Furan ring opening – pyrrole ring closure: a new synthetic route to aryl(heteroaryl)-annulated pyrrolo[1,2-*a*][1,4]diazepines

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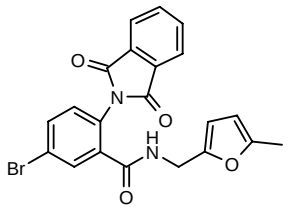
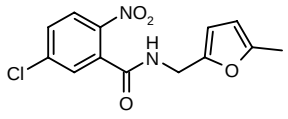


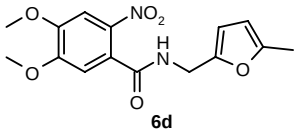
4b

5-Bromo-2-(1,3-dioxo-1,3-dihydro-2*H*-isoindol-2-yl)-*N*-[(5-methyl-2-furyl)methyl]benzamide (4b) was synthesized according to General procedure A from **2a** (2 g, 18 mmol; solution in 50 mL of benzene) and 5-bromo-2-(1,3-dioxo-1,3-dihydro-2*H*-isoindol-2-yl)benzoyl chloride (**3b**) (7.22 g, 19.8 mmol; solution in 50 mL of benzene); eluent: benzene–petroleum ether (1:2); 72% (5.7 g); white solid; mp 134–135 °C (benzene–petroleum ether); δ_H(300 MHz, $CDCl_3$) 2.20 (3H, s, Me), 4.37 (2H, d, ^3J = 5.4 Hz, CH_2), 5.82 (1H, d, ^3J = 3.0 Hz, H_{Fur}), 6.06 (1H, d, ^3J = 3.0 Hz, H_{Fur}), 6.28 (1H, br t, ^3J = 5.4 Hz, NH), 7.24 (1H, d, ^3J = 8.4 Hz, H_{Ar}), 7.70 (1H, dd, ^3J = 8.4 Hz, ^4J = 2.1 Hz, H_{Ar}), 7.74-7.80 (3H, m, H_{Ar}+H_{Pht}), 7.87-7.93 (2H, m, H_{Pht}); δ_C(75 MHz, $CDCl_3$) 13.5, 37.0, 106.2, 108.6, 122.8, 123.9 (2C), 128.8, 131.2, 131.3, 131.7 (2C), 134.2, 134.4 (2C), 135.4, 148.5, 151.9, 165.1, 167.0 (2C); ν_{max} (KBr)/cm^{-1} 3261, 1720, 1628, 1526, 1396, 1372, 1083, 884, 794, 713; *m/z* (EI) 440/438 (M^+, 7/7), 330/328 (22/23), 302/300 (8/10), 193 (21), 165 (10), 111 (56), 110 (100), 104 (14), 95 (31), 75 (12), 45 (17); Found: C, 57.31; H, 3.28; N, 6.37. Calc. for $C_{21}H_{15}BrN_2O_4$: C, 57.42; H, 3.44; N, 6.38%.



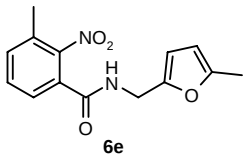
6c

5-Chloro-*N*-[(5-methyl-2-furyl)methyl]-2-nitrobenzamide (6c) was obtained according to General procedure A from **2a** (5 g, 45 mmol; solution in 50 mL of benzene) and 5-chloro-2-nitrobenzoyl chloride (**5b**) (10.9 g, 49.5 mmol; solution in 50 mL of benzene); 91% (12.05 g); white solid; mp 158–159 °C (EtOH); δ_H(300 MHz, $CDCl_3$) 2.27 (3H, s, Me), 4.56 (2H, d, ^3J = 5.4 Hz, CH_2), 5.91 (1H, d, ^3J = 3.0 Hz, H_{Fur}), 6.13 (1H, br t, ^3J = 5.4 Hz, NH), 6.20 (1H, d, ^3J = 3.0 Hz, H_{Fur}), 7.48 (1H, d, ^4J = 2.1 Hz, H_{Ar}), 7.52 (1H, dd, ^3J = 8.7 Hz, ^4J = 2.1 Hz, H_{Ar}), 8.03 (1H, d, ^3J = 8.7 Hz, H_{Ar}); δ_C(75 MHz, $CDCl_3$) 13.5, 37.4, 106.4, 109.1, 126.1, 129.0, 130.5, 134.1, 140.4, 144.4, 148.0, 152.3, 164.7; ν_{max} (KBr)/cm^{-1} 3262, 1639, 1570, 1524, 1345, 842, 790, 719; *m/z* (EI) 278/276 (M^+–18, 7/22%), 170/168 (17/51), 140/138 (11/33), 110 (98), 109 (100), 95 (63), 75 (59), 63 (22), 53 (41), 43 (74); Found: C, 53.21; H, 3.70; N, 9.55. Calc. for $C_{13}H_{11}ClN_2O_4$: C, 52.98; H, 3.76; N, 9.51%.



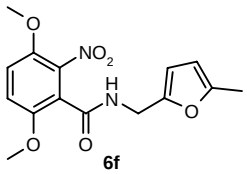
6d

4,5-Dimethoxy-*N*-[(5-methyl-2-furyl)methyl]-2-nitrobenzamide (6d)[1] was synthesized according to General procedure A from **2a** (5 g, 45 mmol; solution in 50 mL of benzene) and 4,5-dimethoxy-2-nitrobenzoyl chloride (**5c**) (12.16 g, 49.5 mmol; solution in 50 mL of benzene); eluent: benzene–petroleum ether (1:1); 84% (12.1 g); white solid.



6e

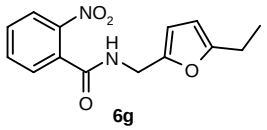
3-Methyl-*N*-[(5-methyl-2-furyl)methyl]-2-nitrobenzamide (6e) was synthesized according to General procedure A from **2a** (5 g, 45 mmol; solution in 50 mL of benzene) and 3-methyl-2-nitrobenzoyl chloride (**5d**) (9.88 g, 49.5 mmol; solution in 50 mL of benzene); eluent: benzene–petroleum ether (1:1); 73% (8.96 g); white solid; mp 78–79 °C (benzene–petroleum ether); δ_H(300 MHz, $CDCl_3$) 2.24 (3H, s, Me), 2.33 (3H, s, Me), 4.45 (2H, d, ^3J = 5.4 Hz, CH_2), 5.87 (1H, d, ^3J = 3.0 Hz, H_{Fur}), 6.12 (1H, d, ^3J = 3.0 Hz, H_{Fur}), 6.47 (1H, br t, ^3J = 5.4 Hz, NH), 7.35-7.39 (3H, m, H_{Ar}); δ_C(75 MHz, $CDCl_3$) 13.5, 17.6, 37.2, 106.4, 108.7, 125.6, 129.6, 130.4, 131.2, 133.7, 148.5, 149.3, 152.1, 165.0; ν_{max} (KBr)/cm^{-1} 3264, 1644, 1540, 1524, 1448, 1360, 1296, 1216, 1064, 1020, 856, 792; *m/z* (EI) 256 (M^+–18, 35%), 183 (31), 169 (52), 148 (42), 141 (25), 135 (11), 118 (39), 104 (13), 95 (63), 89 (52), 77 (32), 65 (63), 51 (46), 43 (100); Found: C, 61.35; H, 5.13; N, 10.35. Calc. for $C_{14}H_{14}N_2O_4$: C, 61.31; H, 5.14; N, 10.21%.



6f

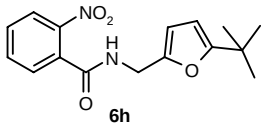
3,6-Dimethoxy-*N*-[(5-methyl-2-furyl)methyl]-2-nitrobenzamide (6f) was synthesized according to General procedure A from **2a** (2 g, 18 mmol; solution in 30 mL of benzene) and 3,6-dimethoxy-2-nitrobenzoyl chloride (**5e**) (4.87 g, 19.8 mmol; solution in 30 mL of benzene); eluent: benzene–petroleum ether (1:1); 68% (3.9 g); colorless plates; mp 104–105 °C (ethyl acetate–petroleum ether); δ_H(300 MHz, $CDCl_3$) 2.26 (3H, s, Me), 3.84 (3H, s, OMe), 3.87 (3H, s, OMe), 4.52 (2H, d, ^3J = 5.4 Hz, CH_2), 5.89 (1H, d, ^3J = 3.0 Hz, H_{Fur}), 6.14 (1H, d, ^3J = 3.0 Hz, H_{Fur}), 7.02 (1H, d, ^3J = 9.3 Hz, H_{Ar}), 7.08 (1H, d, ^3J = 9.3 Hz, H_{Ar}), 7.18 (1H, br t, ^3J = 5.4 Hz, NH); δ_C(75 MHz, $CDCl_3$) 13.5, 37.0, 57.0, 57.1, 106.3, 108.2, 114.3, 115.8, 117.5, 141.5, 145.3,

148.8, 150.1, 151.8, 161.4; ν_{max} (KBr)/cm^{-1} 3344, 1643, 1541, 1485, 1363, 1268, 1076, 940, 825, 802; *m/z* (EI) 302 (M^+–18, 60%), 229 (23), 215 (40), 200 (20), 194 (78), 166 (33), 163 (34), 151 (18), 136 (55), 125 (32), 122 (36), 111 (24), 110 (91), 95 (100), 81 (29), 65 (20), 59 (31), 45 (34), 43 (17); Found: C, 56.40; H, 4.96; N, 8.75. Calc. for $C_{15}H_{16}N_2O_6$: C, 56.25; H, 5.04; N, 8.75%.



6g

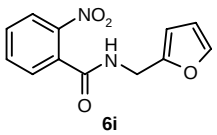
***N*-[(5-Ethyl-2-furyl)methyl]-2-nitrobenzamide (6g)** was obtained according to General procedure A from 5-ethylfurfurylamine (**2b**) (5 g, 40 mmol; solution in 50 mL of benzene) and **5a** (8.2 g, 44 mmol; solution in 50 mL of benzene); 82% (8.94 g); white solid; mp 78–79 °C (CH_2Cl_2–petroleum ether); δ_H(300 MHz, $CDCl_3$) 1.18 (3H, t, ^3J = 7.5 Hz, CH_2*Me*), 2.57 (2H, q, ^3J = 7.5 Hz, *CH_2*Me), 4.47 (2H, d, ^3J = 5.4 Hz, CH_2), 5.87 (1H, d, ^3J = 3.0 Hz, H_{Fur}), 6.15 (1H, d, ^3J = 3.0 Hz, H_{Fur}), 6.51 (1H, br t, ^3J = 5.4 Hz, NH), 7.42-7.44 (1H, m, H_{Ar}), 7.47-7.53 (1H, m, H_{Ar}), 7.56-7.62 (1H, m, H_{Ar}), 7.93-7.96 (1H, m, H_{Ar}); δ_C(75 MHz, $CDCl_3$) 12.0, 21.2, 37.2, 104.7, 108.4, 124.3, 128.7, 130.3, 132.5, 133.5, 146.2, 148.3, 157.7, 166.1; ν_{max} (KBr)/cm^{-1} 3276, 1636, 1524, 1352, 1292, 1256, 1188, 1020, 856, 808, 788, 748; *m/z* (EI) 256 (M^+–18, 30%), 183 (11), 169 (28), 155 (41), 150 (23), 141 (13), 134 (64), 124 (65), 104 (52), 94 (23), 91 (16), 76 (80), 65 (43), 51 (100), 43 (60); Found: C, 61.46; H, 5.23; N, 10.30. Calc. for $C_{14}H_{14}N_2O_4$: C, 61.31; H, 5.14; N, 10.21%.



6h

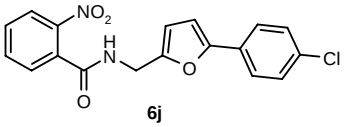
***N*-[(5-*tert*-Butyl-2-furyl)methyl]-2-nitrobenzamide (6h)** was synthesized according to General procedure A from 5-*tert*-butylfurfurylamine (**2c**) (5 g, 32.6 mmol; solution in 50 mL of benzene) and **5a** (6.66 g, 35.9 mmol; solution in 50 mL of benzene); eluent: benzene–petroleum ether (1:2); 86% (8.5 g); white solid; mp 114–115 °C (acetone–petroleum ether); δ_H(300 MHz, $CDCl_3$) 1.25 (9H, s, t-Bu), 4.58 (2H, d, ^3J = 5.4 Hz, CH_2), 5.88 (1H, d, ^3J = 3.0 Hz, H_{Fur}), 6.14 (1H, br t, ^3J = 5.4 Hz, NH), 6.18 (1H, d, ^3J = 3.0 Hz, H_{Fur}), 7.48-7.51 (1H, m, H_{Ar}), 7.52-7.58 (1H, m, H_{Ar}), 7.62-7.67 (1H, m, H_{Ar}), 8.02-8.05 (1H, m, H_{Ar}); δ_C(75 MHz, $CDCl_3$) 29.0 (3C), 32.6, 37.4, 102.7, 108.3, 124.5, 128.7, 130.5, 132.7, 133.7, 146.5, 148.1, 164.4, 166.1; ν_{max} (KBr)/cm^{-1} 3259, 1650, 1525, 1346, 1307, 1205, 1129, 1039, 1013, 860, 793, 749; *m/z* (EI) 302 (M^+, 2%), 284 (5), 197 (10), 152 (34), 150 (34), 136 (99), 121 (78), 104 (55), 91 (33), 76 (85), 65 (43), 51

(100), 43 (99); Found: C, 63.58; H, 6.03; N, 9.31. Calc. for $C_{16}H_{18}N_2O_4$: C, 63.57; H, 6.00; N, 9.27%.



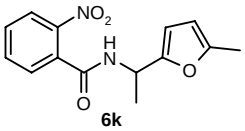
6i

***N*-(2-Furylmethyl)-2-nitrobenzamide (6i)** was obtained according to General procedure A from furfurylamine (**2e**) (5 g, 51.5 mmol; solution in 50 mL of benzene) and **5a** (10.51 g, 56.65 mmol; solution in 50 mL of benzene); 92% (11.63 g); white solid; mp 108–110 °C (EtOH); δ_H(300 MHz, $CDCl_3$) 4.56 (2H, d, ^3J = 5.7 Hz, CH_2), 6.29 (1H, dd, ^3J = 3.3 Hz, ^4J = 0.9 Hz, H_{Fur}), 6.32 (1H, dd, ^3J = 1.8 Hz, ^3J = 3.3 Hz, H_{Fur}), 6.42 (1H, br t, ^3J = 5.7 Hz, NH), 7.34 (1H, dd, ^3J = 1.8 Hz, ^4J = 0.9 Hz, H_{Fur}), 7.44-7.47 (1H, m, H_{Ar}), 7.50-7.56 (1H, m, H_{Ar}), 7.59-7.65 (1H, m, H_{Ar}), 7.98-8.01 (1H, m, H_{Ar}); δ_C(75 MHz, $CDCl_3$) 37.1, 107.9, 110.5, 124.5, 128.7, 130.5, 132.4, 133.7, 142.3, 146.1, 150.3, 166.2; ν_{max} (KBr)/cm^{-1} 3272, 1648, 1560, 1528, 1444, 1352, 1308, 1260, 1152, 1076, 1016, 792, 748; *m/z* (EI) 228 (M^+–18, 8%), 155 (13), 134 (27), 128 (76), 121 (15), 104 (35), 96 (56), 81 (49), 76 (72), 69 (12), 65 (30), 53 (88), 50 (100), 41 (42); Found: C, 58.46; H, 4.12; N, 11.46. Calc. for $C_{12}H_{10}N_2O_4$: C, 58.54; H, 4.09; N, 11.38%.



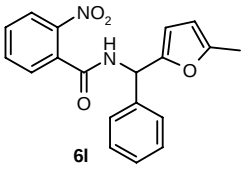
6j

***N*-[(5-(4-Chlorophenyl)-2-furyl)methyl]-2-nitrobenzamide (6j)** was synthesized according to General procedure A from 5-(4-chlorophenyl)furfurylamine (**2d**) (5 g, 24.08 mmol; solution in 50 mL of benzene) and **5a** (4.92 g, 26.5 mmol; solution in 50 mL of benzene); 82% (7.02 g); beige needles; mp 156–157 °C (EtOH); δ_H(300 MHz, $CDCl_3$) 4.62 (2H, d, ^3J = 5.4 Hz, CH_2), 6.38 (1H, d, ^3J = 3.3 Hz, H_{Fur}), 6.43 (1H, br t, ^3J = 5.4 Hz, NH), 6.54 (1H, d, ^3J = 3.3 Hz, H_{Fur}), 7.30 (2H, d, ^3J = 8.7 Hz, H_{Ar}), 7.45-7.49 (1H, m, H_{Ar}), 7.51-7.57 (1H, m, H_{Ar}), 7.54 (2H, d, ^3J = 8.7 Hz, H_{Ar}), 7.58-7.63 (1H, m, H_{Ar}), 7.98-8.01 (1H, m, H_{Ar}); δ_C(75 MHz, $CDCl_3$) 37.2, 106.3, 110.2, 124.5, 124.9 (2C), 128.7, 128.8 (2C), 129.0, 130.5, 132.4, 133.0, 133.7, 146.5, 150.2, 152.7, 166.3; ν_{max} (KBr)/cm^{-1} 3264, 1644, 1556, 1524, 1480, 1352, 1316, 1092, 832, 792, 788, 724; *m/z* (EI) 358/356 (M^+, 5/16%), 340/338 (33/100), 265 (10), 231 (26), 207/205 (27/81), 191 (22), 149 (42), 134 (18), 128 (31), 115 (20), 104 (27), 75 (47), 63 (17), 51 (53); Found: C, 60.61; H, 3.63; N, 7.90. Calc. for $C_{18}H_{13}ClN_2O_4$: C, 60.60; H, 3.67; N, 7.85%.



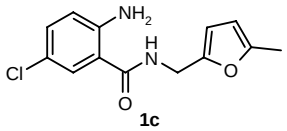
6k

***N*-[1-(5-Methyl-2-furyl)ethyl]-2-nitrobenzamide (6k)** was obtained according to General procedure A from [1-(5-methyl-2-furyl)ethyl]amine (**2f**) (5 g, 40 mmol; solution in 50 mL of benzene) and **5a** (8.16 g, 44 mmol; solution in 50 mL of benzene); eluent: benzene; 63% (6.9 g); colorless needles; mp 123–124 °C (CH_2Cl_2-petroleum); δ_H(300 MHz, $CDCl_3$) 1.60 (3H, d, ^3J = 6.9 Hz, CH*Me*), 2.26 (3H, s, Me), 5.34 (1H, dq, ^3J = 6.9 Hz, ^3J = 8.4 Hz, *CH*Me), 5.89 (1H, d, ^3J = 3.0 Hz, H_{Fur}), 6.00 (1H, d, ^3J = 8.4 Hz, NH), 6.14 (1H, d, ^3J = 3.0 Hz, H_{Fur}), 7.51-7.60 (2H, m, H_{Ar}), 7.63-7.68 (1H, m, H_{Ar}), 8.05-8.08 (1H, m, H_{Ar}); δ_C(75 MHz, $CDCl_3$) 13.5, 19.0, 43.7, 106.0, 106.7, 124.4, 128.7, 130.3, 132.7, 133.6, 146.2, 151.7, 152.6, 165.5; ν_{max} (KBr)/cm^{-1} 3224, 1635, 1525, 1448, 1347, 1106, 1022, 904, 856, 800; *m/z* (EI) 274 (M^+, 2%), 256 (24), 212 (14), 159 (47), 150 (51), 134 (57), 124 (100), 108 (76), 104 (46), 90 (17), 76 (50), 65 (22), 51 (72), 43 (89); Found: C, 61.71; H, 5.22; N, 10.00. Calc. for $C_{14}H_{14}N_2O_4$: C, 61.31; H, 5.14; N, 10.21%.



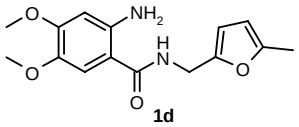
6l

***N*-[(5-Methyl-2-furyl)(phenyl)methyl]-2-nitrobenzamide (6l)** was synthesized according to General procedure A from [(5-methyl-2-furyl)(phenyl)methyl]amine (**2g**) (5 g, 26.7 mmol; solution in 50 mL of benzene) and **5a** (5.45 g, 29.37 mmol; solution in 50 mL of benzene); 90% (8.05 g); white solid; mp 152–153 °C (benzene–petroleum ether); δ_H(300 MHz, $CDCl_3$) 2.20 (3H, s, Me), 5.91 (1H, d, ^3J = 3.0 Hz, H_{Fur}), 6.09 (1H, d, ^3J = 3.0 Hz, H_{Fur}), 6.36 (1H, d, ^3J = 8.1 Hz, CH), 7.25-7.35 (3H, m, H_{Ar}), 7.38-7.42 (2H, m, H_{Ar}), 7.58-7.64 (2H, m, H_{Ar}), 7.68-7.73 (1H, m, H_{Ar}), 7.97-8.00 (1H, m, H_{Ar}), 8.54 (1H, d, ^3J = 8.1 Hz, NH); δ_C(75 MHz, $CDCl_3$) 13.6, 52.1, 106.8, 109.0, 124.6, 128.0 (2C), 128.1 (2C), 129.0, 129.8, 131.0, 133.5, 134.0, 140.4, 147.6, 152.3, 152.5, 165.9; ν_{max} (KBr)/cm^{-1} 3308, 1644, 1540, 1448, 1360, 1220, 1204, 1024, 952, 856, 784, 736; *m/z* (EI) 318 (M^+–18, 17%), 221 (100), 186 (78), 170 (74), 150 (18), 134 (29), 104 (49), 90 (27), 77 (38), 65 (18), 51 (50), 43 (56); Found: C, 68.08; H, 4.91; N, 8.15. Calc. for $C_{19}H_{16}N_2O_4$: C, 67.85; H, 4.79; N, 8.33%.



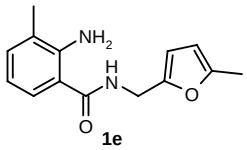
1c

2-Amino-5-chloro-*N*-[(5-methyl-2-furyl)methyl]benzamide (1c) was synthesized according to General procedure C from **6c** (1 g, 3.4 mmol); 89% (0.8 g); colorless plates, mp 108–109 °C (CH_2Cl_2–petroleum ether); δ_H(300 MHz, $CDCl_3$) 2.28 (3H, s, Me), 4.50 (2H, d, ^3J = 5.4 Hz, CH_2), 5.91 (1H, d, ^3J = 3.0 Hz, H_{Fur}), 6.15 (1H, d, ^3J = 3.0 Hz, H_{Fur}), 6.25 (1H, br t, ^3J = 5.4 Hz, NH), 6.61 (1H, d, ^3J = 8.7 Hz, H_{Ar}), 7.13 (1H, dd, ^3J = 8.7 Hz, ^4J = 2.4 Hz, H_{Ar}), 7.27 (1H, d, ^4J = 2.4 Hz, H_{Ar}); δ_C(75 MHz, $CDCl_3$) 13.5, 36.8, 106.3, 108.6, 116.5, 118.5, 120.8, 126.8, 132.1, 147.2, 148.9, 152.1, 167.8; ν_{max} (KBr)/cm^{-1} 3459, 3358, 3282, 1621, 1535, 1251, 1150, 1017, 904, 819, 787, 748; *m/z* (EI) 266/264 (M^+, 3/10%), 156/154 (3/14), 110 (100), 95 (68), 43 (14); Found: C, 58.82; H, 5.00; N, 10.68. Calc. for $C_{13}H_{13}ClN_2O_2$: C, 58.99; H, 4.95; N, 10.58%.



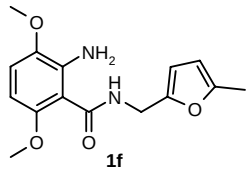
1d

2-Amino-4,5-dimethoxy-*N*-[(5-methyl-2-furyl)methyl]benzamide (1d)[1] was obtained according to General procedure C from **6d** (1 g, 3.12 mmol); 89% (0.81 g); white solid.



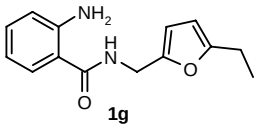
1e

2-Amino-3-methyl-*N*-[(5-methyl-2-furyl)methyl]benzamide (1e) was synthesized according to General procedure C from **6e** (1 g, 3.65 mmol); 75% (0.67 g); colorless needles, mp 102–103 °C (petroleum ether); δ_H(300 MHz, $CDCl_3$) 2.14 (3H, s, Me), 2.26 (3H, s, Me), 4.51 (2H, d, ^3J = 5.4 Hz, CH_2), 5.58 (2H, br s, NH_2), 5.89 (1H, d, ^3J = 3.0 Hz, H_{Fur}), 6.13 (1H, d, ^3J = 3.0 Hz, H_{Fur}), 6.37 (1H, br t, ^3J = 5.4 Hz, NH), 6.53-6.58 (1H, m, H_{Ar}), 7.09-7.12 (1H, m, H_{Ar}), 7.20-7.23 (1H, m, H_{Ar}); δ_C(75 MHz, $CDCl_3$) 13.6, 17.5, 36.8, 106.3, 108.4, 115.2, 115.9, 123.7, 125.1, 133.2, 147.1, 149.4, 152.0, 169.4; ν_{max} (KBr)/cm^{-1} 3420, 3340, 1640, 1616, 1576, 1520, 1460, 1332, 1256, 1188, 788, 756; *m/z* (EI) 244 (M^+, 48%), 134 (30), 110 (100), 95 (56), 77 (37), 65 (13), 43 (48); Found: C, 68.81; H, 6.55; N, 11.58. Calc. for $C_{14}H_{16}N_2O_2$: C, 68.83; H, 6.60; N, 11.47%.



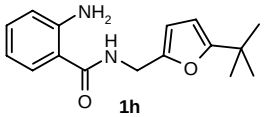
1f

2-Amino-3,6-dimethoxy-*N*-[(5-methyl-2-furyl)methyl]benzamide (1f) was synthesized according to General procedure C from **6f** (1 g, 3.12 mmol); residue was poured into water and extracted with diethyl ether (3×30 mL); the combined organic fractions were dried over Na_2SO_4. Solvent was removed using rotor evaporator. Residue was distilled under vacuum. Product was isolated as light-yellow oil (0.8 g, 89%) and used for further transformations without additional purification.



1g

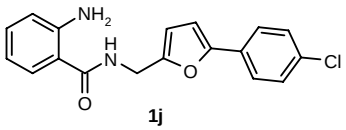
2-Amino-*N*-[(5-ethyl-2-furyl)methyl]benzamide (1g) was synthesized according to General procedure C from **6g** (1 g, 3.65 mmol); 94% (0.84 g); white solid, mp 70–71 °C (EtOH); δ_H(300 MHz, $CDCl_3$) 1.21 (3H, t, ^3J = 7.5 Hz, $CH_2\mathit{Me}$), 2.61 (2H, q, ^3J = 7.5 Hz, $\mathit{CH_2}$Me), 4.52 (2H, d, ^3J = 5.4 Hz, CH_2), 5.52 (2H, br s, NH_2), 5.90 (1H, d, ^3J = 3.0 Hz, H_{Fur}), 6.15 (1H, d, ^3J = 3.0 Hz, H_{Fur}), 6.35 (1H, br t, ^3J = 5.4 Hz, NH), 6.58-6.67 (2H, m, H_{Ar}), 7.15-7.21 (1H, m, H_{Ar}), 7.29-7.32 (1H, m, H_{Ar}); δ_C(75 MHz, $CDCl_3$) 12.0, 21.3, 36.8, 104.6, 108.1, 115.6, 116.5, 117.2, 127.2, 132.3, 148.8, 149.2, 157.7, 168.9; ν_{max} (KBr)/cm^{-1} 3416, 3284, 1624, 1588, 1524, 1448, 1288, 1256, 1188, 1156, 1024, 792, 752; *m/z* (EI) 244 (M^+, 12%), 124 (100), 120 (35), 109 (38), 92 (31), 65 (47), 52 (15), 43 (25); Found: C, 68.87; H, 6.67; N, 11.56. Calc. for $C_{14}H_{16}N_2O_2$: C, 68.83; H, 6.60; N, 11.47%.



1h

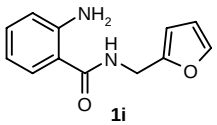
2-Amino-*N*-[(5-*tert*-butyl-2-furyl)methyl]benzamide (1h) was synthesized according to General procedure C from **6h** (1 g, 3.31 mmol); 92% (0.83 g); white solid, mp 79–80 °C (EtOH); δ_H(300 MHz, $CDCl_3$) 1.24 (9H, s, t-Bu), 4.53 (2H, d, ^3J = 5.4 Hz, CH_2), 5.51 (2H, br s, NH_2), 5.88 (1H, d, ^3J = 3.0 Hz, H_{Fur}), 6.13 (1H, d, ^3J = 3.0 Hz, H_{Fur}), 6.37 (1H, br t, ^3J = 5.4 Hz, NH), 6.59-6.67 (2H, m, H_{Ar}), 7.15-7.21 (1H, m, H_{Ar}), 7.29-7.32 (1H, m, H_{Ar}); δ_C(75 MHz, $CDCl_3$) 29.0 (3C), 32.5, 36.9, 102.6, 107.7, 115.8, 116.5, 117.2, 127.1, 132.3, 148.7, 149.0, 164.1, 168.9; ν_{max} (KBr)/cm^{-1} 3477, 3374, 3281, 1632, 1582, 1554, 1419, 1302, 1263, 1207, 1157, 1025, 982,

792, 750; *m/z* (EI) 272 (M^+, 14%), 152 (100), 137 (31), 121 (17), 120 (56), 92 (27), 65 (30), 43 (42); Found: C, 70.89; H, 7.56; N, 10.29. Calc. for $C_{16}H_{20}N_2O_2$: C, 70.56; H, 7.40; N, 10.29%.



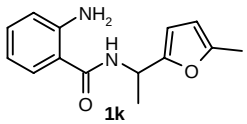
1j

2-Amino-*N*-{[5-(4-chlorophenyl)-2-furyl]methyl}benzamide (1j) was synthesized according to General procedure C from **6j** (1 g, 2.8 mmol); 93% (0.85 g); colorless plates, mp 163–164 °C (EtOH); δ_H(300 MHz, $CDCl_3$) 4.63 (2H, d, ^3J = 5.4 Hz, CH_2), 5.53 (2H, br s, NH_2), 6.35 (1H, d, ^3J = 3.3 Hz, H_{Fur}), 6.42 (1H, br t, ^3J = 5.4 Hz, NH), 6.56 (1H, d, ^3J = 3.3 Hz, H_{Fur}), 6.60-6.69 (2H, m, H_{Ar}), 7.17-7.23 (1H, m, H_{Ar}), 7.30-7.35 (3H, m, H_{Ar}), 7.56 (2H, d, ^3J = 8.7 Hz, H_{Ar}); δ_C(75 MHz, $CDCl_3$) 36.8, 106.3, 109.9, 115.4, 116.6, 117.3, 123.6, 124.9 (2C), 127.2, 128.8 (2C), 132.5, 133.0, 148.8, 151.2, 152.6, 169.0; ν_{max} (KBr)/cm^{-1} 3480, 3368, 3304, 1628, 1580, 1536, 1484, 1424, 1268, 1160, 1016, 824, 788, 752; *m/z* (EI) 328/326 (M^+, 5/14%), 208/206 (33/100), 191 (26), 172 (16), 128 (20), 120 (40), 99 (16), 92 (28), 65 (18), 43 (20); Found: C, 66.45; H, 4.73; N, 8.55. Calc. for $C_{18}H_{15}ClN_2O_2$: C, 66.16; H, 4.63; N, 8.57%.



1i

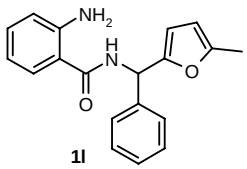
2-Amino-*N*-[(2-furyl)methyl]benzamide (1i) was synthesized according to General procedure C from **6i** (1 g, 4.06 mmol); 90% (0.79 g); white solid, mp 87–88 °C (aq. EtOH); δ_H(300 MHz, $CDCl_3$) 4.57 (2H, d, ^3J = 5.4 Hz, CH_2), 5.53 (2H, br s, NH_2), 6.26 (1H, dd, ^3J = 3.3 Hz, ^4J = 0.6 Hz, H_{Fur}), 6.32 (1H, dd, ^3J = 1.8 Hz, ^3J = 3.3 Hz, H_{Fur}), 6.41 (1H, br t, ^3J = 5.4 Hz, NH), 6.58-6.67 (2H, m, H_{Ar}), 7.16-7.21 (1H, m, H_{Ar}), 7.29-7.32 (1H, m, H_{Ar}), 7.36 (1H, dd, ^3J = 1.8 Hz, ^4J = 0.6 Hz, H_{Fur}); δ_C(75 MHz, $CDCl_3$) 36.6, 107.5, 110.4, 115.4, 116.5, 117.3, 127.2, 132.4, 142.2, 148.8, 151.3, 169.0; ν_{max} (KBr)/cm^{-1} 3420, 3300, 1624, 1588, 1532, 1448, 1296, 1260, 1196, 1152, 1012, 752; *m/z* (EI) 216 (M^+, 11%), 120 (46), 96(100), 92 (53), 81 (41), 65 (83), 52 (61); Found: C, 66.72; H, 5.65; N, 13.01. Calc. for $C_{12}H_{12}N_2O_2$: C, 66.65; H, 5.59; N, 12.95%.



1k

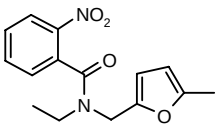
2-Amino-*N*-[1-(5-methyl-2-furyl)ethyl]benzamide (1k) was synthesized according to General procedure C from **6k** (1 g, 3.65 mmol); 96% (0.85 g); white solid, mp 93–94 °C (aq. EtOH);

δ_H(300 MHz, $CDCl_3$) 1.54 (3H, d, ^3J = 6.9 Hz, CH*Me*), 2.26 (3H, s, Me), 5.30 (1H, dq, ^3J = 6.9 Hz, ^3J = 7.2 Hz, *CH*Me), 5.52 (2H, br s, NH_2), 5.89 (1H, d, ^3J = 3.0 Hz, H_{Fur}), 6.09 (1H, d, ^3J = 3.0 Hz, H_{Fur}), 6.23 (1H, br d, ^3J = 7.2 Hz, NH), 6.60-6.68 (2H, m, H_{Ar}), 7.16-7.22 (1H, m, H_{Ar}), 7.29-7.32 (1H, m, H_{Ar}); δ_C(75 MHz, $CDCl_3$) 13.5, 19.6, 42.9, 105.9, 106.3, 115.8, 116.4, 117.2, 127.1, 132.2, 148.7, 151.6, 153.5, 168.2; ν_{max} (KBr)/cm^{-1} 3418, 3293, 1619, 1587, 1526, 1448, 1311, 1257, 1218, 1156, 1018, 941, 781, 748; *m/z* (EI) 244 (M^+, 13%), 124 (100), 120 (41), 109 (69), 92 (25), 65 (35), 53 (11), 43 (34); Found: C, 69.10; H, 6.75; N, 11.23. Calc. for $C_{14}H_{16}N_2O_2$: C, 68.83; H, 6.60; N, 11.47%.



1l

2-Amino-*N*-[(5-methyl-2-furyl)(phenyl)methyl]benzamide (1l) was synthesized according to General procedure C from **6l** (1 g, 2.97 mmol); 91% (0.83 g); white solid, mp 138–139 °C (aq. EtOH); δ_H(300 MHz, $CDCl_3$) 2.28 (3H, s, Me), 5.56 (2H, br s, NH_2), 5.91 (1H, d, ^3J = 3.0 Hz, H_{Fur}), 6.04 (1H, d, ^3J = 3.0 Hz, H_{Fur}), 6.37 (1H, d, ^3J = 7.8 Hz, CH), 6.62-6.68 (2H, m, H_{Ar}), 6.78 (1H, br d, ^3J = 7.8 Hz, NH), 7.18-7.21 (1H, m, H_{Ar}), 7.26-7.37 (5H, m, H_{Ar}), 7.39-7.42 (1H, m, H_{Ar}); δ_C(75 MHz, $CDCl_3$) 13.6, 51.2, 106.2, 108.7, 115.2, 116.4, 117.3, 126.9 (2C), 127.2 (2C), 127.6, 128.6, 132.5, 139.7, 149.0, 151.5, 152.3, 168.1; ν_{max} (KBr)/cm^{-1} 3428, 3304, 1620, 1588, 1520, 1452, 1316, 1256, 1160, 1024, 792, 748, 700; *m/z* (EI) 306 (M^+, 28%), 187 (85), 186 (50), 171 (100), 128 (31), 120 (94), 104 (20), 92 (80), 77 (23), 65 (82), 51 (18), 43 (68); Found: C, 74.78; H, 5.94; N, 8.99. Calc. for $C_{19}H_{18}N_2O_2$: C, 74.49; H, 5.92; N, 9.14%.



7b

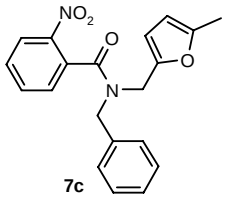
***N*-Ethyl-*N*-[(5-methyl-2-furyl)methyl]-2-nitrobenzamide (7b)** was synthesized according to General procedure D using ethyl bromide (2.51 g, 23 mmol); eluent: benzene–petroleum ether (1:1). Product was isolated as white solid by recrystallization from petroleum ether below 0 °C; 83% (2.76 g,); mp 62–63 °C. According to NMR spectra, this compound exists as two rotamers in a ratio of 1.5:1.

The major rotamer: δ_H(300 MHz, $CDCl_3$, 45 °C) 1.19 (3H, t, ^3J = 7.2 Hz, CH_2*Me*), 2.19 (3H, s, Me), 3.55 (2H, br s, *CH_2*Me), 4.13 (2H, s, CH_2), 5.81 (1H, d, ^3J = 3.0 Hz, H_{Fur}), 5.94 (1H, d, ^3J = 3.0 Hz, H_{Fur}), 7.44-7.53 (2H, m, H_{Ar}), 7.61-7.67 (1H, m, H_{Ar}), 8.10-8.13 (1H, m, H_{Ar}); δ_C(75

MHz, $CDCl_3$, 45 °C) 11.3, 13.2, 39.4, 45.0, 106.0, 109.4, 124.4, 128.0, 128.5, 129.5, 133.0, 133.9, 145.2, 147.3, 152.3, 167.0;

The minor rotamer: δ_H(300 MHz, $CDCl_3$, 45 °C) 0.98 (3H, t, ^3J = 7.2 Hz, CH_2*Me*), 2.24 (3H, s, Me), 3.10 (2H, q, ^3J = 7.2 Hz, *CH_2*Me), 4.69 (2H, s, CH_2), 5.89 (1H, d, ^3J = 3.0 Hz, H_{Fur}), 6.23 (1H, d, ^3J = 3.0 Hz, H_{Fur}), 7.33-7.36 (1H, m, H_{Ar}), 7.44-7.53 (1H, m, H_{Ar}), 7.61-7.67 (1H, m, H_{Ar}), 8.09-8.12 (1H, m, H_{Ar}); δ_C(75 MHz, $CDCl_3$, 45 °C) 12.9, 13.3, 40.0, 42.7, 106.3, 109.5, 124.5, 128.0, 128.5, 129.5, 133.1, 134.0, 145.1, 148.2, 151.6, 167.2.

ν_{max} (KBr)/cm^{-1} 1636, 1559, 1520, 1426, 1346, 1273, 1223, 1148, 1068, 1027, 972, 820, 793, 767; *m/z* (EI) 288 (M^+, 17%), 272 (14), 271 (49), 178 (13), 150 (65), 138 (100), 137 (99), 122 (76), 110 (21), 104 (51), 95 (62), 81 (16), 76 (69), 65 (50), 56 (50), 51 (62); Found: C, 62.59; H, 5.48; N, 9.84. Calc. for $C_{15}H_{16}N_2O_4$: C, 62.49; H, 5.59; N, 9.72%.



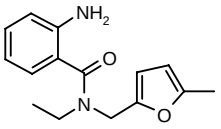
7c

***N*-Benzyl-*N*-[(5-methyl-2-furyl)methyl]-2-nitrobenzamide (7c)** was synthesized according to General procedure D using benzyl chloride (2.91 g, 23 mmol); eluent: benzene–petroleum ether (1:1). 62% (2.5 g); colorless needles; mp 88–89 °C (petroleum ether–diethyl ether); according to NMR spectra, this compound exists as two rotamers in a ratio of 2:1.

The major rotamer: δ_H(300 MHz, $CDCl_3$) 2.25 (3H, s, Me), 4.07 (2H, s, CH_{2Fur}), 4.67 (2H, s, CH_{2Ph}), 5.86 (1H, d, ^3J = 3.0 Hz, H_{Fur}), 5.93 (1H, d, ^3J = 3.0 Hz, H_{Fur}), 7.12-7.15 (1H, m, H_{Ar}), 7.25-7.46 (5H, m, H_{Ar}), 7.57-7.62 (1H, m, H_{Ar}), 7.70-7.76 (1H, m, H_{Ar}), 8.20-8.23 (1H, m, H_{Ar}); δ_C(75 MHz, $CDCl_3$) 13.4, 44.1, 46.8, 106.1, 110.2, 124.6, 127.3, 127.5, 128.6 (2C), 128.8 (2C), 129.8 (2C), 134.2, 136.1, 145.2, 146.6, 152.6, 167.8;

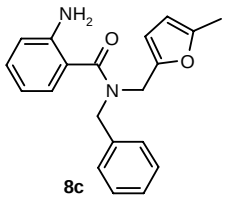
The minor rotamer: δ_H(300 MHz, $CDCl_3$) 2.29 (3H, s, Me), 4.30 (2H, s, CH_{2Fur}), 5.18 (2H, s, CH_{2Ph}), 5.93 (1H, d, ^3J = 3.0 Hz, H_{Fur}), 6.22 (1H, d, ^3J = 3.0 Hz, H_{Fur}), 7.25-7.45 (4H, m, H_{Ar}), 7.49-7.66 (4H, m, H_{Ar}), 7.60-7.66 (1H, m, H_{Ar}), 8.16-8.19 (1H, m, H_{Ar}); δ_C(75 MHz, $CDCl_3$) 13.6, 40.1, 51.5, 106.3, 110.1, 124.7, 127.7, 128.1, 128.7 (2C), 128.8 (2C), 132.7 (2C), 134.3, 135.5, 145.0, 147.6, 152.0, 167.9.

ν_{max} (KBr)/cm^{-1} 1639, 1529, 1445, 1353, 1258, 1219, 1022, 991, 771, 733; *m/z* (EI) 350 (M^+, 1%), 200 (63), 150 (77), 121 (20), 104 (20), 95 (100), 91 (97), 76 (27), 65 (36), 57 (16), 51 (55), 43 (51); Found: C, 68.78; H, 5.14; N, 7.95. Calc. for $C_{20}H_{18}N_2O_4$: C, 68.56; H, 5.18; N, 8.00%.



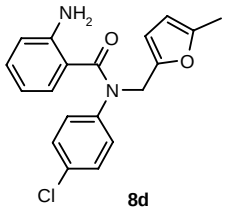
8b

2-Amino-*N*-ethyl-*N*-[(5-methyl-2-furyl)methyl]benzamide (8b) was synthesized according to General procedure C from **7b** (1 g, 3.47 mmol). Product was extracted with diethyl ether (4×20 mL). The combined organic phases dried over anhydrous Na_2SO_4. Solvent was evaporated under reduced pressure. Eluent: CH_2Cl_2–petroleum ether (1:2). Aniline **8b** was isolated as light-yellow oil in 76% yield (0.68 g); δ_H(300 MHz, $CDCl_3$, 45 °C) 1.11 (3H, t, ^3J = 6.9 Hz, CH_2Me), 2.26 (3H, s, Me), 3.42 (2H, q, ^3J = 6.9 Hz, CH_2Me), 4.16 (2H, br s, CH_2), 4.52 (2H, s, NH_2), 5.88 (1H, d, ^3J = 3.0 Hz, H_{Fur}), 6.10 (1H, d, ^3J = 3.0 Hz, H_{Fur}), 6.67-6.72 (2H, m, H_{Ar}), 7.09-7.18 (2H, m, H_{Ar}); δ_C(75 MHz, $CDCl_3$, 45 °C) 12.9, 13.4, 41.3, 42.9, 106.2, 109.1, 116.5, 117.4, 121.0, 127.5, 130.2, 145.0, 148.9, 151.9, 170.9; ν_{max} (KBr)/cm^{-1} 3459, 3359, 1647, 1495, 1217, 1146, 1073, 1021, 980, 866, 791; *m/z* (EI) 258 (M^+, 11%), 138 (99), 120 (100), 110 (18), 95 (50), 92 (55), 65 (61), 56 (14), 45 (13); Found: C, 69.57; H, 6.85; N, 10.85. Calc. for $C_{15}H_{18}N_2O_2$: C, 69.74; H, 7.02; N, 10.84%.



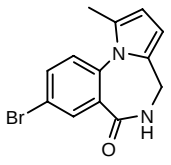
8c

2-Amino-*N*-benzyl-*N*-[(5-methyl-2-furyl)methyl]benzamide (8c) was synthesized according to General procedure C from **7c** (1 g, 2.85 mmol); eluent: CH_2Cl_2–petroleum ether (1:1); 85% (0.77 g); white powder, mp 68–69 °C (aq. EtOH); δ_H(300 MHz, $CDCl_3$, 45 °C) 2.27 (3H, s, Me), 4.30 (2H, s, CH_2), 4.45 (2H, s, CH_2), 4.63 (2H, s, NH_2), 5.89 (1H, d, ^3J = 3.0 Hz, H_{Fur}), 6.06 (1H, d, ^3J = 3.0 Hz, H_{Fur}), 6.67-6.72 (2H, m, H_{Ar}), 7.12-7.17 (1H, m, H_{Ar}), 7.25-7.36 (6H, m, H_{Ar}); δ_C(75 MHz, $CDCl_3$, 45 °C) 13.5, 42.7, 49.3, 106.2, 109.6, 116.6, 117.4, 120.3, 127.4, 127.7, 127.9, 128.6 (3C), 130.5, 136.9, 145.3, 148.4, 152.1, 171.4; ν_{max} (KBr)/cm^{-1} 3472, 3356, 1618, 1493, 1447, 1259, 1137, 1023, 988, 795, 749; *m/z* (EI) 229 (M^+–91, 13%), 200 (30), 120 (100), 110 (11), 95 (34), 92 (23), 91 (25), 65 (27), 43 (12); Found: C, 75.10; H, 6.21; N, 8.87. Calc. for $C_{20}H_{20}N_2O_2$: C, 74.98; H, 6.29; N, 8.74%.



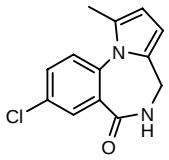
8d

2-Amino-*N*-(4-chlorophenyl)-*N*-[(5-methyl-2-furyl)methyl]benzamide (8d) was synthesized according to General procedure C from **7d** (1 g, 2.7 mmol); eluent: ethyl acetate–petroleum ether (1:2). (0.66 g, 72%). Product was isolated as light-yellow solid by recrystallization from petroleum ether below 0 °C; 72% (0.66 g,); mp 96–97 °C; δ_H(300 MHz, $CDCl_3$) 2.25 (3H, s, Me), 4.75 (2H, br s, CH_2), 4.96 (2H, s, NH_2), 5.86 (1H, d, ^3J = 3.0 Hz, H_{Fur}), 6.10 (1H, d, ^3J = 3.0 Hz, H_{Fur}), 6.35-6.40 (1H, m, H_{Ar}), 6.74-6.77 (1H, m, H_{Ar}), 6.94-7.02 (3H, m, H_{Ar}), 7.11-7.16 (2H, m, H_{Ar}); δ_C(75 MHz, $CDCl_3$) 13.5, 46.5, 106.3, 109.7, 116.5, 116.9, 119.4, 128.2 (2C), 129.0 (2C), 129.5, 130.7, 132.2, 142.1, 146.5, 148.6, 151.8, 170.6; ν_{max} (KBr)/cm^{-1} 3440, 3348, 1620, 1588, 1568, 1488, 1408, 1392, 1380, 1288, 1196, 1092, 1026, 1012, 780, 752 ; *m/z* (EI) 340 (M^+, 35%), 246 (15), 220 (100), 170 (38), 120 (72), 101 (40), 95 (87), 59 (49), 43 (72); Found: C, 66.77; H, 5.17; N, 8.06. Calc. for $C_{19}H_{17}ClN_2O_2$: C, 66.96; H, 5.03; N, 8.22%.



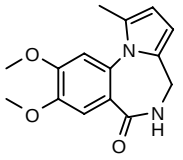
13b

8-Bromo-1-methyl-4,5-dihydro-6*H*-pyrrolo[1,2-*a*][1,4]benzodiazepin-6-one (13b) was synthesized according to General procedure E from **1b** (1g, 3.23 mmol); eluent: benzene; 65% (0.61 g); colorless needles; mp 201–202 °C (benzene–petroleum ether); δ_H(300 MHz, $CDCl_3$) 2.28 (3H, s, Me), 4.09 (2H, d, ^3J = 6.3 Hz, CH_2), 6.00-6.03 (2H, m, H_{Pyr}), 7.15 (1H, d, ^3J = 8.7 Hz, H_{Ar}), 7.63 (1H, br t, ^3J = 6.3 Hz, NH), 7.65 (1H, dd, ^3J = 8.7 Hz, ^4J = 2.4 Hz, H_{Ar}), 8.07 (1H, d, ^4J = 2.4 Hz, H_{Ar}); δ_C(75 MHz, $CDCl_3$) 14.0, 37.9, 105.4, 109.9, 119.7, 126.4, 129.4, 130.9, 132.4, 134.0, 134.4, 134.8, 169.3; ν_{max} (KBr)/cm^{-1} 3186, 1649, 1477, 1424, 1391, 1323, 1204, 1085, 995, 822, 787, 726; *m/z* (EI) 292/290 (M^+, 98/100%), 277/275 (47/49), 263/261 (29/30), 168 (40), 167 (48), 154 (21), 127 (14), 77 (16), 74 (27), 63 (10), 59 (41), 43 (48); Found: C, 53.83; H, 3.85; N, 9.67. Calc. for $C_{13}H_{11}BrN_2O$: C, 53.63; H, 3.81; N, 9.62%.



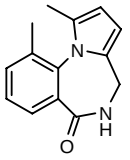
13c

8-Chloro-1-methyl-4,5-dihydro-6*H*-pyrrolo[1,2-*a*][1,4]benzodiazepin-6-one (13c) was obtained according to General procedure E from **1c** (1 g, 3.77 mmol); eluent: benzene; 75% (0.7 g); white solid; mp 195–196 °C (benzene–petroleum ether); δ_H(300 MHz, $CDCl_3$) 2.28 (3H, s, Me), 4.08 (1H, dd, ^2J = 15.6 Hz, ^3J = 5.7 Hz, CH_2), 4.12 (1H, dd, ^2J = 15.6 Hz, ^3J = 6.6 Hz, CH_2), 6.01 (2H, s, H_{Pyr}), 7.21 (1H, d, ^3J = 8.7 Hz, H_{Ar}), 7.50 (1H, dd, ^3J = 8.7 Hz, ^4J = 2.4 Hz, H_{Ar}), 7.92 (1H, d, ^4J = 2.4 Hz, H_{Ar}), 8.18 (1H, br dd, ^3J = 5.7 Hz, ^3J = 6.6 Hz, NH); δ_C(75 MHz, $CDCl_3$) 14.0, 37.9, 105.4, 109.9, 126.2, 129.4, 130.7, 131.1, 131.5, 132.0, 132.4, 134.4, 169.5; ν_{max} (KBr)/cm^{-1} 3237, 1619, 1480, 1329, 1205, 1124, 938, 896, 832, 796, 730; *m/z* (EI) 248/246 (M^+, 33/100%), 233/231 (24/74), 219/217 (15/47), 204/202 (6/18), 190/188 (8/26), 168 (45), 154 (19), 110 (16), 75 (52), 63 (25), 51 (42); Found: C, 63.09; H, 4.40; N, 11.18. Calc. for $C_{13}H_{11}ClN_2O$: C, 63.29; H, 4.49; N, 11.36%.



13d

8,9-Dimethoxy-1-methyl-4,5-dihydro-6*H*-pyrrolo[1,2-*a*][1,4]benzodiazepin-6-one (13d)[1] was obtained according to General procedure E from **1d** (1 g, 3.44 mmol); eluent: benzene; 78% (0.73 g); beige prisms.

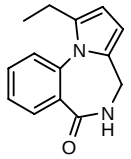


13e

1,10-Dimethyl-4,5-dihydro-6*H*-pyrrolo[1,2-*a*][1,4]benzodiazepin-6-one (13e) was synthesized according to General procedure E from **1e** (1g, 4.09 mmol); product was isolated by column chromatography on silica gel (eluent: ethyl acetate–benzene–petroleum ether, 9:2:6); 11% (0.1 g); white solid; mp 191–192 °C (ethyl acetate–petroleum ether); δ_H(300 MHz, $CDCl_3$) 2.06 (3H, s, Me), 2.18 (3H, s, Me), 4.08 (2H, d, ^3J = 6.0 Hz, CH_2), 5.96 (1H, d, ^3J = 3.3 Hz, H_{Pyr}), 6.02 (1H, d, ^3J = 3.3 Hz, H_{Pyr}), 7.31-7.36 (1H, m, H_{Ar}), 7.41-7.44 (1H, m, H_{Ar}), 7.70-7.73 (1H, m, H_{Ar}), 7.79 (1H, br t, ^3J = 6.0 Hz, NH); δ_C(75 MHz, $CDCl_3$) 12.9, 18.2, 38.3, 105.1, 108.2, 127.1, 127.8, 131.5, 131.7, 132.8, 133.7, 133.9, 134.9, 170.9; ν_{max} (KBr)/cm^{-1} 3308, 1652, 1616,

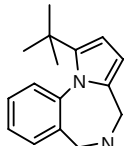
1584, 1472, 1404, 1328, 1200, 1072, 996, 772; *m/z* (EI) 226 (M^+, 100%), 211 (80), 196 (13), 182 (43), 168 (90), 154 (14), 115 (11), 89 (23), 77 (23), 63 (30), 51 (38); Found: C, 74.51; H, 6.03; N, 12.40. Calc. for $C_{14}H_{14}N_2O$: C, 74.31; H, 6.24; N, 12.38%.

Compound **13e** was also synthesized from 2-amino-*N*-(2,5-dioxohexyl)-3-methylbenzamide (**14e**) (0.2 g, 0.76 mmol) similarly to the preparation of **13f** from **14f**, 75% (0.13 g), as well as from **24e** (1 g, 3.42 mmol) according to General procedure H (eluent: ethyl acetate–petroleum ether (1:2)); 80% (0.62 g);



13g

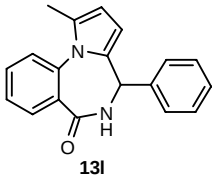
1-Ethyl-4,5-dihydro-6*H*-pyrrolo[1,2-*a*][1,4]benzodiazepin-6-one (13g) was synthesized according to General procedure E from **1g** (1g, 4.1 mmol); eluent: benzene; 70% (0.65 g); white solid; mp 181–182 °C (benzene–petroleum ether); δ_H(300 MHz, $CDCl_3$) 1.17 (3H, t, ^3J = 7.5 Hz, CH_2*Me*), 2.54 (1H, dq, ^2J = 15.0 Hz, ^3J = 7.5 Hz, *CH*$_2$Me), 2.79 (1H, dq, ^2J = 15.0 Hz, ^3J = 7.5 Hz, *CH*$_2$Me), 4.09 (2H, d, ^3J = 6.0 Hz, CH_2), 6.04 (1H, d, ^3J = 3.3 Hz, H_{Pyr}), 6.06 (1H, d, ^3J = 3.3 Hz, H_{Pyr}), 7.27-7.31 (1H, m, H_{Ar}), 7.35-7.41 (1H, m, H_{Ar}), 7.51-7.56 (1H, m, H_{Ar}), 7.90 (1H, br t, ^3J = 6.0 Hz, NH), 7.93-7.96 (1H, m, H_{Ar}); δ_C(75 MHz, $CDCl_3$): 13.1, 21.1, 38.0, 104.9, 107.5, 124.9, 126.2, 129.4, 131.2, 131.4, 132.7, 135.9, 136.1, 170.7; ν_{max} (KBr)/cm^{-1} 3172, 1664, 1604, 1516, 1468, 1416, 1340, 1324, 1268, 1208, 764; *m/z* (EI) 226 (M^+, 55%), 211 (35), 197 (42), 182 (33), 168 (61), 154 (25), 127 (12), 115 (15), 102 (19), 90 (17), 77 (57), 63 (42), 51 (81), 38 (100); Found: C, 74.49; H, 6.02; N, 12.33. Calc. for $C_{14}H_{14}N_2O$: C, 74.31; H, 6.24; N, 12.38%.



13h

1-*tert*-Butyl-4,5-dihydro-6*H*-pyrrolo[1,2-*a*][1,4]benzodiazepin-6-one (13h) was synthesized according to General procedure H from **(24h)** (1 g, 3.12 mmol); product was isolated by column chromatography on silica gel (eluent: acetone–petroleum ether, 2:5); 19% (0.15 g); colorless plates, mp 218–219 °C (acetone–petroleum ether); δ_H(300 MHz, $CDCl_3$) 1.22 (9H, s, *t*-Bu), 3.96 (1H, dd, ^2J = 15.6 Hz, ^3J = 6.0 Hz, CH_2), 4.00 (1H, dd, ^2J = 15.6 Hz, ^3J = 6.3 Hz, CH_2), 6.01 (1H, d, ^3J = 3.3 Hz, H_{Pyr}), 6.13 (1H, d, ^3J = 3.3 Hz, H_{Pyr}), 7.03 (1H, br dd, ^3J = 6.0 Hz, ^3J = 6.3 Hz, NH), 7.39-7.54 (3H, m, H_{Ar}), 7.84-7.87 (1H, m, H_{Ar}); δ_C(75 MHz, $CDCl_3$) 32.2 (3C), 33.0,

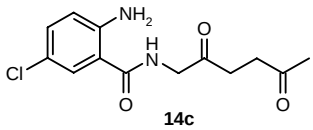
38.5, 104.6, 108.6, 127.0, 127.7, 129.9, 130.1, 130.5, 134.8, 138.4, 144.8, 170.6; ν_{max} (KBr)/cm^{-1} 3180, 1664, 1604, 1476, 1404, 1368, 1340, 1277, 1252, 1220, 1188, 1152, 1064, 976, 940, 764; *m/z* (EI) 254 (M$^+$, 50%), 239 (100), 210 (22), 196 (23), 181 (14), 77 (21), 43 (28); Found: C, 75.61; H, 7.32; N, 10.92. Calc. for $C_{16}H_{18}N_2O$: C, 75.56; H, 7.13; N, 11.01%.



13l

1-Methyl-4-phenyl-4,5-dihydro-6*H*-pyrrolo[1,2-*a*][1,4]benzodiazepin-6-one (13l) was synthesized according to General procedure H from **24l** (1 g, 2.82 mmol); eluent: ethyl acetate–petroleum ether (1:2); 67% (0.55 g); colorless prisms; mp 185–186 °C (petroleum ether–acetone); product was obtained as a mixture of two conformer.

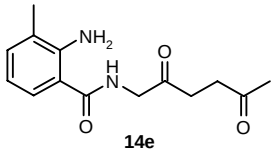
δ_H(600 MHz, DMSO-d$_6$) conformer A, 58%: 2.26 (3H, s, Me), 5.57 (1H, d, ^3J = 7.6 Hz, CH), 6.09 (1H, d, ^3J = 3.3 Hz, H$_{Fur}$), 6.25 (1H, d, ^3J = 3.3 Hz, H$_{Fur}$), 6.92-6.99 (3H, m, H$_{Ar}$), 7.01-7.06 (2H, m, H$_{Ar}$), 7.08-7.12 (1H, m, H$_{Ar}$), 7.14-7.17 (1H, m, H$_{Ar}$), 7.27-7.31 (1H, m, H$_{Ar}$), 7.50-7.53 (1H, m, H$_{Ar}$), 9.23 (1H, d, ^3J = 7.6 Hz, NH); conformer B, 42%: 2.29 (3H, s, Me), 5.24 (1H, d, ^3J = 3.5 Hz, H$_{Fur}$), 5.30 (1H, d, ^3J = 5.6 Hz, CH), 5.94 (1H, d, ^3J = 3.5 Hz, H$_{Fur}$), 7.37-7.43 (3H, m, H$_{Ar}$), 7.47-7.50 (2H, m, H$_{Ar}$), 7.55-7.59 (2H, m, H$_{Ar}$), 7.65-7.69 (1H, m, H$_{Ar}$), 7.84-7.87 (1H, m, H$_{Ar}$), 8.74 (1H, d, ^3J = 5.6 Hz, NH); δ_C(150.9 MHz, DMSO-d$_6$, conformer A / conformer B) 14.3/14.2, 51.5/53.4, 107.8/105.4, 109.9/109.6, 124.9/125.6, 126.1/126.9, 126.3/128.9 (2C), 126.8/128.7, 128.1/128.8 (2C), 129.4/129.5, 130.9/131.2, 131.1/130.6, 131.4/132.0, 134.4/138.0, 135.4/135.4, 140.1/134.4, 169.0/168.6; ν_{max} (KBr)/cm^{-1} 3168, 1640, 1604, 1488, 1460, 1404, 1324, 868, 768; *m/z* (EI) 288 (M$^+$, 100%), 273 (84), 230 (24), 211 (56), 184 (57), 167 (13), 101 (23), 77 (32), 59 (30), 43 (67); Found: C, 79.24; H, 5.77; N, 9.56. Calc. for $C_{19}H_{16}N_2O$: C, 79.14; H, 5.59; N, 9.71%.



14c

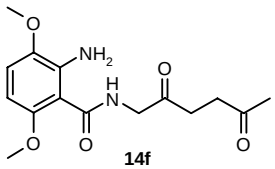
2-Amino-5-chloro-*N*-(2,5-dioxohexyl)benzamide (14c) was obtained according to General procedure E from **1c** (1 g, 3.77 mmol) but reaction mixture was stirred for 1 h (increase of reaction time leads to decrease of yield of **14c**); product was isolated by column chromatography on Al_2O_3 (eluent: ethyl acetate–petroleum ether, 1:2); 15% (0.16 g); white powder; mp 94–95 °C (ethyl acetate–petroleum ether); δ_H(300 MHz, $CDCl_3$) 2.17 (3H, s, Me), 2.67-2.72 (2H, m, CH_2), 2.79-2.83 (2H, m, CH_2), 4.31 (2H, d, ^3J = 4.8 Hz, CH_2), 5.49 (2H, br s, NH_2), 6.59 (1H, d, ^3J =

8.7 Hz, H_{Ar}), 6.89 (1H, br t, ^3J = 4.8 Hz, NH), 7.12 (1H, dd, ^3J = 8.7 Hz, ^4J = 2.4 Hz, H_{Ar}), 7.36 (1H, d, ^4J = 2.4 Hz, H_{Ar}); δ_C(75 MHz, $CDCl_3$) 29.7, 33.5, 37.0, 49.3, 116.0, 118.5, 120.9, 127.1, 132.4, 147.2, 168.0, 204.4, 206.9; ν_{max} (KBr)/cm^{-1} 3457, 3344, 1719, 1632, 1538, 1407, 1366, 1258, 1165, 1092, 1004, 833; *m/z* (EI) 284/282 (M^+, 13/40%), 266/264 (5/16), 239 (11), 184 (39), 156 (45), 154 (100), 138 (23), 128/126 (20/58), 120 (25), 99 (86), 95 (20), 89 (32), 71 (13), 45 (23), 43 (13); Found: C, 55.25; H, 5.16; N, 10.02. Calc. for $C_{13}H_{15}ClN_2O_3$: C, 55.23; H, 5.35; N, 9.91%.



14e

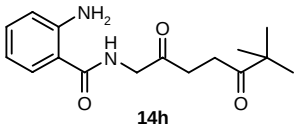
2-Amino-3-methyl-*N*-(2,5-dioxohexyl)benzamide (14e) was synthesized according to General procedure E from **1e** (1g, 4.09 mmol); product was isolated by column chromatography on silica gel (eluent: ethyl acetate–benzene–petroleum ether, 9:2:6); 20% (0.21 g); flakes; mp 102–103 °C (ethyl acetate–petroleum ether); δ_H(300 MHz, $CDCl_3$) 2.12 (3H, s, Me), 2.16 (3H, s, Me), 2.67-2.71 (2H, m, CH_2), 2.76-2.80 (2H, m, CH_2), 4.31 (2H, d, ^3J = 4.8 Hz, CH_2), 5.57 (2H, br s, NH_2), 6.54-6.59 (1H, m, H_{Ar}), 6.89 (1H, br t, ^3J = 4.8 Hz, NH), 7.09-7.12 (1H, m, H_{Ar}), 7.28-7.31 (1H, m, H_{Ar}); δ_C(75 MHz, $CDCl_3$) 17.4, 29.7, 33.4, 36.9, 49.3, 114.5, 115.9, 123.6, 125.3, 133.3, 147.1, 169.5, 204.6, 206.8; ν_{max} (KBr)/cm^{-1} 3420, 3336, 1708, 1616, 1532, 1404, 1368, 1260, 1188, 1088, 1000, 744; *m/z* (EI) 262 (M^+, 8%), 134 (100), 106 (32), 99 (14), 77 (50), 51 (17), 43 (97); Found: C, 64.21; H, 7.01; N, 10.76. Calc. for $C_{14}H_{18}N_2O_3$: C, 64.11; H, 6.92; N, 10.68%.



14f

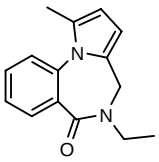
2-Amino-3,6-dimethoxy-*N*-(2,5-dioxohexyl)benzamide (14f) was synthesized according to General procedure E from **1f** (1g, 3.44 mmol); reaction time was 2 h; reaction mixture was poured into water (100 mL), neutralized to pH ~ 7 with $NaHCO_3$ and extracted with ethyl acetate (4×30 mL). The combined organic fractions were dried over Na_2SO_4. Solvent was evaporated under reduced pressure. Product **14f** was isolated by column chromatography on Al_2O_3 (eluent: ethyl acetate–petroleum ether, 1:1); 32% (0.34 g); white solid; mp 104–105 °C (ethyl acetate–petroleum ether); δ_H(300 MHz, $CDCl_3$) 2.18 (3H, s, Me), 2.70-2.75 (2H, m, CH_2), 2.78-2.82 (2H, m, CH_2), 3.79 (3H, s, OMe), 3.87 (3H, s, OMe), 4.34 (2H, d, ^3J = 4.8 Hz, CH_2), 6.08 (1H, d, ^3J = 8.7 Hz, H_{Ar}), 6.68 (1H, d, ^3J = 8.7 Hz, H_{Ar}), 8.74 (1H, br t, ^3J = 4.8 Hz, NH); δ_C(75 MHz,

$CDCl_3$) 29.7, 33.4, 36.8, 49.5, 55.9, 56.0, 96.0, 103.1, 111.3, 142.0, 142.7, 153.0, 168.3, 204.7, 206.8; ν_{max} (KBr)/cm^{-1} 3504, 3347, 3314, 1710, 1628, 1534, 1458, 1407, 1357, 1268, 1226, 1157, 1094, 966, 769; *m/z* (EI) 308 (M^+, 17%), 181 (20), 180 (100), 165 (25), 150 (43), 122 (16), 45 (22), 43 (16); Found: C, 58.63; H, 6.43; N, 9.20. Calc. for $C_{15}H_{20}N_2O_5$: C, 58.43; H, 6.54; N, 9.09%.



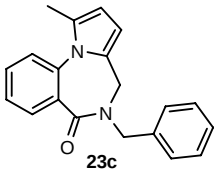
14h

2-Amino-*N*-(6,6-dimethyl-2,5-dioxoheptyl)benzamide (14h) was synthesized according to General procedure E from **1h** (1g, 3.67 mmol); reaction time was 4 h. Product **14h** was isolated by column chromatography on Al_2O_3 (eluent: ethyl acetate–petroleum ether, 1:1); 57% (0.6 g); white solid; mp 128–129°C; δ_H(300 MHz, $CDCl_3$): 1.15 (9H, s, t-Bu), 2.66-2.70 (2H, m, CH_2), 2.85-2.89 (2H, m, CH_2), 4.35 (2H, d, ^3J = 4.5 Hz, CH_2), 5.51 (2H, br s, NH_2), 6.60-6.66 (2H, m, H_{Ar}), 6.86 (1H, br t, ^3J = 4.5 Hz, NH), 7.15-7.21 (1H, m, H_{Ar}), 7.38-7.41 (1H, m, H_{Ar}); δ_C(75 MHz, $CDCl_3$) 26.5 (3C), 30.8, 33.6, 43.8, 49.4, 115.1, 116.6, 117.2, 127.5, 132.5, 148.8, 169.0, 204.8 (2C); ν_{max} (KBr)/cm^{-1} 3444, 3375, 3346, 1732, 1694, 1616, 1528, 1400, 1304, 1267, 1157, 1061, 995, 759; *m/z* (EI) 290 (M^+, 11%), 120 (100), 92 (18), 65 (15), 57 (14); Found: C, 66.37; H, 7.89; N, 9.57. Calc. for $C_{16}H_{22}N_2O_3$: C, 66.19; H, 7.64; N, 9.65%.



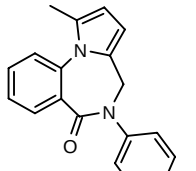
23b

5-Ethyl-1-methyl-4,5-dihydro-6*H*-pyrrolo[1,2-*a*][1,4]benzodiazepin-6-one (23b) was synthesized according to General procedure F using ethyl bromide (2.05 g, 18.84 mmol); 6 h; eluent: CH_2Cl_2, 93 % (2.1 g); colorless needles; mp 156–157 °C (CH_2Cl_2–petroleum ether); δ_H(300 MHz, $CDCl_3$) 1.20 (3H, t, ^3J = 7.2 Hz, CH_2*Me*), 2.31 (3H, s, Me), 3.46 (1H, dq, ^2J = 14.4 Hz, ^3J = 7.2 Hz, *CH*$_2$Me), 3.74 (1H, dq, ^2J = 14.4 Hz, ^3J = 7.2 Hz, *CH*$_2$Me), 4.02 (1H, d, ^2J = 15.6 Hz, CH_2), 4.22 (1H, d, ^2J = 15.6 Hz, CH_2), 5.99 (1H, d, ^3J = 3.3 Hz, H_{Pyr}), 6.03 (1H, d, ^3J = 3.3 Hz, H_{Pyr}), 7.22-7.25 (1H, m, H_{Ar}), 7.33-7.38 (1H, m, H_{Ar}), 7.47-7.53 (1H, m, H_{Ar}), 7.92-7.95 (1H, m, H_{Ar}); δ_C(75 MHz, $CDCl_3$) 13.1, 14.0, 42.3, 43.8, 104.9, 109.3, 124.3, 126.1, 129.1, 130.8, 131.0, 131.5, 131.6, 135.2, 167.3; ν_{max} (KBr)/cm^{-1} 1618, 1470, 1300, 1211, 1144, 771, 713; *m/z* (EI) 240 (M^+, 100%), 225 (61), 197 (51), 184 (28), 168 (43), 154 (89), 99 (24), 84 (19), 77 (31), 63 (15), 51 (34), 42 (69); Found: C, 74.89; H, 6.71; N, 11.49. Calc. for $C_{15}H_{16}N_2O$: C, 74.97; H, 6.71; N, 11.66%.



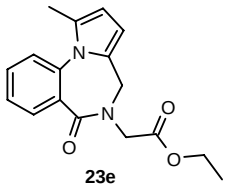
23c

5-Benzyl-1-methyl-4,5-dihydro-6*H*-pyrrolo[1,2-*a*][1,4]benzodiazepin-6-one (23c) was synthesized according to General procedure F using benzyl chloride (2.38 g, 18.84 mmol); 48 h; eluent: CH_2Cl_2, 85 % (2.41 g); colorless prisms; mp 132–133 °C (CH_2Cl_2–petroleum ether); δ_H(300 MHz, $CDCl_3$) 2.33 (3H, s, Me), 3.95 (1H, d, ^2J = 15.6 Hz, CH_2), 4.15 (1H, d, ^2J = 15.6 Hz, CH_2), 4.23 (1H, d, ^2J = 15.0 Hz, CH_2), 5.28 (1H, d, ^2J = 15.0 Hz, CH_2), 5.92 (1H, d, ^3J = 3.3 Hz, H_{Pyr}), 6.00 (1H, d, ^3J = 3.3 Hz, H_{Pyr}), 7.25-7.36 (6H, m, H_{Ar}), 7.37-7.43 (1H, m, H_{Ar}), 7.51-7.57 (1H, m, H_{Ar}), 8.02-8.05 (1H, m, H_{Ar}); δ_C(75 MHz, $CDCl_3$) 13.9, 43.2, 50.1, 105.3, 109.3, 124.4, 126.1, 127.5, 128.1(2C), 128.6(2C), 129.3, 130.7, 131.0, 131.6, 135.3, 136.6(2C), 168.0; ν_{max} (KBr)/cm^{-1} 1630, 1471, 1403, 1237, 1143, 1025, 936, 762; *m/z* (EI) 302 (M^+, 22%), 197 (80), 182 (17), 168 (31), 154 (100), 91 (71), 77 (32), 65 (28), 51 (32); Found: C, 79.68; H, 5.96; N, 9.33. Calc. for $C_{20}H_{18}N_2O$: C, 79.44; H, 6.00; N, 9.26%.



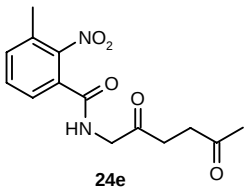
23d

5-(4-Chlorophenyl)-1-methyl-4,5-dihydro-6*H*-pyrrolo[1,2-*a*][1,4]benzodiazepin-6-one (23d) was synthesized according to General procedure H from **25d** (1 g, 2.57 mmol); eluent: benzene–petroleum ether (1:2); 77% (0.64 g); white solid; mp 129–130 °C (petroleum ether–acetone); δ_H(300 MHz, $CDCl_3$) 2.36 (3H, s, Me), 4.37 (1H, d, ^2J = 15.6 Hz, CH_2), 4.67 (1H, d, ^2J = 15.6 Hz, CH_2), 6.07 (2H, s, H_{Pyr}), 7.26 (2H, d, ^3J = 8.7 Hz, H_{Ar}), 7.29-7.32 (1H, m, H_{Ar}), 7.36 (2H, d, ^3J = 8.7 Hz, H_{Ar}), 7.39-7.44 (1H, m, H_{Ar}), 7.55-7.60 (1H, m, H_{Ar}), 7.98-8.01 (1H, m, H_{Ar}); δ_C(75 MHz, $CDCl_3$) 14.0, 47.8, 105.6, 109.7, 124.5, 126.3, 127.5 (2C), 129.3 (2C), 129.6, 130.7, 130.8, 131.4, 131.8, 132.6, 135.3, 141.3, 167.6; ν_{max} (KBr)/cm^{-1} 1644, 1492, 1460, 1408, 1384, 1336, 1196, 1160, 1092, 1012, 816, 764, 712; *m/z* (EI) 324/322 (M^+, 36/100%), 309/307 (34/98), 196 (44), 183 (65), 168 (75), 154 (85), 141 (15), 127 (16), 110 (23), 77 (22), 59 (20), 51 (33), 43 (44); Found: C, 70.93; H, 4.73; N, 8.51. Calc. for $C_{19}H_{15}ClN_2O$: C, 70.70; H, 4.68; N, 8.68%.



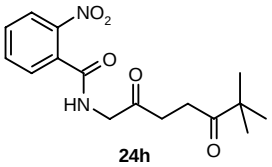
23e

5-(Ethoxycarbonylmethyl)-1-methyl-4,5-dihydro-6*H*-pyrrolo[1,2-*a*][1,4]benzodiazepin-6-one (23e) was synthesized according to General procedure F using ethyl iodoacetate (4.03 g, 18.84 mmol); 24 h; eluent: benzene-petroleum ether (1:2), 67 % (1.9 g); light-yellow oil; δ_H(300 MHz, $CDCl_3$) 1.26 (3H, t, ^3J = 7.2 Hz, CH_2*Me*), 2.31 (3H, s, Me), 3.81 (1H, d, ^2J = 17.7 Hz, CH_2), 4.01 (1H, d, ^2J = 15.9 Hz, CH_2), 4.11-4.27 (2H, m, *CH*$_2$Me), 4.44 (1H, d, ^2J = 15.9 Hz, CH_2), 4.81 (1H, d, ^2J = 17.7 Hz, CH_2), 6.01 (1H, d, ^3J = 3.3 Hz, H_{Pyr}), 6.04 (1H, d, ^3J = 3.3 Hz, H_{Pyr}), 7.24-7.27 (1H, m, H_{Ar}), 7.35-7.40 (1H, m, H_{Ar}), 7.51-7.56 (1H, m, H_{Ar}), 7.95-7.98 (1H, m, H_{Ar}); δ_C(75 MHz, $CDCl_3$) 13.9, 14.0, 45.1, 48.5, 61.3, 105.3, 109.4, 124.4, 126.1, 129.5, 129.8, 130.5, 131.3, 131.7, 135.3, 168.1, 169.0; ν_{max} (KBr)/cm^{-1} 1754, 1657, 1149, 1112, 1026, 933, 860, 770; *m/z* (EI) 298 (M^+, 36%), 211 (37), 196 (13), 184 (29), 167 (24), 154 (25), 77 (15), 51 (18), 42 (100); Found: C, 68.20; H, 6.26; N, 9.12. Calc. for $C_{17}H_{18}N_2O_3$: C, 68.44; H, 6.08; N, 9.39%.



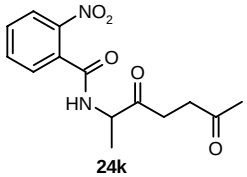
24e

3-Methyl-*N*-(2,5-dioxohexyl)-2-nitrobenzamide (24e) was synthesized according to General procedure G from **6e** (1 g, 3.64 mmol); eluent: CH_2Cl_2–petroleum ether (1:1); 79% (0.84 g); colorless plates; mp 101–102 °C (CH_2Cl_2–petroleum ether); δ_H(300 MHz, $CDCl_3$) 2.16 (3H, s, Me), 2.35 (3H, s, Me), 2.67-2.71 (2H, m, CH_2), 2.80-2.82 (2H, m, CH_2), 4.31 (2H, d, ^3J = 4.5 Hz, CH_2), 6.89 (1H, br t, ^3J = 4.5 Hz, NH), 7.36-7.47 (3H, m, H_{Ar}); δ_C(75 MHz, $CDCl_3$) 17.5, 29.6, 33.4, 37.0, 49.5, 125.6, 129.1, 130.4, 131.3, 133.9, 149.5, 165.0, 203.9, 206.8; ν_{max} (KBr)/cm^{-1} 3300, 1728, 1708, 1640, 1528, 1432, 1368, 1296, 1192, 1088, 812, 776; *m/z* (EI) 262 (M^+–30, 5%), 176 (53), 164 (97), 148 (40), 134 (39), 118 (55), 106 (39), 99 (100), 89 (63), 77 (38), 71 (45), 65 (87), 59 (21), 55 (55), 51 (33), 43 (51); Found: C, 57.76; H, 5.78; N, 9.64. Calc. for $C_{14}H_{16}N_2O_5$: C, 57.53; H, 5.52; N, 9.58.



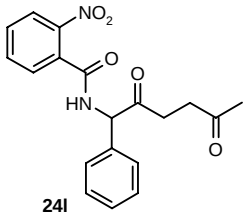
24h

***N*-(6,6-dimethyl-2,5-dioxohexyl)-2-nitrobenzamide (24h)** was synthesized according to General procedure G from **6h** (1 g, 3.3 mmol); reaction time 48 h; product was extracted with ethyl acetate; eluent: benzene–petroleum ether (1:1); 43% (0.46 g); colorless prisms; mp 79–80 °C (petroleum ether–acetone); δ_H(300 MHz, $CDCl_3$) 1.15 (9H, s, t-Bu), 2.68-2.72 (2H, m, CH_2), 2.87-2.91 (2H, m, CH_2), 4.42 (2H, d, ^3J = 4.8 Hz, CH_2), 6.68 (1H, br t, ^3J = 4.8 Hz, NH), 7.53-7.59 (2H, m, H_{Ar}), 7.63-7.68 (1H, m, H_{Ar}), 8.01-8.05 (1H, m, H_{Ar}); δ_C(75 MHz, $CDCl_3$) 26.4 (3C), 30.8, 33.7, 43.8, 49.6, 124.5, 128.7, 130.6, 132.3, 133.6, 146.5, 166.2, 204.0, 214.4; ν_{max} (KBr)/cm^{-1} 3236, 1732, 1704, 1636, 1568, 1524, 1344, 1092, 1052, 1024, 856, 796, 712; *m/z* (EI) 320 (M^+, 2%), 263 (62), 235 (15), 162 (60), 150 (85), 141 (78), 134 (61), 120 (43), 113 (83), 104 (64), 92 (25), 76 (55), 65 (40), 55 (100), 51 (75), 43 (63); Found: C, 60.17; H, 6.43; N, 8.53. Calc. for $C_{16}H_{20}N_2O_5$: C, 59.99; H, 6.29; N, 8.74%.



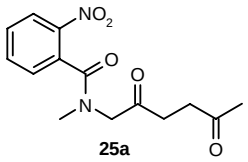
24k

***N*-(2,5-Dioxohept-6-yl)-2-nitrobenzamide (24k)** was synthesized according to General procedure G from **6k** (1 g, 3.64 mmol); eluent: CH_2Cl_2–petroleum ether (1:2); 42% (0.45 g); white solid; mp 90–91 °C (CH_2Cl_2–petroleum ether); δ_H(300 MHz, $CDCl_3$) 1.49 (3H, d, ^3J = 7.2 Hz, CH*Me*), 2.15 (3H, s, Me), 2.68-2.90 (4H, m, CH_2CH_2), 4.79 (1H, dq, ^3J = 6.9 Hz, ^3J = 7.2 Hz, CH), 6.83 (1H, br d, ^3J = 6.9 Hz, NH), 7.48-7.51 (1H, m, H_{Ar}), 7.52-7.58 (1H, m, H_{Ar}), 7.61-7.67 (1H, m, H_{Ar}), 8.00-8.03 (1H, m, H_{Ar}); δ_C(75 MHz, $CDCl_3$) 17.1, 29.7, 32.6, 36.9, 54.6, 124.5, 128.7, 130.5, 132.4, 133.7, 146.3, 165.8, 206.9, 207.4; ν_{max} (KBr)/cm^{-1} 3292, 1724, 1712, 1640, 1520, 1444, 1352, 1176, 856, 796, 752, 712; *m/z* (EI) 262 (M^+–30, 4%), 193 (55), 176 (24), 150 (100), 134 (37), 120 (48), 104 (33), 99 (76), 92 (32), 76 (67), 71 (27), 59 (26), 51 (83), 43 (54); Found: C, 57.62; H, 5.63; N, 9.50. Calc. for $C_{14}H_{16}N_2O_5$: C, 57.53; H, 5.52; N, 9.58%.



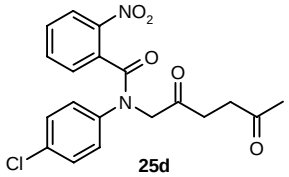
24l

***N*-(2,5-Dioxo-1-phenylhexyl)-2-nitrobenzamide (24l)** was synthesized according to General procedure G from **6l** (1 g, 2.97 mmol); eluent: CH_2Cl_2–petroleum ether (1:2); 40% (0.42 g); white solid; mp 94–95 °C (CH_2Cl_2–petroleum ether); δ_H(300 MHz, $CDCl_3$) 2.14 (3H, s, Me), 2.57-2.85 (4H, m, CH_2CH_2), 5.79 (1H, d, ^3J = 6.0 Hz, CH), 7.15 (1H, br d, ^3J = 6.0 Hz, NH), 7.35-7.42 (5H, m, H_{Ar}), 7.50-7.52 (1H, m, H_{Ar}), 7.53-7.59 (1H, m, H_{Ar}), 7.62-7.67 (1H, m, H_{Ar}), 8.01-8.04 (1H, m, H_{Ar}); δ_C(75 MHz, $CDCl_3$) 29.6, 33.4, 36.9, 63.4, 124.5, 128.1 (2C), 128.8 (2C), 129.2 (2C), 130.6, 132.2, 133.5, 135.7, 146.4, 165.3, 204.3, 206.3; ν_{max} (KBr)/cm^{-1} 3336, 1712, 1640, 1540, 1456, 1348, 1168, 856, 788, 740, 704; *m/z* (EI) 324 (M^+–30, 2%), 255 (85), 239 (31), 222 (19), 165 (26), 150 (100), 134 (53), 120 (62), 104 (87), 99 (86), 92 (44), 77 (43), 65 (29), 51 (48), 43 (67); Found: C, 64.73; H, 5.29; N, 7.67. Calc. for $C_{19}H_{18}N_2O_5$: C, 64.40; H, 5.12; N, 7.91%.



25a

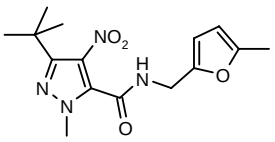
***N*-methyl-(*N*-(2,5-Dioxohexyl)-2-nitrobenzamide (25a)** was obtained according to General procedure H from **7a** (1 g, 3.64 mmol); eluent: ethyl acetate–petroleum ether (1:1). Product was isolated as light-yellow oil (0.75 g, 70%) and used for further transformations without additional purification.



25d

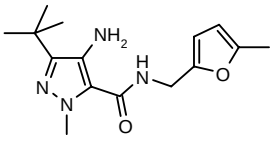
***N*-(4-chlorophenyl)-(*N*-(2,5-Dioxohexyl)-2-nitrobenzamide (25d)** was synthesized according to General procedure G from **7d** (1 g, 2.7 mmol); reaction time 5 h; eluent: ethyl acetate–petroleum ether (1:2); 80% (0.84 g); white solid; mp 108–109 °C (acetone–petroleum ether); δ_H(300 MHz, $CDCl_3$) 2.19 (3H, s, Me), 2.75-2.79 (2H, m, CH_2), 2.84-2.88 (2H, m, CH_2), 4.72 (2H, s, CH_2), 7.08-7.16 (4H, m, H_{Ar}), 7.36-7.41 (2H, m, H_{Ar}), 7.45-7.50 (1H, m, H_{Ar}), 7.95-7.98 (1H, m, H_{Ar}); δ_C(75 MHz, $CDCl_3$) 29.7, 33.5, 37.1, 58.8, 124.4, 128.4 (2C), 129.5 (2C), 129.6, 129.8, 132.4, 133.5, 133.6, 140.8, 145.9, 167.1, 203.4, 206.8; ν_{max} (KBr)/cm^{-1} 1716, 1648, 1528,

1496, 1428, 1352, 1092, 852, 788, 768, 736; *m/z* (EI) 390/388 (M^+, 5/16%), 289 (15), 255 (10), 150 (100), 140 (55), 134 (20), 120 (37), 110 (34), 99 (78), 92 (22), 76 (29), 59 (27), 51 (26), 43 (67); Found: C, 58.93; H, 4.55; N, 7.02. Calc. for $C_{19}H_{17}ClN_2O_5$: C, 58.69; H, 4.41; N, 7.20%.



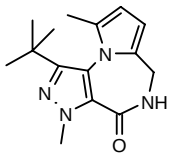
27b

3-*tert*-Butyl-1-methyl-*N*-[(5-methyl-2-furyl)methyl]-4-nitro-1*H*-pyrazole-5-carboxamide (27b) was synthesized according to General procedure A from **2a** (5 g, 45 mmol; solution in 50 mL of benzene) and 3-*tert*-butyl-1-methyl-4-nitro-1*H*-pyrazole-5-carbonyl chloride **26b** (12.16 g, 49.5 mmol; solution in 50 mL of benzene); 88% (12.7 g); colorless needles; mp 176–177 °C (CH_2Cl_2–petroleum ether); δ_H(300 MHz, $CDCl_3$) 1.35 (9H, s, *t*-Bu), 2.24 (3H, s, Me), 3.89 (3H, s, Me), 4.53 (2H, d, ^3J = 5.7 Hz, CH_2), 5.88 (1H, d, ^3J = 3.0 Hz, H_{Fur}), 6.16 (1H, d, ^3J = 3.0 Hz, H_{Fur}), 7.01 (1H, br t, ^3J = 5.7 Hz, NH); δ_C(75 MHz, $CDCl_3$) 13.5, 28.5 (3C), 33.8, 37.2, 39.1, 106.4, 109.0, 131.1, 136.3, 147.7, 152.4, 154.1, 158.0; ν_{max} (KBr)/cm^{-1} 3222, 1644, 1596, 1540, 1492, 1436, 1416, 1348, 1292, 1224, 1196, 1016, 888, 800, 776; *m/z* (EI) 302 (M^+-18, 62%), 136 (86), 122 (13), 110 (95), 95 (100), 83 (48), 67 (64), 57 (88), 53 (44), 43 (96); Found: C, 56.39; H, 6.10; N, 17.73. Calc. for $C_{15}H_{20}N_4O_4$: C, 56.24; H, 6.29; N, 17.49.



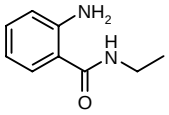
28b

4-Amino-3-*tert*-butyl-1-methyl-*N*-[(5-methyl-2-furyl)methyl]-1*H*-pyrazole-5-carboxamide (28b) was synthesized according to General procedure C from **27b** (1 g, 3.12 mmol); 87% (0.79 g); white solid; mp 81–82 °C (ethyl acetate–petroleum ether); δ_H(300 MHz, $CDCl_3$) 1.34 (9H, s, *t*-Bu), 2.24 (3H, s, Me), 2.86 (2H, br s, NH_2), 4.07 (3H, s, Me), 4.48 (2H, d, ^3J = 5.7 Hz, CH_2), 5.87 (1H, d, ^3J = 3.0 Hz, H_{Fur}), 6.10 (1H, d, ^3J = 3.0 Hz, H_{Fur}), 9.00 (1H, br t, ^3J = 5.7 Hz, NH); δ_C(75 MHz, $CDCl_3$) 13.6, 29.4 (3C), 32.4, 35.7, 39.9, 106.2, 108.0, 123.4, 128.7, 149.7, 151.4, 151.8, 160.4; ν_{max} (KBr)/cm^{-1} 3400, 3268, 3232, 1652, 1544, 1444, 1368, 1340, 1292, 1256, 1216, 1020, 796; *m/z* (EI) 290 (M^+, 8%), 110 (33), 95 (100), 69 (14), 53 (15), 43 (28); Found: C, 61.98; H, 7.83; N, 19.43. Calc. for $C_{15}H_{22}N_4O_2$: C, 62.05; H, 7.64; N, 19.30%.

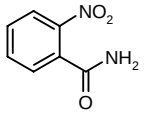


29b

1-*tert*-Butyl-3,9-dimethyl-5,6-dihydropyrazolo[3,4-*f*]pyrrolo[1,2-*a*][1,4]diazepin-4(3H)-one (29b) was synthesized according to General procedure E from **28b** (1 g, 3.44 mmol); eluent: benzene; 76% (0.72 g); white solid; mp 185–186 °C (benzene–petroleum ether); δ_H(300 MHz, $CDCl_3$) 1.32 (9H, s, *t*-Bu), 2.27 (3H, s, Me), 4.02 (1H, dd, ^2J = 15.6 Hz, ^3J = 6.3 Hz, CH_2), 4.04 (3H, s, Me), 4.06 (1H, dd, ^2J = 15.6 Hz, ^3J = 5.1 Hz, CH_2), 5.95 (1H, d, ^3J = 3.3 Hz, H_{Pyr}), 6.01 (1H, d, ^3J = 3.3 Hz, H_{Pyr}), 7.20 (1H, br dd, ^3J = 5.1 Hz, ^3J = 5.7 Hz, NH); δ_C(75 MHz, $CDCl_3$) 14.6, 30.4(3C), 33.3, 38.8, 39.0, 105.9, 108.3, 119.1, 130.4, 131.9, 132.3, 151.9, 162.9; ν_{max} (KBr)/cm^{-1} 3208, 1660, 1520, 1488, 1404, 1364, 1340, 1236, 1208, 992, 784, 744; *m/z* (EI) 272 (M^+, 61%), 257 (33), 228 (24), 103 (10), 92 (14), 77 (36), 65 (29), 57 (14), 52 (42), 41 (100); Found: C, 66.49; H, 7.54; N, 20.70. Calc. for $C_{15}H_{20}N_4O$: C, 66.15; H, 7.40; N, 20.57%.



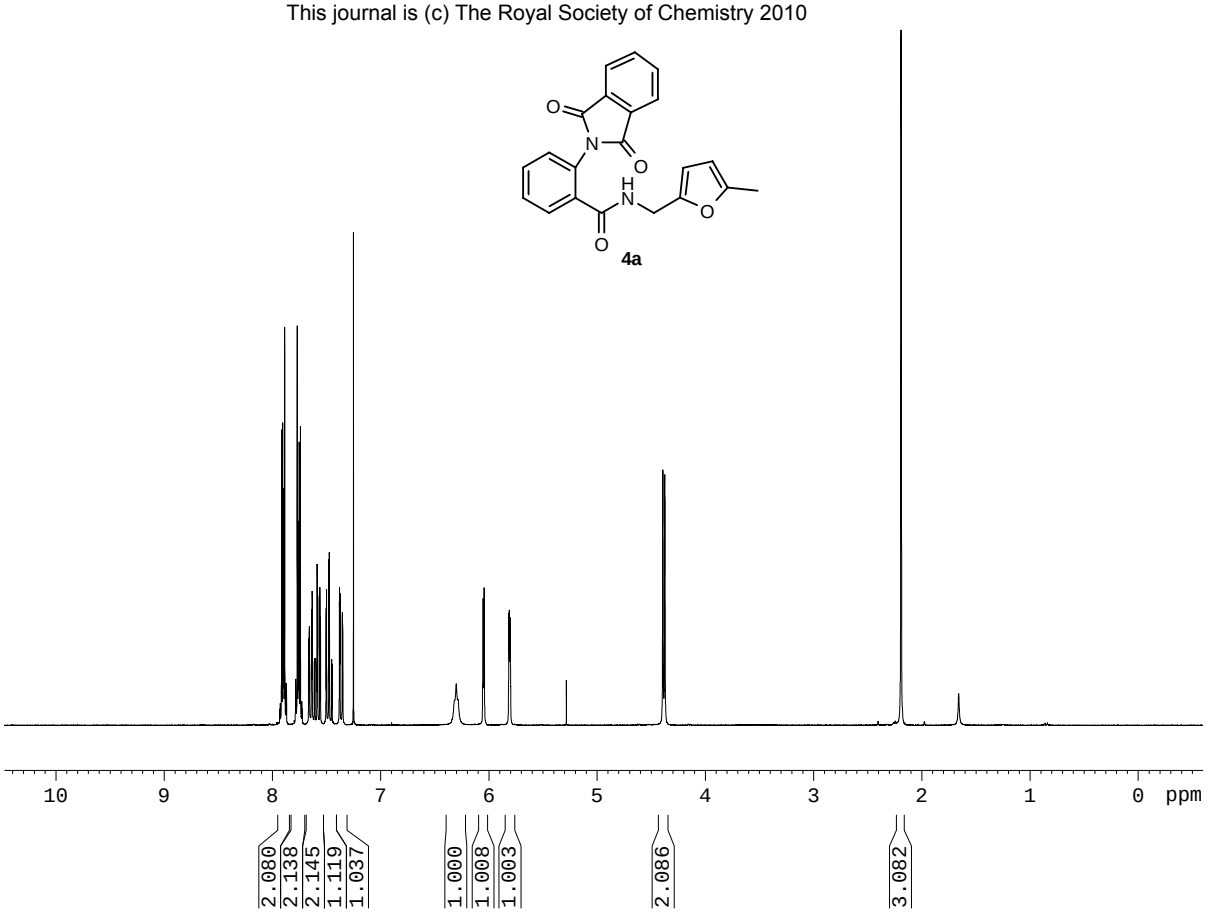
2-Amino-*N*-ethylbenzamide (1m) was isolated when General procedure E was applied to **8b**; white solid; mp 99–100 °C (CCl_4–petroleum ether); δ_H(300 MHz, $CDCl_3$) 1.22 (3H, t, ^3J = 7.2 Hz, Me), 3.44 (2H, dq, ^3J = 5.7 Hz, ^3J = 7.2 Hz, CH_2), 5.48 (2H, br s, NH_2), 6.02 (1H, br d, ^3J = 5.7 Hz, NH), 6.60-6.68 (2H, m, H_{Ar}), 7.15-7.21 (1H, m, H_{Ar}), 7.27-7.30 (1H, m, H_{Ar}); δ_C(75 MHz, $CDCl_3$) 14.8, 34.4, 116.3, 116.5, 117.1, 127.0, 132.0, 148.5, 169.2; ν_{max} (KBr)/cm^{-1} 3422, 3308, 1620, 1588, 1537, 1308, 1261, 1153, 1033, 856, 746; *m/z* (EI) 164 (M^+, 100%), 120 (93), 119 (52), 92 (94), 65 (52), 45 (53), 43 (29); Found: C, 65.63; H, 7.30; N, 16.91. Calc. for $C_9H_{12}N_2O$: C, 65.83; H, 7.37; N, 17.06%.

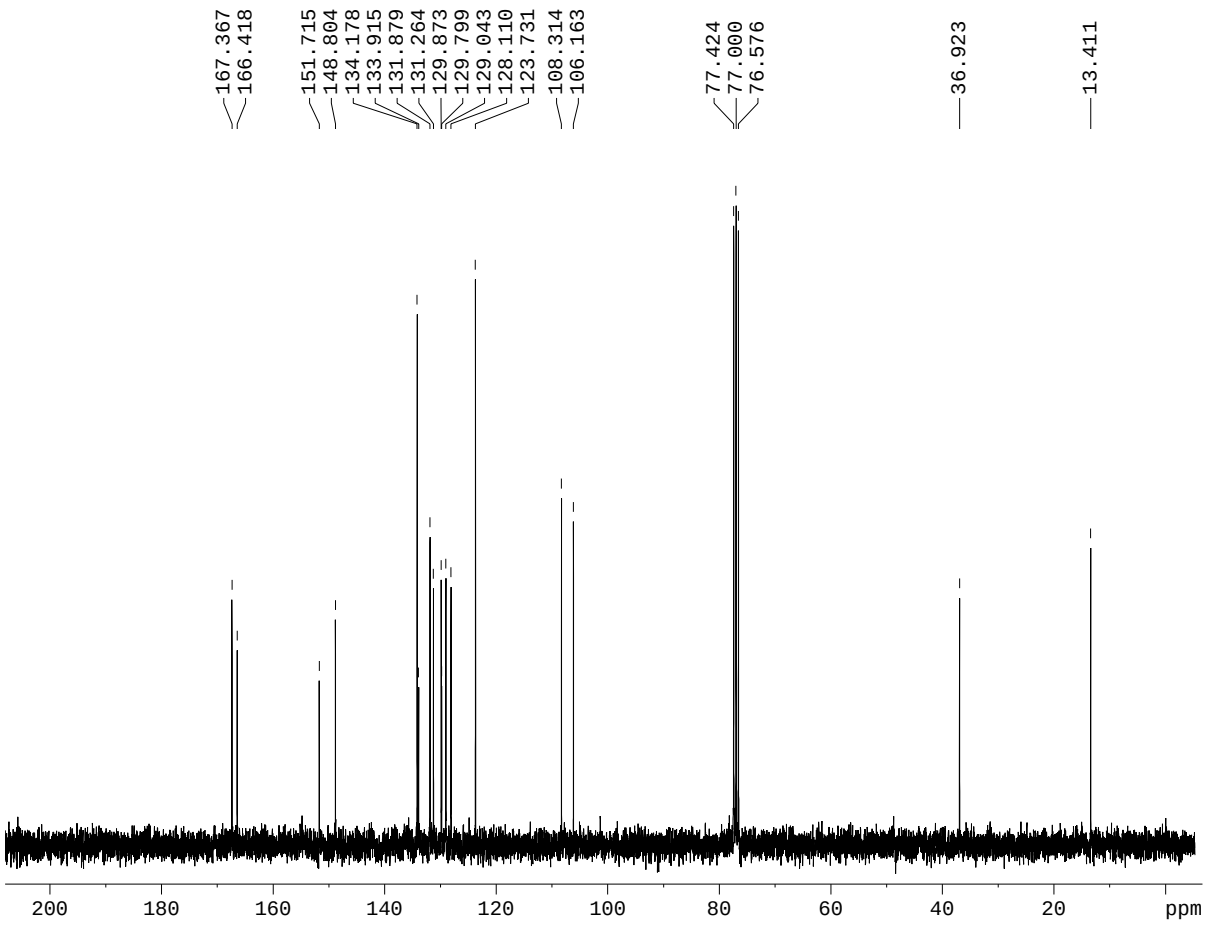


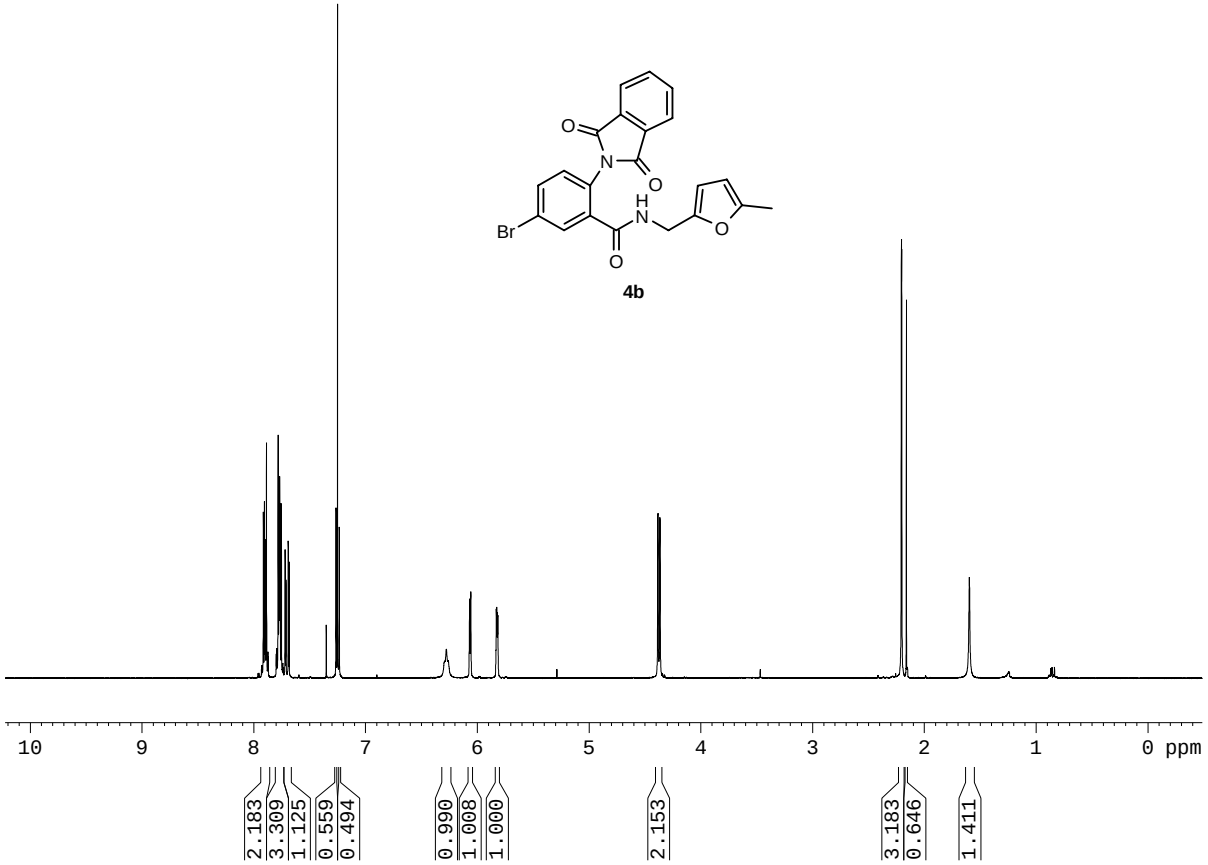
2-Nitrobenzamide was isolated as by-product in transformation of **6a** into **24a**; white solid; mp 176–177 °C (acetone–petroleum ether); δ_H(300 MHz, $CDCl_3$) 7.62-7.70 (3H, m, H_{Ar}+NH), 7.74-7.79 (1H, m, H_{Ar}), 7.97-8.00 (1H, m, H_{Ar}), 8.12 (1H, br s, NH); δ_C(75 MHz, $CDCl_3$) 123.9, 128.8, 130.5, 132.6, 133.3, 147.2, 167.1; ν_{max} (KBr)/cm^{-1} 3364, 3176, 1656, 1576, 1528, 1488, 1444, 1408, 1360, 1120, 860, 788, 696; *m/z* (EI) 166 (M^+, 80%), 150 (100), 118 (24), 104 (15),

92 (41), 76 (72), 65 (49), 51 (94), 43 (23); Found: C, 50.38; H, 3.69; N, 16.73. Calc. for $C_7H_6N_2O_3$: C, 50.61; H, 3.64; N, 16.86%.

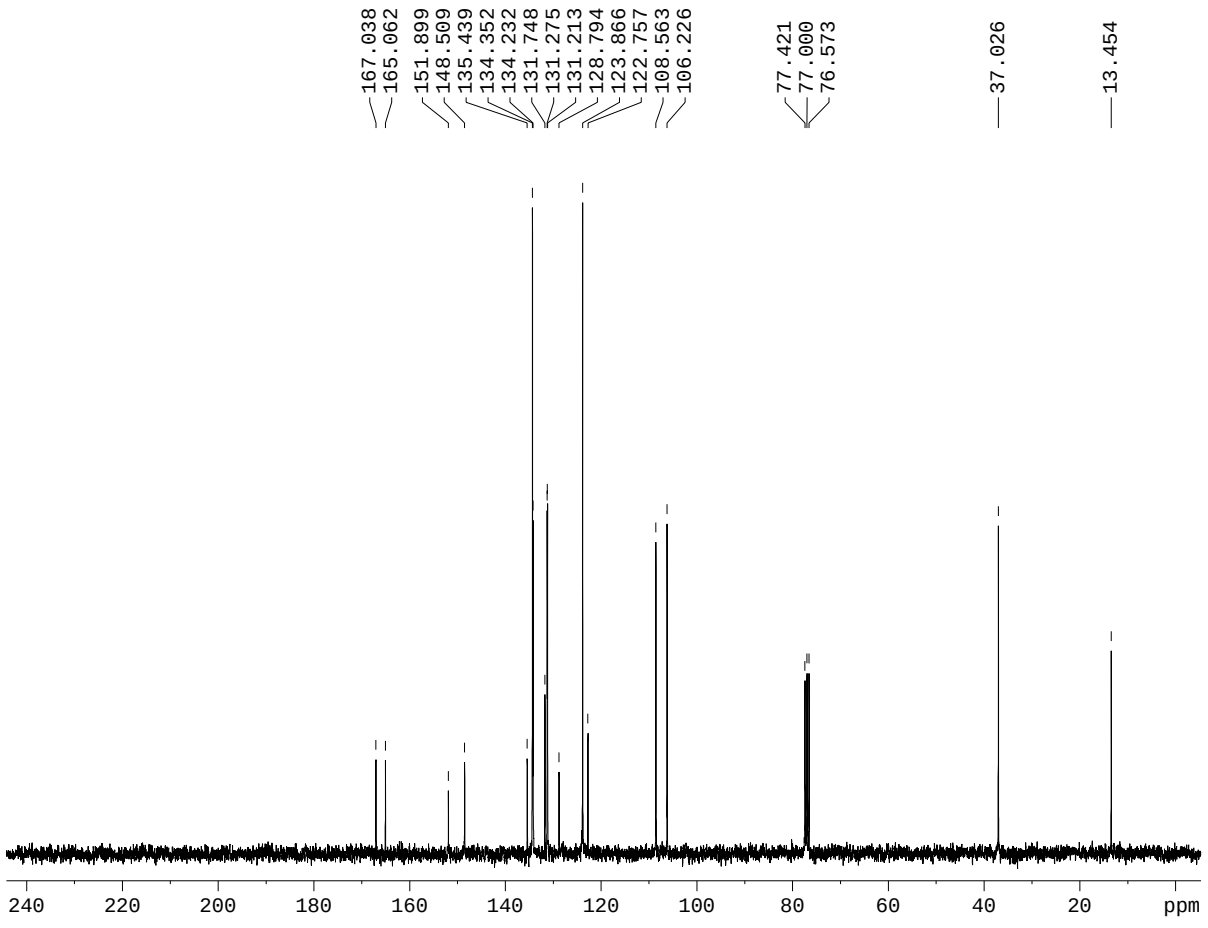
1. 1. T. A. Stroganova, A. V. Butin, V. K. Vasilin, T. A. Nevolina and G. D. Krapivin, *Synlett*, 2007, 1106-1108.

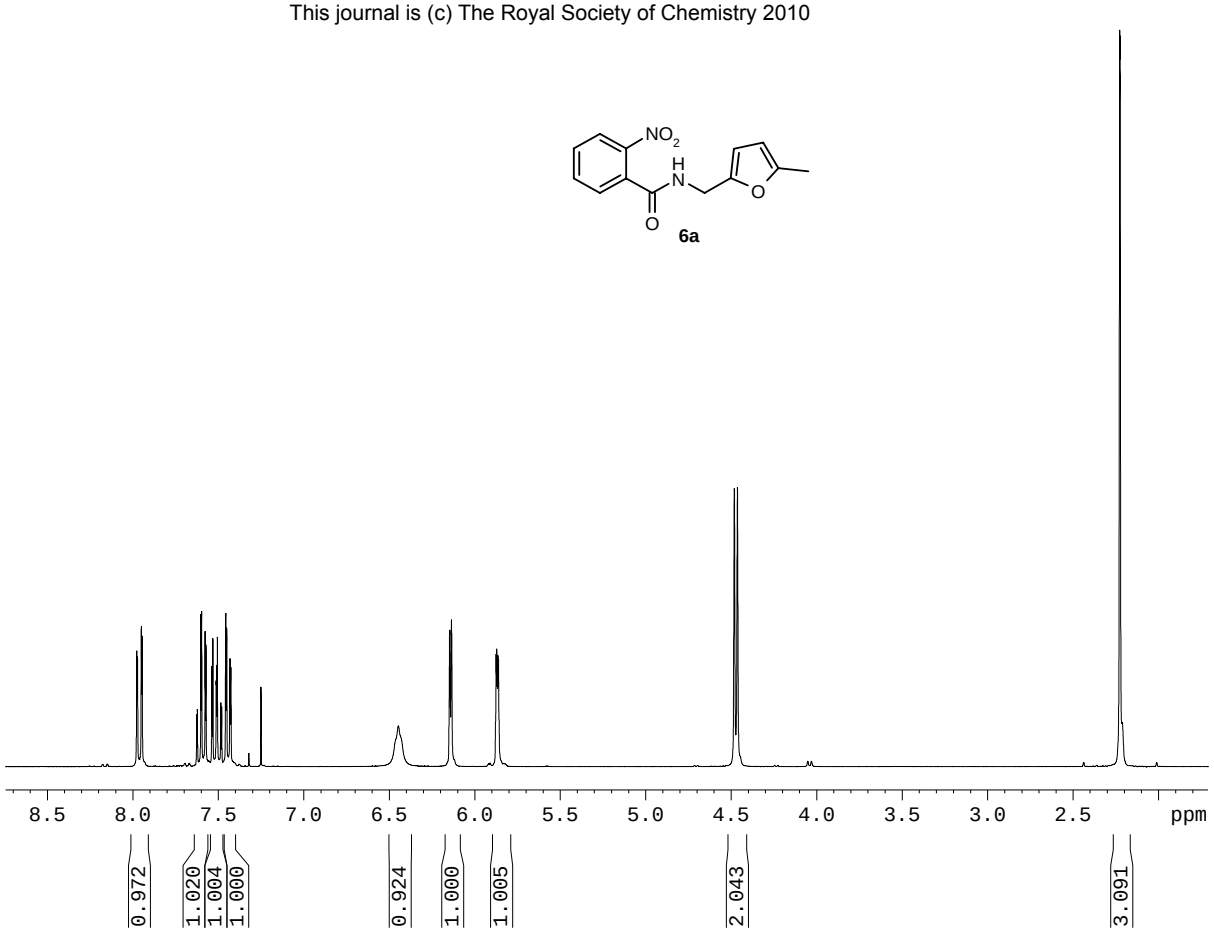

O
N
O
H
N
O
O
4a
10
9
8
7
6
5
4
3
2
1
0
ppm
2.080
2.138
2.145
1.119
1.037
1.000
1.008
1.003
2.086
3.082

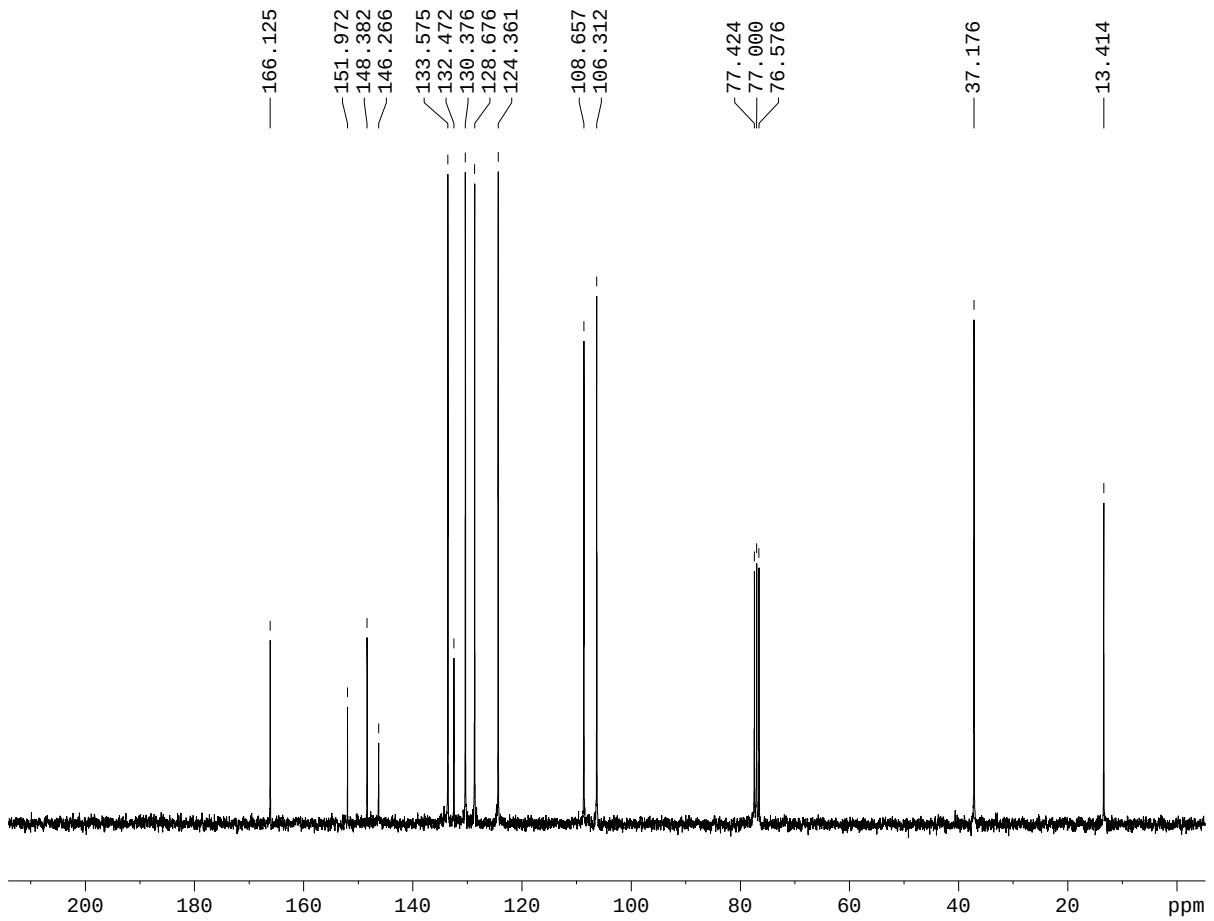

167.367
166.418
151.715
148.804
134.178
133.915
131.879
131.264
129.873
129.799
129.043
128.110
123.731
108.314
106.163
77.424
77.000
76.576
36.923
13.411
200
180
160
140
120
100
80
60
40
20
ppm

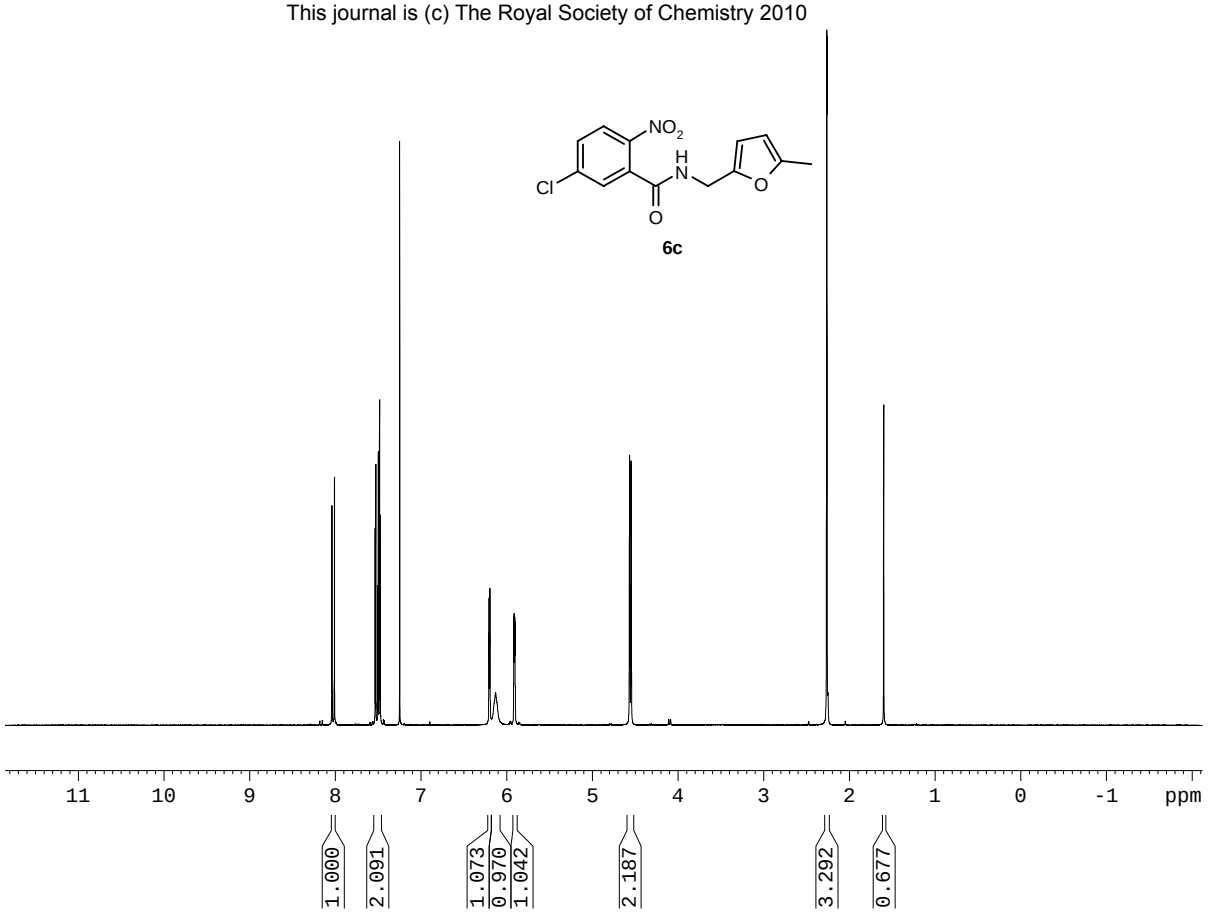

O
N
O
H
N
O
Br
O
10
9
8
7
6
5
4
3
2
1
0 ppm
2.183
3.309
1.125
0.559
0.494
0.990
1.008
1.000
2.153
3.183
0.646
1.411

4b

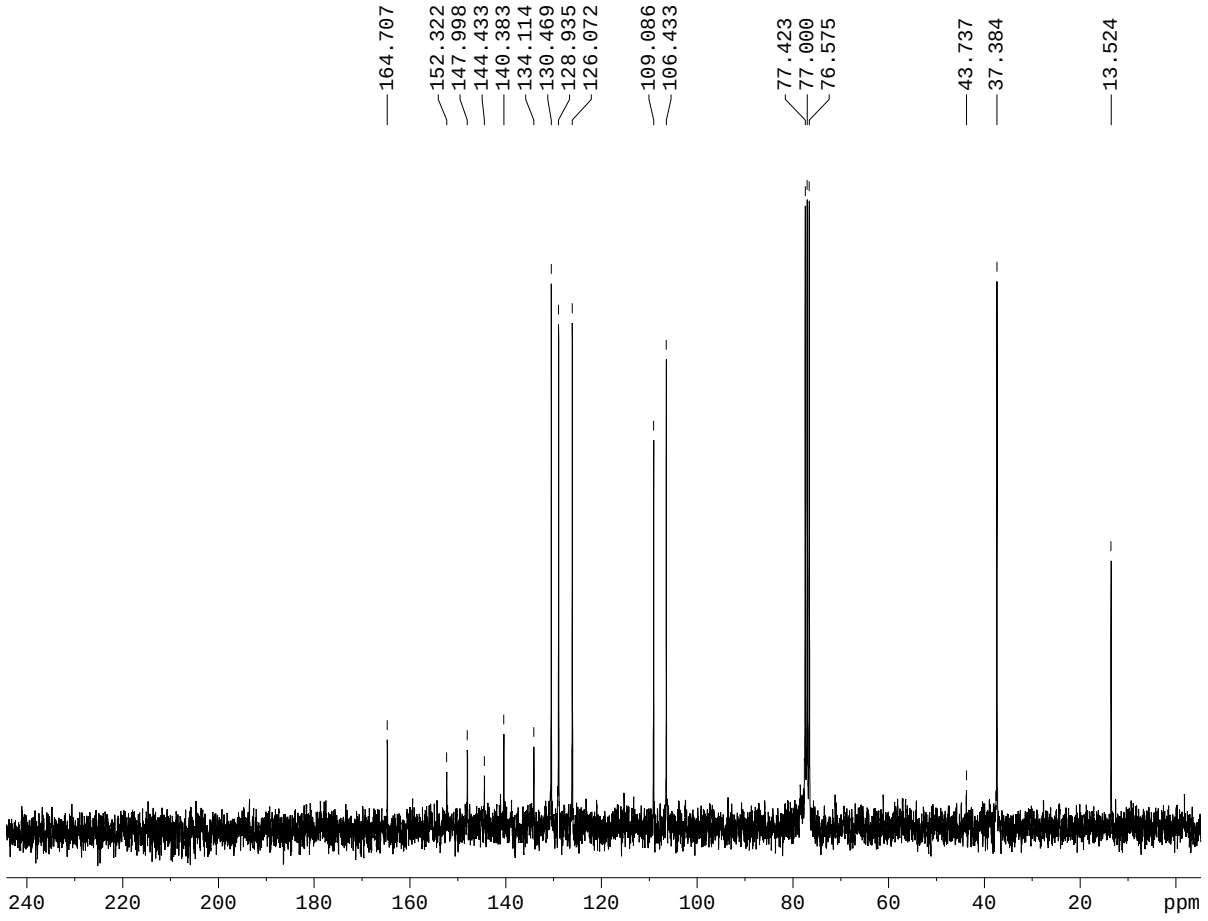

167.038
165.062
151.899
148.509
135.439
134.352
134.232
131.748
131.275
131.213
128.794
123.866
122.757
108.563
106.226
77.421
77.000
76.573
37.026
13.454
240
220
200
180
160
140
120
100
80
60
40
20
ppm

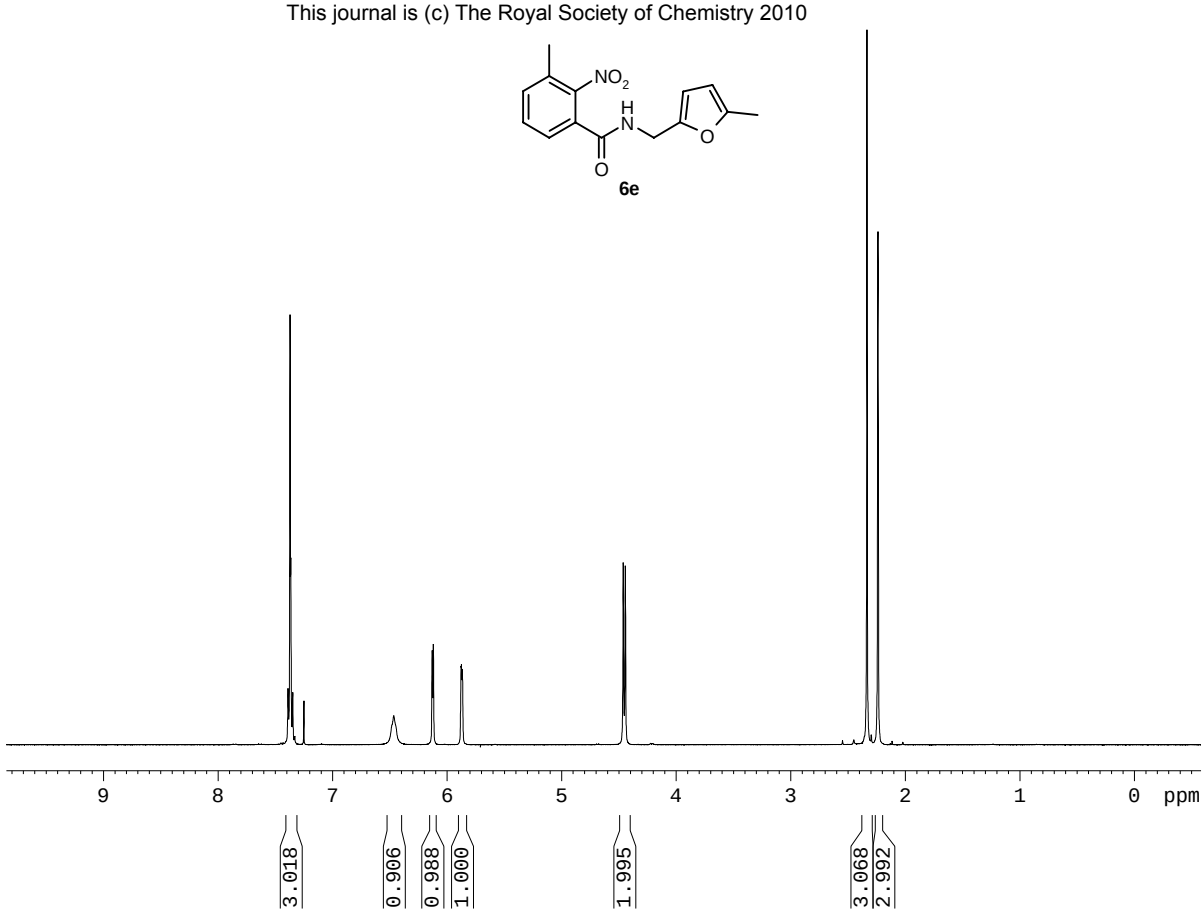

NO2
H
N
O
O
6a
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
ppm
0.972
1.020
1.004
1.000
0.924
1.000
1.005
2.043
3.091

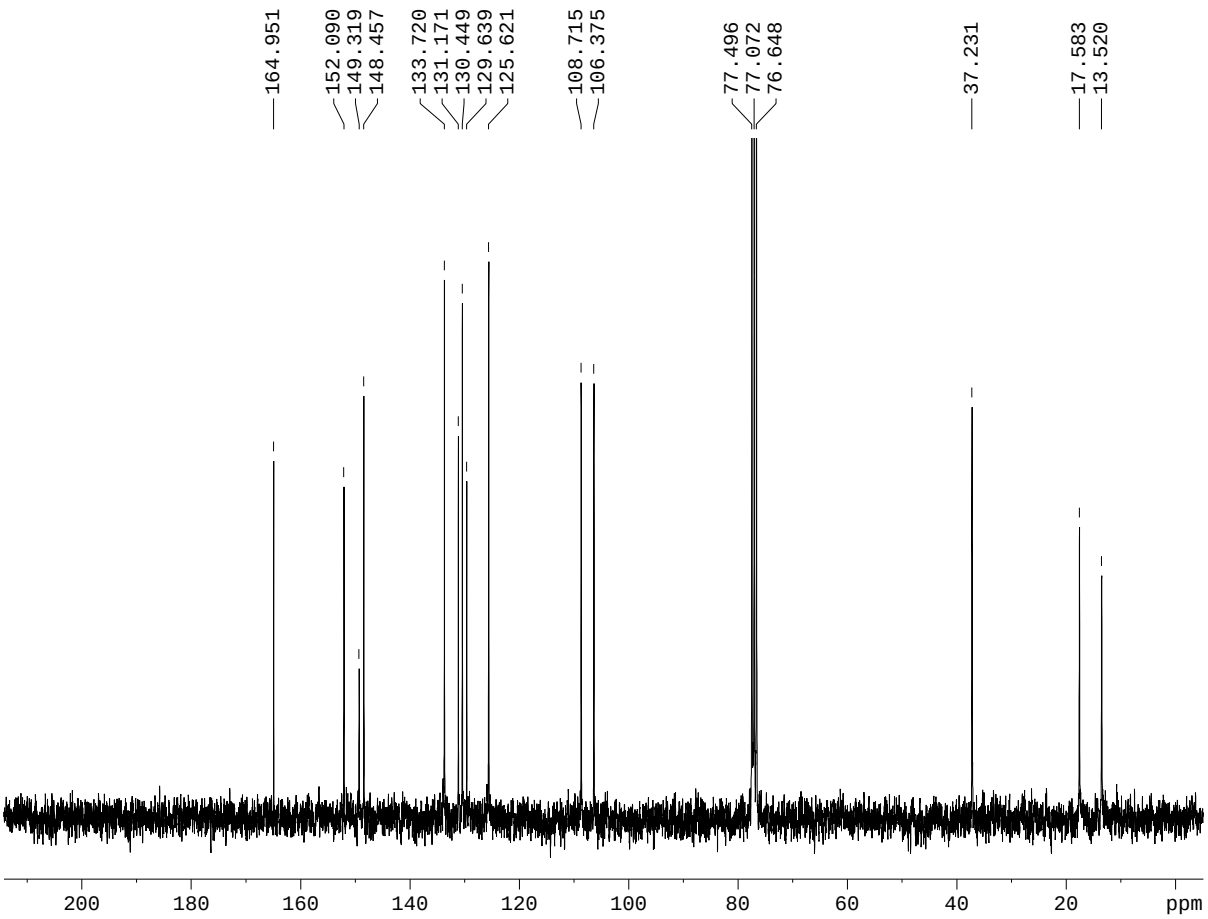

166.125
151.972
148.382
146.266
133.575
132.472
130.376
128.676
124.361
108.657
106.312
77.424
77.000
76.576
37.176
13.414
200
180
160
140
120
100
80
60
40
20
ppm

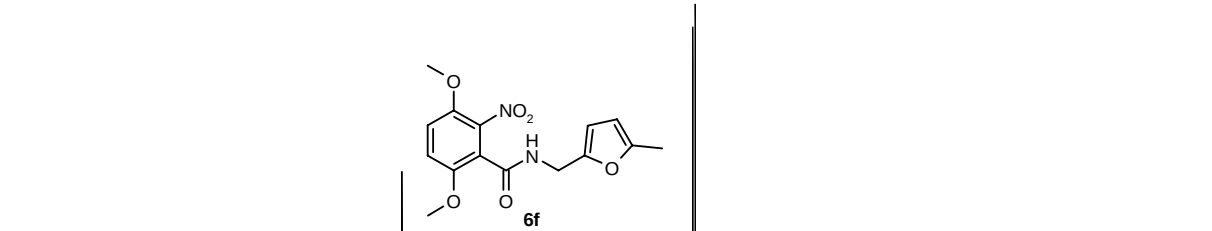

NO2
H
N
Cl
O
O
11 10 9 8 7 6 5 4 3 2 1 0 -1 ppm
1.000
2.091
1.073
0.970
1.042
2.187
3.292
0.677

6c


164.707
152.322
147.998
144.433
140.383
134.114
130.469
128.935
126.072
109.086
106.433
77.423
77.000
76.575
43.737
37.384
13.524
240 220 200 180 160 140 120 100 80 60 40 20 ppm

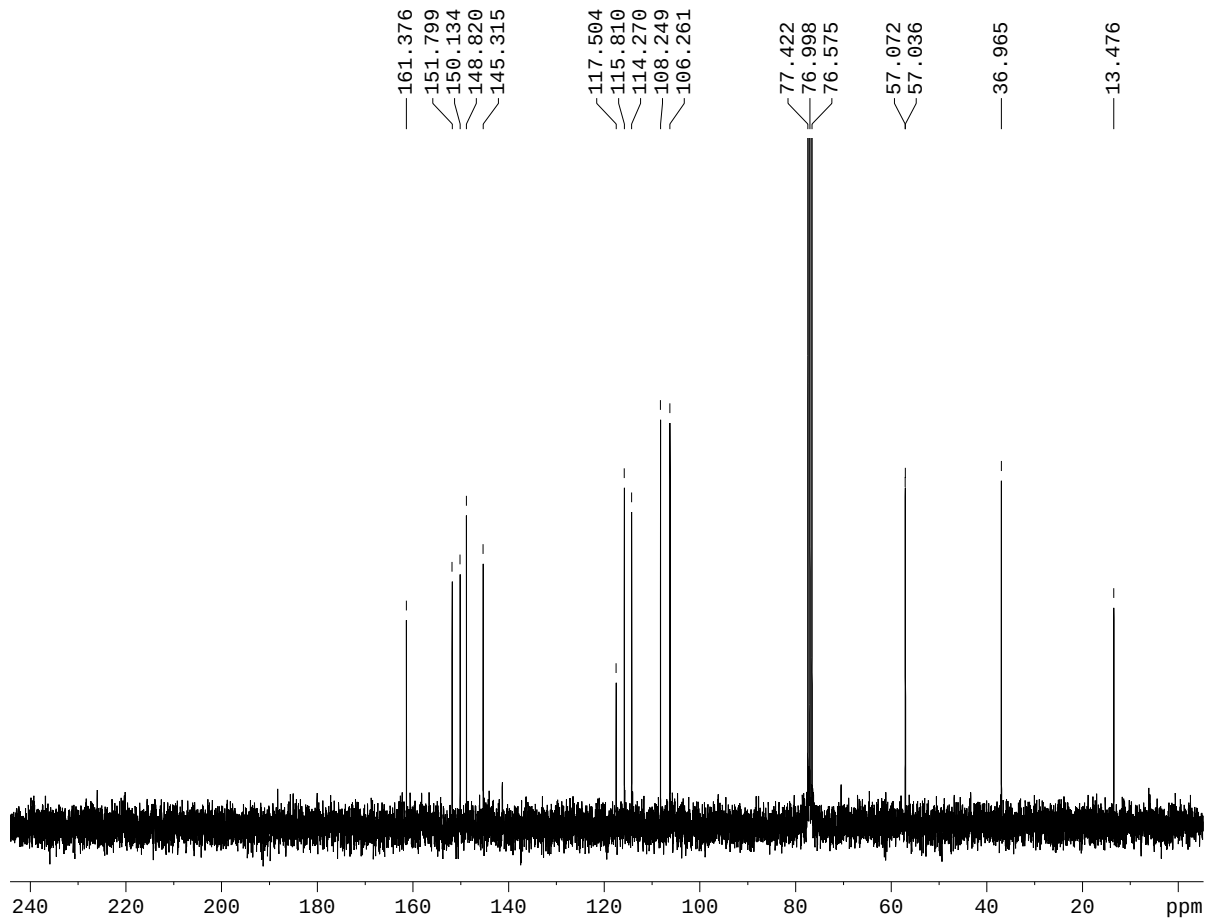

NO2
H
N
O
O
6e
9
8
7
6
5
4
3
2
1
0
ppm
3.018
0.906
0.988
1.000
1.995
3.068
2.992

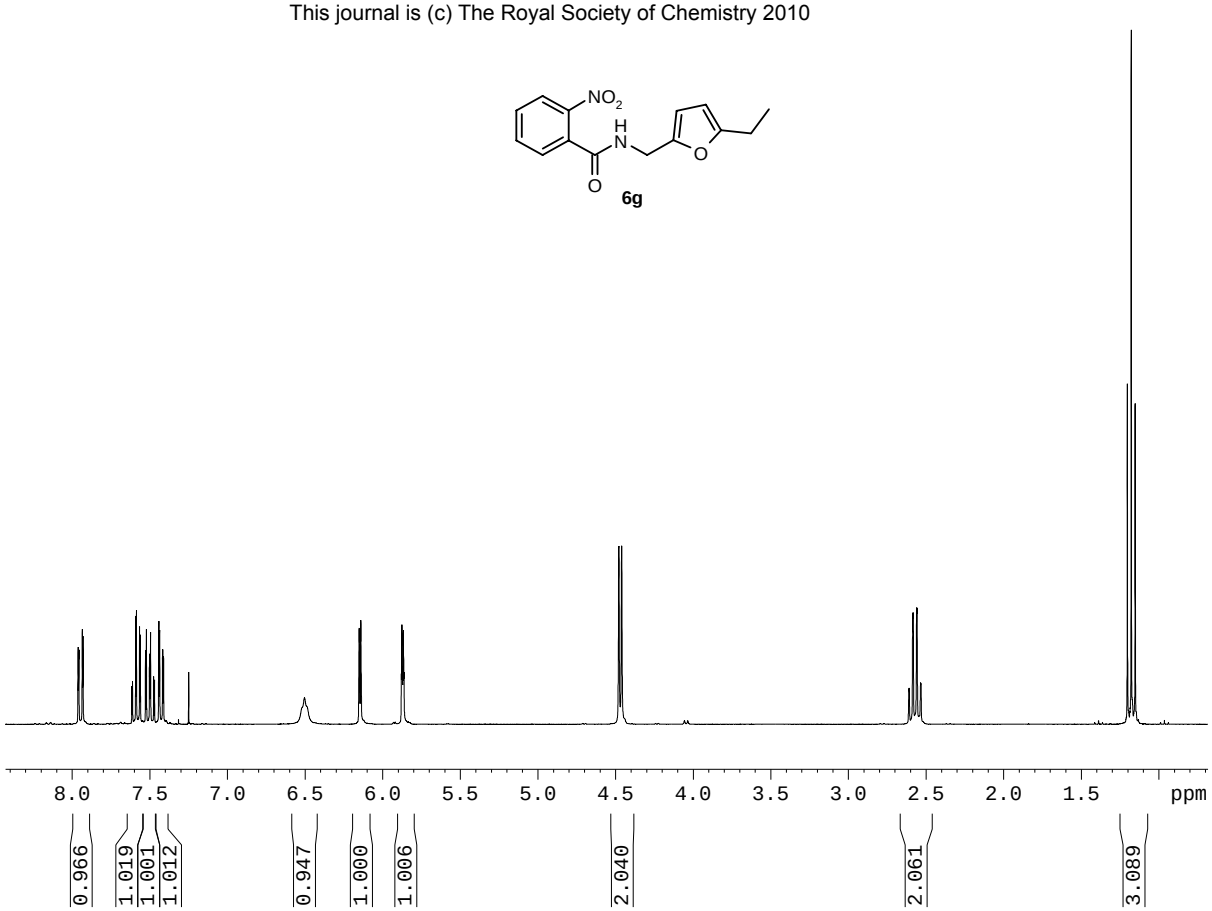

164.951
152.090
149.319
148.457
133.720
131.171
130.449
129.639
125.621
108.715
106.375
77.496
77.072
76.648
37.231
17.583
13.520
200
180
160
140
120
100
80
60
40
20
ppm

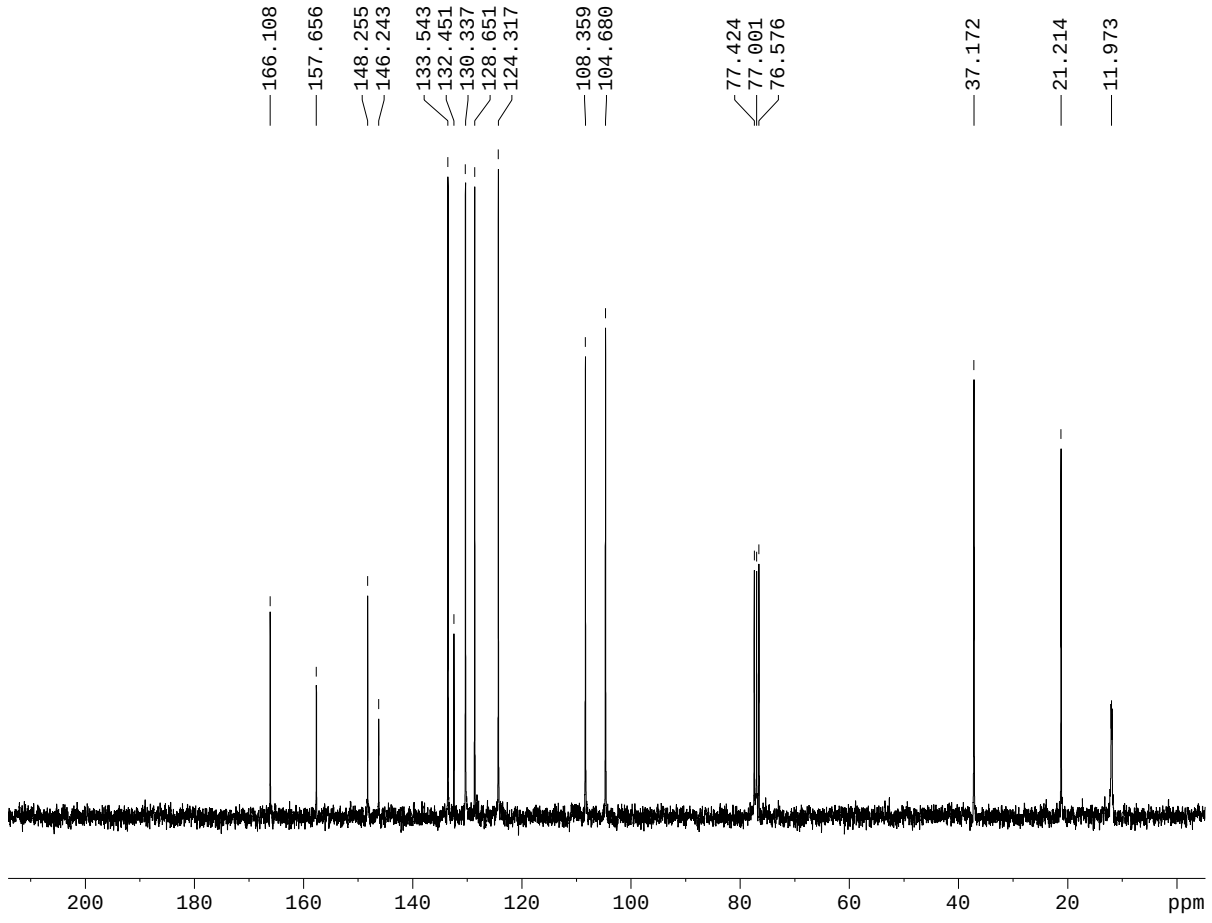

O
NO2
H
N
O
O
O
O

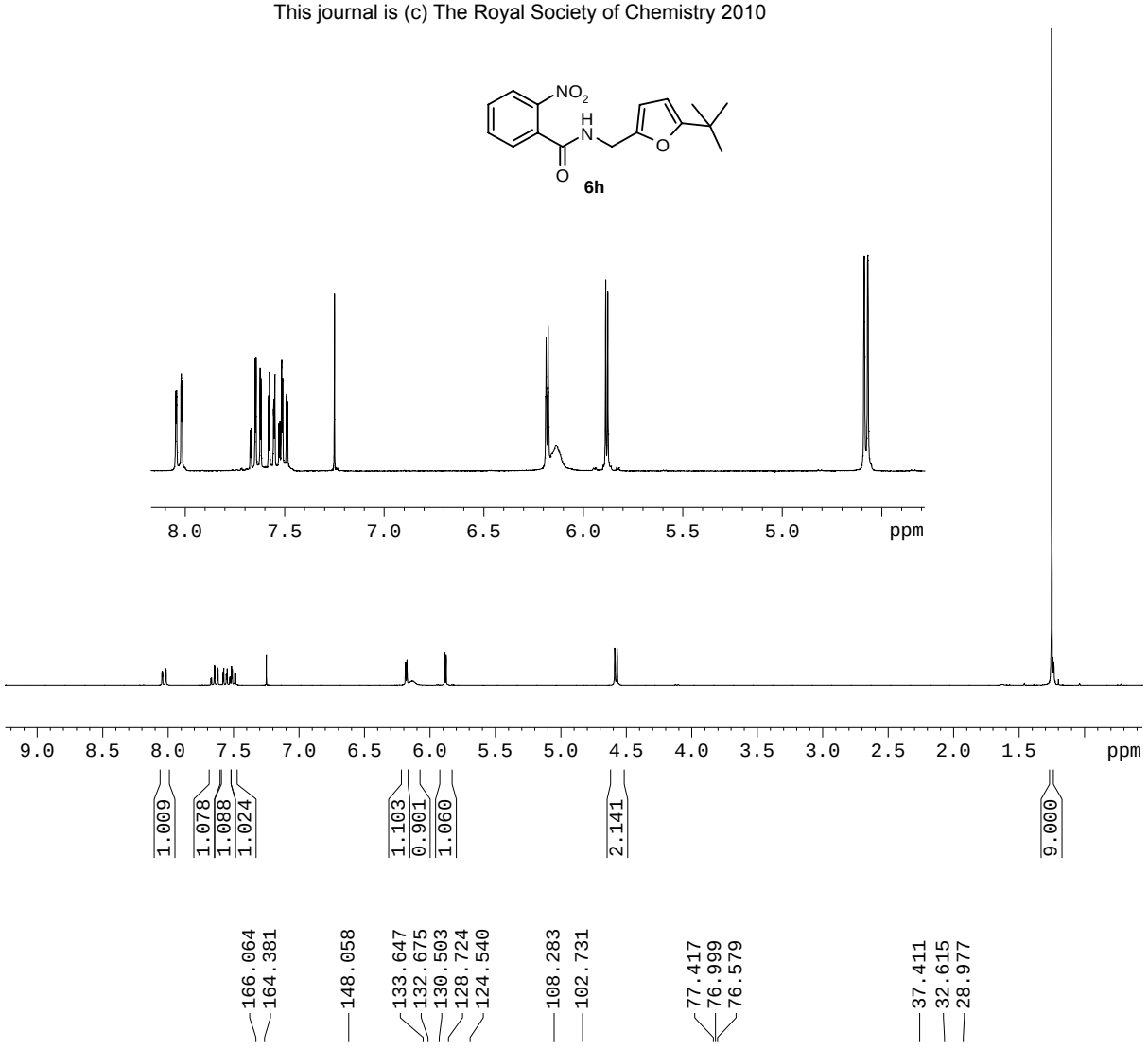
6f

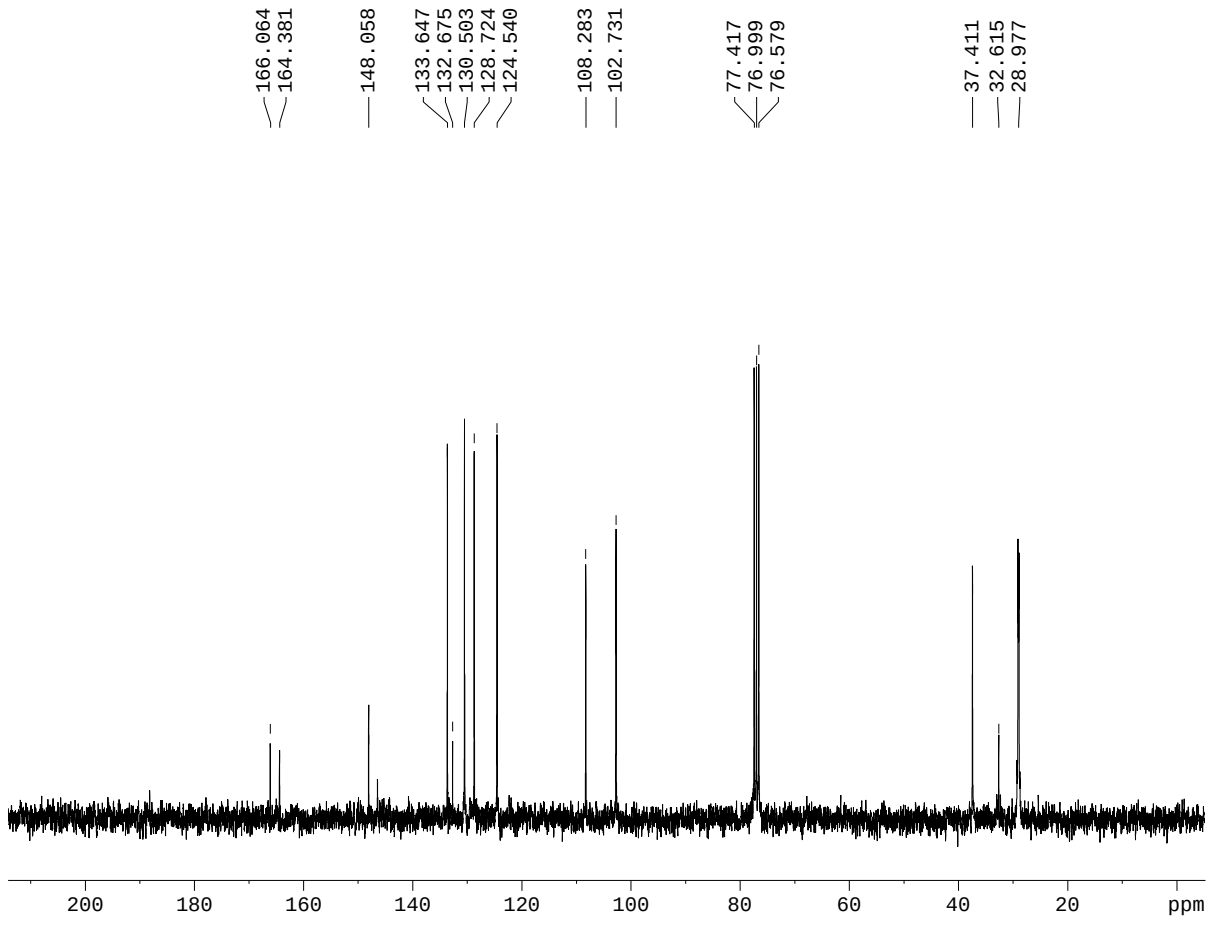
11 10 9 8 7 6 5 4 3 2 1 0 -1 ppm
0.865
2.069
0.970
0.990
2.013
6.139
3.000
0.821

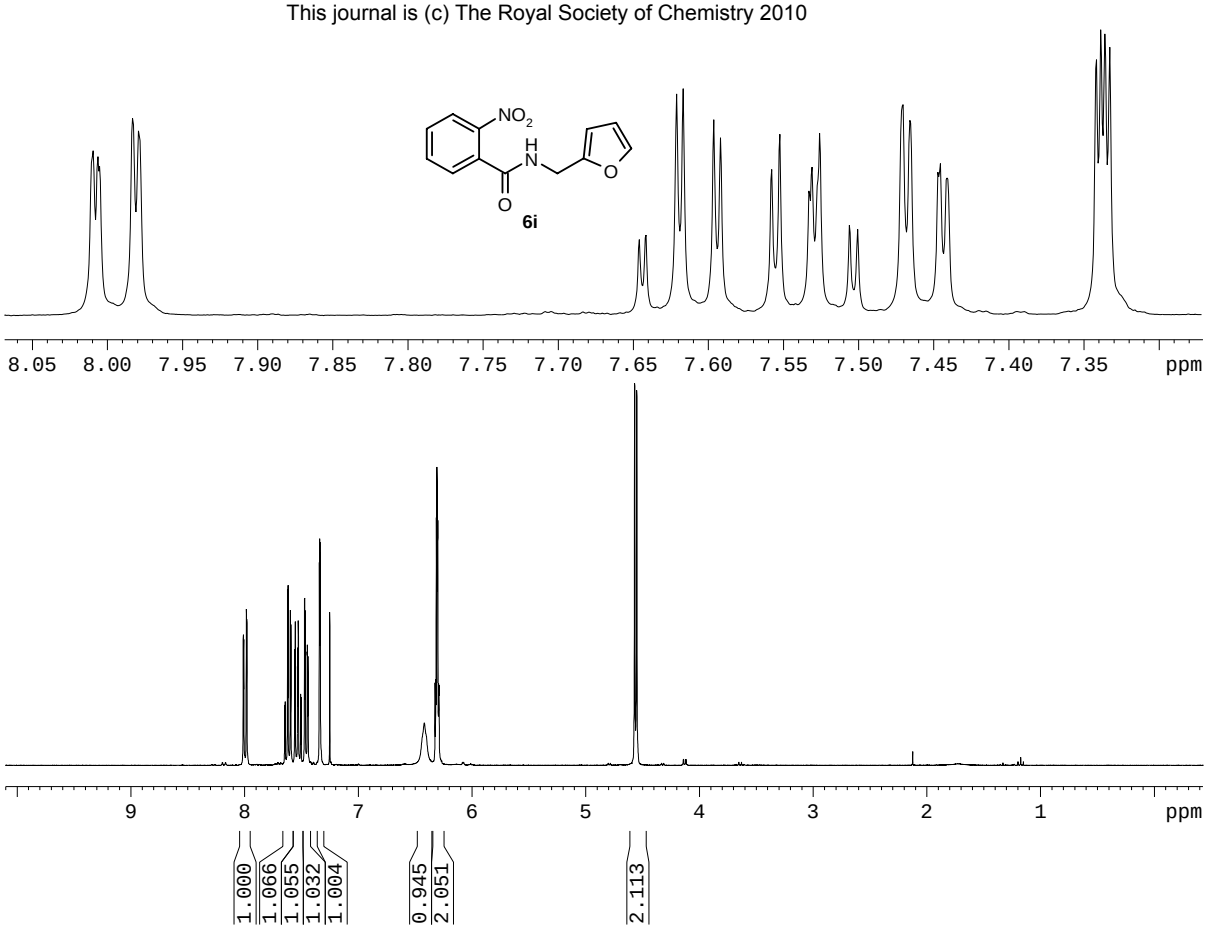

161.376
151.799
150.134
148.820
145.315
117.504
115.810
114.270
108.249
106.261
77.422
76.998
76.575
57.072
57.036
36.965
13.476
240 220 200 180 160 140 120 100 80 60 40 20 ppm

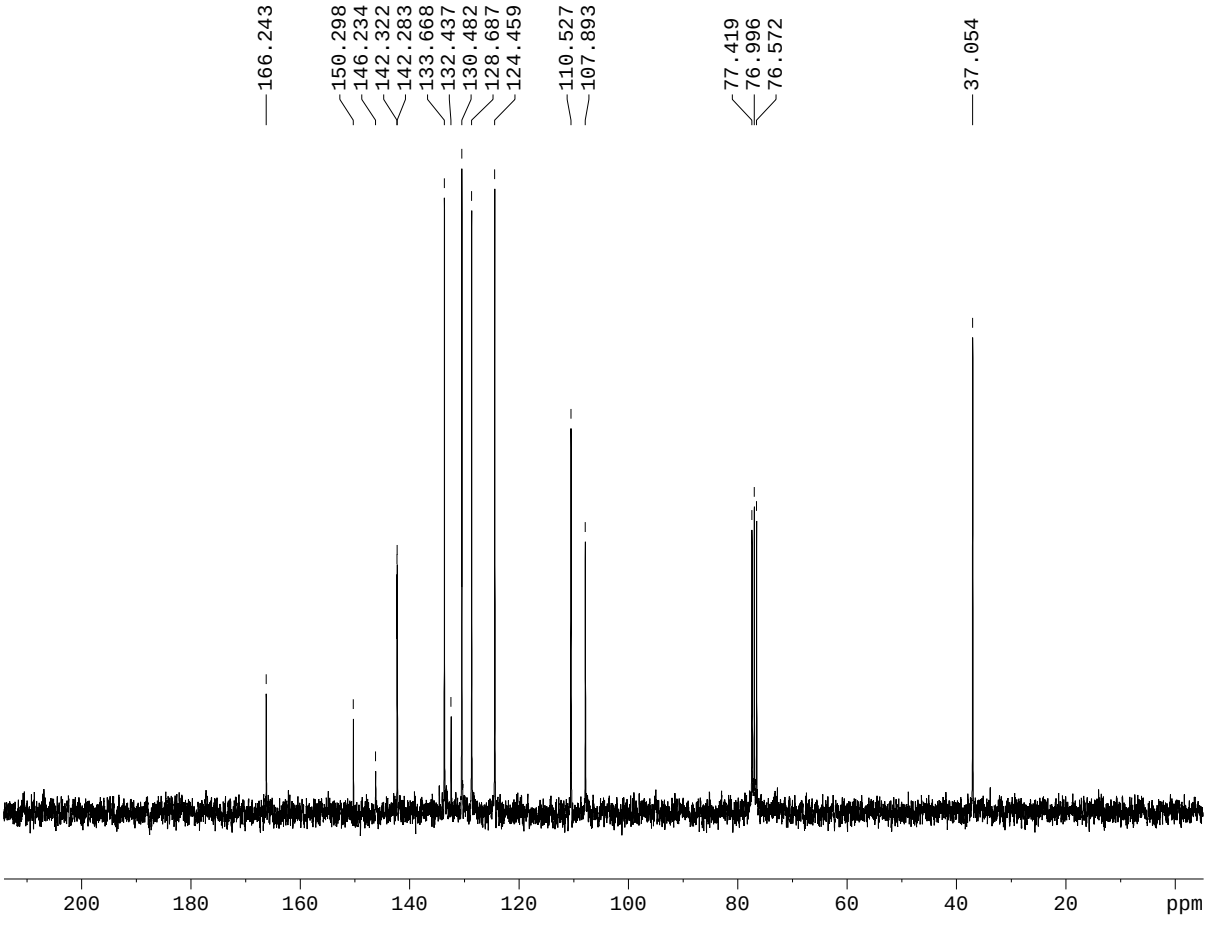

NO2
H
N
O
O
6g
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
ppm
0.966
1.019
1.001
1.012
0.947
1.000
1.006
2.040
2.061
3.089

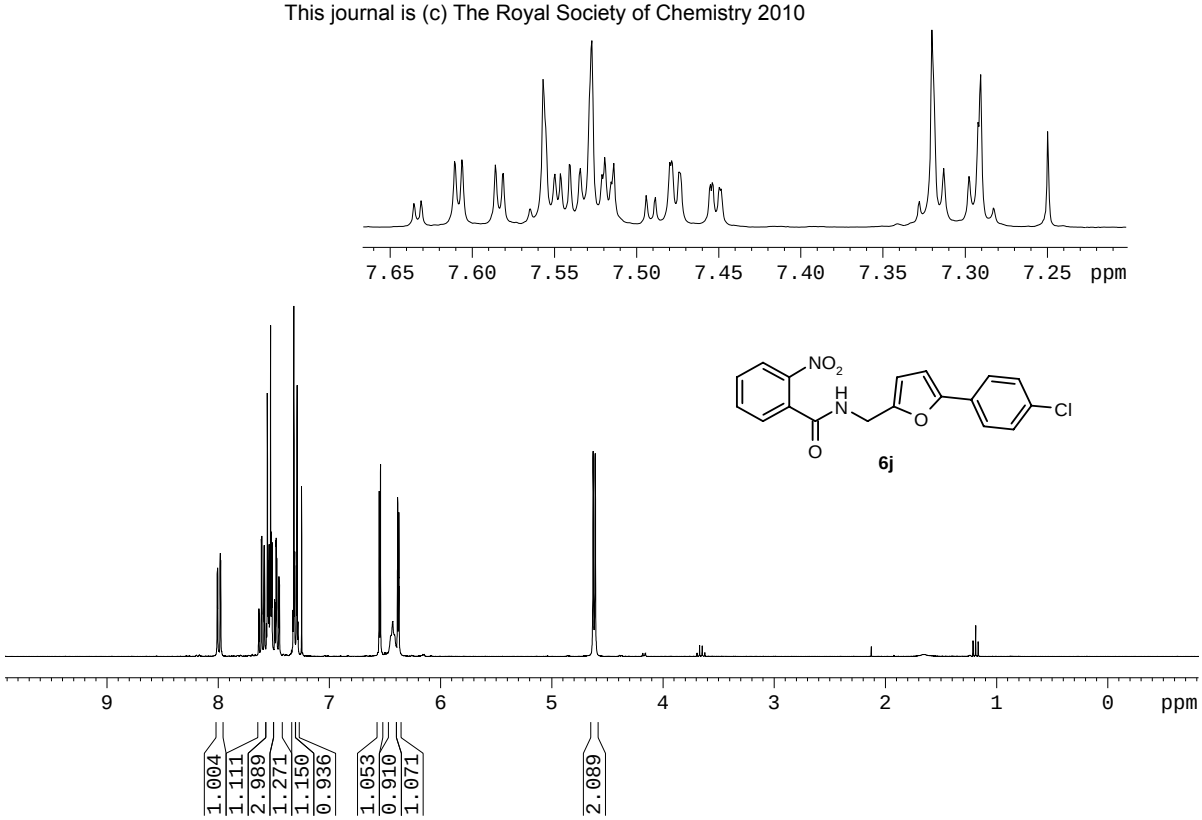

166.108
157.656
148.255
146.243
133.543
132.451
130.337
128.651
124.317
108.359
104.680
77.424
77.001
76.576
37.172
21.214
11.973
200
180
160
140
120
100
80
60
40
20
ppm

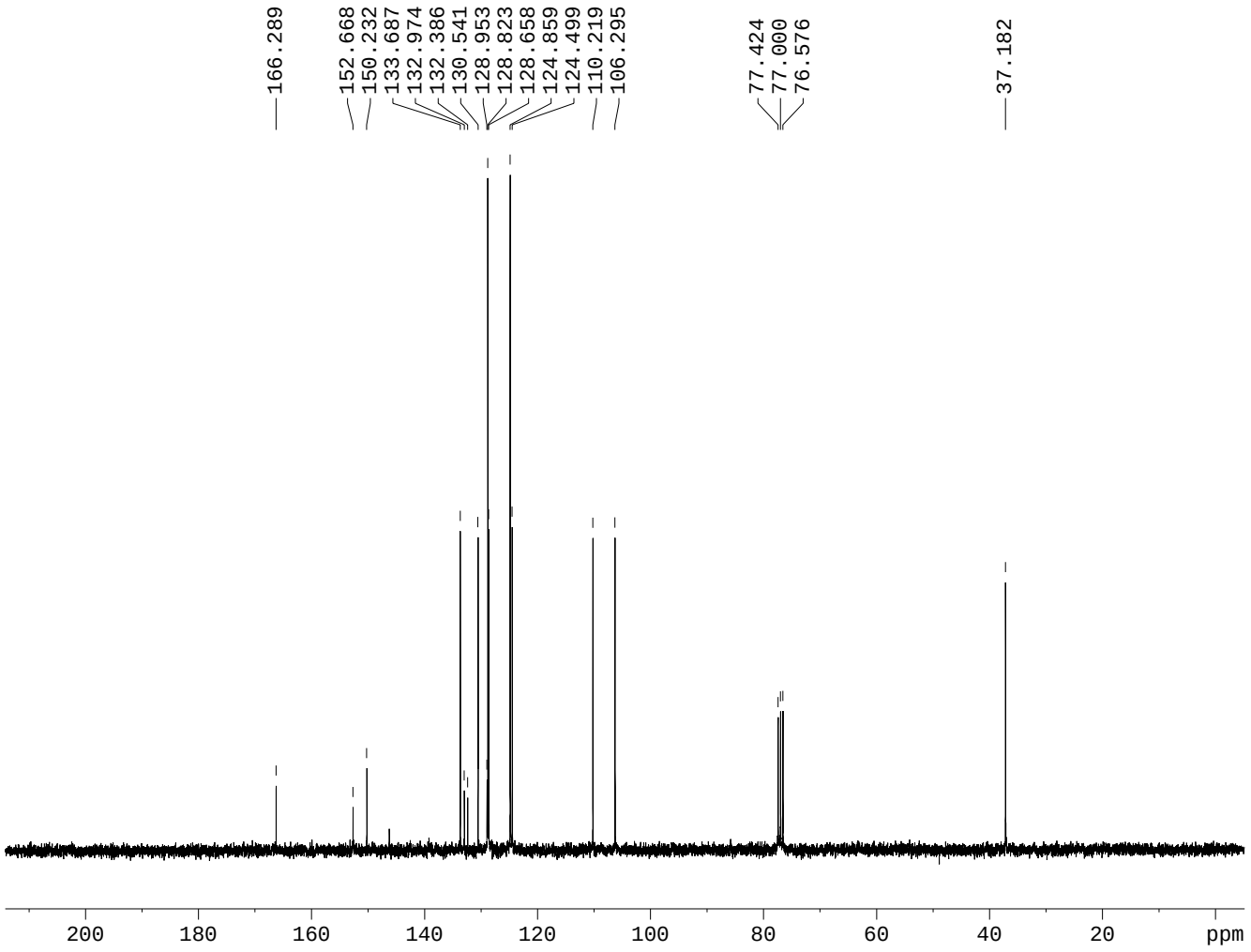

NO2
H
N
O
O
6h
8.0
7.5
7.0
6.5
6.0
5.5
5.0
ppm
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
ppm
1.009
1.078
1.088
1.024
1.103
0.901
1.060
2.141
9.000

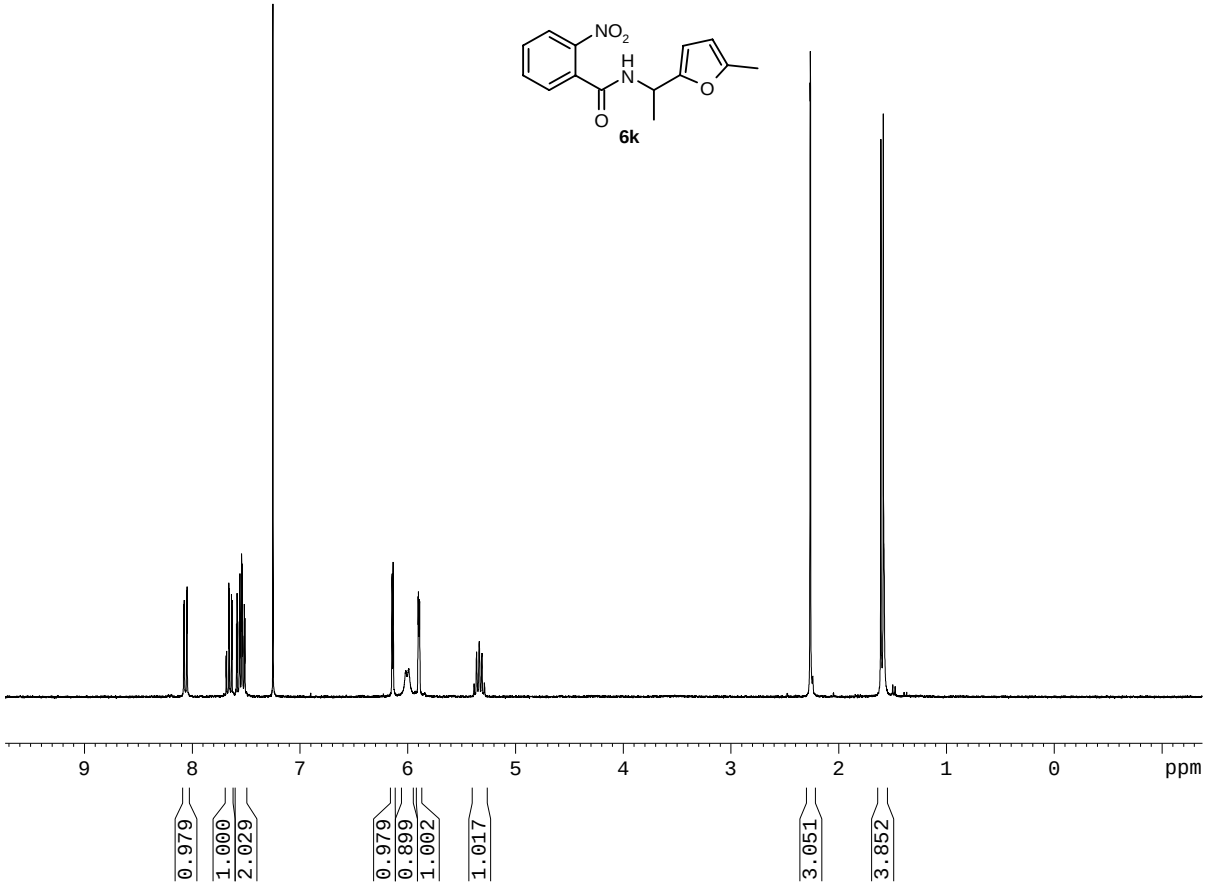

166.064
164.381
148.058
133.647
132.675
130.503
128.724
124.540
108.283
102.731
77.417
76.999
76.579
37.411
32.615
28.977
200
180
160
140
120
100
80
60
40
20
ppm

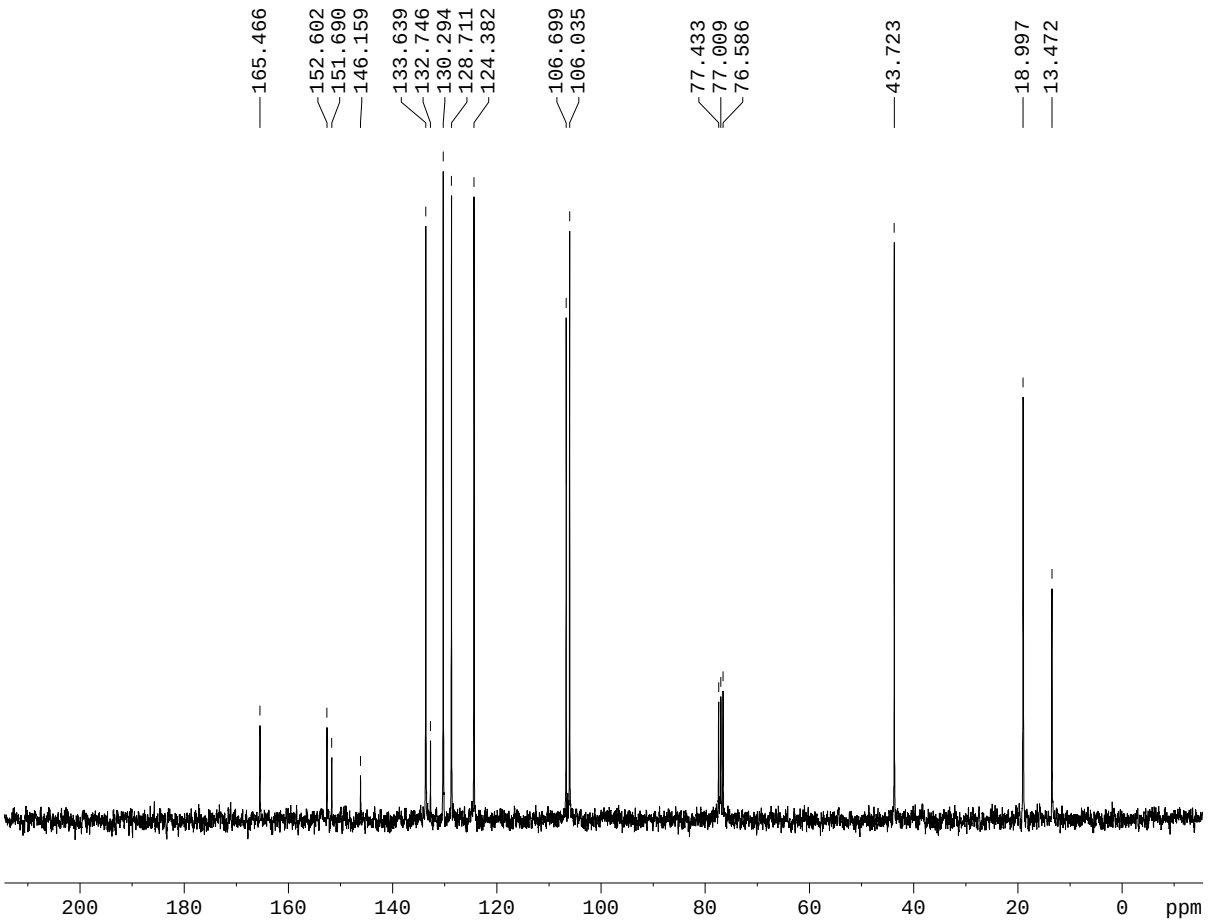

NO2
H
N
O
O
6i
8.05 8.00 7.95 7.90 7.85 7.80 7.75 7.70 7.65 7.60 7.55 7.50 7.45 7.40 7.35 ppm
9 8 7 6 5 4 3 2 1 ppm
1.000
1.066
1.055
1.032
1.004
0.945
2.051
2.113

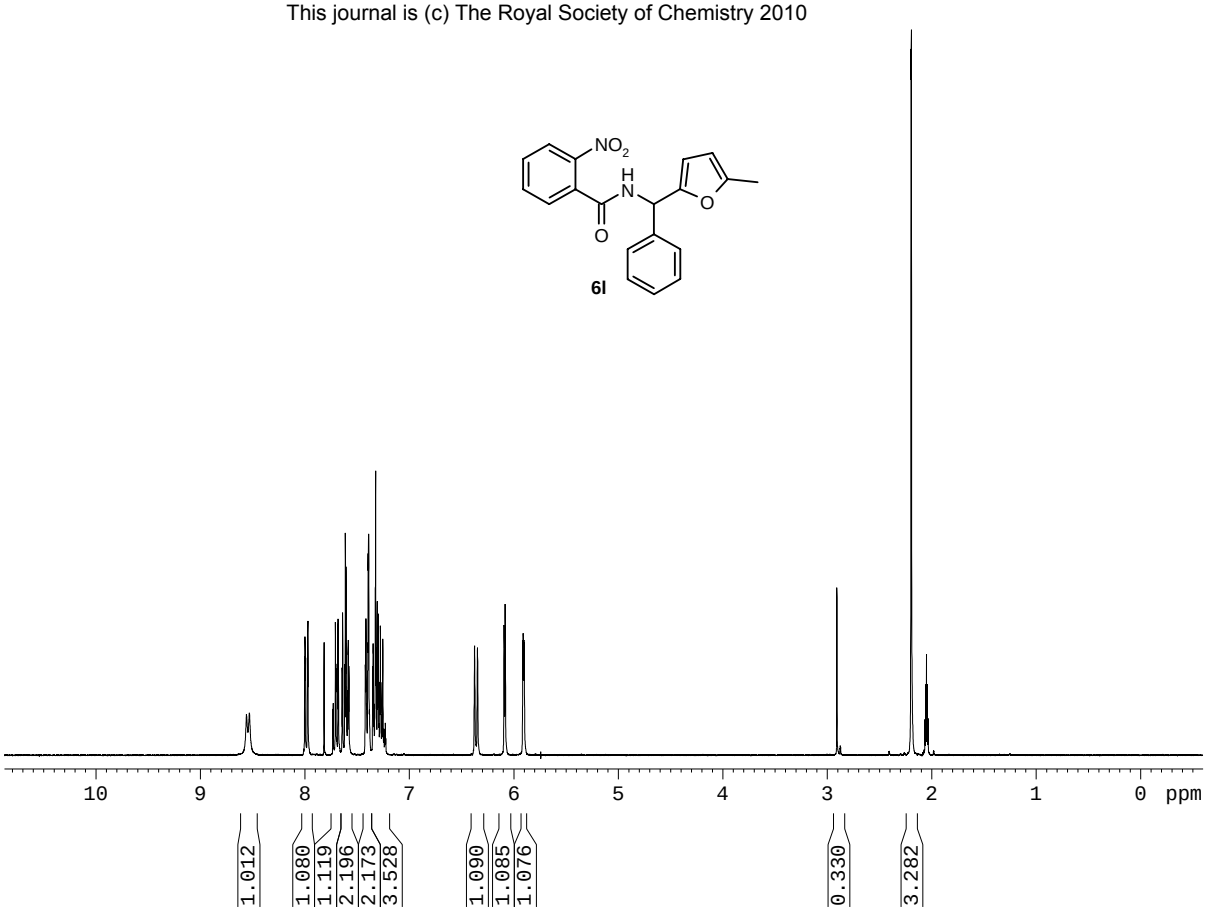

166.243
150.298
146.234
142.322
142.283
133.668
132.437
130.482
128.687
124.459
110.527
107.893
77.419
76.996
76.572
37.054
200 180 160 140 120 100 80 60 40 20 ppm

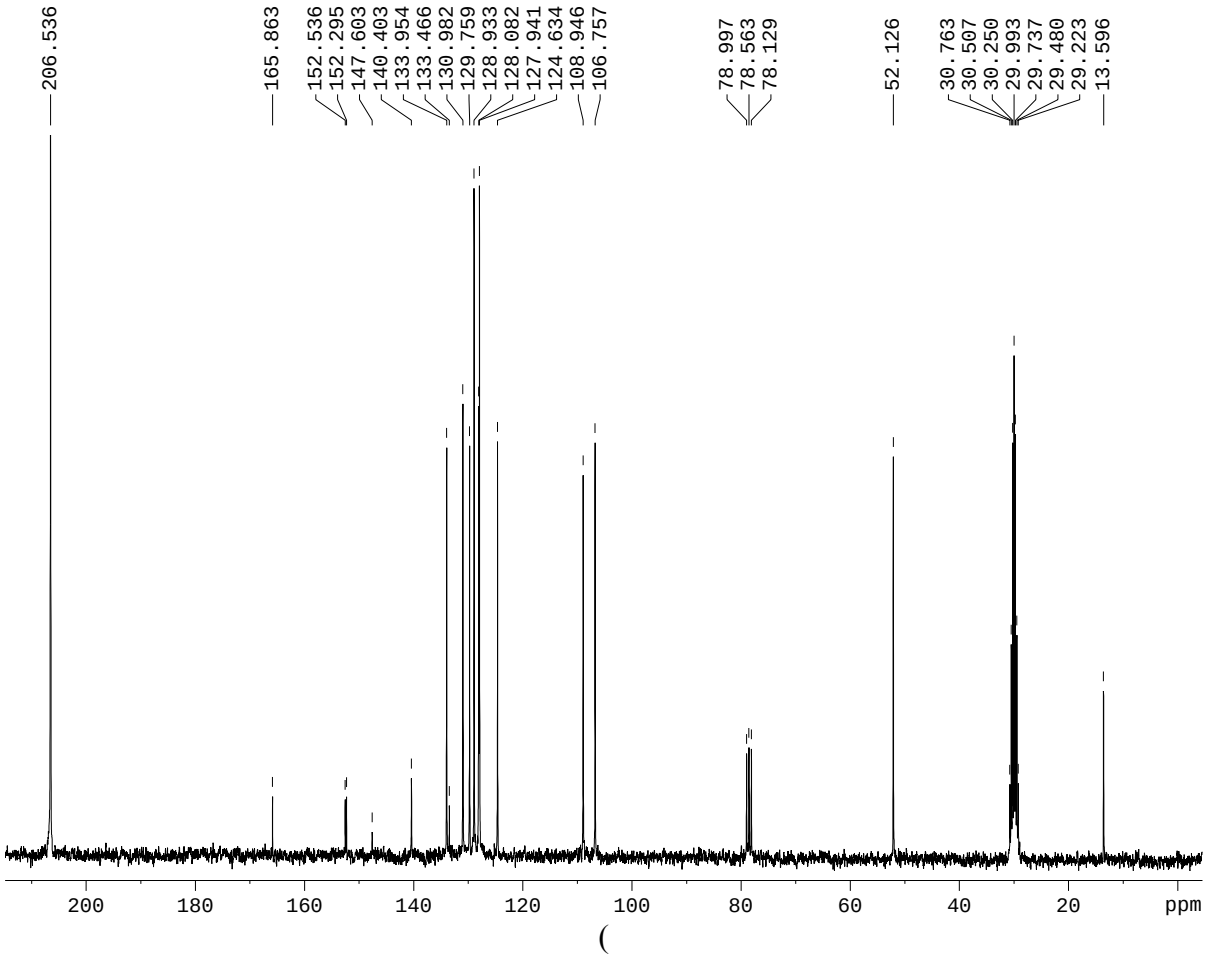

7.65 7.60 7.55 7.50 7.45 7.40 7.35 7.30 7.25 ppm
NO2
H
N
O
O
Cl
6j
9 8 7 6 5 4 3 2 1 0 ppm
1.004 1.111 2.989 1.271 1.150 0.936 1.053 0.910 1.071 2.089


166.289
152.668
150.232
133.687
132.974
132.386
130.541
128.953
128.823
128.658
124.859
124.499
110.219
106.295
77.424
77.000
76.576
37.182
200 180 160 140 120 100 80 60 40 20 ppm

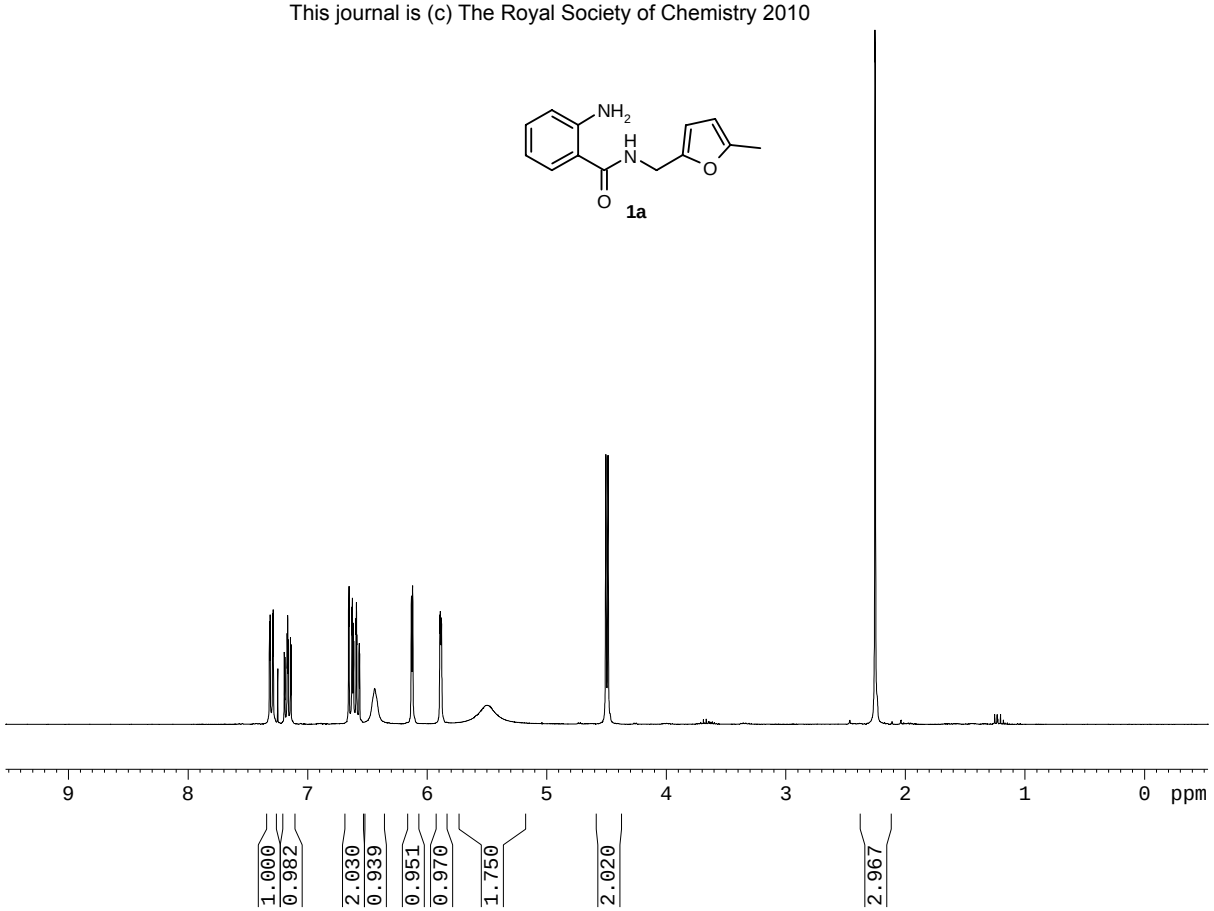

NO2
H
N
O
O
6k
9
8
7
6
5
4
3
2
1
0
ppm
0.979
1.000
2.029
0.979
0.899
1.002
1.017
3.051
3.852

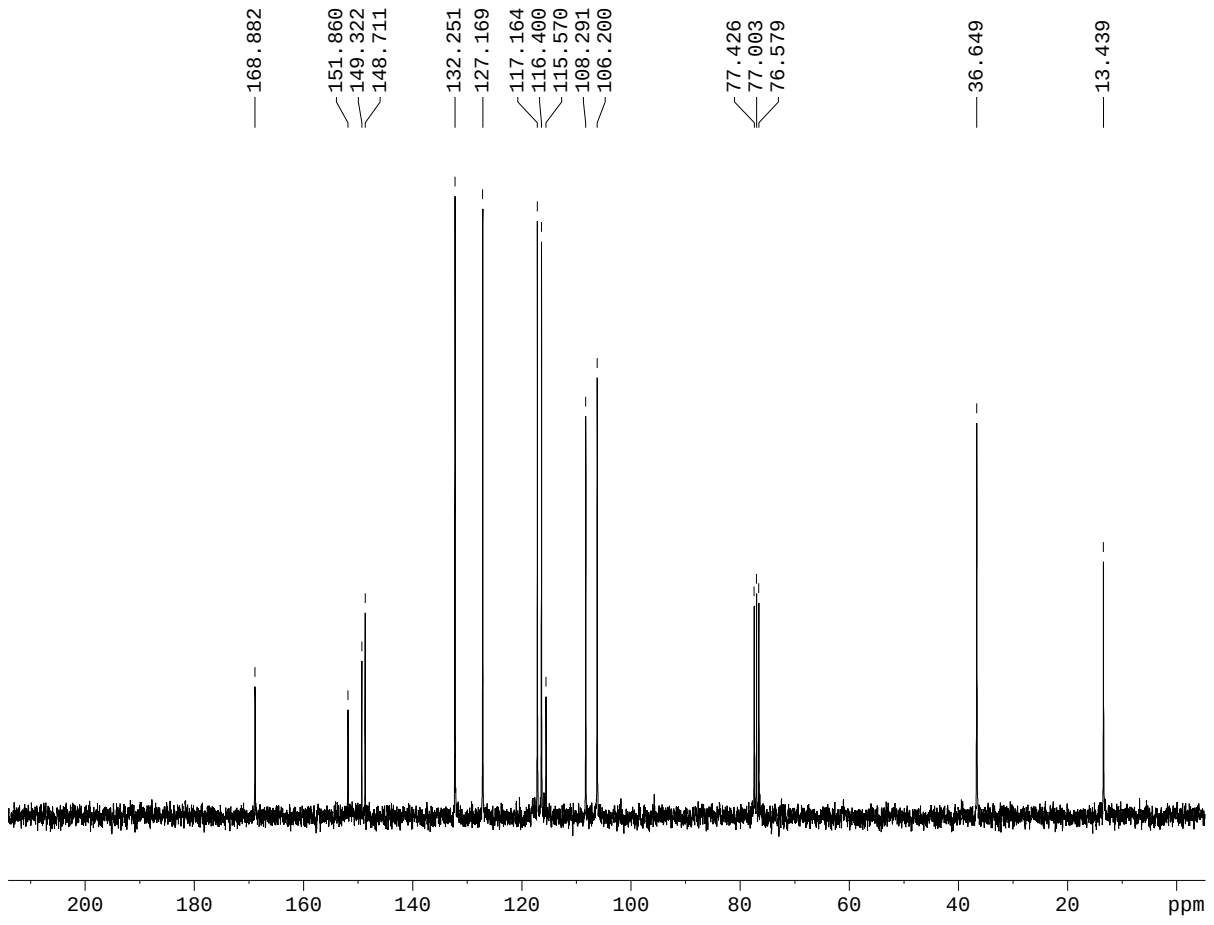

165.466
152.602
151.690
146.159
133.639
132.746
130.294
128.711
124.382
106.699
106.035
77.433
77.009
76.586
43.723
18.997
13.472
200
180
160
140
120
100
80
60
40
20
0
ppm

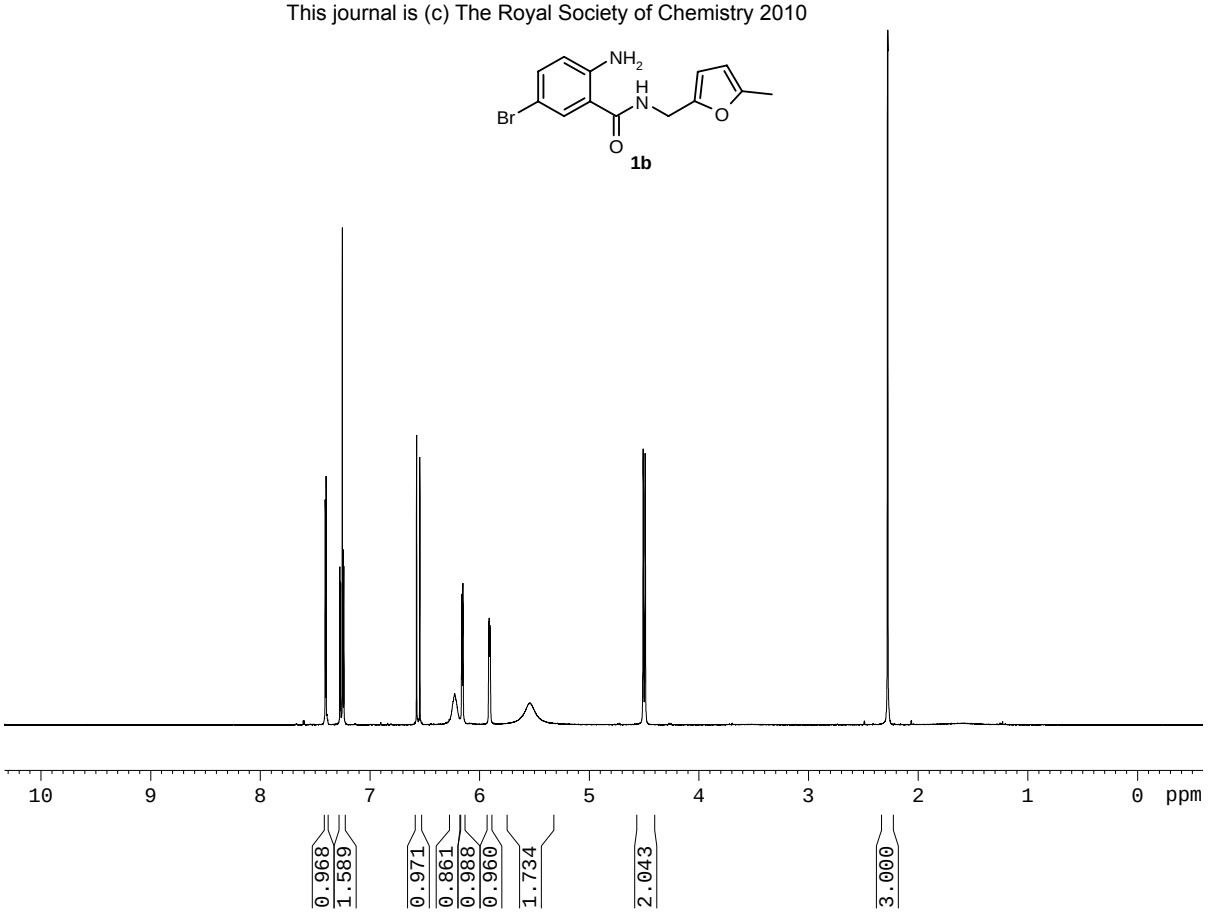

NO2
H
N
O
O
6l
10
9
8
7
6
5
4
3
2
1
0
ppm
1.012
1.080
1.119
2.196
2.173
3.528
1.090
1.085
1.076
0.330
3.282

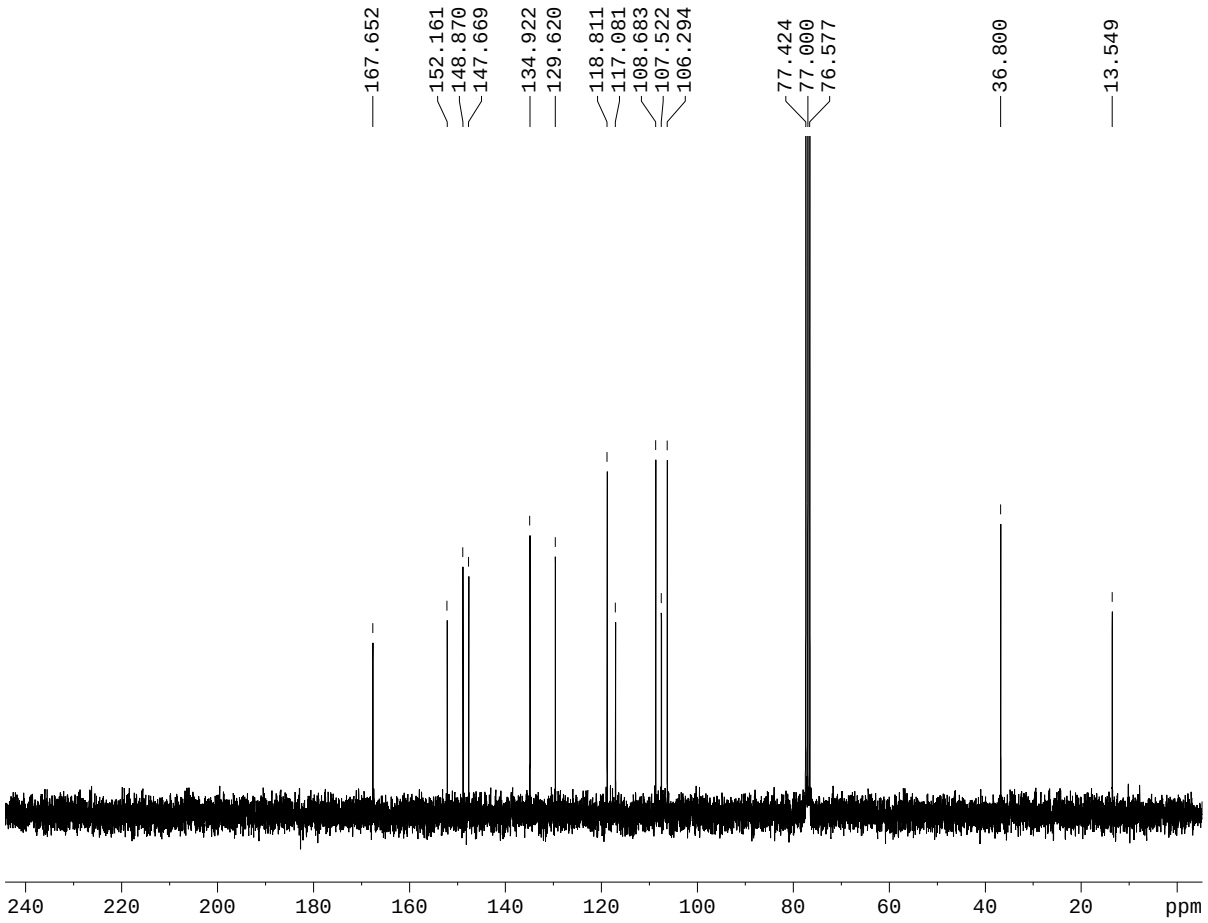

206.536
165.863
152.536
152.295
147.603
140.403
133.954
133.466
130.982
129.759
128.933
128.082
127.941
124.634
108.946
106.757
78.997
78.563
78.129
52.126
30.763
30.507
30.250
29.993
29.737
29.480
29.223
13.596
200
180
160
140
120
100
80
60
40
20
ppm

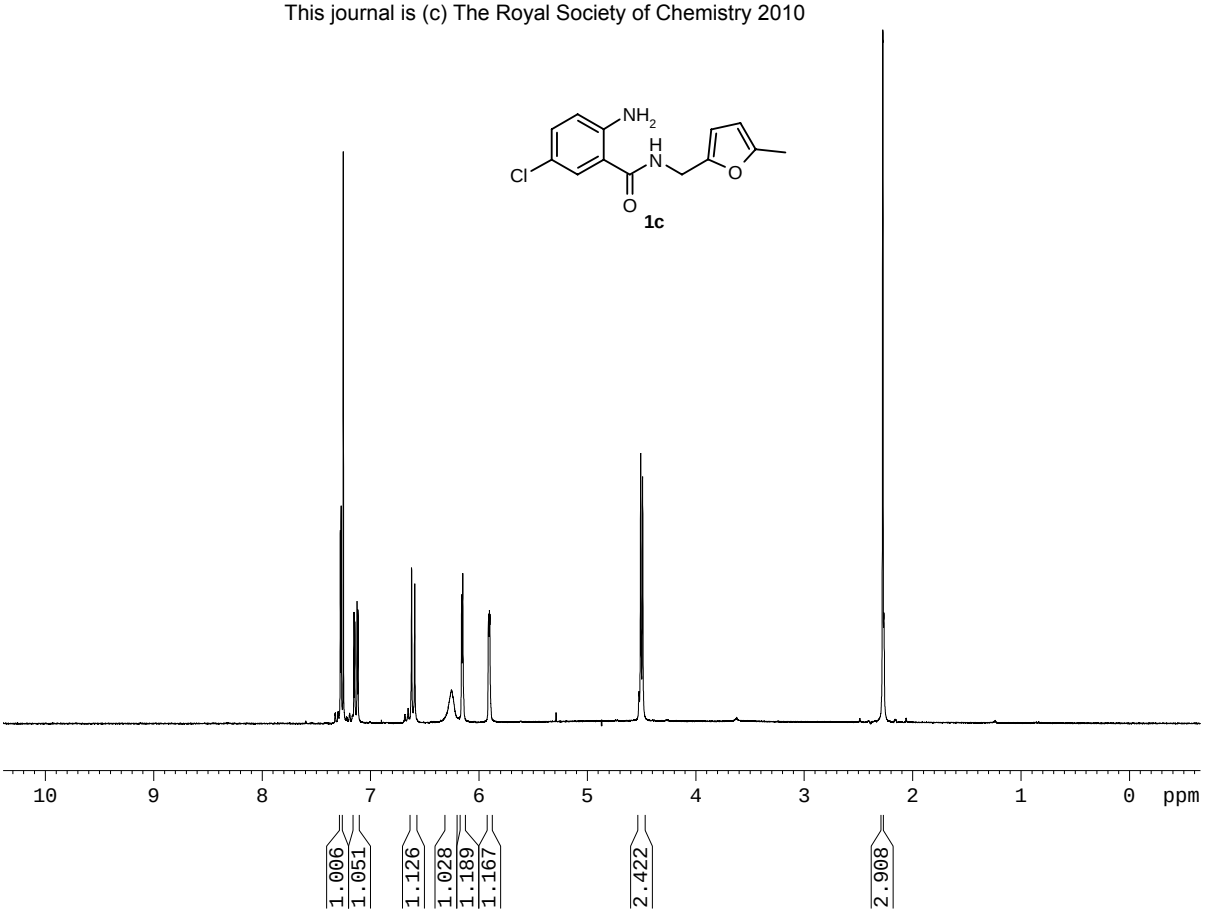
(

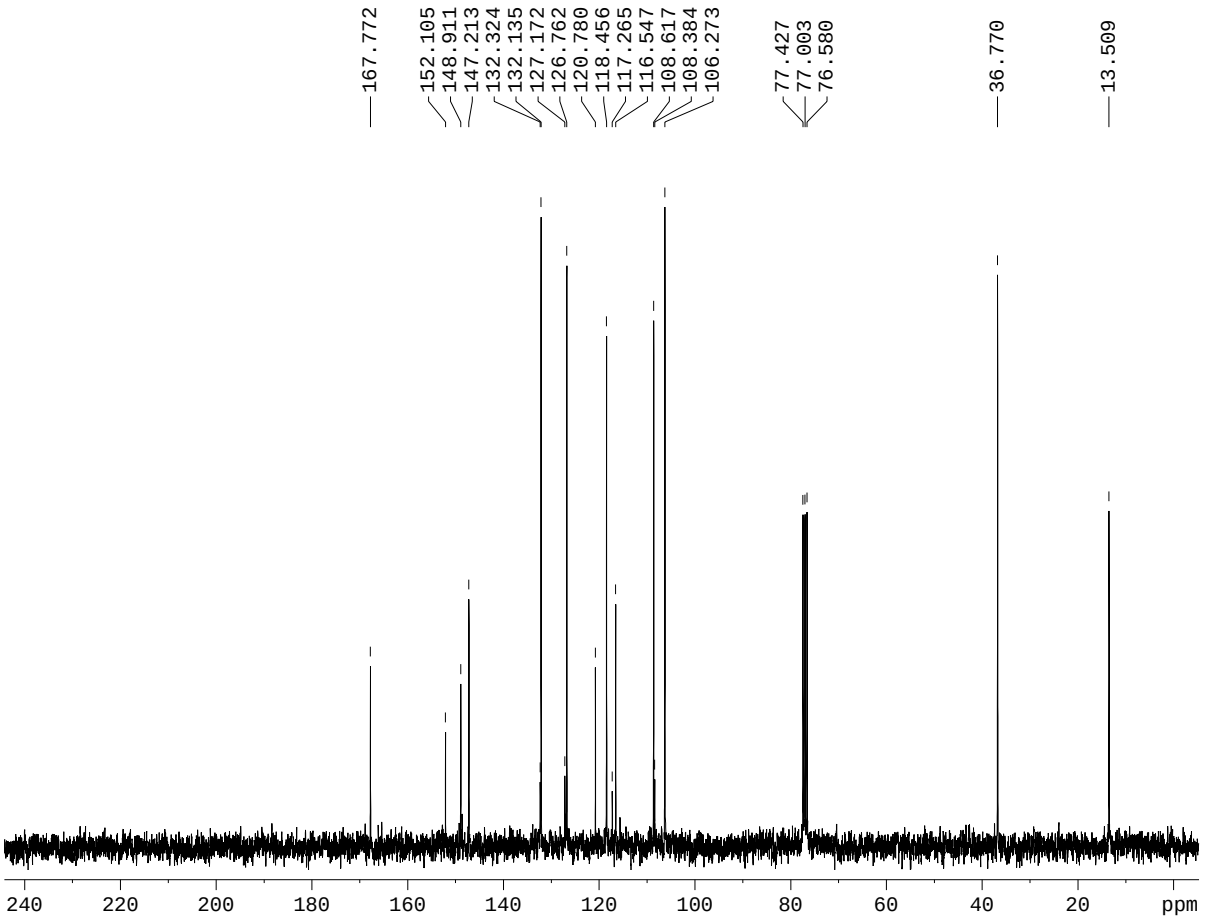

NH2
H
N
O
O
1a
9
8
7
6
5
4
3
2
1
0
ppm
1.000
0.982
2.030
0.939
0.951
0.970
1.750
2.020
2.967

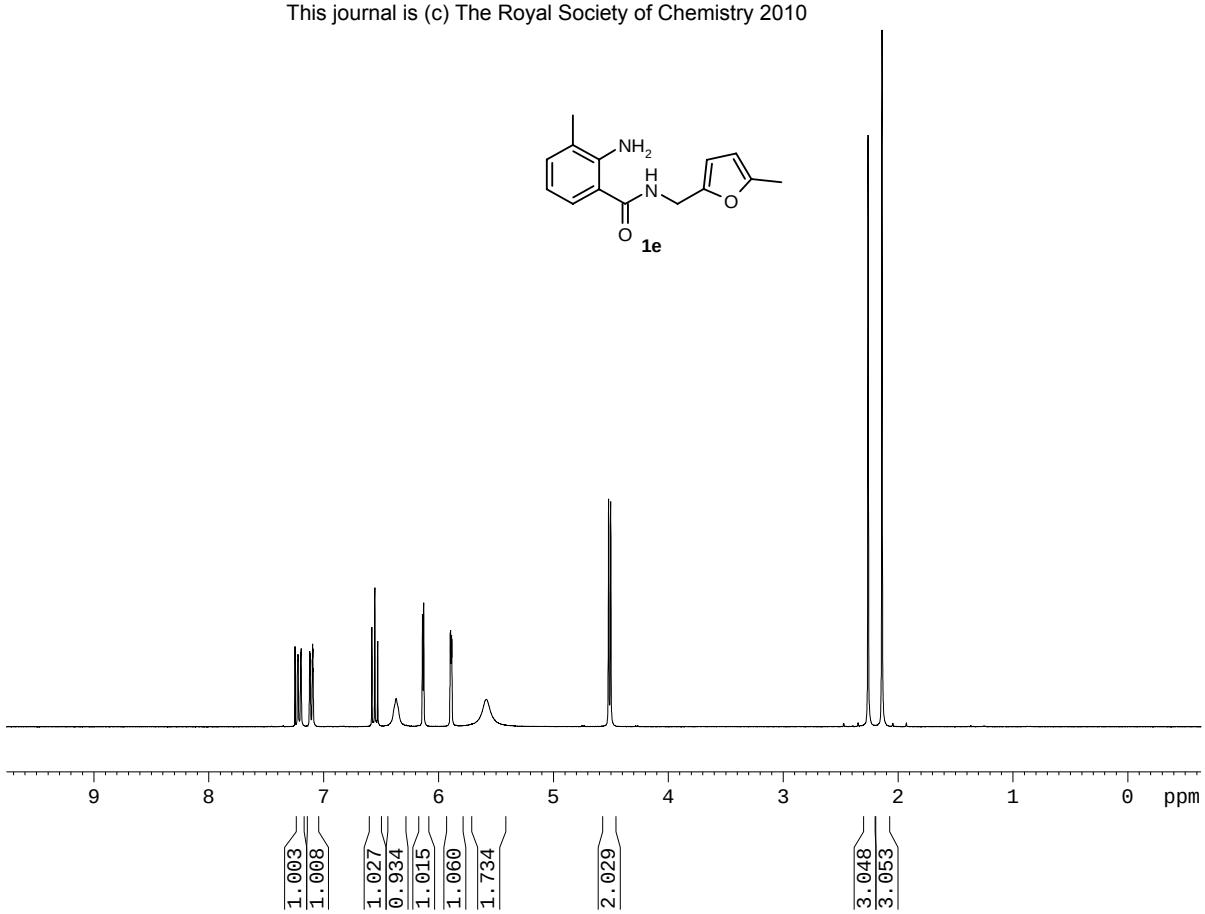

168.882
151.860
149.322
148.711
132.251
127.169
117.164
116.400
115.570
108.291
106.200
77.426
77.003
76.579
36.649
13.439
200
180
160
140
120
100
80
60
40
20
ppm

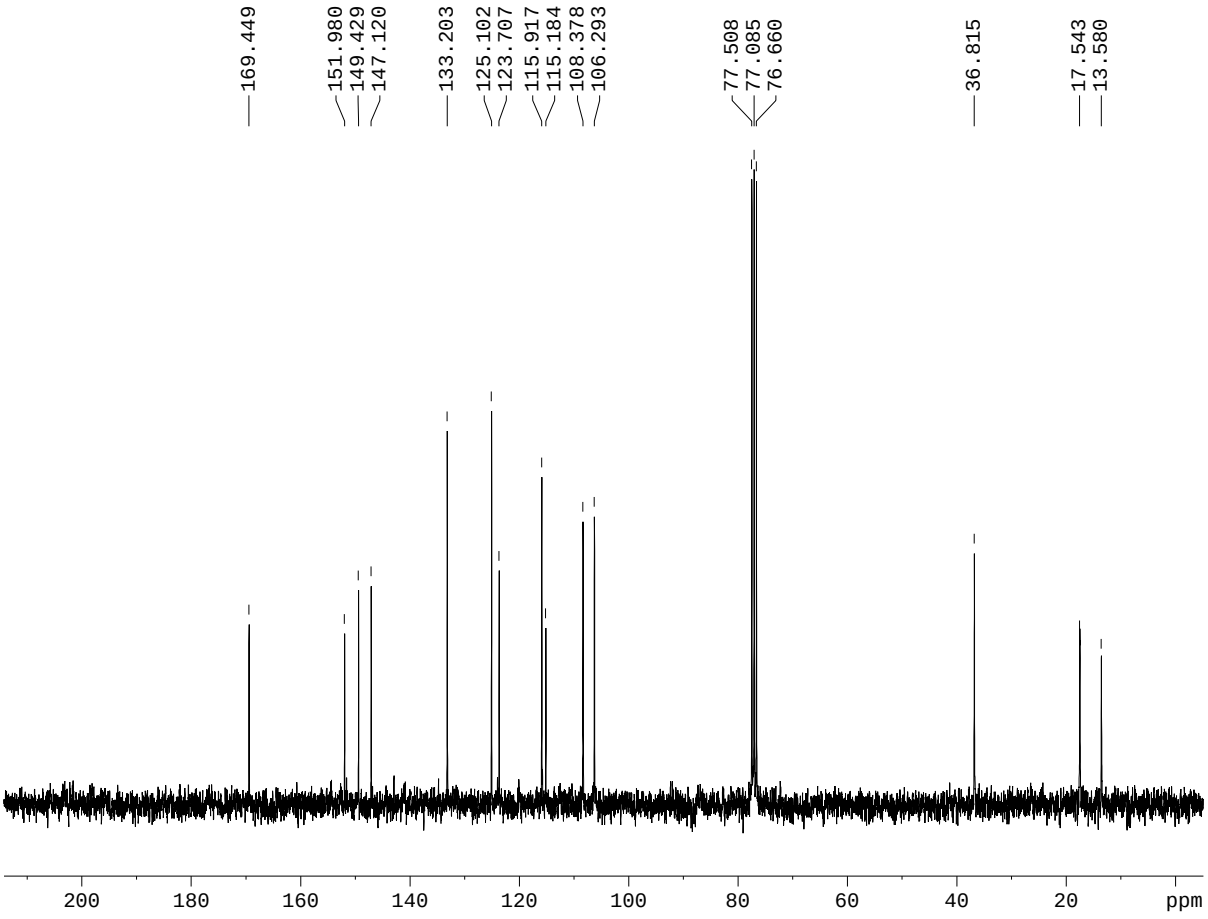

NH2
H
N
Br
O
O
1b
10 9 8 7 6 5 4 3 2 1 0 ppm
0.968
1.589
0.971
0.861
0.988
0.960
1.734
2.043
3.000

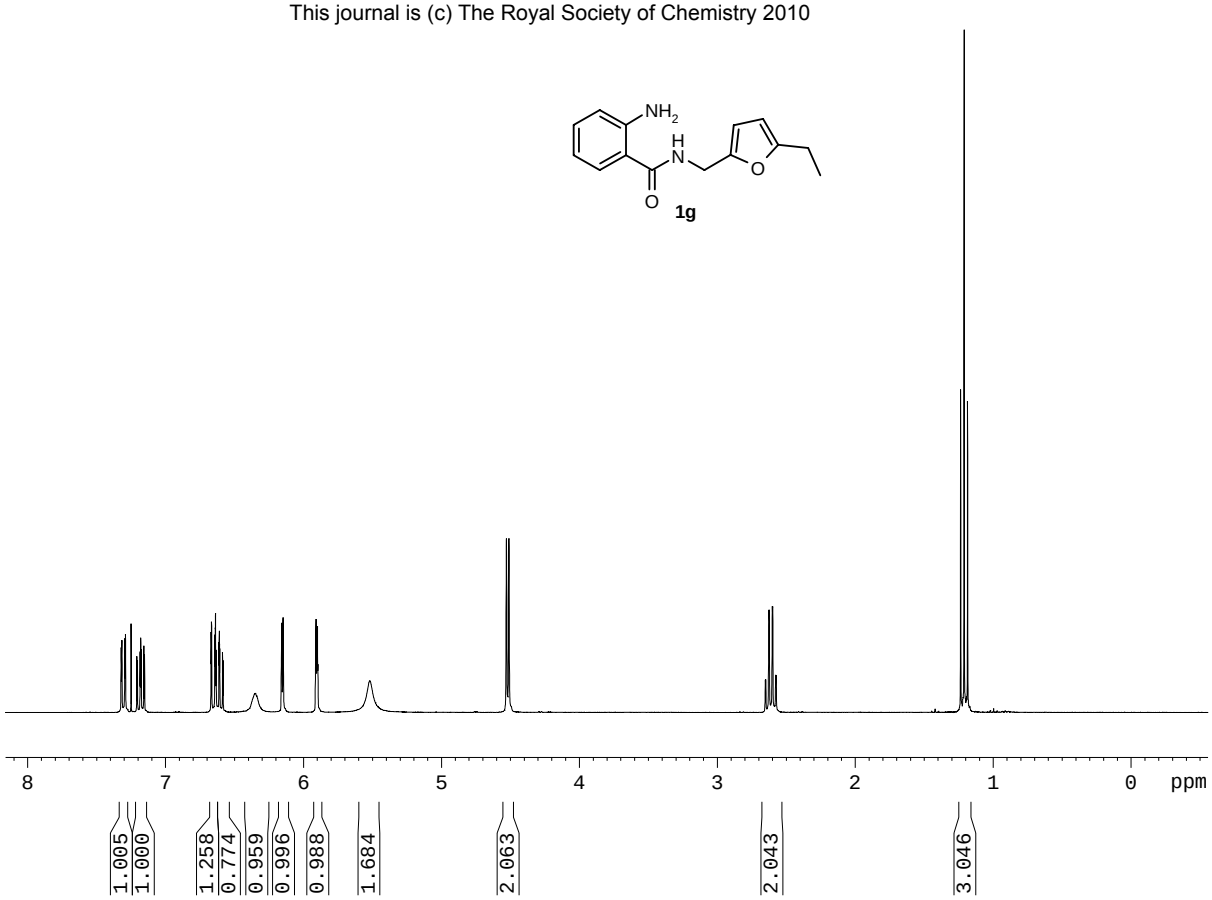

167.652
152.161
148.870
147.669
134.922
129.620
118.811
117.081
108.683
107.522
106.294
77.424
77.000
76.577
36.800
13.549
240 220 200 180 160 140 120 100 80 60 40 20 ppm

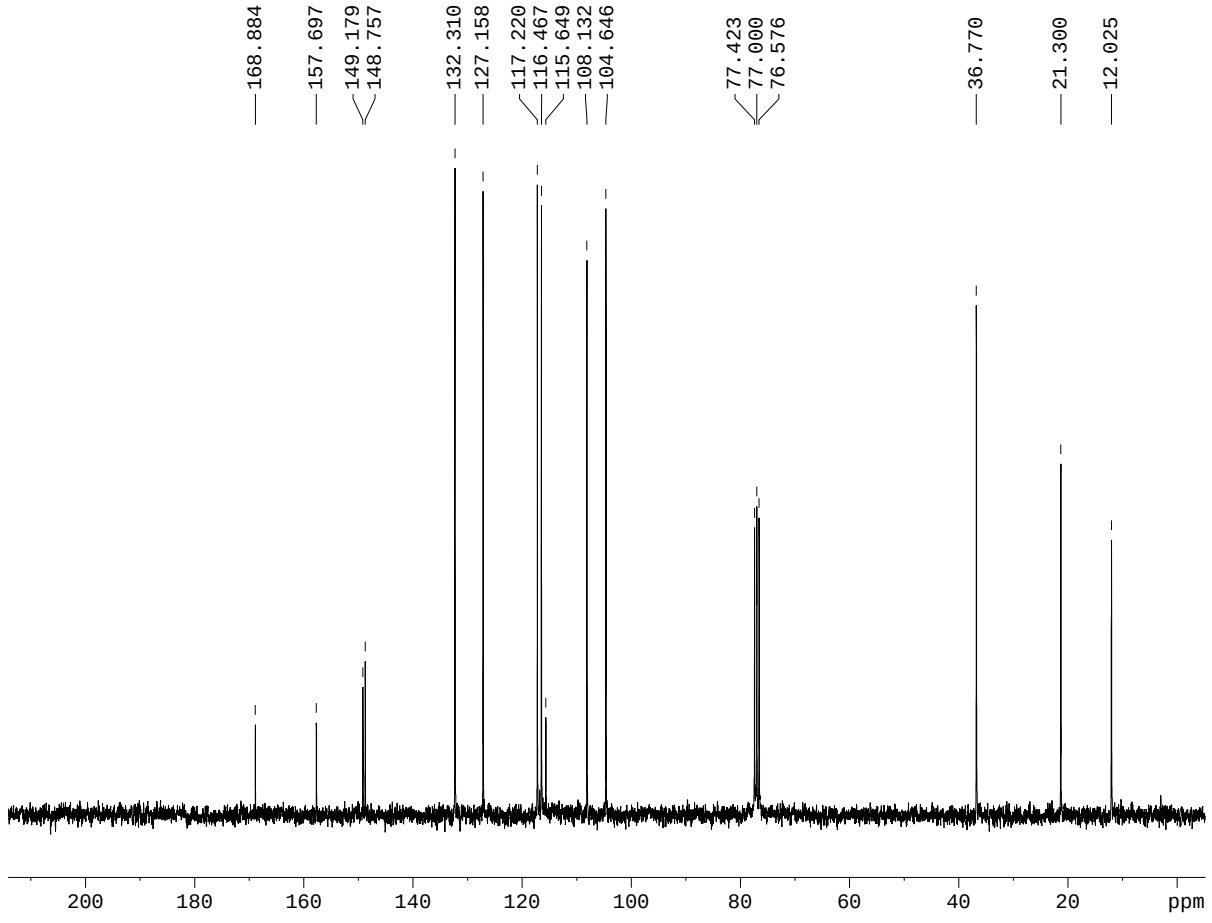

NH2
H
N
Cl
O
O
1c
10
9
8
7
6
5
4
3
2
1
0
ppm
1.006
1.051
1.126
1.028
1.189
1.167
2.422
2.908

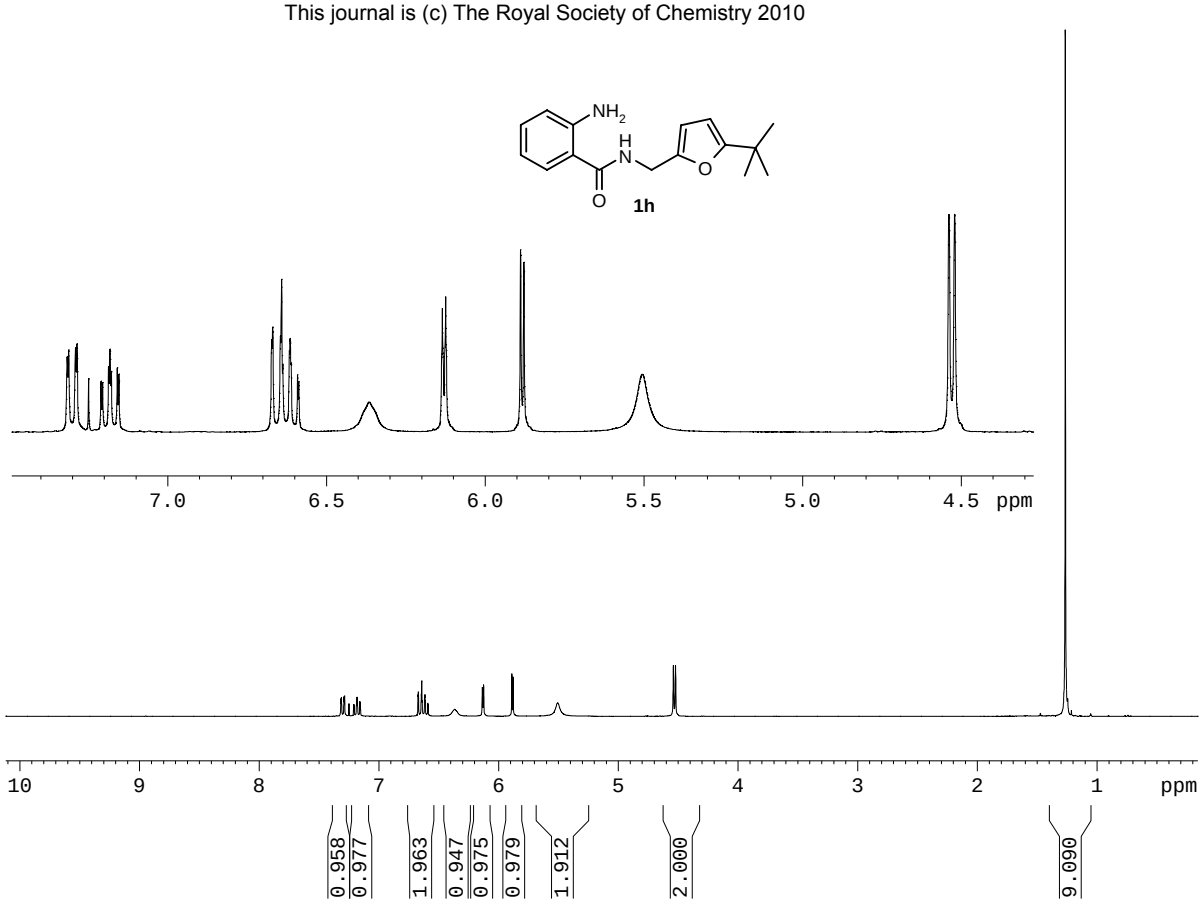

167.772
152.105
148.911
147.213
132.324
132.135
127.172
126.762
120.780
118.456
117.265
116.547
108.617
108.384
106.273
77.427
77.003
76.580
36.770
13.509
240
220
200
180
160
140
120
100
80
60
40
20
ppm

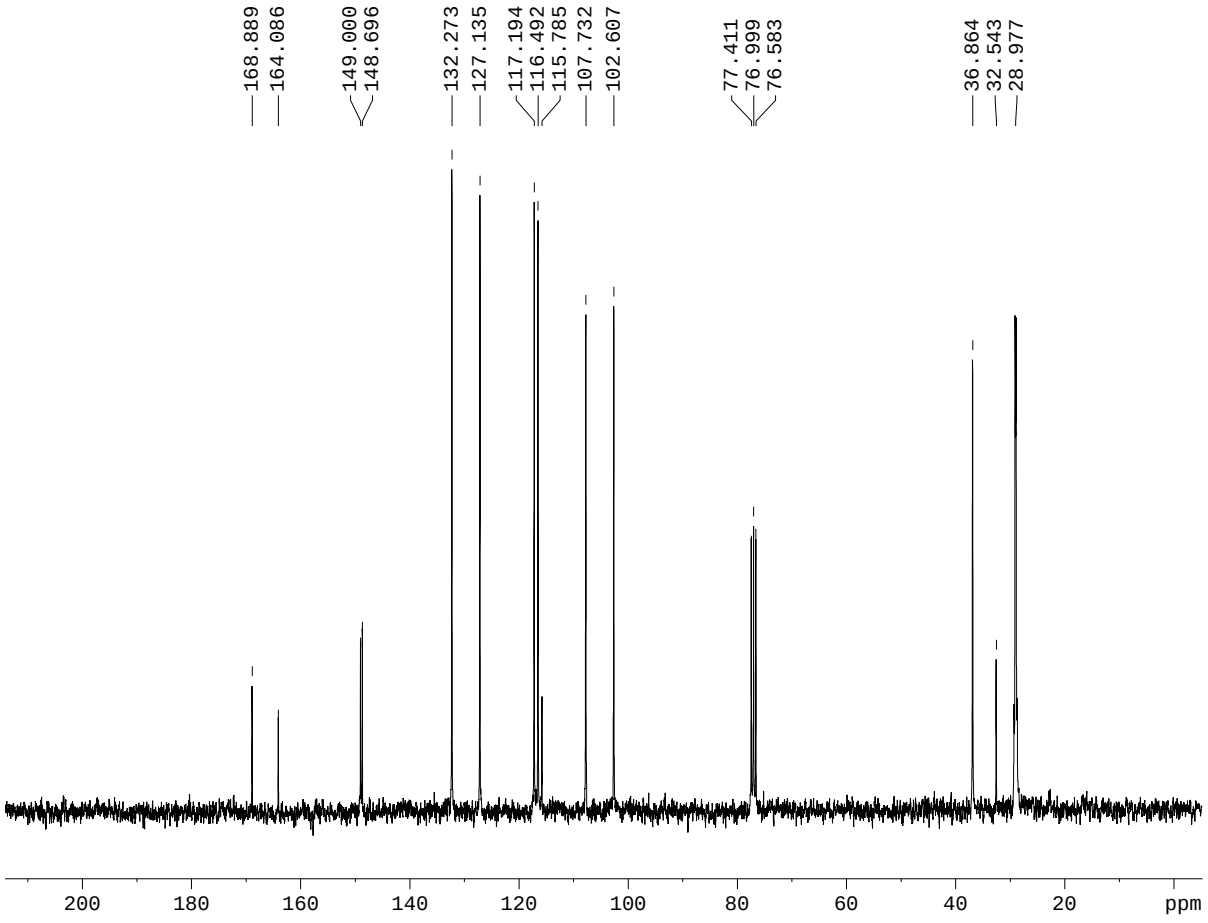

NH2
H
N
O
O
1e
9
8
7
6
5
4
3
2
1
0
ppm
1.003
1.008
1.027
0.934
1.015
1.060
1.734
2.029
3.048
3.053

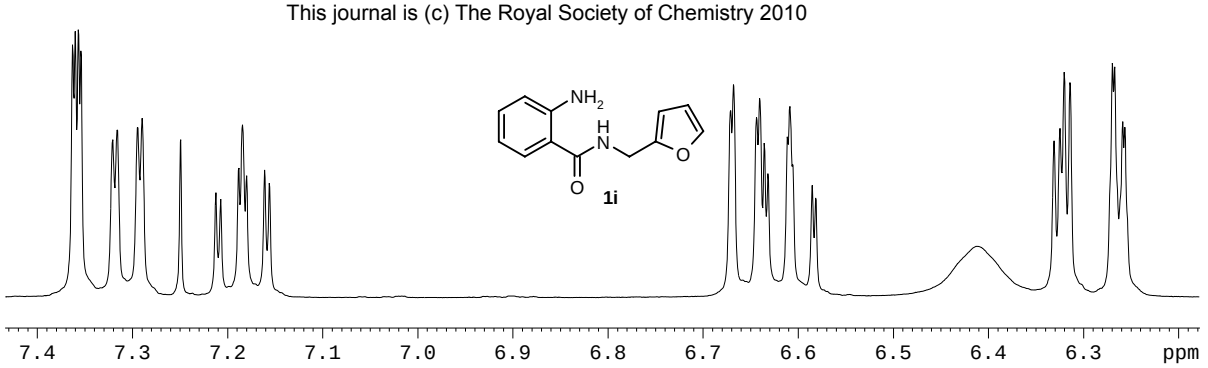

169.449
151.980
149.429
147.120
133.203
125.102
123.707
115.917
115.184
108.378
106.293
77.508
77.085
76.660
36.815
17.543
13.580
200
180
160
140
120
100
80
60
40
20
ppm


NH2
H
N
O
O
1g
8
7
6
5
4
3
2
1
0
ppm
1.005
1.000
1.258
0.774
0.959
0.996
0.988
1.684
2.063
2.043
3.046


168.884
157.697
149.179
148.757
132.310
127.158
117.220
116.467
115.649
108.132
104.646
77.423
77.000
76.576
36.770
21.300
12.025
200
180
160
140
120
100
80
60
40
20
ppm

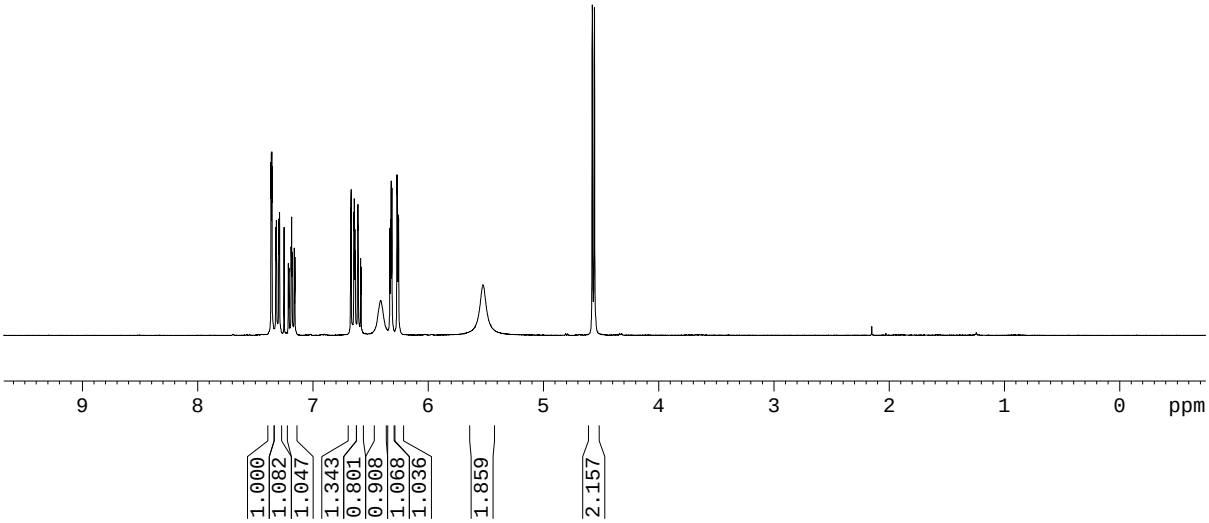

NH2
H
N
O
O
1h
7.0
6.5
6.0
5.5
5.0
4.5 ppm
10
9
8
7
6
5
4
3
2
1
ppm
0.958
0.977
1.963
0.947
0.975
0.979
1.912
2.000
9.090

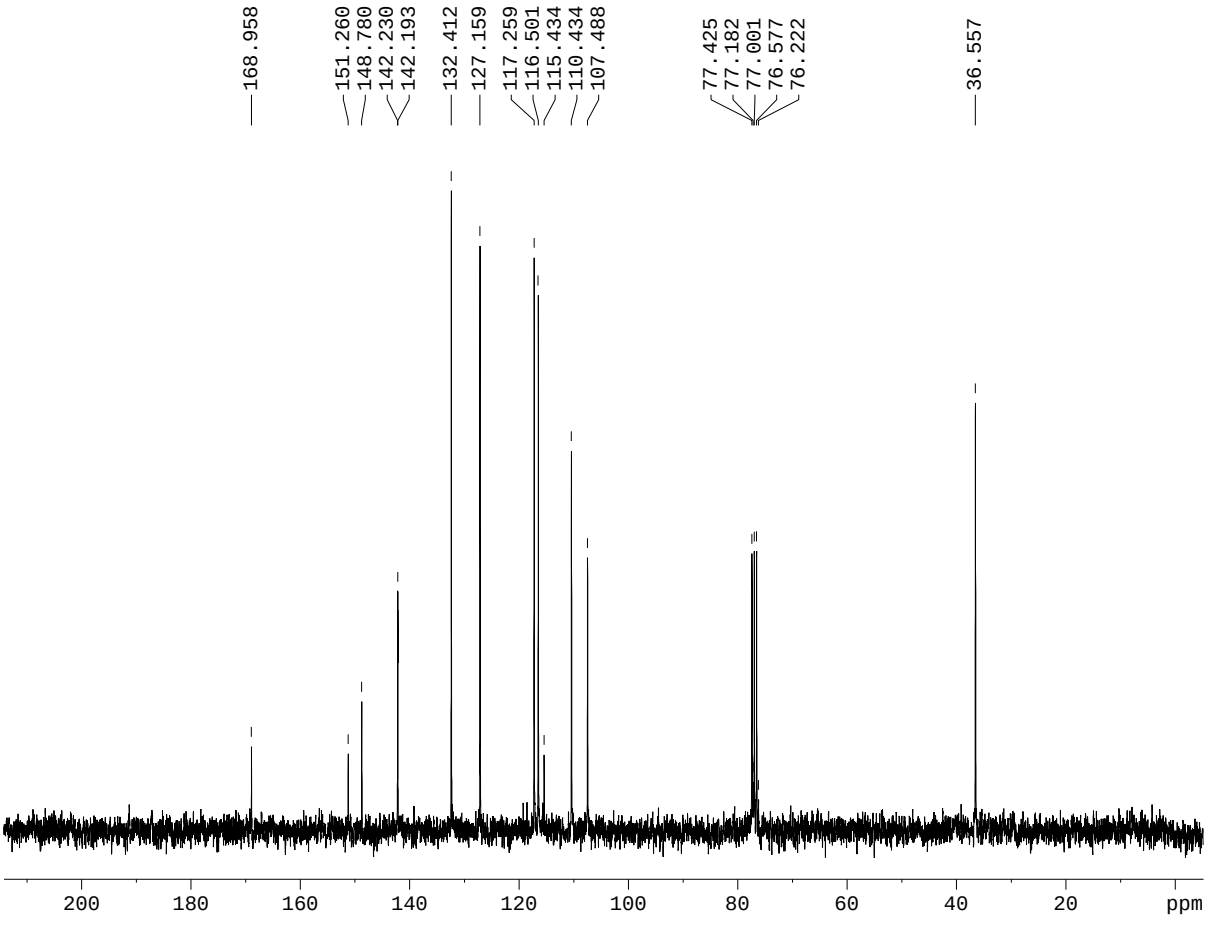

168.889
164.086
149.000
148.696
132.273
127.135
117.194
116.492
115.785
107.732
102.607
77.411
76.999
76.583
36.864
32.543
28.977
200
180
160
140
120
100
80
60
40
20
ppm

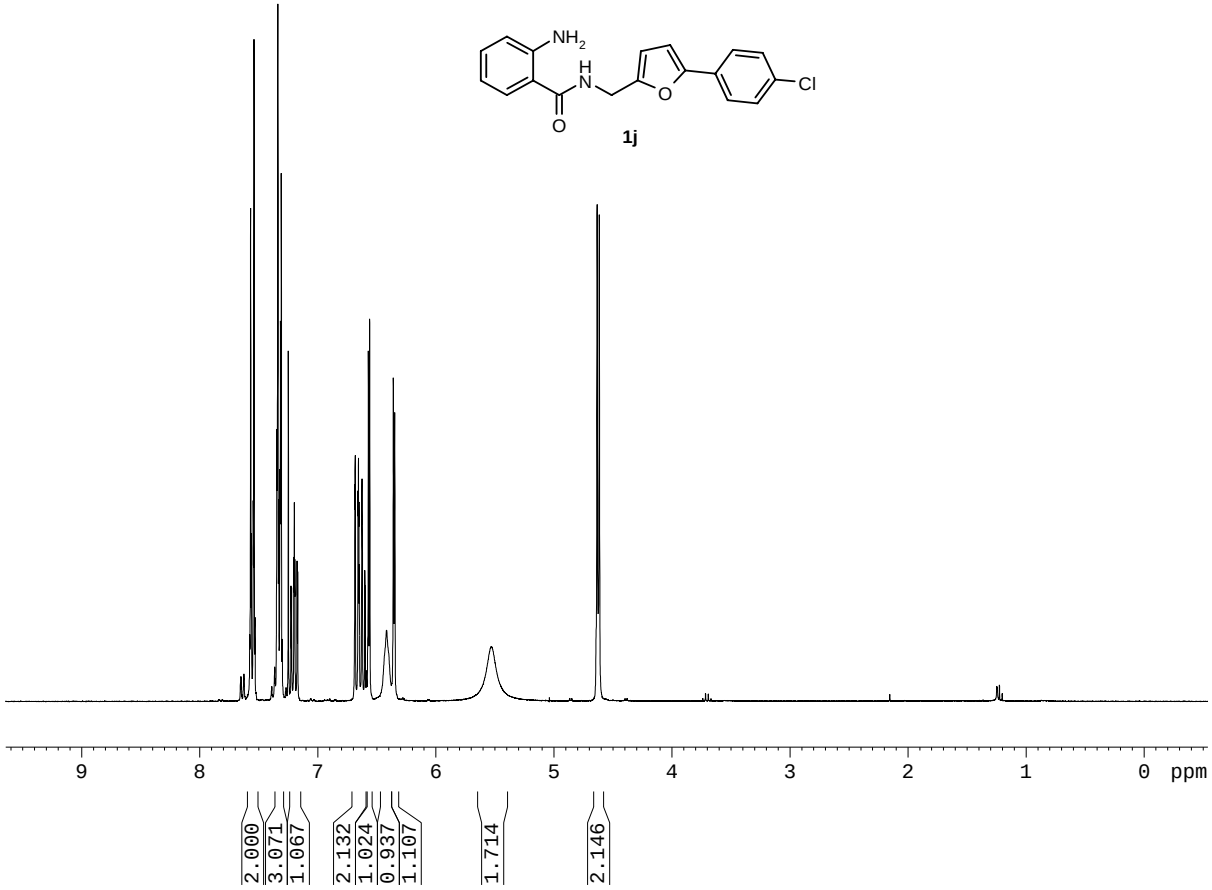

NH2
H
N
O
O

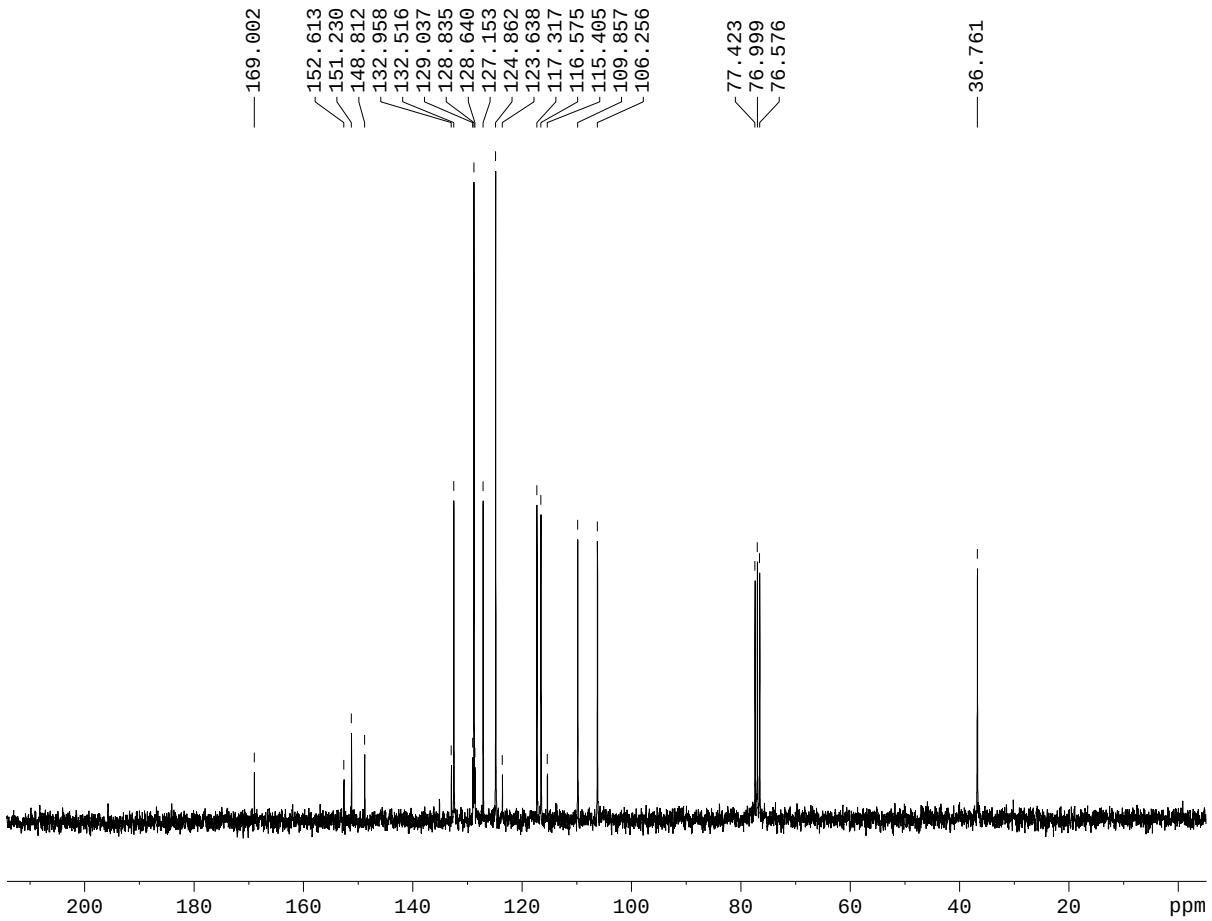
1i

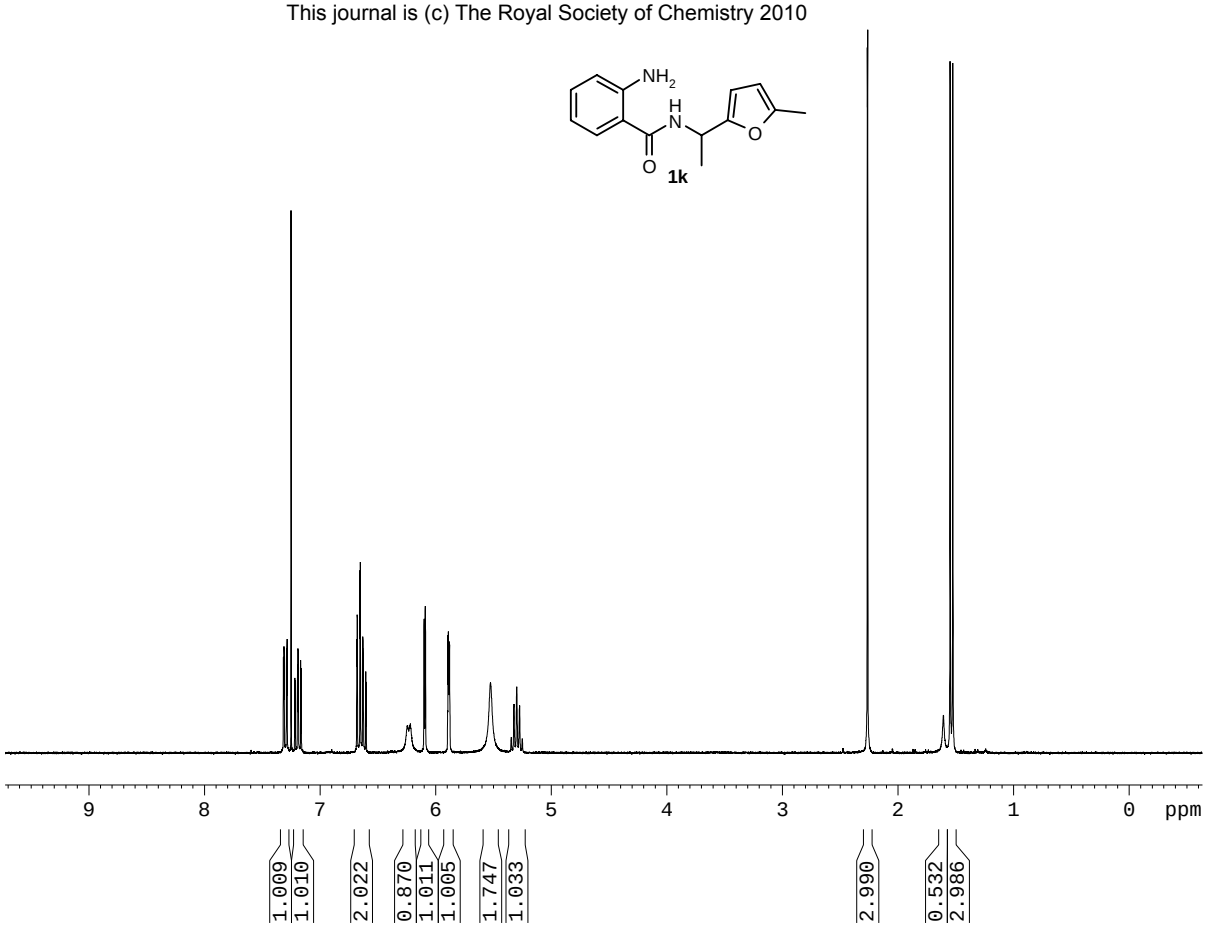
7.4
7.3
7.2
7.1
7.0
6.9
6.8
6.7
6.6
6.5
6.4
6.3
ppm

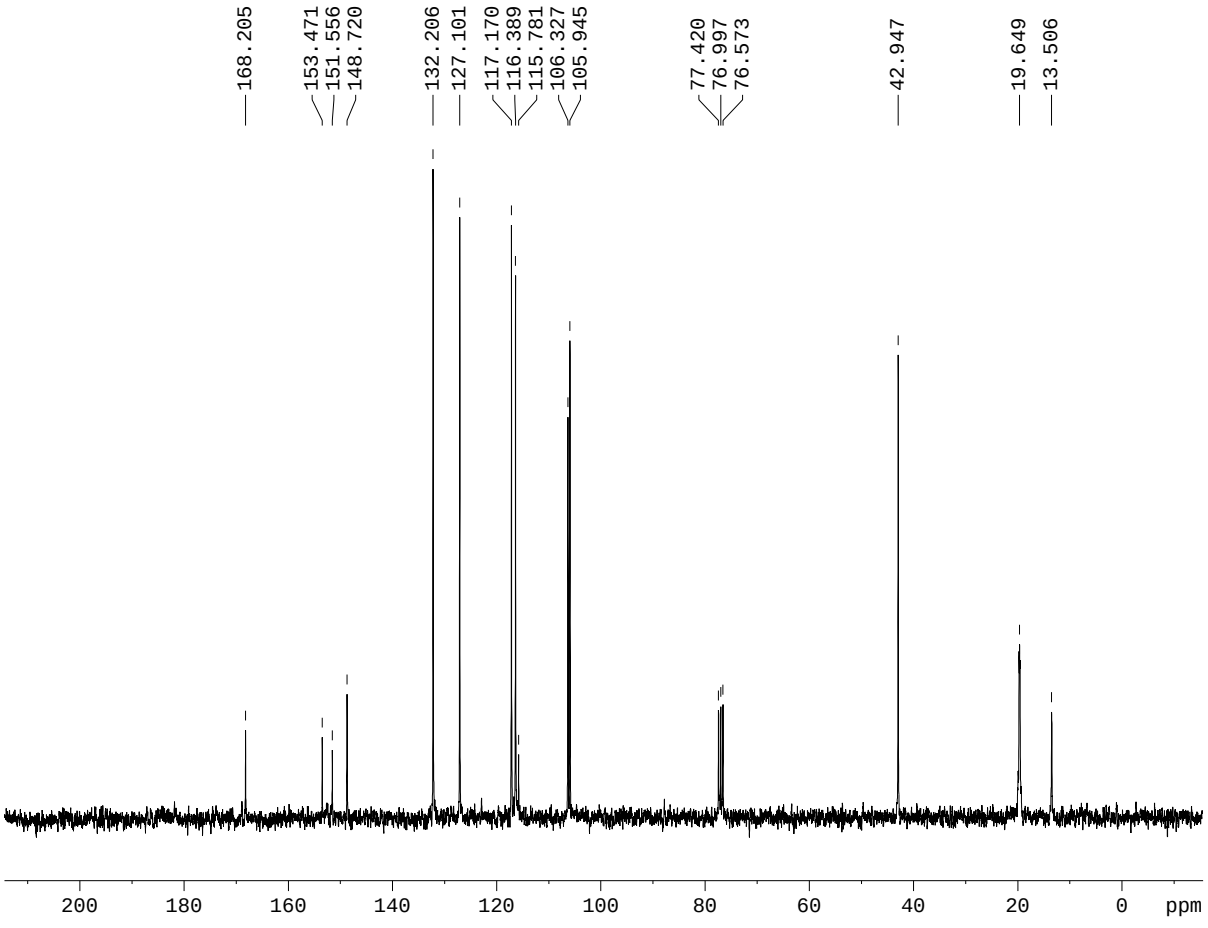

9
8
7
6
5
4
3
2
1
0
ppm
1.000
1.082
1.047
1.343
0.801
0.908
1.068
1.036
1.859
2.157

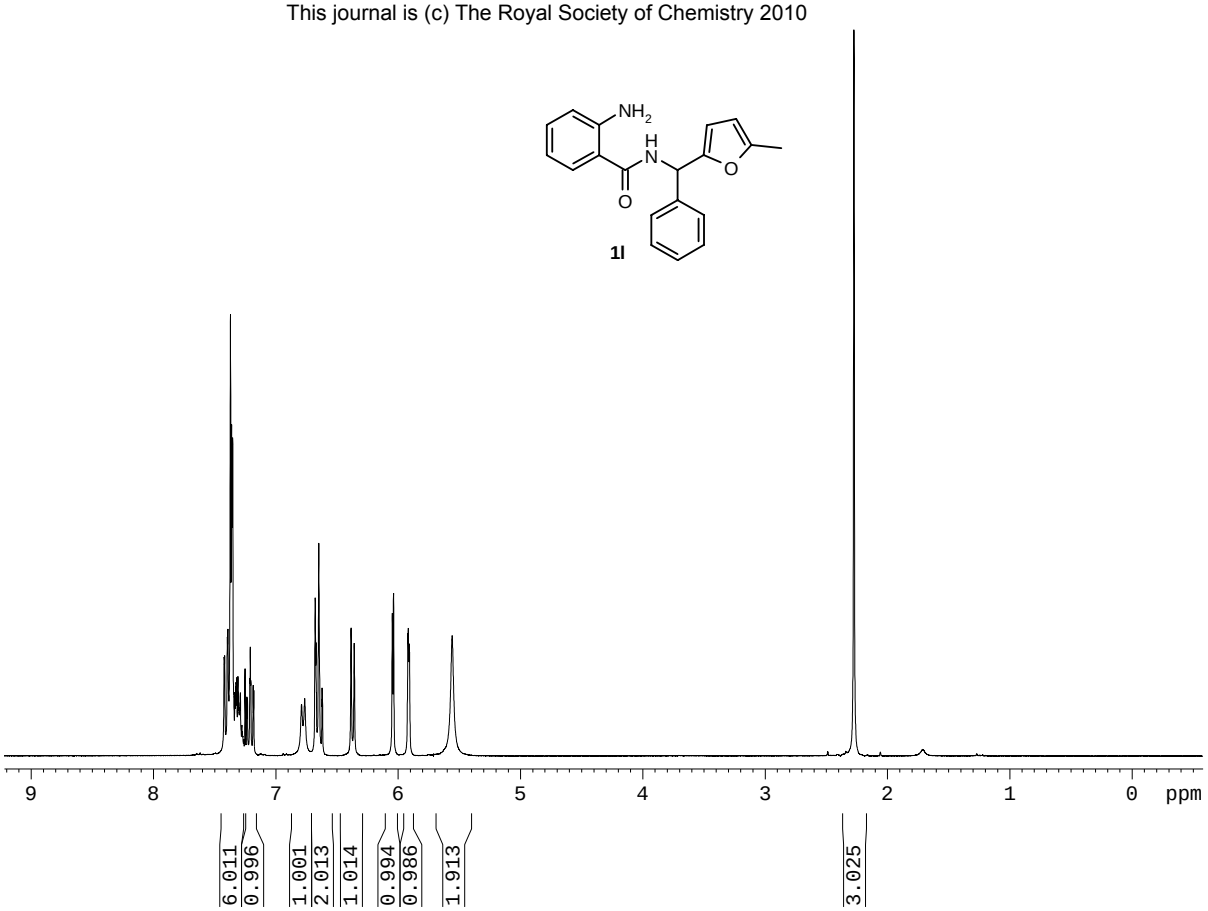

168.958
151.260
148.780
142.230
142.193
132.412
127.159
117.259
116.501
115.434
110.434
107.488
77.425
77.182
77.001
76.577
76.222
36.557
200
180
160
140
120
100
80
60
40
20
ppm

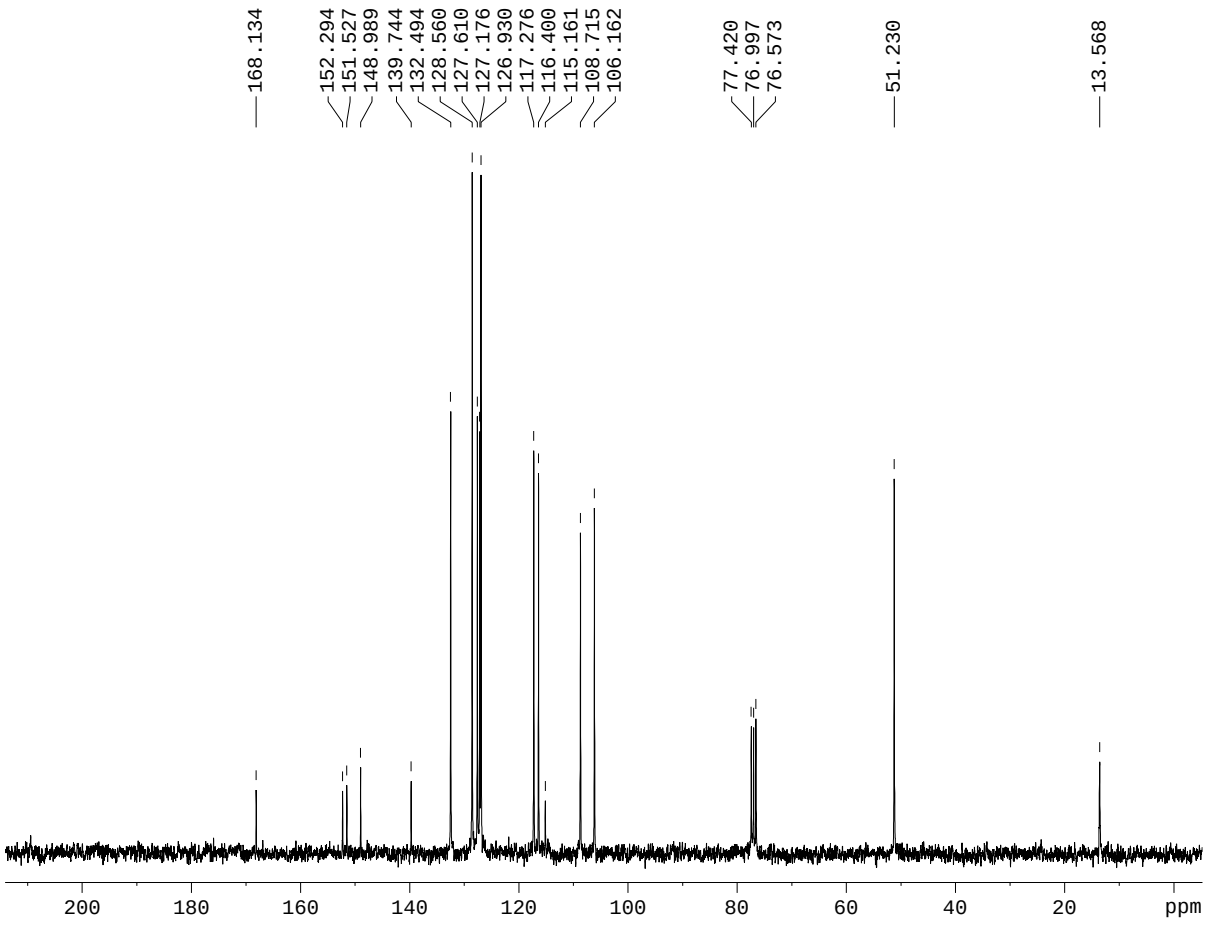

NH2
H
N
O
O
Cl
1j
9
8
7
6
5
4
3
2
1
0
ppm
2.000
3.071
1.067
2.132
1.024
0.937
1.107
1.714
2.146

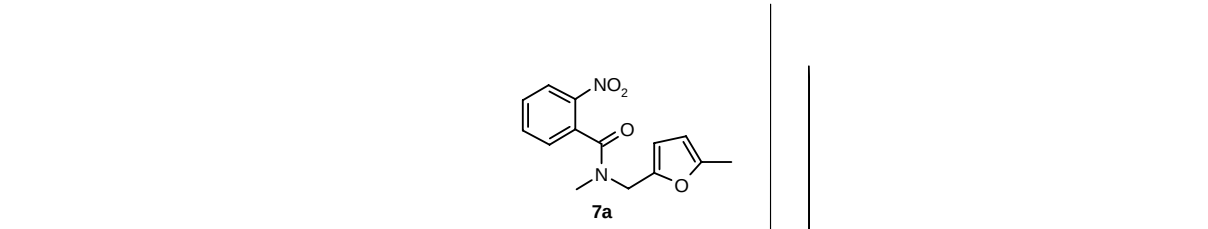

169.002
152.613
151.230
148.812
132.958
132.516
129.037
128.835
128.640
127.153
124.862
123.638
117.317
116.575
115.405
109.857
106.256
77.423
76.999
76.576
36.761
200
180
160
140
120
100
80
60
40
20
ppm


NH2
H
N
O
O
1k
9
8
7
6
5
4
3
2
1
0
ppm
1.009
1.010
2.022
0.870
1.011
1.005
1.747
1.033
2.990
0.532
2.986


168.205
153.471
151.556
148.720
132.206
127.101
117.170
116.389
115.781
106.327
105.945
77.420
76.997
76.573
42.947
19.649
13.506
200
180
160
140
120
100
80
60
40
20
0
ppm

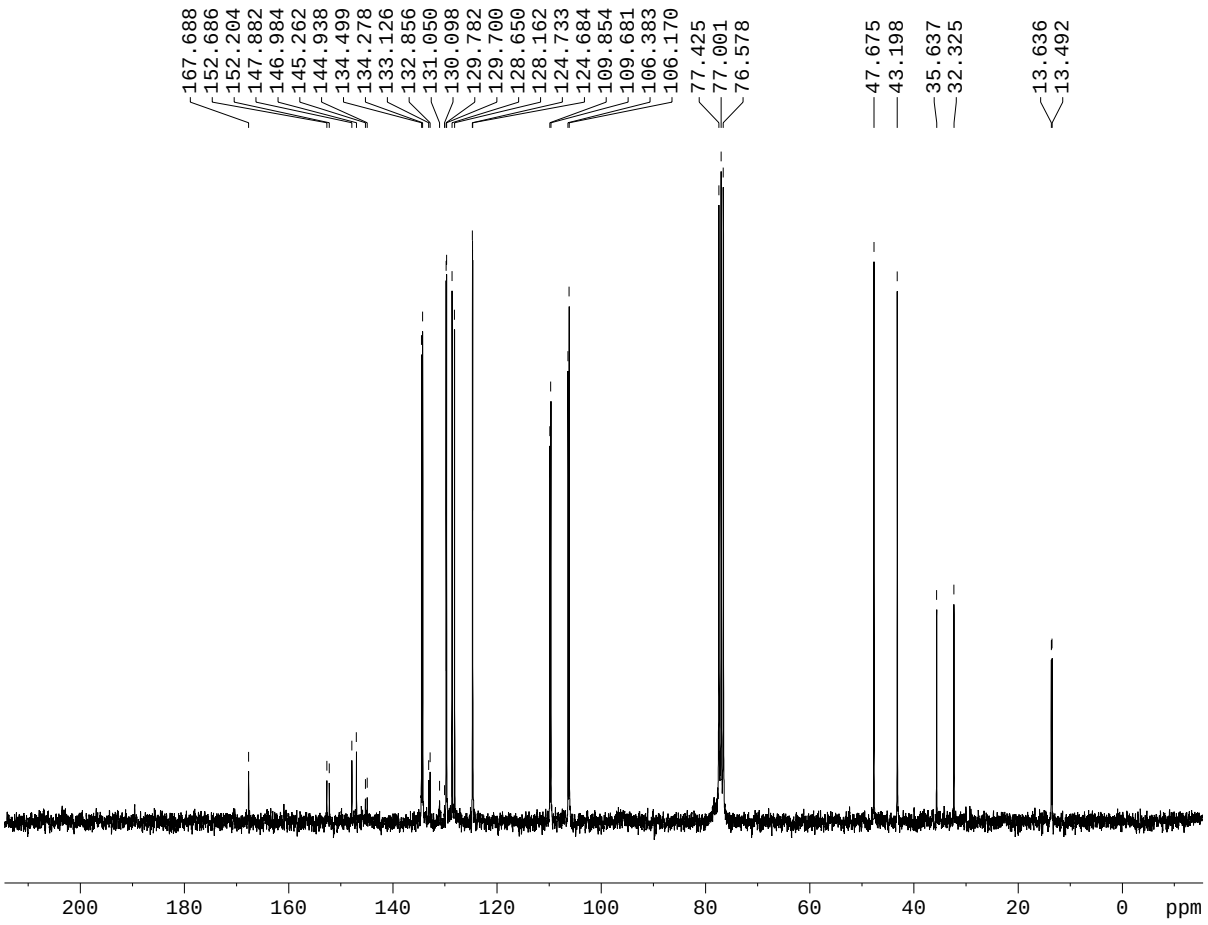

NH2
H
N
O
O
1l
9
8
7
6
5
4
3
2
1
0
ppm
6.011
0.996
1.001
2.013
1.014
0.994
0.986
1.913
3.025

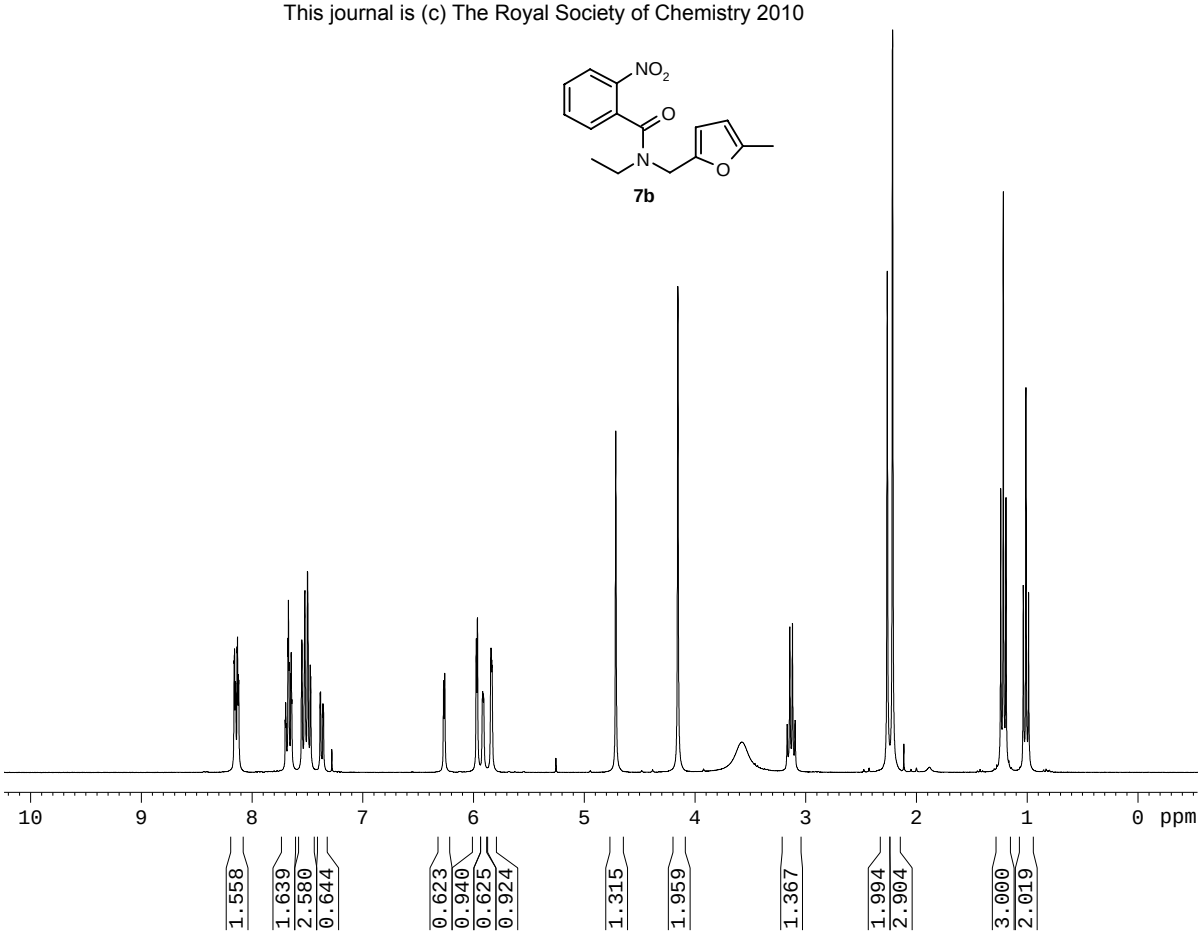

168.134
152.294
151.527
148.989
139.744
132.494
128.560
127.610
127.176
126.930
117.276
116.400
115.161
108.715
106.162
77.420
76.997
76.573
51.230
13.568
200
180
160
140
120
100
80
60
40
20
ppm

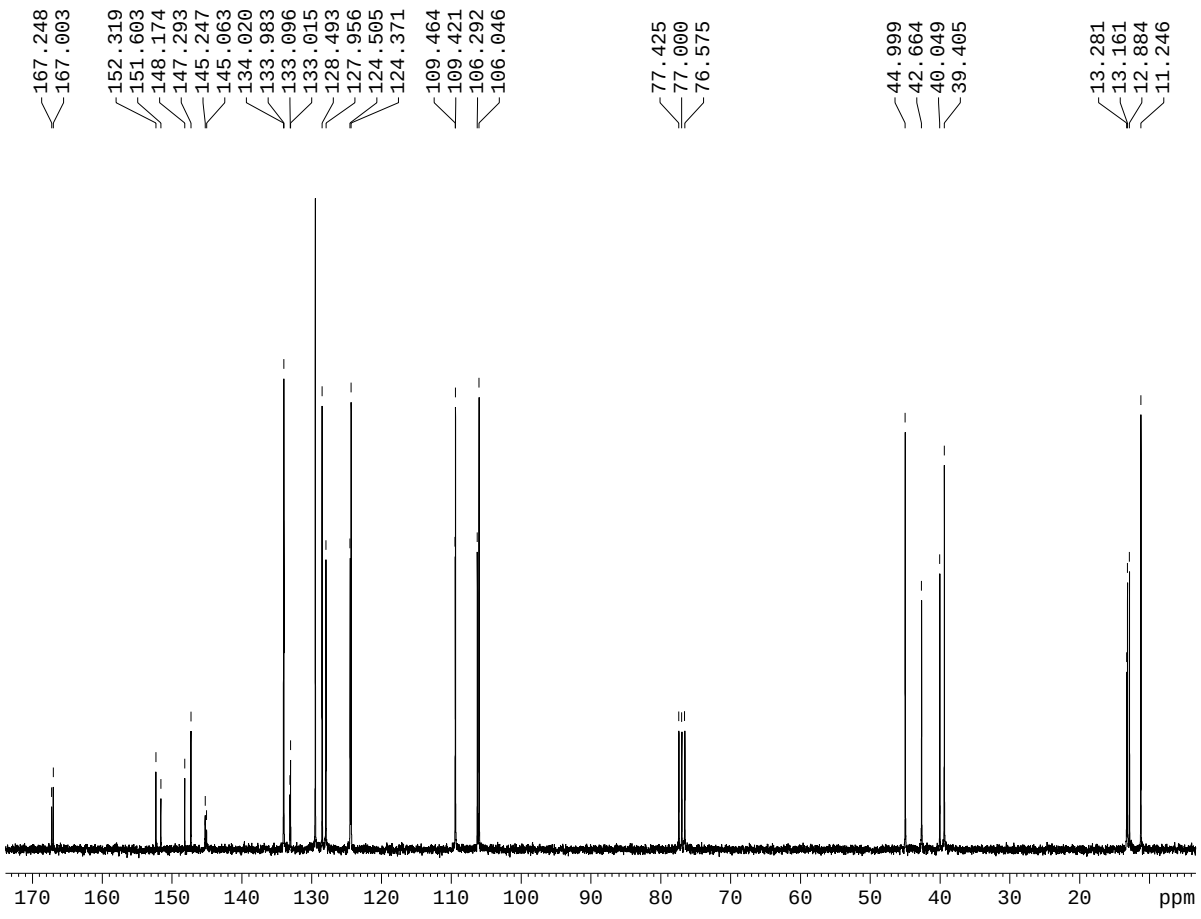

NO2
O
N
O

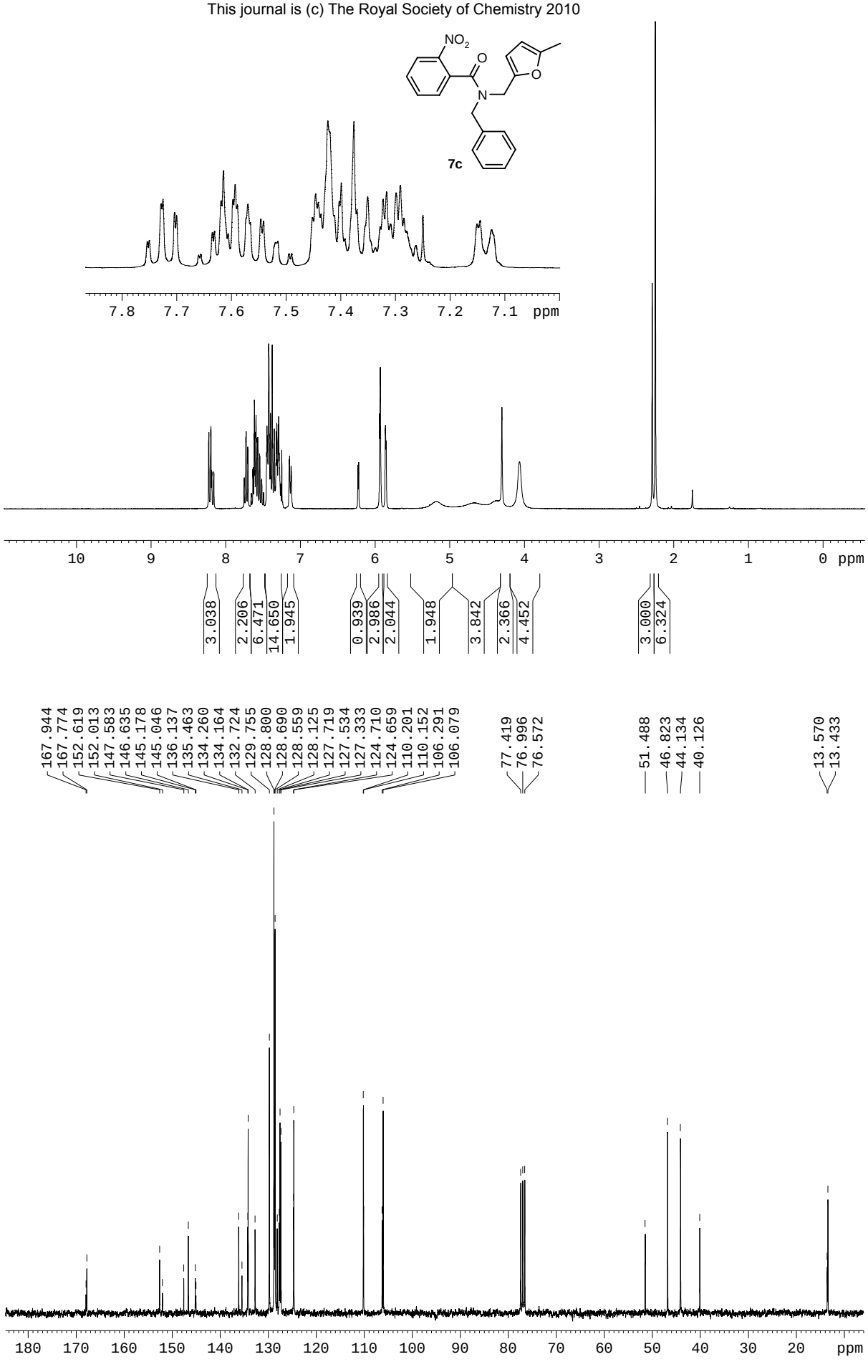
7a

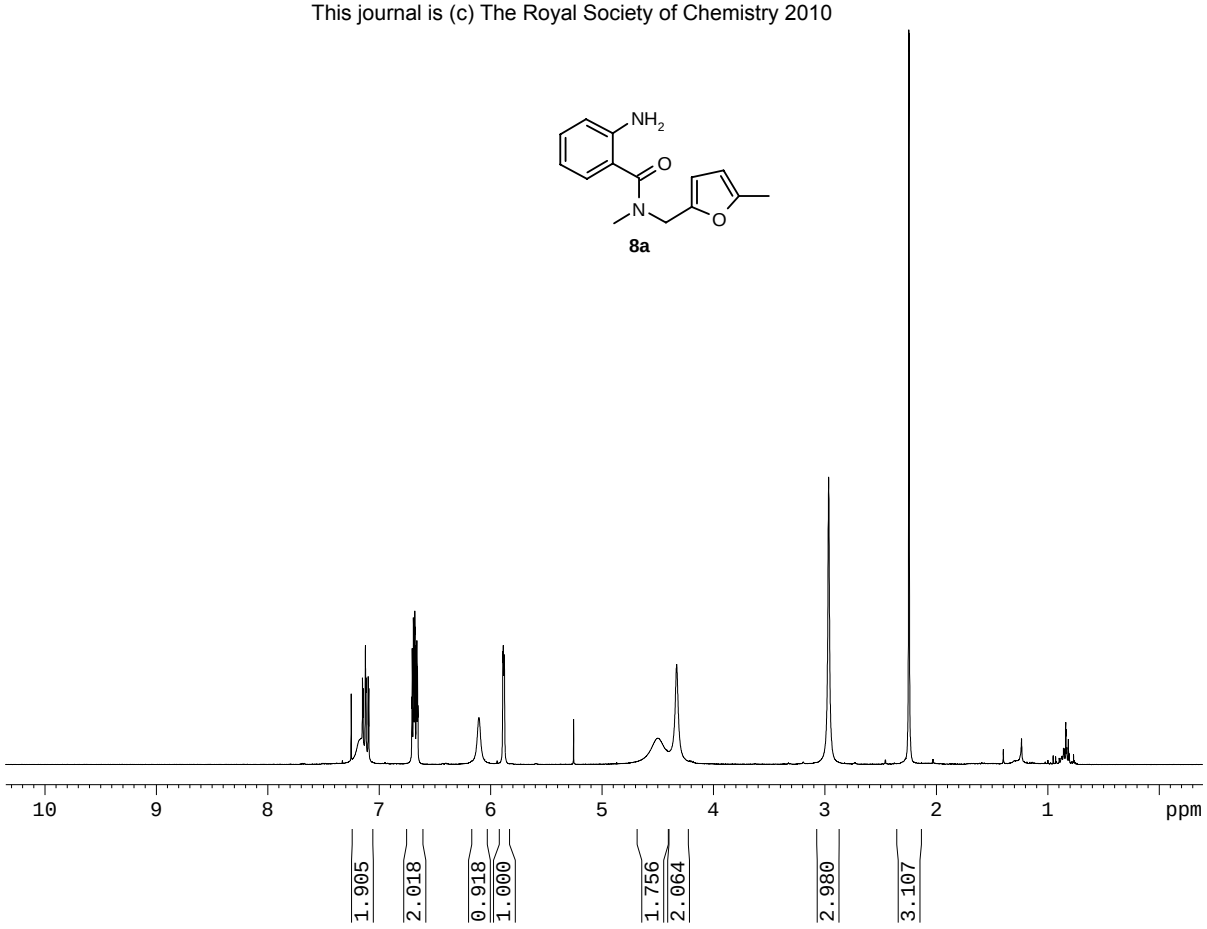
9
8
7
6
5
4
3
2
1
0
ppm
2.013
2.023
3.082
1.000
0.990
1.027
0.987
1.037
1.874
1.894
3.105
2.973
3.001
3.114
0.789

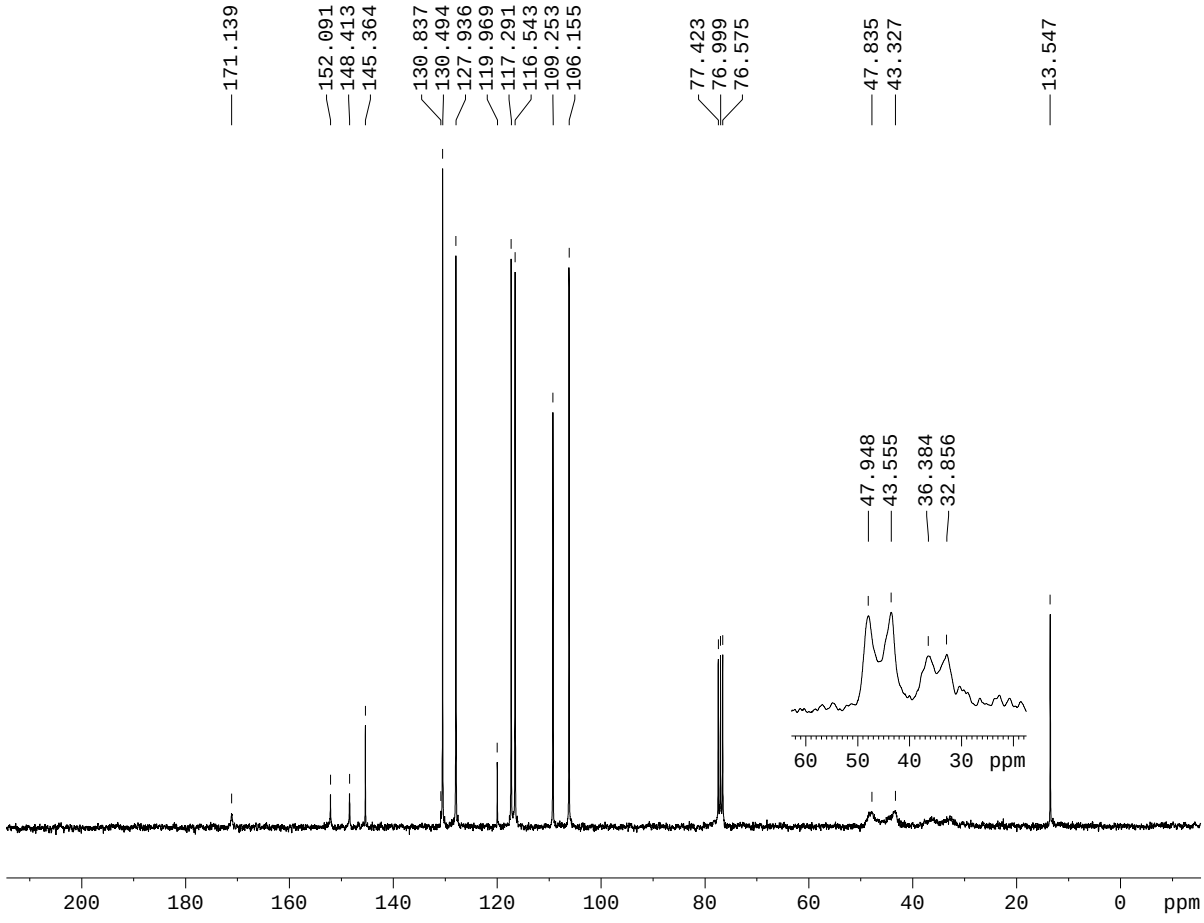

167.688
152.686
152.204
147.882
146.984
145.262
144.938
134.499
134.278
133.126
132.856
131.050
130.098
129.782
129.700
128.650
128.162
124.733
124.684
109.854
109.681
106.383
106.170
77.425
77.001
76.578
47.675
43.198
35.637
32.325
13.636
13.492
200
180
160
140
120
100
80
60
40
20
0
ppm

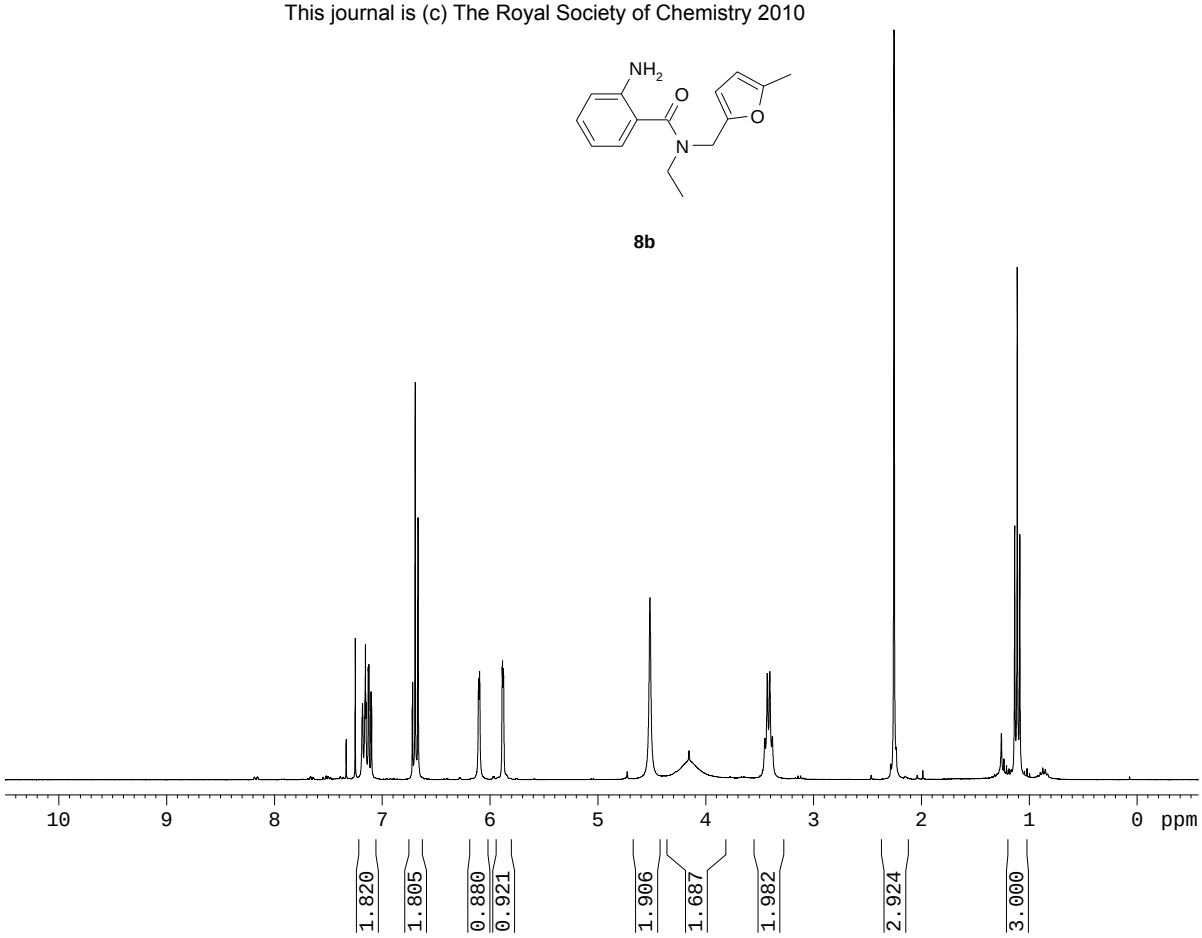

NO2
O
N
O
7b
10 9 8 7 6 5 4 3 2 1 0 ppm
1.558 1.639 2.580 0.644 0.623 0.940 0.625 0.924 1.315 1.959 1.367 1.994 2.904 3.000 2.019


167.248 167.003 152.319 151.603 148.174 147.293 145.247 145.063 134.020 133.983 133.096 133.015 128.493 127.956 124.505 124.371 109.464 109.421 106.292 106.046 77.425 77.000 76.575 44.999 42.664 40.049 39.405 13.281 13.161 12.884 11.246
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

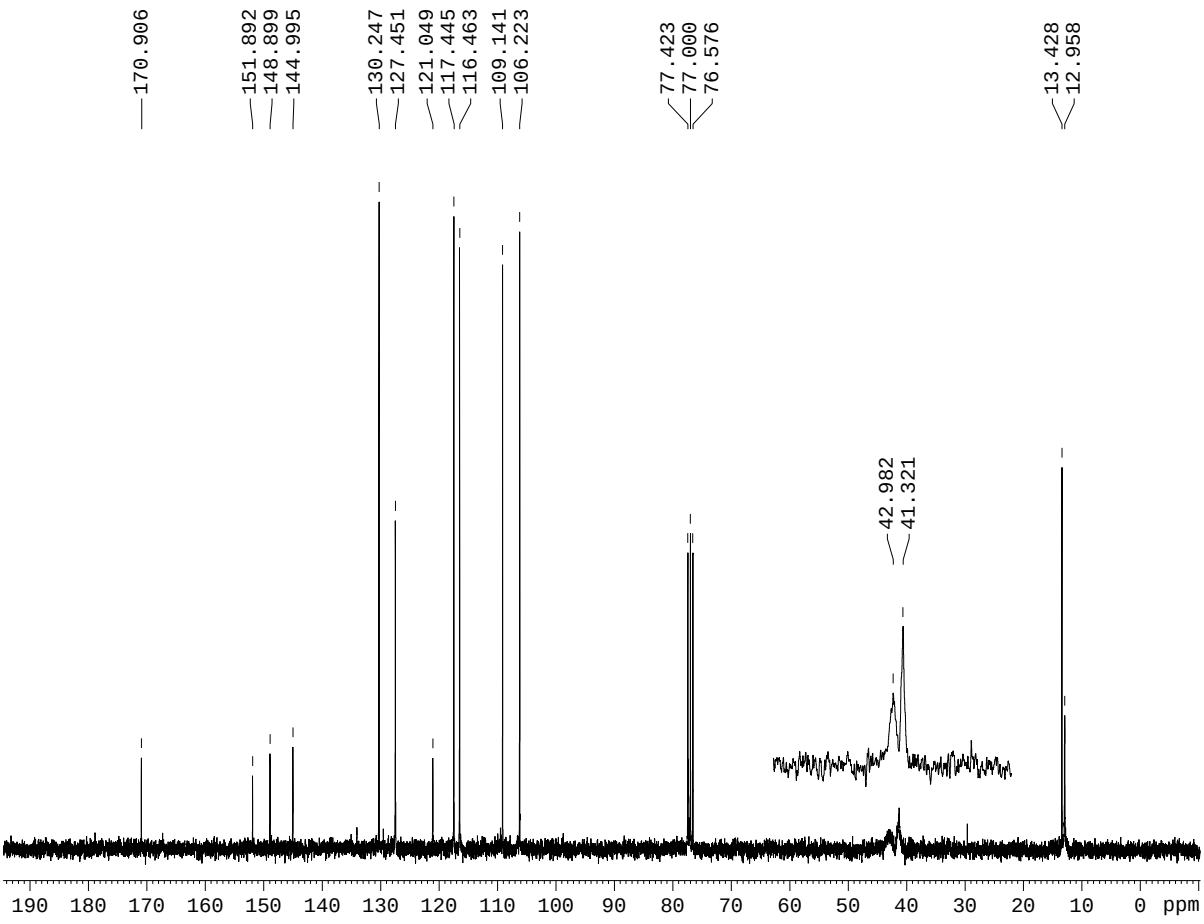

NO2
O
N
O
7c
7.8 7.7 7.6 7.5 7.4 7.3 7.2 7.1 ppm
10 9 8 7 6 5 4 3 2 1 0 ppm
3.038 2.206 6.471 14.650 1.945 0.939 2.986 2.044 1.948 3.842 2.366 4.452 3.000 6.324
167.944 167.774 152.619 152.013 147.583 146.635 145.178 145.046 136.137 135.463 134.260 134.164 132.724 129.755 128.800 128.690 128.559 128.125 127.719 127.534 127.333 124.710 124.659 110.201 110.152 106.291 106.079
77.419 76.996 76.572
51.488 46.823 44.134 40.126
13.570 13.433
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

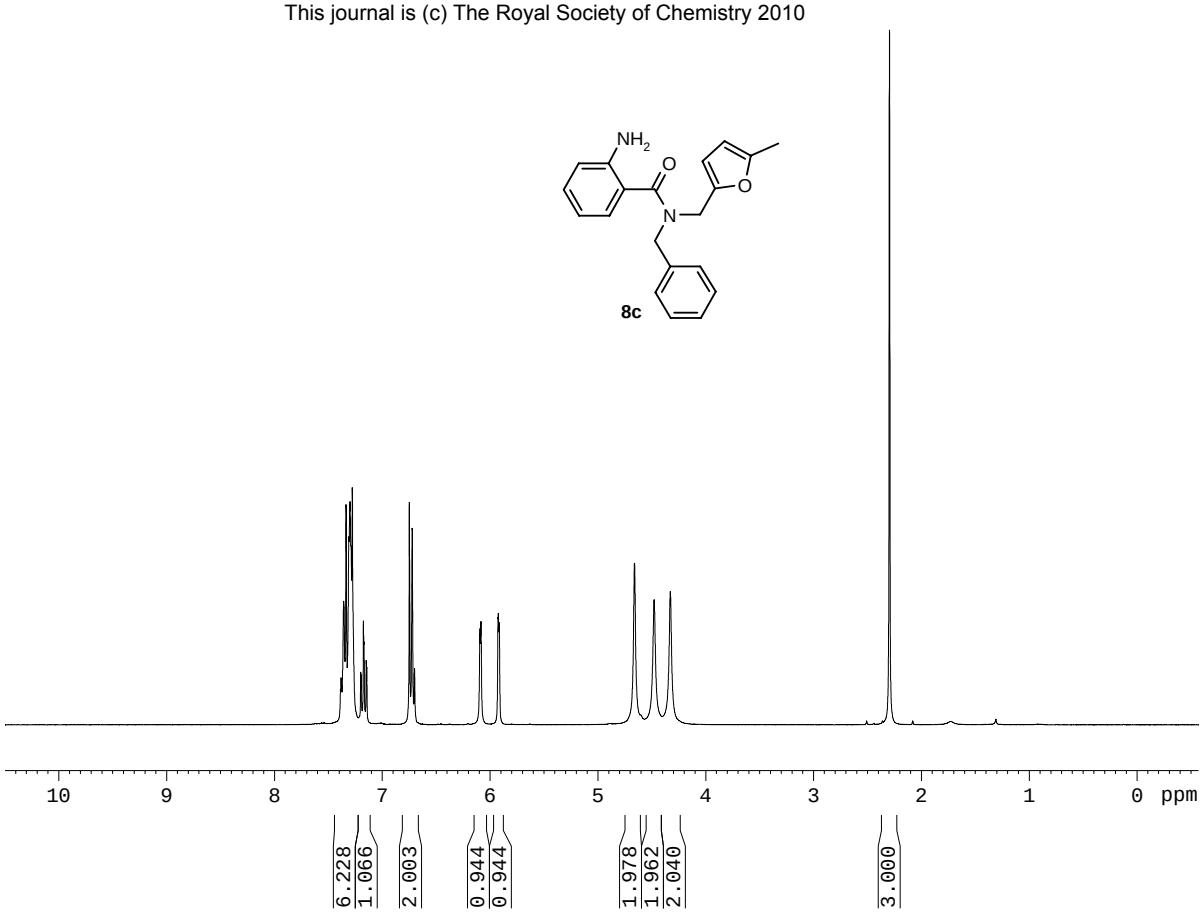

NH2
O
N
O
8a
10
9
8
7
6
5
4
3
2
1
ppm
1.905
2.018
0.918
1.000
1.756
2.064
2.980
3.107

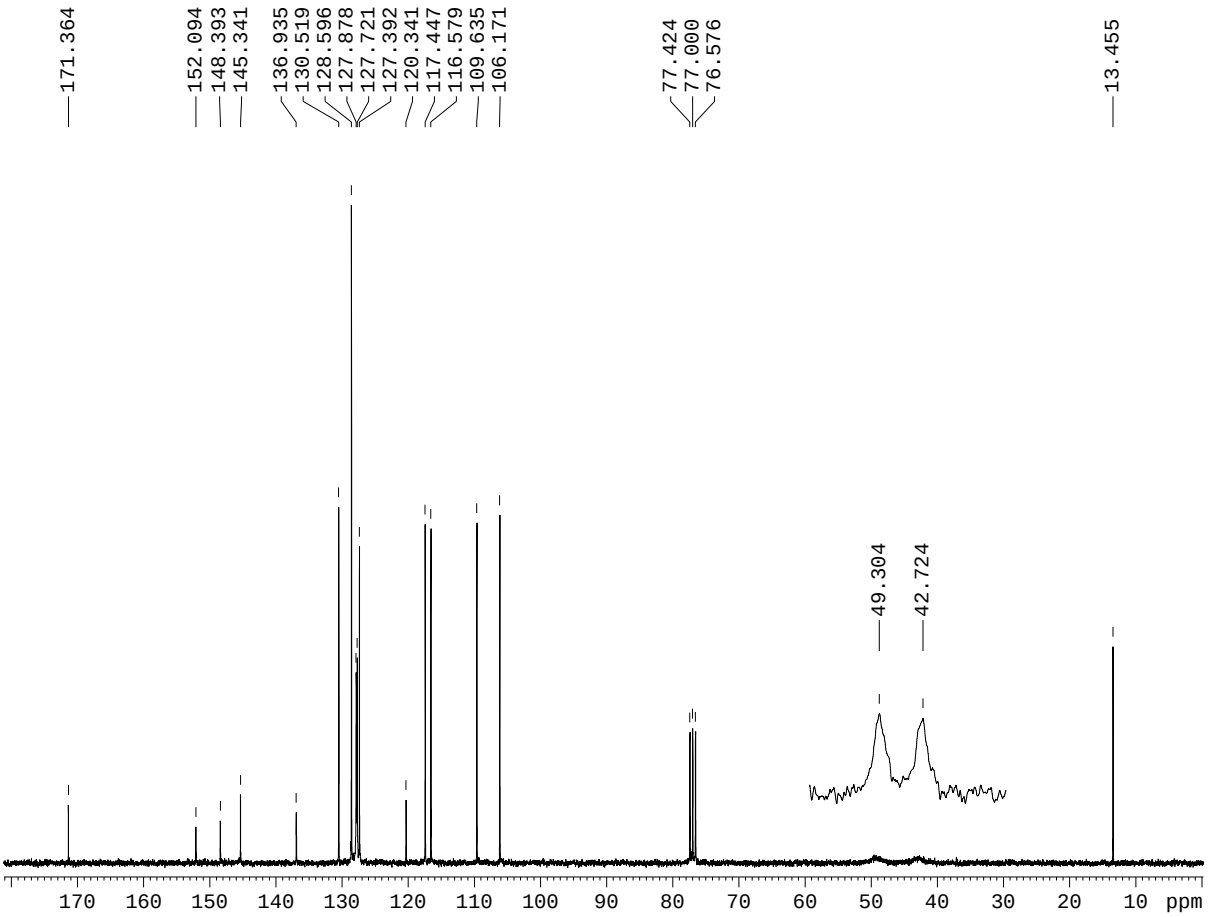

171.139
152.091
148.413
145.364
130.837
130.494
127.936
119.969
117.291
116.543
109.253
106.155
77.423
76.999
76.575
47.835
43.327
13.547
47.948
43.555
36.384
32.856
60
50
40
30
ppm
200
180
160
140
120
100
80
60
40
20
0
ppm

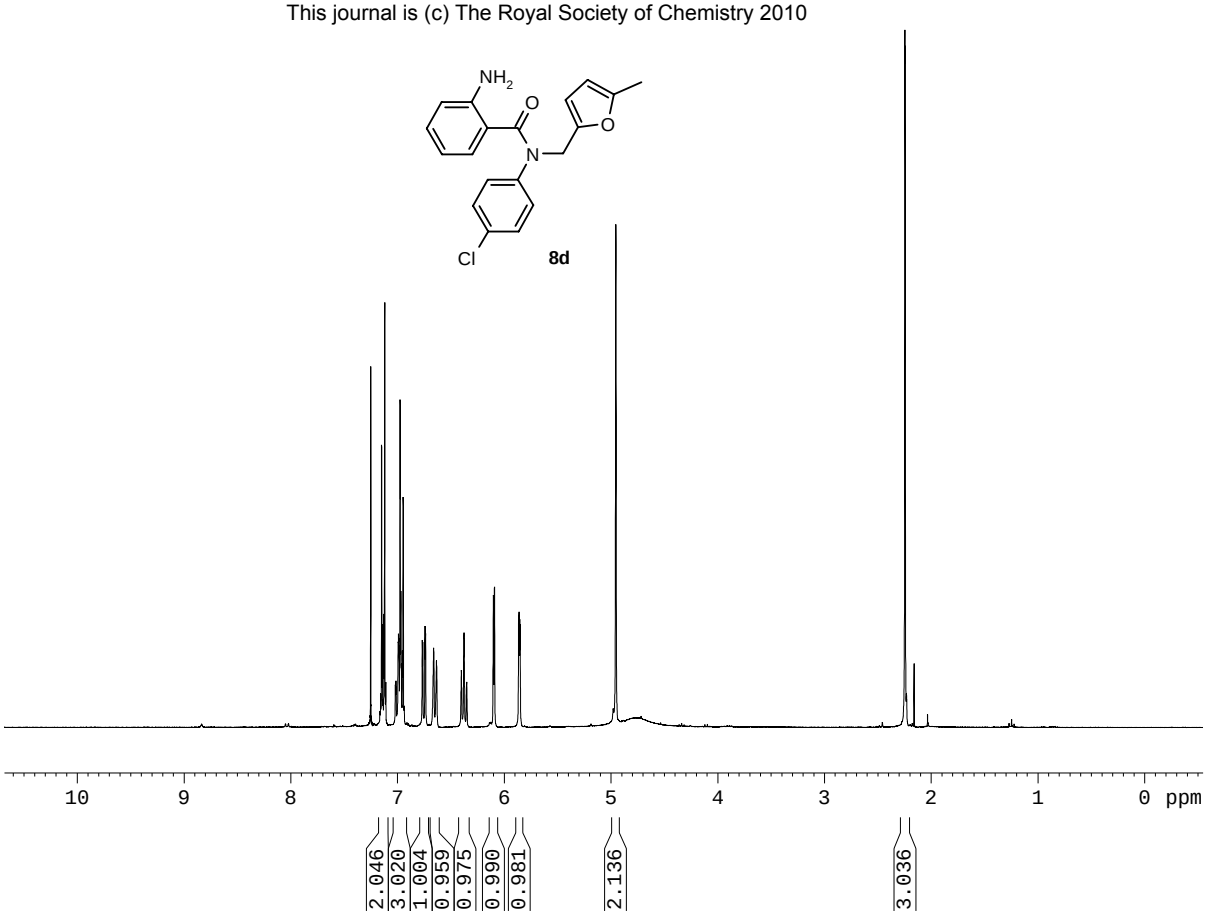

NH2
O
N
O
10 9 8 7 6 5 4 3 2 1 0 ppm
1.820
1.805
0.880
0.921
1.906
1.687
1.982
2.924
3.000

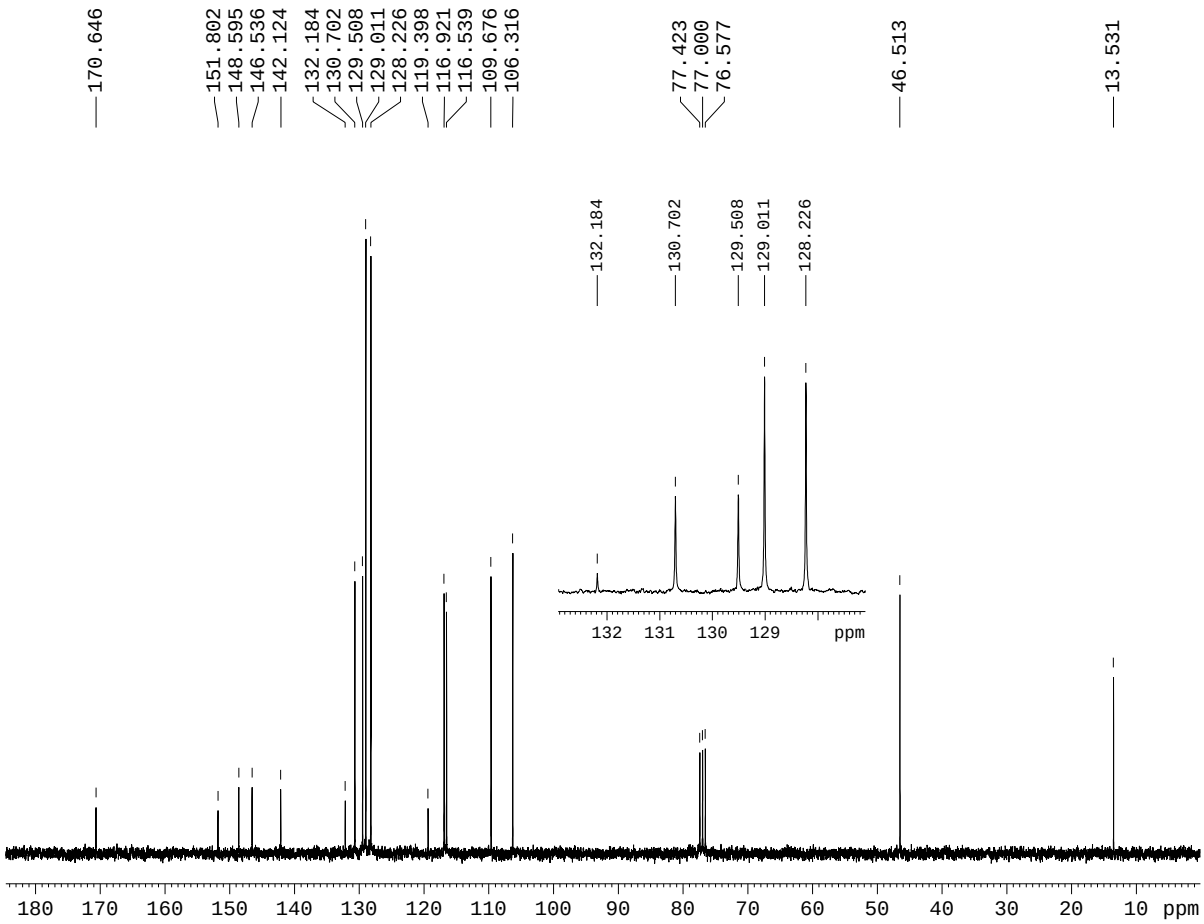
8b

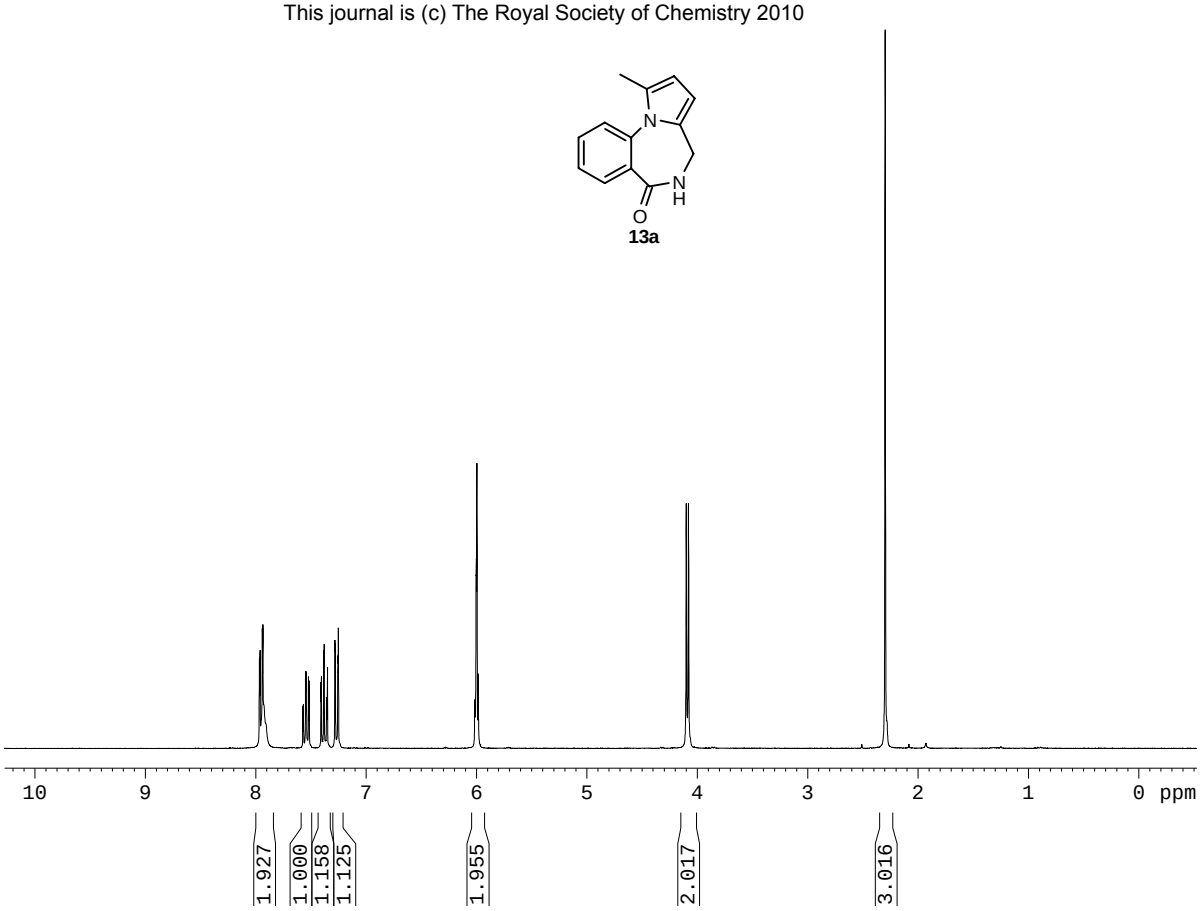

170.906
151.892
148.899
144.995
130.247
127.451
121.049
117.445
116.463
109.141
106.223
77.423
77.000
76.576
42.982
41.321
13.428
12.958
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

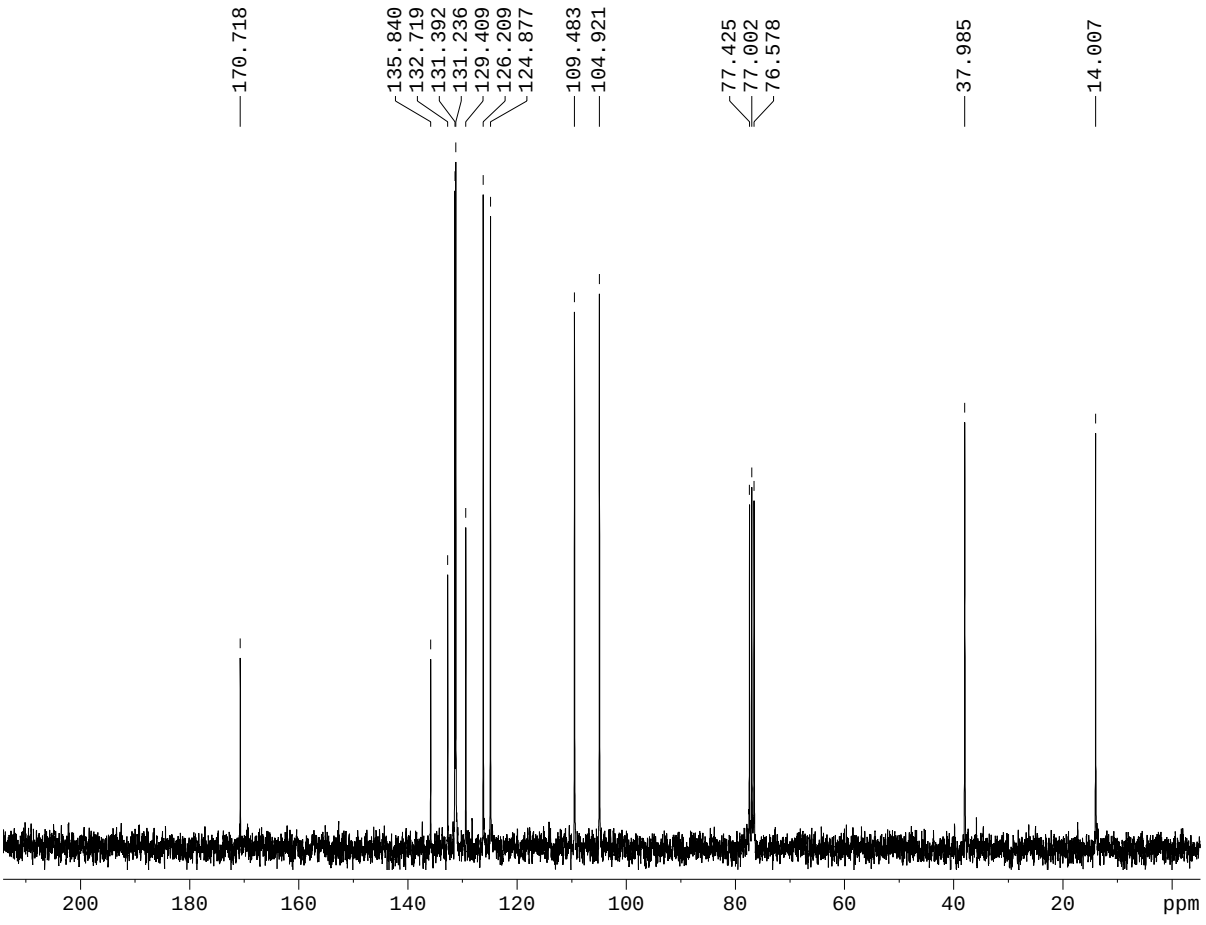

NH2
O
N
O
8c
10 9 8 7 6 5 4 3 2 1 0 ppm
6.228
1.066
2.003
0.944
0.944
1.978
1.962
2.040
3.000

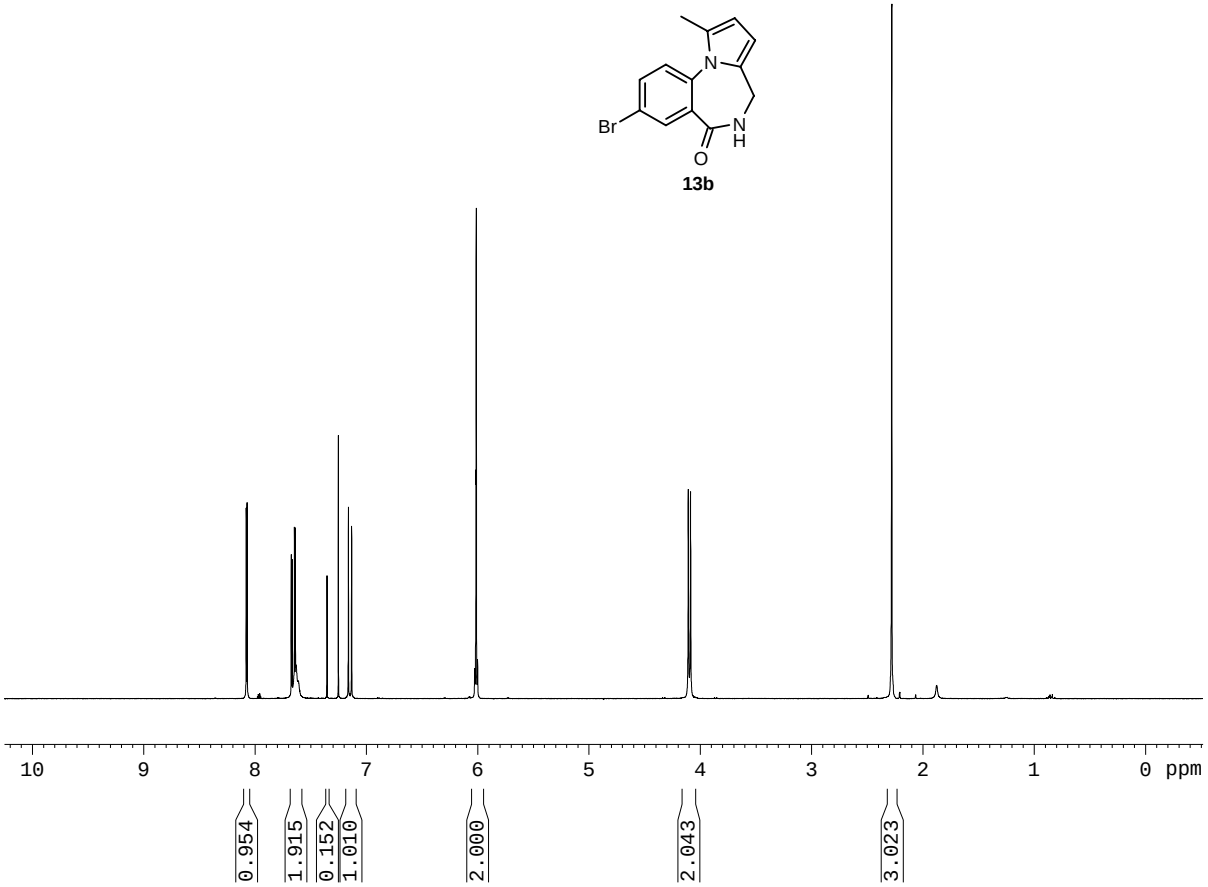

171.364
152.094
148.393
145.341
136.935
130.519
128.596
127.878
127.721
127.392
120.341
117.447
116.579
109.635
106.171
77.424
77.000
76.576
13.455
49.304
42.724
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm


NH2
O
N
O
Cl
8d
10 9 8 7 6 5 4 3 2 1 0 ppm
2.046
3.020
1.004
0.959
0.975
0.990
0.981
2.136
3.036

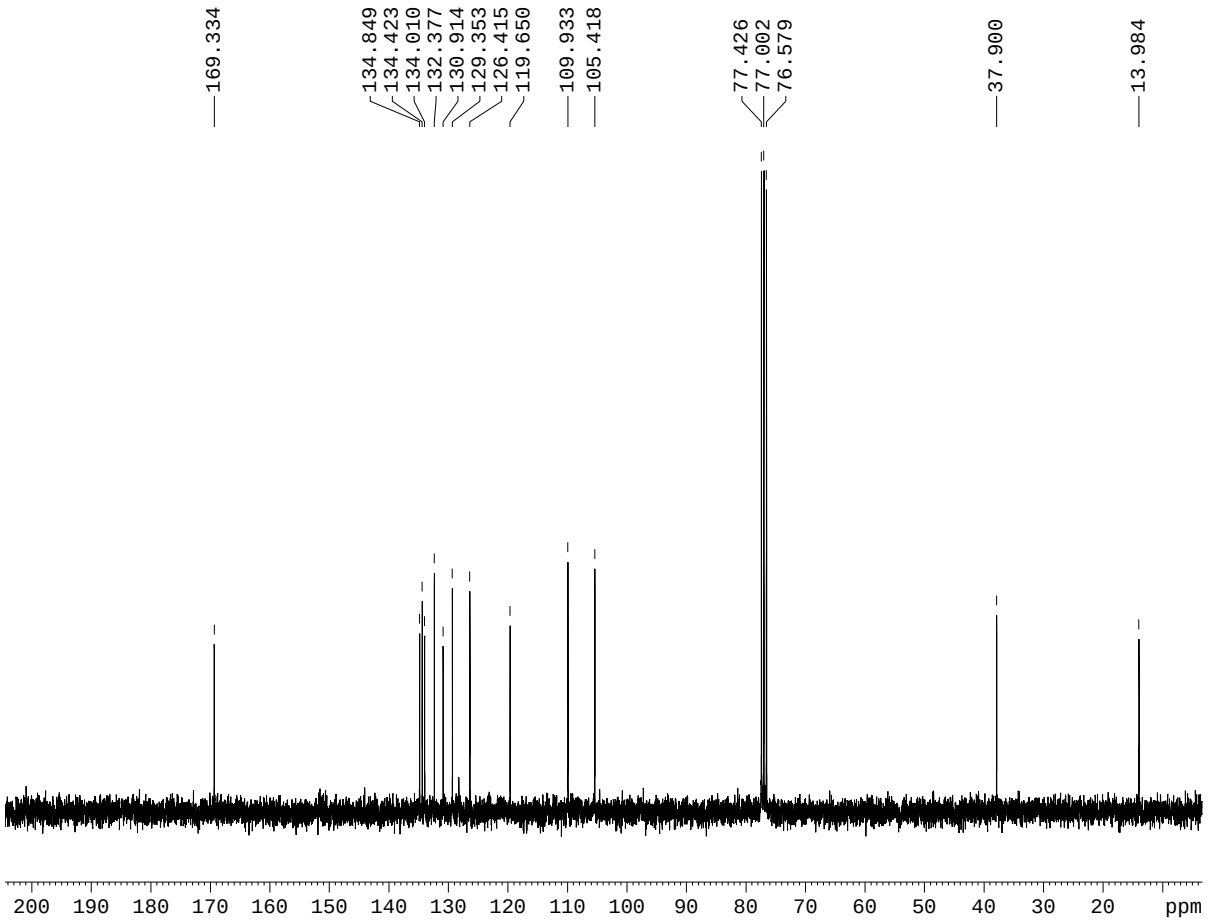

170.646
151.802
148.595
146.536
142.124
132.184
130.702
129.508
129.011
128.226
119.398
116.921
116.539
109.676
106.316
77.423
77.000
76.577
46.513
13.531
132 131 130 129 ppm
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

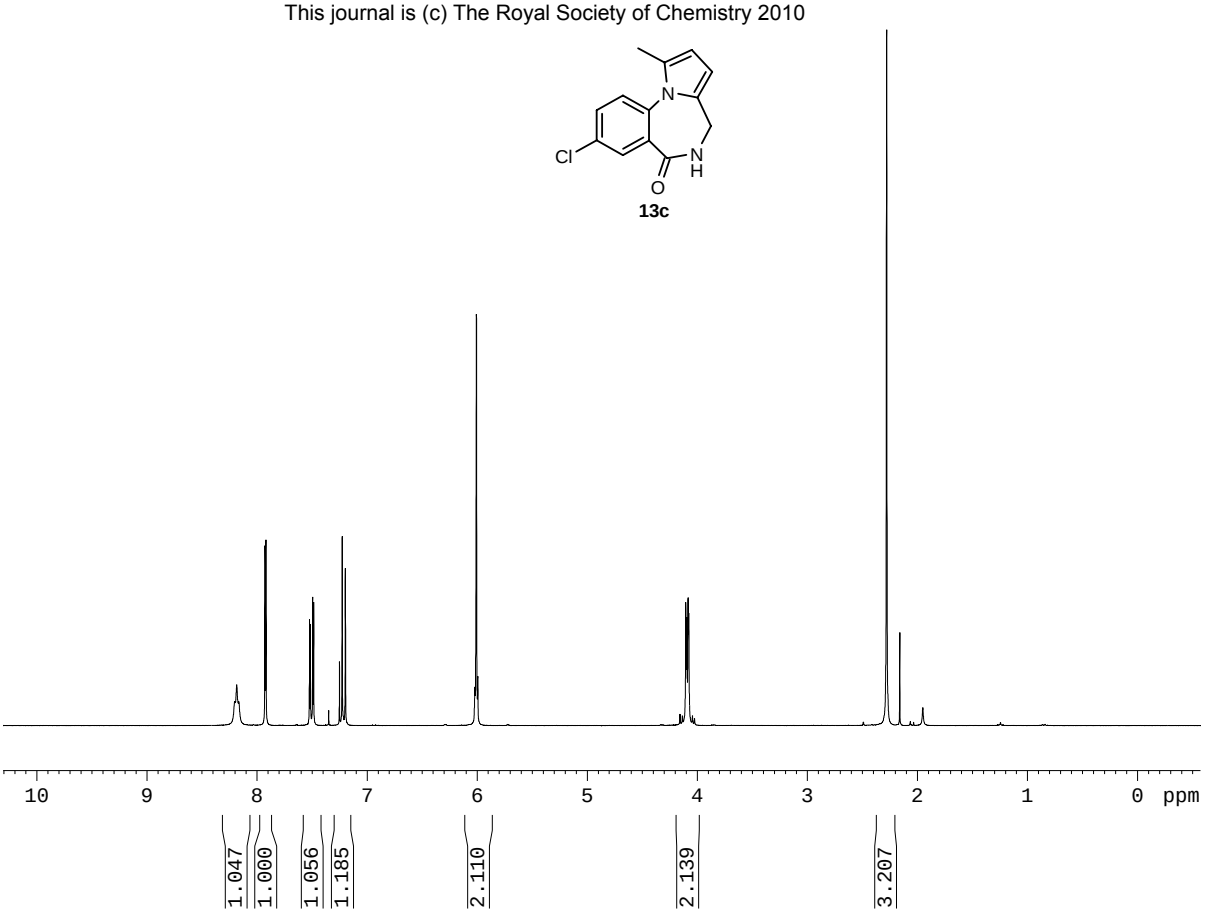

N
N
H
O
13a
10
9
8
7
6
5
4
3
2
1
0 ppm
1.927
1.000
1.158
1.125
1.955
2.017
3.016


170.718
135.840
132.719
131.392
131.236
129.409
126.209
124.877
109.483
104.921
77.425
77.002
76.578
37.985
14.007
200
180
160
140
120
100
80
60
40
20
ppm

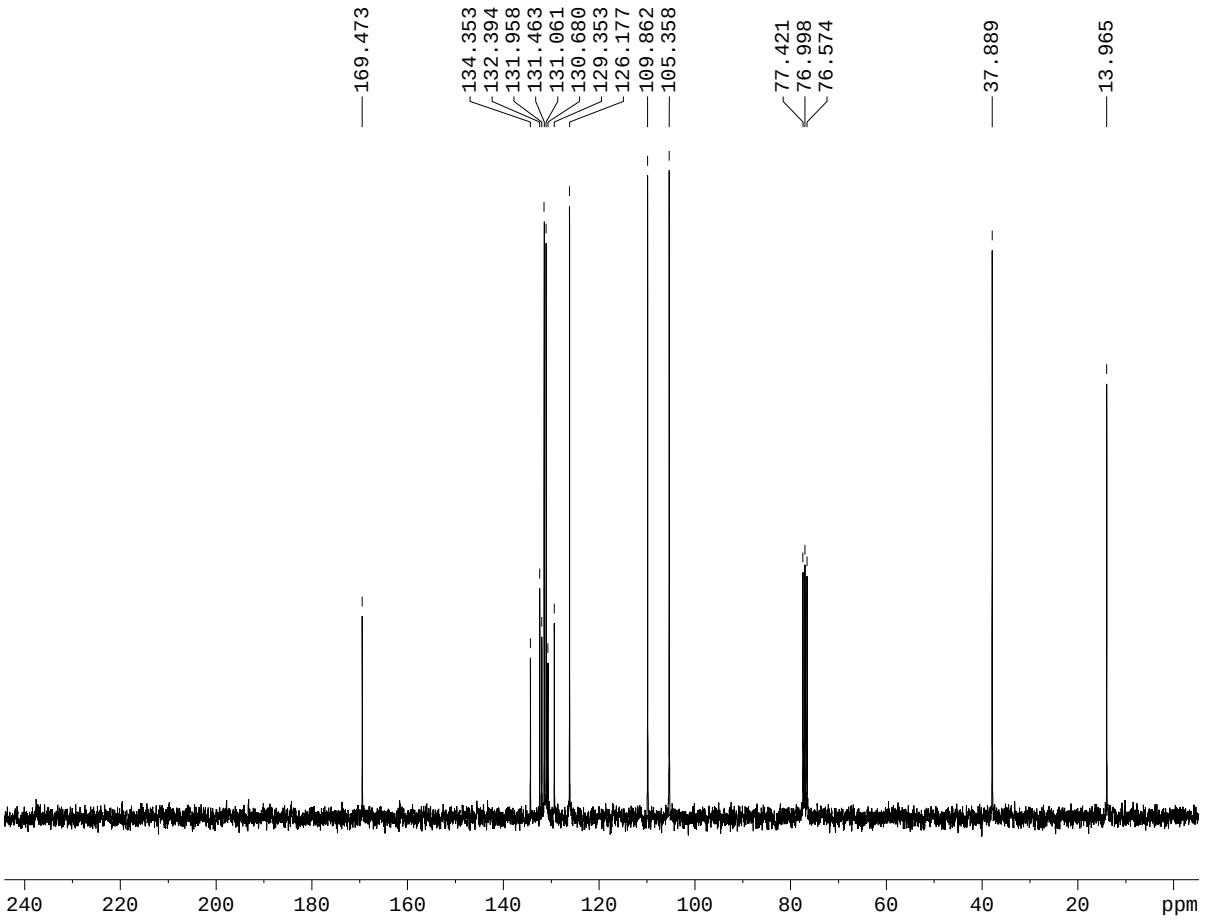

Br
N
N
H
O
10
9
8
7
6
5
4
3
2
1
0 ppm
0.954
1.915
0.152
1.010
2.000
2.043
3.023

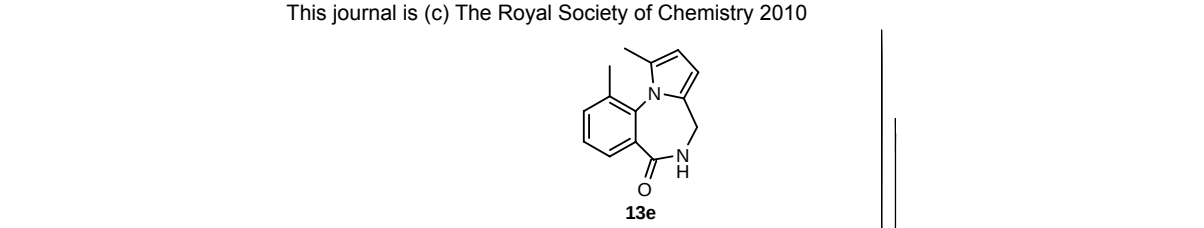
13b


169.334
134.849
134.423
134.010
132.377
130.914
129.353
126.415
119.650
109.933
105.418
77.426
77.002
76.579
37.900
13.984
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm


Cl
N
N
H
O
10
9
8
7
6
5
4
3
2
1
0
ppm
1.047
1.000
1.056
1.185
2.110
2.139
3.207

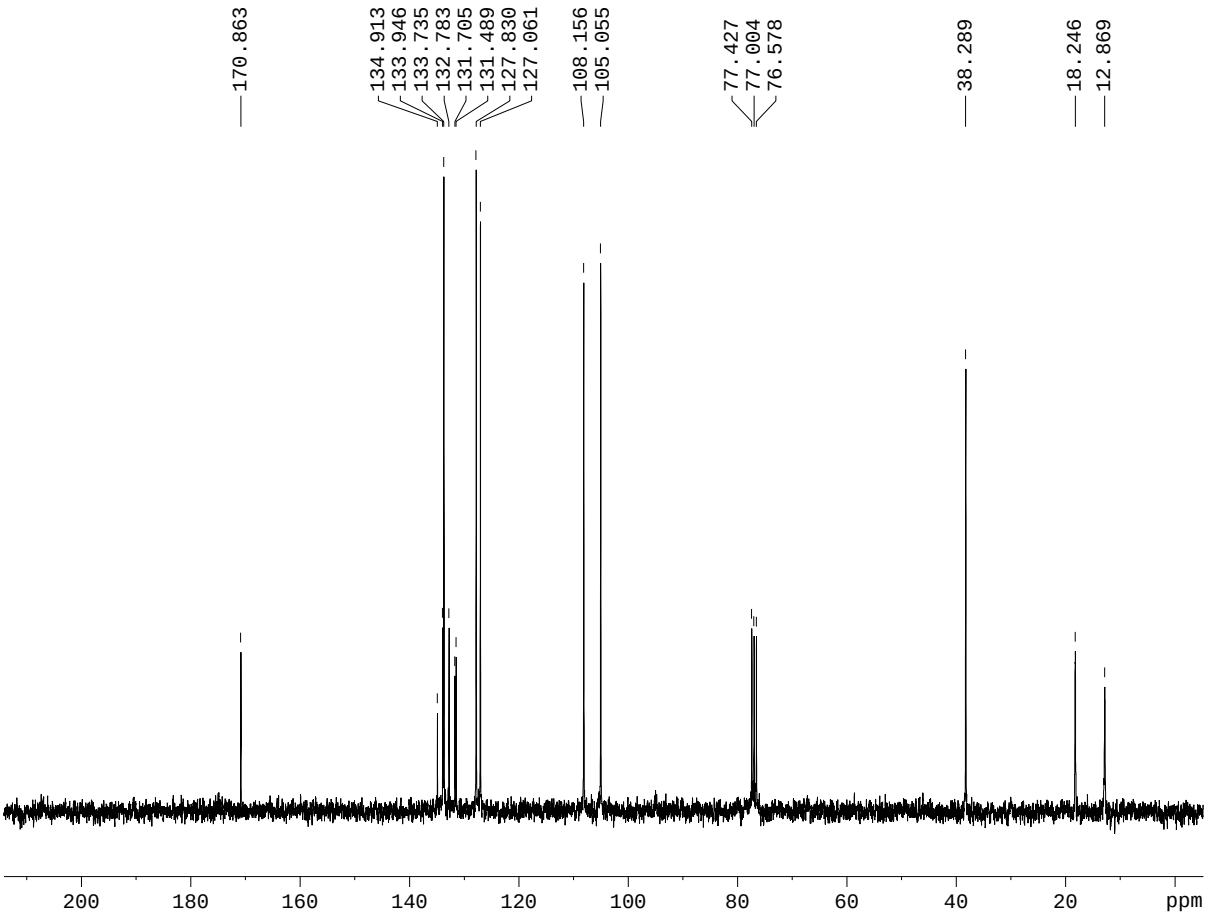
13c

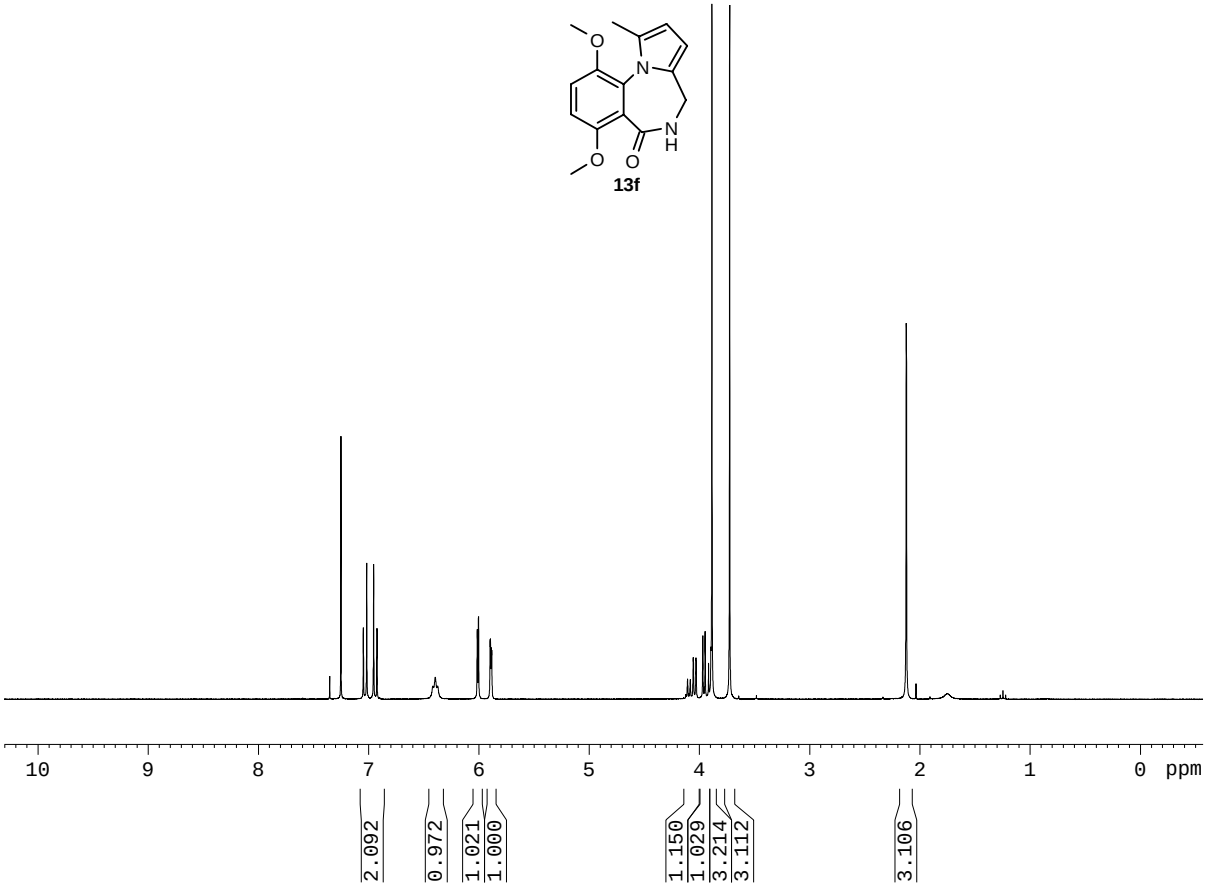

169.473
134.353
132.394
131.958
131.463
131.061
130.680
129.353
126.177
109.862
105.358
77.421
76.998
76.574
37.889
13.965
240
220
200
180
160
140
120
100
80
60
40
20
ppm

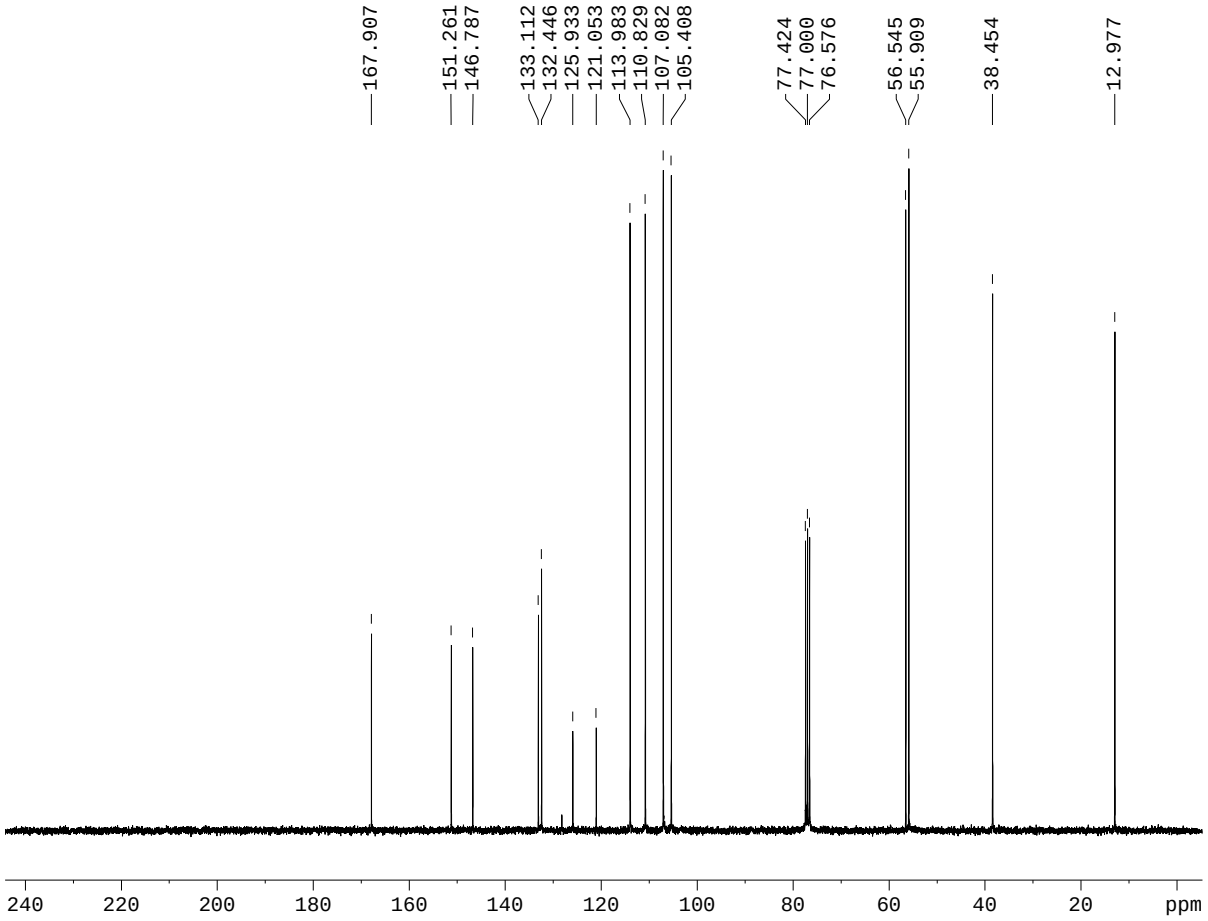

N
N
H
O

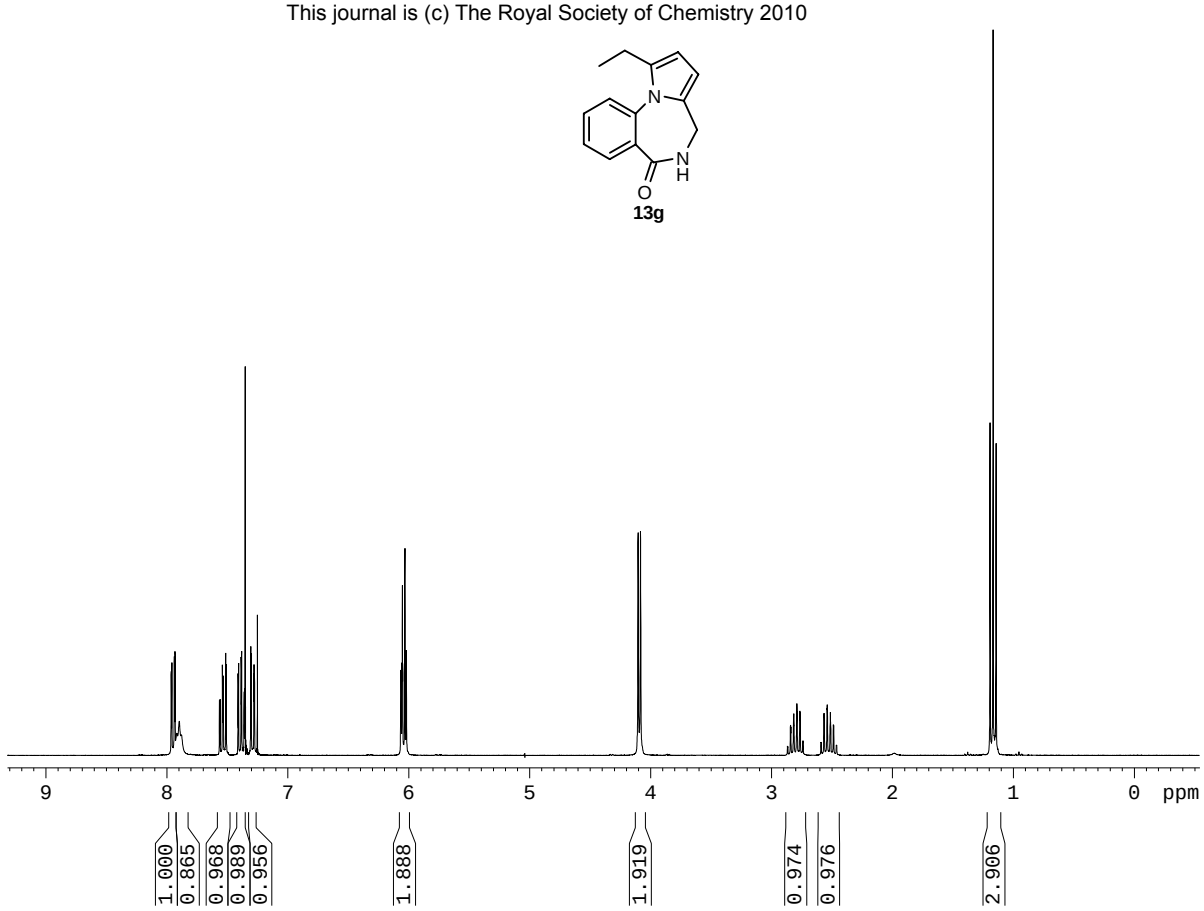
13e

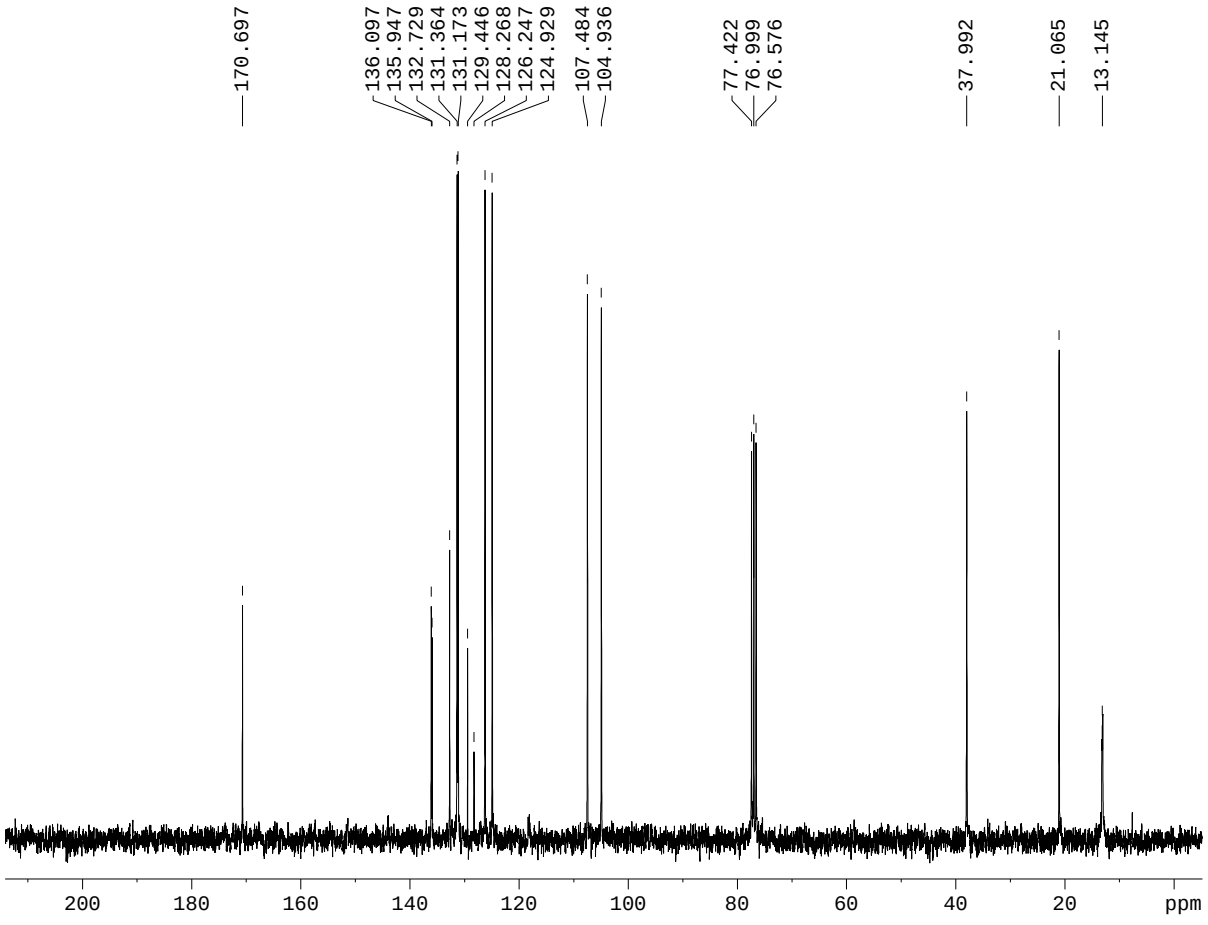
9
8
7
6
5
4
3
2
1
0
ppm
0.912
1.000
0.979
0.968
0.969
0.962
1.941
2.904
3.046

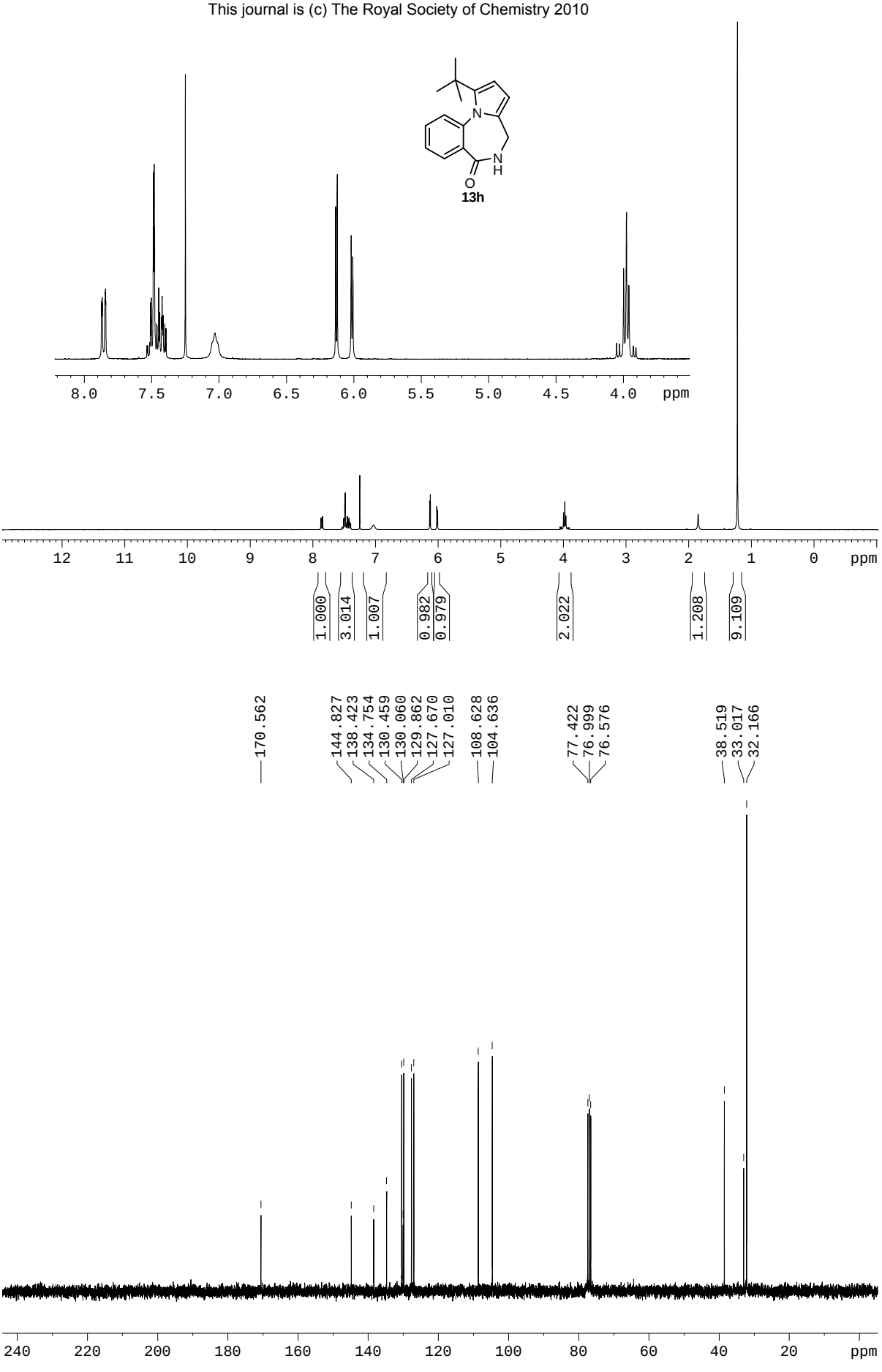

170.863
134.913
133.946
133.735
132.783
131.705
131.489
127.830
127.061
108.156
105.055
77.427
77.004
76.578
38.289
18.246
12.869
200
180
160
140
120
100
80
60
40
20
ppm

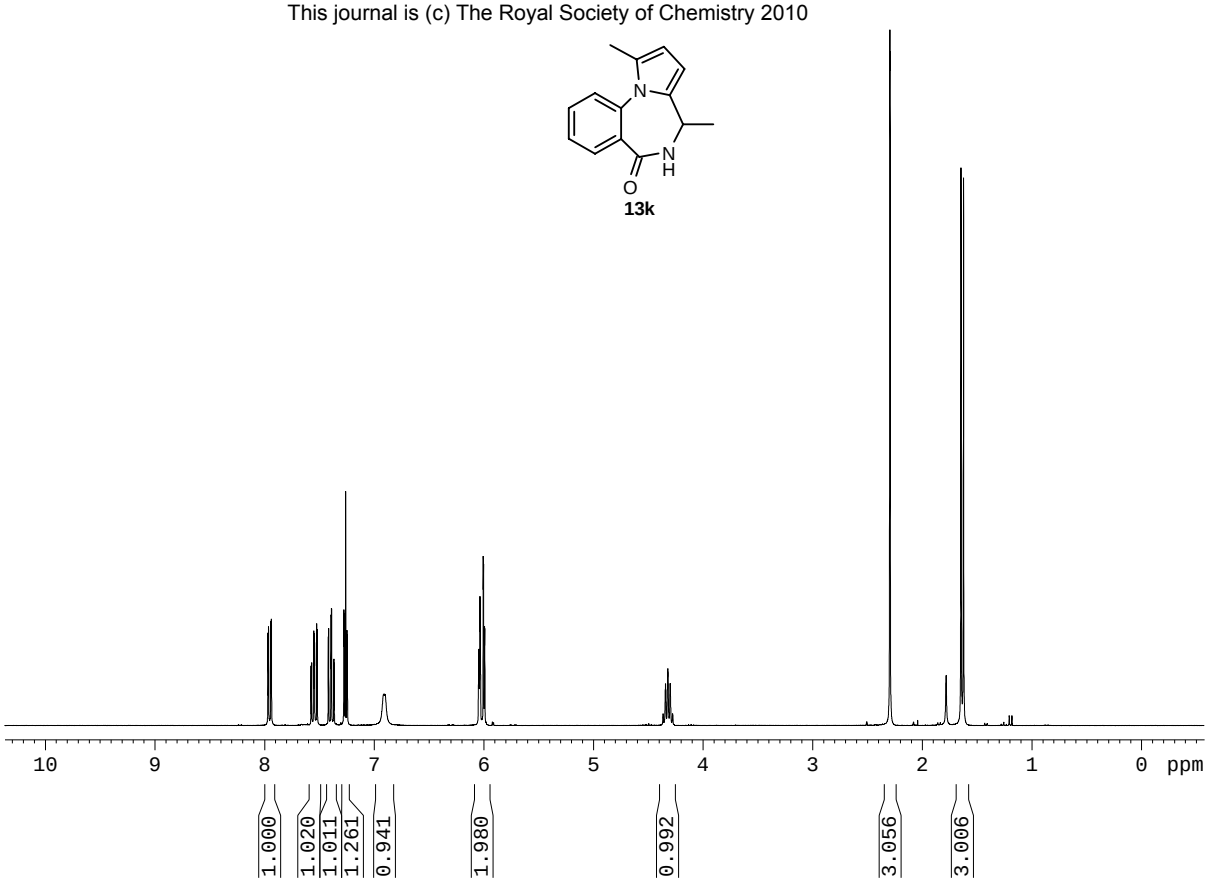

O
N
N
H
O
O
13f
10
9
8
7
6
5
4
3
2
1
0
ppm
2.092
0.972
1.021
1.000
1.150
1.029
3.214
3.112
3.106

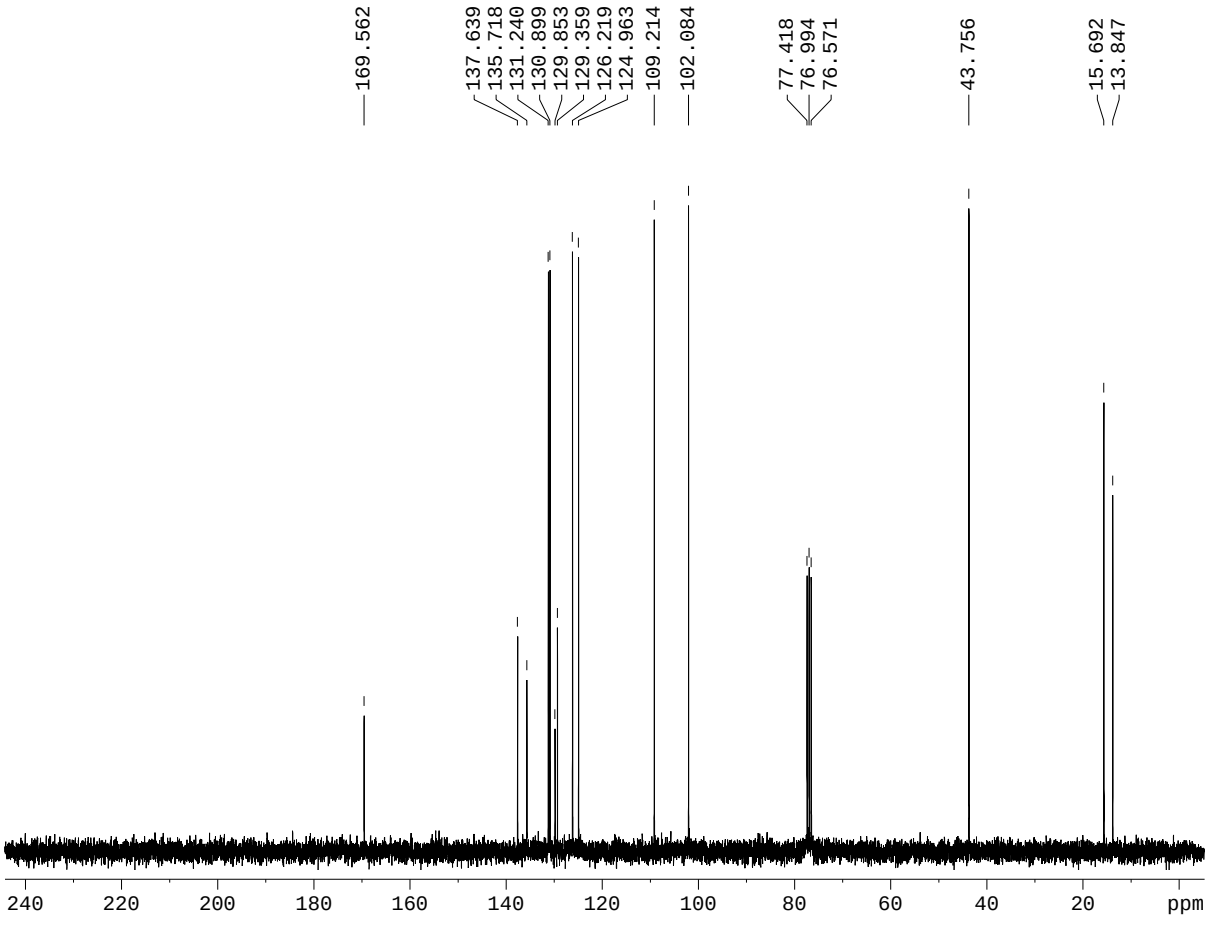

167.907
151.261
146.787
133.112
132.446
125.933
121.053
113.983
110.829
107.082
105.408
77.424
77.000
76.576
56.545
55.909
38.454
12.977
240
220
200
180
160
140
120
100
80
60
40
20
ppm

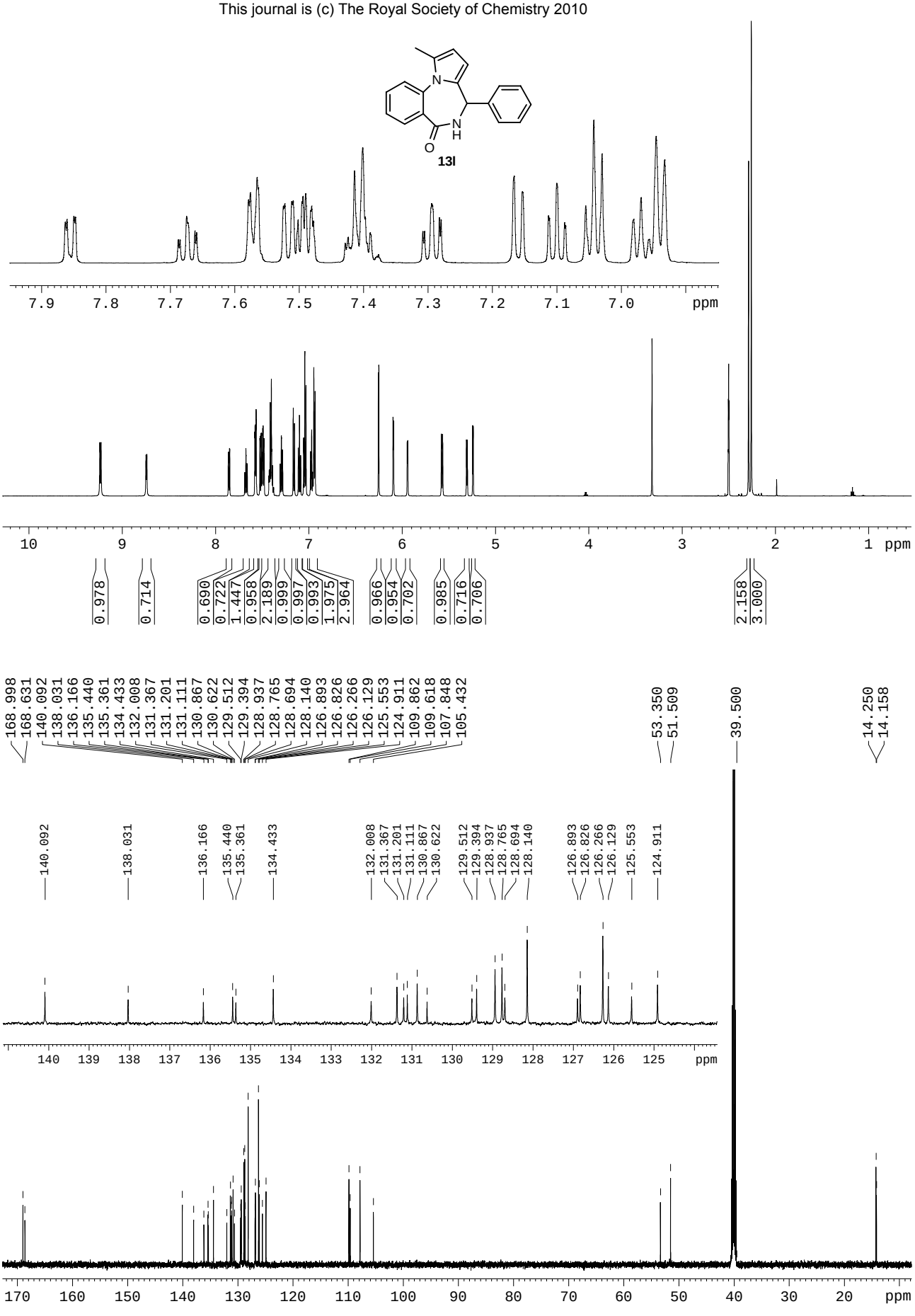

N
N
H
O
13g
9
8
7
6
5
4
3
2
1
0
ppm
1.000
0.865
0.968
0.989
0.956
1.888
1.919
0.974
0.976
2.906

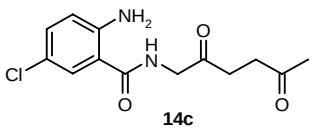

170.697
136.097
135.947
132.729
131.364
131.173
129.446
128.268
126.247
124.929
107.484
104.936
77.422
76.999
76.576
37.992
21.065
13.145
200
180
160
140
120
100
80
60
40
20
ppm


13h
8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 ppm
12 11 10 9 8 7 6 5 4 3 2 1 0 ppm
1.000
3.014
1.007
0.982
0.979
2.022
1.208
9.109
170.562
144.827
138.423
134.754
130.459
130.060
129.862
127.670
127.010
108.628
104.636
77.422
76.999
76.576
38.519
33.017
32.166
240 220 200 180 160 140 120 100 80 60 40 20 ppm


N
N
H
O
13k
10 9 8 7 6 5 4 3 2 1 0 ppm
1.000
1.020
1.011
1.261
0.941
1.980
0.992
3.056
3.006

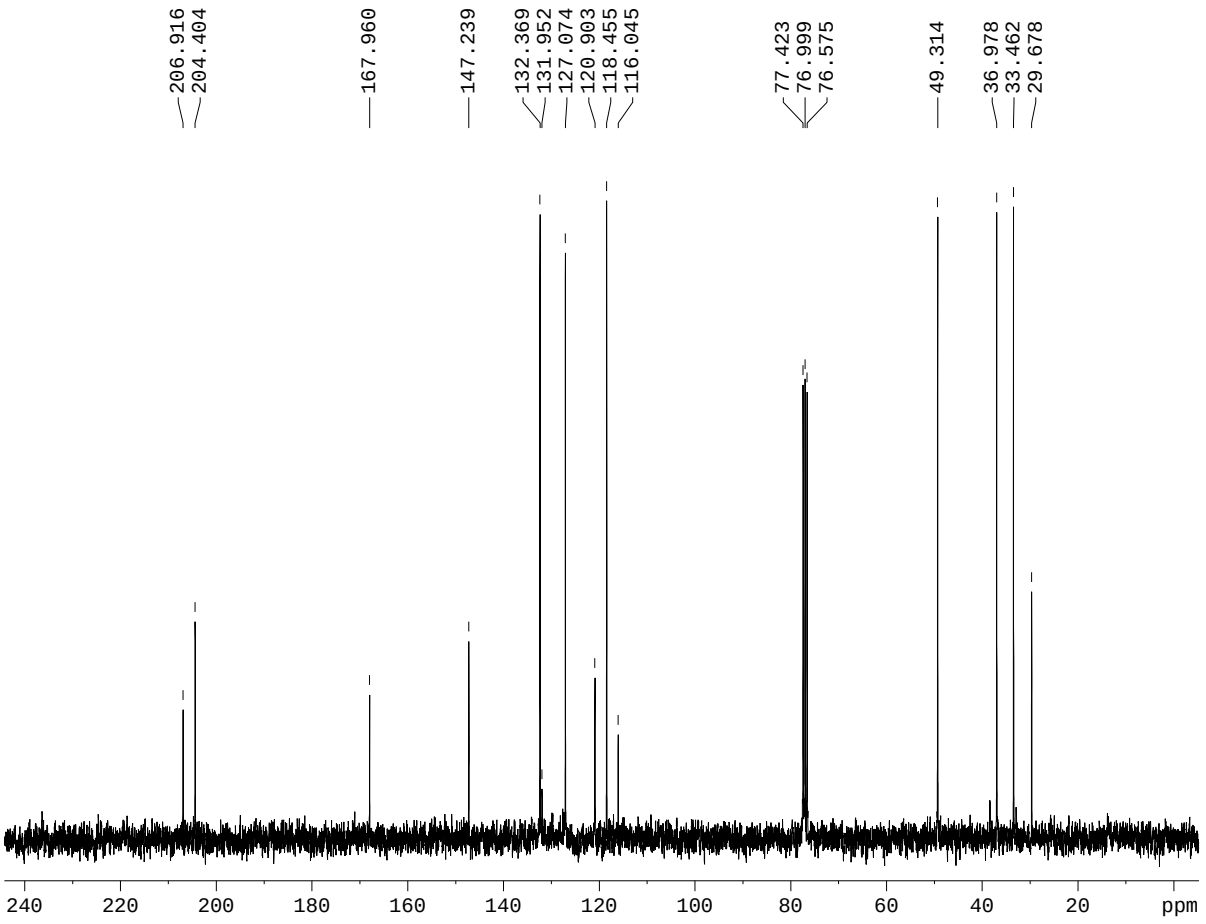

169.562
137.639
135.718
131.240
130.899
129.853
129.359
126.219
124.963
109.214
102.084
77.418
76.994
76.571
43.756
15.692
13.847
240 220 200 180 160 140 120 100 80 60 40 20 ppm

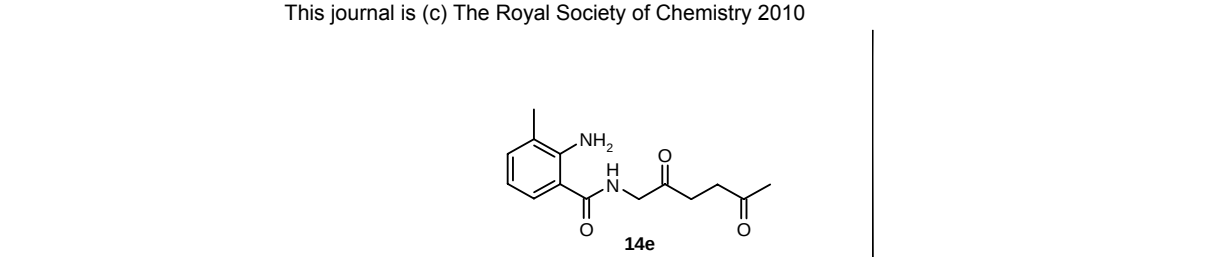

13l
7.9 7.8 7.7 7.6 7.5 7.4 7.3 7.2 7.1 7.0 ppm
10 9 8 7 6 5 4 3 2 1 ppm
0.978 0.714 0.690 0.722 1.447 0.958 2.189 0.999 0.997 0.993 1.975 2.964 0.966 0.954 0.702 0.985 0.716 0.706 2.158 3.000
168.998 168.631 140.092 138.031 136.166 135.440 135.361 134.433 132.008 131.367 131.201 131.111 130.867 130.622 129.512 129.394 128.937 128.765 128.694 128.140 126.826 126.266 126.129 125.553 124.911 109.862 109.618 107.848 105.432
53.350 51.509 39.500 14.250 14.158
140 139 138 137 136 135 134 133 132 131 130 129 128 127 126 125 ppm
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm


NH2
Cl
H
N
O
O
O

14c

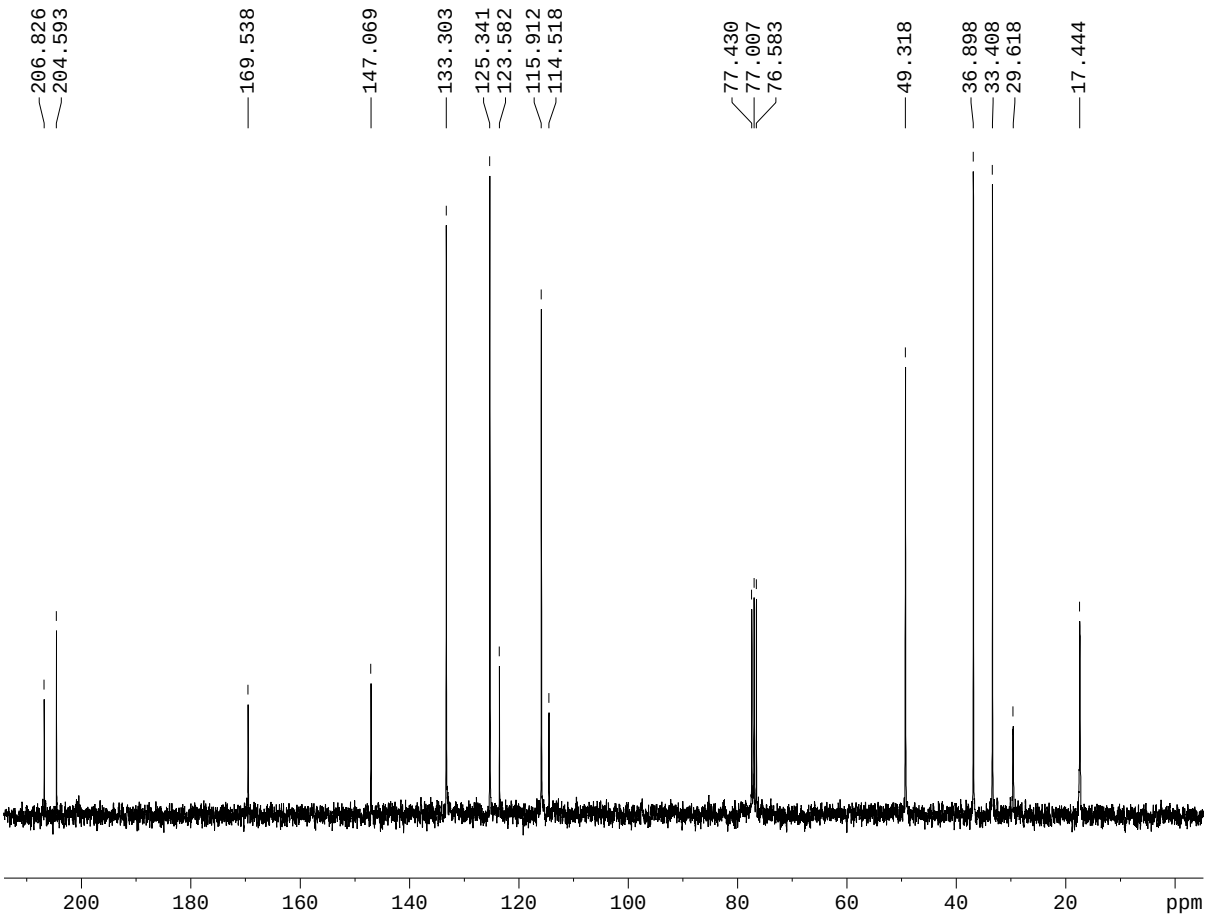
10
9
8
7
6
5
4
3
2
1
0 ppm
1.000
1.037
1.040
1.016
1.917
2.051
4.125
2.997

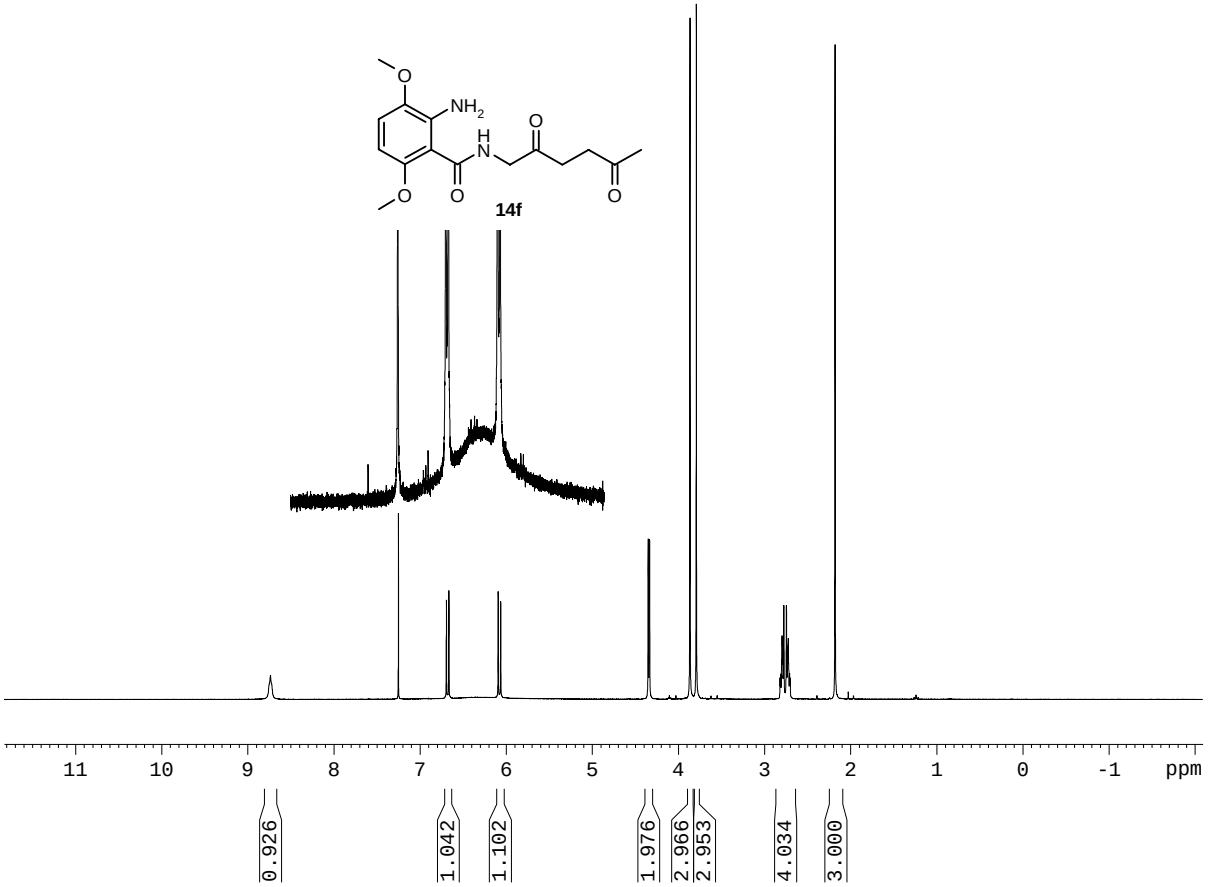

206.916
204.404
167.960
147.239
132.369
131.952
127.074
120.903
118.455
116.045
77.423
76.999
76.575
49.314
36.978
33.462
29.678
240
220
200
180
160
140
120
100
80
60
40
20
ppm

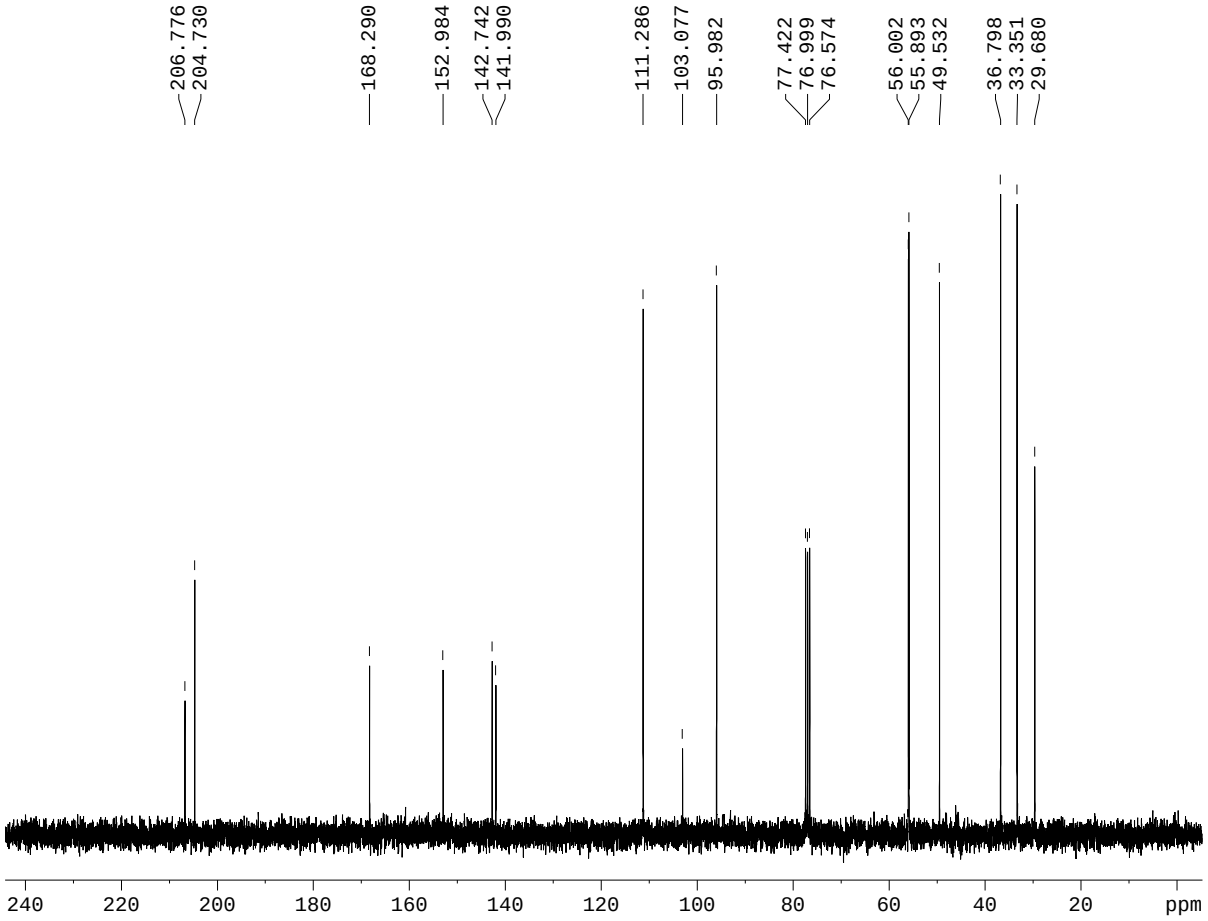

NH2
H
N
O
O
O

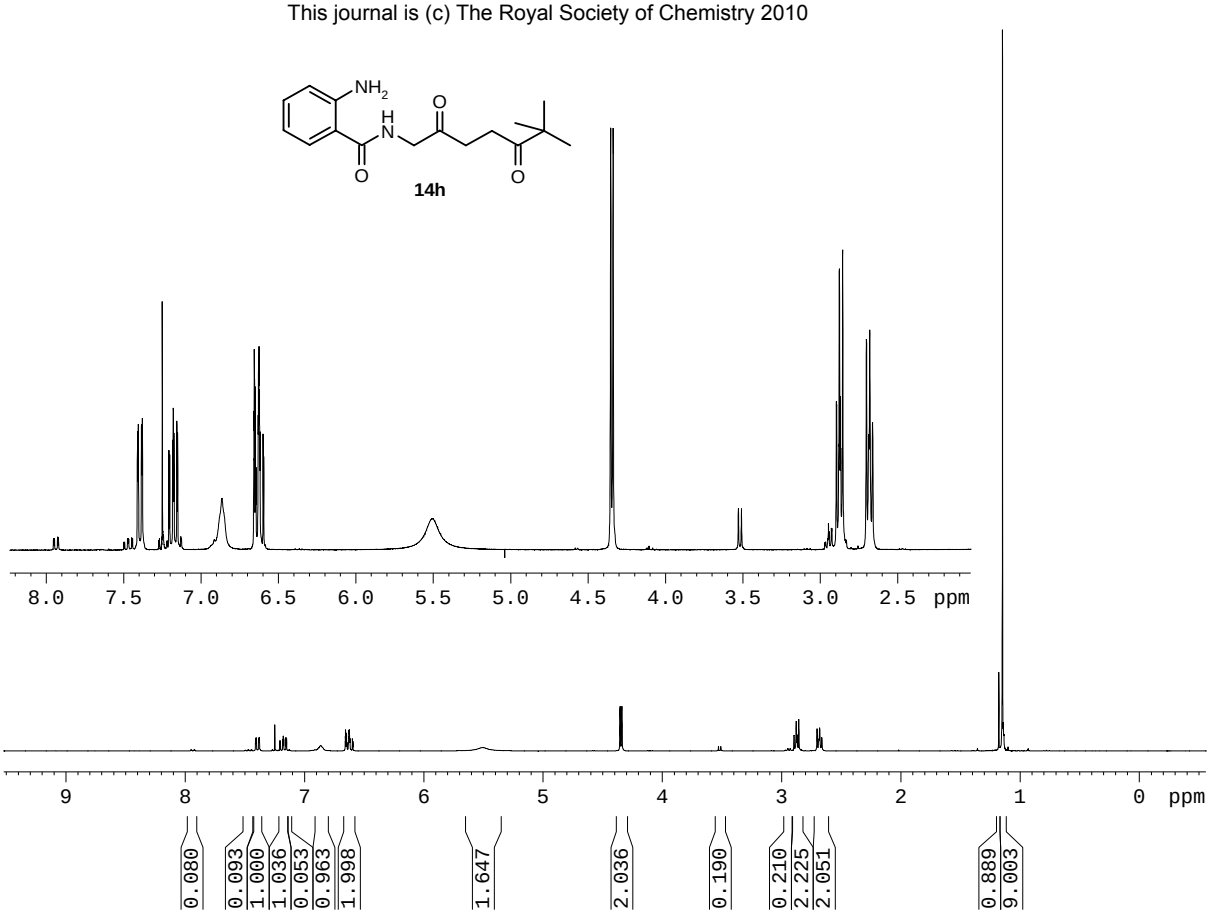
14e

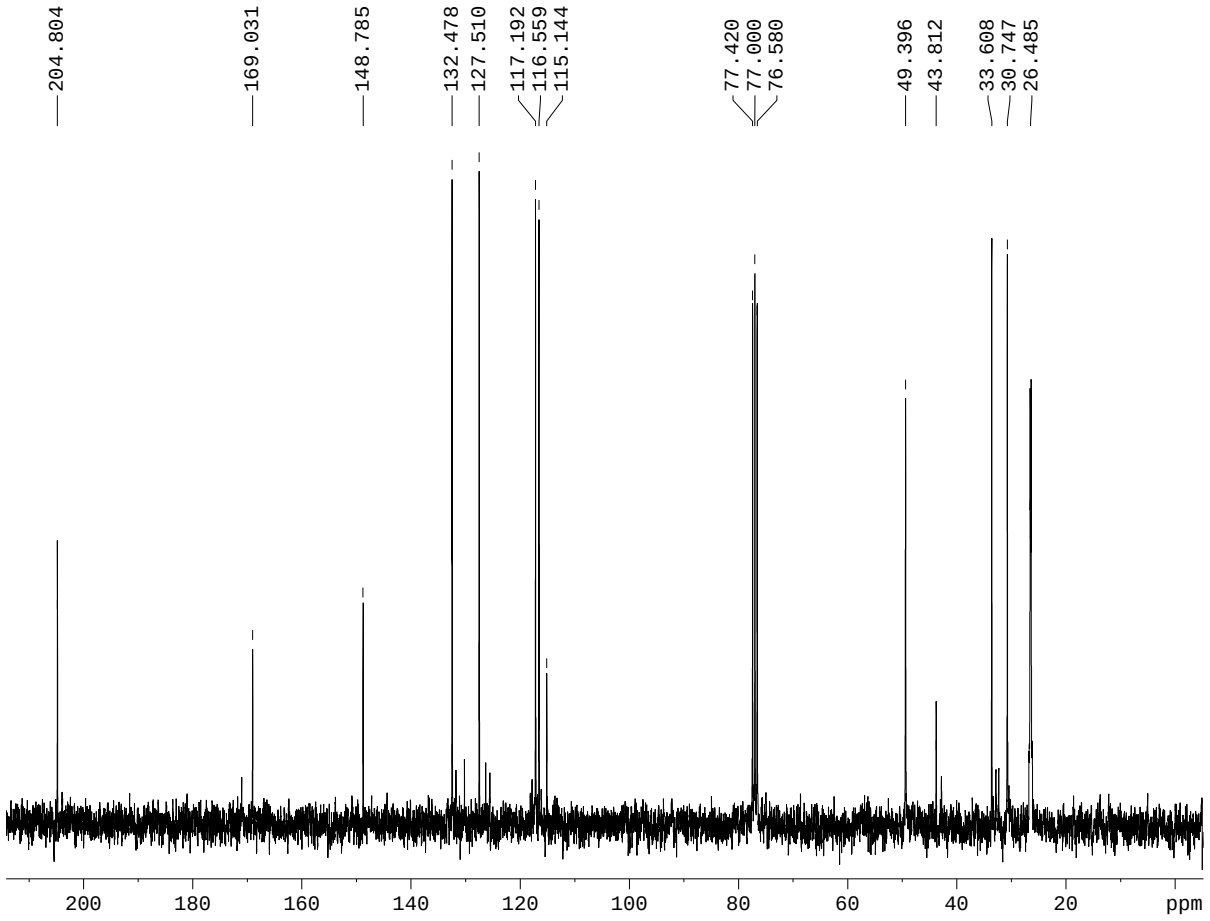
9
8
7
6
5
4
3
2
1
0
ppm
1.000
1.004
0.968
0.984
1.778
1.969
3.957
5.915

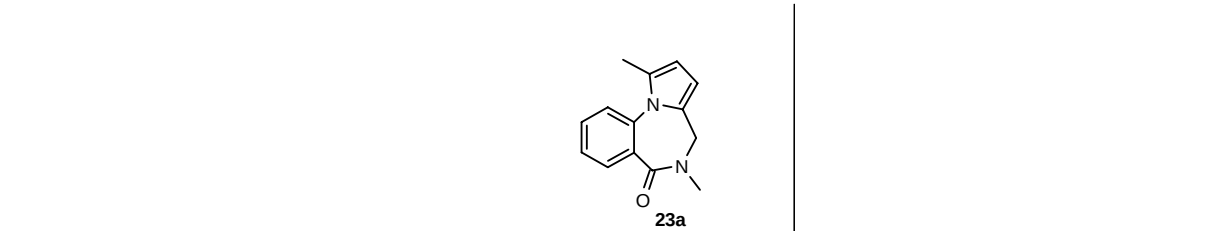

206.826
204.593
169.538
147.069
133.303
125.341
123.582
115.912
114.518
77.430
77.007
76.583
49.318
36.898
33.408
29.618
17.444
200
180
160
140
120
100
80
60
40
20
ppm


O
NH2
H
N
O
O
O
O
O
14f
11
10
9
8
7
6
5
4
3
2
1
0
-1
ppm
0.926
1.042
1.102
1.976
2.966
2.953
4.034
3.000


206.776
204.730
168.290
152.984
142.742
141.990
111.286
103.077
95.982
77.422
76.999
76.574
56.002
55.893
49.532
36.798
33.351
29.680
240
220
200
180
160
140
120
100
80
60
40
20
ppm

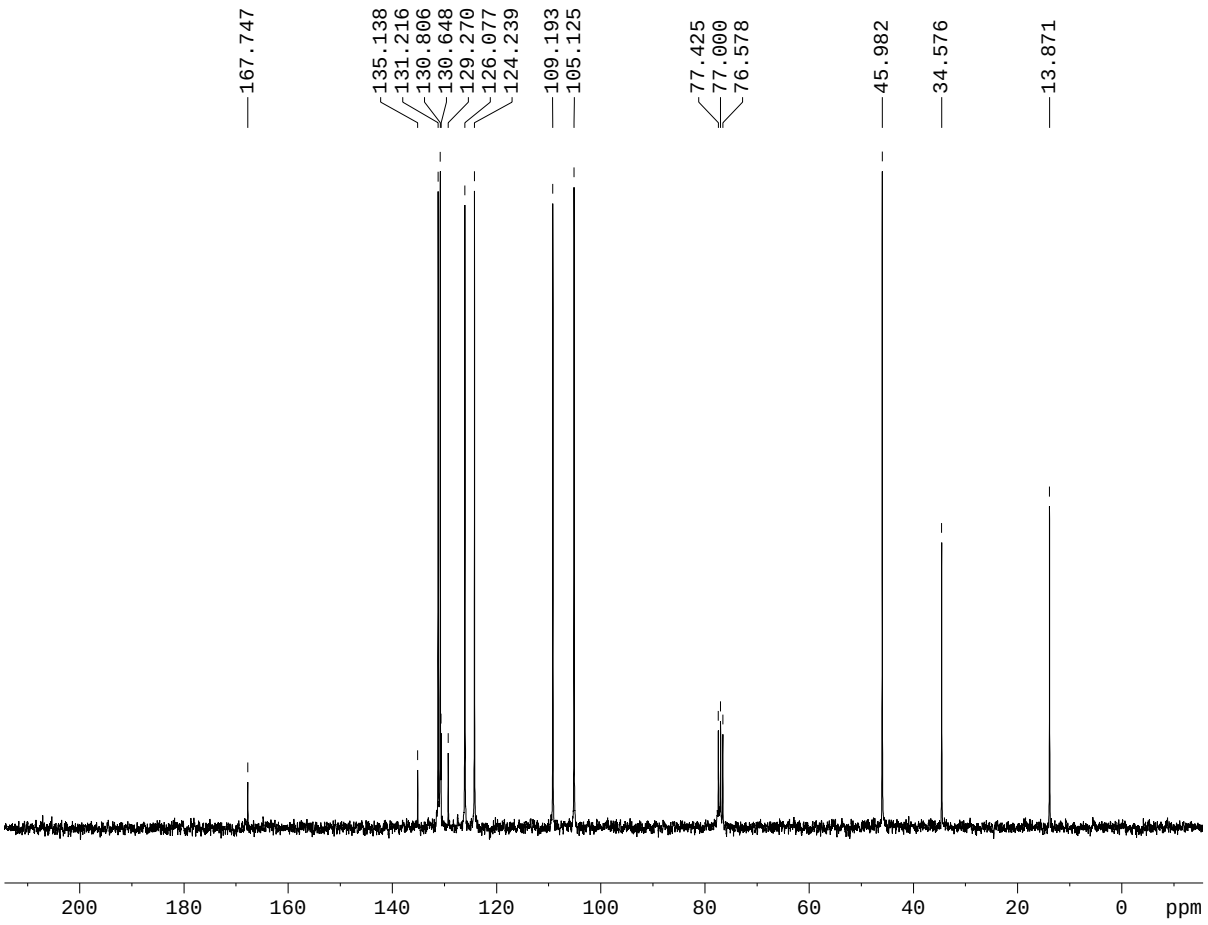

NH2
H
N
O
O
O
O
14h
8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 ppm
9 8 7 6 5 4 3 2 1 0 ppm
0.080
0.093
1.000
1.036
0.053
0.963
1.998
1.647
2.036
0.190
0.210
2.225
2.051
0.889
9.003

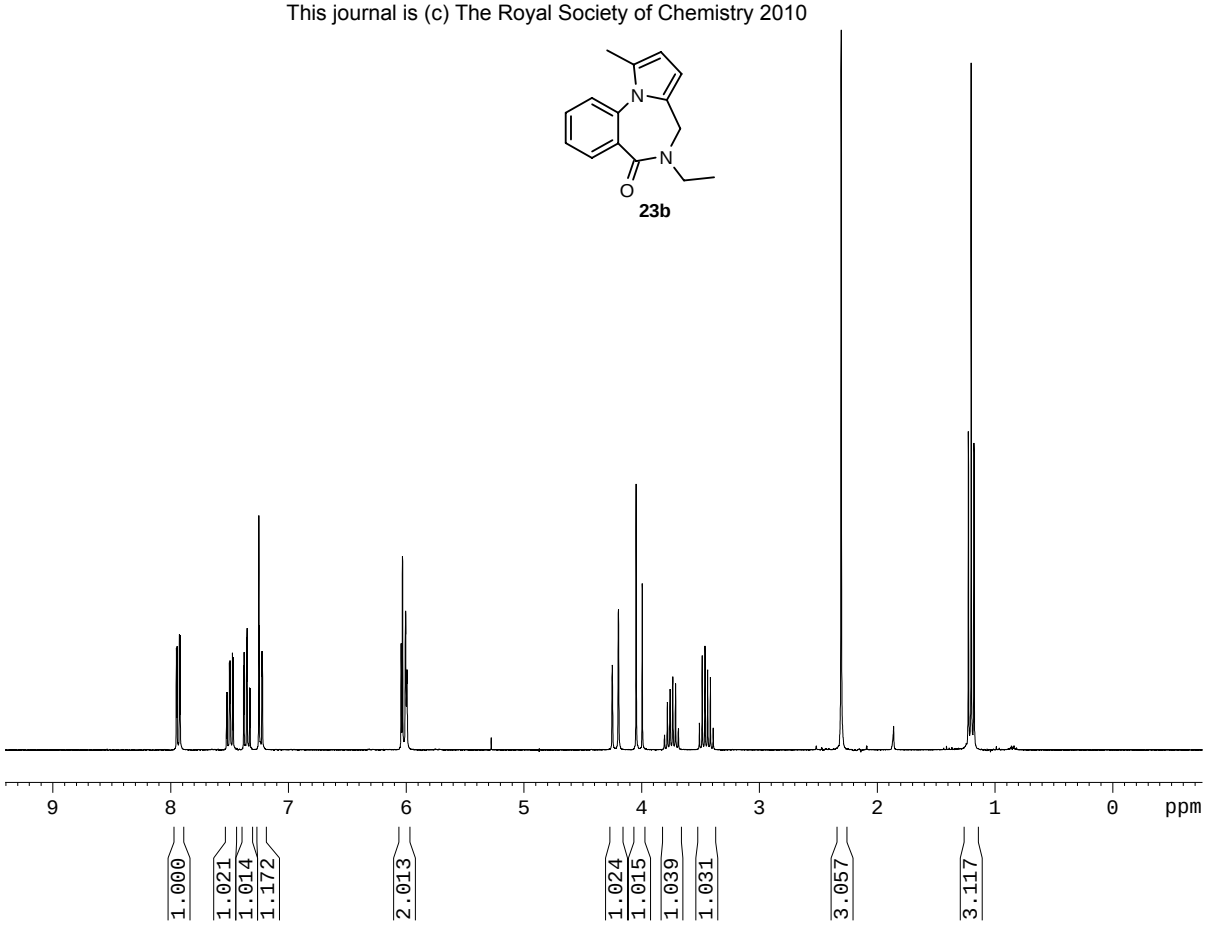

204.804
169.031
148.785
132.478
127.510
117.192
116.559
115.144
77.420
77.000
76.580
49.396
43.812
33.608
30.747
26.485
200 180 160 140 120 100 80 60 40 20 ppm

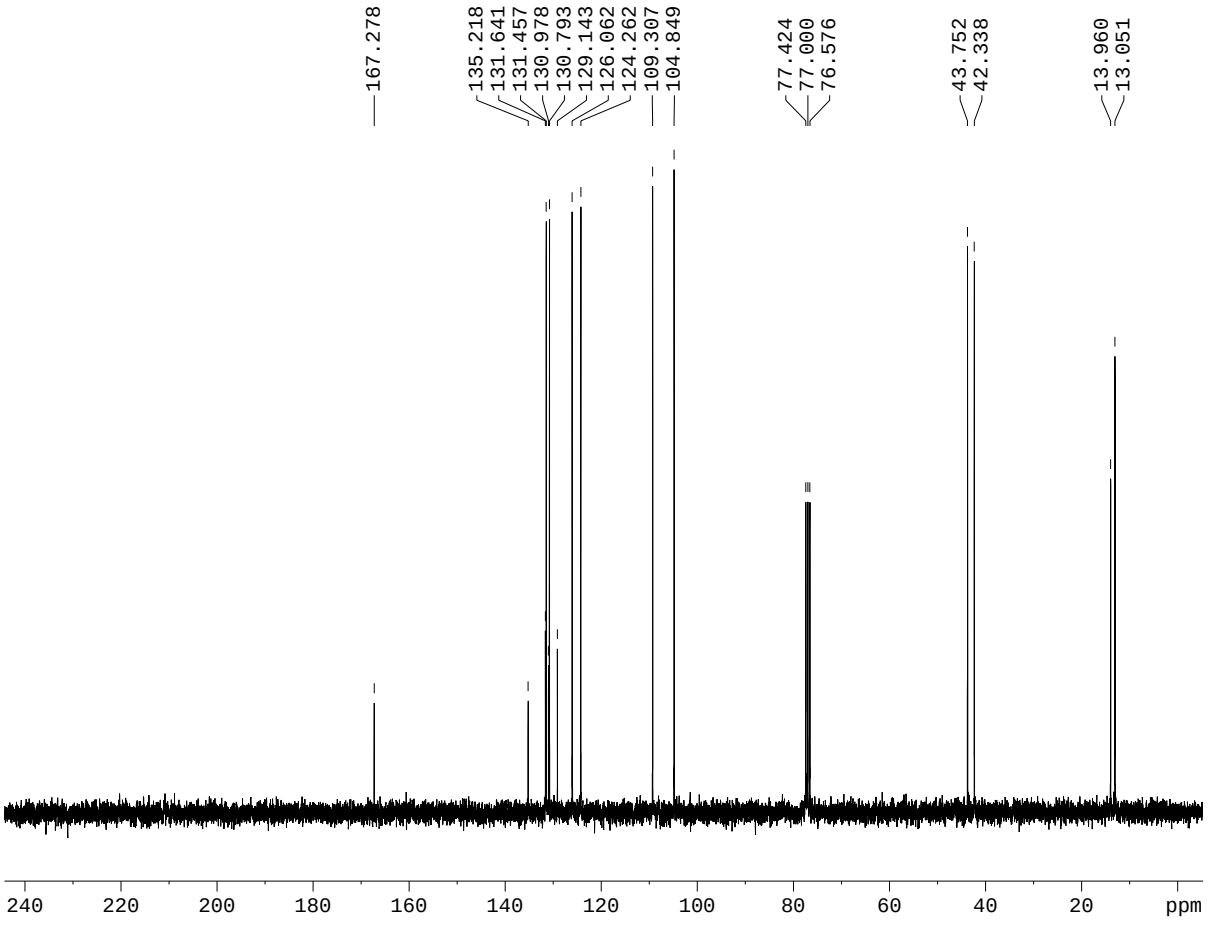

N
N
O

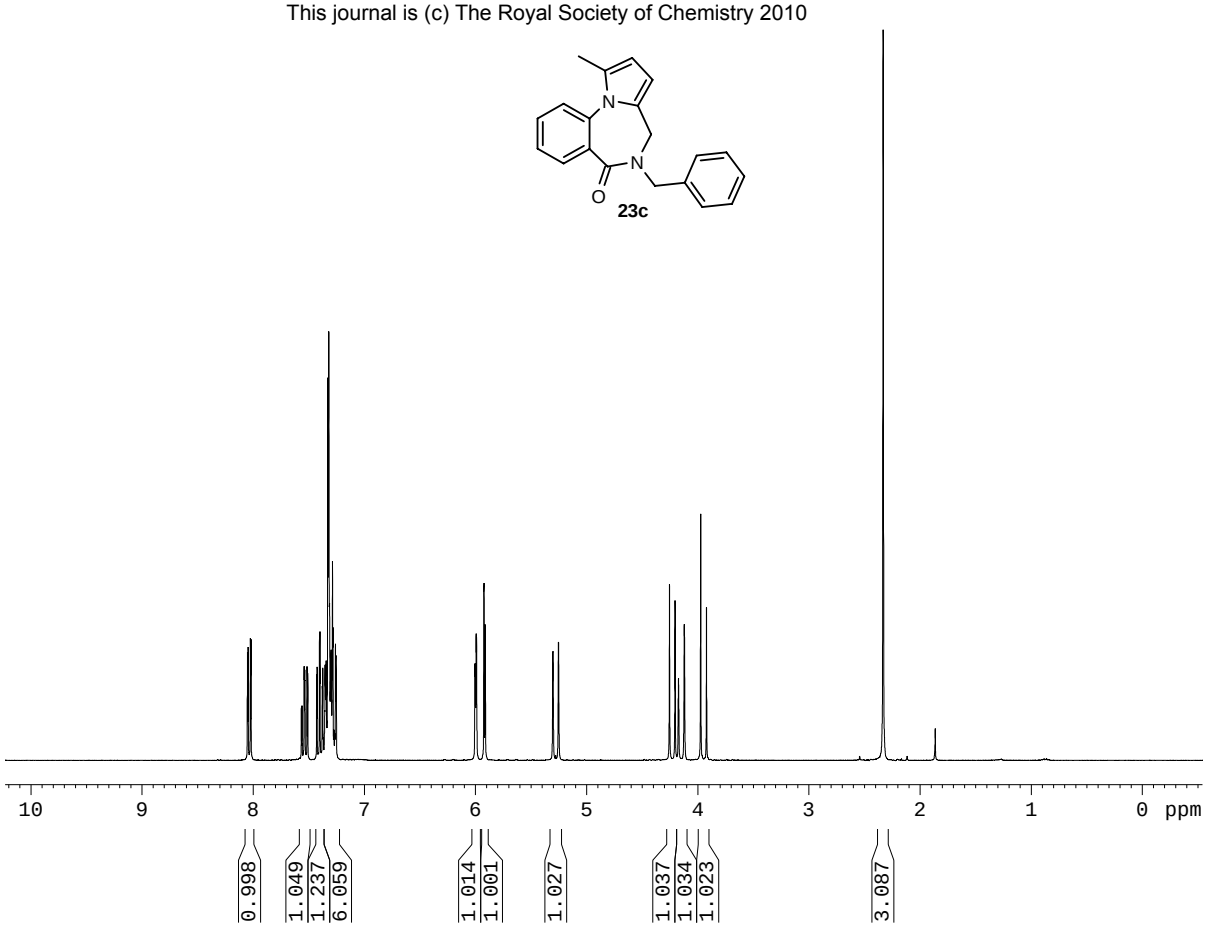
23a

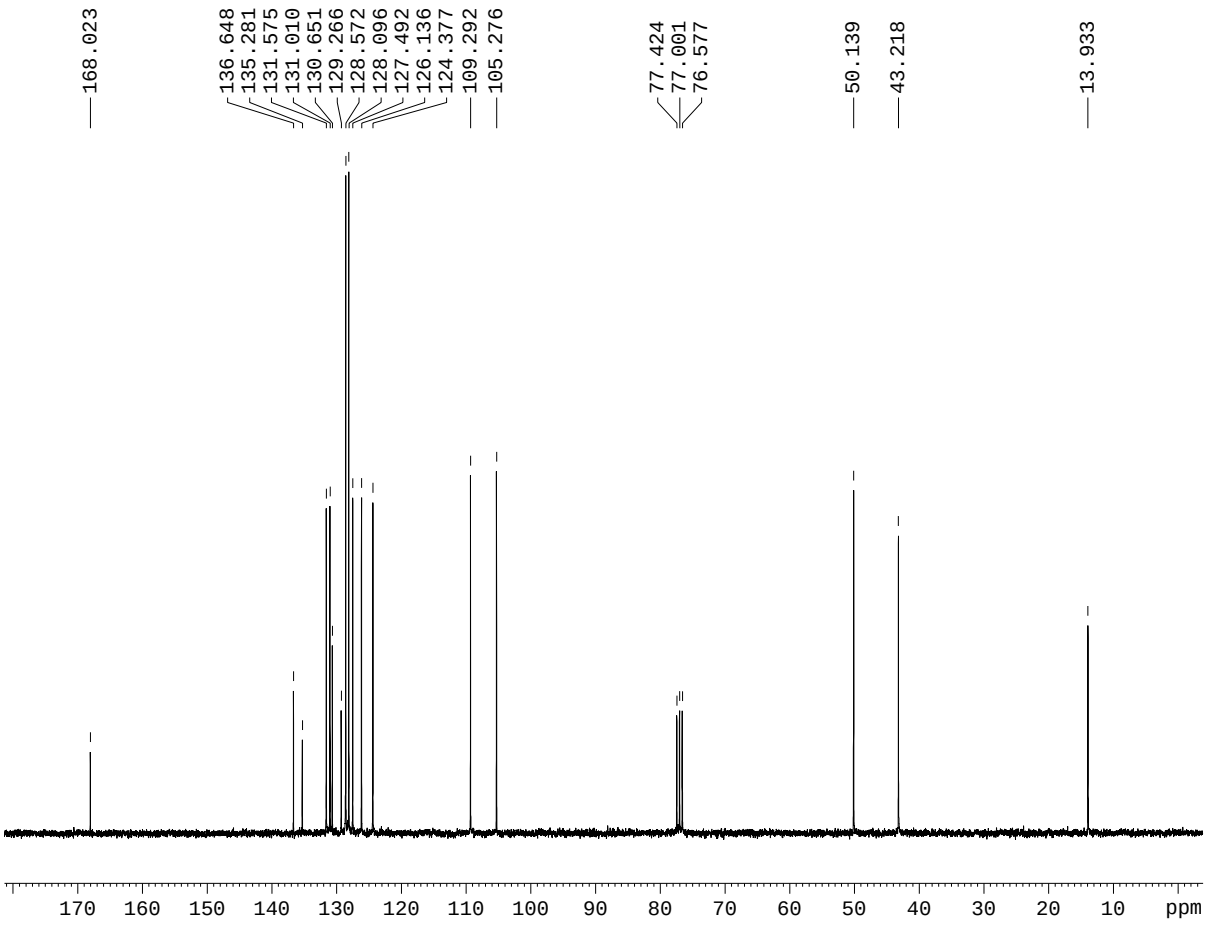
10
9
8
7
6
5
4
3
2
1
0
ppm
1.000
1.017
1.019
1.411
0.999
1.007
1.020
1.023
3.051
3.052

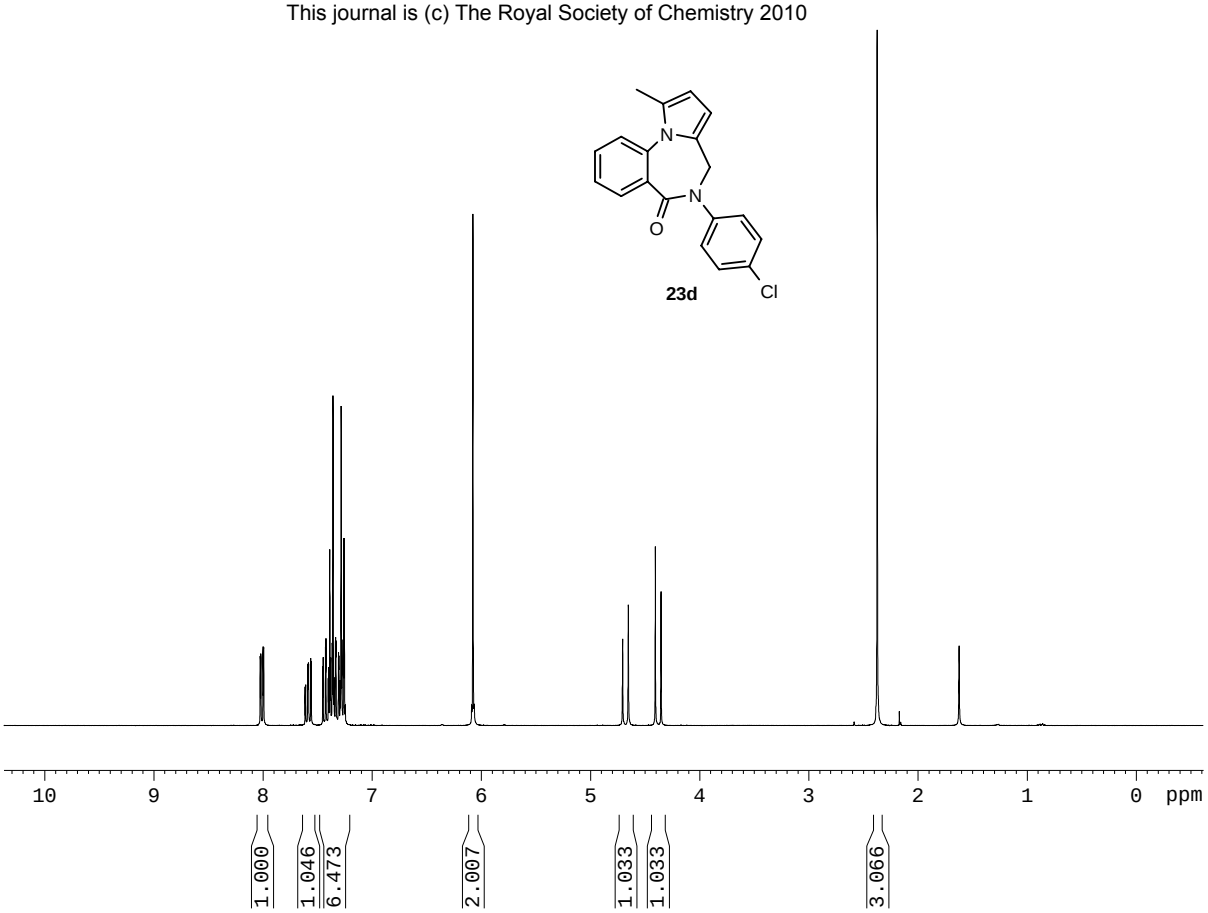

167.747
135.138
131.216
130.806
130.648
129.270
126.077
124.239
109.193
105.125
77.425
77.000
76.578
45.982
34.576
13.871
200
180
160
140
120
100
80
60
40
20
0
ppm

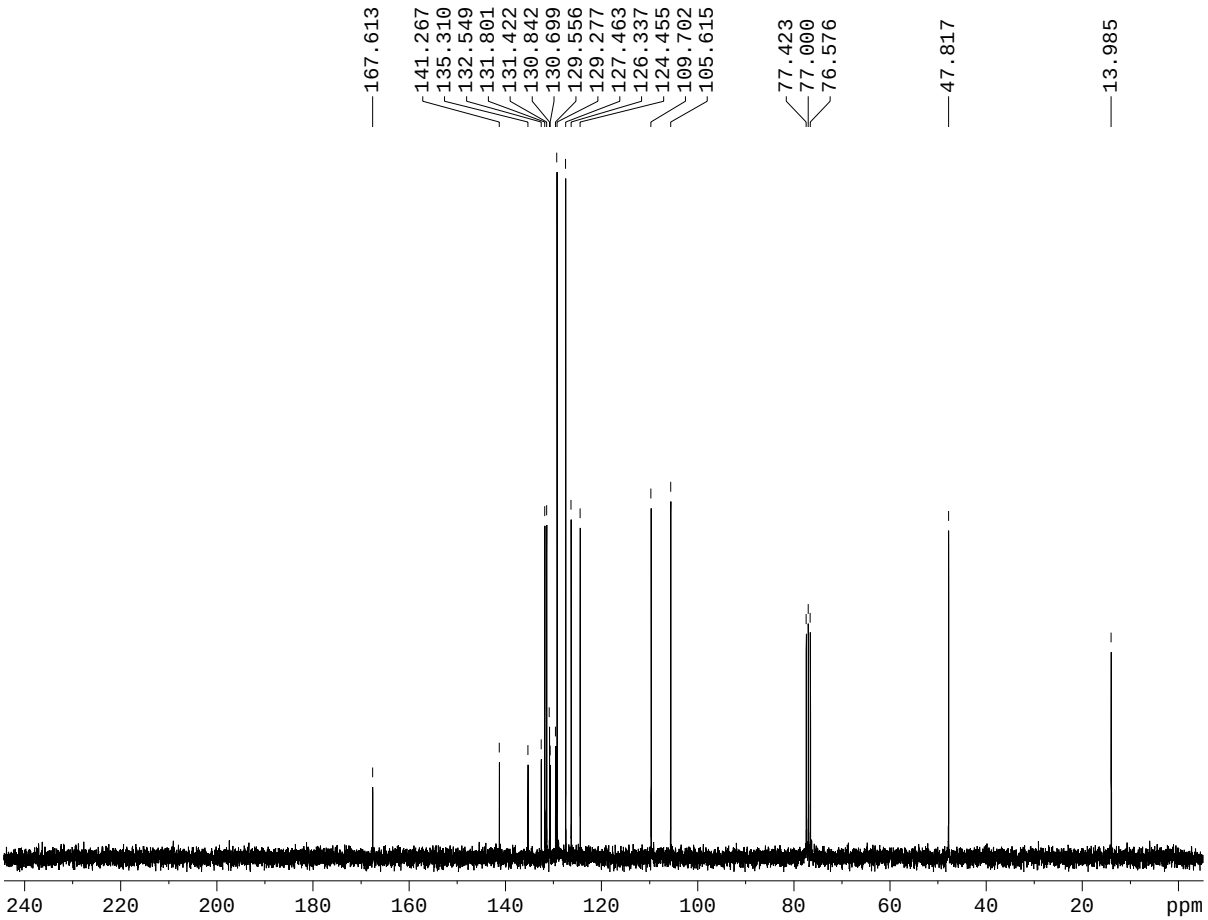

N
N
O
23b
9
8
7
6
5
4
3
2
1
0
ppm
1.000
1.021
1.014
1.172
2.013
1.024
1.015
1.039
1.031
3.057
3.117

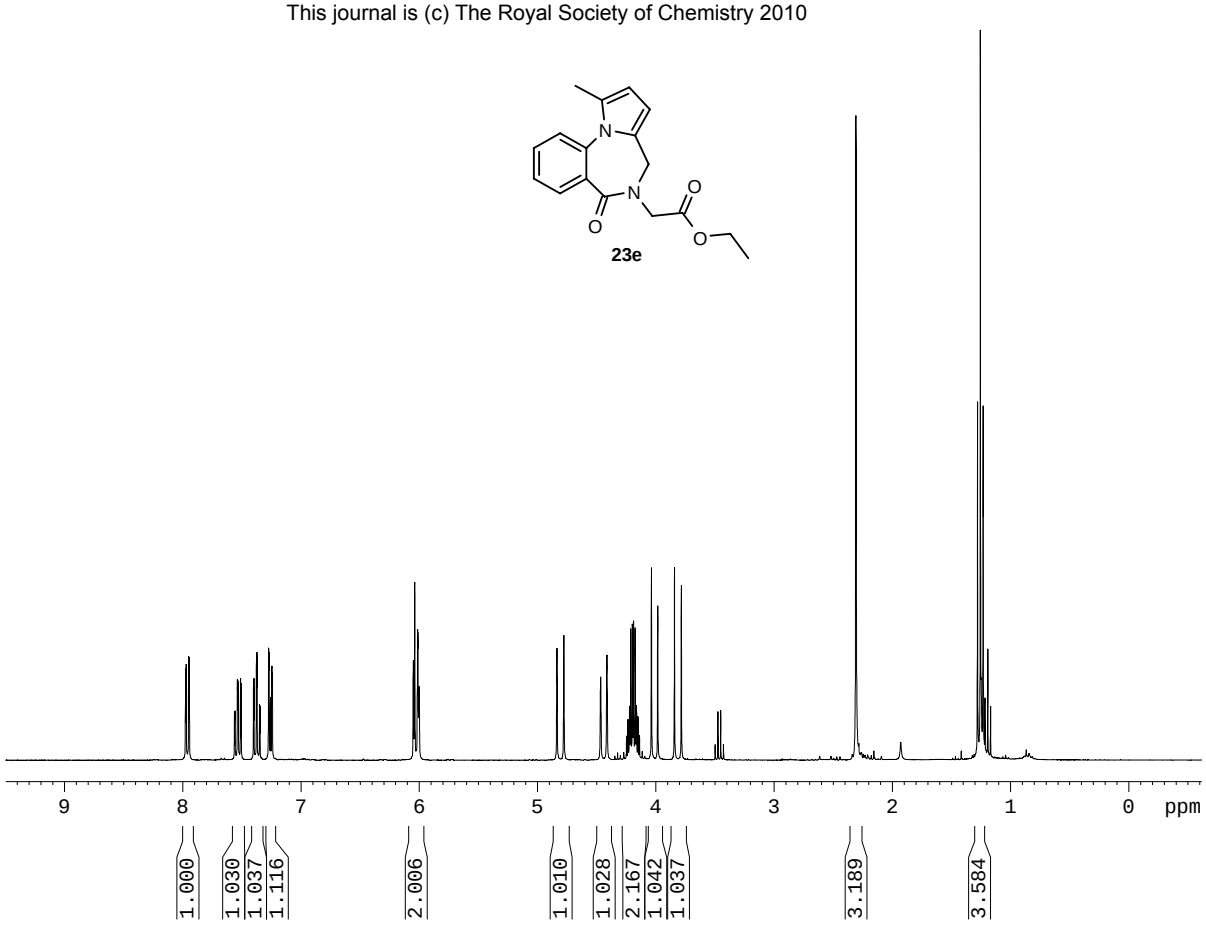

167.278
135.218
131.641
131.457
130.978
130.793
129.143
126.062
124.262
109.307
104.849
77.424
77.000
76.576
43.752
42.338
13.960
13.051
240
220
200
180
160
140
120
100
80
60
40
20
ppm

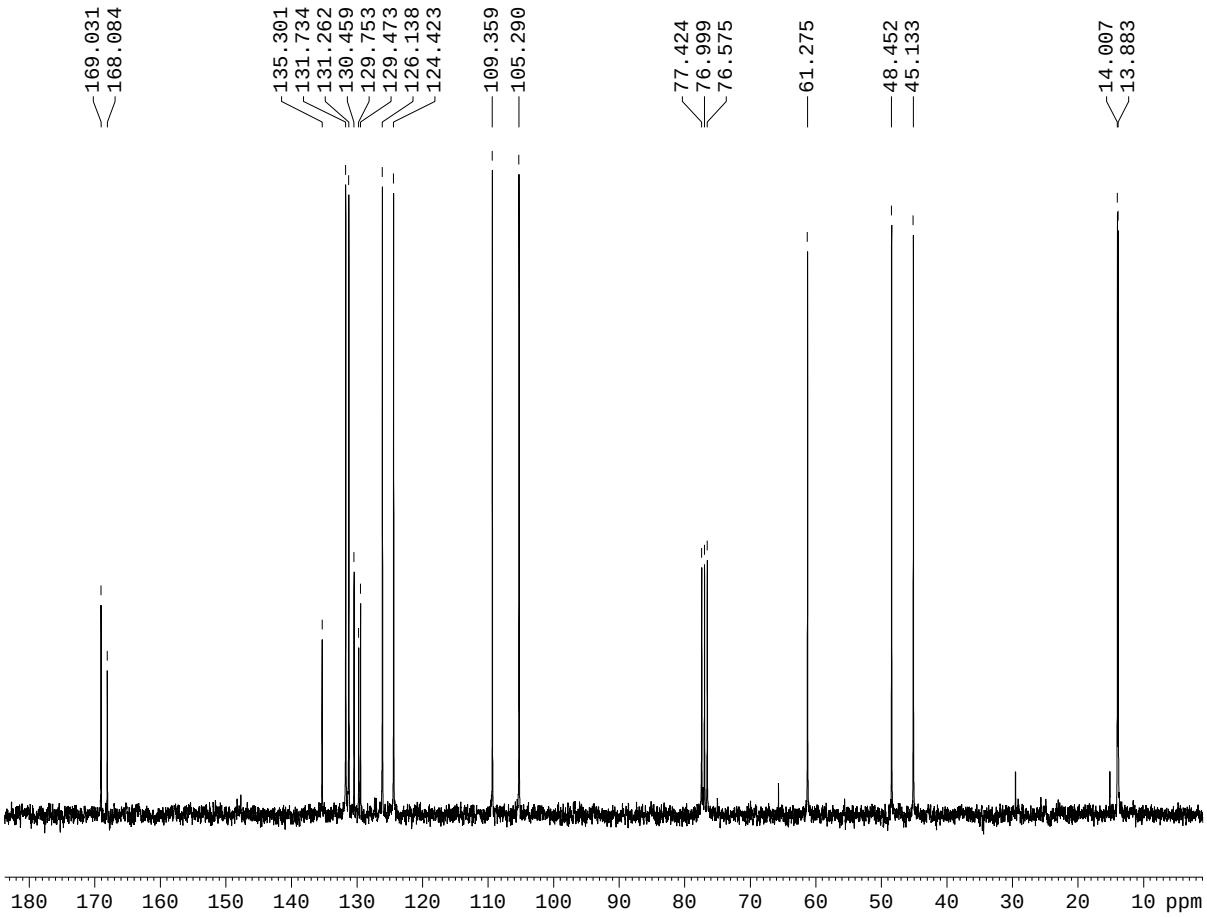

N
N
O
23c
10 9 8 7 6 5 4 3 2 1 0 ppm
0.998
1.049
1.237
6.059
1.014
1.001
1.027
1.037
1.034
1.023
3.087

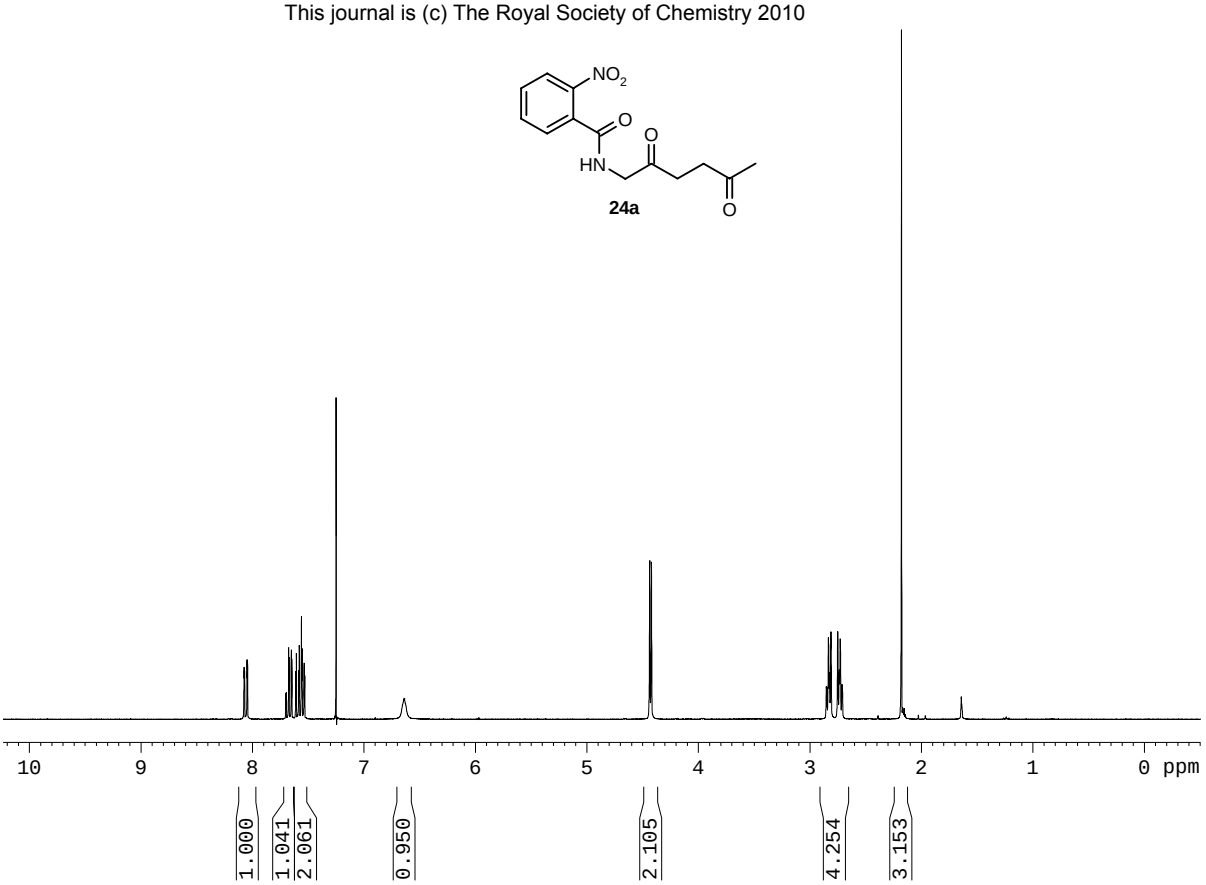

168.023
136.648
135.281
131.575
131.010
130.651
129.266
128.572
128.096
127.492
126.136
124.377
109.292
105.276
77.424
77.001
76.577
50.139
43.218
13.933
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm


N
N
O
Cl
23d
10
9
8
7
6
5
4
3
2
1
0
ppm
1.000
1.046
6.473
2.007
1.033
1.033
3.066

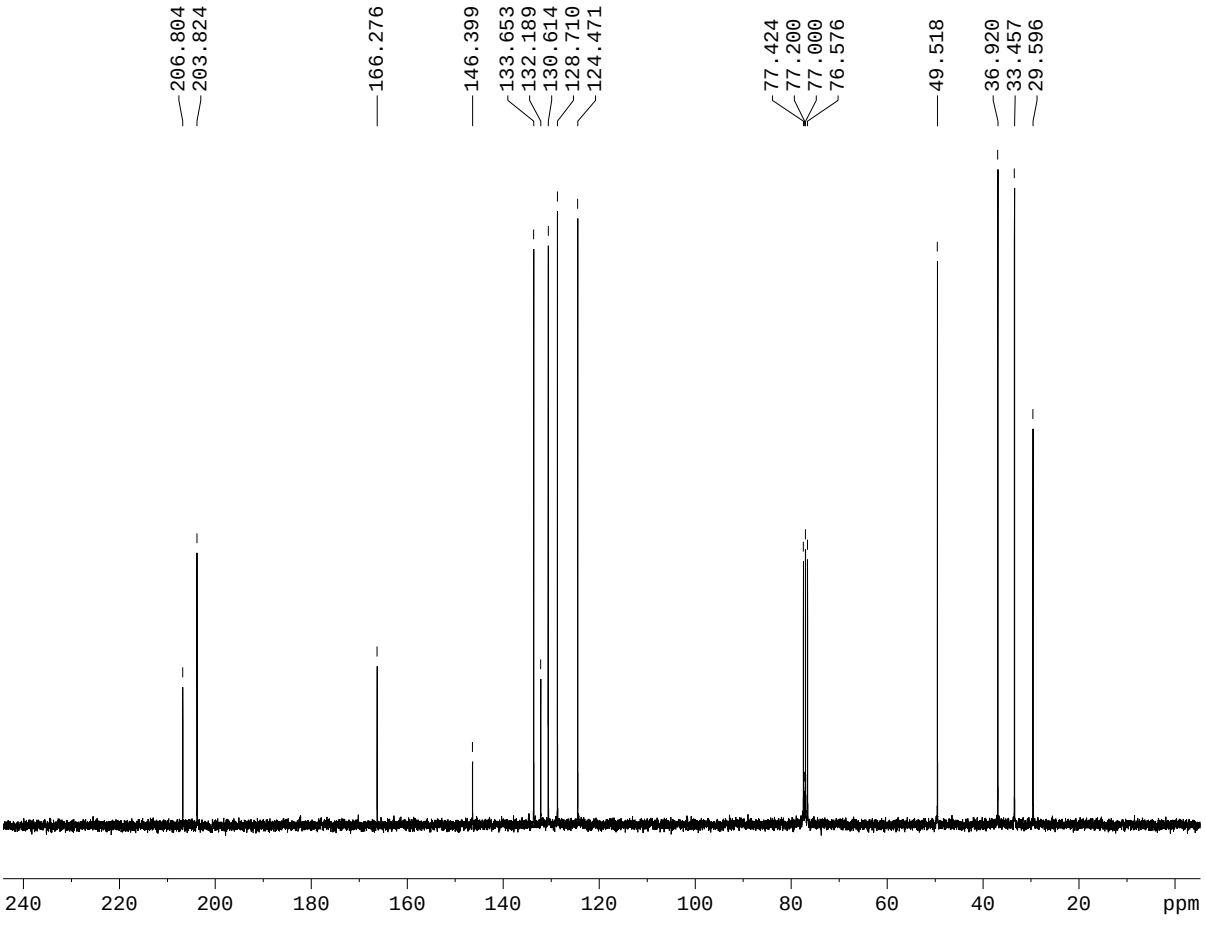

167.613
141.267
135.310
132.549
131.801
131.422
130.842
130.699
129.556
129.277
127.463
126.337
124.455
109.702
105.615
77.423
77.000
76.576
47.817
13.985
240
220
200
180
160
140
120
100
80
60
40
20
ppm

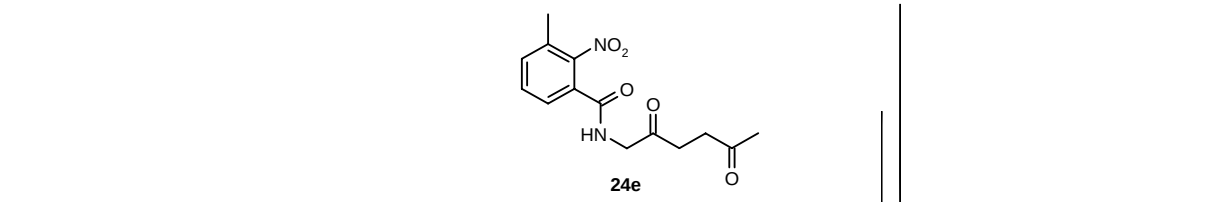

23e
9 8 7 6 5 4 3 2 1 0 ppm
1.000
1.030
1.037
1.116
2.006
1.010
1.028
2.167
1.042
1.037
3.189
3.584


169.031
168.084
135.301
131.734
131.262
130.459
129.753
129.473
126.138
124.423
109.359
105.290
77.424
76.999
76.575
61.275
48.452
45.133
14.007
13.883
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm


NO2
O
O
HN
O
10
9
8
7
6
5
4
3
2
1
0 ppm
1.000
1.041
2.061
0.950
2.105
4.254
3.153

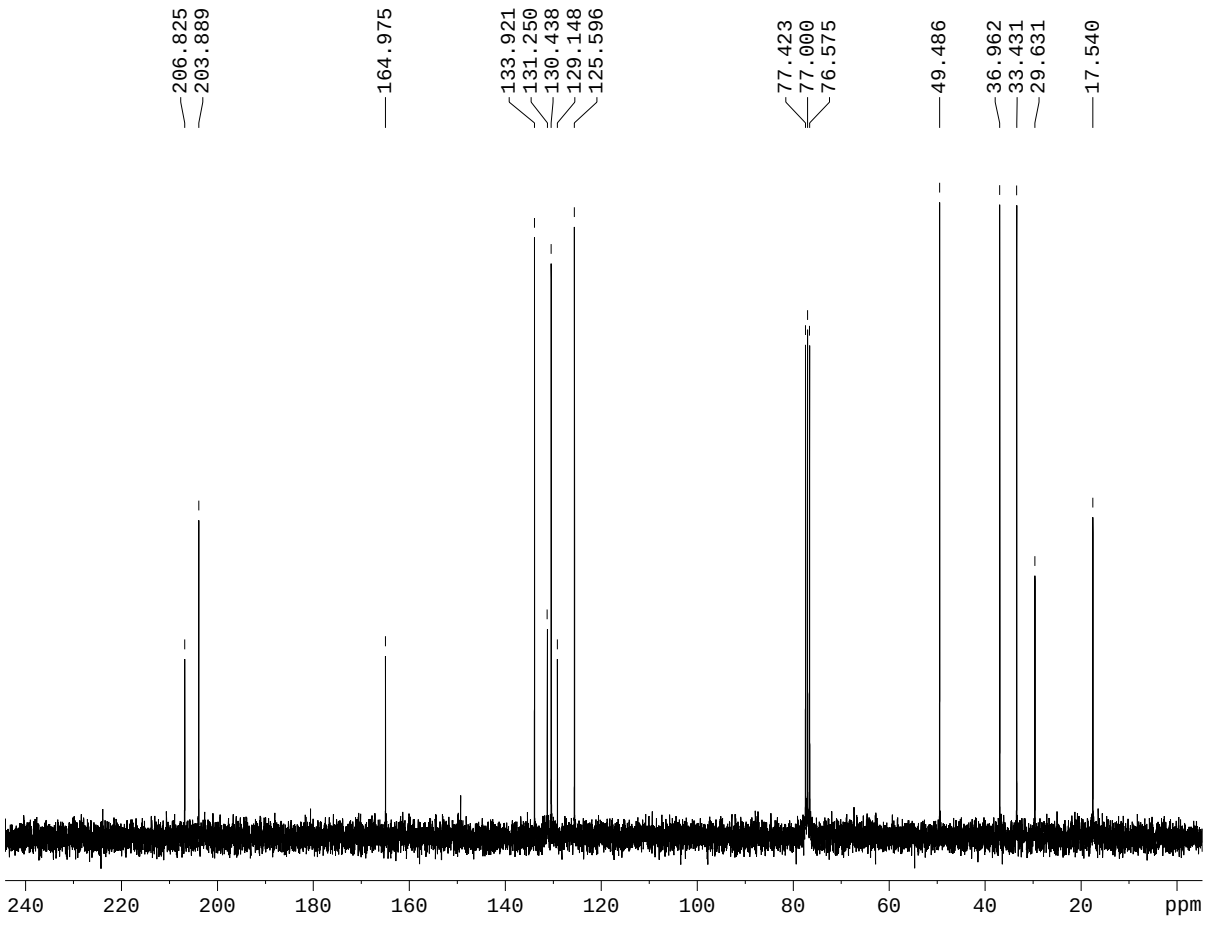
24a

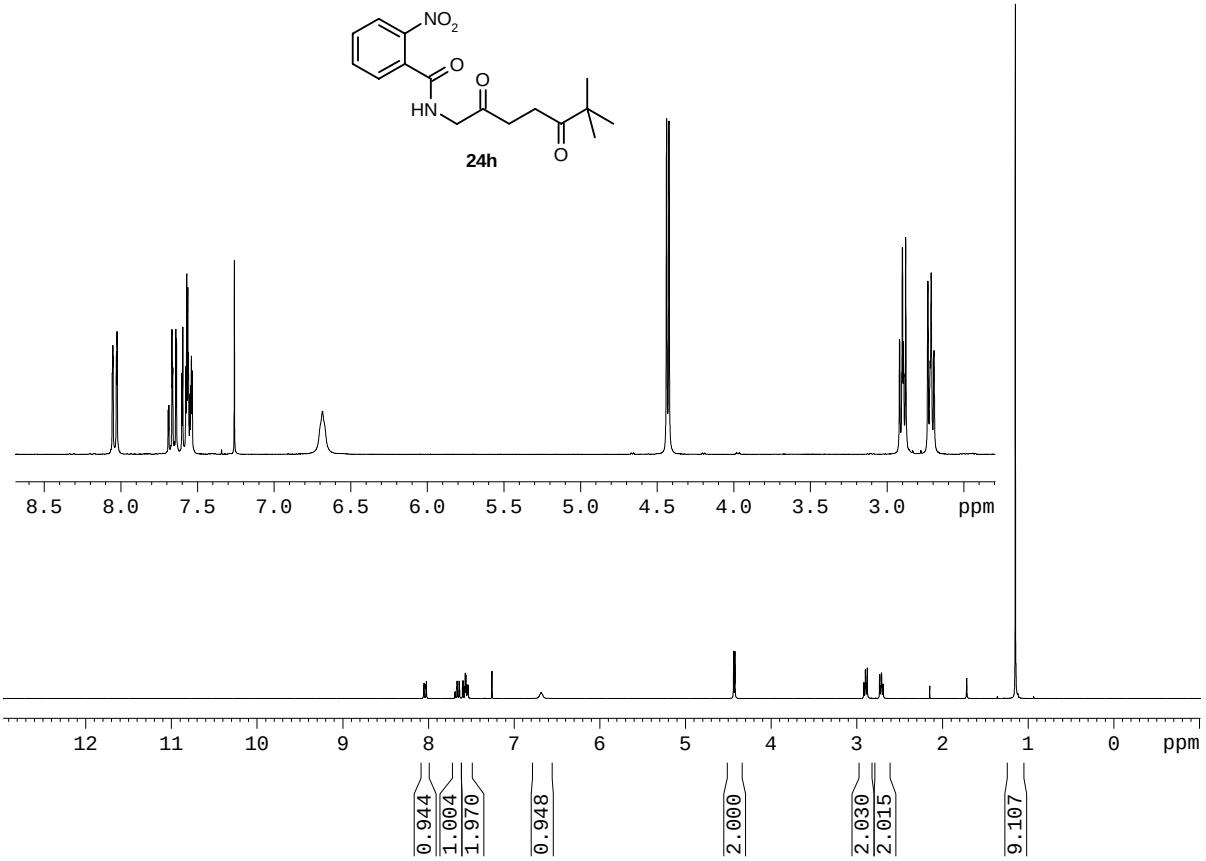

206.804
203.824
166.276
146.399
133.653
132.189
130.614
128.710
124.471
77.424
77.200
77.000
76.576
49.518
36.920
33.457
29.596
240
220
200
180
160
140
120
100
80
60
40
20
ppm

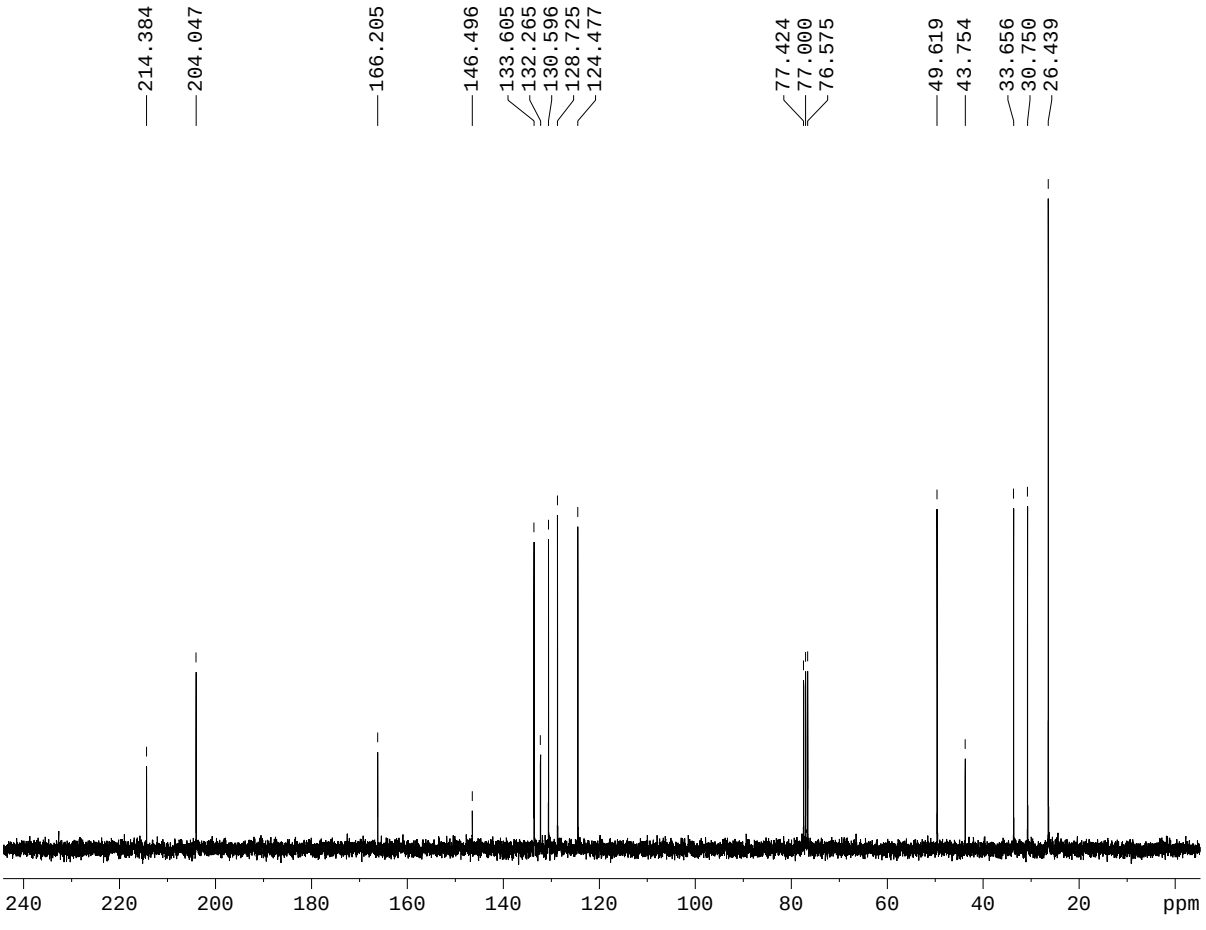

NO2
O
O
HN
O

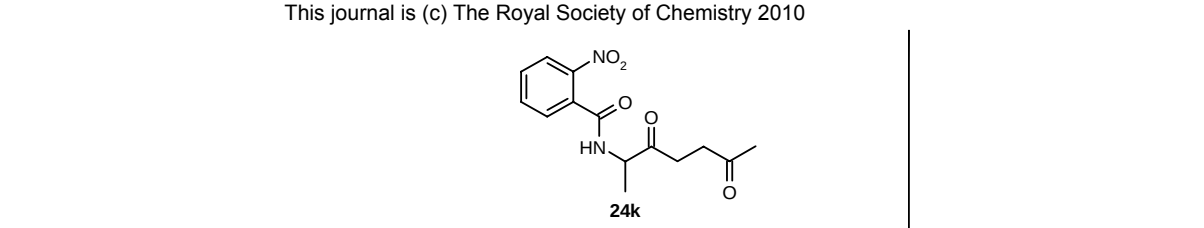
24e

11
10
9
8
7
6
5
4
3
2
1
0
ppm
3.038
0.935
2.019
2.030
2.008
3.036
3.000


206.825
203.889
164.975
133.921
131.250
130.438
129.148
125.596
77.423
77.000
76.575
49.486
36.962
33.431
29.631
17.540
240
220
200
180
160
140
120
100
80
60
40
20
ppm

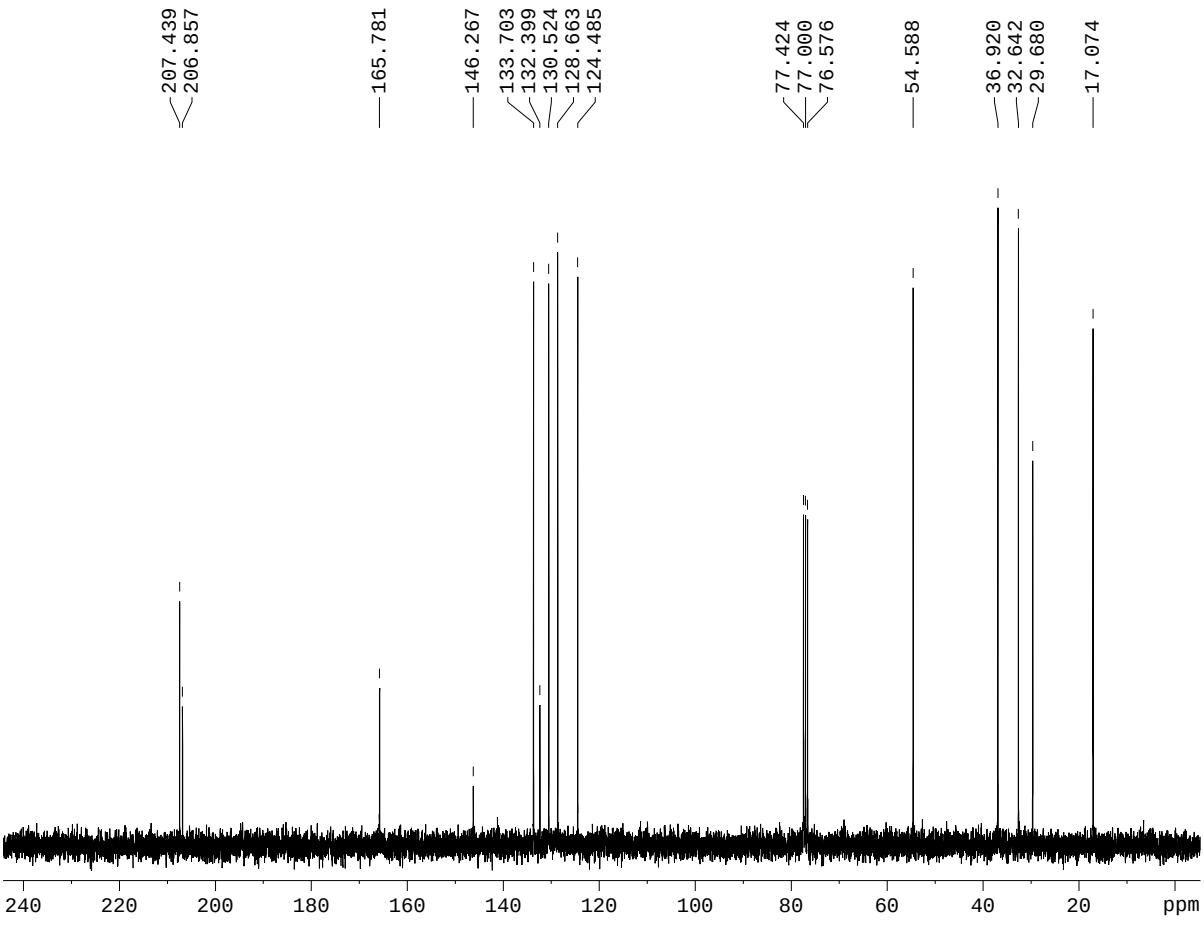

NO2
O
HN
O
O
24h
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 ppm
12 11 10 9 8 7 6 5 4 3 2 1 0 ppm
0.944
1.004
1.970
0.948
2.000
2.030
2.015
9.107

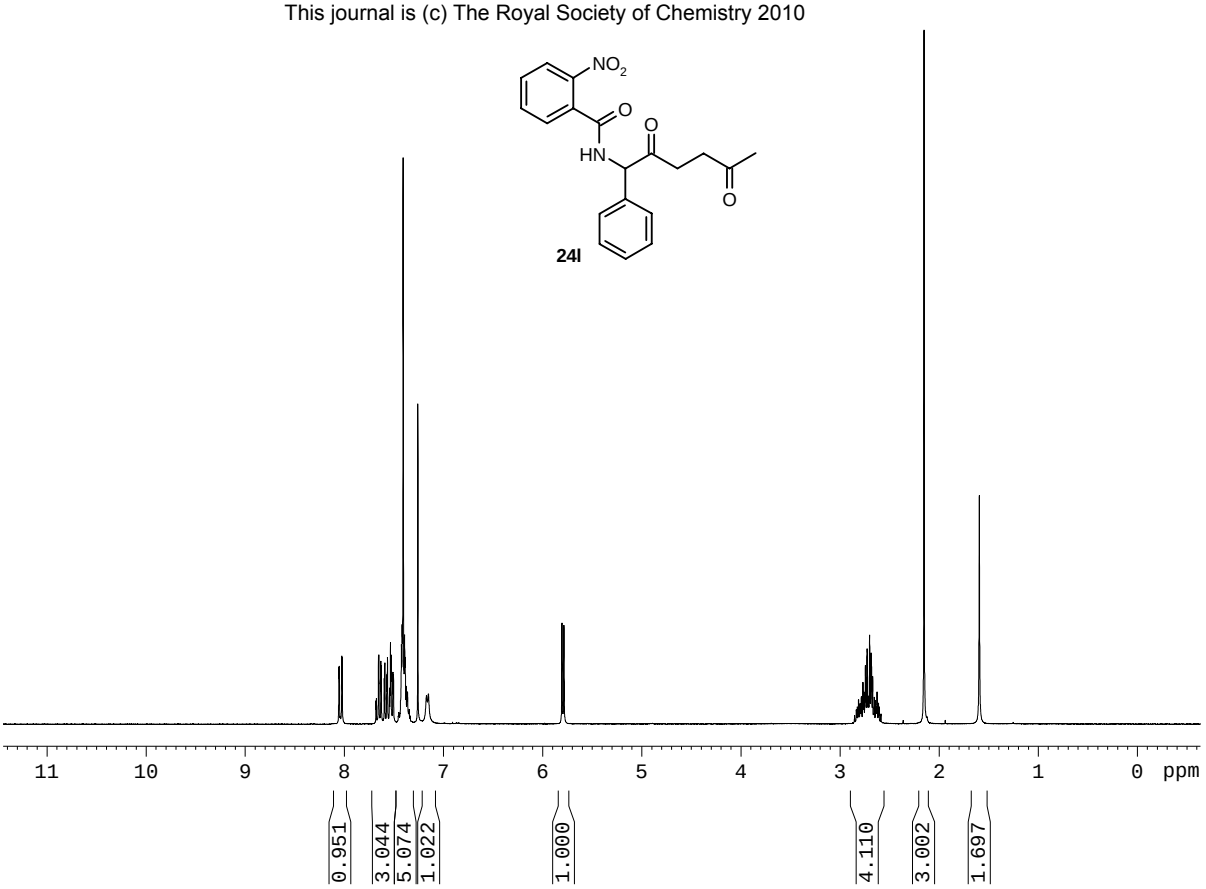

214.384
204.047
166.205
146.496
133.605
132.265
130.596
128.725
124.477
77.424
77.000
76.575
49.619
43.754
33.656
30.750
26.439
240 220 200 180 160 140 120 100 80 60 40 20 ppm

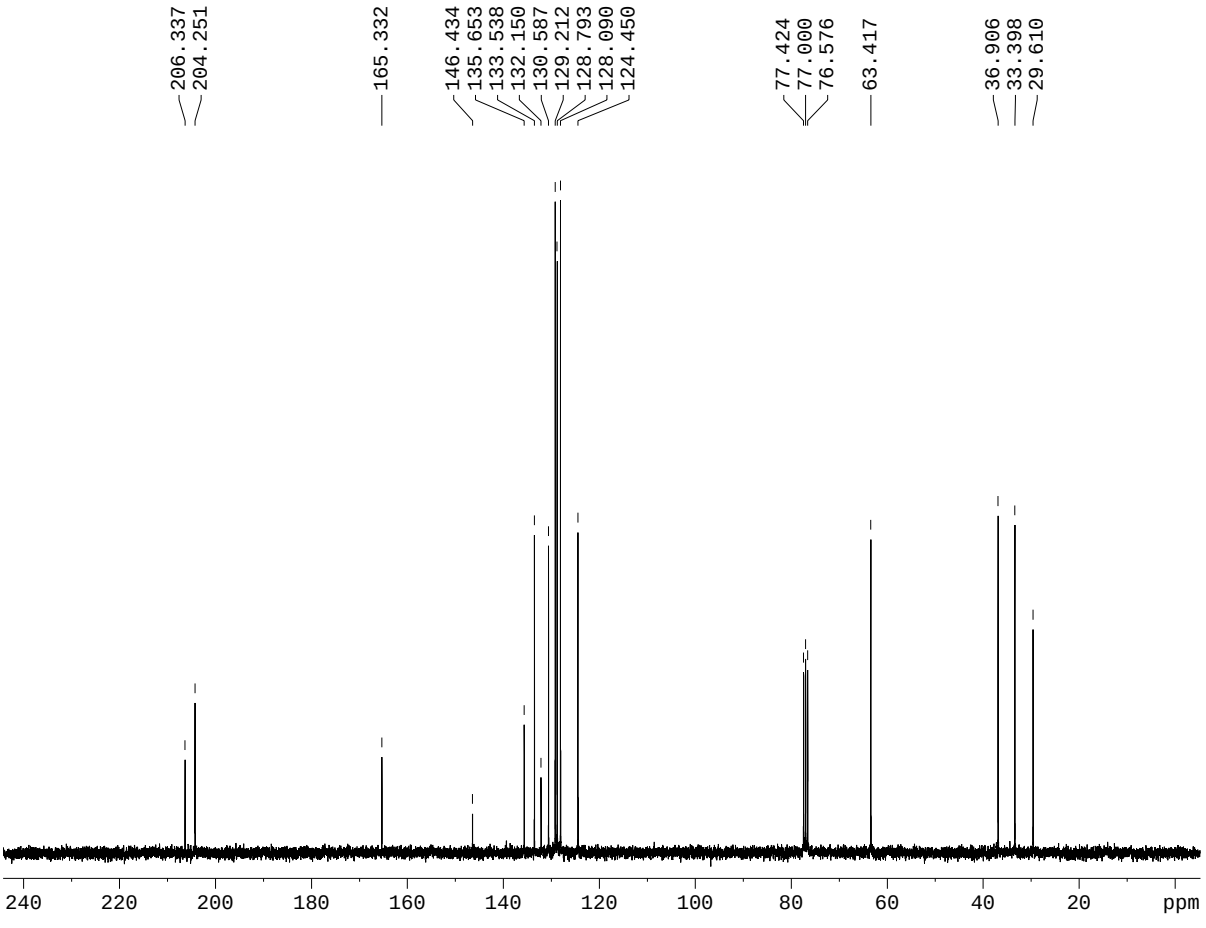

NO2
O
HN
O
O

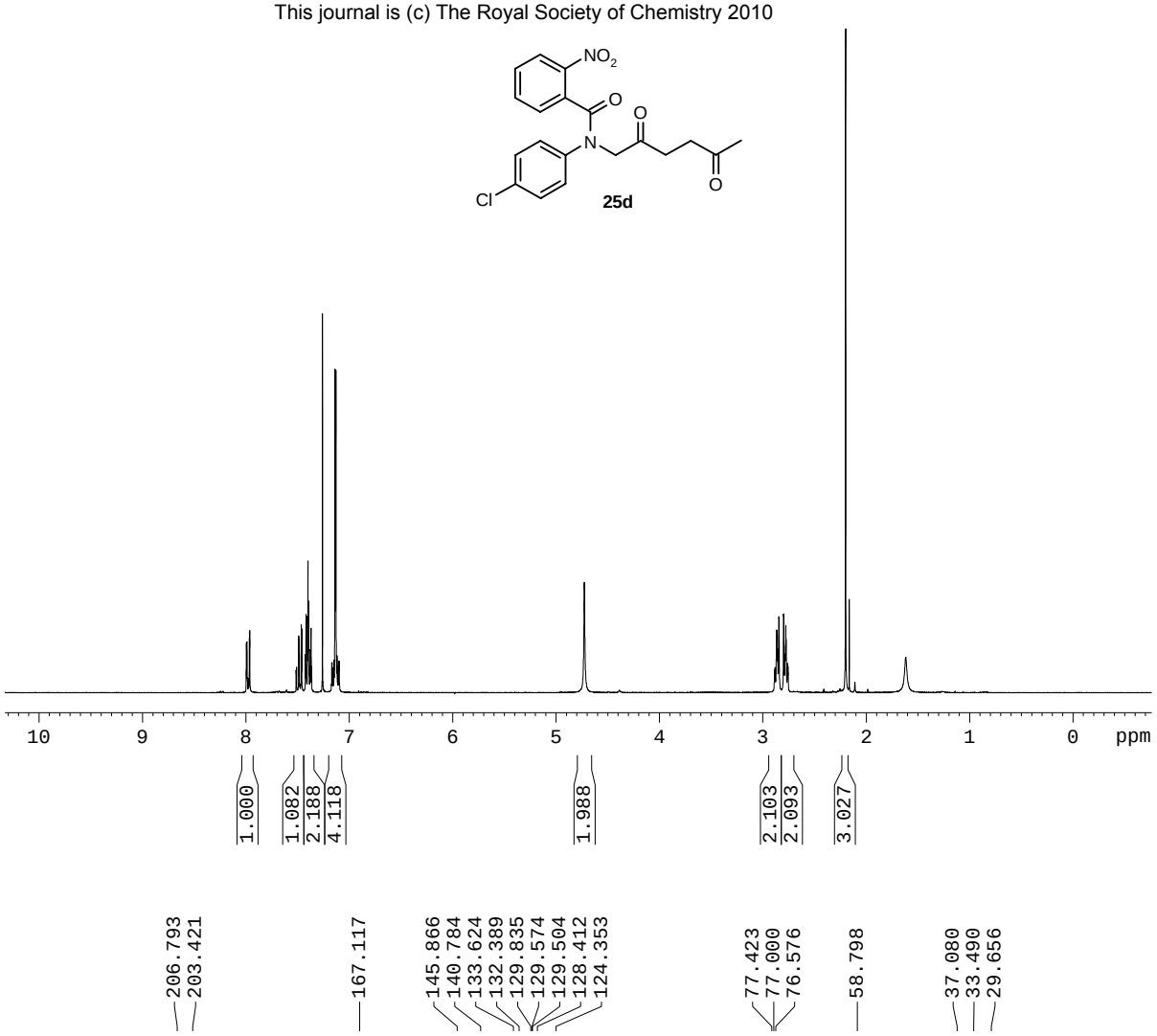
24k

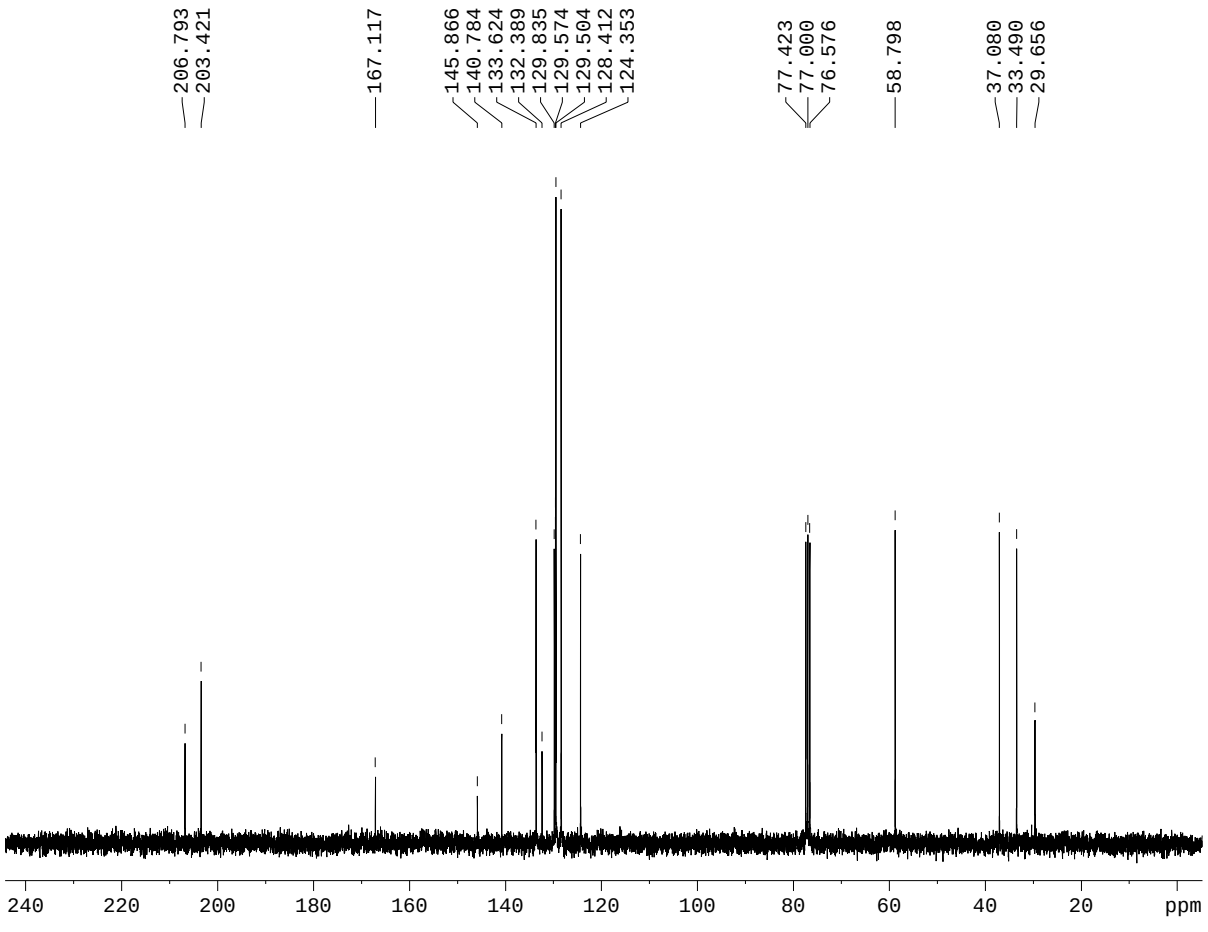
11
10
9
8
7
6
5
4
3
2
1
0
ppm
0.954
1.008
1.052
0.945
0.939
0.978
4.005
2.987
3.000

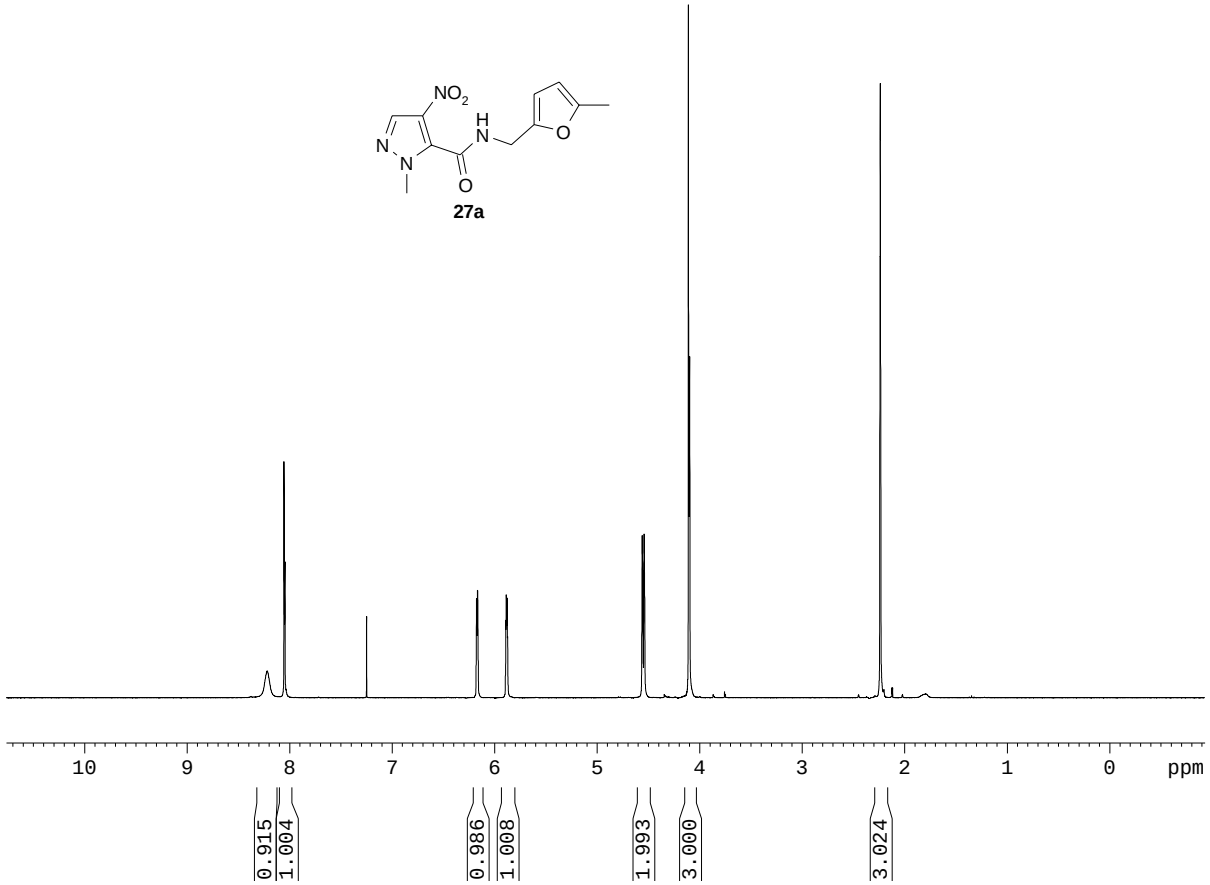

207.439
206.857
165.781
146.267
133.703
132.399
130.524
128.663
124.485
77.424
77.000
76.576
54.588
36.920
32.642
29.680
17.074
240
220
200
180
160
140
120
100
80
60
40
20
ppm

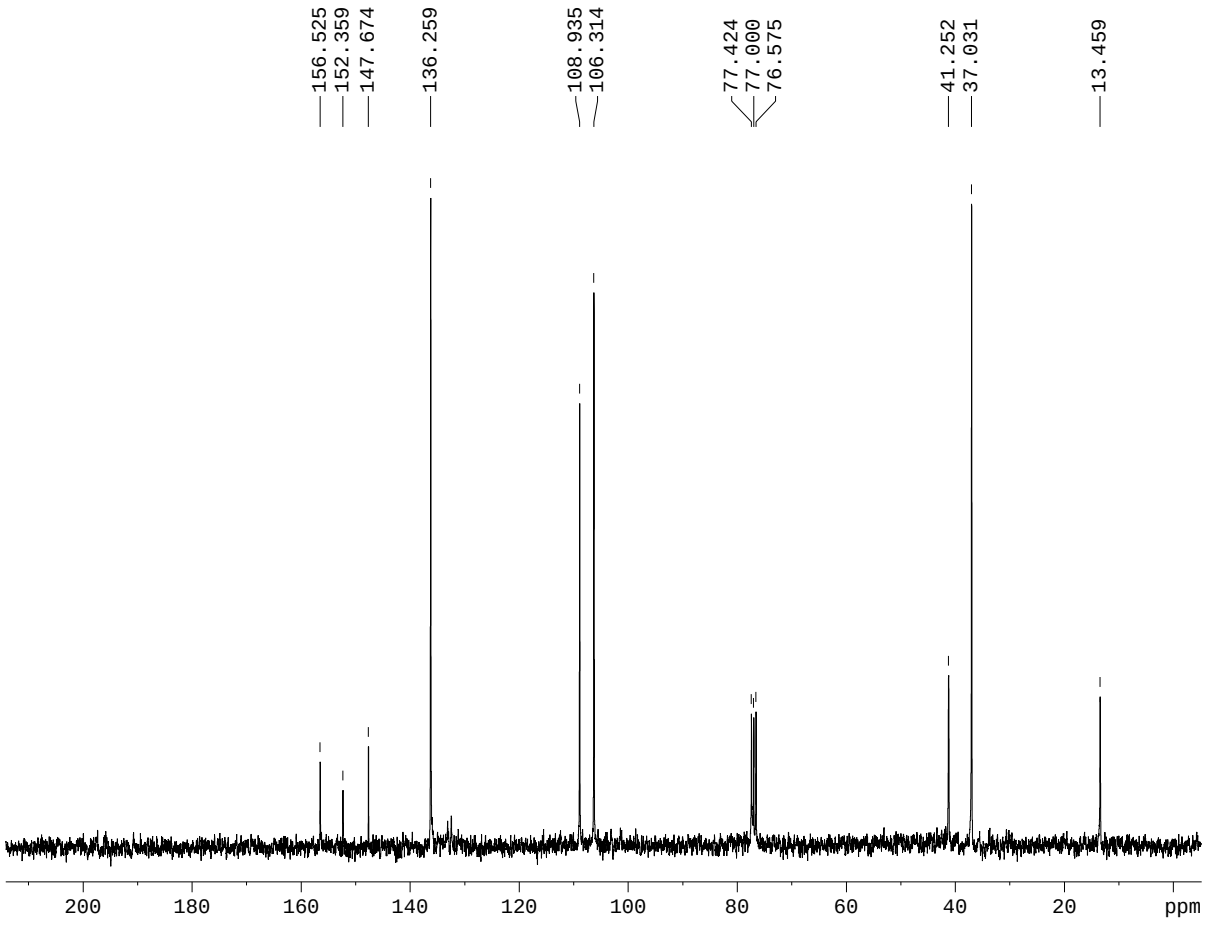

NO2
O
HN
O
O
24l
11 10 9 8 7 6 5 4 3 2 1 0 ppm
0.951
3.044
5.074
1.022
1.000
4.110
3.002
1.697

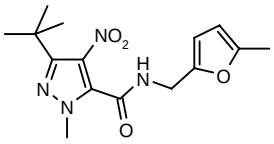

206.337
204.251
165.332
146.434
135.653
133.538
132.150
130.587
129.212
128.793
128.090
124.450
77.424
77.000
76.576
63.417
36.906
33.398
29.610
240 220 200 180 160 140 120 100 80 60 40 20 ppm


NO2
O
N
O
O
Cl
25d
10
9
8
7
6
5
4
3
2
1
0
ppm
1.000
1.082
2.188
4.118
1.988
2.103
2.093
3.027


206.793
203.421
167.117
145.866
140.784
133.624
132.389
129.835
129.574
129.504
128.412
124.353
77.423
77.000
76.576
58.798
37.080
33.490
29.656
240
220
200
180
160
140
120
100
80
60
40
20
ppm

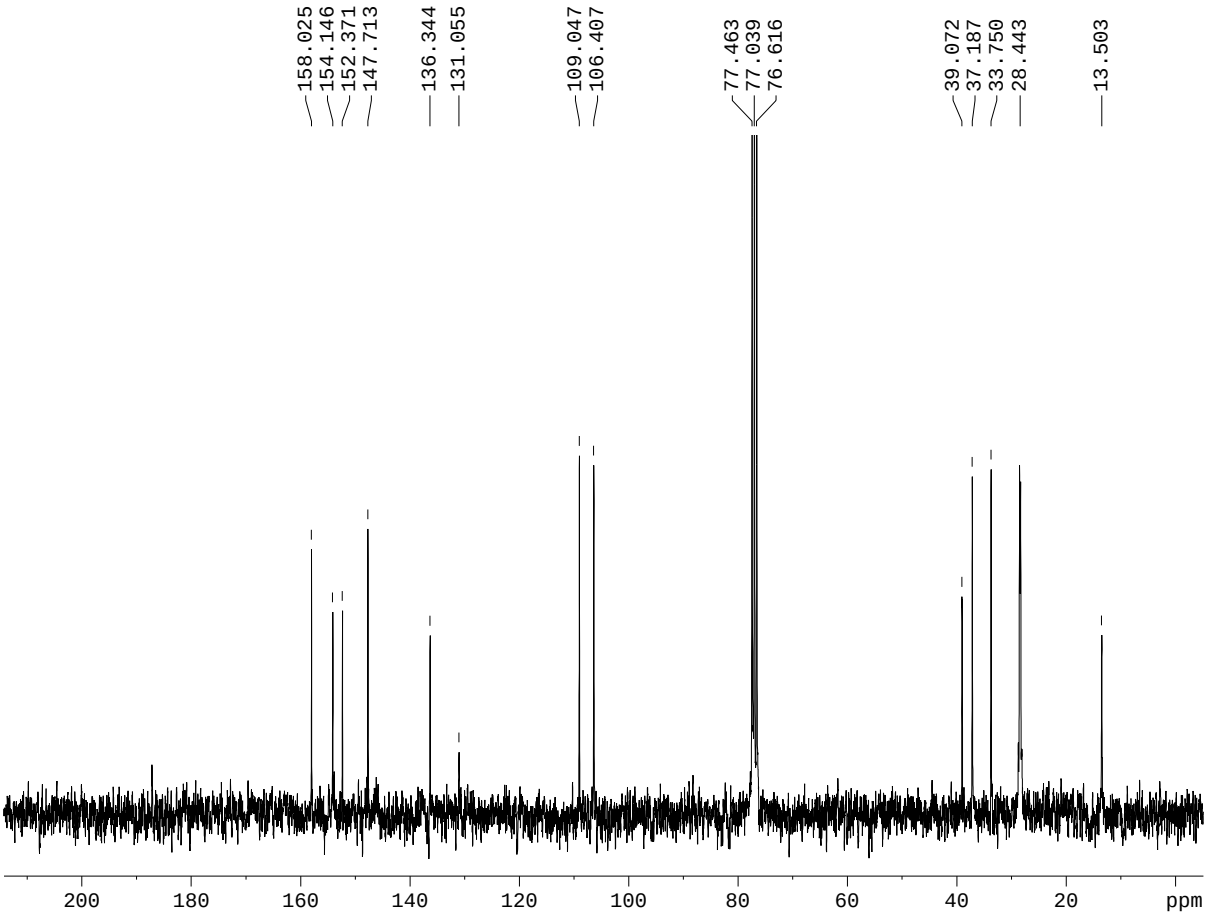

NO2
H
N
N
N
O
O
27a
10
9
8
7
6
5
4
3
2
1
0
ppm
0.915
1.004
0.986
1.008
1.993
3.000
3.024

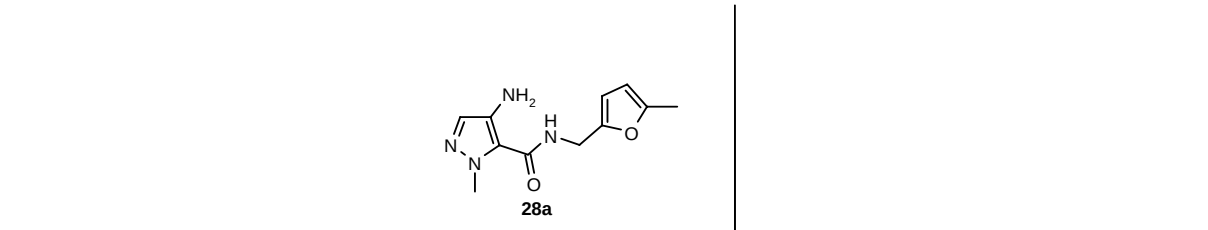

156.525
152.359
147.674
136.259
108.935
106.314
77.424
77.000
76.575
41.252
37.031
13.459
200
180
160
140
120
100
80
60
40
20
ppm


NO2
H
N
N
N
O
O

27b

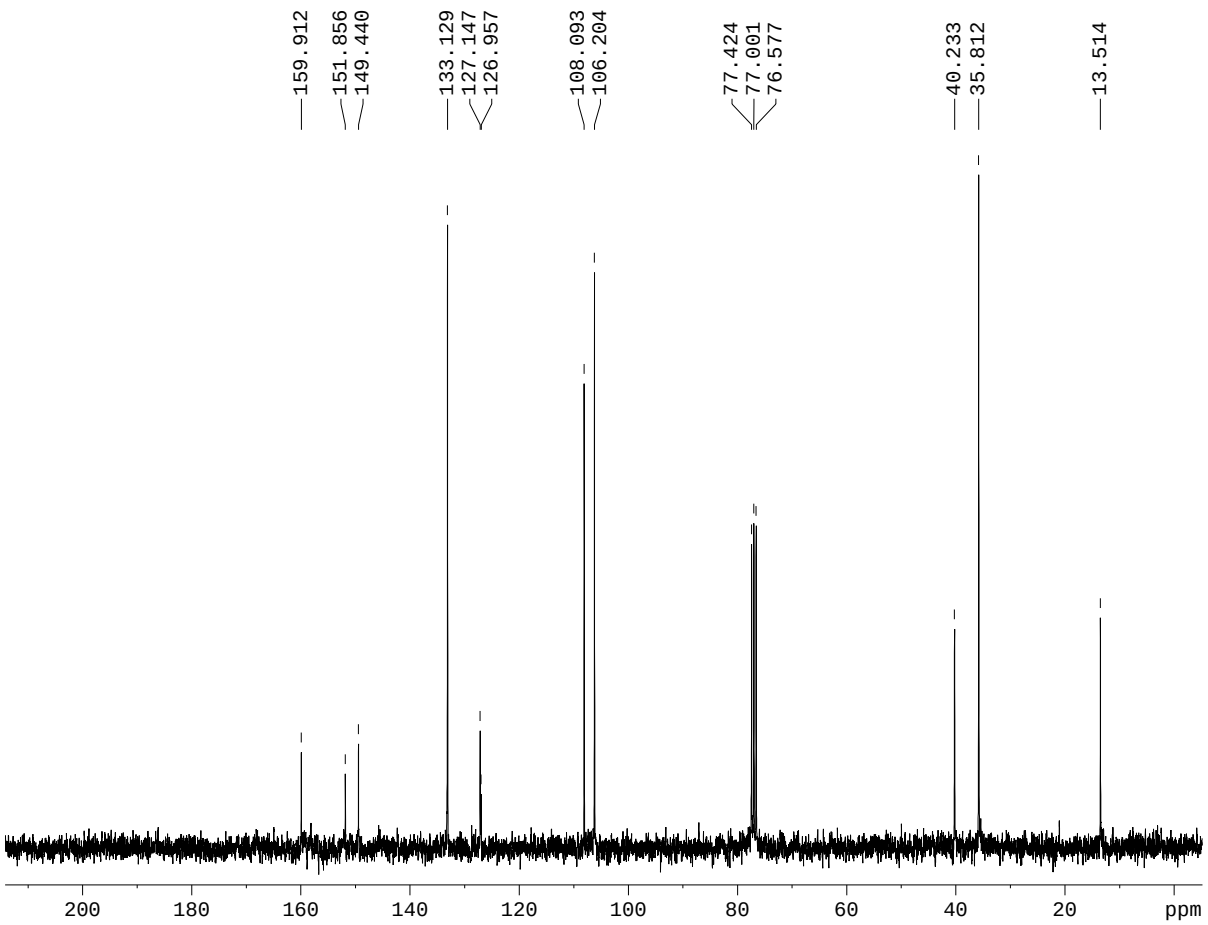
9
8
7
6
5
4
3
2
1
0
ppm
0.940
1.000
1.039
2.000
3.017
3.076
9.050

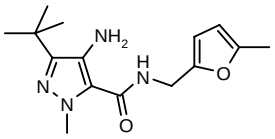

158.025
154.146
152.371
147.713
136.344
131.055
109.047
106.407
77.463
77.039
76.616
39.072
37.187
33.750
28.443
13.503
200
180
160
140
120
100
80
60
40
20
ppm


NH2
H
N
N
N
O
O

28a

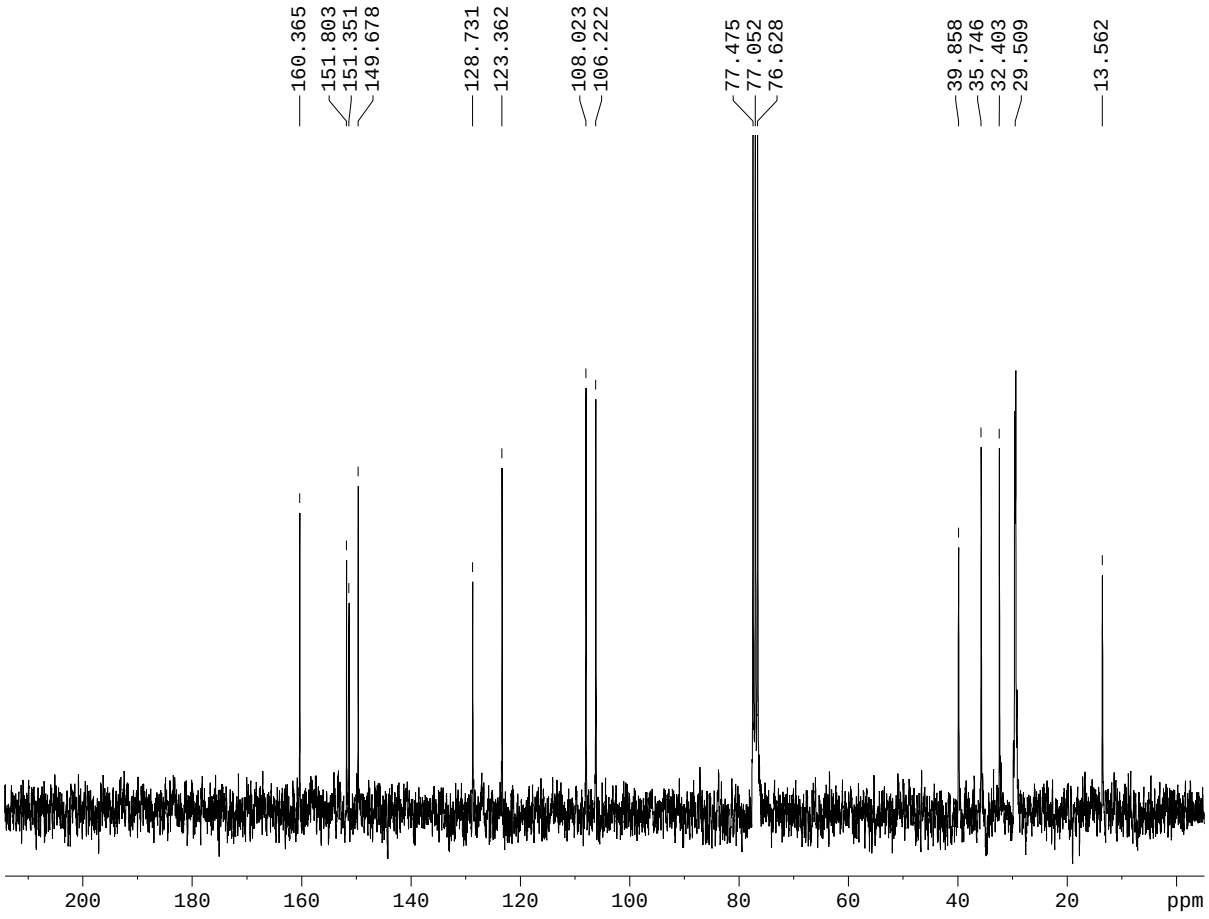
10
9
8
7
6
5
4
3
2
1
ppm
0.977
1.000
1.020
1.011
2.045
3.052
1.958
3.136

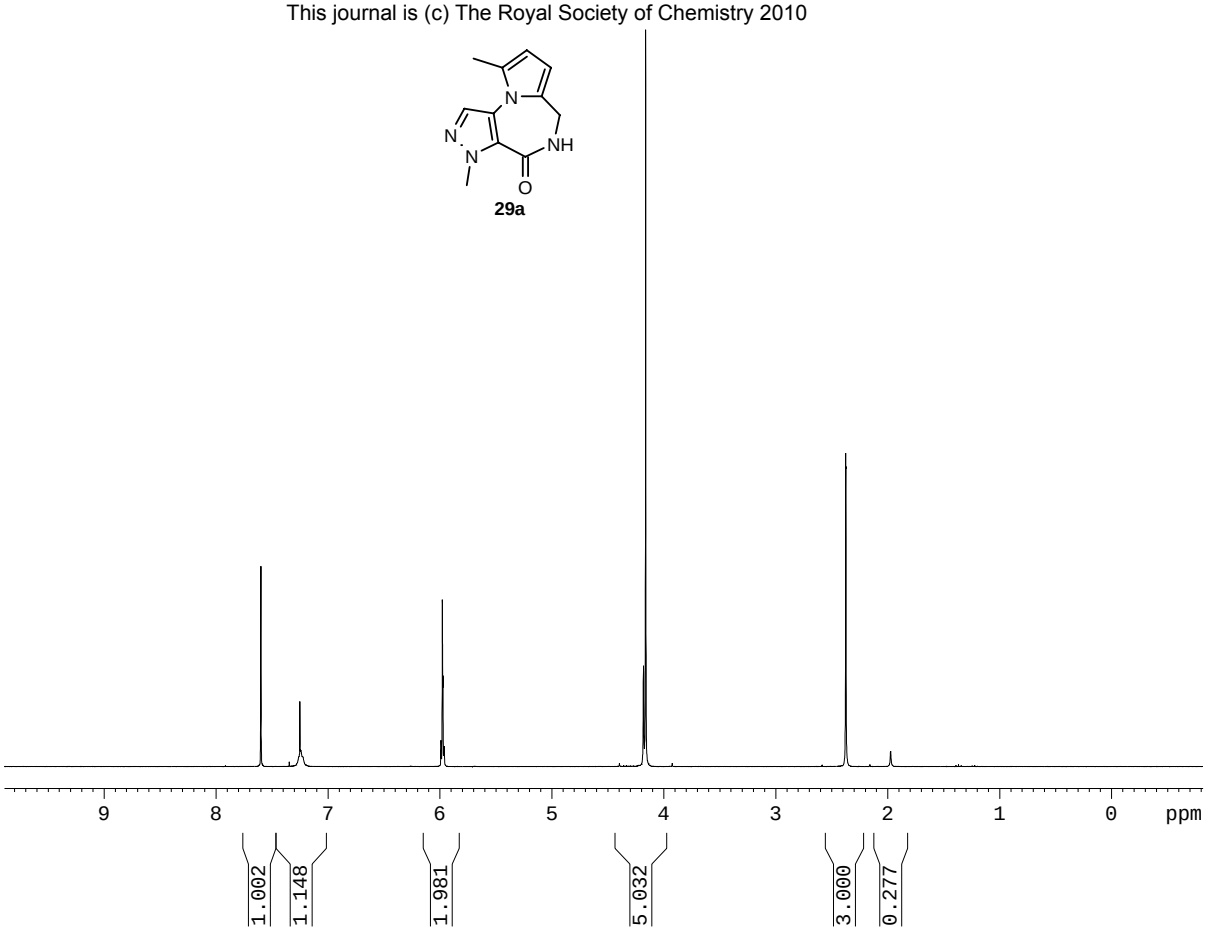

159.912
151.856
149.440
133.129
127.147
126.957
108.093
106.204
77.424
77.001
76.577
40.233
35.812
13.514
200
180
160
140
120
100
80
60
40
20
ppm

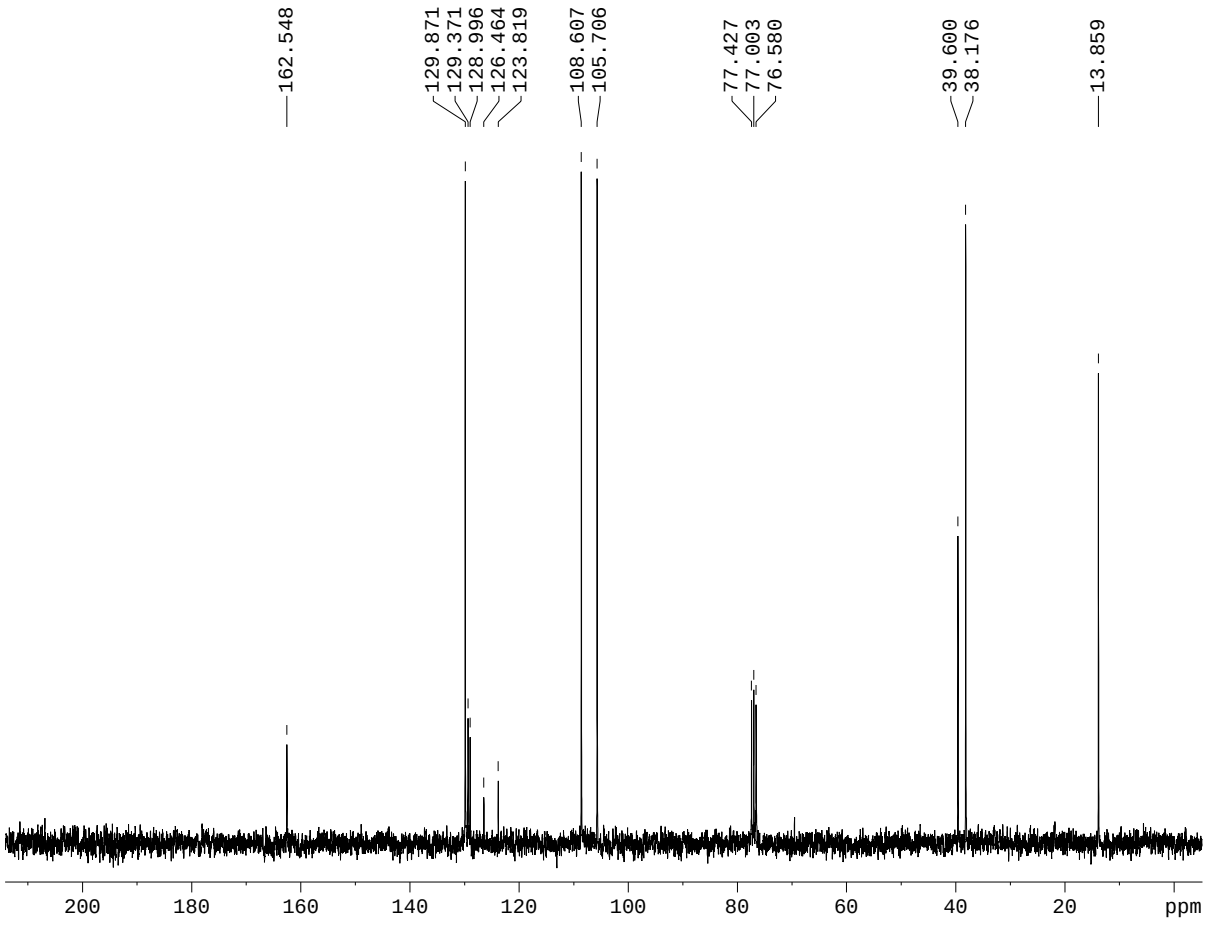

NH2
H
N
N
N
O
O

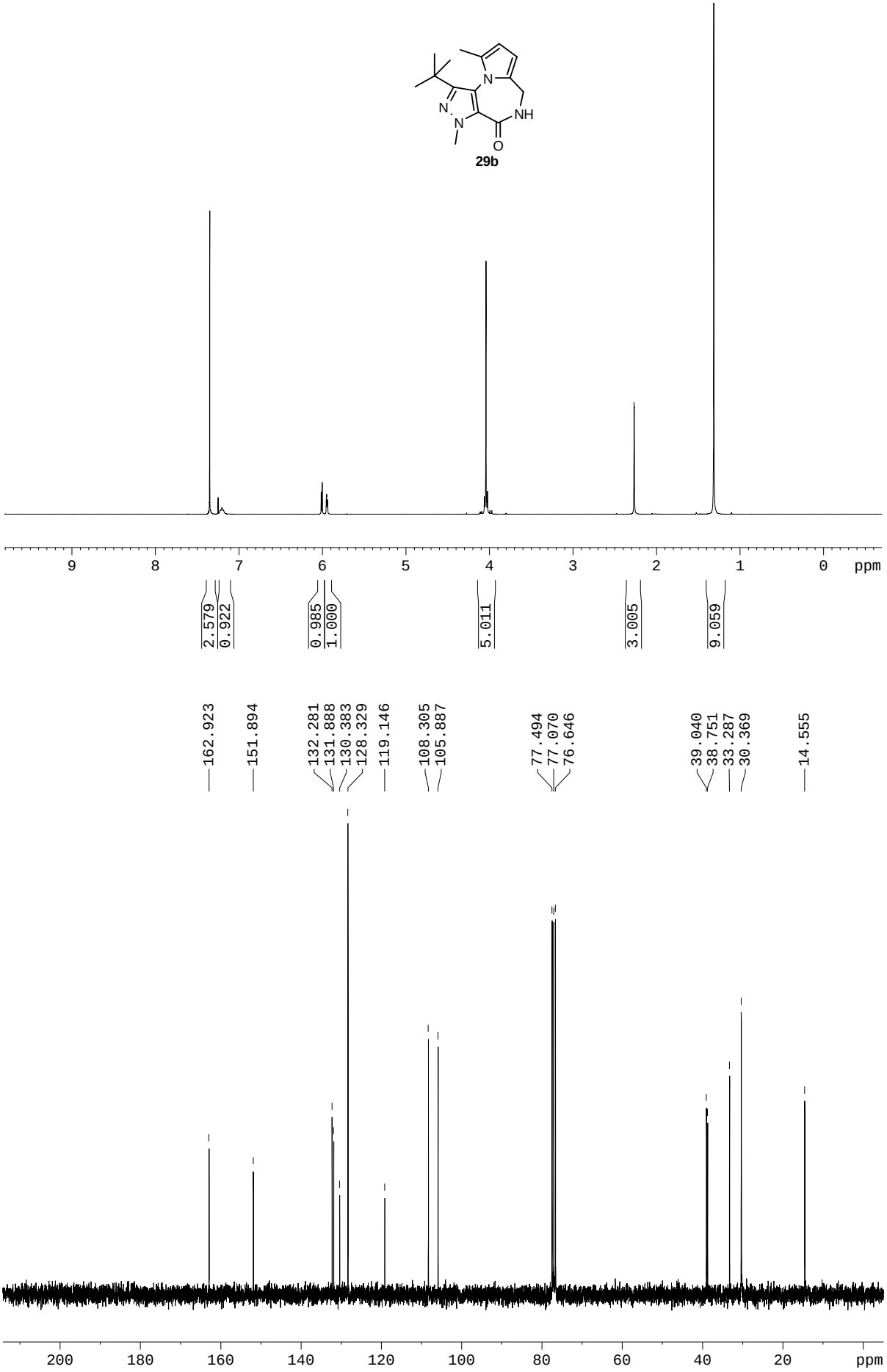
28b

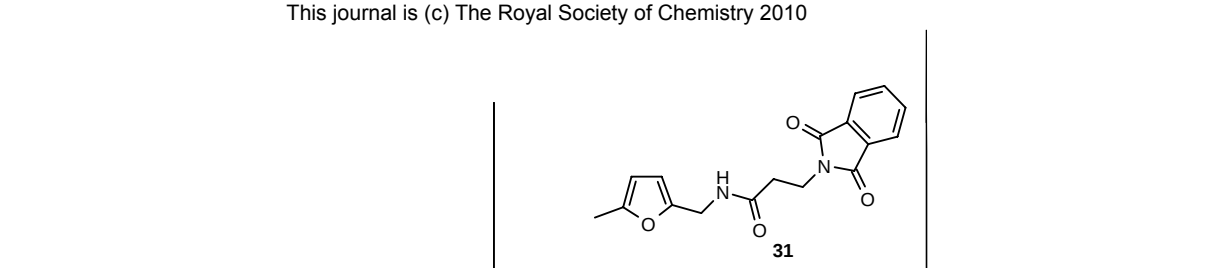
10
9
8
7
6
5
4
3
2
1
0
ppm
0.935
0.999
1.007
2.037
3.092
2.008
3.097
9.283


160.365
151.803
151.351
149.678
128.731
123.362
108.023
106.222
77.475
77.052
76.628
39.858
35.746
32.403
29.509
13.562
200
180
160
140
120
100
80
60
40
20
ppm

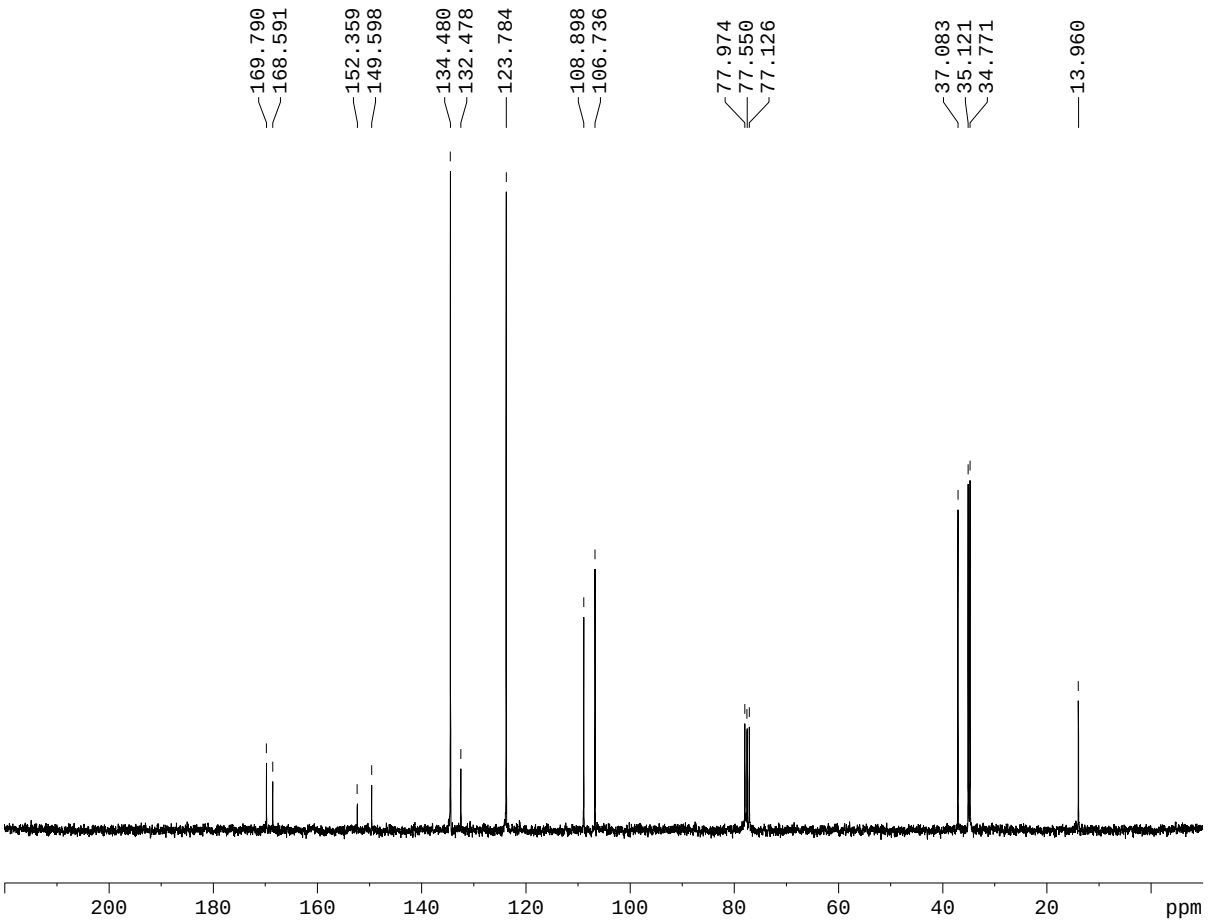

N
N
N
NH
O
29a
9
8
7
6
5
4
3
2
1
0
ppm
1.002
1.148
1.981
5.032
3.000
0.277

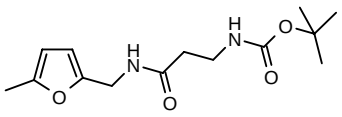

162.548
129.871
129.371
128.996
126.464
123.819
108.607
105.706
77.427
77.003
76.580
39.600
38.176
13.859
200
180
160
140
120
100
80
60
40
20
ppm


N
N
N
NH
O
29b
9
8
7
6
5
4
3
2
1
0
ppm
2.579
0.922
0.985
1.000
5.011
3.005
9.059
162.923
151.894
132.281
131.888
130.383
128.329
119.146
108.305
105.887
77.494
77.070
76.646
39.040
38.751
33.287
30.369
14.555
200
180
160
140
120
100
80
60
40
20
ppm


O
N
O
H
N
O
O
31

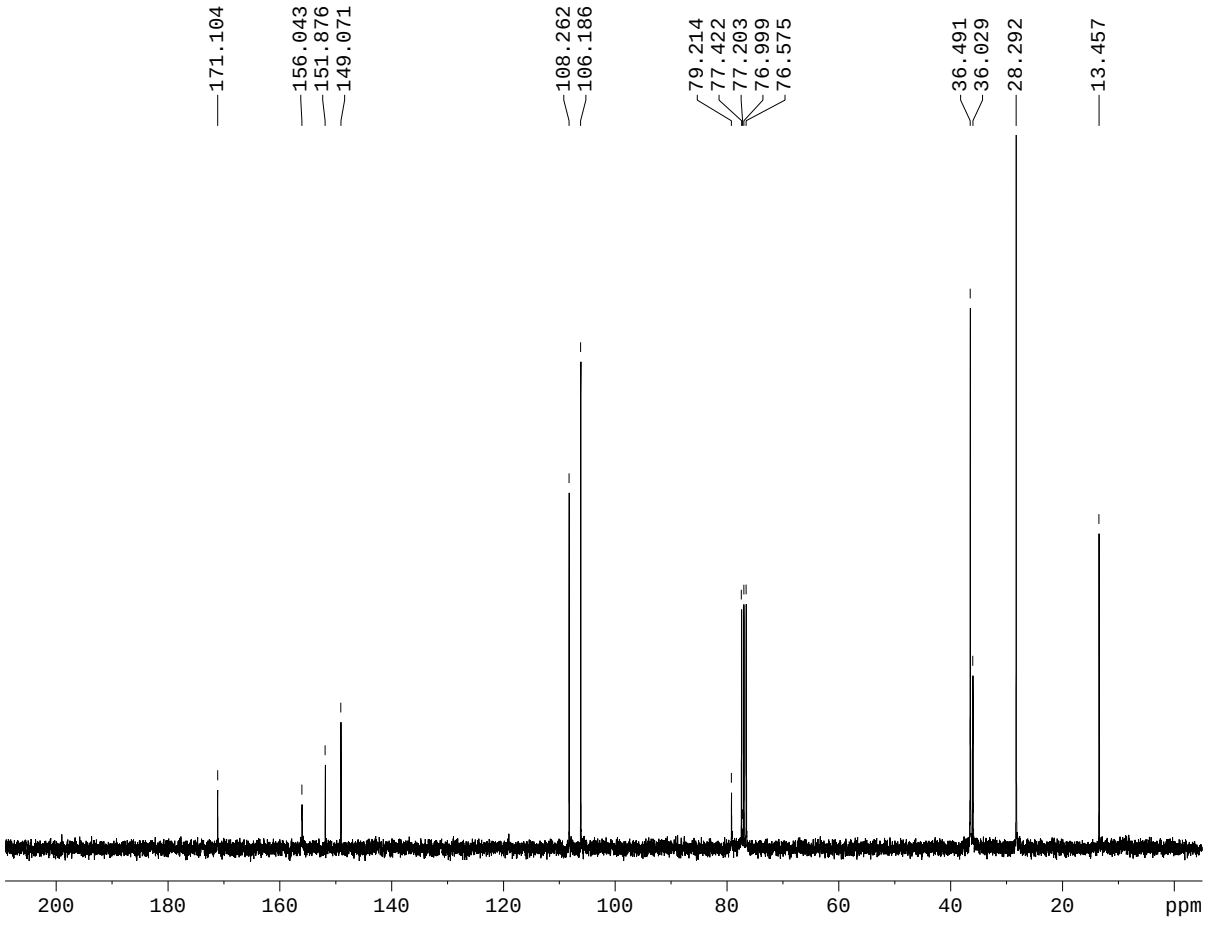
12
11
10
9
8
7
6
5
4
3
2
1
0
ppm
2.009
2.026
1.021
0.893
1.017
1.978
2.000
1.982
3.011

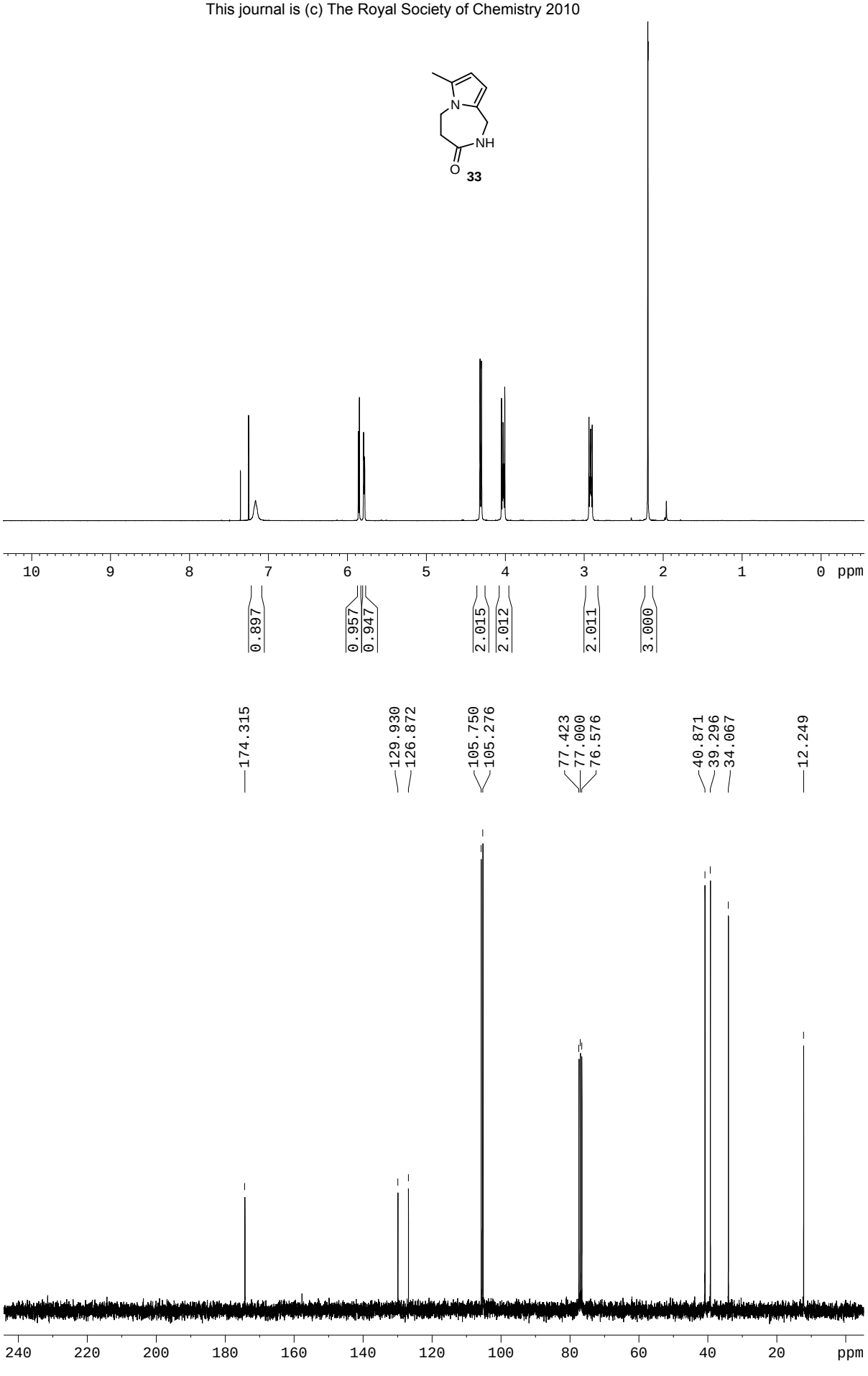

169.790
168.591
152.359
149.598
134.480
132.478
123.784
108.898
106.736
77.974
77.550
77.126
37.083
35.121
34.771
13.960
200
180
160
140
120
100
80
60
40
20
ppm

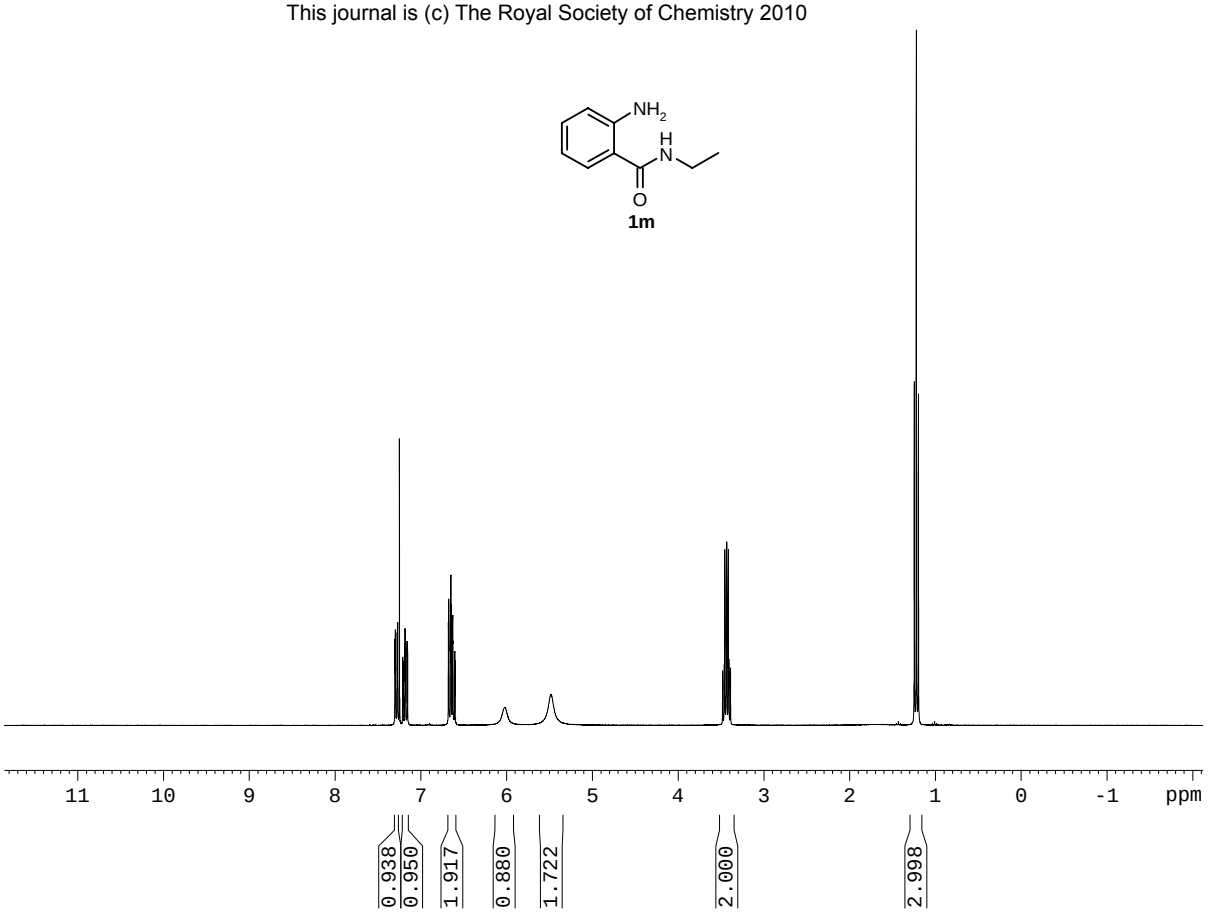


32

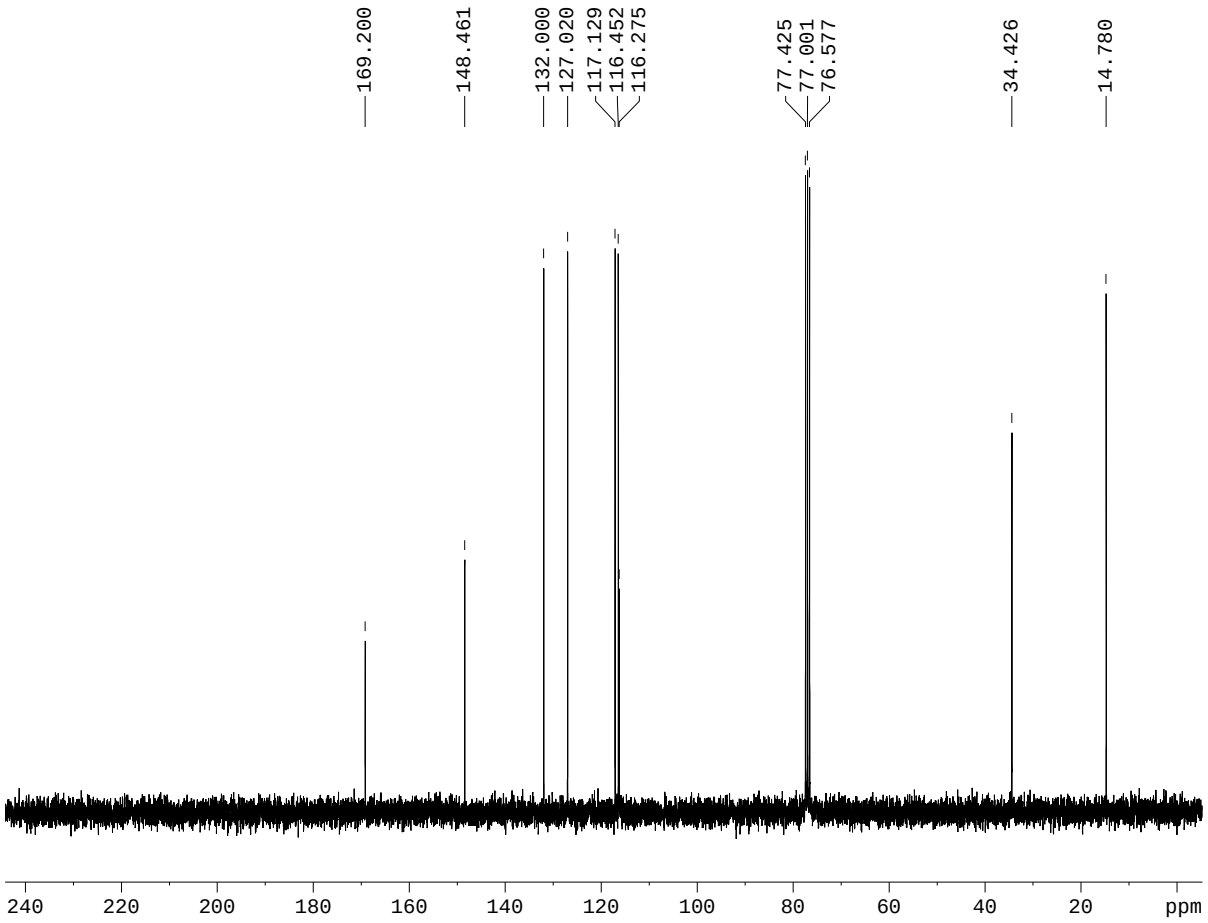
10
9
8
7
6
5
4
3
2
1
0
ppm
1.805
0.978
0.858
2.000
2.040
2.012
3.061
9.184

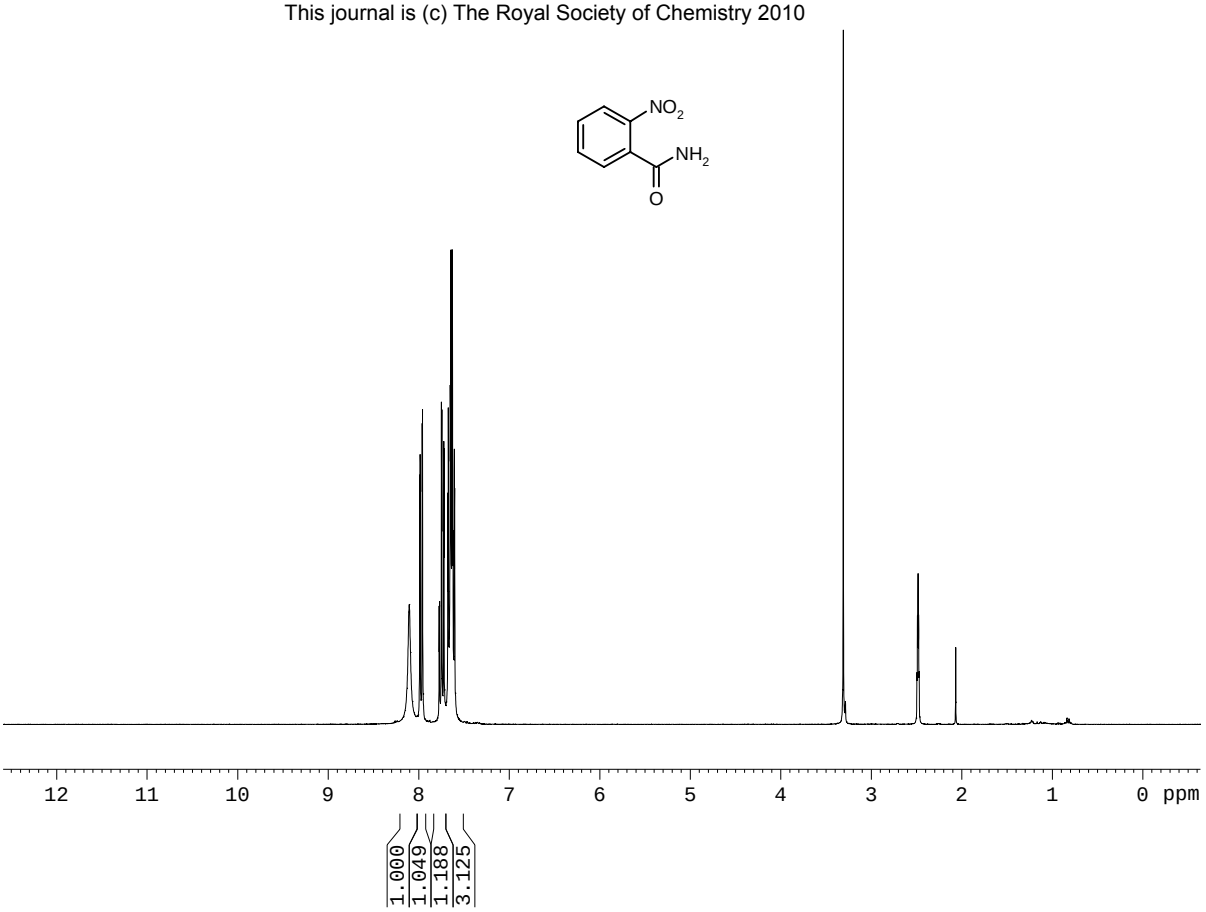

171.104
156.043
151.876
149.071
108.262
106.186
79.214
77.422
77.203
76.999
76.575
36.491
36.029
28.292
13.457
200
180
160
140
120
100
80
60
40
20
ppm

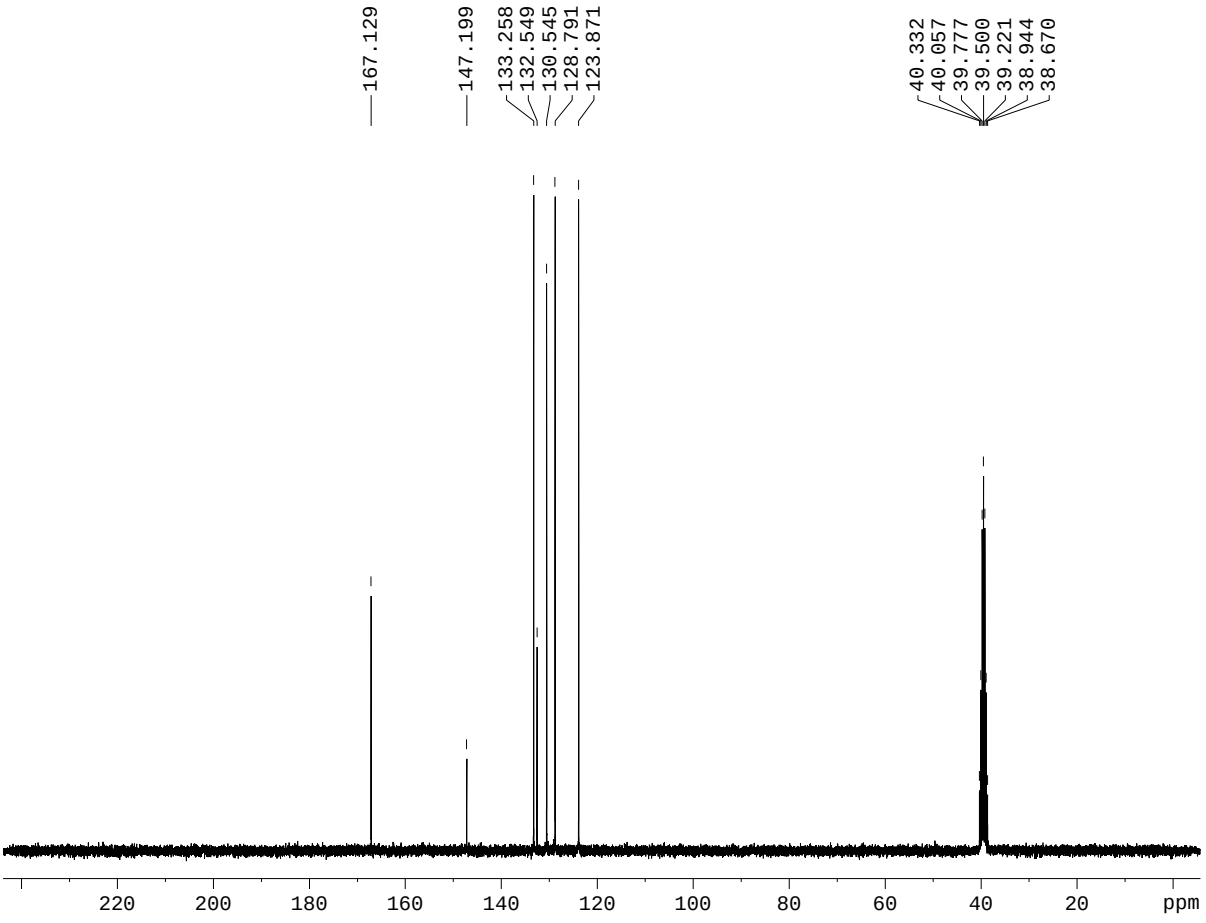

N
NH
O
33
10 9 8 7 6 5 4 3 2 1 0 ppm
0.897
0.957
0.947
2.015
2.012
2.011
3.000
174.315
129.930
126.872
105.750
105.276
77.423
77.000
76.576
40.871
39.296
34.067
12.249
240 220 200 180 160 140 120 100 80 60 40 20 ppm


NH2
H
N
O
11
10
9
8
7
6
5
4
3
2
1
0
-1
ppm
0.938
0.950
1.917
0.880
1.722
2.000
2.998

1m

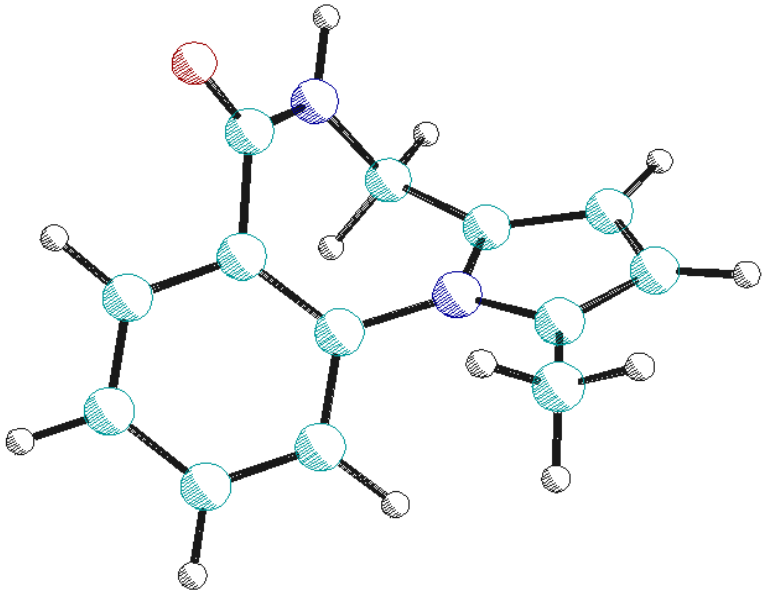

169.200
148.461
132.000
127.020
117.129
116.452
116.275
77.425
77.001
76.577
34.426
14.780
240
220
200
180
160
140
120
100
80
60
40
20
ppm


NO2
NH2
O
12
11
10
9
8
7
6
5
4
3
2
1
0 ppm
1.000
1.049
1.188
3.125


167.129
147.199
133.258
132.549
130.545
128.791
123.871
40.332
40.057
39.777
39.500
39.221
38.944
38.670
220
200
180
160
140
120
100
80
60
40
20
ppm

Results of *ab initio* calculations at MP2/6-311G** level

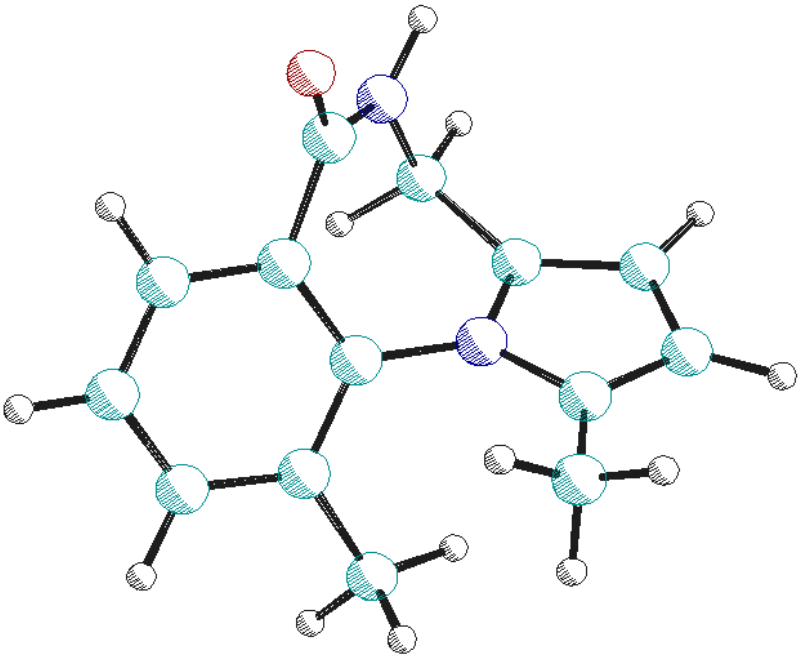
1-Methyl-4,5-dihydro-6*H*-pyrrolo[1,2-*a*][1,4]benzodiazepin-6-one (13a)



HF=-683.1872066|MP2=-685.5318556|RMSD=7.712e-009|RMSF=3.327e-00

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.452805	-0.524003	0.285716
2	6	0	1.285311	0.560251	-0.063583
3	6	0	2.673228	0.423403	0.100401
4	6	0	3.226953	-0.738150	0.637943
5	6	0	2.391059	-1.796737	1.012436
6	6	0	1.010913	-1.684644	0.844087
7	7	0	-0.949659	-0.466711	0.089599
8	6	0	-1.726645	0.611361	0.479156
9	6	0	-1.756339	-1.455758	-0.456982
10	6	0	-3.062837	-0.986831	-0.394129
11	6	0	-3.047058	0.308180	0.187858
12	6	0	-1.043260	1.834550	0.977500
13	6	0	-1.223073	-2.714565	-1.065815
14	7	0	-0.243882	2.458400	-0.075183
15	6	0	0.823564	1.859005	-0.679118
16	8	0	1.430855	2.360931	-1.615780
17	1	0	3.304100	1.250276	-0.211082
18	1	0	4.302772	-0.819620	0.761655
19	1	0	2.808012	-2.699924	1.448631
20	1	0	0.349151	-2.486323	1.153805
21	1	0	-3.926814	-1.524046	-0.762706
22	1	0	-3.893602	0.956583	0.371243
23	1	0	-0.390670	1.612379	1.831037
24	1	0	-1.787794	2.561680	1.309483
25	1	0	-1.966043	-3.104383	-1.766583
26	1	0	-0.297492	-2.528099	-1.619734
27	1	0	-1.019984	-3.497575	-0.327518
28	1	0	-0.601426	3.273412	-0.555724

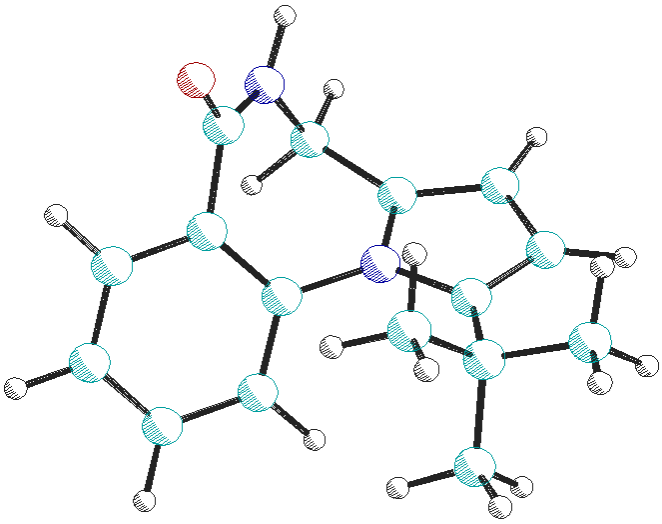
1,10-Dimethyl-4,5-dihydro-6*H*-pyrrolo[1,2-*a*][1,4]benzodiazepin-6-one (13e)



HF=-722.2258602|MP2=-724.7304019|RMSD=8.136e-009|RMSF=1.055e-006

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.444379	-0.430233	-0.097217
2	6	0	-1.303519	0.648056	0.205517
3	6	0	-2.684696	0.426462	0.273877
4	6	0	-3.210629	-0.832470	-0.019401
5	6	0	-2.355629	-1.870393	-0.397324
6	6	0	-0.965551	-1.689502	-0.460255
7	7	0	0.960220	-0.223685	-0.065896
8	6	0	1.587658	0.768781	-0.798642
9	6	0	1.895169	-0.928891	0.677049
10	6	0	3.138838	-0.383525	0.374546
11	6	0	2.948743	0.685698	-0.538967
12	6	0	0.725198	1.801272	-1.435059
13	6	0	1.520856	-1.989234	1.663233
14	7	0	0.026360	2.590843	-0.417245
15	6	0	-0.835292	2.050671	0.501327
16	8	0	-1.280419	2.682858	1.449616
17	6	0	-0.093742	-2.808031	-0.976135
18	1	0	0.431249	3.473346	-0.130705
19	1	0	-3.326895	1.256411	0.552277
20	1	0	-4.282646	-1.000929	0.029767
21	1	0	-2.767671	-2.838692	-0.673524
22	1	0	4.075836	-0.712353	0.804712
23	1	0	3.706652	1.337377	-0.953601
24	1	0	1.333813	2.485282	-2.030828
25	1	0	-0.021388	1.351796	-2.100384
26	1	0	2.238465	-1.976520	2.488089
27	1	0	1.528575	-2.994530	1.230928
28	1	0	0.524858	-1.805086	2.078652
29	1	0	-0.557229	-3.241958	-1.867398
30	1	0	0.011506	-3.607380	-0.236263
31	1	0	0.904020	-2.451695	-1.241973

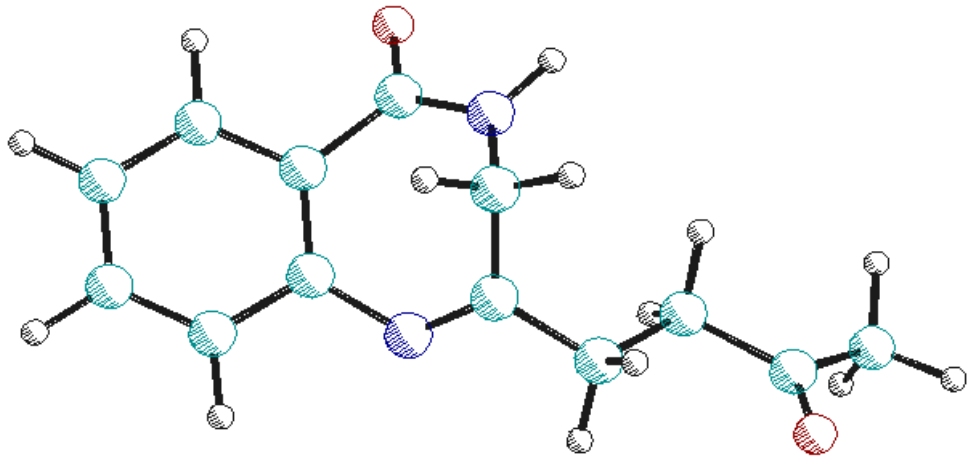
1-*tert*-Butyl-4,5-dihydro-6*H*-pyrrolo[1,2-*a*][1,4]benzodiazepin-6-one (13h)



HF=-800.3011282|MP2=-803.1199492|RMSD=9.022e-009|RMSF=2.740e-006

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.611860	0.484938	-0.488974
2	6	0	1.807947	0.339220	0.238706
3	6	0	2.700804	1.419360	0.298840
4	6	0	2.451168	2.593447	-0.414017
5	6	0	1.302073	2.695062	-1.208773
6	6	0	0.394293	1.635431	-1.258485
7	7	0	-0.351111	-0.559456	-0.489899
8	6	0	-0.006502	-1.828098	-0.926857
9	6	0	-1.718975	-0.496285	-0.221374
10	6	0	-2.226153	-1.759107	-0.540384
11	6	0	-1.162083	-2.590452	-0.970132
12	6	0	1.442213	-2.154148	-1.041769
13	6	0	-2.426626	0.635657	0.501107
14	7	0	2.101672	-2.065145	0.264290
15	6	0	2.180150	-0.909060	0.994201
16	8	0	2.597684	-0.864603	2.143224
17	6	0	-3.702742	0.054945	1.136094
18	6	0	-1.551963	1.191446	1.638517
19	6	0	-2.867978	1.783380	-0.426109
20	1	0	2.222367	-2.911221	0.806700
21	1	0	3.595550	1.311193	0.904983
22	1	0	3.154028	3.419756	-0.361634
23	1	0	1.123307	3.585894	-1.804322
24	1	0	-0.483050	1.677071	-1.893963
25	1	0	-3.254423	-2.064319	-0.411608
26	1	0	-1.218346	-3.632659	-1.256010
27	1	0	1.959356	-1.484810	-1.739430
28	1	0	1.563181	-3.175426	-1.410220
29	1	0	-3.464661	-0.777242	1.805043
30	1	0	-4.204480	0.837964	1.714753
31	1	0	-4.401832	-0.297957	0.371314
32	1	0	-1.224893	0.384700	2.303503
33	1	0	-0.664562	1.707156	1.263221
34	1	0	-2.135184	1.910333	2.226163
35	1	0	-3.399097	1.389689	-1.299293
36	1	0	-3.545987	2.452511	0.117359
37	1	0	-2.021585	2.381973	-0.766636

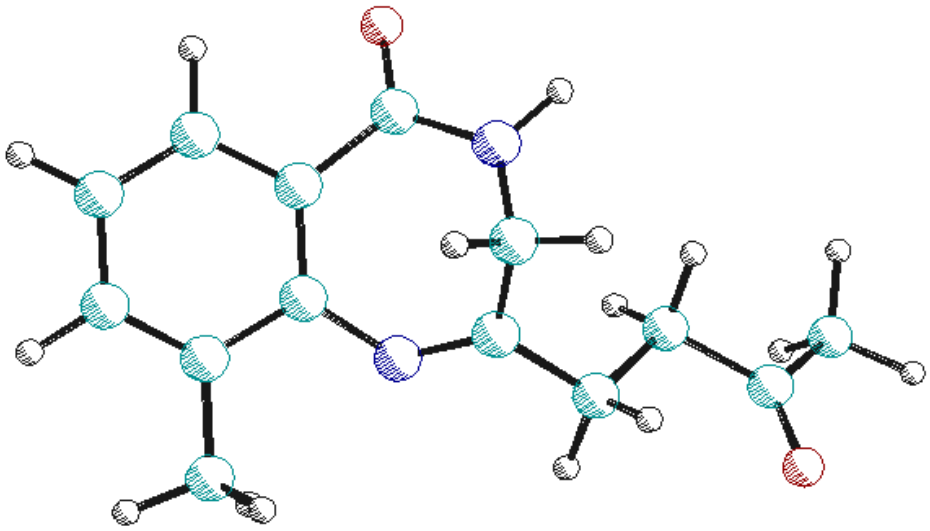
2-(3-Oxobutyl)-3,4-dihydro-5*H*-1,4-benzodiazepin-5-one (15a)



HF=-759.245452|MP2=-761.7880905|RMSD= 5.687e-009|RMSF=6.396e-006

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.892732	-1.669812	0.078787
2	6	0	-1.979561	-2.562854	0.149772
3	6	0	-1.784562	-3.939956	0.194201
4	6	0	-0.480775	-4.453393	0.243128
5	6	0	0.605741	-3.583080	0.223889
6	6	0	0.423890	-2.191719	0.116168
7	7	0	-1.247294	-0.301984	0.103075
8	6	0	-0.603800	0.543881	-0.625139
9	6	0	0.559756	0.125296	-1.499429
10	7	0	1.672783	-0.246815	-0.643975
11	6	0	1.691608	-1.383875	0.120897
12	8	0	2.691286	-1.741812	0.729179
13	6	0	-0.957166	1.998729	-0.538809
14	6	0	0.120281	2.772754	0.226242
15	6	0	-0.162713	4.269090	0.277183
16	8	0	-1.005547	4.784040	-0.433801
17	6	0	0.663575	5.065155	1.266565
18	1	0	2.553487	0.245575	-0.706046
19	1	0	-2.976479	-2.131798	0.165936
20	1	0	-2.640780	-4.607736	0.226587
21	1	0	-0.315882	-5.524995	0.307380
22	1	0	1.622543	-3.955789	0.297560
23	1	0	0.261229	-0.718679	-2.136060
24	1	0	0.882079	0.946908	-2.143486
25	1	0	-1.062247	2.431484	-1.540434
26	1	0	-1.915832	2.094925	-0.023306
27	1	0	1.108886	2.647599	-0.238313
28	1	0	0.217578	2.383645	1.247478
29	1	0	0.550054	6.131896	1.070812
30	1	0	1.717494	4.776430	1.214341
31	1	0	0.312295	4.843004	2.280099

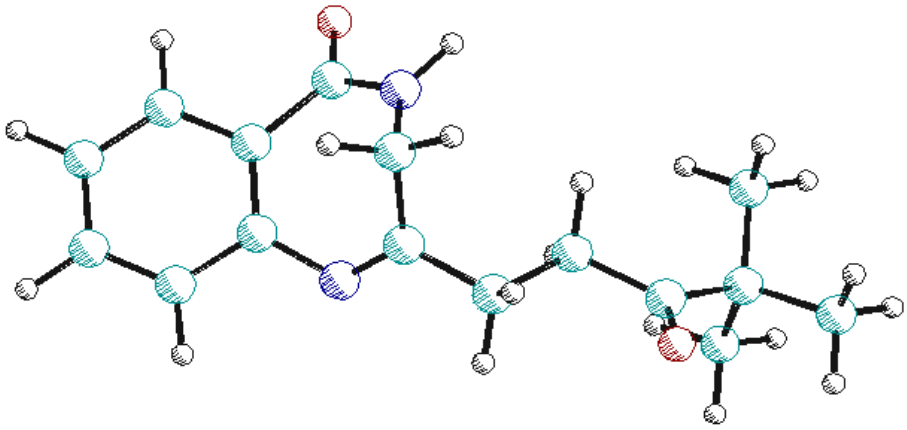
9-Methyl-2-(3-oxobutyl)-3,4-dihydro-5*H*-1,4-benzodiazepin-5-one (15e)



HF=-798.2900149|MP2=-800.9897074|RMSD=5.540e-009|RMSF=4.064e-006

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.611357	-0.540491	-0.100910
2	6	0	-2.602862	-1.546656	-0.219807
3	6	0	-3.947783	-1.176431	-0.287165
4	6	0	-4.324745	0.172341	-0.303575
5	6	0	-3.351388	1.163373	-0.224445
6	6	0	-1.992617	0.824306	-0.096323
7	7	0	-0.279786	-1.007646	-0.145035
8	6	0	0.614257	-0.494478	0.628550
9	6	0	0.285066	0.638996	1.576912
10	7	0	0.038535	1.832820	0.788173
11	6	0	-1.054089	1.995825	-0.024166
12	8	0	-1.277849	3.050301	-0.604073
13	6	0	2.036766	-0.954548	0.510622
14	6	0	2.897380	0.110335	-0.175647
15	6	0	4.363443	-0.295144	-0.264601
16	8	0	4.804670	-1.236943	0.367417
17	6	0	5.226043	0.540837	-1.187809
18	1	0	0.624177	2.649839	0.894640
19	6	0	-2.190444	-2.994888	-0.247881
20	1	0	-4.705021	-1.953678	-0.360519
21	1	0	-5.373438	0.444314	-0.384075
22	1	0	-3.612589	2.216000	-0.264085
23	1	0	1.116735	0.841199	2.256170
24	1	0	-0.599749	0.380858	2.174181
25	1	0	2.058061	-1.877330	-0.074485
26	1	0	2.456953	-1.167807	1.500374
27	1	0	2.514099	0.321222	-1.181861
28	1	0	2.859468	1.065840	0.366659
29	1	0	6.279140	0.316341	-1.015424
30	1	0	4.969047	0.301595	-2.225441
31	1	0	5.033055	1.607515	-1.040101
32	1	0	-3.051550	-3.634569	-0.458775
33	1	0	-1.758120	-3.300019	0.710722
34	1	0	-1.422104	-3.154655	-1.009215

2-(4,4-Dimethyl-3-oxopentyl)-3,4-dihydro-5*H*-1,4-benzodiazepin-5-one (15h)

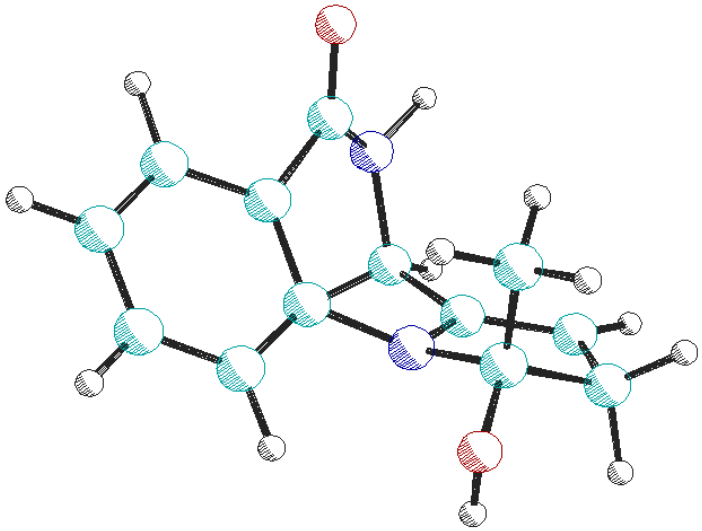


HF=-876.3734914|MP2=-879.3810528|RMSD=4.874e-009|RMSF=8.162e-006

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.622891	-0.849894	0.186859
2	6	0	3.570104	-1.851615	0.474935
3	6	0	4.916218	-1.546752	0.652566
4	6	0	5.333682	-0.208695	0.617470
5	6	0	4.402736	0.799662	0.383048
6	6	0	3.049356	0.500341	0.139683
7	7	0	1.287587	-1.303738	0.096284
8	6	0	0.496223	-0.804245	-0.789424
9	6	0	0.941878	0.292754	-1.733745
10	7	0	1.135187	1.512445	-0.969332
11	6	0	2.164868	1.695198	-0.083757
12	8	0	2.378110	2.774433	0.452367
13	6	0	-0.934910	-1.249371	-0.825035
14	6	0	-1.847734	-0.150157	-0.270123
15	6	0	-3.322391	-0.535878	-0.354994
16	8	0	-3.683957	-1.435670	-1.094349
17	6	0	-4.312830	0.229979	0.526055
18	1	0	0.593542	2.339943	-1.178845
19	6	0	-5.737680	-0.034064	0.037828
20	6	0	-4.017059	1.735681	0.496858
21	6	0	-4.154696	-0.301730	1.962104
22	1	0	3.206422	-2.872381	0.550484
23	1	0	5.629944	-2.340995	0.852248
24	1	0	6.376756	0.044414	0.783564
25	1	0	4.696579	1.844598	0.387625
26	1	0	1.874274	-0.002632	-2.233751
27	1	0	0.184901	0.483597	-2.498166
28	1	0	-1.244154	-1.485767	-1.849456
29	1	0	-1.035563	-2.153682	-0.219328
30	1	0	-1.727054	0.783446	-0.837150
31	1	0	-1.567961	0.084753	0.762576
32	1	0	-5.868750	0.320395	-0.989234
33	1	0	-5.961922	-1.102903	0.052933
34	1	0	-6.451902	0.489296	0.682327
35	1	0	-4.081172	2.130905	-0.523334
36	1	0	-4.757087	2.263240	1.108290
37	1	0	-3.026460	1.968178	0.898975
38	1	0	-4.353047	-1.377976	2.000143
39	1	0	-3.150900	-0.117825	2.357921
40	1	0	-4.873028	0.203054	2.617406

1-Hydroxy-1-methyl-1,2,4,5-tetrahydro-6*H*-pyrrolo[1,2-*a*][1,4]benzodiazepin-6-one (16a)

Isomer 1

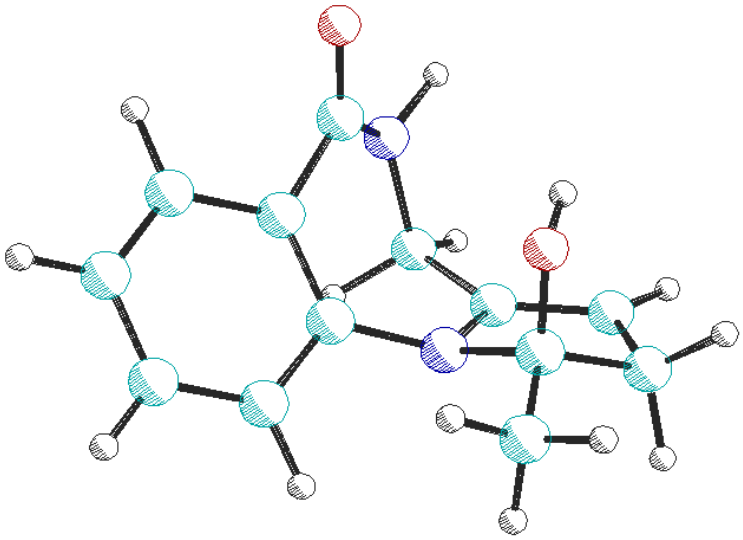


HF=-759.2281885|MP2=-761.7891554|RMSD=5.500e-009|RMSF=1.060e-005

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.553172	-0.573986	-0.386599
2	6	0	-1.473078	0.412174	0.045511
3	6	0	-2.828299	0.068247	0.193340
4	6	0	-3.285571	-1.218973	-0.081025
5	6	0	-2.375276	-2.196073	-0.499799
6	6	0	-1.029209	-1.871257	-0.658700
7	7	0	0.842310	-0.360529	-0.526360
8	6	0	1.374712	0.903562	-0.817630
9	6	0	1.781943	-1.034999	0.421392
10	6	0	3.110206	-0.282898	0.156428
11	6	0	2.667278	1.021687	-0.444348
12	6	0	0.469307	1.918613	-1.432742
13	6	0	1.300591	-0.869642	1.852420
14	7	0	-0.358251	2.546785	-0.408140
15	6	0	-1.138169	1.821719	0.457735
16	8	0	-1.617413	2.312769	1.470747
17	1	0	-0.024403	3.415451	-0.009123
18	8	0	1.872114	-2.417582	0.179137
19	1	0	2.196940	-2.505881	-0.723857
20	1	0	-3.508671	0.834786	0.551832
21	1	0	-4.337924	-1.459583	0.037591
22	1	0	-2.712207	-3.205675	-0.717918
23	1	0	-0.316461	-2.619347	-0.983781
24	1	0	3.715890	-0.863954	-0.556729
25	1	0	3.690454	-0.189569	1.079896
26	1	0	3.303063	1.869202	-0.666993
27	1	0	-0.173917	1.454637	-2.188358
28	1	0	1.054963	2.702780	-1.917779
29	1	0	1.220525	0.195454	2.091464
30	1	0	2.015499	-1.342150	2.531639
31	1	0	0.322656	-1.340485	1.978640

1-Hydroxy-1-methyl-1,2,4,5-tetrahydro-6*H*-pyrrolo[1,2-*a*][1,4]benzodiazepin-6-one (16a)

Isomer 2

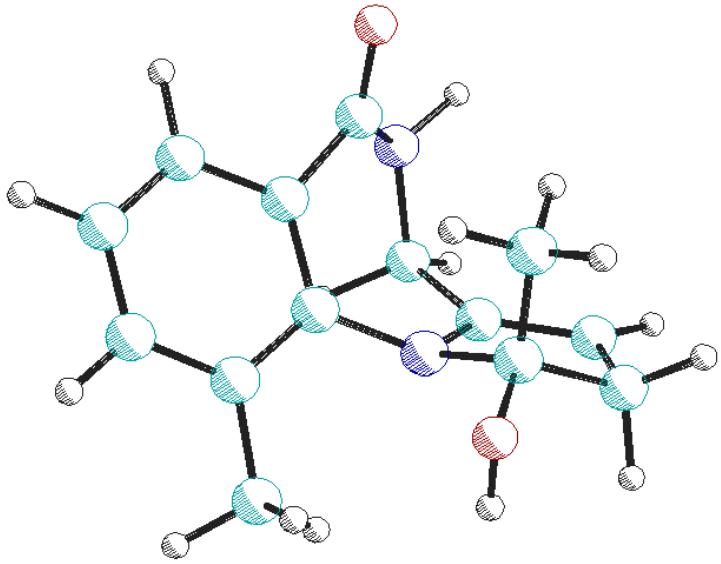


HF=-759.2260966|MP2=-761.7883427|RMSD=5.817e-009|RMSF=2.657e-005

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.577826	-0.588065	-0.416712
2	6	0	-1.445747	0.399243	0.101330
3	6	0	-2.806701	0.097984	0.274852
4	6	0	-3.321854	-1.146150	-0.086724
5	6	0	-2.469365	-2.116247	-0.626703
6	6	0	-1.115608	-1.828973	-0.801503
7	7	0	0.824338	-0.415437	-0.568677
8	6	0	1.371572	0.833932	-0.915614
9	6	0	1.735407	-0.987323	0.465378
10	6	0	3.090242	-0.391548	0.028943
11	6	0	2.681414	0.920828	-0.590402
12	6	0	0.450713	1.876198	-1.458353
13	6	0	1.708401	-2.498182	0.542464
14	7	0	-0.284880	2.497130	-0.358591
15	6	0	-1.027998	1.774424	0.544396
16	8	0	-1.411011	2.250918	1.603867
17	1	0	0.097420	3.349755	0.031955
18	8	0	1.365218	-0.525283	1.750497
19	1	0	1.456142	0.435704	1.731601
20	1	0	-3.446613	0.861087	0.707845
21	1	0	-4.377823	-1.358261	0.052504
22	1	0	-2.859064	-3.083700	-0.930699
23	1	0	-0.446727	-2.560180	-1.243929
24	1	0	3.569740	-1.048075	-0.710364
25	1	0	3.748096	-0.305609	0.899068
26	1	0	3.331835	1.752519	-0.828200
27	1	0	-0.256390	1.441127	-2.172479
28	1	0	1.015905	2.659008	-1.968915
29	1	0	1.908249	-2.934142	-0.438456
30	1	0	0.737022	-2.837847	0.909123
31	1	0	2.476443	-2.825050	1.248795

1-Hydroxy-1,10-dimethyl-1,2,4,5-tetrahydro-6*H*-pyrrolo[1,2-*a*][1,4]benzodiazepin-6-one

(16e) Isomer 1

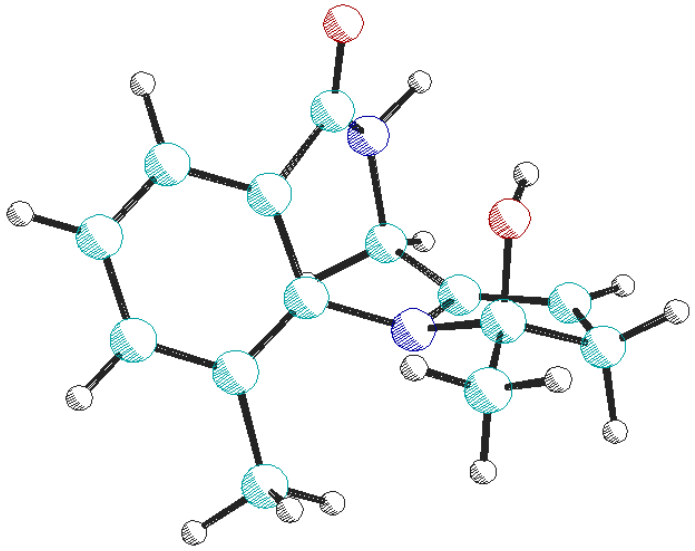


HF=-798.2658657|MP2=-800.9876061|RMSD=5.897e-009|RMSF=3.837e-005

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.577849	-0.046926	0.539435
2	6	0	-1.399506	-0.070645	-0.614437
3	6	0	-2.752013	0.287259	-0.522929
4	6	0	-3.310642	0.626157	0.708340
5	6	0	-2.515548	0.588945	1.855166
6	6	0	-1.155415	0.251998	1.796375
7	7	0	0.823928	-0.297417	0.485306
8	6	0	1.347191	-1.272524	-0.384369
9	6	0	1.768943	0.869197	0.410147
10	6	0	3.102431	0.158349	0.084690
11	6	0	2.655329	-1.071258	-0.656516
12	6	0	0.401035	-2.264034	-0.975938
13	6	0	1.344591	1.832884	-0.685558
14	7	0	-0.290866	-1.651106	-2.110746
15	6	0	-0.938726	-0.441616	-1.998386
16	8	0	-1.225192	0.239808	-2.973042
17	6	0	-0.370827	0.171215	3.081705
18	1	0	0.139781	-1.774339	-3.019863
19	8	0	1.801967	1.608826	1.599574
20	1	0	-3.344937	0.296179	-1.432518
21	1	0	-4.360210	0.897614	0.777599
22	1	0	-2.953870	0.815551	2.824717
23	1	0	3.766297	0.820193	-0.479871
24	1	0	3.609218	-0.103971	1.027965
25	1	0	3.283356	-1.738940	-1.232334
26	1	0	0.941451	-3.138805	-1.344674
27	1	0	-0.334708	-2.599097	-0.237499
28	1	0	1.315343	1.319397	-1.650395
29	1	0	0.354447	2.239711	-0.465972
30	1	0	2.064462	2.654680	-0.734721
31	1	0	-1.022569	-0.177952	3.888141
32	1	0	0.462564	-0.527373	2.974322
33	1	0	0.028756	1.149086	3.361662
34	1	0	2.111038	1.004649	2.282899

1-Hydroxy-1,10-dimethyl-1,2,4,5-tetrahydro-6*H*-pyrrolo[1,2-*a*][1,4]benzodiazepin-6-one

(16e) Isomer 2

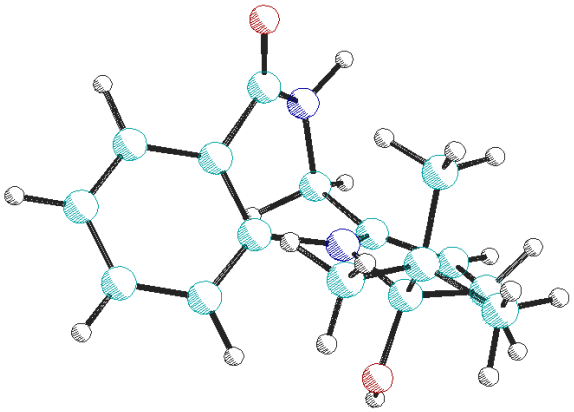


HF=-798.2644693|MP2=-800.9869335|RMSD=4.512e-009|RMSF=1.921e-005

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.581767	-0.553400	0.022077
2	6	0	-1.355784	0.571356	-0.347676
3	6	0	-2.741822	0.569433	-0.142156
4	6	0	-3.374364	-0.560790	0.375374
5	6	0	-2.619733	-1.698813	0.667059
6	6	0	-1.228338	-1.721356	0.488122
7	7	0	0.841813	-0.553990	-0.051398
8	6	0	1.501047	0.020739	-1.158012
9	6	0	1.616388	-0.096484	1.143654
10	6	0	3.044385	-0.055182	0.562134
11	6	0	2.786218	0.332362	-0.872913
12	6	0	0.679633	0.364133	-2.356668
13	6	0	1.442648	-0.976451	2.359859
14	7	0	-0.022326	1.623033	-2.096741
15	6	0	-0.797566	1.818695	-0.972949
16	8	0	-1.105097	2.936361	-0.583053
17	6	0	-0.476171	-3.005352	0.738947
18	1	0	0.446868	2.470219	-2.395605
19	8	0	1.189196	1.192207	1.540558
20	1	0	-3.303572	1.463093	-0.397066
21	1	0	-4.449525	-0.562666	0.530886
22	1	0	-3.114021	-2.598914	1.026811
23	1	0	3.651658	0.659634	1.125637
24	1	0	3.509560	-1.048279	0.634507
25	1	0	3.508707	0.725176	-1.576524
26	1	0	1.312595	0.506884	-3.235294
27	1	0	-0.048869	-0.422303	-2.578714
28	1	0	1.756311	-1.998586	2.145909
29	1	0	2.053532	-0.570340	3.170467
30	1	0	0.397079	-0.966778	2.679440
31	1	0	-1.049181	-3.847164	0.337818
32	1	0	0.502392	-2.977799	0.255994
33	1	0	-0.326956	-3.184729	1.808107
34	1	0	1.375569	1.787353	0.803451

1-*tert*-Butyl-1-hydroxy-1,2,4,5-tetrahydro-6*H*-pyrrolo[1,2-*a*][1,4]benzodiazepin-6-one (16h)

Isomer 1

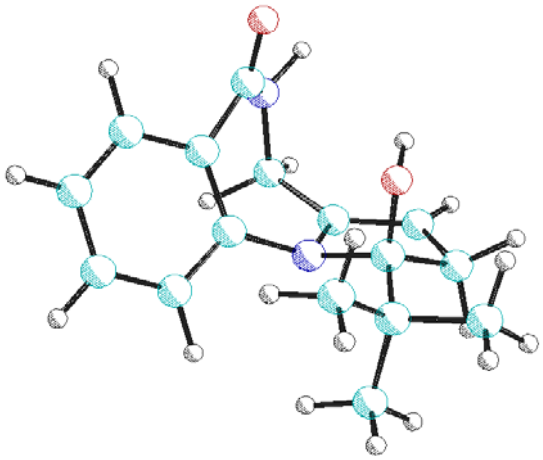


HF=-876.3467025|MP2=-879.3809113|RMSD=9.389e-009|RMSF=6.744e-00

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.867827	0.559461	-0.221126
2	6	0	-1.683802	0.571869	0.933680
3	6	0	-3.077129	0.656214	0.810257
4	6	0	-3.675186	0.770812	-0.445373
5	6	0	-2.868989	0.786325	-1.589287
6	6	0	-1.479114	0.699908	-1.481985
7	7	0	0.530164	0.402013	-0.062538
8	6	0	1.268680	1.322226	0.697922
9	6	0	1.437071	-0.315079	-0.981247
10	6	0	2.838338	0.008572	-0.379496
11	6	0	2.599011	1.192730	0.515571
12	6	0	0.507809	2.180533	1.655659
13	6	0	1.146159	-1.833464	-1.072155
14	7	0	-0.160210	1.348523	2.651382
15	6	0	-1.125472	0.429731	2.321109
16	8	0	-1.551696	-0.399198	3.112899
17	1	0	0.330220	1.147536	3.513851
18	8	0	1.363394	0.208148	-2.306756
19	6	0	1.018249	-2.423238	0.337096
20	6	0	-0.149437	-2.140359	-1.839627
21	6	0	2.304528	-2.507423	-1.824955
22	1	0	1.666537	1.121861	-2.242209
23	1	0	-3.676211	0.624923	1.716006
24	1	0	-4.755814	0.835321	-0.532134
25	1	0	-3.318923	0.884431	-2.573666
26	1	0	-0.856574	0.698288	-2.367478
27	1	0	3.542747	0.177455	-1.201024
28	1	0	3.217762	-0.833493	0.208852
29	1	0	3.358739	1.749541	1.048474
30	1	0	-0.243268	2.785546	1.136091
31	1	0	1.191494	2.857711	2.172523
32	1	0	0.165880	-1.991081	0.870373
33	1	0	1.916542	-2.258120	0.940764
34	1	0	0.862728	-3.505226	0.260257
35	1	0	-1.035961	-1.813577	-1.292816
36	1	0	-0.222189	-3.225899	-1.973490
37	1	0	-0.146866	-1.671379	-2.826674
38	1	0	3.253563	-2.415712	-1.288065
39	1	0	2.420194	-2.070913	-2.820839
40	1	0	2.088805	-3.575466	-1.936104

1-*tert*-Butyl-1-hydroxy-1,2,4,5-tetrahydro-6*H*-pyrrolo[1,2-*a*][1,4]benzodiazepin-6-one (16h)

Isomer 2



HF=-876.3351363|MP2=-879.3738153|RMSD=4.837e-009|RMSF=1.530e-006

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.745472	0.605523	-0.538408
2	6	0	1.879534	0.304963	0.247088
3	6	0	2.830483	1.303406	0.510699
4	6	0	2.713217	2.571255	-0.058948
5	6	0	1.637092	2.846730	-0.910606
6	6	0	0.674200	1.865978	-1.154033
7	7	0	-0.315723	-0.326513	-0.772000
8	6	0	0.040839	-1.661877	-1.072461
9	6	0	-1.460123	-0.440717	0.202957
10	6	0	-2.128572	-1.750852	-0.288144
11	6	0	-0.962444	-2.531221	-0.825625
12	6	0	1.468340	-1.965180	-1.395169
13	6	0	-2.430952	0.759606	0.282998
14	7	0	2.218699	-2.060978	-0.138608
15	6	0	2.186493	-1.055262	0.804396
16	8	0	2.502224	-1.236151	1.971374
17	1	0	2.281635	-2.983445	0.276979
18	8	0	-0.948666	-0.619122	1.511737
19	6	0	-2.893462	1.204187	-1.107757
20	6	0	-3.668154	0.310998	1.083007
21	6	0	-1.811427	1.944156	1.042631
22	1	0	-0.473614	-1.460207	1.510417
23	1	0	3.669586	1.055192	1.154412
24	1	0	3.459934	3.332358	0.148053
25	1	0	1.552745	3.815968	-1.394297
26	1	0	-0.157536	2.070188	-1.818623
27	1	0	-2.869220	-1.543834	-1.070054
28	1	0	-2.637823	-2.232863	0.551344
29	1	0	-0.938452	-3.593410	-1.033205
30	1	0	1.915228	-1.195813	-2.031947
31	1	0	1.549308	-2.926647	-1.907203
32	1	0	-3.411538	0.400253	-1.639721
33	1	0	-2.061666	1.532746	-1.731713
34	1	0	-3.596222	2.038300	-1.000339
35	1	0	-4.249325	-0.444783	0.545478
36	1	0	-4.319567	1.176266	1.247491
37	1	0	-3.373021	-0.090885	2.055805
38	1	0	-0.925104	2.343072	0.549115
39	1	0	-1.532695	1.645049	2.055331
40	1	0	-2.555167	2.746967	1.106295