Supplementary Material (ESI) for Organic & Biomolecular Chemistry

A Nitro Enolate Approach to the Synthesis of 4,5-Disubstituted-2-Aminoimidazoles. Pilot Library Assembly and Screening for Antibiotic and Antibiofilm Activity.

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Supplementary Information

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α-nitro ketones synthesis

2-nitro-6-phenylhexan-3-one: 4-Phenylbutyric acid (0.100 g, 0.61 mmol) and CDI (0.100 g, 0.61 mmol) were added together and then reacted with nitroethane (0.050 g, 0.67 mmol) and DBU (0.185 g, 1.22 mmol) according to the general procedure. Purification by column chromatography gave 0.063 g (47%) as a yellow oil: ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.30 (m, 2H), 7.16 (m, 3H), 5.19 (q, *J* = 6.8 Hz, 1H), 2.64 (m, 4H), 1.98 (m, 2H), 1.69 (d, *J* = 7.6 Hz, 3H) ppm; ^{13}C NMR (100 MHz, $CDCl_3$) δ 199.6, 141.9, 128.8, 128.7, 126.5, 89.0, 38.4, 34.8, 24.8, 15.2 ppm; IR ν_{max} (cm^{-1}) 2922, 2851, 1730, 1559, 1454, 1118; HRMS (FAB) calcd for $C_{12}H_{15}NO_3$ (MNa^+) 244.0944, found 244.0940.

5-nitro-1-phenylheptan-4-one: 4-Phenylbutyric acid (0.100 g, 0.61 mmol) and CDI (0.100 g, 0.61 mmol) were added together and then reacted with nitropropane (0.054 g, 0.60 mmol) and DBU (0.093 g, 0.61 mmol) according to the general procedure. Purification by column chromatography gave 0.038 g (27%) as a yellow oil: ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.30 (m, 2H), 7.16 (m, 3H), 5.02 (dd, *J* = 4.8, 10.0 Hz, 1H), 2.63 (m, 4H), 1.97 (m, 2H), 1.26 (m, 2H), 1.01 (t, *J* = 7.2 Hz, 3H) ppm; ^{13}C NMR (100 MHz, $CDCl_3$) δ 199.6, 141.1, 128.8, 128.7, 126.4, 95.8, 38.8, 34.8, 24.8, 23.5, 10.6 ppm; IR ν_{max} (cm^{-1}) 2918, 2849, 1730, 1559, 1454, 1368, 801, 744, 700; HRMS (FAB) calcd for $C_{13}H_{17}NO_3$ (MNa^+) 258.1101, found 258.1098.

5-nitro-1-phenyloctan-4-one: 4-Phenylbutyric acid (0.100 g, 0.61 mmol) and CDI (0.128 g, 0.79 mmol) were added together and then reacted with nitrobutane (0.069 g, 0.67 mmol) and DBU (0.139 g, 0.91 mmol) according to the general procedure. Purification by column chromatography gave 0.076 g (50%) as a yellow oil: ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.30 (m, 2H), 7.17 (m, 3H), 5.11 (dd, *J* = 4.4, 10.0 Hz, 1H), 2.63 (m, 4H), 1.96 (m, 2H), 1.38 (m, 4H), 0.97 (t, *J* = 6.8 Hz, 3H) ppm; ^{13}C NMR (100 MHz, $CDCl_3$) δ 199.3, 141.1, 128.8, 128.7, 126.4, 94.3, 38.7, 34.8, 31.8, 24.8, 19.4, 13.6 ppm; IR ν_{max} (cm^{-1}) 2917, 2849, 1730, 1551, 1454, 1362, 1030, 746, 700; HRMS

(FAB) calcd for $C_{14}H_{19}NO_3$ (MNa^+) 272.1257, found 272.1251.

5-nitro-1-phenylnonan-4-one: 4-Phenylbutyric acid (0.100 g, 0.61 mmol) and CDI (0.128 g, 0.79 mmol) were added together and then reacted with nitropentane (0.078 g, 0.67 mmol) and DBU (0.185 g, 1.22 mmol) according to the general procedure. Purification by column chromatography gave 0.074 g (46%) as a yellow oil: ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.30 (m, 2H), 7.17 (m, 3H), 5.08 (dd, *J* = 4.4, 10.0 Hz, 1H), 2.63 (m, 4H), 1.96 (m, 2H), 1.33 (m, 6H), 0.91 (t, *J* = 6.8 Hz, 3H) ppm; ^{13}C NMR (100 MHz, $CDCl_3$) δ 199.2, 141.1, 128.8, 128.7, 126.4, 94.5, 38.7, 34.8, 29.6, 28.1, 24.8, 22.2, 13.8 ppm; IR ν_{max} (cm^{-1}) 2918, 2849, 1730, 1559, 1454, 1363, 1020, 743, 699; HRMS (FAB) calcd for $C_{15}H_{21}NO_3$ (MNa^+) 286.1414, found 286.1414.

5-nitro-1-phenyldecan-4-one: 4-Phenylbutyric acid (0.100 g, 0.61 mmol) and CDI (0.128 g, 0.79 mmol) were added together and then reacted with nitrohexane (0.120 g, 0.91 mmol) and DBU (0.232 g, 1.52 mmol) according to the general procedure. Purification by column chromatography gave 0.038 g (23%) as a yellow oil: ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.30 (m, 2H), 7.16 (m, 3H), 5.08 (dd, *J* = 4.2, 9.9 Hz, 1H), 2.64 (m, 4H), 1.96 (m, 2H), 1.32 (m, 8H), 0.89 (t, *J* = 6.6 Hz, 3H) ppm; ^{13}C NMR (100 MHz, $CDCl_3$) δ 199.3, 141.1, 128.8, 128.7, 126.4, 94.5, 38.7, 34.8, 31.2, 29.9, 25.7, 24.8, 22.4, 14.1 ppm; IR ν_{max} (cm^{-1}) 3027, 2928, 2859, 1731, 1559, 1455, 1363, 1030, 746, 700; HRMS (FAB) calcd for $C_{16}H_{23}NO_3$ (MNa^+) 300.1570, found 300.1580.

2-nitro-7-phenylheptan-3-one: 5-Phenylpentanoic acid (0.100 g, 0.56 mmol) and CDI (0.182 g, 1.12 mmol) were added together and then reacted with nitroethane (0.063 g, 0.84 mmol) and DBU (0.214 g, 1.40 mmol) according to the general procedure. Purification by column chromatography gave 0.046 g (35%) as a yellow oil: ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.28 (m, 2H), 7.17(m, 3H), 5.20 (q, *J* = 6.8 Hz, 1H), 2.63 (m, 4H), 1.69 (d, *J* = 6.8 Hz, 3H), 1.66 (m, 4H) ppm; ^{13}C NMR (100 MHz, $CDCl_3$) δ 199.6, 142.0, 128.6, 128.6, 126.1, 89.0, 39.1, 35.9, 30.8, 23.0, 15.2 ppm; IR ν_{max} (cm^{-1}) 3026, 2917, 2849, 1731, 1559, 1453, 1387, 1030, 748, 700; HRMS (FAB)

calcd for $C_{13}H_{17}NO_3$ (MNa^+) 258.1101, found 258.1099.

3-nitro-8-phenyloctan-4-one: 5-Phenylpentanoic acid (0.200 g, 1.12 mmol) and CDI (0.364 g, 2.24 mmol) were added together and then reacted with nitropropane (0.150 g, 1.68 mmol) and DBU (0.427 g, 2.81 mmol) according to the general procedure. Purification by column chromatography gave 0.078 g (28%) as a yellow oil: ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.28 (m, 2H), 7.17 (m, 3H), 5.04 (dd, *J* = 4.8, 10.0 Hz, 1H), 2.62 (m, 4H), 1.65 (m, 6H), 1.02 (t, *J* = 7.2 Hz, 3H) ppm; ^{13}C NMR (100 MHz, $CDCl_3$) δ 199.2, 142.0, 128.6, 128.6, 126.1, 95.8, 38.5, 35.8, 30.8, 23.5, 23.0, 10.6 ppm; IR ν_{max} (cm^{-1}) 2917, 2849, 1730, 1559, 1458, 1369, 1029, 748, 700; HRMS (FAB) calcd for $C_{14}H_{19}NO_3$ (MNa^+) 272.1257, found 272.1256.

6-nitro-1-phenylnonan-5-one: 5-Phenylpentanoic acid (0.150 g, 0.84 mmol) and CDI (0.273 g, 1.68 mmol) were added together and then reacted with nitrobutane (0.130 g, 1.26 mmol) and DBU (0.320 g, 2.10 mmol) according to the general procedure. Purification by column chromatography gave 0.046 g (21%) as a yellow oil: ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.28 (m, 2H), 7.17 (m, 3H), 5.12 (dd, *J* = 4.8, 10.4 Hz, 1H), 2.62 (m, 4H), 1.65 (m, 6H), 1.39 (m, 2H), 0.98 (t, *J* = 7.2 Hz, 3H) ppm; ^{13}C NMR (100 MHz, $CDCl_3$) δ 199.3, 142.0, 128.6, 128.6, 126.1, 94.3, 39.3, 35.8, 31.8, 30.7, 23.0, 19.4, 13.6 ppm; IR ν_{max} (cm^{-1}) 3027, 2918, 2849, 1730, 1559, 1454, 1375, 1030, 749, 700; HRMS (FAB) calcd for $C_{15}H_{21}NO_3$ (MNa^+) 286.1414, found 286.1410.

6-nitro-1-phenyldecan-5-one: 5-Phenylpentanoic acid (0.150 g, 0.84 mmol) and CDI (0.273 g, 1.68 mmol) were added together and then reacted with nitropentane (0.148 g, 1.26 mmol) and DBU (0.320 g, 2.10 mmol) according to the general procedure. Purification by column chromatography gave 0.054 g (23%) as a yellow oil: ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.28 (m, 2H), 7.17 (m, 3H), 5.10 (dd, *J* = 4.8, 10.0 Hz, 1H), 2.62 (m, 4H), 1.65 (m, 6H), 1.35 (m, 4H), 0.92 (t, *J* = 7.2 Hz, 3H) ppm; ^{13}C NMR (100 MHz, $CDCl_3$) δ 199.3, 142.0, 128.6, 128.6, 126.1, 94.5, 39.4, 35.8, 30.7, 29.6, 28.1,

23.0, 22.2, 13.9 ppm; IR ν_{max} (cm^{-1}) 3027, 2930, 2861, 1731, 1559, 1454, 1363, 1030, 748, 700; HRMS (FAB) calcd for $C_{16}H_{23}NO_3$ (MNa^+) 300.1570, found 300.1568.

6-nitro-1-phenylundecan-5-one: 5-Phenylpentanoic acid (0.150 g, 0.84 mmol) and CDI (0.273 g, 1.68 mmol) were added together and then reacted with nitrohexane (0.166 g, 1.26 mmol) and DBU (0.320 g, 2.10 mmol) according to the general procedure. Purification by column chromatography gave 0.060 g (25%) as a yellow oil: ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.30 (m, 2H), 7.17 (m, 3H), 5.10 (dd, *J* = 4.4, 10.0 Hz, 1H), 2.62 (m, 4H), 1.64 (m, 6H), 1.32 (m, 6H), 0.89 (t, *J* = 7.6 Hz, 3H) ppm; ^{13}C NMR (100 MHz, $CDCl_3$) δ 199.3, 142.0, 128.6, 128.6, 126.1, 94.6, 39.4, 35.8, 31.2, 30.8, 29.9, 25.7, 23.0, 22.4, 14.1 ppm; IR ν_{max} (cm^{-1}) 3027, 2930, 2859, 1731, 1559, 1454, 1363, 1030, 748, 700; HRMS (FAB) calcd for $C_{17}H_{25}NO_3$ (MNa^+) 314.1727, found 314.1723.

6-nitro-1-phenyldodecan-5-one: 5-Phenylpentanoic acid (0.150 g, 0.84 mmol) and CDI (0.273 g, 1.68 mmol) were added together and then reacted with nitroheptane (0.183 g, 1.26 mmol) and DBU (0.320 g, 2.10 mmol) according to the general procedure. Purification by column chromatography gave 0.080 g (31%) as a yellow oil: ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.26 (m, 2H), 7.17 (m, 3H), 5.10 (dd, *J* = 4.8, 10.4 Hz, 1H), 2.62 (m, 4H), 1.64 (m, 6H), 1.28 (m, 8H), 0.88 (t, *J* = 7.2 Hz, 3H) ppm; ^{13}C NMR (100 MHz, $CDCl_3$) δ 199.3, 142.0, 128.6, 128.6, 126.1, 94.6, 39.4, 35.8, 31.5, 30.8, 29.9, 28.7, 26.0, 23.0, 22.7, 14.2 ppm; IR ν_{max} (cm^{-1}) 2926, 2857, 1731, 1559, 1454, 1363, 1030, 749, 700; HRMS (FAB) calcd for $C_{18}H_{27}NO_3$ (MNa^+) 328.1883, found 328.1879.

5-nitro-12-phenyldodecan-6-one: 7-Phenylheptanoic acid (0.150 g, 0.73 mmol) and CDI (0.236 g, 1.45 mmol) were added together and then reacted with nitropentane (0.128 g, 1.09 mmol) and DBU (0.277 g, 1.82 mmol) according to the general procedure. Purification by column chromatography gave 0.044 g (20%) as a yellow oil: ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.27 (m, 2H), 7.18 (m, 3H), 5.11 (dd, *J* = 4.4, 10.0

Hz, 1H), 2.60 (m, 4H), 1.61 (m, 6H), 1.33 (m, 8H) 0.92 (t, *J* = 6.8 Hz, 3H) ppm; ^{13}C NMR (100 MHz, $CDCl_3$) δ 199.5, 142.8, 128.6, 128.5, 126.0, 94.5, 39.5, 36.0, 31.4, 29.6, 29.1, 28.9, 28.1, 23.3, 22.2, 13.9 ppm; IR ν_{max} (cm^{-1}) 3026, 2931, 2858, 1732, 1555, 1454, 1364, 1030, 748, 699; HRMS (FAB) calcd for $C_{18}H_{27}NO_3$ (MNa^+) 328.1883, found 328.1879.

8-nitro-1-phenyltridecan-7-one: 7-Phenylheptanoic acid (0.150 g, 0.73 mmol) and CDI (0.236 g, 1.45 mmol) were added together and then reacted with nitrohexane (0.143 g, 1.09 mmol) and DBU (0.277 g, 1.82 mmol) according to the general procedure. Purification by column chromatography gave 0.076 g (32%) as a yellow oil: ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.28 (m, 2H), 7.18 (m, 3H), 5.12 (dd, *J* = 4.8, 10.4 Hz, 1H), 2.60 (m, 4H), 1.61 (m, 6H), 1.33 (m, 10H) 0.90 (t, *J* = 6.4 Hz, 3H) ppm; ^{13}C NMR (100 MHz, $CDCl_3$) δ 199.5, 142.8, 128.6, 128.5, 125.9, 94.6, 39.5, 36.0, 31.4, 31.2, 29.9, 29.1, 28.9, 25.7, 23.3, 22.5, 14.1 ppm; IR ν_{max} (cm^{-1}) 3027, 2931, 2858, 1731, 1554, 1454, 1366, 1099, 747, 699; HRMS (FAB) calcd for $C_{19}H_{29}NO_3$ (MNa^+) 342.2040, found 342.2038.

8-nitro-1-phenyltetradecan-7-one: 7-Phenylheptanoic acid (0.150 g, 0.73 mmol) and CDI (0.236 g, 1.45 mmol) were added together and then reacted with nitroheptane (0.158 g, 1.09 mmol) and DBU (0.277 g, 1.82 mmol) according to the general procedure. Purification by column chromatography gave 0.096 g (40%) as a yellow oil: ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.28 (m, 2H), 7.18 (m, 3H), 5.12 (dd, *J* = 4.4, 10.0 Hz, 1H), 2.60 (m, 4H), 1.62 (m, 6H), 1.34 (m, 12H) 0.90 (t, *J* = 7.2 Hz, 3H) ppm; ^{13}C NMR (100 MHz, $CDCl_3$) δ 199.5, 142.8, 128.6, 128.5, 125.9, 94.6, 39.5, 36.0, 31.5, 31.4, 29.9, 29.1, 28.9, 28.8, 26.0, 23.3, 22.7, 14.2 ppm; IR ν_{max} (cm^{-1}) 3027, 2930, 2858, 1732, 1559, 1454, 1367, 1030, 748, 700; HRMS (FAB) calcd for $C_{20}H_{31}NO_3$ (MNa^+) 356.2196, found 356.2198.

2-aminoimidazole synthesis

5-methyl-4-(3-phenylpropyl)-1H-imidazol-2-amine: 2-Nitro-6-phenylhexan-3-one (0.063 g, 0.28 mmol) reacted with concentrated HCl (1.40 mmol) and palladium, 5 wt. % on activated carbon (0.121 g, 0.057 mmol) under H_2, then reacted with cyanamide (0.060 g, 1.4 mmol) according to the general procedure. Purification by column chromatography gave 0.019 g (31%) over two steps as a yellow oil: ^{1}H NMR (400 MHz, CD_3OD) δ 7.25 (m, 2H), 7.18 (m, 3H), 2.63 (t, *J* = 7.2 Hz, 2H), 2.46 (t, *J* = 7.6 Hz, 2H), 2.00 (s, 3H) 1.88 (m, 2H) ppm; ^{13}C NMR (100 MHz, CD_3OD) δ 146.3, 141.6, 128.2, 128.2, 125.8, 121.6, 117.7, 34.8, 30.3, 22.6, 7.5 ppm; IR ν_{max} (cm^{-1}) 3313, 3169, 2941, 2795, 1680, 1624, 1453, 1181, 1018, 750, 700; HRMS (FAB) calcd for $C_{13}H_{17}N_3$ (MH^+) 216.1495, found 216.1502.

5-ethyl-4-(3-phenylpropyl)-1H-imidazol-2-amine: 5-Nitro-1-phenylheptan-4-one (0.049 g, 0.21 mmol) reacted with concentrated HCl (1.04 mmol) and palladium, 5 wt. % on activated carbon (0.089 g, 0.040 mmol) under H_2, then reacted with cyanamide (0.044 g, 1.04 mmol) according to the general procedure. Purification by column chromatography gave 0.026 g (55%) over two steps as a yellow oil: ^{1}H NMR (400 MHz, CD_3OD) δ 7.23 (m, 2H), 7.18 (m, 3H), 2.62 (t, *J* = 7.2 Hz, 2H), 2.42 (m, 4H), 1.87 (m, 2H), 1.14 (t, *J* = 7.8 Hz, 3H) ppm; ^{13}C NMR (75 MHz, CD_3OD) δ 146.4, 141.6, 128.4, 128.3, 125.8, 123.6, 121.0, 34.9, 30.7, 22.6, 16.6, 13.1 ppm; IR ν_{max} (cm^{-1}) 3340, 3026, 2930, 2850, 1679, 1603, 1453, 1030, 748, 699; HRMS (FAB) calcd for $C_{14}H_{19}N_3$ (MH^+) 230.1652, found 230.1654.

4-(3-phenylpropyl)-5-propyl-1H-imidazol-2-amine: 5-Nitro-1-phenyloctan-4-one (0.076 g, 0.30 mmol) reacted with concentrated HCl (1.52 mmol) and palladium, 5 wt. % on activated carbon (0.130 g, 0.061 mmol) under H_2, then reacted with cyanamide (0.064 g, 1.52 mmol) according to the general procedure. Purification by column chromatography gave 0.030 g (41%) over two steps as a yellow oil: ^{1}H NMR (300

MHz, CD_3OD) δ 7.23 (m, 2H), 7.19 (m, 3H), 2.64 (t, *J* = 7.2 Hz, 2H), 2.46 (t, *J* = 7.5 Hz, 2H), 2.36 (t, *J* = 7.5 Hz, 2H), 1.87 (m, 2H), 1.56 (m, 2H), 0.90 (t, *J* = 7.2 Hz, 3H) ppm; ^{13}C NMR (100 MHz, CD_3OD) δ 146.4, 141.6, 128.4, 128.3, 125.8, 122.0, 121.9, 34.9, 30.7, 25.0, 22.6, 22.2, 12.6 ppm; IR ν_{max} (cm^{-1}) 3157, 2929, 1677, 1453, 1181, 1028, 745, 698; HRMS (FAB) calcd for $C_{15}H_{21}N_3$ (MH^+) 244.1808, found 244.1809.

5-butyl-4-(3-phenylpropyl)-1H-imidazol-2-amine: 5-Nitro-1-phenylnonan-4-one: (0.074 g, 0.28 mmol) reacted with concentrated HCl (1.40 mmol) and palladium, 5 wt. % on activated carbon (0.120 g, 0.056 mmol) under H_2, then reacted with cyanamide (0.059 g, 1.40 mmol) according to the general procedure. Purification by column chromatography gave 0.054 g (75%) over two steps as a yellow oil: ^1H NMR (400 MHz, CD_3OD) δ 7.26 (m, 2H), 7.19 (m, 3H), 2.64 (t, *J* = 7.6 Hz, 2H), 2.46 (t, *J* = 7.2 Hz, 2H), 2.38 (t, *J* = 7.6 Hz, 2H), 1.88 (m, 2H), 1.50 (m, 2H), 1.32 (m, 2H), 0.92 (t, *J* = 7.2 Hz, 3H) ppm; ^{13}C NMR (100 MHz, CD_3OD) δ 146.4, 141.6, 128.4, 128.3, 125.8, 122.2, 121.7, 34.9, 31.1, 30.7, 22.8, 22.6, 21.9, 12.9 ppm; IR ν_{max} (cm^{-1}) 3318, 3169, 2929, 1680, 1453, 1181, 1021, 747, 700; HRMS (FAB) calcd for $C_{16}H_{23}N_3$ (MH^+) 258.1965, found 258.1971.

5-pentyl-4-(3-phenylpropyl)-1H-imidazol-2-amine: 5-Nitro-1-phenyldecan-4-one (0.031 g, 0.11 mmol) reacted with concentrated HCl (0.55 mmol) and palladium, 5 wt. % on activated carbon (0.048 g, 0.022 mmol) under H_2, then reacted with cyanamide (0.024 g, 0.55 mmol) according to the general procedure. Purification by column chromatography gave 0.016 g (53%) over two steps as a yellow oil: ^1H NMR (400 MHz, CD_3OD) δ 7.25 (m, 2H), 7.18 (m, 3H), 2.63 (t, *J* = 7.6 Hz, 2H), 2.45 (t, *J* = 8.0 Hz, 2H), 2.36 (t, *J* = 7.6 Hz, 2H), 1.88 (m, 2H), 1.52 (m, 2H), 1.27 (m, 4H), 0.89 (t, *J* = 7.2 Hz, 3H) ppm; ^{13}C NMR (100 MHz, CD_3OD) δ 146.4, 141.6, 128.7, 128.3, 125.9, 122.2, 121.7, 34.9, 31.0, 30.7, 28.6, 23.1, 22.6, 22.2, 13.2 ppm; IR ν_{max} (cm^{-1}) 3157, 2929, 2858, 1677, 1453, 1030, 748, 700; HRMS (FAB) calcd for $C_{17}H_{25}N_3$ (MH^+) 272.2121, found 272.2125.

5-methyl-4-(4-phenylbutyl)-1H-imidazol-2-amine: 2-Nitro-7-phenylheptan-3-one (0.045 g, 0.19 mmol) reacted with concentrated HCl (0.95 mmol) and palladium, 5 wt. % on activated carbon (0.081 g, 0.040 mmol) under H_2, then reacted with cyanamide (0.040 g, 0.95 mmol) according to the general procedure. Purification by column chromatography gave 0.036 g (82%) over two steps as a yellow oil: ^{1}H NMR (400 MHz, CD_3OD) δ 7.24 (m, 2H), 7.17 (m, 3H), 2.63 (t, *J* = 7.2 Hz, 2H), 2.46 (t, *J* = 7.6 Hz, 2H), 2.04 (s, 3H) 1.58 (m, 4H) ppm; ^{13}C NMR (100 MHz, CD_3OD) δ 146.3, 142.2, 128.2, 128.2, 125.6, 121.8, 117.6, 35.3, 30.7, 28.3, 22.9, 7.5 ppm; IR ν_{max} (cm^{-1}) 3164, 2926, 1680, 1453, 1030, 749; HRMS (FAB) calcd for $C_{14}H_{19}N_3$ (MH^+) 230.1652, found 230.1657.

5-ethyl-4-(4-phenylbutyl)-1H-imidazol-2-amine: 3-Nitro-8-phenyloctan-4-one: (0.078 g, 0.31 mmol) reacted with concentrated HCl (1.55 mmol) and palladium, 5 wt. % on activated carbon (0.133 g, 0.063 mmol) under H_2, then reacted with cyanamide (0.066 g, 1.56 mmol) according to the general procedure. Purification by column chromatography gave 0.051 g (67%) over two steps as a yellow oil: ^{1}H NMR (400 MHz, CD_3OD) δ 7.23 (m, 2H), 7.16 (m, 3H), 2.62 (t, *J* = 7.6 Hz, 2H), 2.45 (m, 4H), 1.58 (m, 4H), 1.13 (t, *J* = 7.6 Hz, 3H) ppm; ^{13}C NMR (100 MHz, CD_3OD) δ 146.4, 142.2, 128.3, 128.2, 125.6, 123.5, 121.2, 35.3, 30.7, 28.6, 22.9, 16.6, 13.2 ppm; IR ν_{max} (cm^{-1}) 3157, 2936, 2790, 1680, 1454, 1202, 1030, 749, 700; HRMS (FAB) calcd for $C_{15}H_{21}N_3$ (MH^+) 244.1808, found 244.1811.

4-(4-phenylbutyl)-5-propyl-1H-imidazol-2-amine: 6-Nitro-1-phenylnonan-5-one (0.046 g, 0.17 mmol) reacted with concentrated HCl (0.85 mmol) and palladium, 5 wt. % on activated carbon (0.074 g, 0.035 mmol) under H_2, then reacted with cyanamide (0.037 g, 0.87 mmol) according to the general procedure. Purification by column chromatography gave 0.032 g (71%) over two steps as a yellow oil: ^{1}H NMR (400 MHz, CD_3OD) δ 7.23 (m, 2H), 7.17 (m, 3H), 2.62 (t, *J* = 7.2 Hz, 2H), 2.44 (t, *J* = 7.6 Hz, 2H), 2.39 (t, *J* = 7.6 Hz, 2H), 1.56 (m, 6H), 0.91 (t, *J* = 7.2 Hz, 3H) ppm; ^{13}C NMR (100 MHz, CD_3OD) δ 146.4, 142.2, 128.2, 128.2, 125.7, 122.1, 121.9, 35.3,

30.7, 28.5, 25.0, 23.0, 22.2, 12.6 ppm; IR ν_{max} (cm^{-1}) 3161, 2934, 2793, 1680, 1454, 1202, 1181, 1020, 749, 700; HRMS (FAB) calcd for $C_{16}H_{23}N_3$ (MH^+) 258.1965, found 258.1977.

5-butyl-4-(4-phenylbutyl)-1H-imidazol-2-amine: 6-Nitro-1-phenyldecan-5-one (0.047 g, 0.17 mmol) reacted with concentrated HCl (0.85 mmol) and palladium, 5 wt. % on activated carbon (0.072 g, 0.034 mmol) under H_2, then reacted with cyanamide (0.036 g, 0.85 mmol) according to the general procedure. Purification by column chromatography gave 0.020 g (43%) over two steps as a yellow oil: ^{1}H NMR (400 MHz, CD_3OD) δ 7.24 (m, 2H), 7.17 (m, 3H), 2.64 (t, *J* = 6.8 Hz, 2H), 2.44 (m, 4H), 1.65 (m, 6H), 1.32 (m, 2H), 0.92 (t, *J* = 7.2 Hz, 3H) ppm; ^{13}C NMR (100 MHz, CD_3OD) δ 146.4, 142.2, 128.3, 128.2, 125.8, 122.2, 121.7, 35.3, 31.2, 30.7, 28.5, 22.9, 22.8, 21.9, 12.9 ppm; IR ν_{max} (cm^{-1}) 3165, 2929, 1680, 1453, 1030; HRMS (FAB) calcd for $C_{17}H_{25}N_3$ (MH^+) 272.2121, found 272.2132.

5-pentyl-4-(4-phenylbutyl)-1H-imidazol-2-amine: 6-Nitro-1-phenylundecan-5-one (0.060 g, 0.21 mmol) reacted with concentrated HCl (1.05 mmol) and palladium, 5 wt. % on activated carbon (0.088 g, 0.040 mmol) under H_2, then reacted with cyanamide (0.043 g, 1.03 mmol) according to the general procedure. Purification by column chromatography gave 0.064 g (97%) over two steps as a yellow oil: ^{1}H NMR (400 MHz, CD_3OD) δ 7.24 (m, 2H), 7.17 (m, 3H), 2.64 (t, *J* = 6.8 Hz, 2H), 2.45 (m, 4H), 1.52 (m, 6H), 1.30 (m, 4H), 0.89 (t, *J* = 7.2 Hz, 3H) ppm; ^{13}C NMR (100 MHz, CD_3OD) δ 146.4, 142.2, 128.2, 128.2, 125.7, 122.1, 121.9, 35.3, 31.1, 30.7, 28.7, 28.5, 23.0, 23.0, 22.2, 13.2 ppm; IR ν_{max} (cm^{-1}) 3159, 2929, 2858, 1680, 1453, 1202, 1181, 1030, 749, 699; HRMS (FAB) calcd for $C_{18}H_{27}N_3$ (MH^+) 286.2278, found 286.2283.

5-hexyl-4-(4-phenylbutyl)-1H-imidazol-2-amine: 6-Nitro-1-phenyldodecan-5-one (0.040 g, 0.13 mmol) reacted with concentrated HCl (0.65 mmol) and palladium, 5 wt. % on activated carbon (0.056 g, 0.026 mmol) under H_2, then reacted with cyanamide (0.028 g, 0.65 mmol) according to the general procedure. Purification by column

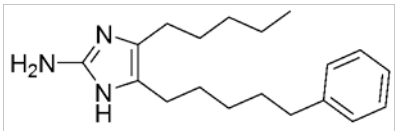
chromatography gave 0.030 g (77%) over two steps as a yellow oil: ^{1}H NMR (400 MHz, CD_3OD) δ 7.24 (m, 2H), 7.16 (m, 3H), 2.63 (t, *J* = 7.2 Hz, 2H), 2.45 (m, 4H), 1.60 (m, 6H), 1.28 (m, 6H), 0.88 (t, *J* = 6.8 Hz, 3H) ppm; ^{13}C NMR (100 MHz, CD_3OD) δ 146.4, 142.2, 128.2, 128.2, 125.7, 122.1, 121.8, 35.3, 31.5, 30.7, 29.0, 28.7, 28.5, 23.1, 23.0, 22.4, 13.3 ppm; IR ν_{max} (cm^{-1}) 3166, 2930, 2857, 1680, 1454, 1202, 1181, 1029, 748, 699; HRMS (FAB) calcd for $C_{19}H_{29}N_3$ (MH^+) 300.2434, found 300.2435.

5-butyl-4-(6-phenylhexyl)-1H-imidazol-2-amine: 5-Nitro-12-phenyldodecan-6-one (0.044 g, 0.14 mmol) reacted with concentrated HCl (0.70 mmol) and palladium, 5 wt. % on activated carbon (0.061 g, 0.029 mmol) under H_2, then reacted with cyanamide (0.030 g, 0.72 mmol) according to the general procedure. Purification by column chromatography gave 0.022 g (51%) over two steps as a yellow oil: ^{1}H NMR (400 MHz, CD_3OD) δ 7.23 (m, 2H), 7.15 (m, 3H), 2.60 (t, *J* = 7.2 Hz, 2H), 2.42 (m, 4H), 1.54 (m, 6H), 1.35 (m, 6H), 0.94 (t, *J* = 7.6 Hz, 3H) ppm; ^{13}C NMR (100 MHz, CD_3OD) δ 146.4, 142.6, 128.2, 128.1, 125.5, 122.1, 122.0, 35.6, 31.3, 31.2, 28.8, 28.7, 28.6, 23.0, 22.8, 21.9, 13.0 ppm; IR ν_{max} (cm^{-1}) 3160, 2928, 2856, 1680, 1453, 1030, 747, 700; HRMS (FAB) calcd for $C_{19}H_{29}N_3$ (MH^+) 300.2434, found 300.2437.

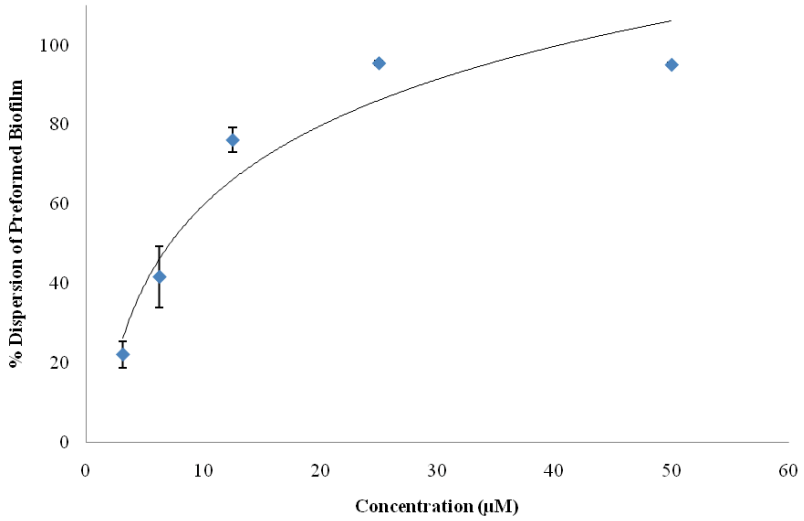
5-pentyl-4-(6-phenylhexyl)-1H-imidazol-2-amine: 8-Nitro-1-phenyltridecan-7-one: (0.076 g, 0.24 mmol) reacted with concentrated HCl (1.20 mmol) and palladium, 5 wt. % on activated carbon (0.101 g, 0.048 mmol) under H_2, then reacted with cyanamide (0.050 g, 1.19 mmol) according to the general procedure. Purification by column chromatography gave 0.031 g (41%) over two steps as a yellow oil: ^{1}H NMR (400 MHz, CD_3OD) δ 7.24 (m, 2H), 7.16 (m, 3H), 2.60 (t, *J* = 7.6 Hz, 2H), 2.42 (m, 4H), 1.55 (m, 6H), 1.35 (m, 8H), 0.91 (t, *J* = 6.8 Hz, 3H) ppm; ^{13}C NMR (100 MHz, CD_3OD) δ 146.4, 142.6, 128.2, 128.1, 125.5, 122.1, 122.0, 35.6, 31.4, 31.1, 28.8, 28.7, 28.7, 28.6, 23.0, 23.0, 22.2, 13.2 ppm; IR ν_{max} (cm^{-1}) 3169, 2928, 1680, 1453, 1202, 1030, 745, 699; HRMS (FAB) calcd for $C_{20}H_{31}N_3$ (MH^+) 314.2591, found 314.2596.

5-hexyl-4-(6-phenylhexyl)-1H-imidazol-2-amine: 8-Nitro-1-phenyltetradecan-7-one (0.096 g, 0.29 mmol) reacted with concentrated HCl (1.45 mmol) and palladium, 5 wt. % on activated carbon (0.123 g, 0.058 mmol) under H_2, then reacted with cyanamide (0.061 g, 1.44 mmol) according to the general procedure. Purification by column chromatography gave 0.019 g (20%) over two steps as a yellow oil: ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.24 (m, 2H), 7.16 (m, 3H), 2.58 (t, *J* = 7.5 Hz, 2H), 2.34 (m, 4H), 1.50 (m, 6H), 1.26 (m, 10H), 0.86 (t, *J* = 6.6 Hz, 3H) ppm; ^{13}C NMR (100 MHz, CD_3OD) δ 146.4, 142.6, 128.2, 128.1, 125.5, 122.1, 122.0, 35.6, 31.5, 31.4, 29.0, 28.8, 28.7, 28.6, 28.6, 23.1, 23.0, 22.5, 13.2 ppm; IR ν_{max} (cm^{-1}) 3158, 2928, 2857, 1680, 1454, 1202, 1029, 748, 699; HRMS (FAB) calcd for $C_{20}H_{31}N_3$ (MH^+) 328.2747, found 328.2753.

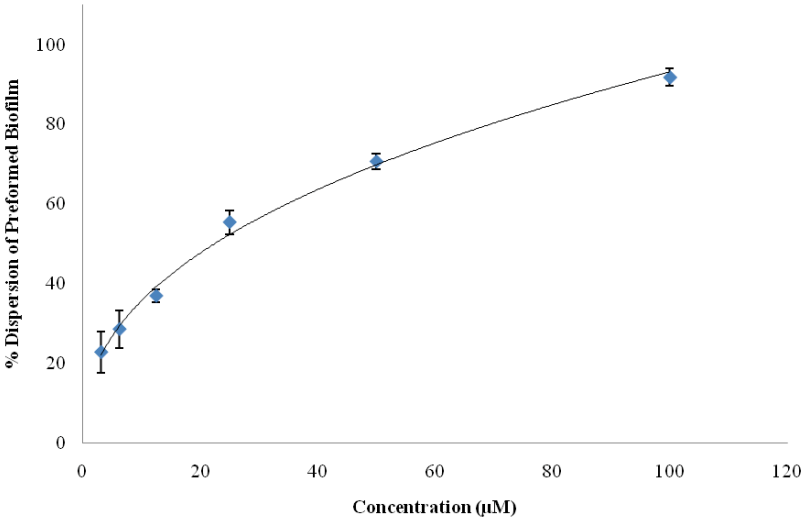
Dispersion Graphs:



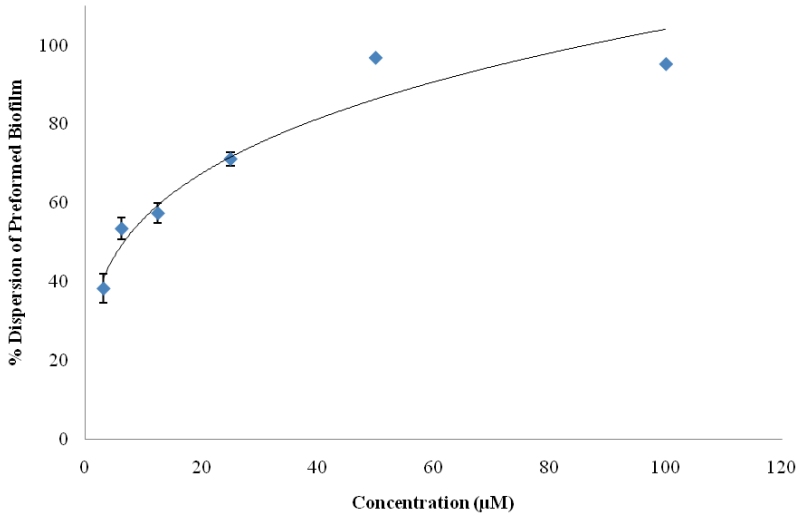
L. anguillarum



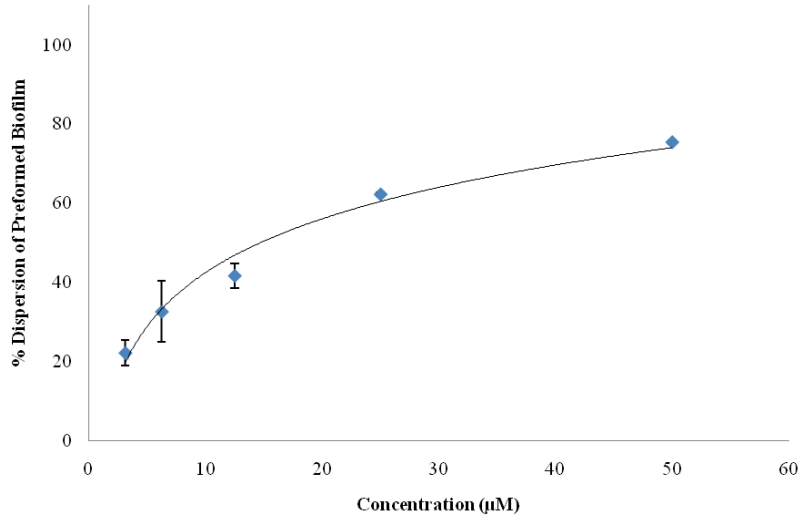
R. salexigens



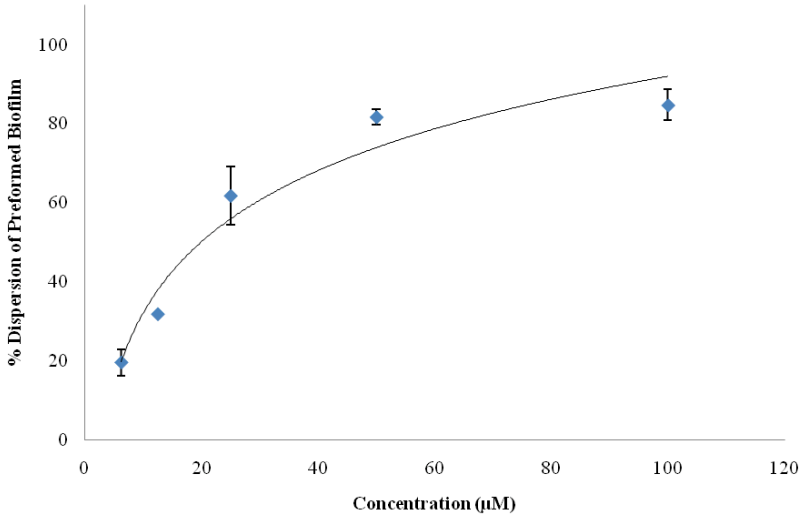
V. cholerae



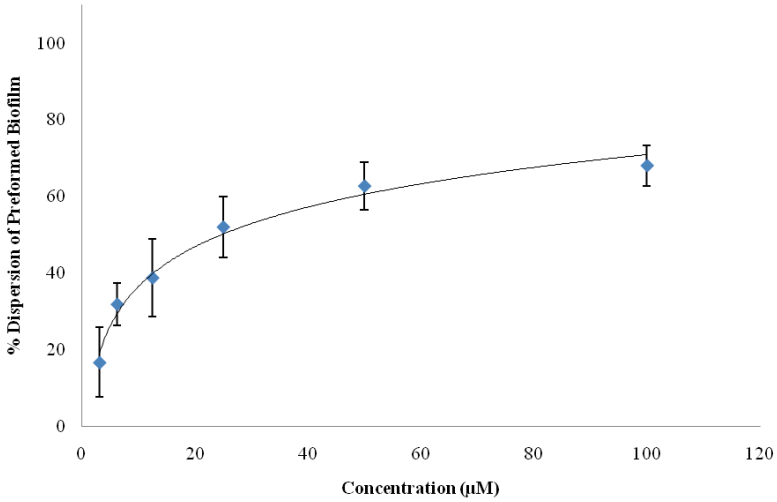
V. vulnificus



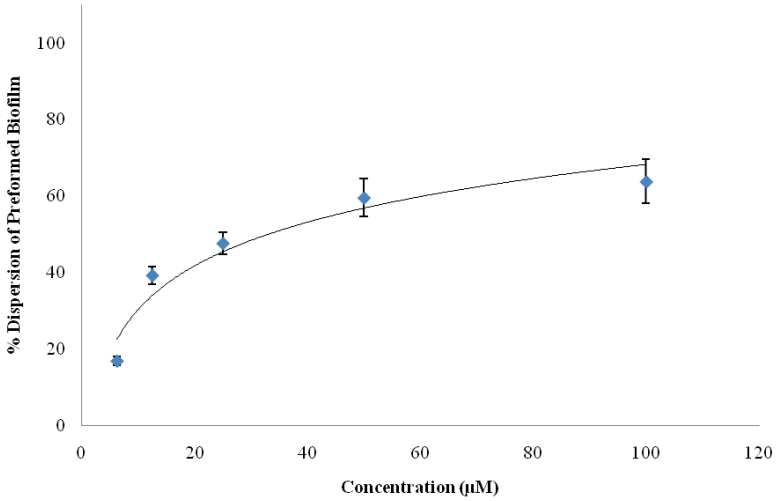
S.aureus (ATCC: 29213)



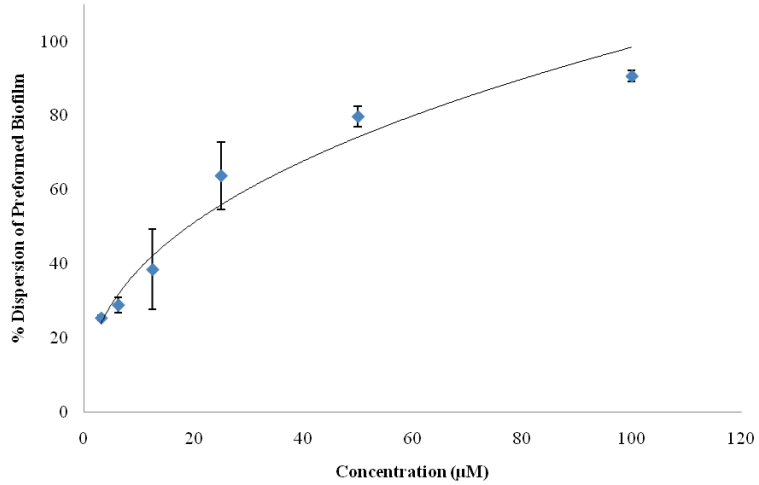
S. epidermidis



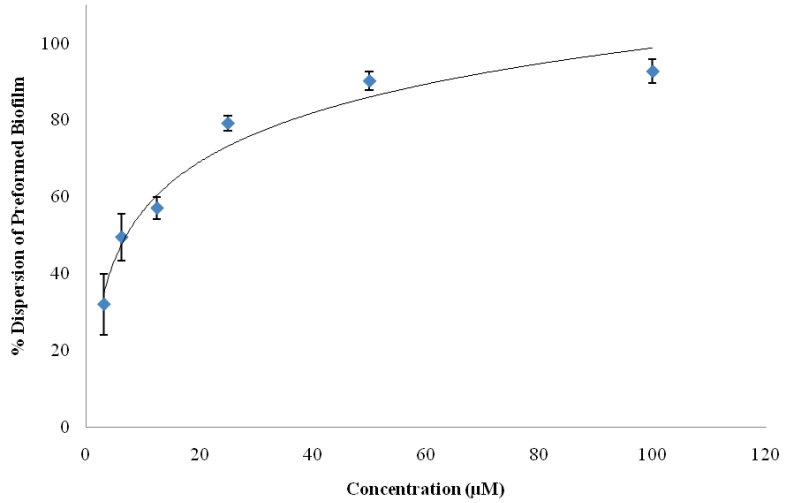
MRSA



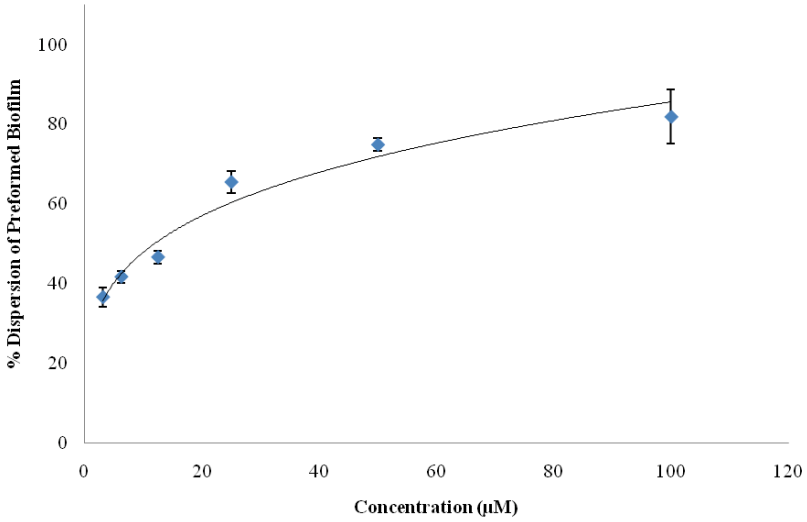
VRE

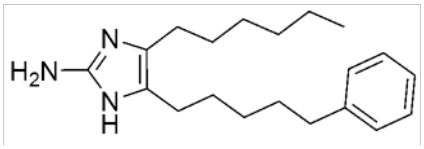


MDRAB

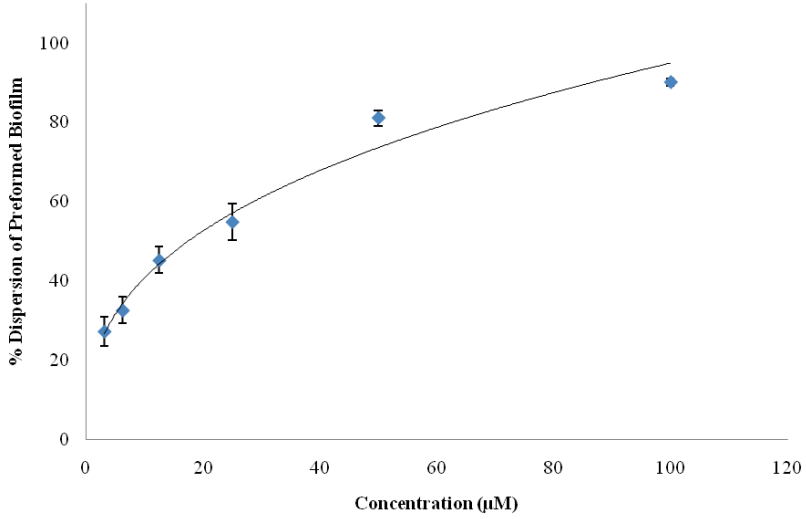


E. coli

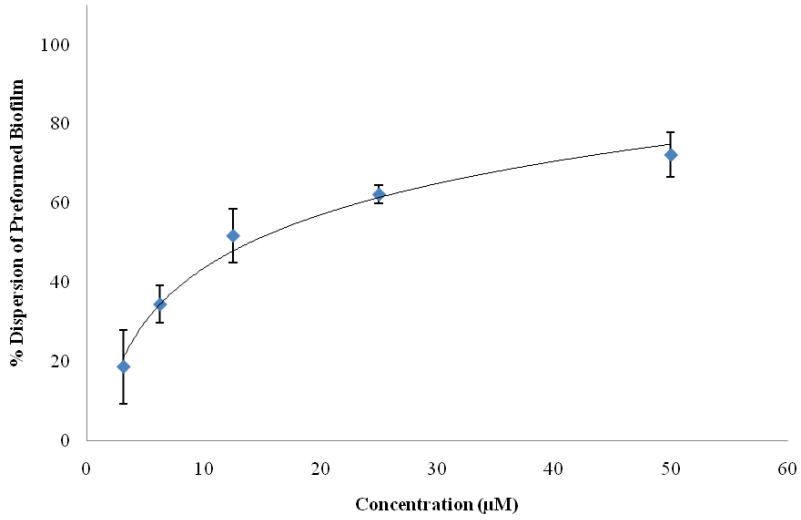




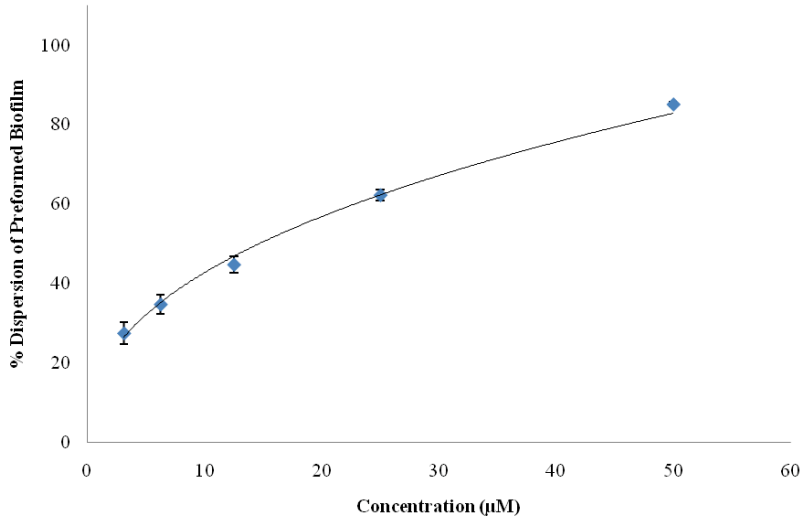
V. cholerae



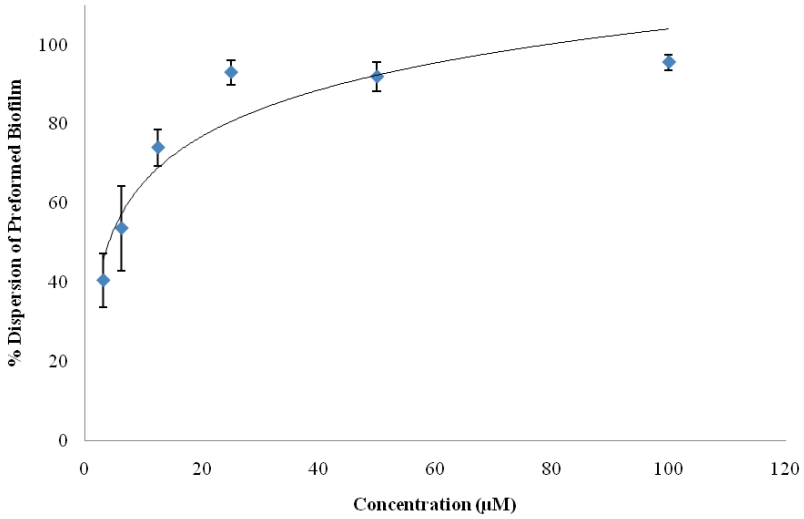
V. vulnificus



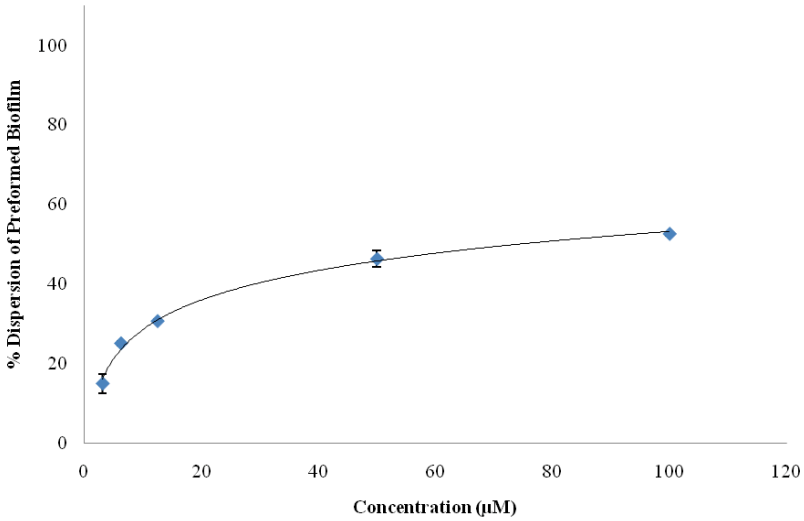
L. anguillarum



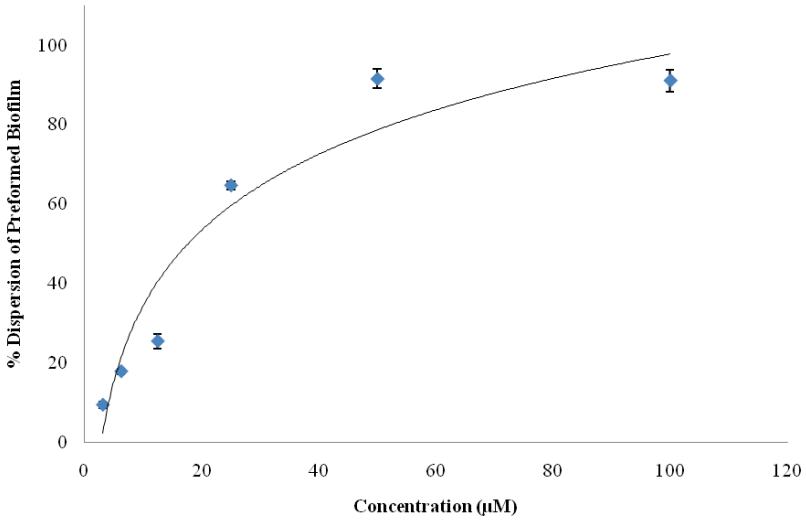
R. salexigens



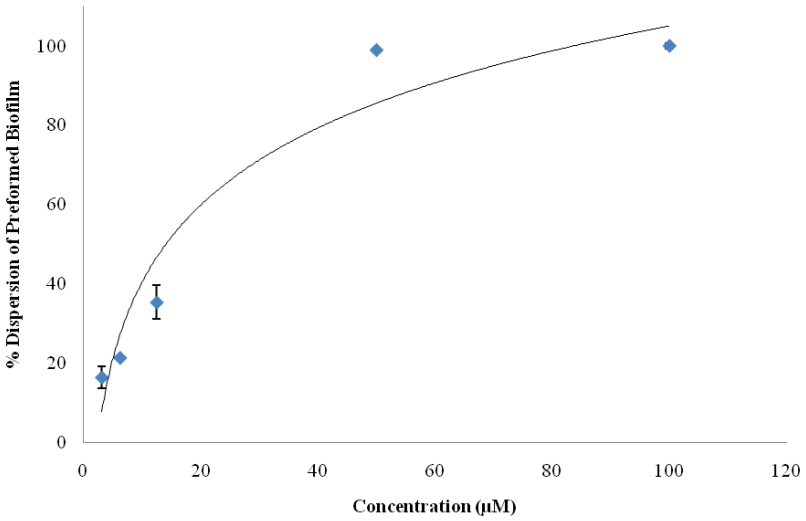
MRSA



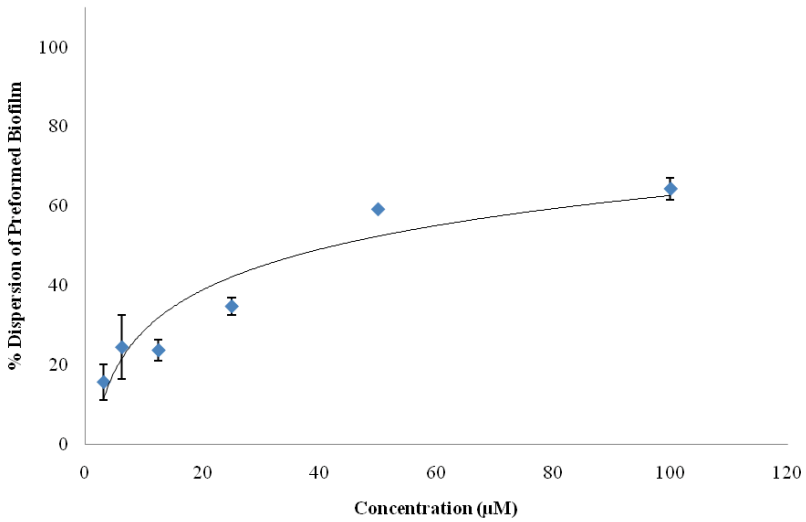
S. epidermidis

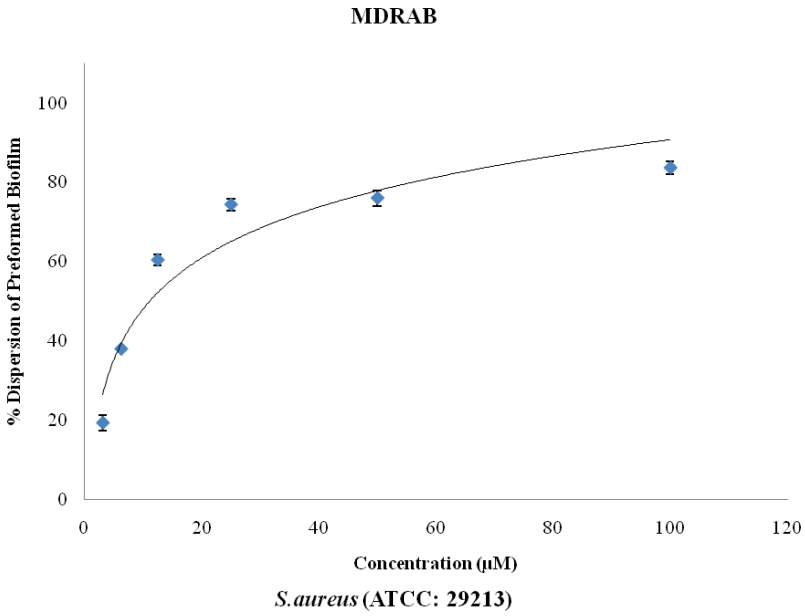


VRE

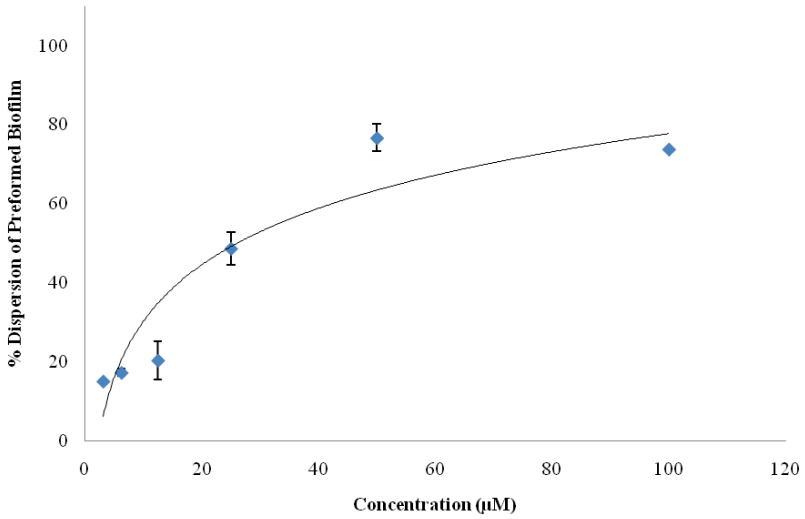


E. coli

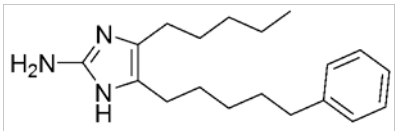


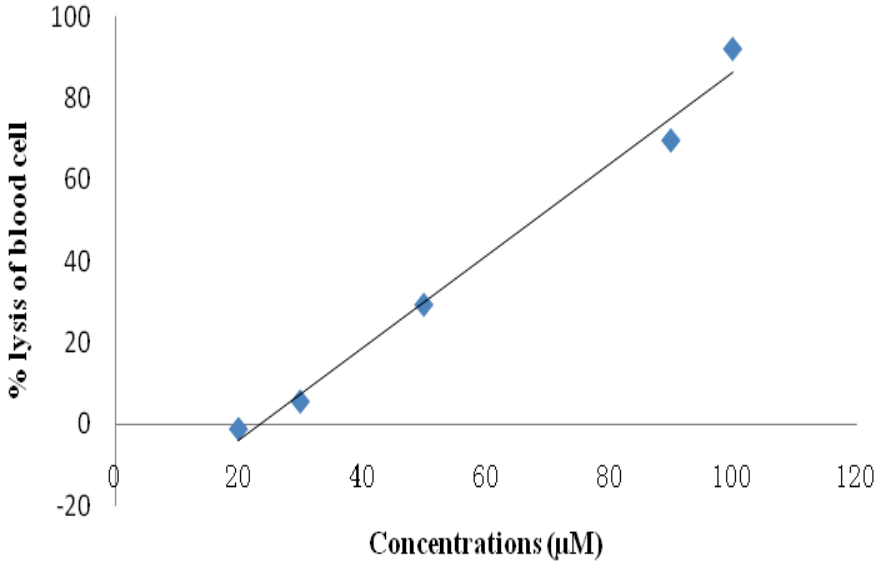


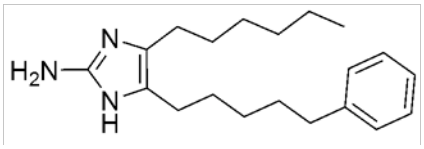
S.aureus (ATCC: 29213)

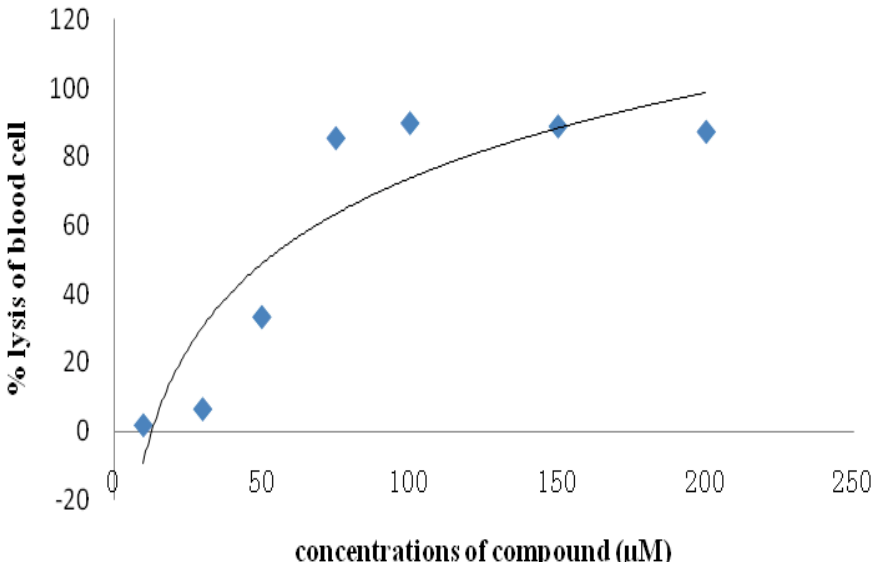


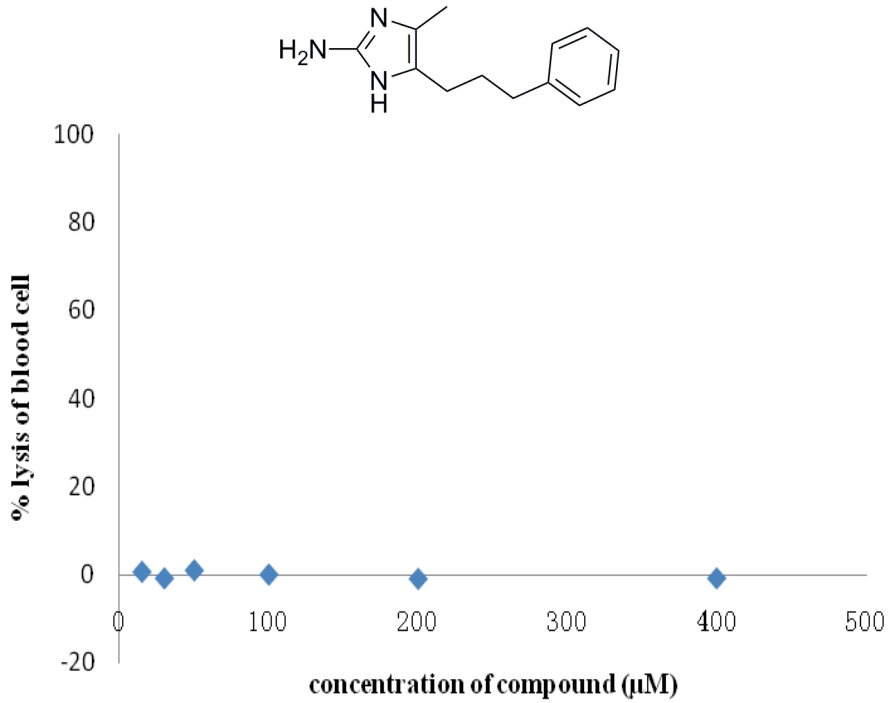
Hemolysis Graphs:



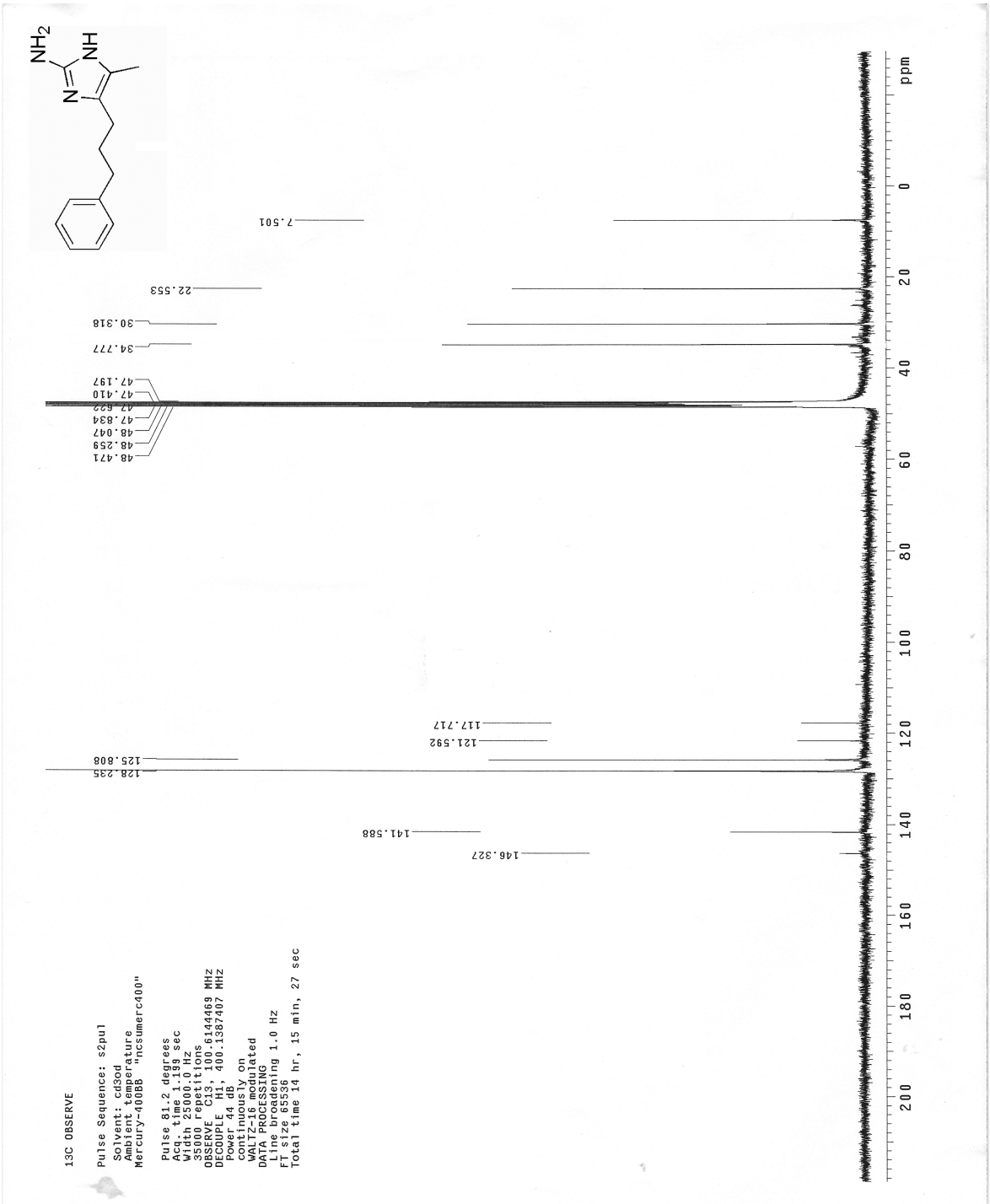


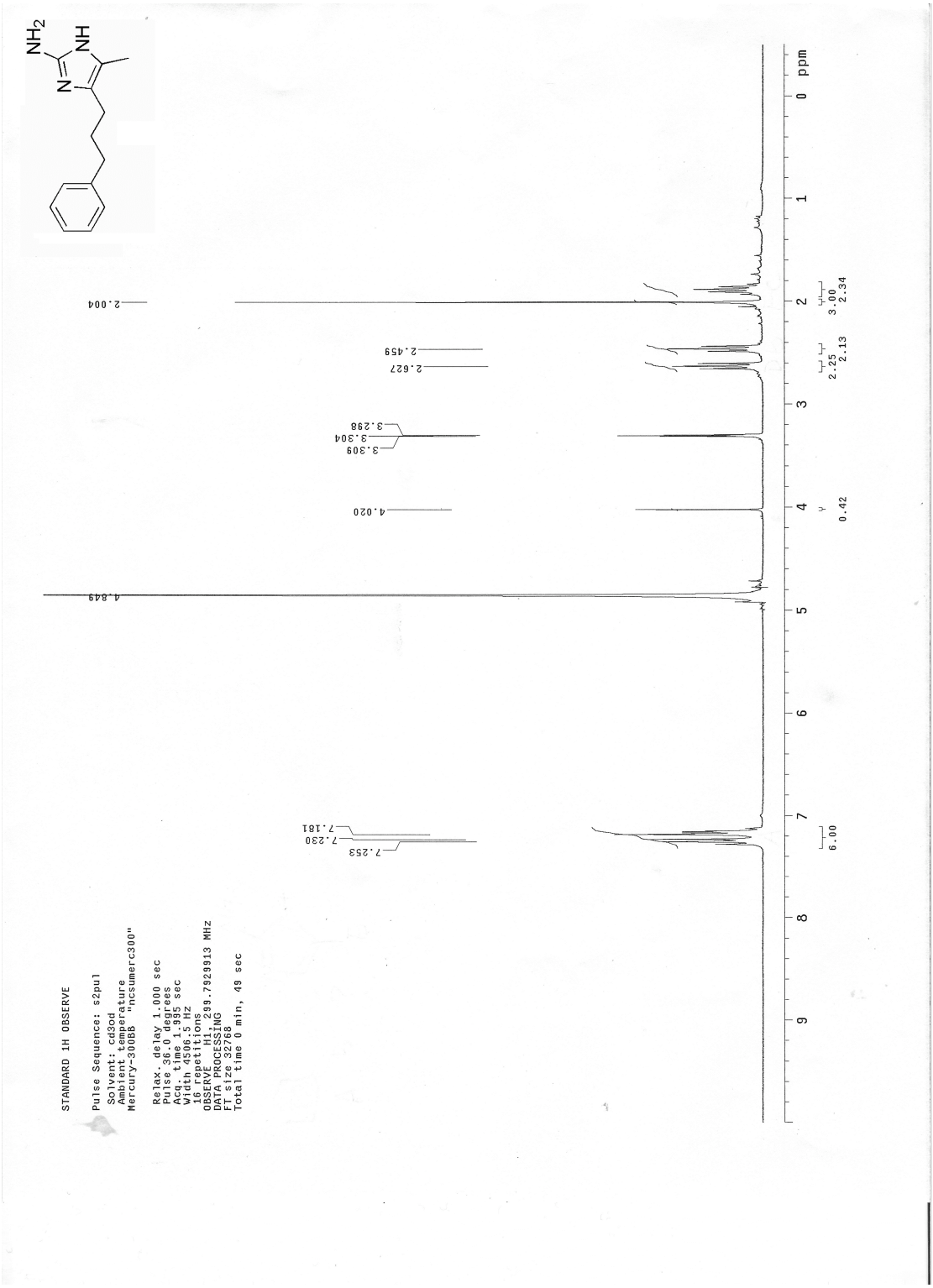






NMR data for 4,5-disubstituted-2-aminoimidazole

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3.309
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7.230
7.253
ppm
0
1
2
3
4
5
6
7
8
9
3.00
2.34
2.25
2.13
0.42
6.00
STANDARD 1H OBSERVE
Pulse Sequence: s2pul
Solvent: cd3od
Ambient temperature
Mercury-300BB "ncsumerc300"
Relax. delay 1.000 sec
Pulse 36.0 degrees
Acq. time 1.995 sec
Width 4806.5 HZ
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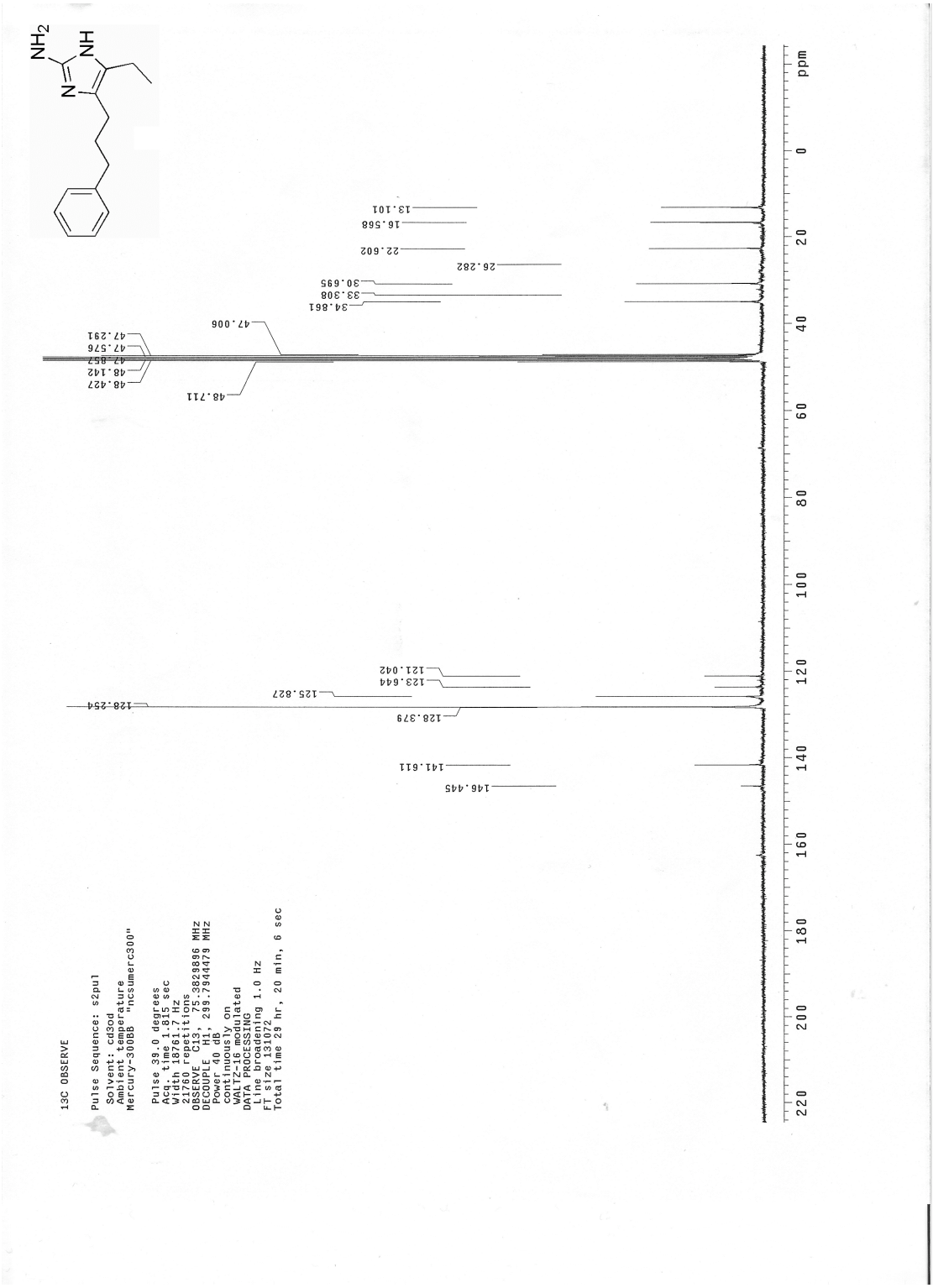
Total time 0 min, 49 sec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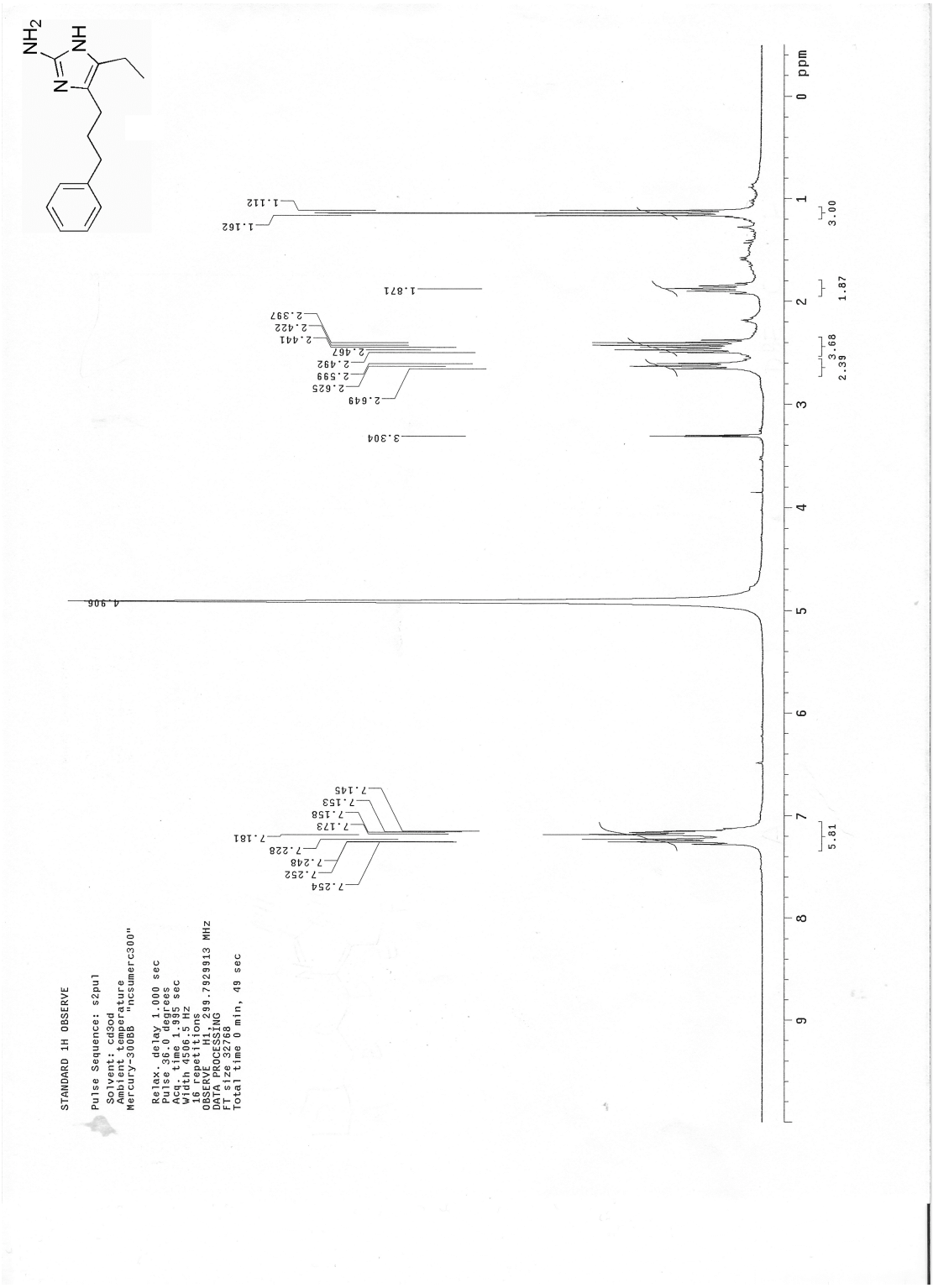
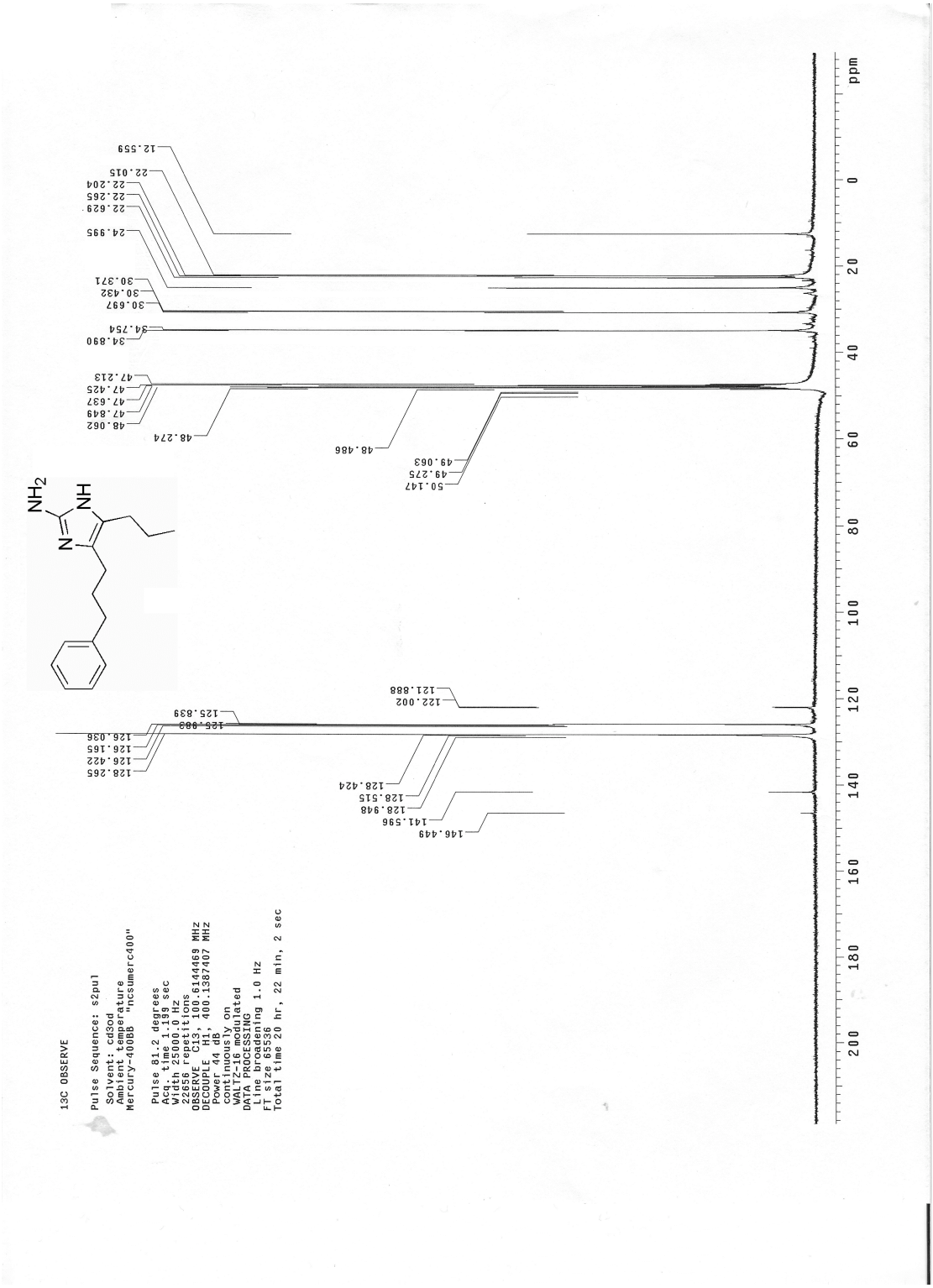
48.142
48.427
48.711
121.042
123.644
125.827
128.254
128.379
141.611
146.445
ppm
13C OBSERVE
Pulse Sequence: s2pul
Solvent: cd3od
Ambient temperature
Mercury-300BB "ncsumerc300"
Pulse 39.0 degrees
Acq. time 1.815 sec
Width 18761.7 Hz
21760 repetitions
OBSERVE C13, 75.3829896 MHz
DECOUPLE H1, 299.7944479 MHz
Power 40 dB
continuously on
WALTZ-16 modulated
Data processing
Line broadening 1.0 Hz
FT size 131072
Total time 29 hr, 20 min, 6 sec

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49.063
49.275
50.147
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125.882
126.036
126.165
126.422
128.265
128.424
128.515
128.948
141.596
146.449
NH2
NH
N
13C OBSERVE
Pulse Sequence: s2pul
Solvent: cd3od
Ambient temperature
Mercury-400BB "ncsumerc400"
Pulse 81.2 degrees
Acq. time 1.194 sec
Width 24000.0 Hz
22656 repetitions
OBSERVE C13, 100.6144469 MHz
DECOUPLE H1, 400.1387407 MHz
Power 44 dB
continuously on
WALTZ-16 modulated
Data processing
Line broadening 1.0 Hz
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Total time 20 hr, 22 min, 2 sec
ppm
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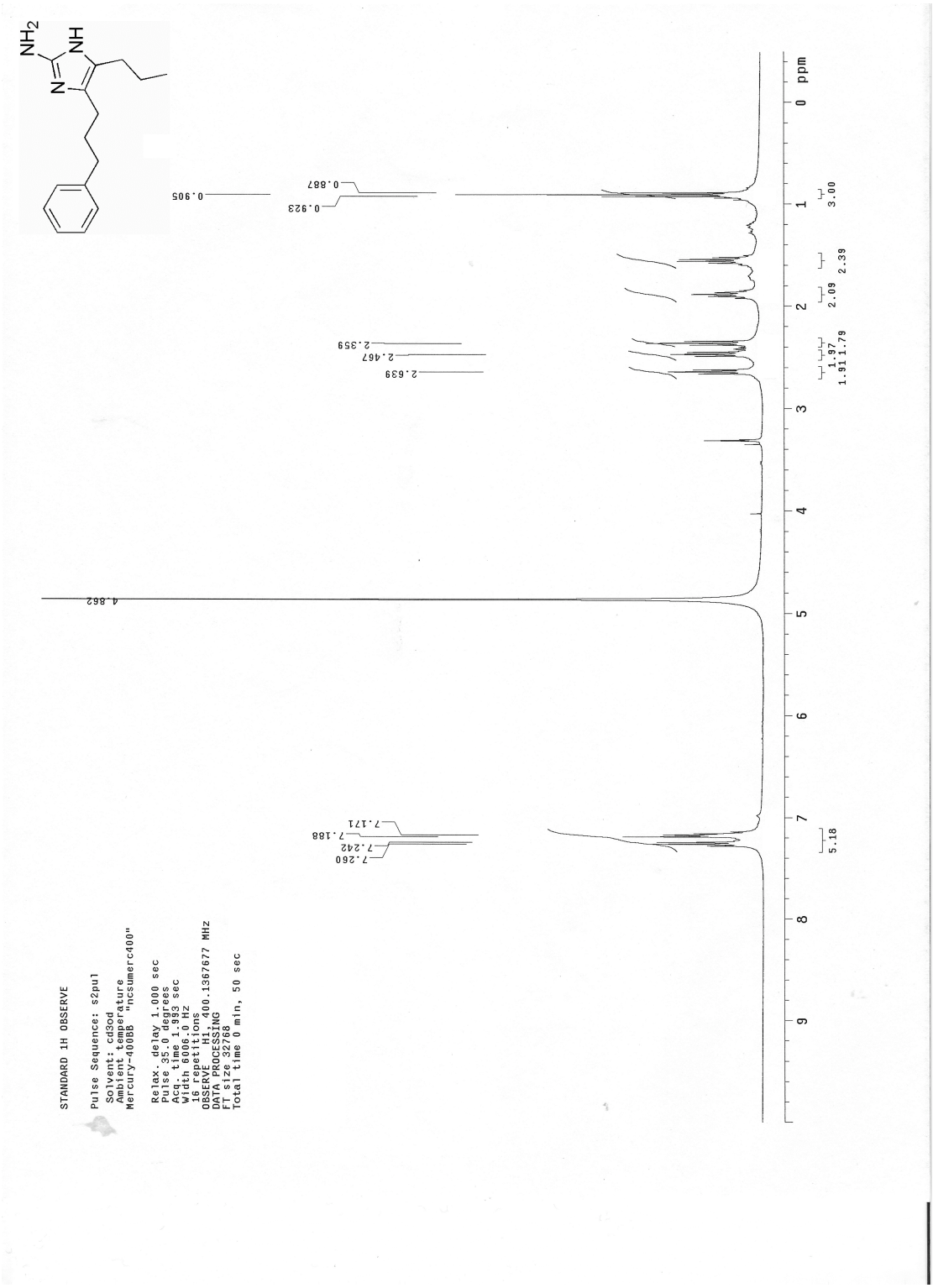
20
40
60
80
100
120
140
160
180
200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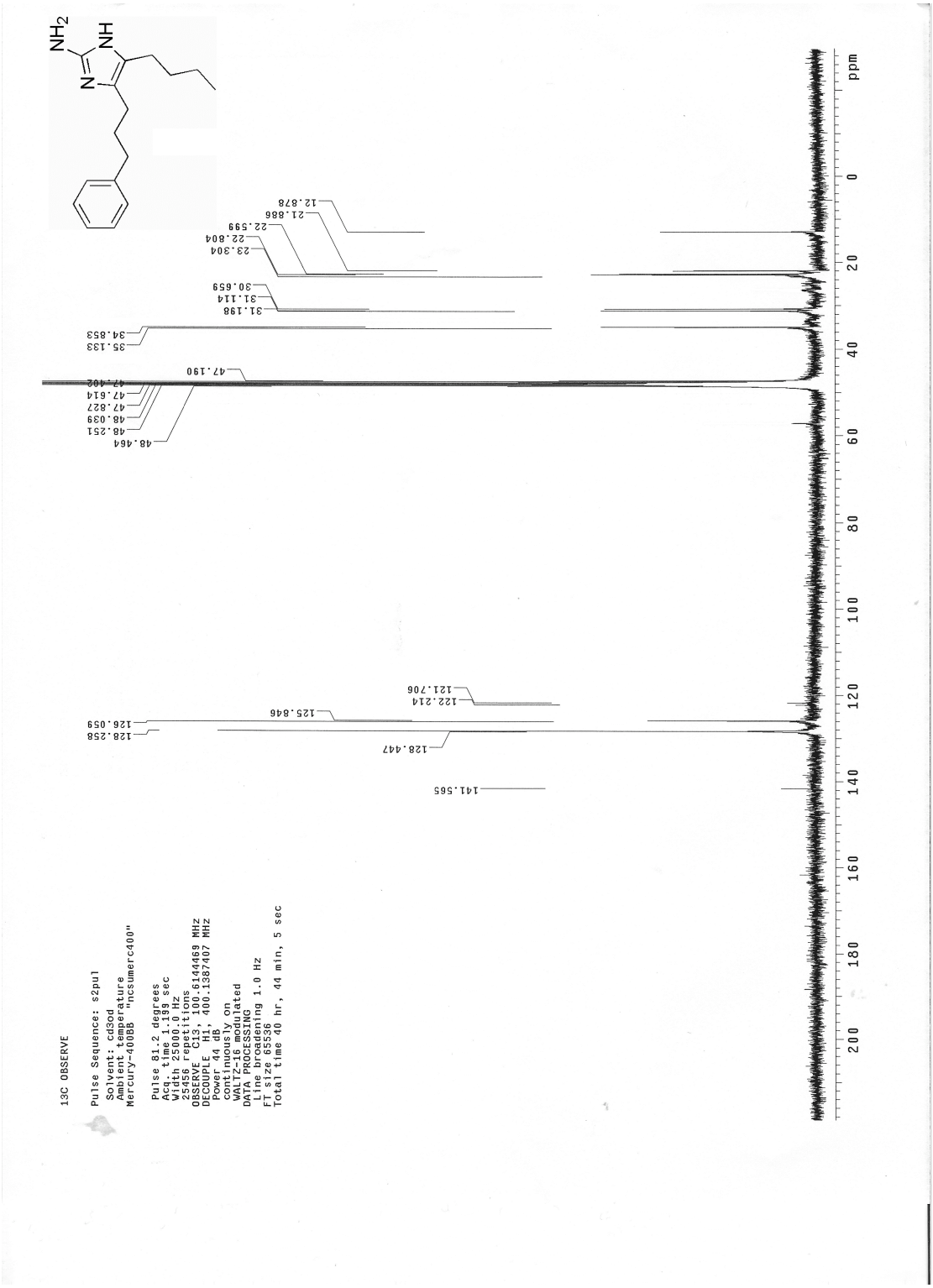
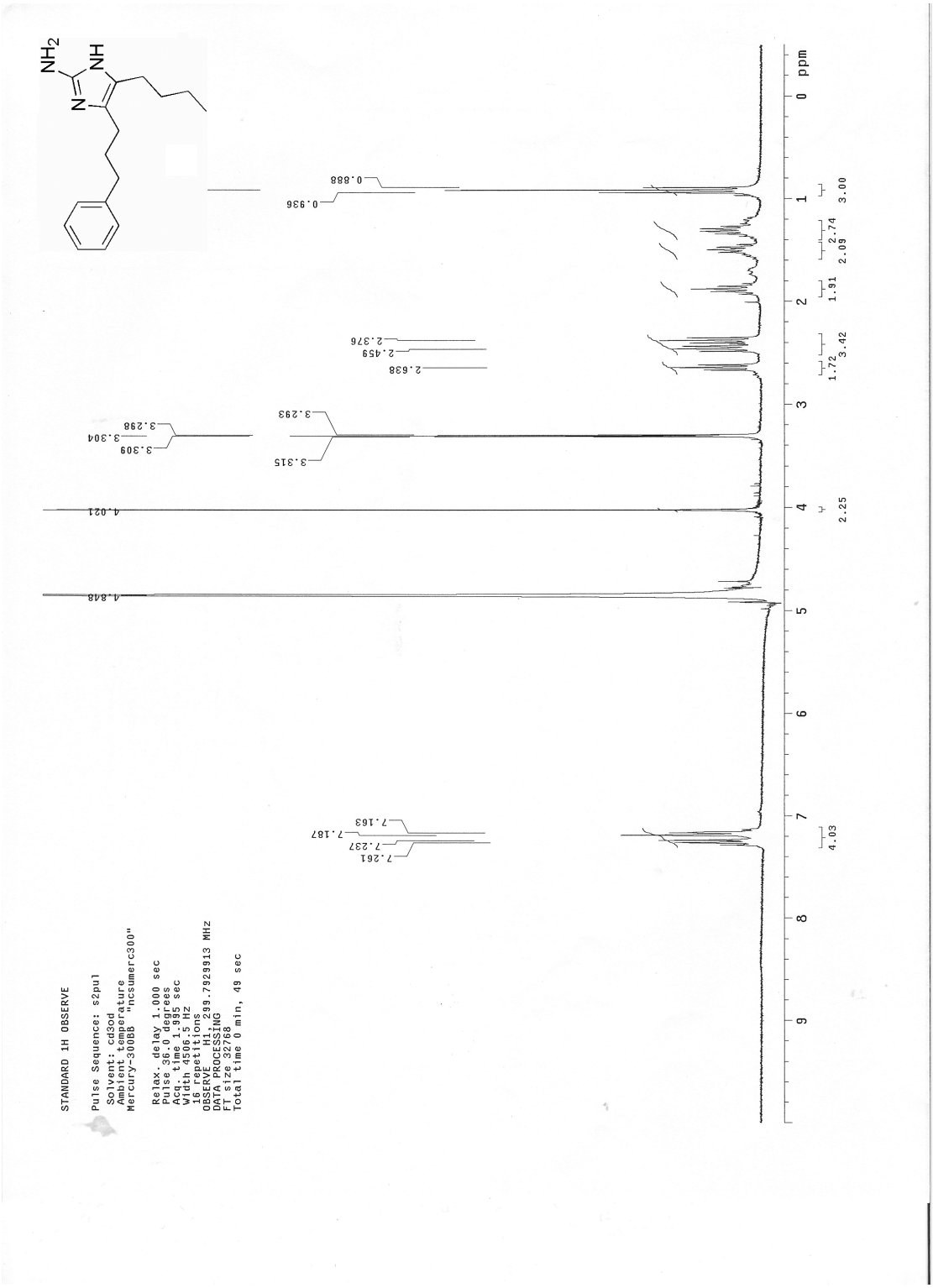
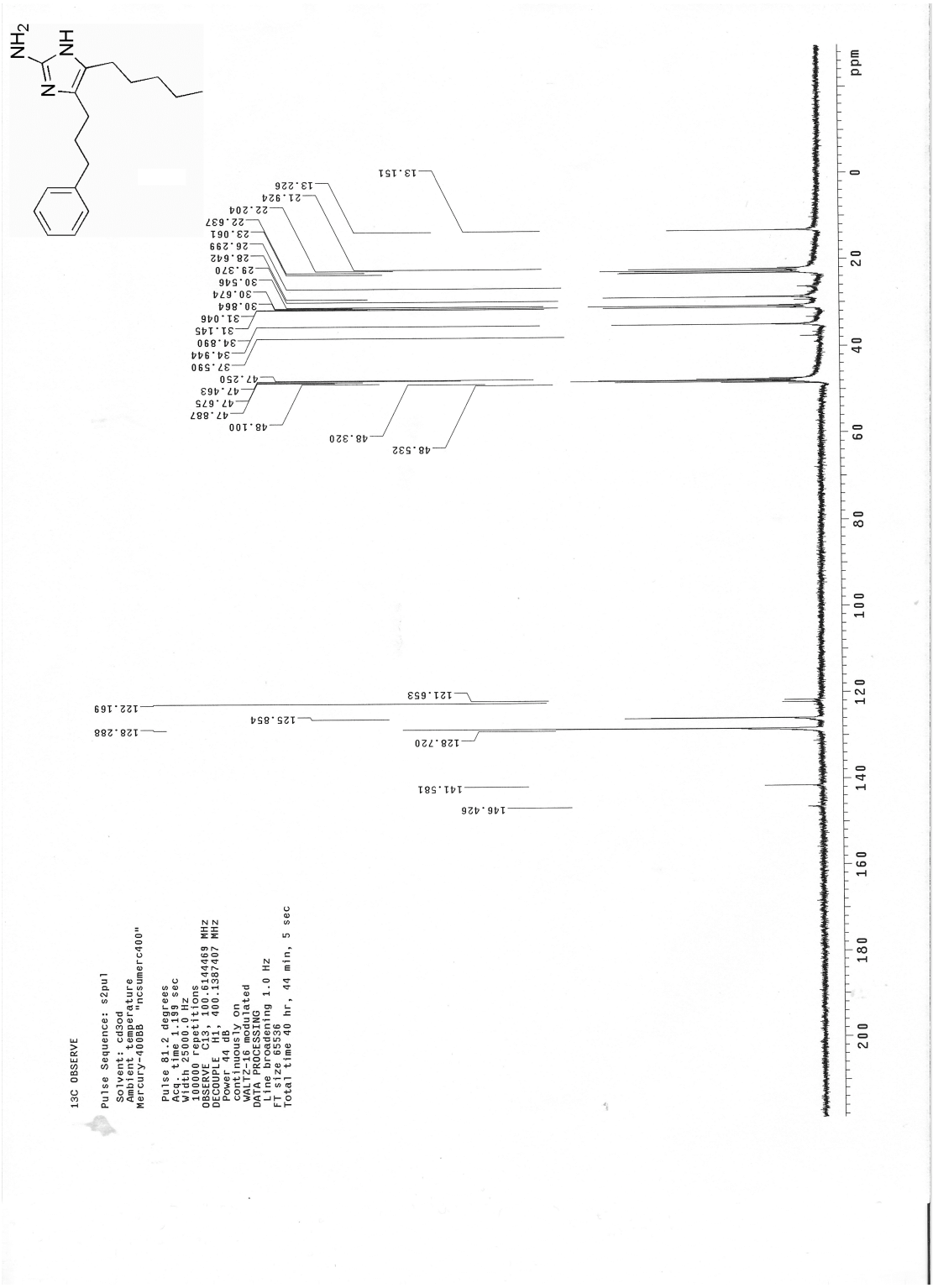
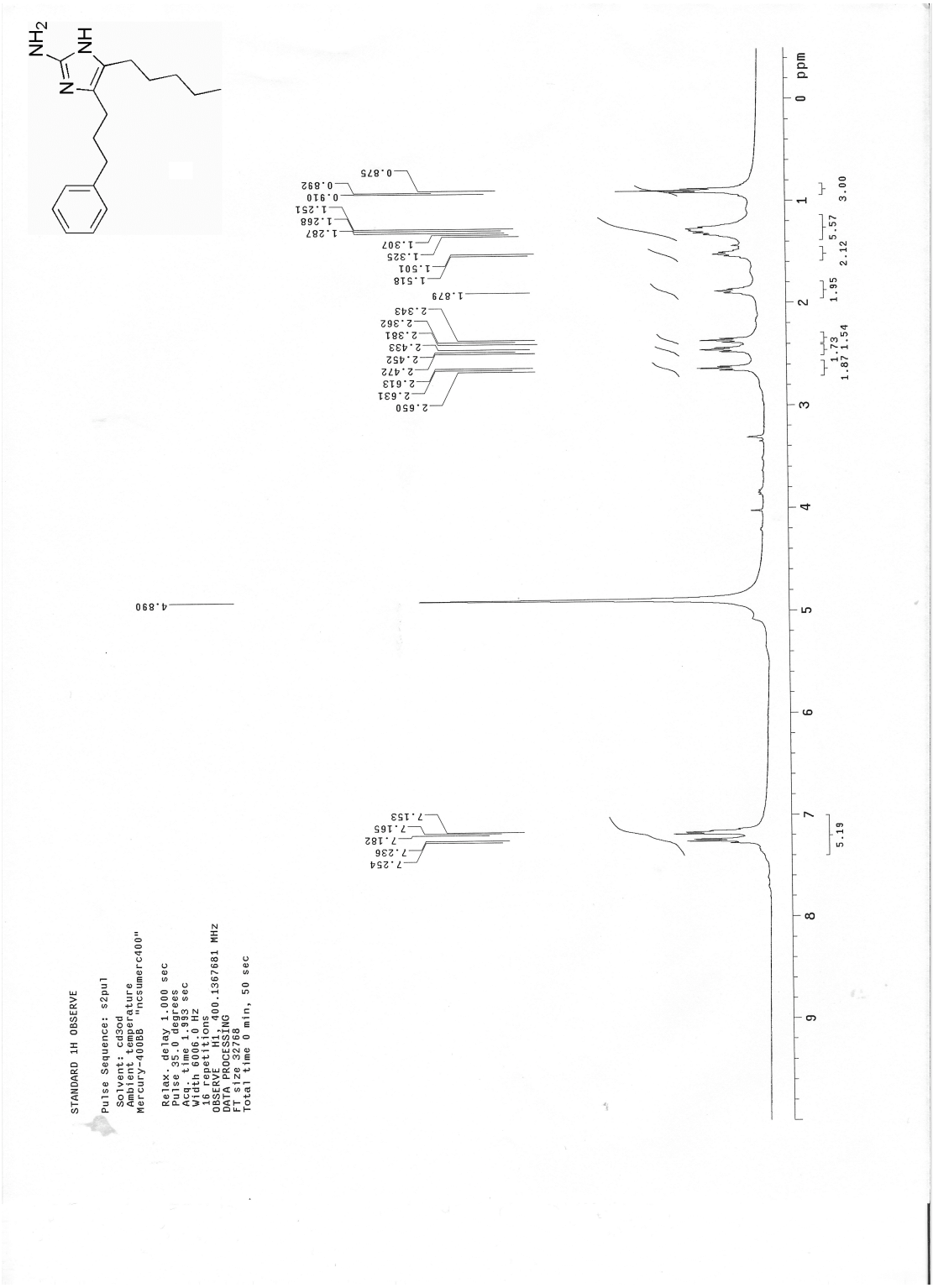
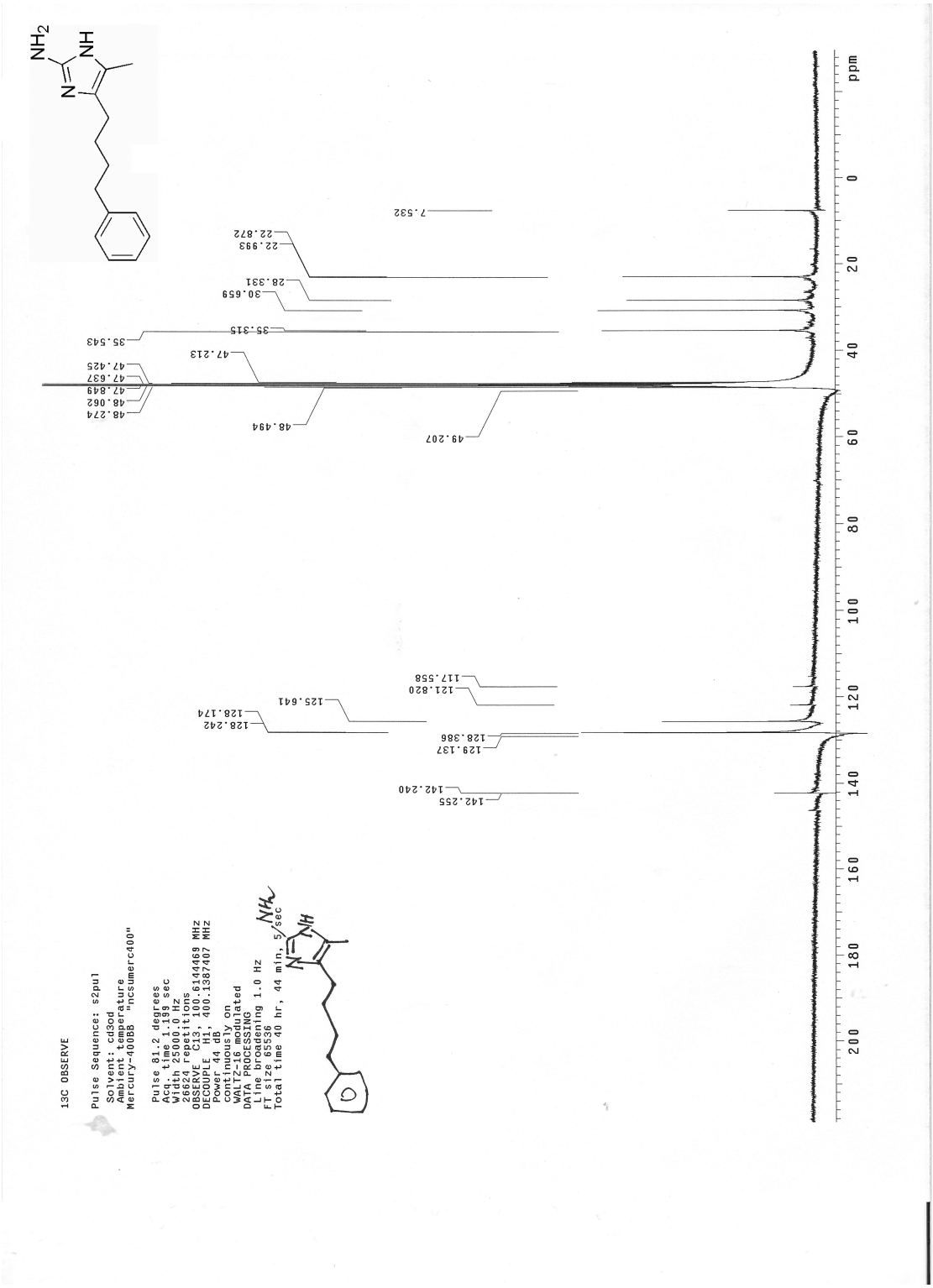
7.242
7.260
ppm
3.00
2.39
2.09
1.97
1.91
1.79
5.18
STANDARD 1H OBSERVE
Pulse Sequence: s2pul
Solvent: cd3od
Ambient temperature
Mercury-400BB "ncsumerc400"
Relax. delay 1.000 sec
Pulse 35.0 degrees
Acq. time 1.495 sec
Width 6006.0 Hz
16 repetitions
OBSERVE H1, 400.1367677 MHz
DATA PROCESSING
FT size 32768
Total time 0 min, 50 sec

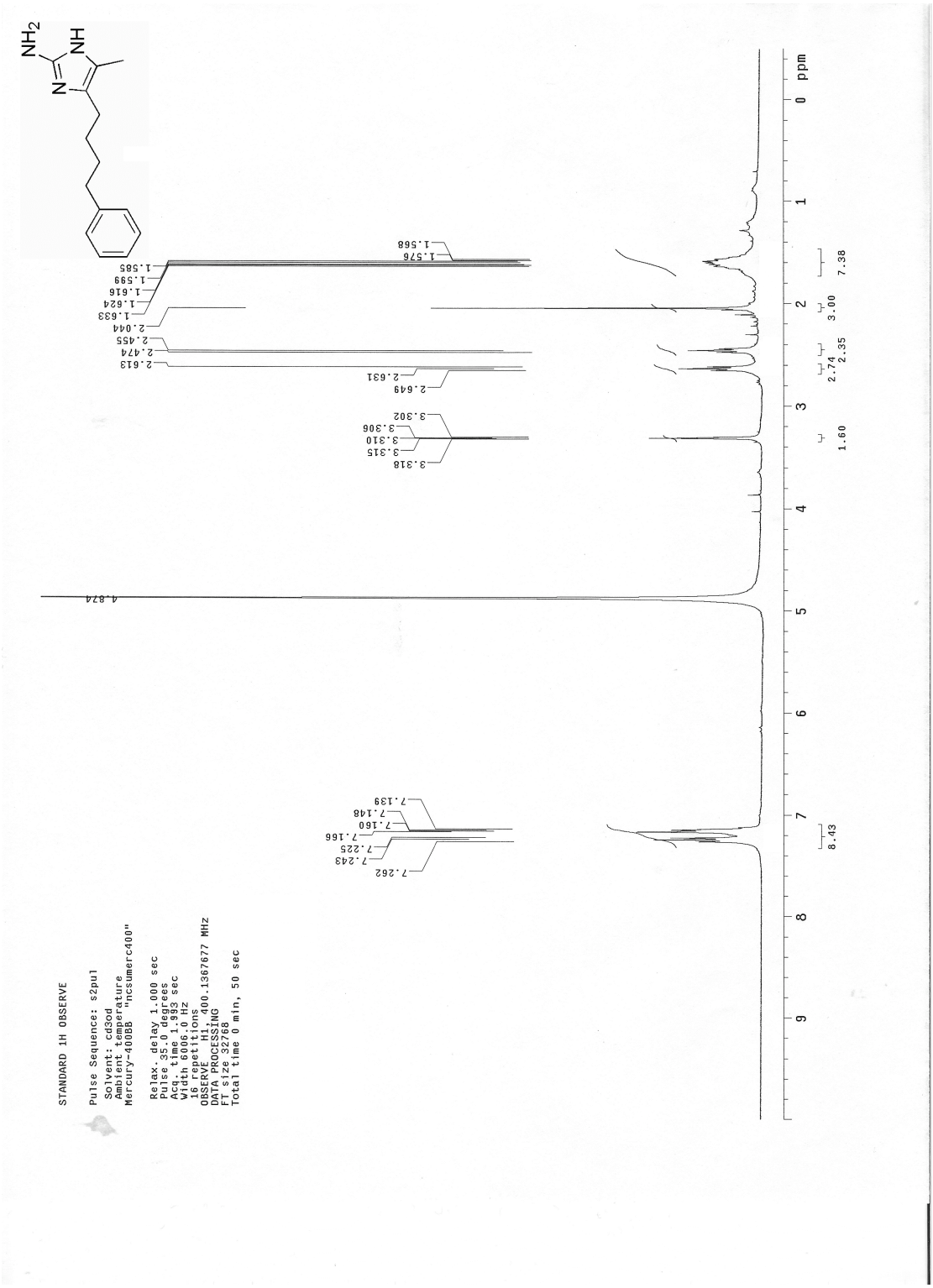


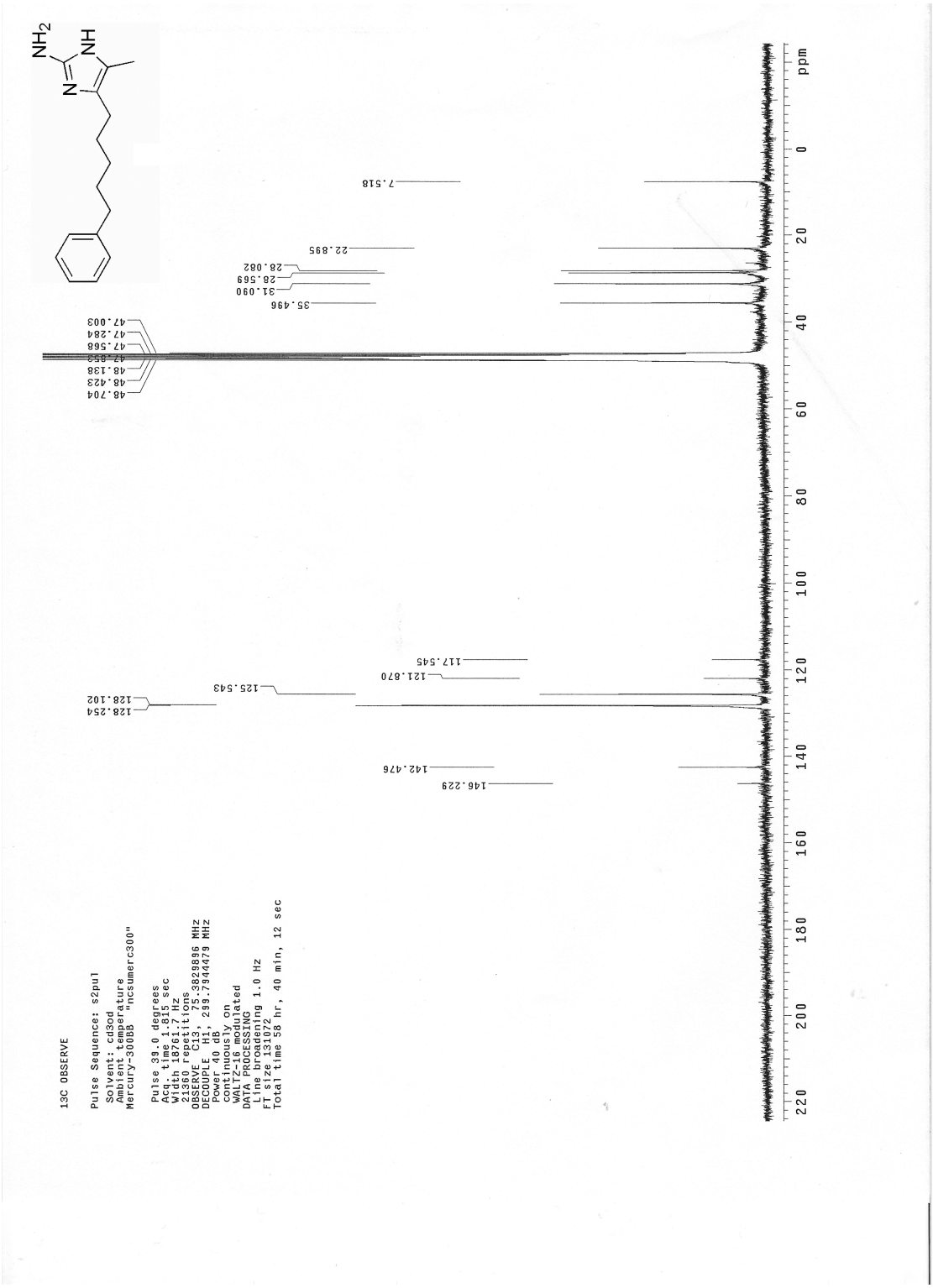

NH2
NH
N
0.888
0.936
2.376
2.459
2.638
3.293
3.298
3.304
3.309
3.315
4.021
4.848
7.163
7.187
7.237
7.261
ppm
STANDARD 1H OBSERVE
Pulse Sequence: s2pul
Solvent: cd3od
Ambient temperature
Mercury-300BB "ncsumerc300"
Relax. delay 1.000 sec
Pulse 36.0 degrees
Acq. time 1.195 sec
Width 4806.5 Hz
16 repetitions
OBSERVE H1, 299.7929913 MHz
DATA PROCESSING
FT size 32768
Total time 0 min, 49 sec

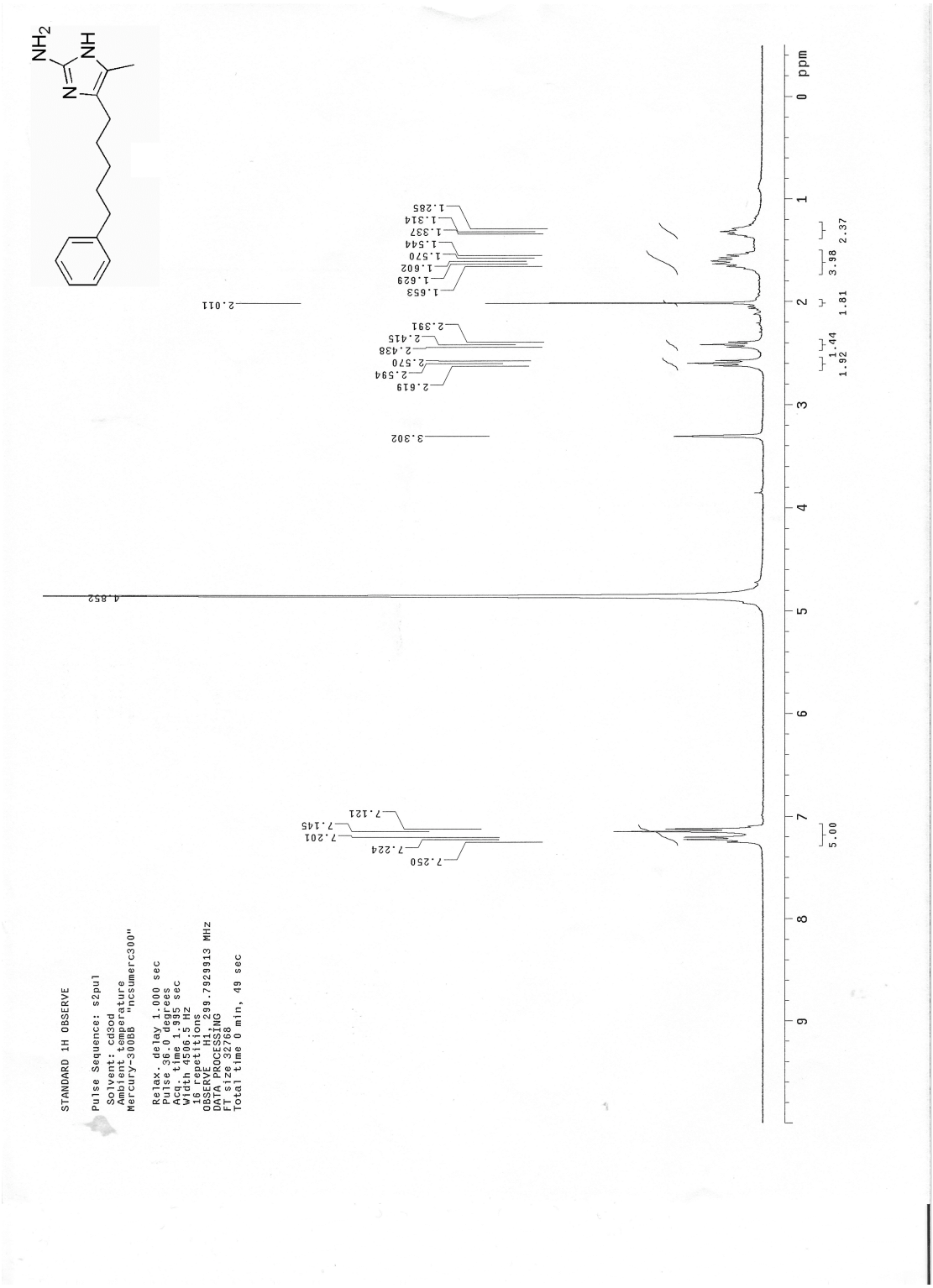


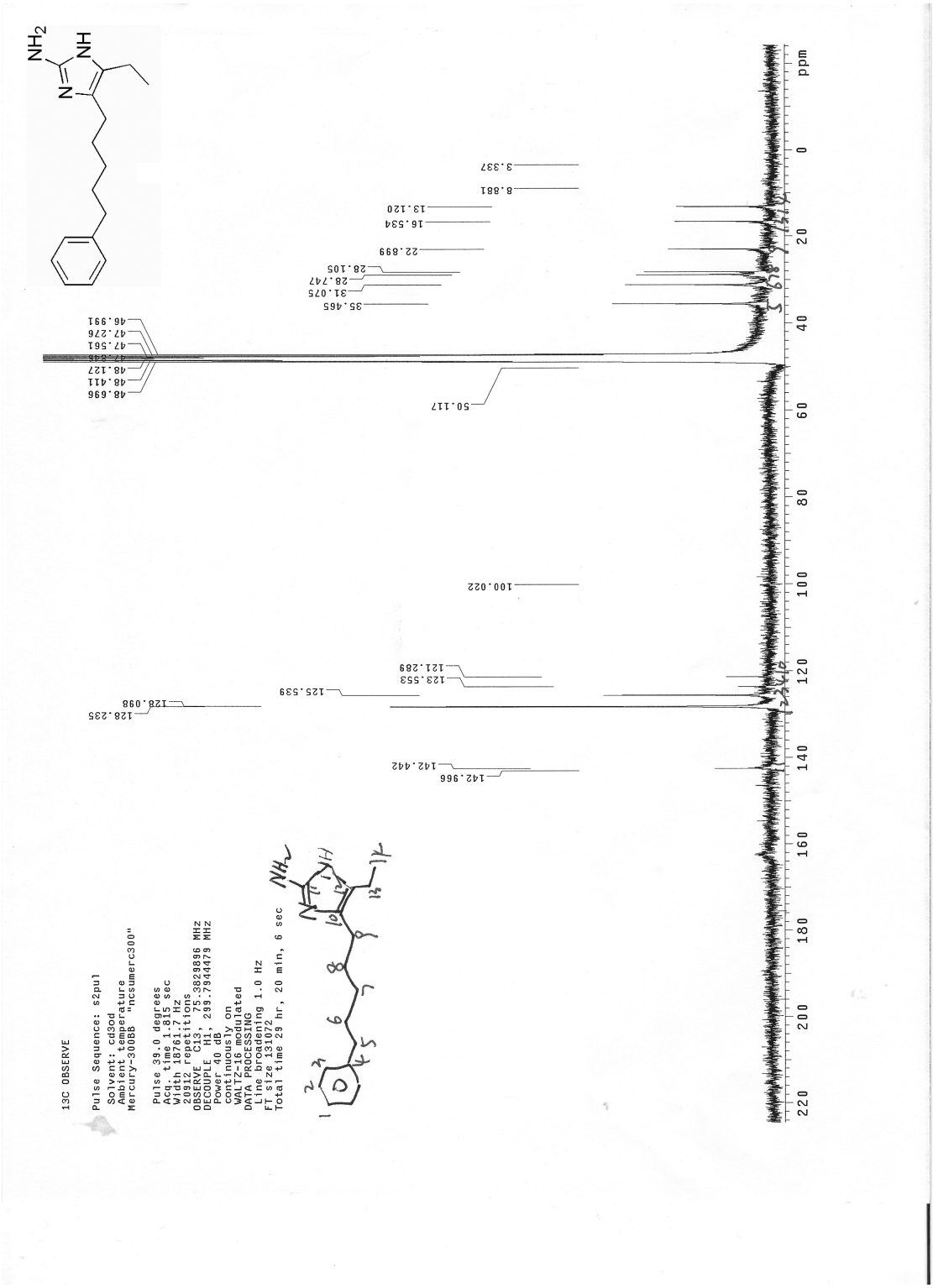


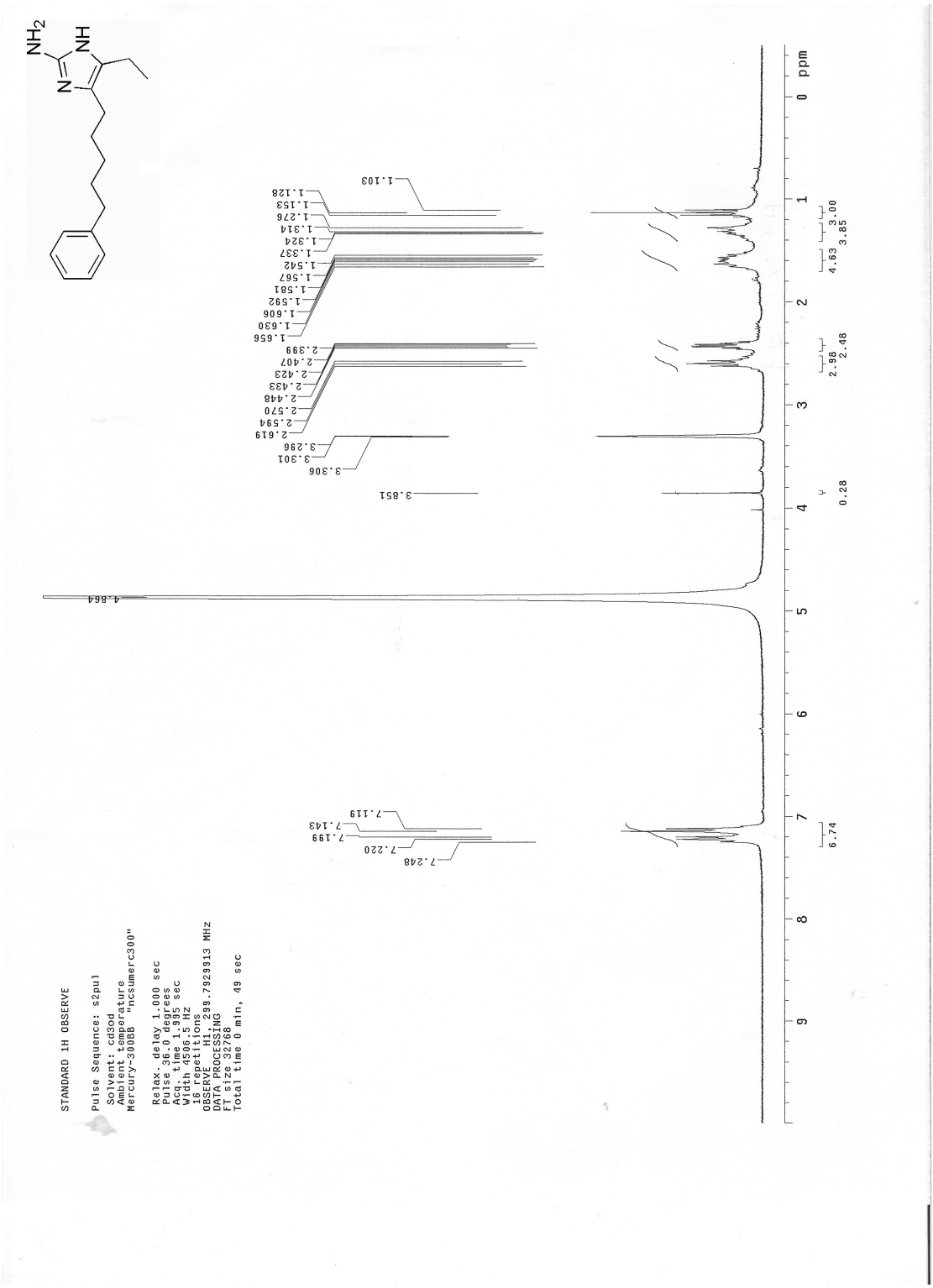

NH2
NH
N
7.532
22.872
22.993
28.331
30.659
35.315
35.543
47.213
47.425
47.637
47.849
48.062
48.274
48.494
49.207
117.558
121.820
125.641
128.174
128.242
128.386
129.137
142.240
142.255
ppm
0
20
40
60
80
100
120
140
160
180
200
13C OBSERVE
Pulse Sequence: s2pul
Solvent: cd3od
Ambient temperature
Mercury-400BB "ncsumerc400"
Pulse 81.2 degrees
Acq. time 1.199 sec
Width 25000.0 Hz
26624 repetitions
OBSERVE C13, 100.6144469 MHz
DECOUPLE H1, 400.1387407 MHz
Power 44 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 65536
Total time 40 hr, 44 min, 5/sec

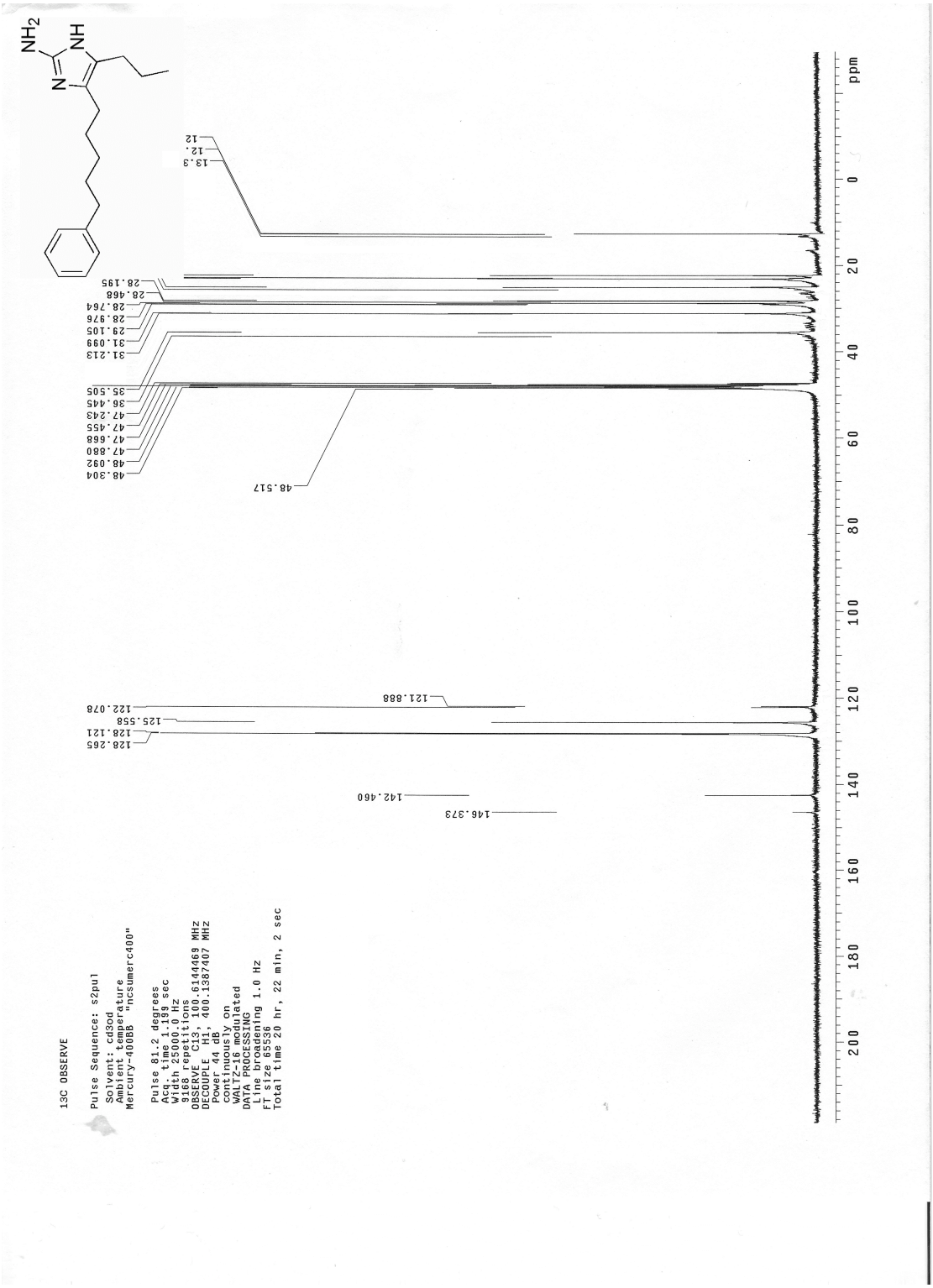

NH2
NH
N
STANDARD 1H OBSERVE
Pulse Sequence: s2pul
Solvent: cdsod
Ambient temperature
Mercury-400BB "ncsumerc400"
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.993 sec
Width 6006.0 Hz
16 repetitions
OBSERVE H1, 400.1367677 MHz
DATA PROCESSING
FT size 32768
Total time 0 min, 50 sec
1.568
1.576
1.585
1.599
1.616
1.624
1.633
2.044
2.455
2.474
2.613
2.631
2.649
3.302
3.306
3.310
3.315
3.318
4.824
7.139
7.148
7.160
7.166
7.225
7.243
7.262
ppm
7.38
3.00
2.35
2.74
1.60
8.43

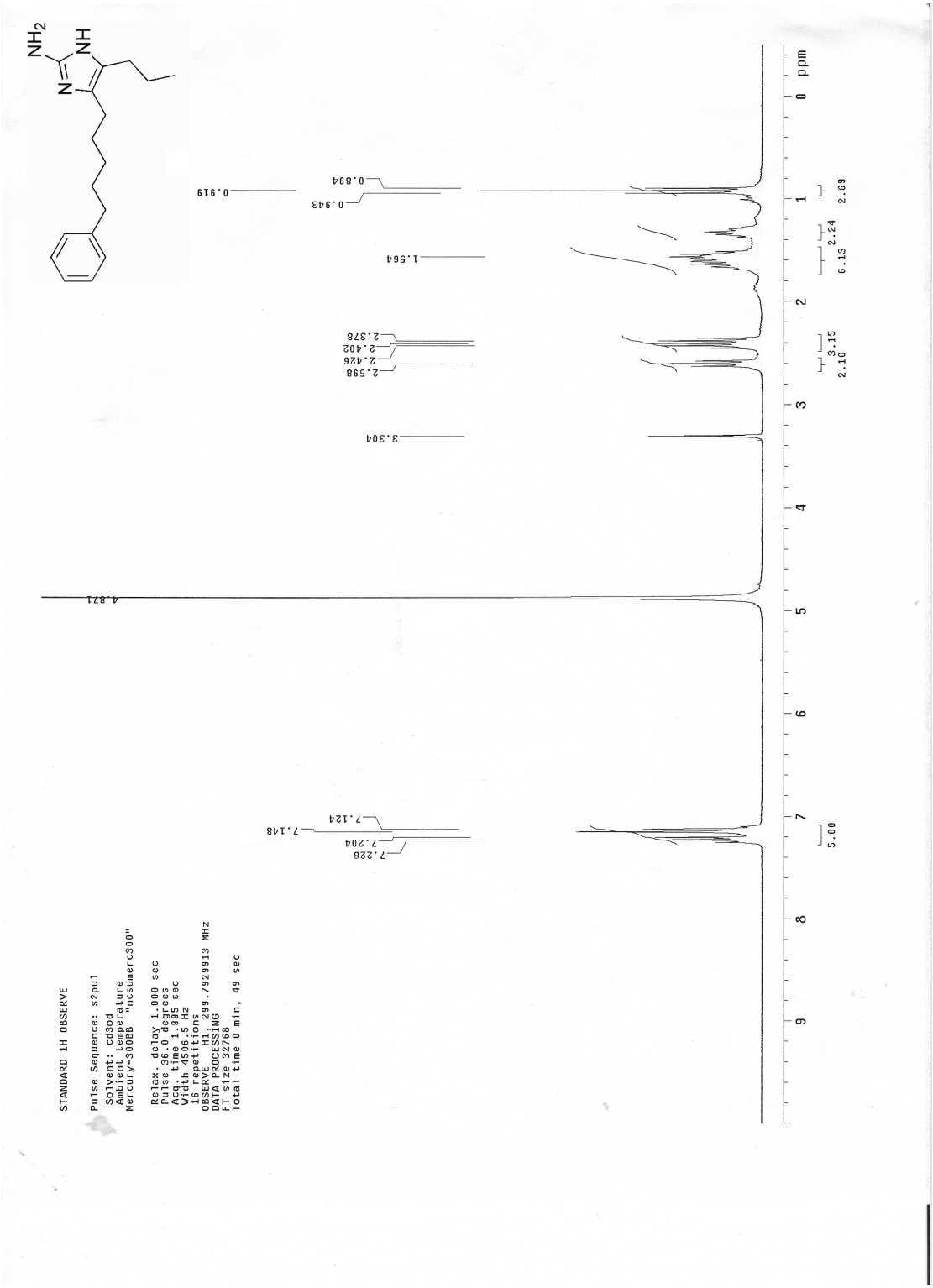

NH2
NH
N
7.518
22.895
28.082
28.569
31.090
35.496
47.003
47.284
47.568
47.853
48.138
48.423
48.704
117.545
121.870
125.543
128.102
128.254
142.476
146.229
ppm
0
20
40
60
80
100
120
140
160
180
200
220
13C OBSERVE
Pulse Sequence: s2pul
Solvent: cd3od
Ambient temperature
Mercury-300BB "ncsumerc300"
Pulse 39.0 degrees
Acq. time 1.815 sec
Width 18817.7 Hz
21360 repetitions
OBSERVE C13, 75.3829896 MHz
DECOUPLE H1, 299.7944479 MHz
Power 40 dB
continuously on
WALTZ-16 modulated
Data processing
Line broadening 1.0 Hz
FT size 131072
Total time 58 hr, 40 min, 12 sec

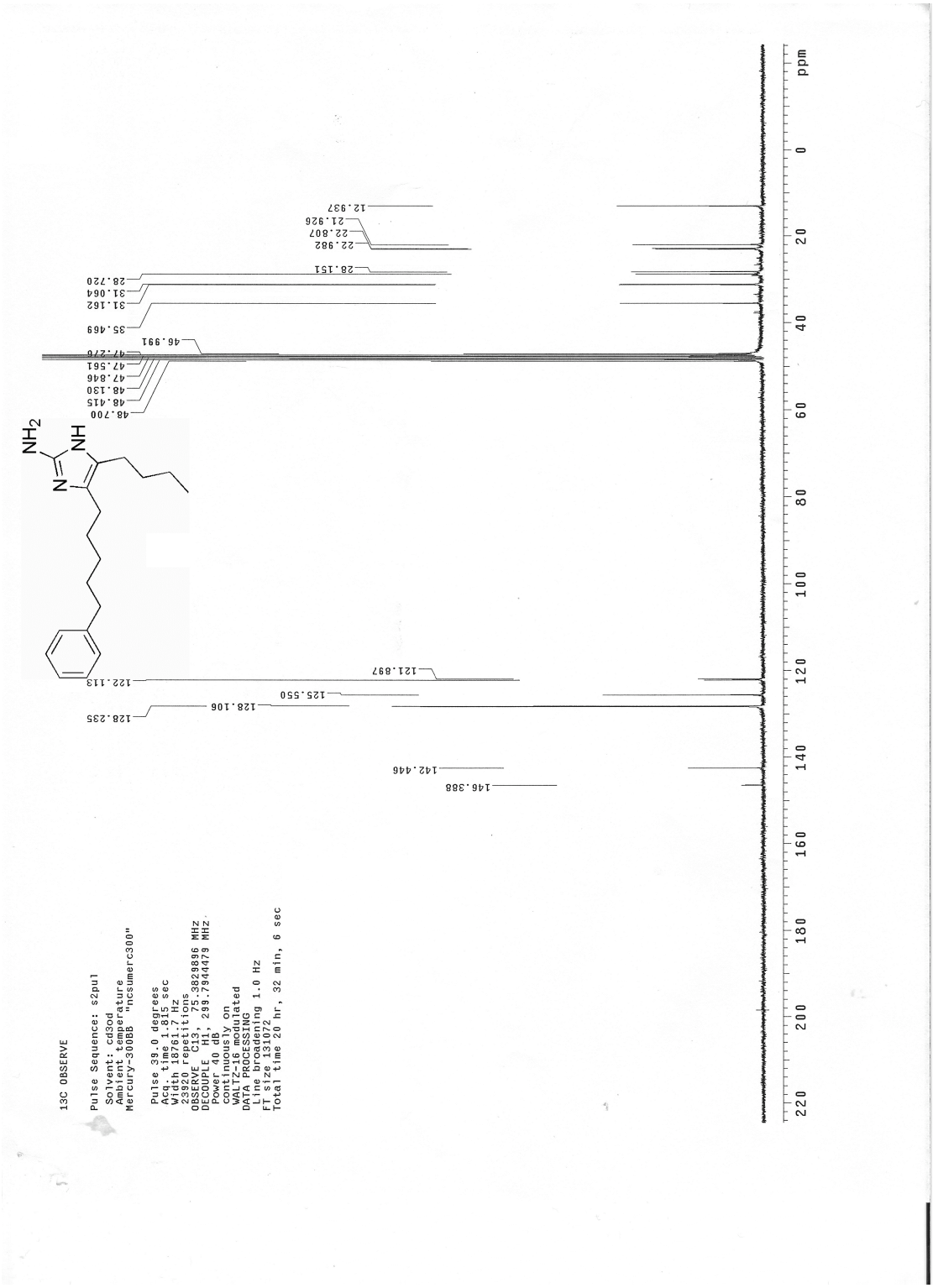

NH2
NH
N
STANDARD 1H OBSERVE
Pulse Sequence: s2pul
Solvent: cd3od
Ambient temperature
Mercury-300BB "ncsumerc300"
Relax. delay 1.000 sec
Pulse 36.0 degrees
Acq. time 1.895 sec
Width 4806.5 HZ
16 repetitions
OBSERVE H1, 299.7929913 MHz
DATA PROCESSING
FT size 32768
Total time 0 min, 49 sec
7.250
7.224
7.201
7.145
7.121
4.852
3.302
2.619
2.594
2.570
2.438
2.415
2.391
2.011
1.653
1.629
1.602
1.570
1.544
1.337
1.314
1.285
ppm
5.00
1.92
1.44
1.81
3.98
2.37

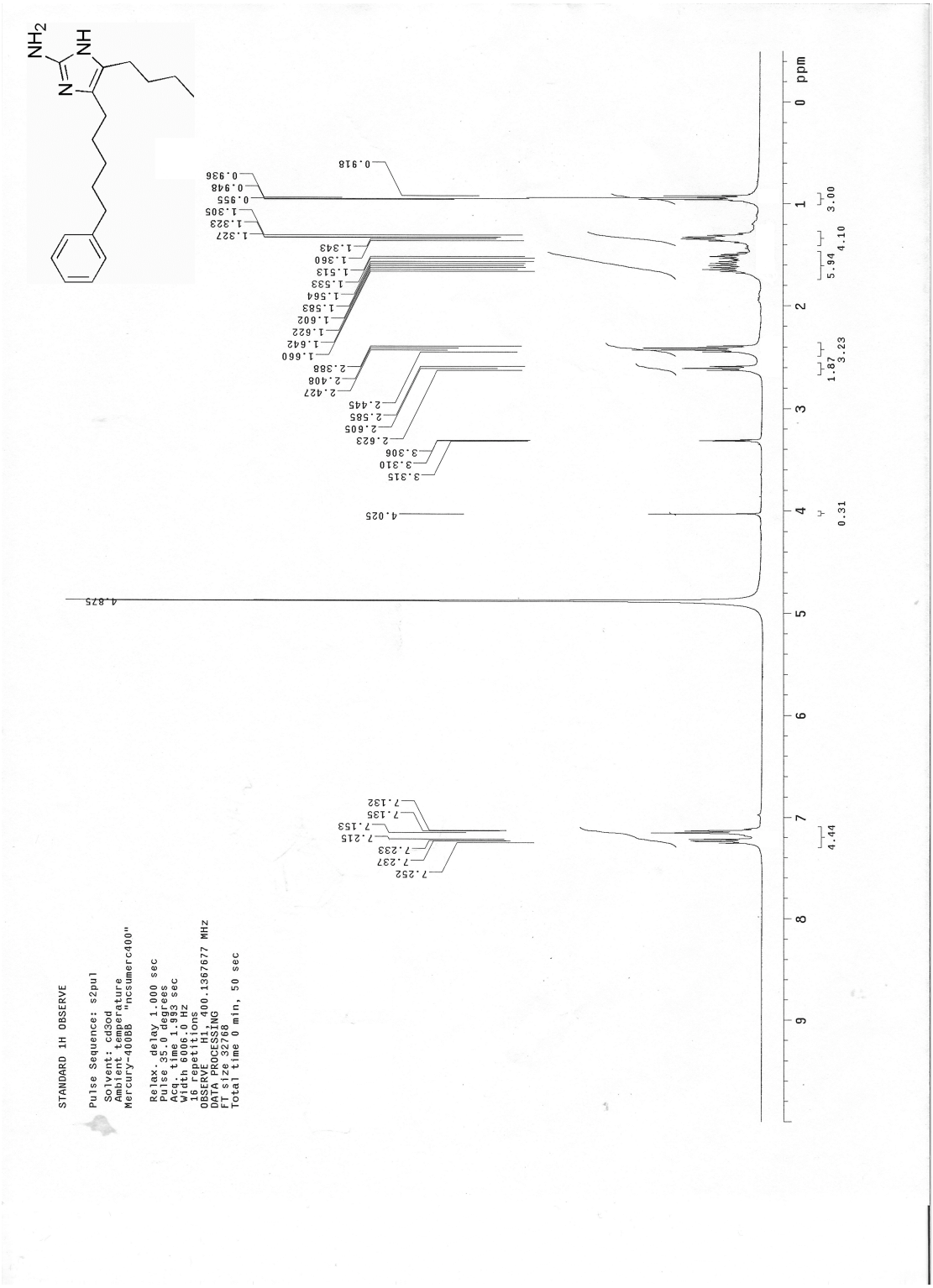

13C OBSERVE
Pulse Sequence: s2pul
Solvent: cd3od
Ambient temperature
Mercury-300BB "ncsumerc300"
Pulse 39.0 degrees
Acq. time 1.815 sec
Width 18761.7 Hz
2000 repetitions
OBSERVE C13, 75.3829896 MHz
DECOUPLE H1, 299.7944479 MHz
Power 40 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 131072
Total time 29 hr, 20 min, 6 sec
ppm
3.337
8.881
13.120
16.534
22.899
28.105
28.747
31.075
35.465
46.991
47.276
47.561
48.127
48.411
48.696
50.117
100.022
121.289
123.553
125.539
128.098
128.235
142.442
142.966

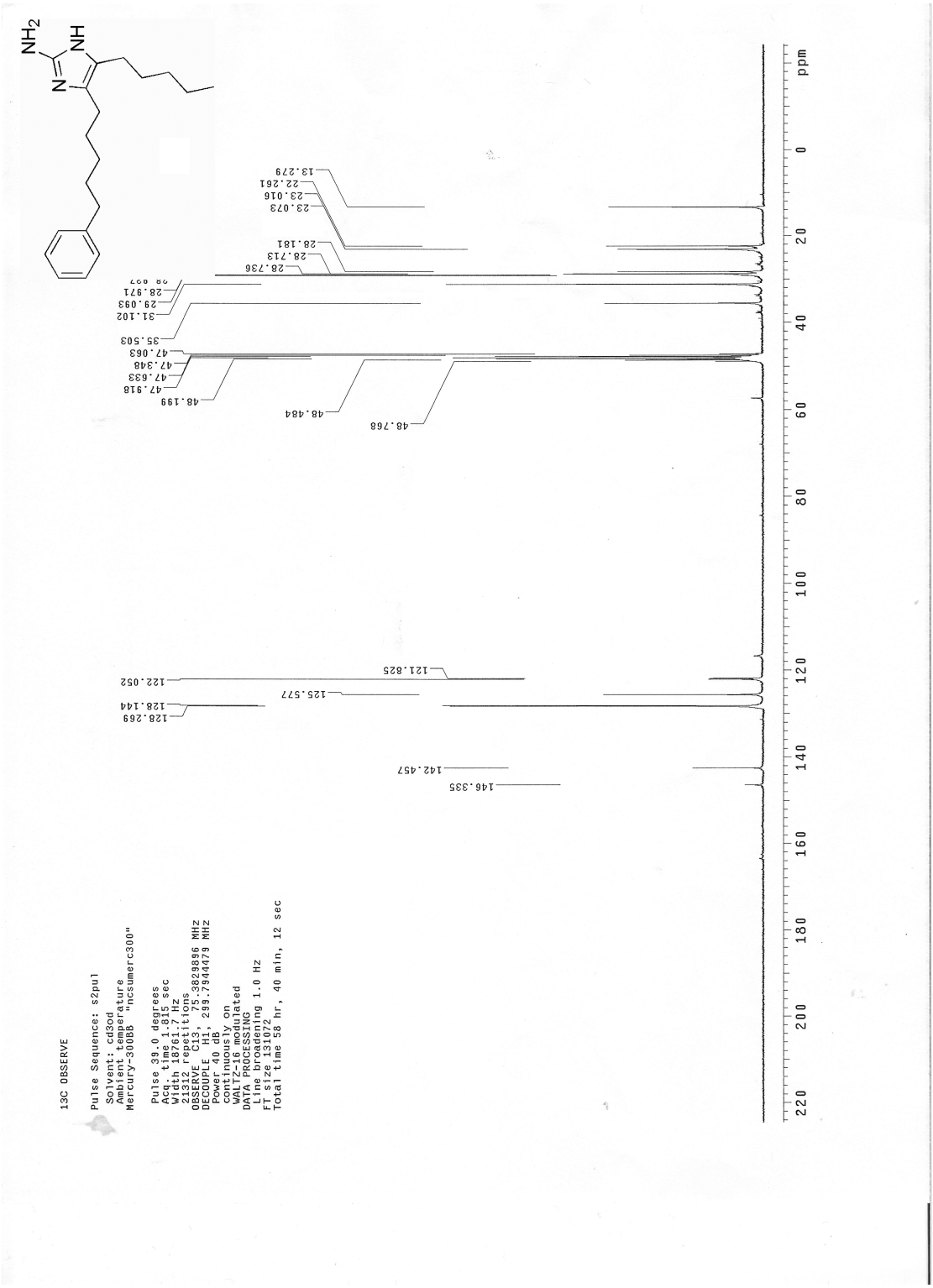

NH2
NH
N
1.103
1.128
1.153
1.276
1.314
1.324
1.337
1.542
1.567
1.581
1.592
1.606
1.630
1.656
2.399
2.407
2.423
2.433
2.448
2.570
2.594
2.619
3.286
3.301
3.306
3.851
4.864
7.119
7.143
7.199
7.220
7.248
ppm
0 1 2 3 4 5 6 7 8 9
4.63 3.00 3.85
2.98 2.48
0.28
6.74
STANDARD 1H OBSERVE
Pulse Sequence: s2pul
Solvent: cd3od
Ambient temperature
Mercury-300BB "ncsumerc300"
Relax. delay 1.000 sec
Pulse 36.0 degrees
Acq. time 1.895 sec
Width 4806.5 HZ
16 repetitions
OBSERVE H1, 299.7929913 MHz
DATA PROCESSING
FT size 32768
Total time 0 min, 49 sec

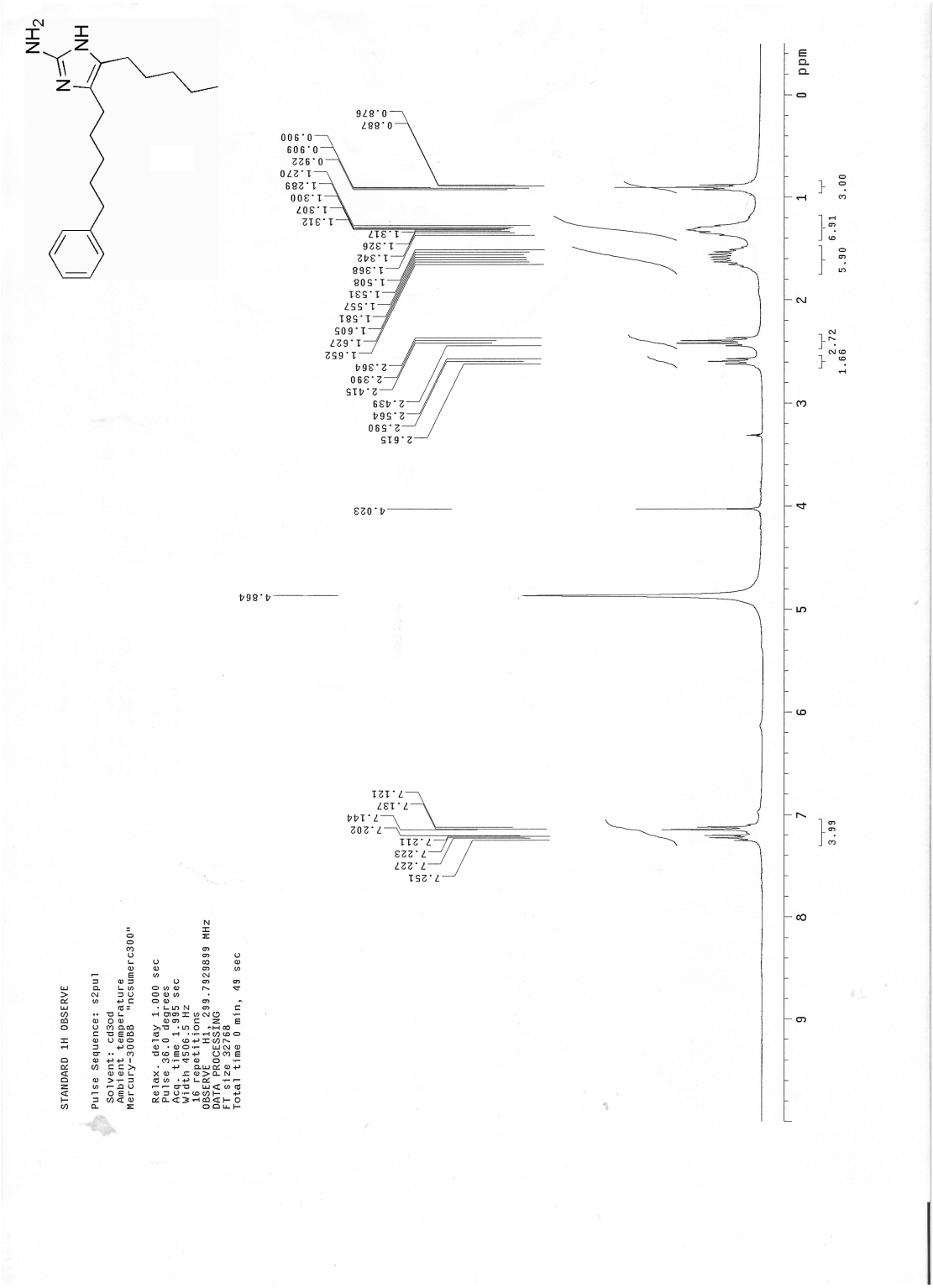

NH2
NH
N
13.3
12.
12
26.195
28.468
28.764
28.976
29.105
31.099
31.213
35.505
36.445
47.243
47.455
47.668
47.880
48.092
48.304
48.517
121.888
122.078
125.558
128.121
128.265
142.460
146.373
ppm
0
20
40
60
80
100
120
140
160
180
200
13C OBSERVE
Pulse Sequence: s2pul
Solvent: cd3od
Ambient temperature
Mercury-400BB "ncsumerc400"
Pulse 81.2 degrees
Acq. time 1.193 sec
Width 25000.0 Hz
9168 repetitions
OBSERVE C13, 100.6144469 MHz
DECOUPLE H1, 400.1387407 MHz
Power 44 dB
continuously on
WALTZ16 modulated
Data processing
Line broadening 1.0 Hz
FT size 65536
Total time 20 hr, 22 min, 2 sec

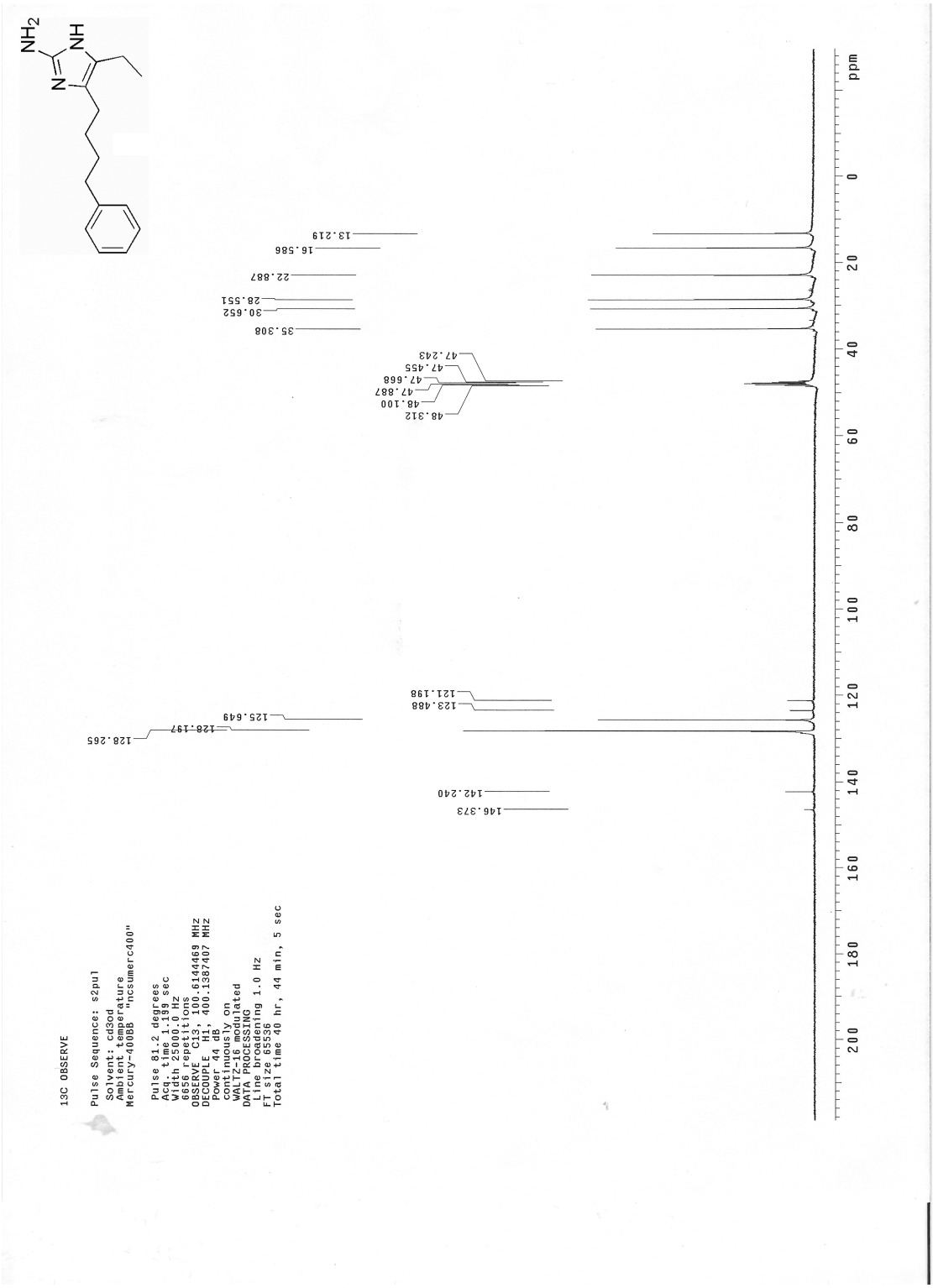

NH2
NH
N
0.919
0.894
0.943
1.564
2.378
2.402
2.426
2.598
3.304
4.821
7.124
7.148
7.204
7.228
ppm
0
1
2
3
4
5
6
7
8
9
2.69
2.24
6.13
3.15
2.10
5.00
STANDARD 1H OBSERVE
Pulse Sequence: s2pul
Solvent: cd3od
Ambient temperature
Mercury-300BB "ncsumerc300"
Relax. delay 1.000 sec
Pulse 30.0 degrees
Acq. time 1.819 sec
Width 4506.5 Hz
16 repetitions
OBSERVE H1, 299.7929913 MHz
DATA PROCESSING
FT size 32768
Total time 0 min, 49 sec

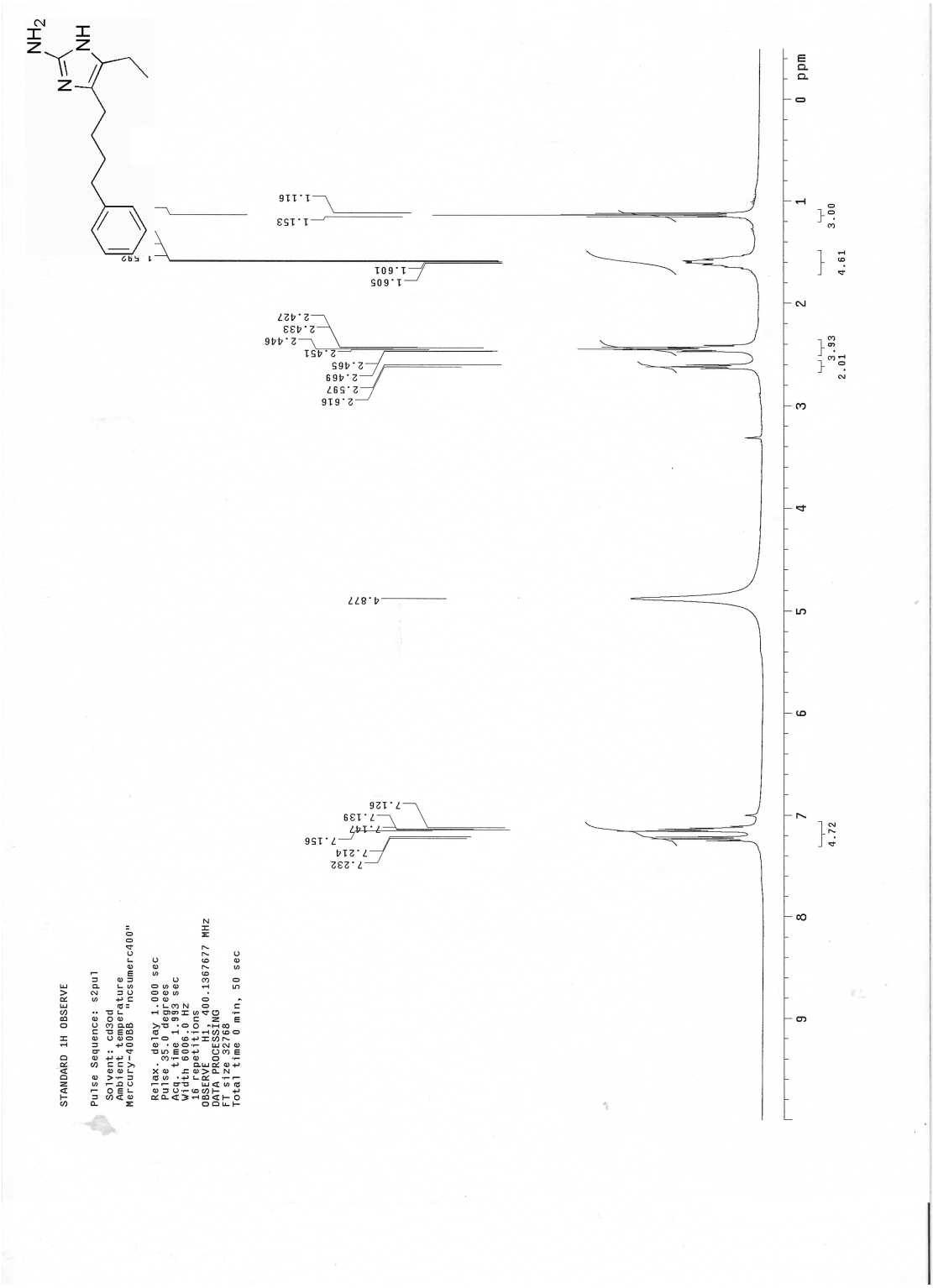

12.937
21.926
22.807
22.982
28.151
28.720
31.064
31.162
35.469
46.991
47.276
47.561
47.846
48.130
48.415
48.700
NH2
NH
N
122.113
121.897
125.550
128.106
128.235
142.446
146.388
ppm
0
20
40
60
80
100
120
140
160
180
200
220
13C OBSERVE
Pulse Sequence: s2pul
Solvent: cd3od
Ambient temperature
Mercury-300BB "ncsumerc300"
Pulse 39.0 degrees
Acq. time 1.815 sec
Width 18761.7 Hz
23920 repetitions
OBSERVE C13, 75.3829896 MHz
DECOUPLE H1, 299.7944479 MHz
Power 40 dB
continuously on
WALTZ16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 131072
Total time 20 hr, 32 min, 6 sec

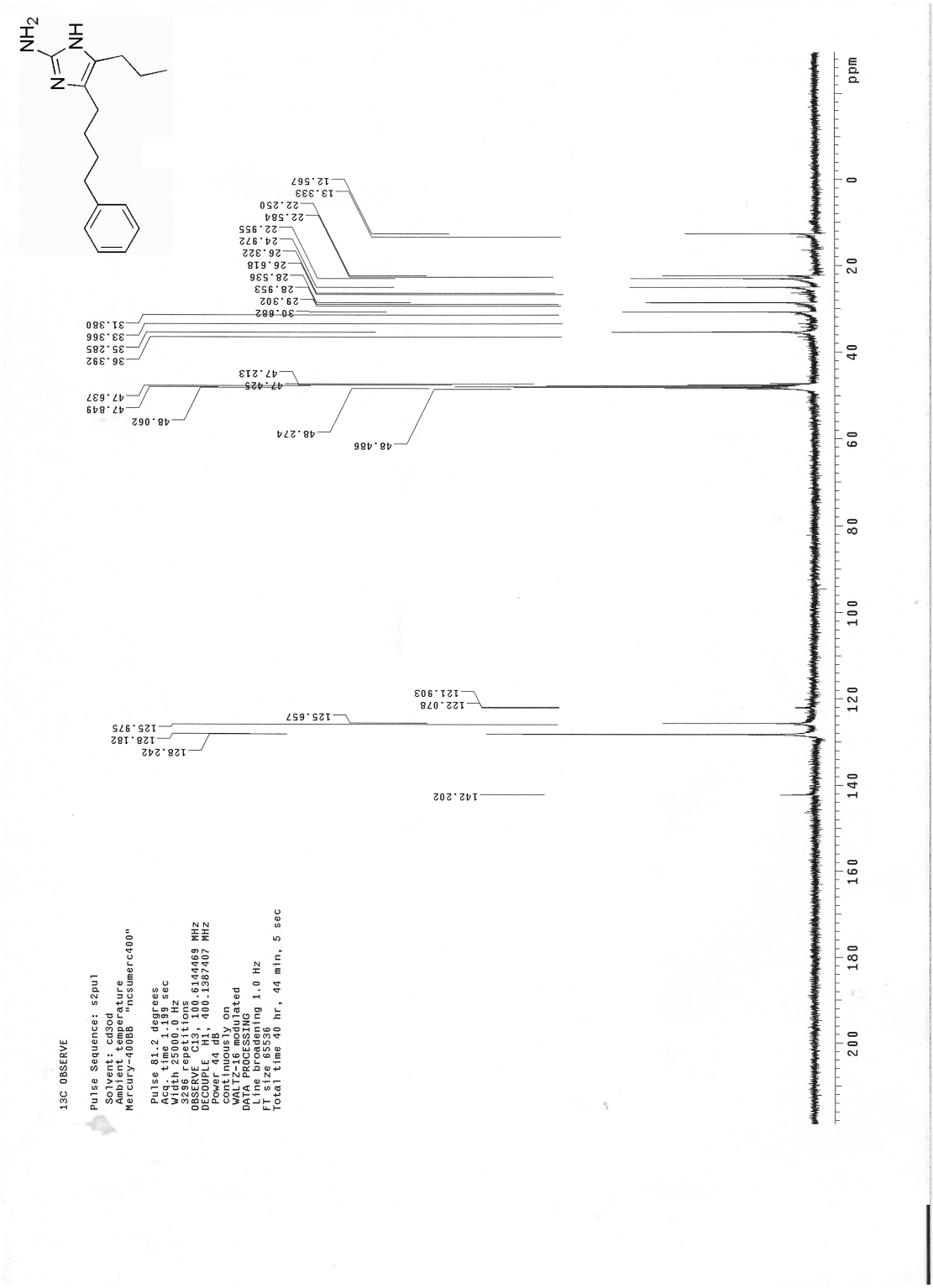

NH2
NH
N
0.918
0.936
0.948
0.955
1.305
1.323
1.327
1.343
1.360
1.513
1.533
1.564
1.583
1.602
1.622
1.642
1.660
2.388
2.408
2.427
2.445
2.585
2.605
2.623
3.306
3.310
3.315
4.025
4.825
7.132
7.135
7.153
7.215
7.233
7.237
7.252
ppm
3.00
4.10
5.94
1.87
3.23
0.31
4.44
STANDARD 1H OBSERVE
Pulse Sequence: s2pul
Solvent: cd3od
Ambient temperature
Mercury-400BB "ncsumerc400"
Relax. delay 1.000 sec
Pulse 35.0 degrees
Acq. time 1.993 sec
Width 6006.0 Hz
16 repetitions
OBSERVE H1, 400.1367677 MHz
DATA PROCESSING
FT size 32768
Total time 0 min, 50 sec

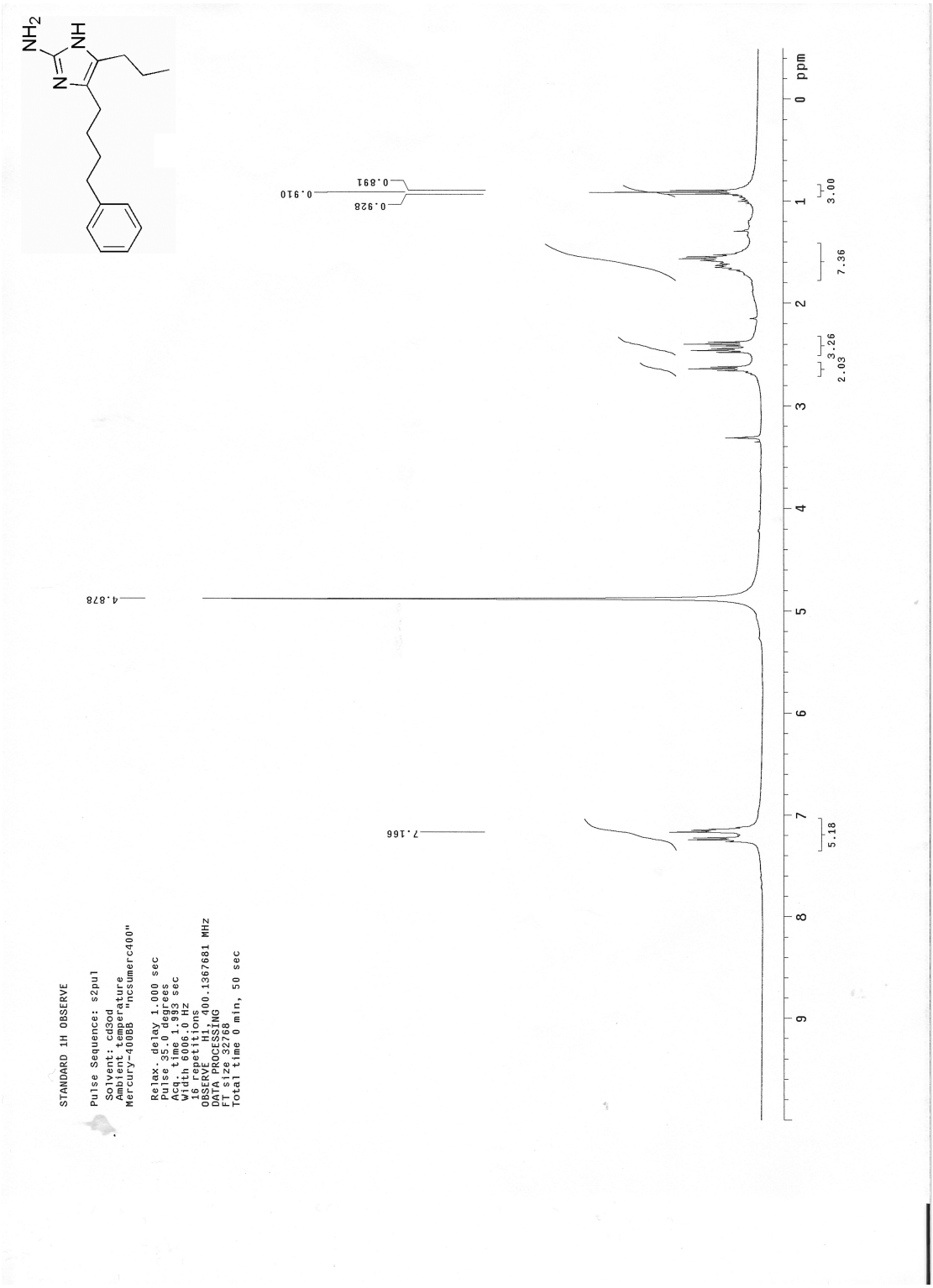

NH2
NH
N
13.279
22.261
23.016
23.073
28.181
28.713
28.736
28.971
29.093
31.102
35.503
47.063
47.348
47.633
47.918
48.199
48.484
48.768
121.825
122.052
125.577
128.144
128.269
142.457
146.335
ppm
0
20
40
60
80
100
120
140
160
180
200
220
13C OBSERVE
Pulse Sequence: s2pul
Solvent: cd3od
Ambient temperature
Mercury-300BB "ncsumerc300"
Pulse 39.0 degrees
Acq. time 1.815 sec
Width 18761.7 Hz
21312 repetitions
OBSERVE C13, 75.3829896 MHz
DECOUPLE H1, 299.7944479 MHz
Power 40 dB
continuously on
WALTZ16 modulated
Data processing
Line broadening 1.0 Hz
FT size 131072
Total time 58 hr, 40 min, 12 sec

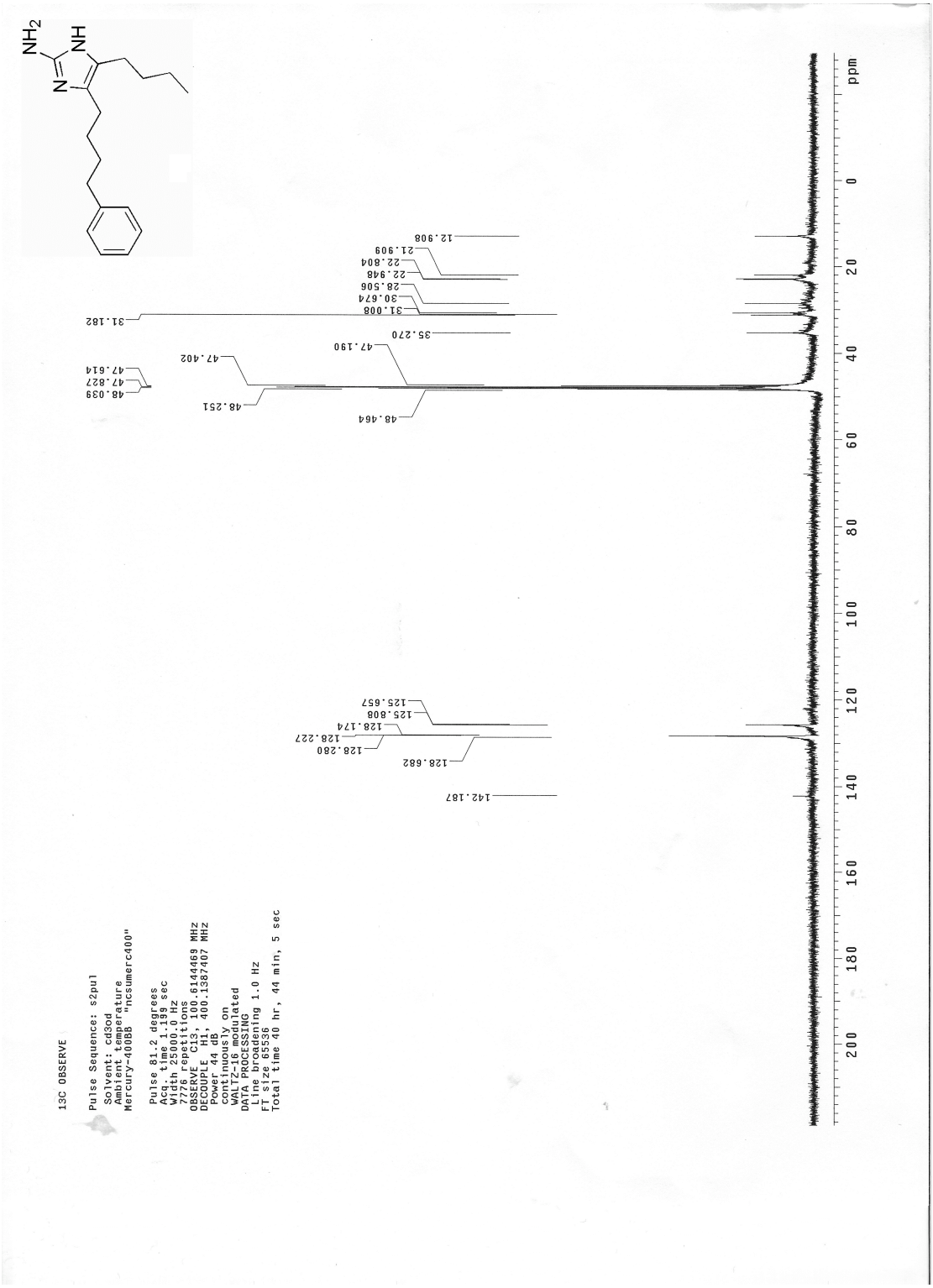

NH2
NH
N
0.876
0.887
0.900
0.909
0.922
1.270
1.289
1.300
1.307
1.312
1.317
1.326
1.342
1.368
1.508
1.531
1.557
1.581
1.605
1.627
1.652
2.364
2.390
2.415
2.439
2.564
2.590
2.615
4.023
4.864
7.121
7.137
7.144
7.202
7.211
7.223
7.227
7.251
ppm
3.00
6.91
5.90
2.72
1.66
3.99
STANDARD 1H OBSERVE
Pulse Sequence: s2pul
Solvent: cd3od
Ambient temperature
Mercury-300BB "ncsumerc300"
Relax. delay 1.000 sec
Pulse 36.0 degrees
Acq. time 1.895 sec
Width 4506.5 Hz
16 repetitions
OBSERVE H1, 299.7929899 MHz
DATA PROCESSING
FT size 32768
Total time 0 min, 49 sec

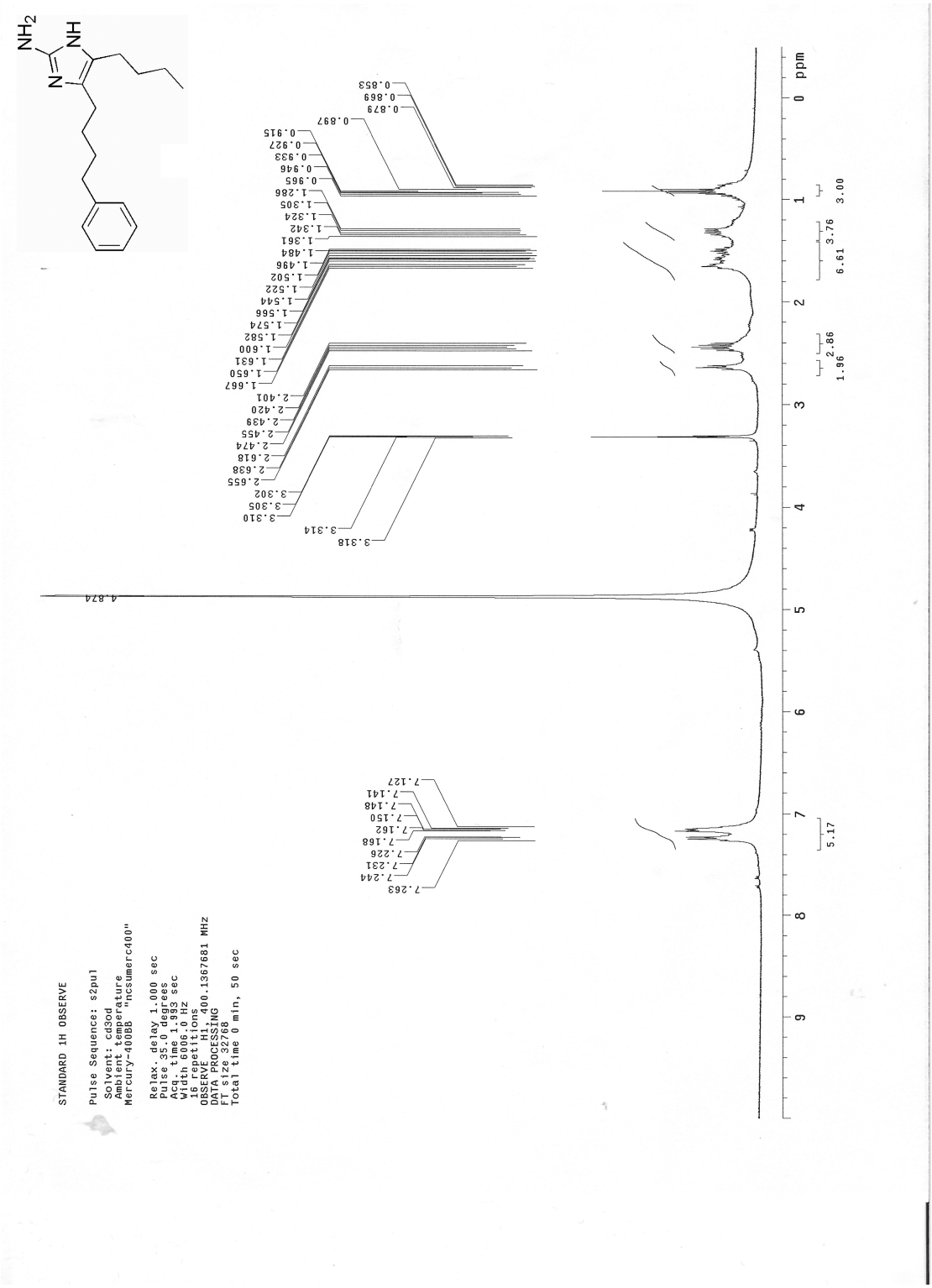

NH2
NH
N
13.219
16.586
22.887
28.551
30.652
35.308
47.243
47.455
47.668
47.887
48.100
48.312
121.198
123.488
125.649
128.197
128.265
142.240
146.373
ppm
0
20
40
60
80
100
120
140
160
180
200
13C OBSERVE
Pulse Sequence: s2pul
Solvent: cd3od
Ambient temperature
Mercury-400BB "ncsumerc400"
Pulse 81.2 degrees
Acq. time 1.339 sec
Width 25000.0 Hz
6656 repetitions
OBSERVE C13, 100.6144469 MHz
DECOUPLE H1, 400.1387407 MHz
Power 44 dB
continuously on
WALTZ16 modulated
Data processing
Line broadening 1.0 Hz
FT size 65536
Total time 40 hr, 44 min, 5 sec

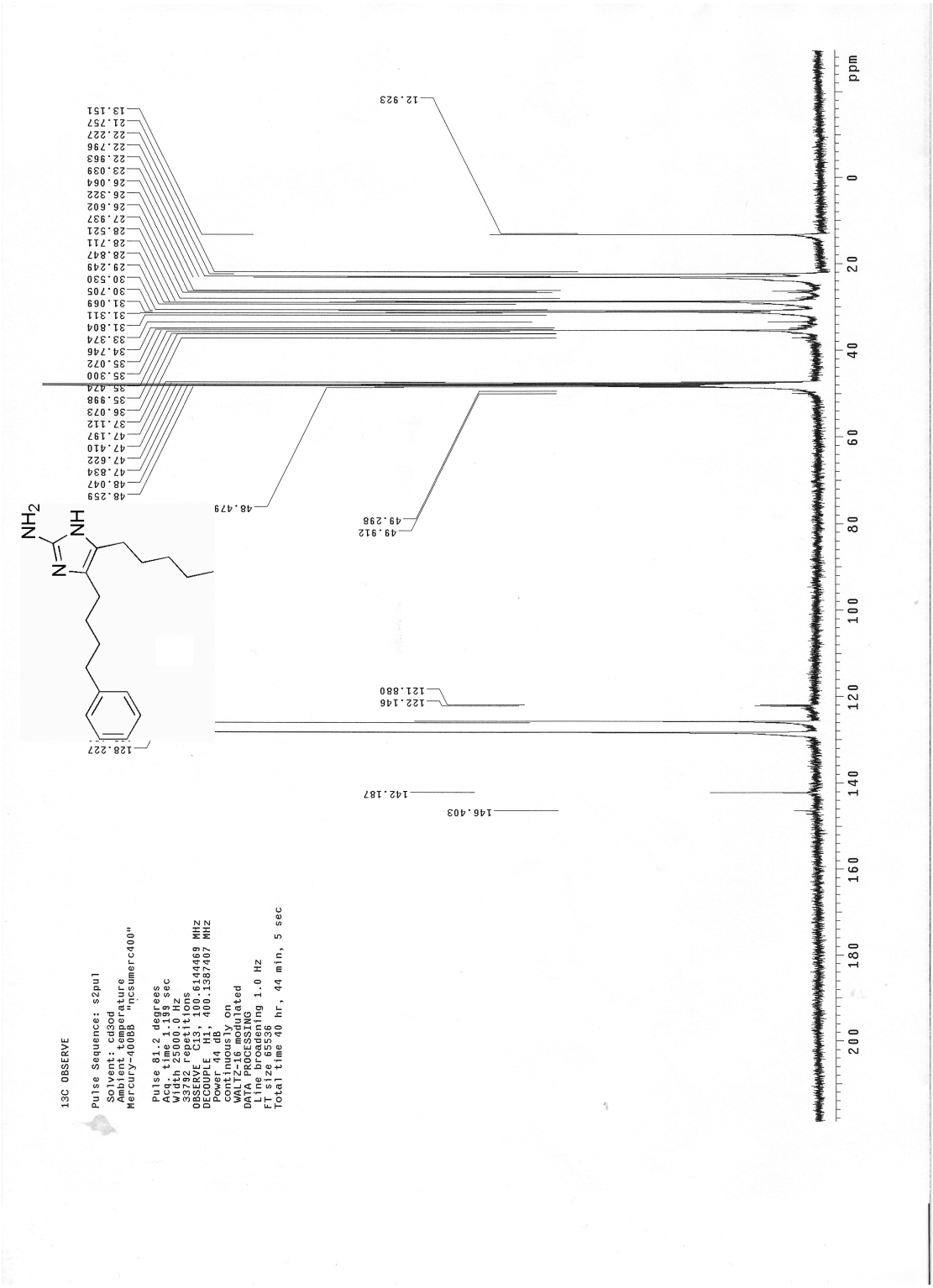

NH2
NH
N
1.592
1.116
1.153
1.601
1.605
2.427
2.433
2.446
2.451
2.465
2.469
2.597
2.616
4.877
7.126
7.139
7.147
7.156
7.214
7.232
ppm
3.00
4.61
3.93
2.01
4.72
STANDARD 1H OBSERVE
Pulse Sequence: s2pul
Solvent: cd3od
Ambient temperature
Mercury-400BB "ncsumerc400"
Relax. delay 1.000 sec
Pulse 35.0 degrees
Acq. time 1.638 sec
Width 6006.0 Hz
16 repetitions
OBSERVE H1, 400.1367677 MHz
DATA PROCESSING
FT size 32768
Total time 0 min, 50 sec

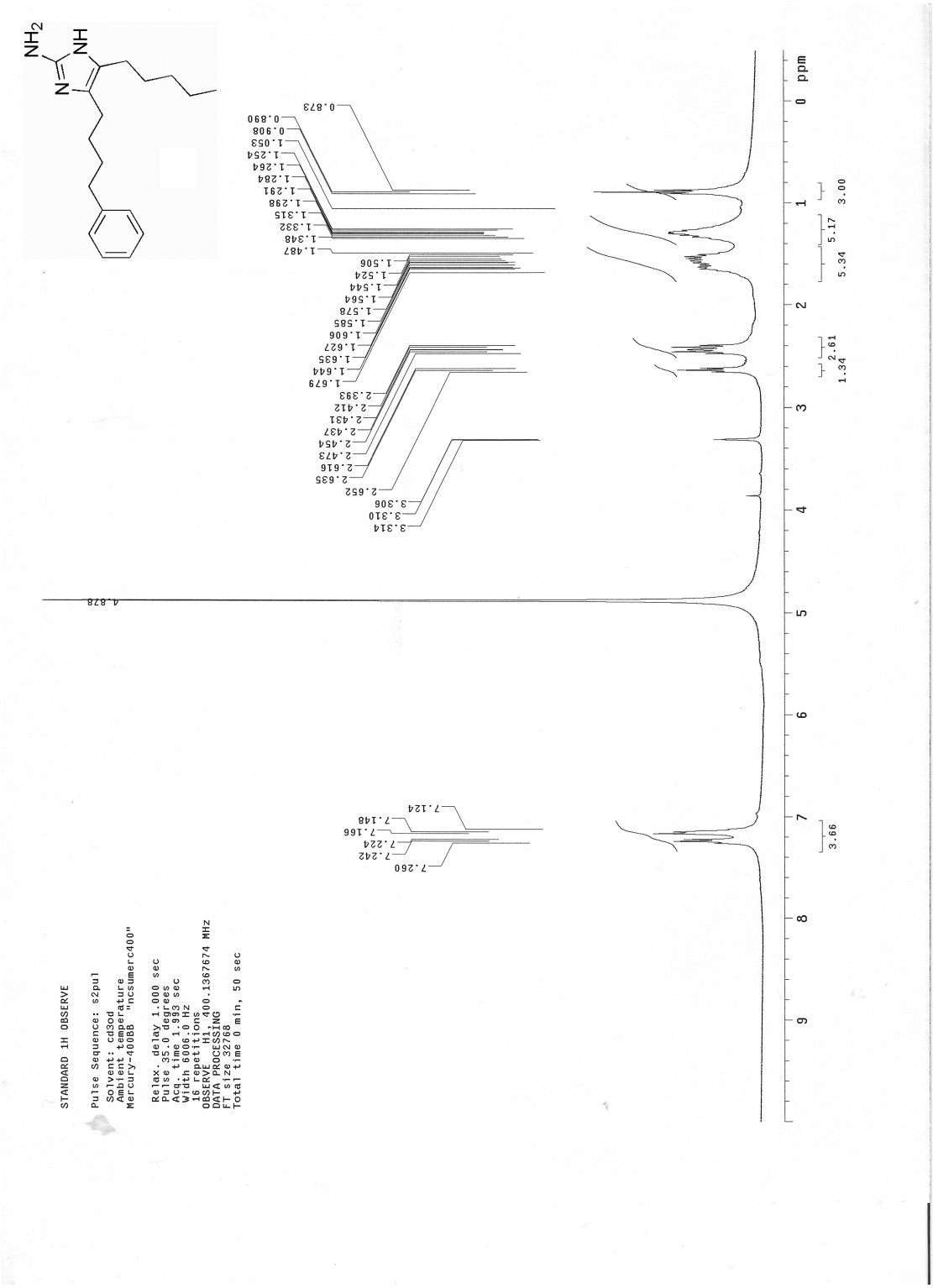

NH2
NH
N
12.567
13.333
22.250
22.584
22.955
24.972
26.322
26.618
28.536
28.953
29.302
30.682
31.380
33.366
35.285
36.392
47.213
47.425
47.637
47.849
48.062
48.274
48.486
121.903
122.078
125.657
125.975
128.182
128.242
142.202
ppm
0
20
40
60
80
100
120
140
160
180
200
13C OBSERVE
Pulse Sequence: s2pul
Solvent: cd3od
Ambient temperature
Mercury-400BB "ncsumerc400"
Pulse 81.2 degrees
Acq. time 1.193 sec
Width 24000.0 Hz
3296 repetitions
OBSERVE C13, 100.6144469 MHz
DECOUPLE H1, 400.1387407 MHz
Power 44 dB
continuously on
WALTZ16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 65536
Total time 40 hr, 44 min, 5 sec

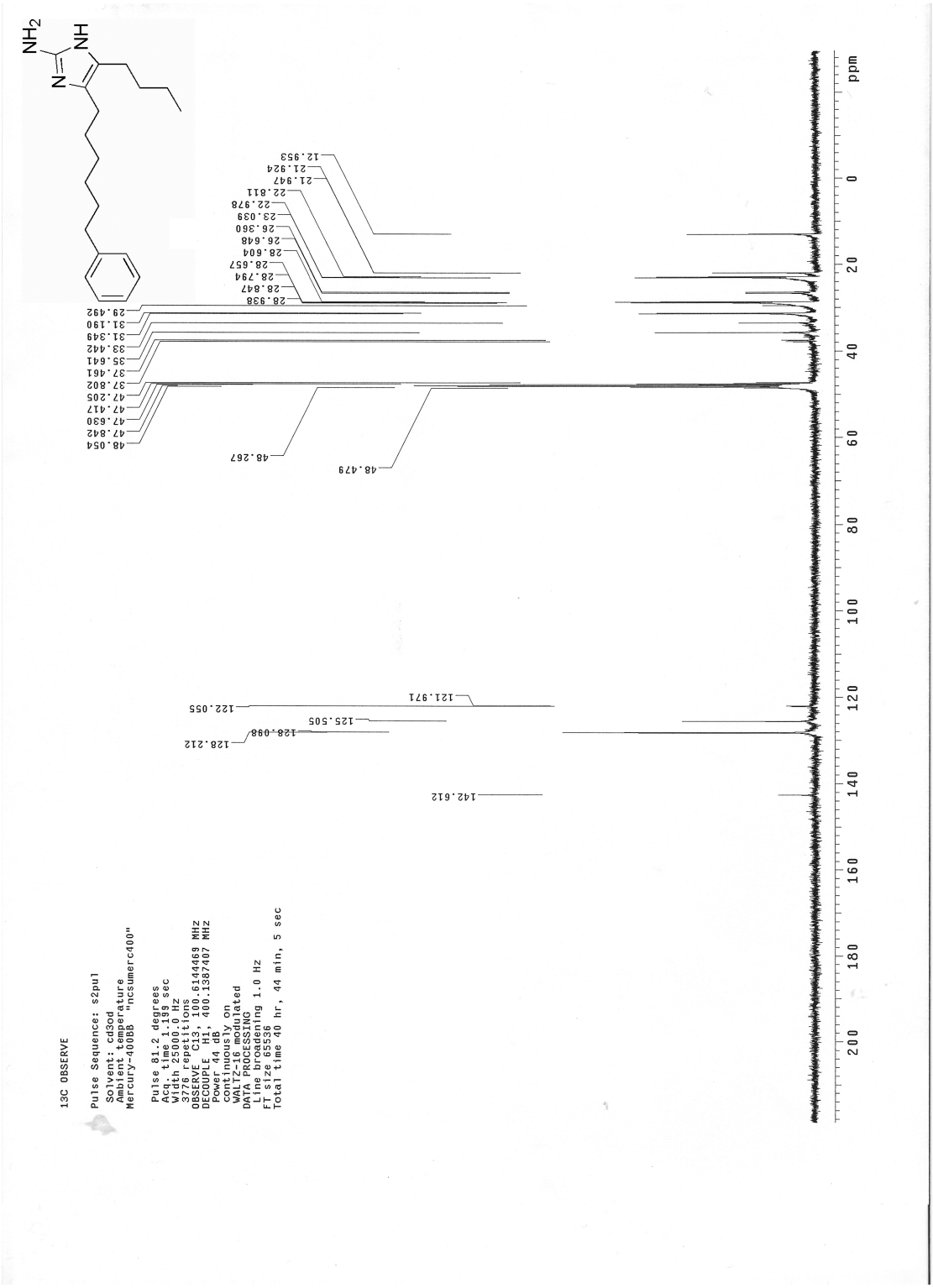

NH2
NH
N
0.928
0.910
0.891
4.878
7.166
3.00
7.36
3.26
2.03
5.18
ppm
STANDARD 1H OBSERVE
Pulse Sequence: s2pul
Solvent: cdsod
Ambient temperature
Mercury-400BB "ncsumerc400"
Relax. delay 1.000 sec
Pulse 35.0 degrees
Acq. time 1.638 sec
Width 6006.0 Hz
16 repetitions
OBSERVE H1, 400.1367681 MHz
DATA PROCESSING
FT size 32768
Total time 0 min, 50 sec

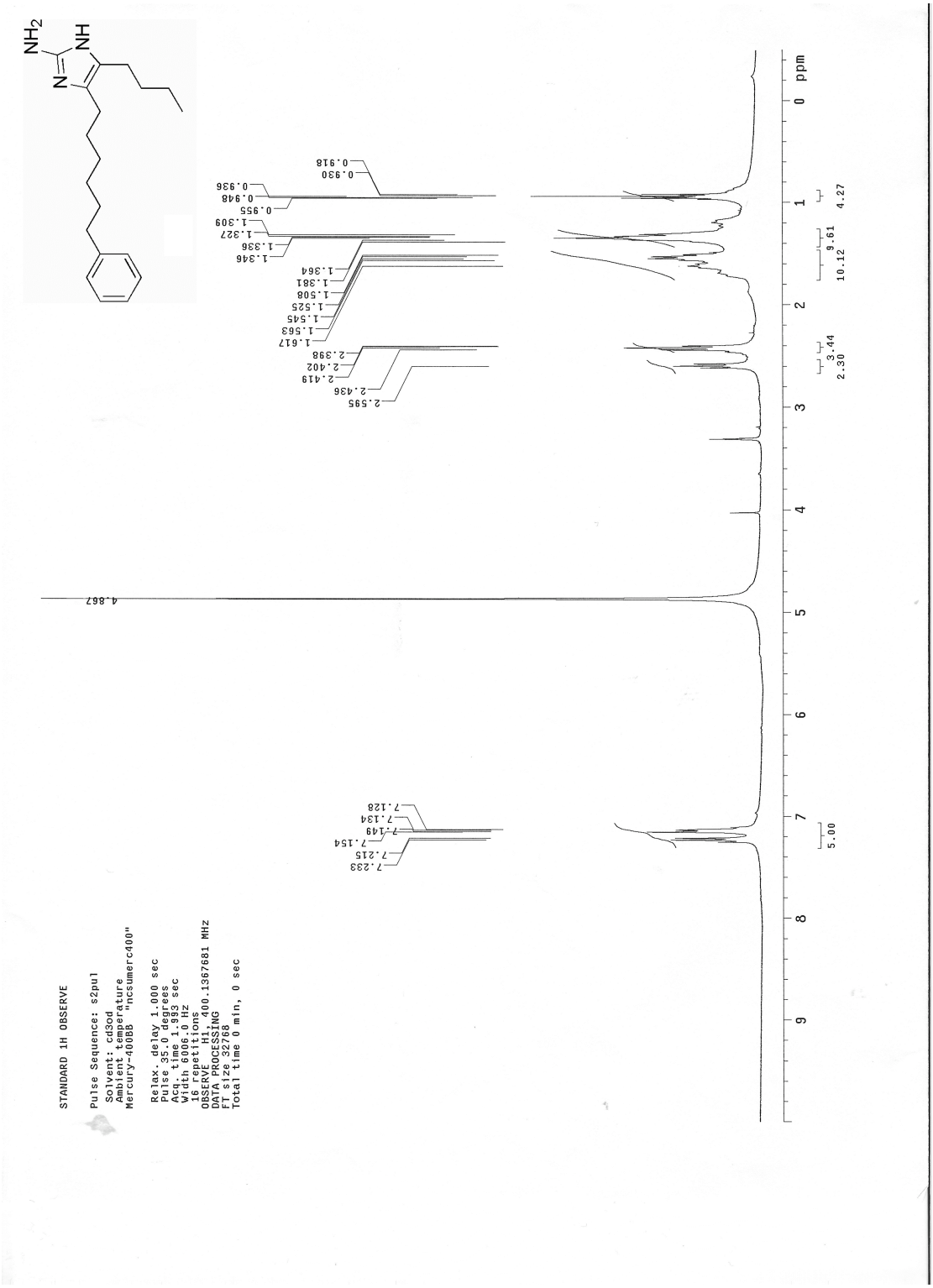


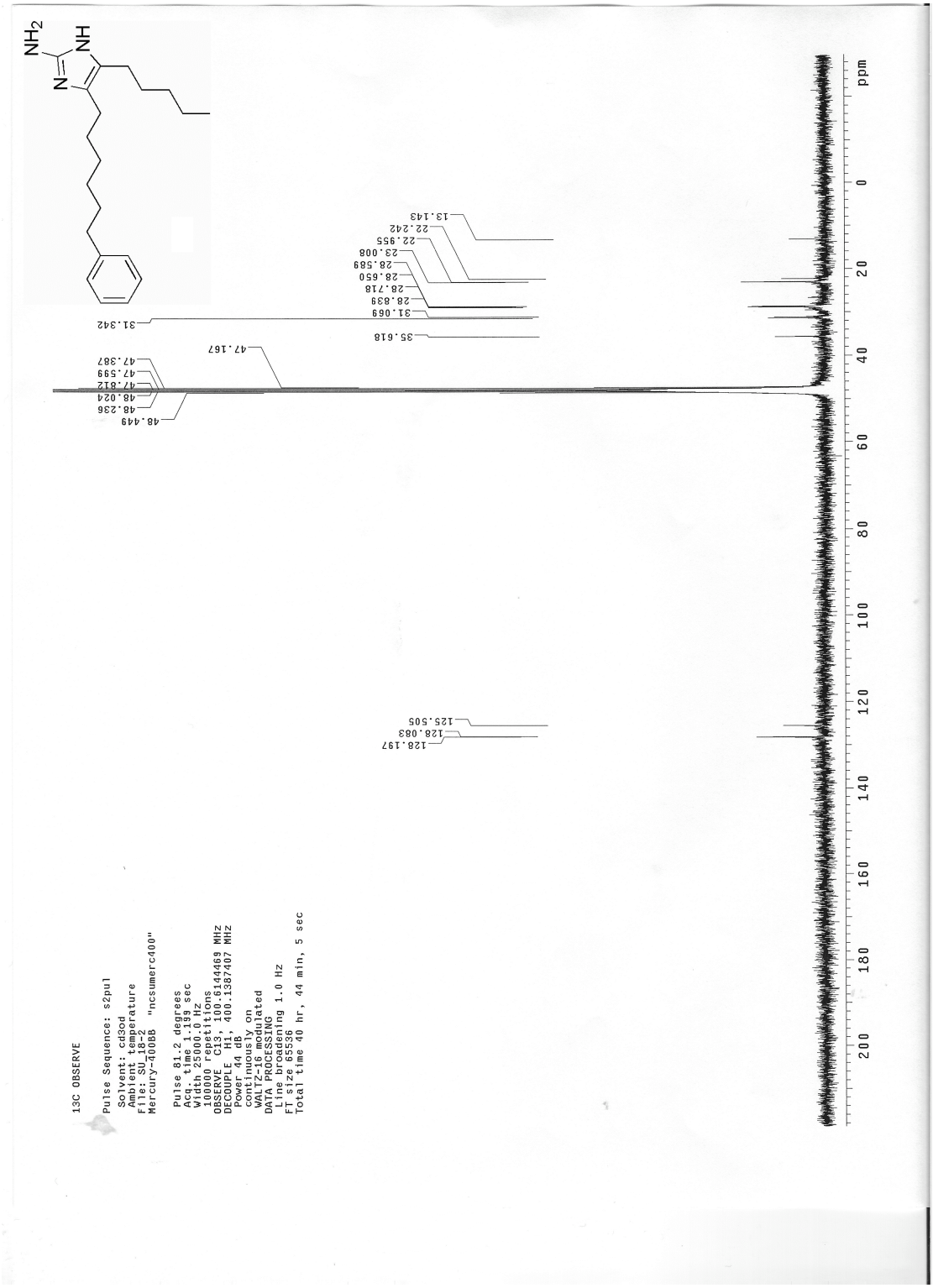

NH2
NH
N
0.853
0.869
0.879
0.897
0.915
0.927
0.933
0.946
0.965
1.286
1.305
1.324
1.342
1.361
1.484
1.496
1.502
1.522
1.544
1.566
1.574
1.582
1.600
1.631
1.650
1.667
2.401
2.420
2.439
2.455
2.474
2.618
2.638
2.655
3.302
3.305
3.310
3.314
3.318
4.824
7.127
7.141
7.148
7.150
7.162
7.166
7.226
7.231
7.244
7.263
ppm
3.00
3.76
6.61
2.86
1.96
5.17
STANDARD 1H OBSERVE
Pulse Sequence: s2pul
Solvent: cd3od
Ambient temperature
Mercury-400BB "ncsumerc400"
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.983 sec
Width 6006.0 Hz
16 repetitions
OBSERVE H1, 400.1367681 MHz
DATA PROCESSING
FT size 32768
Total time 0 min, 50 sec

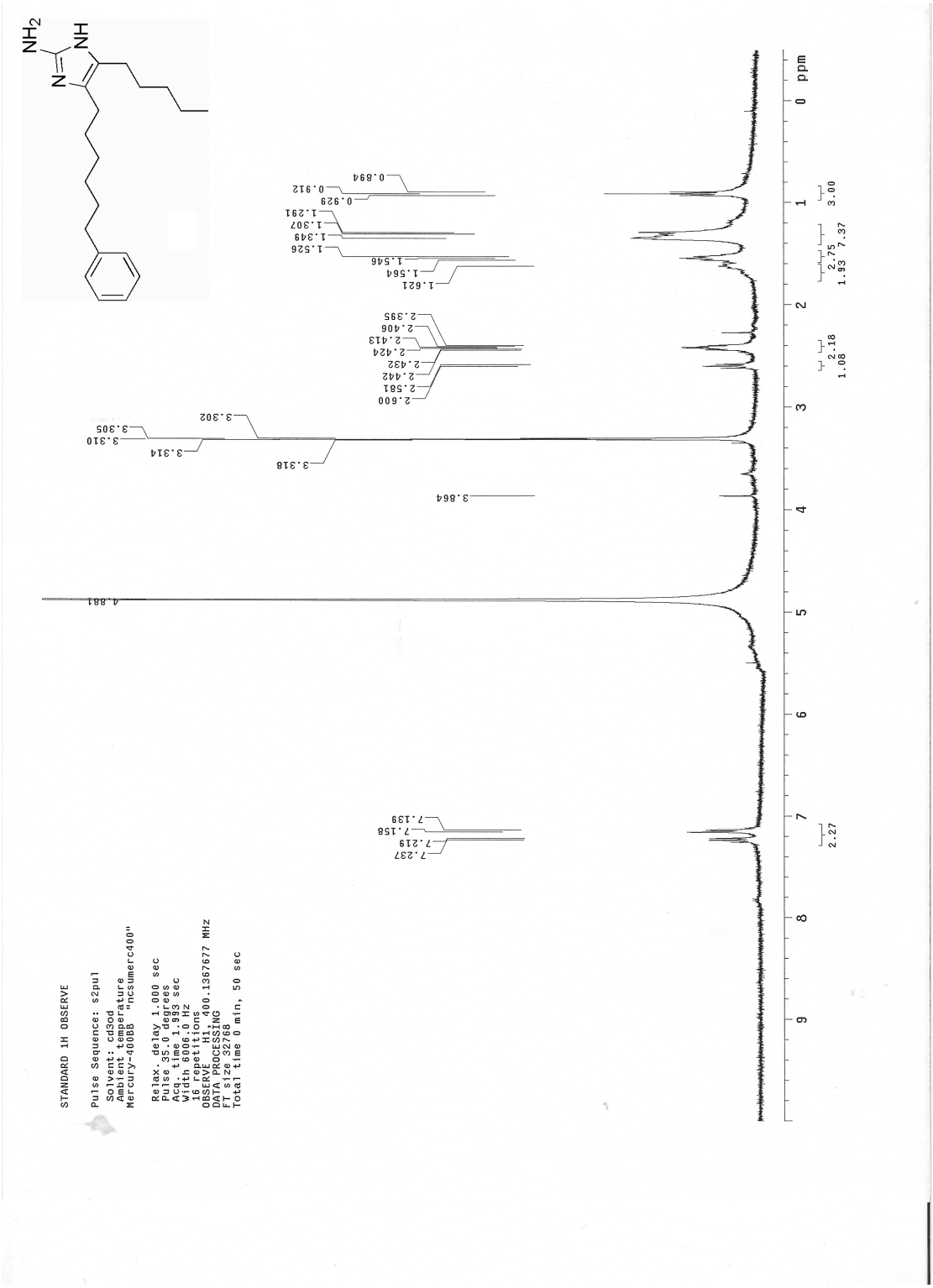

13C OBSERVE
Pulse Sequence: s2pul
Solvent: cd3od
Ambient temperature
Mercury-400BB "hcsumerc400"
Pulse 81.2 degrees
Acq. time 1.199 sec
Width 25000.0 Hz
33792 repetitions
OBSERVE C13, 100.6144469 MHz
DECOUPLE H1, 400.1387407 MHz
Power 44 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 65536
Total time 40 hr, 44 min, 5 sec
ppm
NH2
NH
N
13.151
21.757
22.227
22.796
22.963
23.039
26.064
26.322
26.602
27.937
28.521
28.711
28.847
29.249
30.530
30.705
31.069
31.311
31.804
33.374
34.746
35.072
35.300
35.424
35.998
36.073
37.112
47.197
47.410
47.622
47.834
48.047
48.259
48.479
49.298
49.912
121.880
122.146
128.227
142.187
146.403

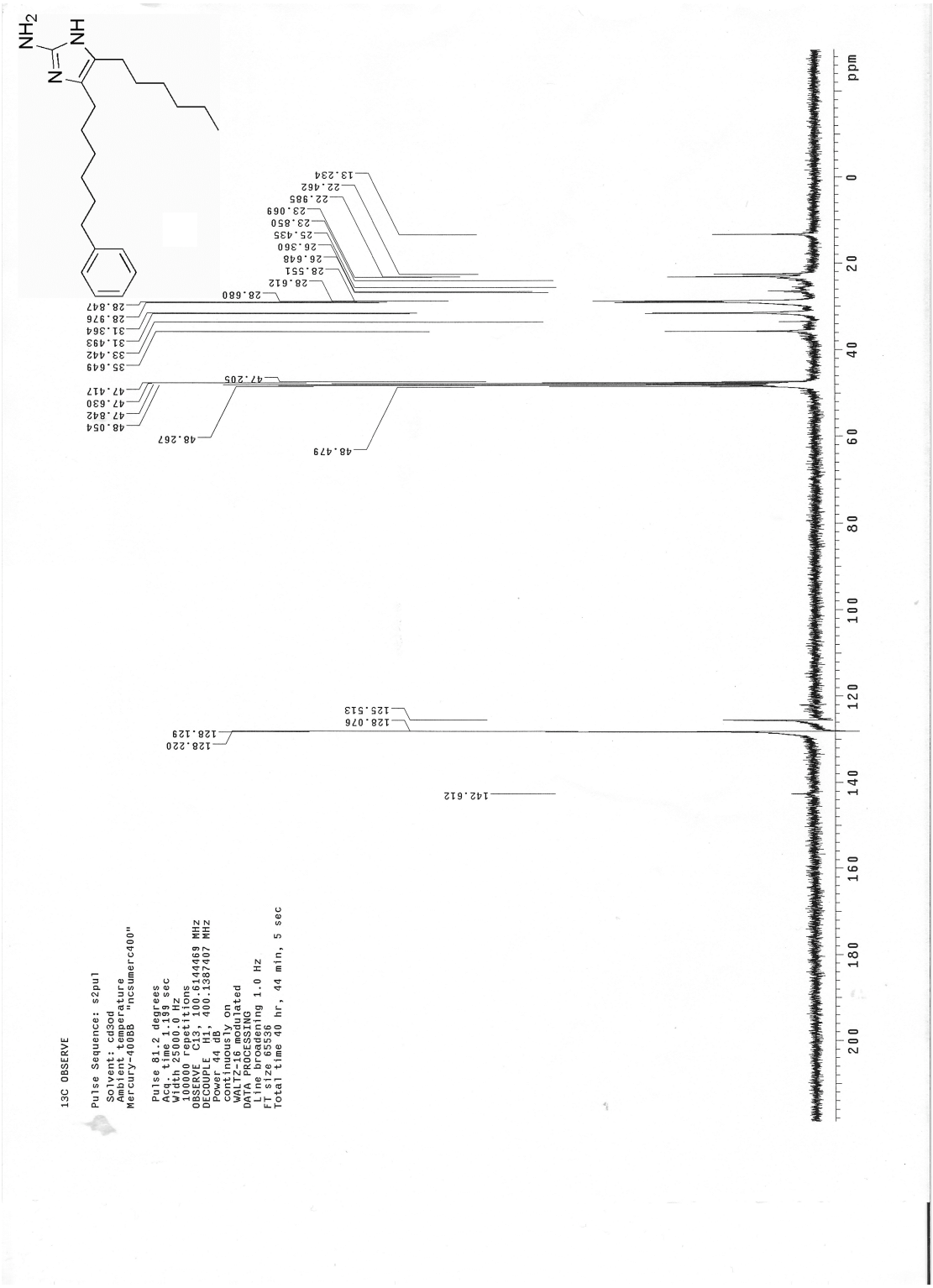

NH2
NH
N
0.873
0.890
0.908
1.053
1.254
1.264
1.284
1.291
1.298
1.315
1.332
1.348
1.487
1.506
1.524
1.544
1.564
1.578
1.585
1.606
1.627
1.635
1.644
1.679
2.393
2.412
2.431
2.437
2.454
2.473
2.616
2.635
2.652
3.306
3.310
3.314
4.878
7.124
7.148
7.166
7.224
7.242
7.260
ppm
3.00
5.17
5.34
2.61
1.34
3.66
STANDARD 1H OBSERVE
Pulse Sequence: s2pul
Solvent: cd3od
Ambient temperature
Mercury-400BB "ncsumerc400"
Relax. delay 1.000 sec
Pulse 85.0 degrees
Acq. time 1.892 sec
Width 6006.0 Hz
16 repetitions
OBSERVE H1, 400.1367674 MHz
DATA PROCESSING
FT size 32768
Total time 0 min, 50 sec

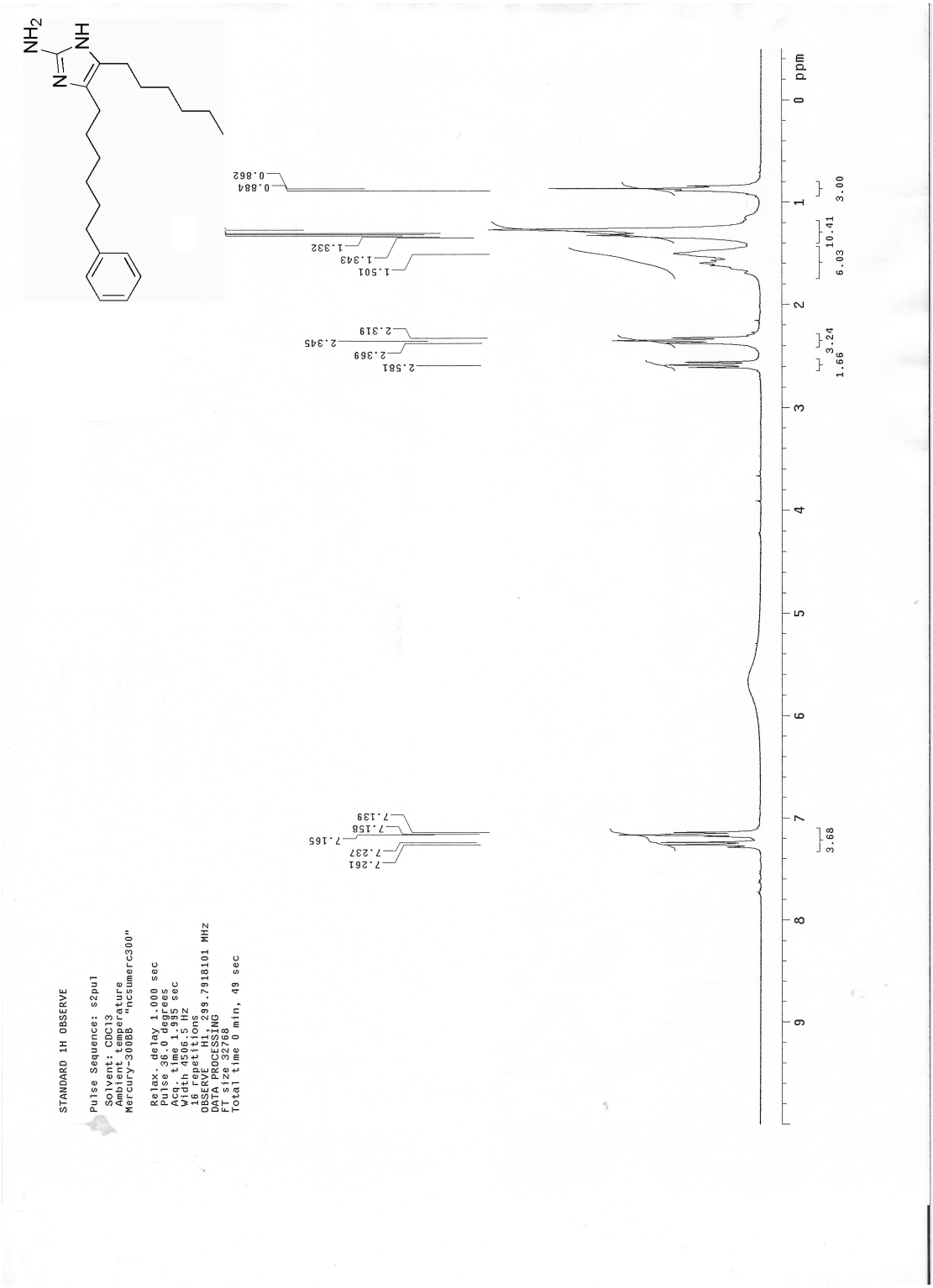

NH2
NH
N
12.953
21.924
21.947
22.811
22.978
23.039
26.360
26.648
28.604
28.657
28.794
28.847
28.938
29.492
31.190
31.349
33.442
35.641
37.461
37.802
47.205
47.417
47.630
47.842
48.054
48.267
48.479
121.971
122.055
125.505
128.088
128.212
142.612
ppm
0
20
40
60
80
100
120
140
160
180
200
13C OBSERVE
Pulse Sequence: s2pul
Solvent: cd3od
Ambient temperature
Mercury-400BB "ncsumerc400"
Pulse 81.2 degrees
Acq. time 1.193 sec
Width 25000.0 Hz
3776 repetitions
OBSERVE C13, 100.6144469 MHz
DECOUPLE H1, 400.1387407 MHz
Power 44 dB
continuously on
WALTZ-16 modulated
Data processing
Line broadening 1.0 Hz
FT size 65536
Total time 40 hr, 44 min, 5 sec

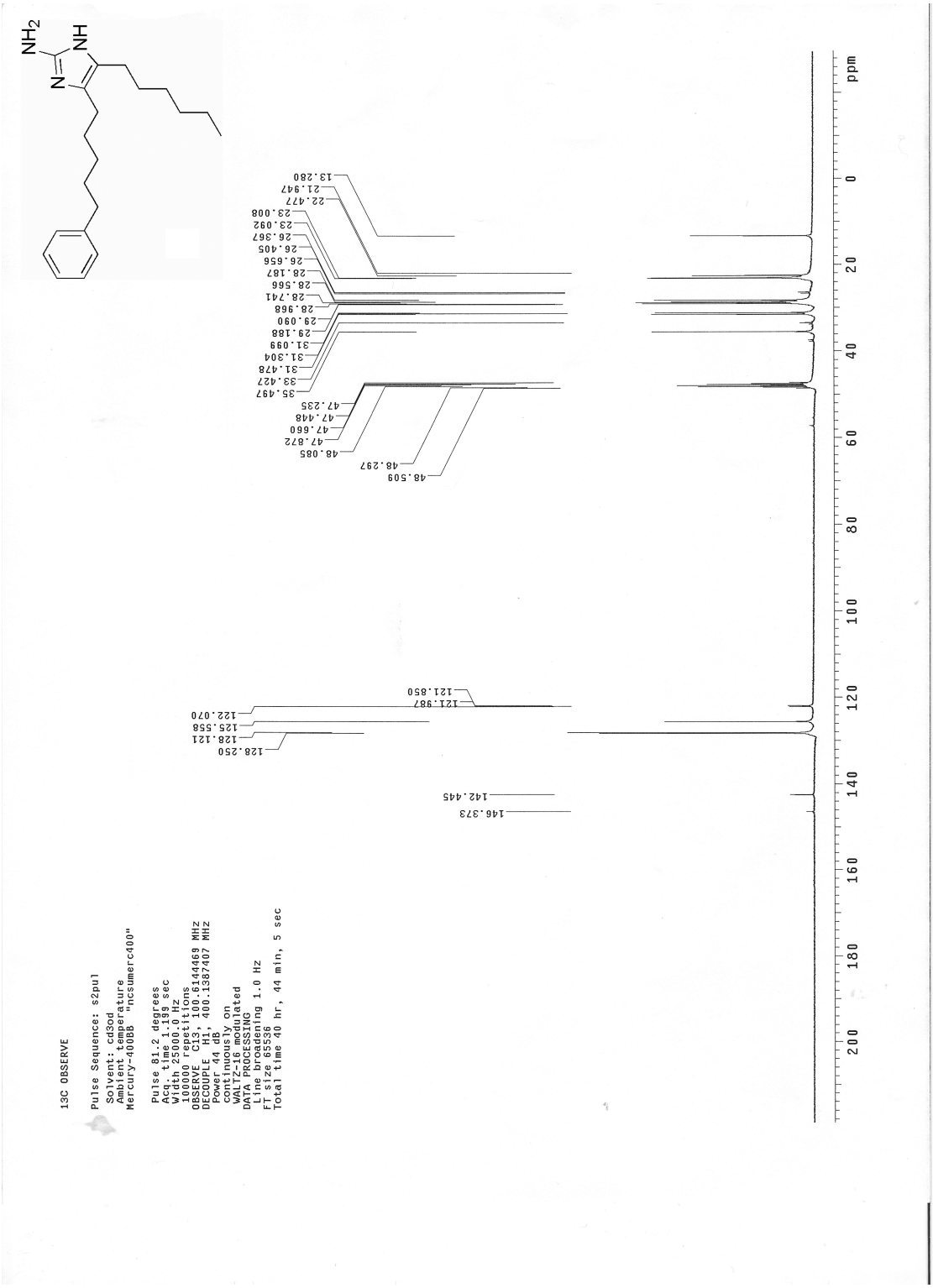

NH2
NH
N
0.918
0.930
0.936
0.948
0.955
1.309
1.327
1.336
1.346
1.364
1.381
1.508
1.525
1.545
1.563
1.617
2.398
2.402
2.419
2.436
2.595
4.867
7.128
7.134
7.149
7.154
7.215
7.233
STANDARD 1H OBSERVE
Pulse Sequence: s2pul
Solvent: cd3od
Ambient temperature
Mercury-400BB "ncstumerc400"
Relax. delay 1.000 sec
Pulse 35.0 degrees
Acq. time 1.638 sec
Width 6006.0 Hz
16 repetitions
OBSERVE H1, 400.1367681 MHz
DATA PROCESSING
FT size 32768
Total time 0 min, 0 sec
ppm
0
1
2
3
4
5
6
7
8
9
4.27
9.61
10.12
3.44
2.30
5.00

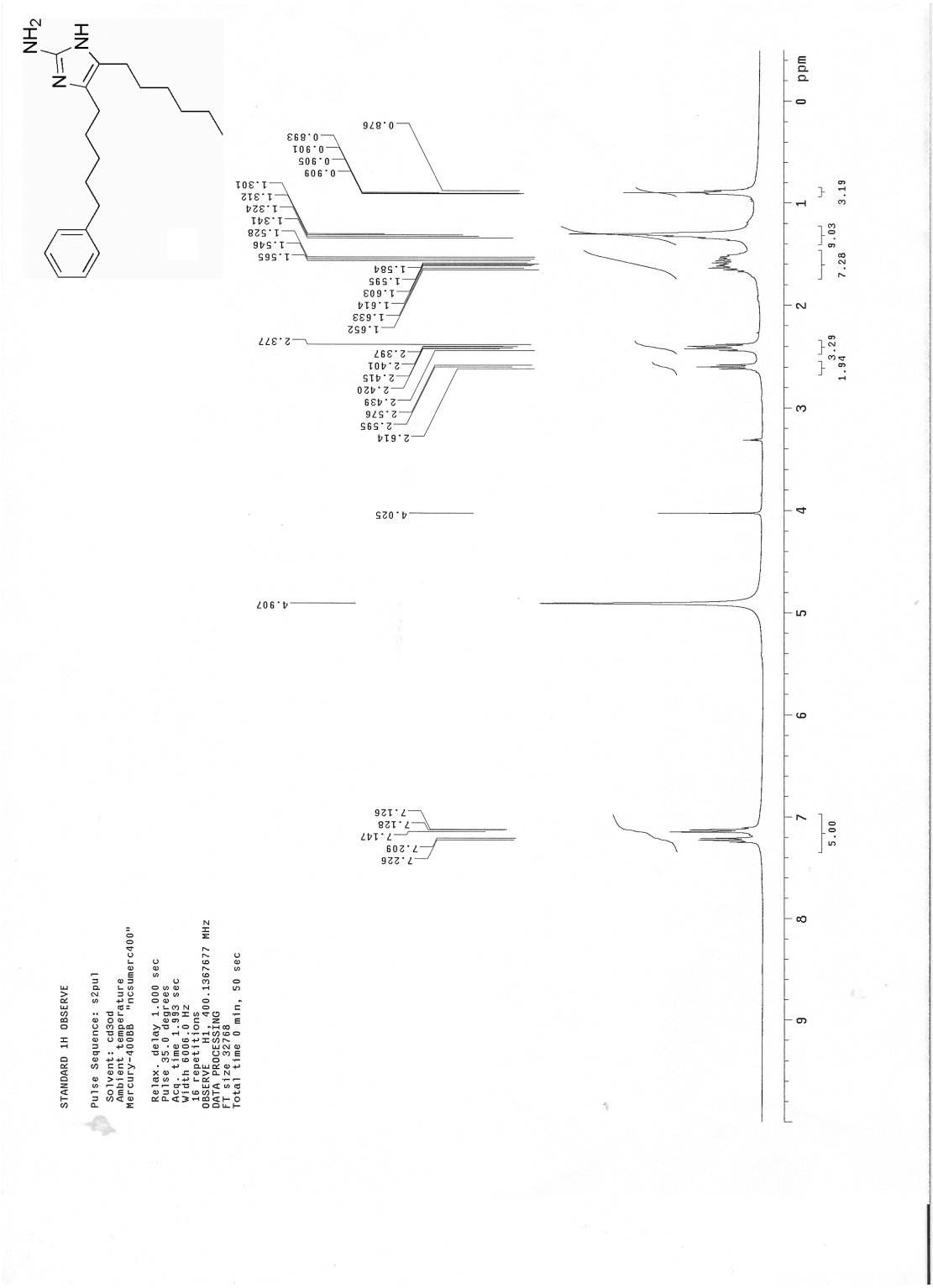

NH2
NH
N
13.143
22.242
22.955
23.008
28.589
28.650
28.718
28.839
31.069
35.618
31.342
47.167
47.387
47.599
47.812
48.024
48.236
48.449
125.505
128.083
128.197
ppm
0
20
40
60
80
100
120
140
160
180
200
13C OBSERVE
Pulse Sequence: s2pul
Solvent: cd3od
Ambient temperature
File: SU_1802
Mercury-400BB "ncsumerc400"
Pulse 81.2 degrees
Acq. time 1.139 sec
Width 25000.0 Hz
100000 repetitions
OBSERVE C13, 100.6144469 MHz
DECOUPLE H1, 400.1387407 MHz
Power 44 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 65536
Total time 40 hr, 44 min, 5 sec

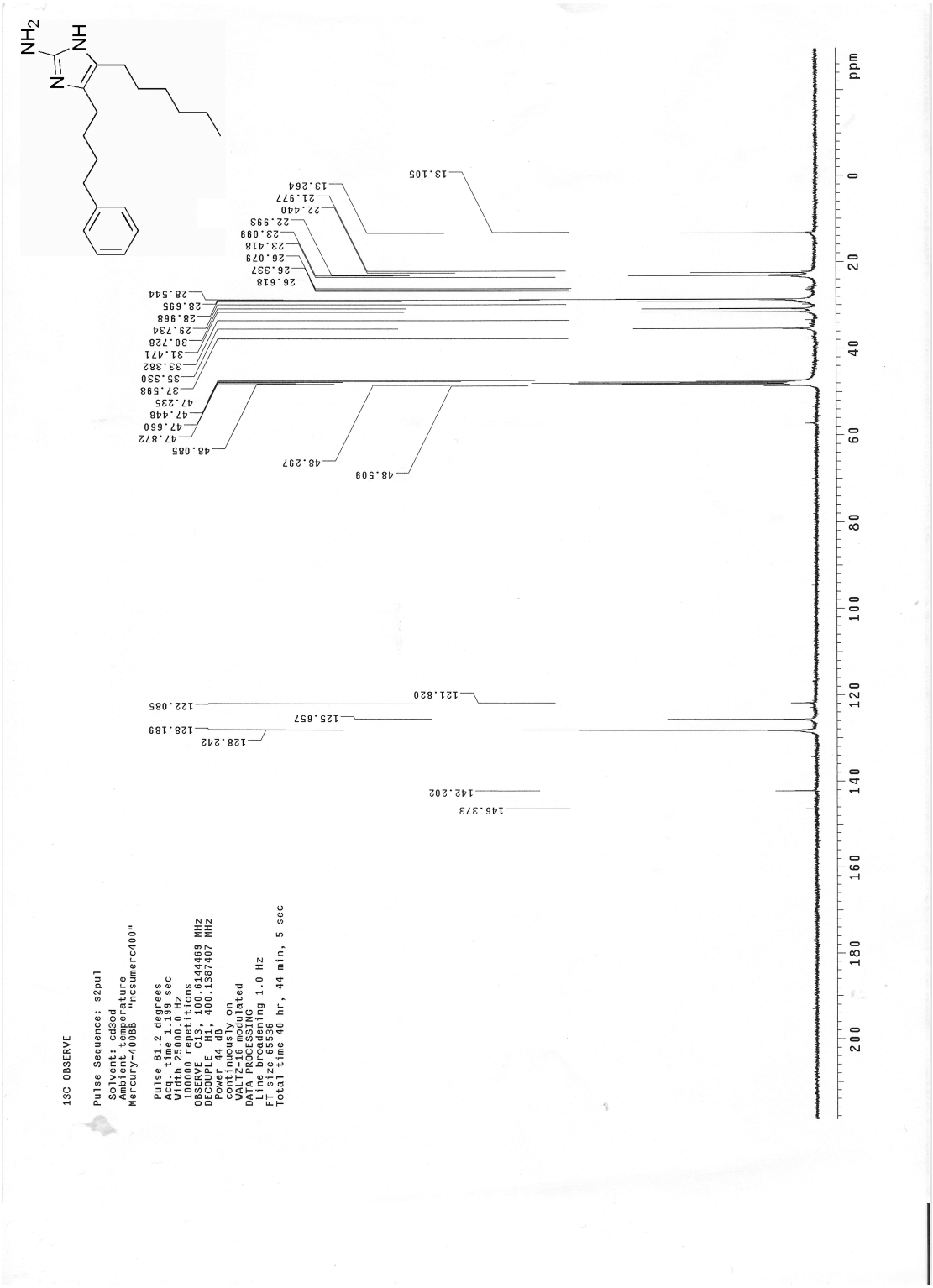

NH2
NH
N
0.894
0.912
0.929
1.291
1.307
1.349
1.526
1.546
1.564
1.621
2.395
2.406
2.413
2.424
2.432
2.442
2.581
2.600
3.302
3.305
3.310
3.314
3.318
3.864
4.881
7.139
7.158
7.219
7.237
ppm
3.00
2.75
1.93
7.37
2.18
1.08
2.27
STANDARD 1H OBSERVE
Pulse Sequence: s2pul
Solvent: cd3od
Ambient temperature
Mercury-400BB "ncsumerc400"
Relax. delay 1.000 sec
Pulse 85.0 degrees
Acq. time 1.638 sec
Width 6006.0 HZ
16 repetitions
OBSERVE H1, 400.1367677 MHz
DATA PROCESSING
FT size 32768
Total time 0 min, 50 sec

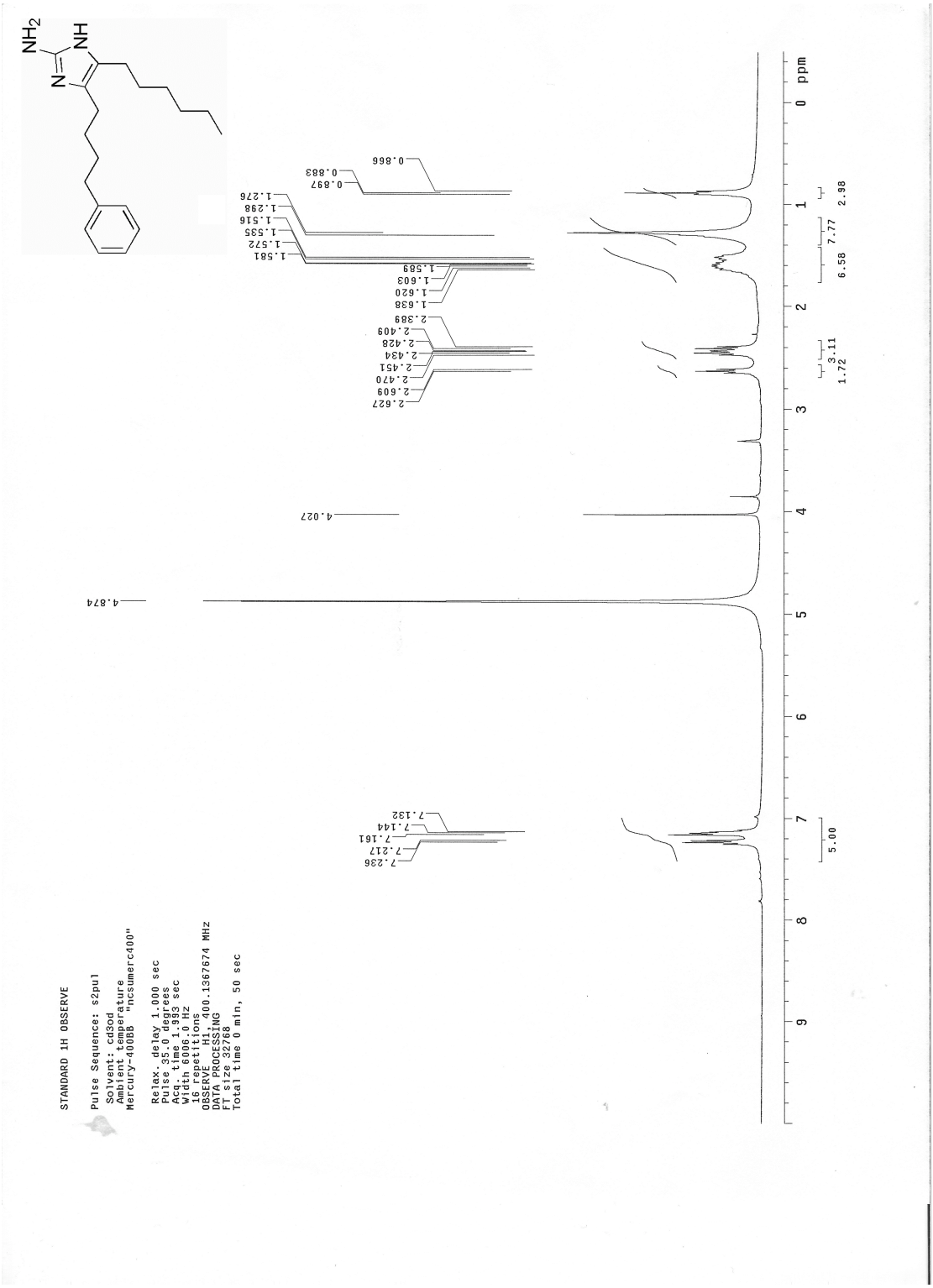

NH2
NH
N
13.234
22.462
22.985
23.069
23.850
25.435
26.360
26.648
28.551
28.612
28.680
28.847
28.976
31.364
31.493
33.442
35.649
47.205
47.417
47.630
47.842
48.054
48.267
48.479
125.513
128.076
128.129
128.220
142.612
ppm
0
20
40
60
80
100
120
140
160
180
200
13C OBSERVE
Pulse Sequence: s2pul
Solvent: cd3od
Ambient temperature
Mercury-400BB "ncsumerc400"
Pulse 81.2 degrees
Acq. time 1.199 sec
Width 25000.0 Hz
100000 repetitions
OBSERVE C13, 100.6144469 MHz
DECOUPLE H1, 400.1387407 MHz
Power 44 dB
continuously on
WALTZ-16 modulated
DATA processing
Line broadening 1.0 Hz
FT size 65536
Total time 40 hr, 44 min, 5 sec


NH2
NH
N
0.862
0.884
1.332
1.343
1.501
2.319
2.345
2.369
2.581
7.139
7.156
7.165
7.237
7.261
ppm
0
1
2
3
4
5
6
7
8
9
3.00
10.41
6.03
3.24
1.66
3.68
STANDARD 1H OBSERVE
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
Mercury-300BB "ncsumerc300"
Relax. delay 1.000 sec
Pulse 30.0 degrees
Acq. time 1.995 sec
Width 4506.5 Hz
16 repetitions
OBSERVE H1, 299.7918101 MHz
DATA PROCESSING
FT size 32768
Total time 0 min, 49 sec

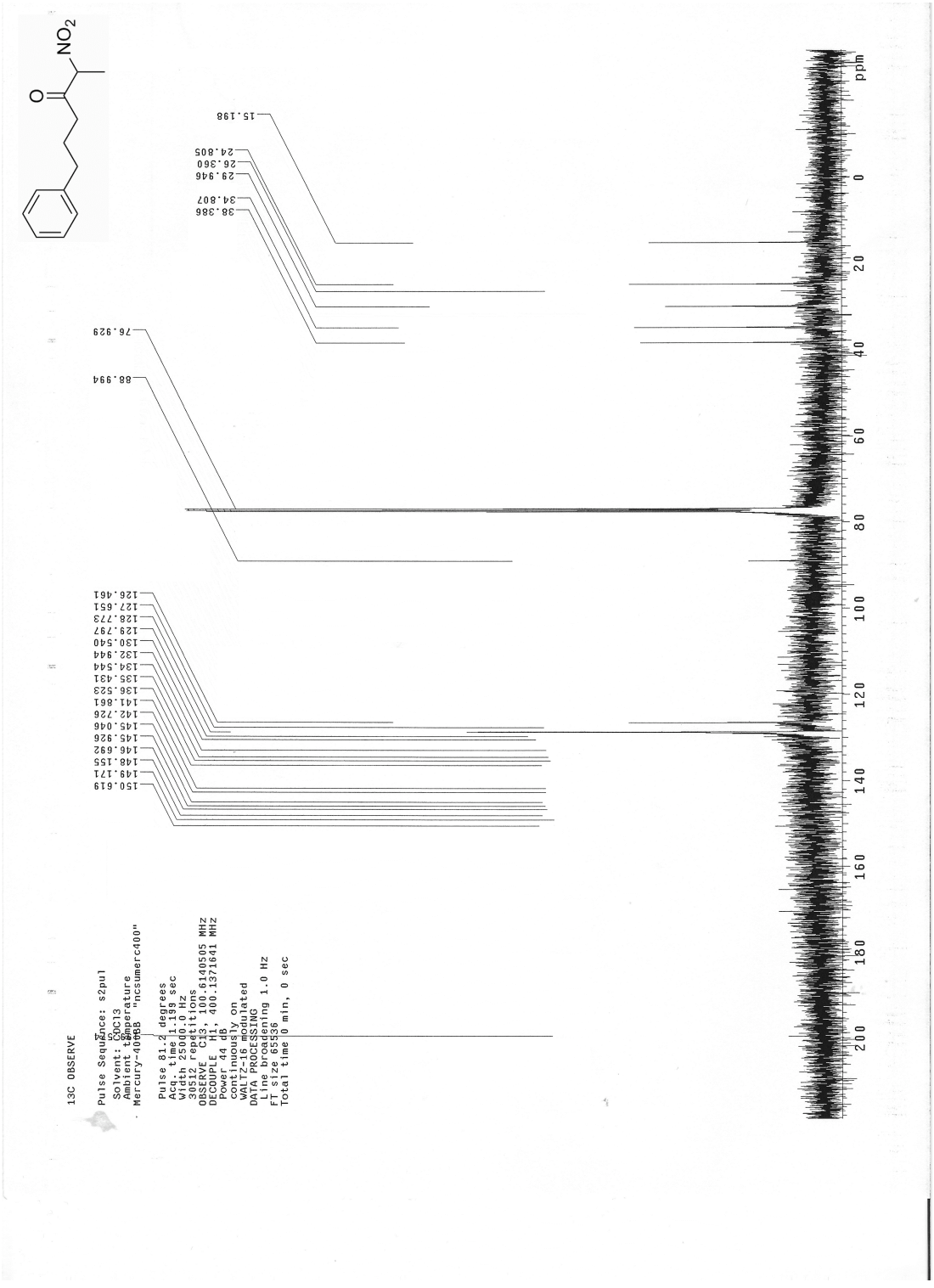

13C OBSERVE
Pulse Sequence: s2pul
Solvent: cd3od
Ambient temperature
Mercury-400BB "ncsumerc400"
Pulse 81.2 degrees
Acq. time 1.193 sec
Width 25000.0 Hz
100000 repetitions
OBSERVE C13, 100.6144469 MHz
DECOUPLE H1, 400.1387407 MHz
Power 44 dB
continuously on
WALTZ-16 modulated
Data processing
Line broadening 1.0 Hz
FT size 65536
Total time 40 hr, 44 min, 5 sec
13.280
21.947
22.477
23.008
23.092
26.367
26.405
26.656
28.187
28.566
28.741
28.968
29.090
29.188
31.099
31.304
31.478
33.427
35.497
47.235
47.448
47.660
47.872
48.085
48.297
48.509
121.850
121.987
122.070
125.558
128.121
128.250
142.445
146.373
ppm
0
20
40
60
80
100
120
140
160
180
200

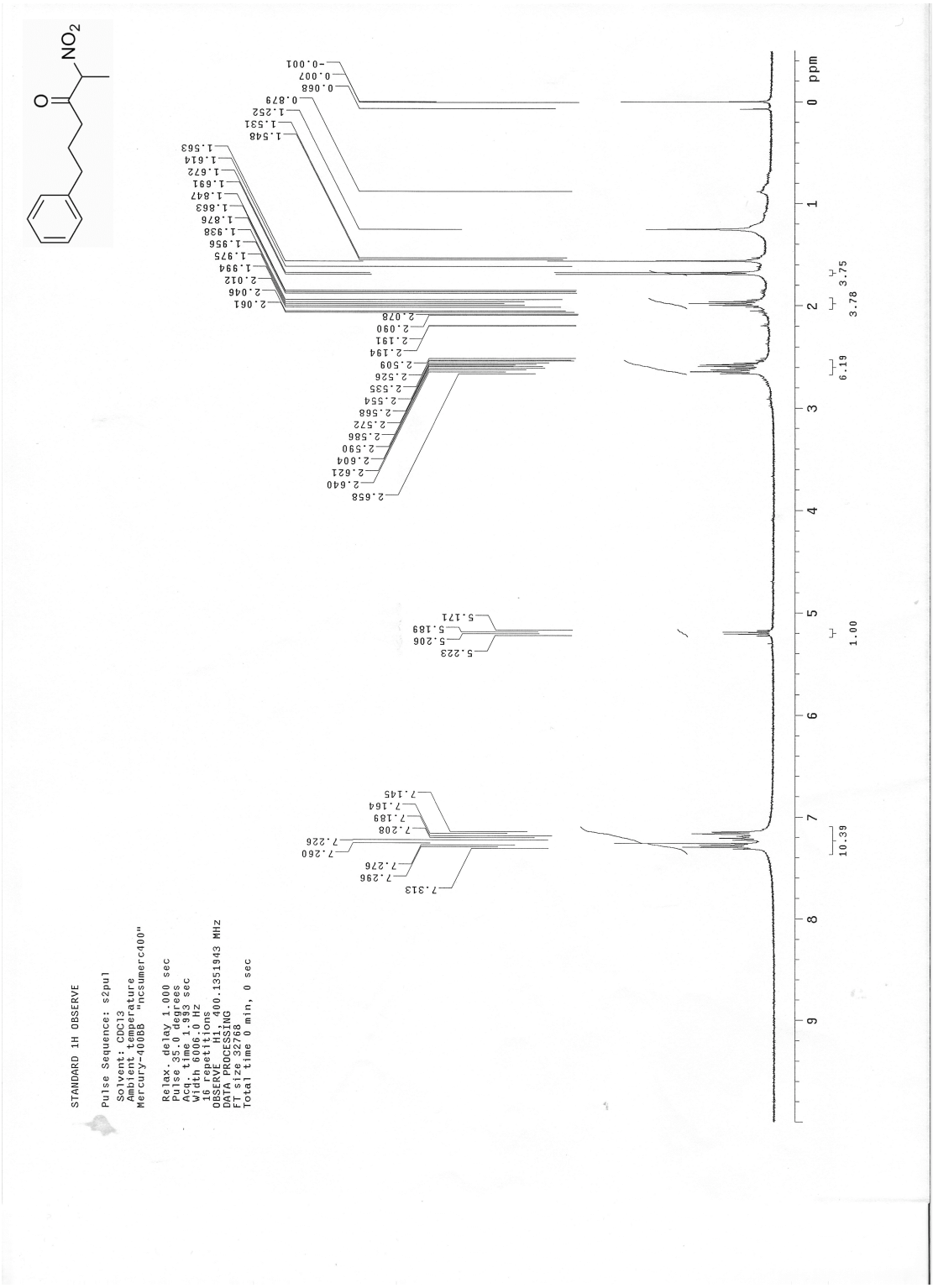

NH2
NH
N
0.876
0.893
0.901
0.905
0.909
1.301
1.312
1.324
1.341
1.528
1.546
1.565
1.584
1.595
1.603
1.614
1.633
1.652
2.377
2.397
2.401
2.415
2.420
2.439
2.576
2.595
2.614
4.025
4.907
7.126
7.128
7.147
7.209
7.226
ppm
3.19
9.03
7.28
3.29
1.94
5.00
STANDARD 1H OBSERVE
Pulse Sequence: s2pul
Solvent: cd3od
Ambient temperature
Mercury-400BB "ncsumerc400"
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.638 sec
Width 6006.0 HZ
16 repetitions
OBSERVE H1, 400.1367677 MHz
DATA PROCESSING
FT size 32768
Total time 0 min, 50 sec

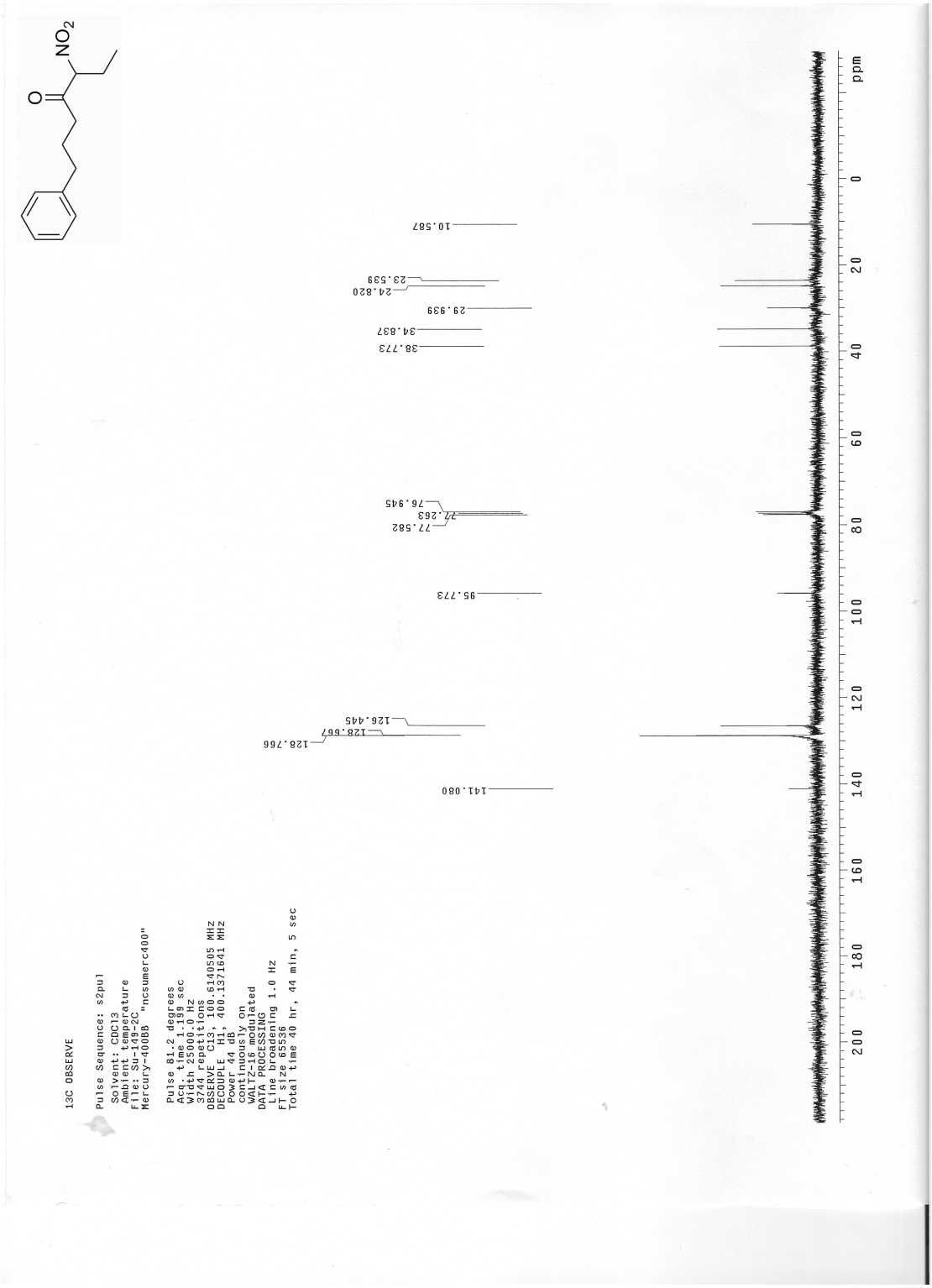

NH2
NH
N
13.105
13.264
21.977
22.440
22.993
23.099
23.418
26.079
26.337
26.618
28.544
28.695
28.968
29.734
30.728
31.471
33.382
35.330
37.598
47.235
47.448
47.660
47.872
48.085
48.297
48.509
121.820
122.085
125.657
128.189
128.242
142.202
146.373
ppm
0
20
40
60
80
100
120
140
160
180
200
13C OBSERVE
Pulse Sequence: s2pul
Solvent: cd3od
Ambient temperature
Mercury-400BB "ncsumerc400"
Pulse 81.2 degrees
Acq. time 1.199 sec
Width 25000.0 Hz
16000 repetitions
OBSERVE C13, 100.6144469 MHz
DECOUPLE H1, 400.1387407 MHz
Power 44 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 65536
Total time 40 hr, 44 min, 5 sec

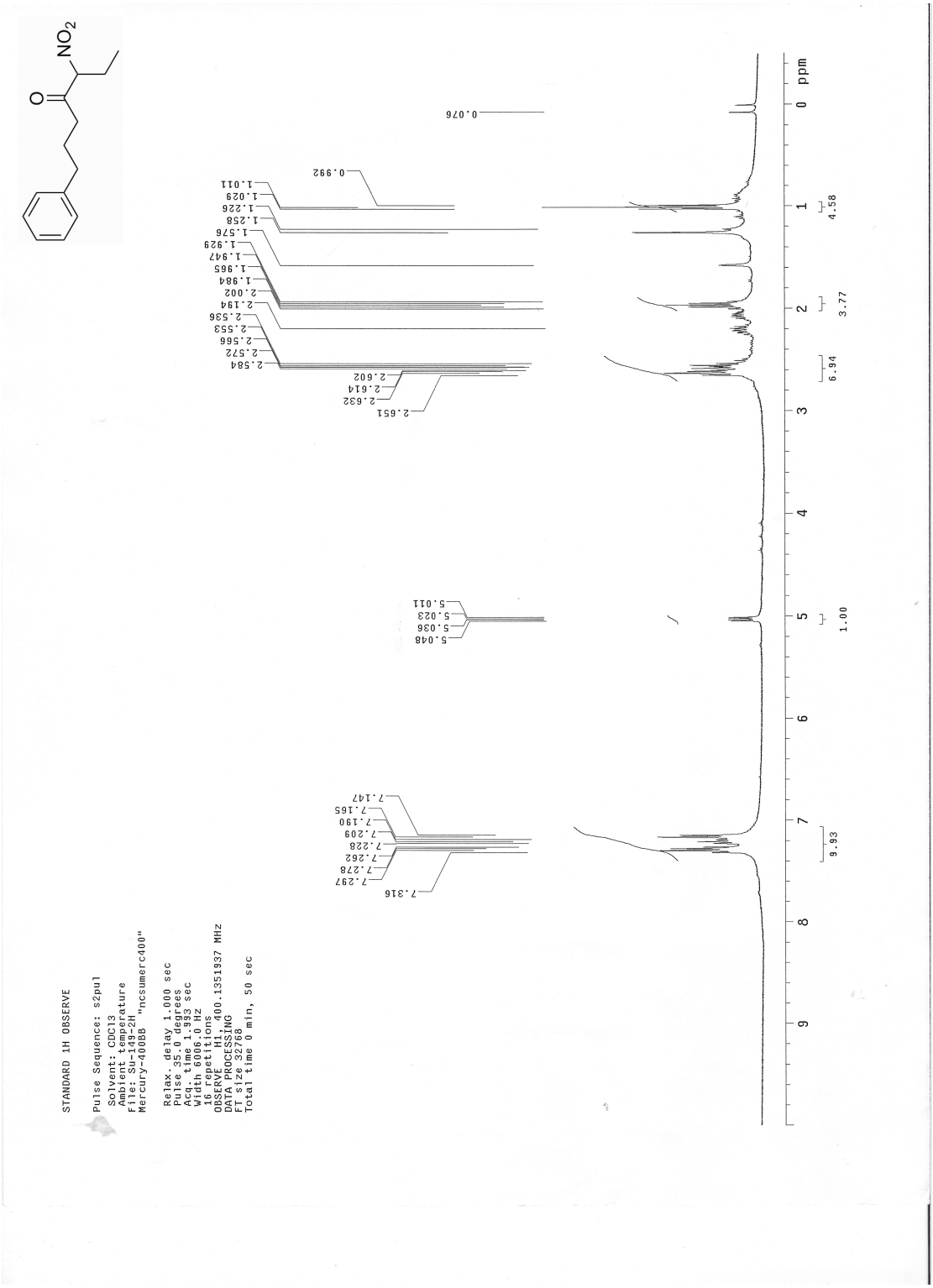

NH2
NH
N
0.866
0.897
0.883
1.276
1.298
1.516
1.535
1.572
1.581
1.589
1.603
1.620
1.638
2.389
2.409
2.428
2.434
2.451
2.470
2.609
2.627
4.027
4.874
7.132
7.144
7.161
7.217
7.236
ppm
2.98
7.77
6.58
3.11
1.72
5.00
STANDARD 1H OBSERVE
Pulse Sequence: s2pul
Solvent: cd3od
Ambient temperature
Mercury-400BB "ncsumerc400"
Relax. delay 1.000 sec
Pulse 35.0 degrees
Acq. time 1.193 sec
Width 6006.0 Hz
16 repetitions
OBSERVE H1, 400.1367674 MHz
DATA PROCESSING
FT size 32768
Total time 0 min, 50 sec

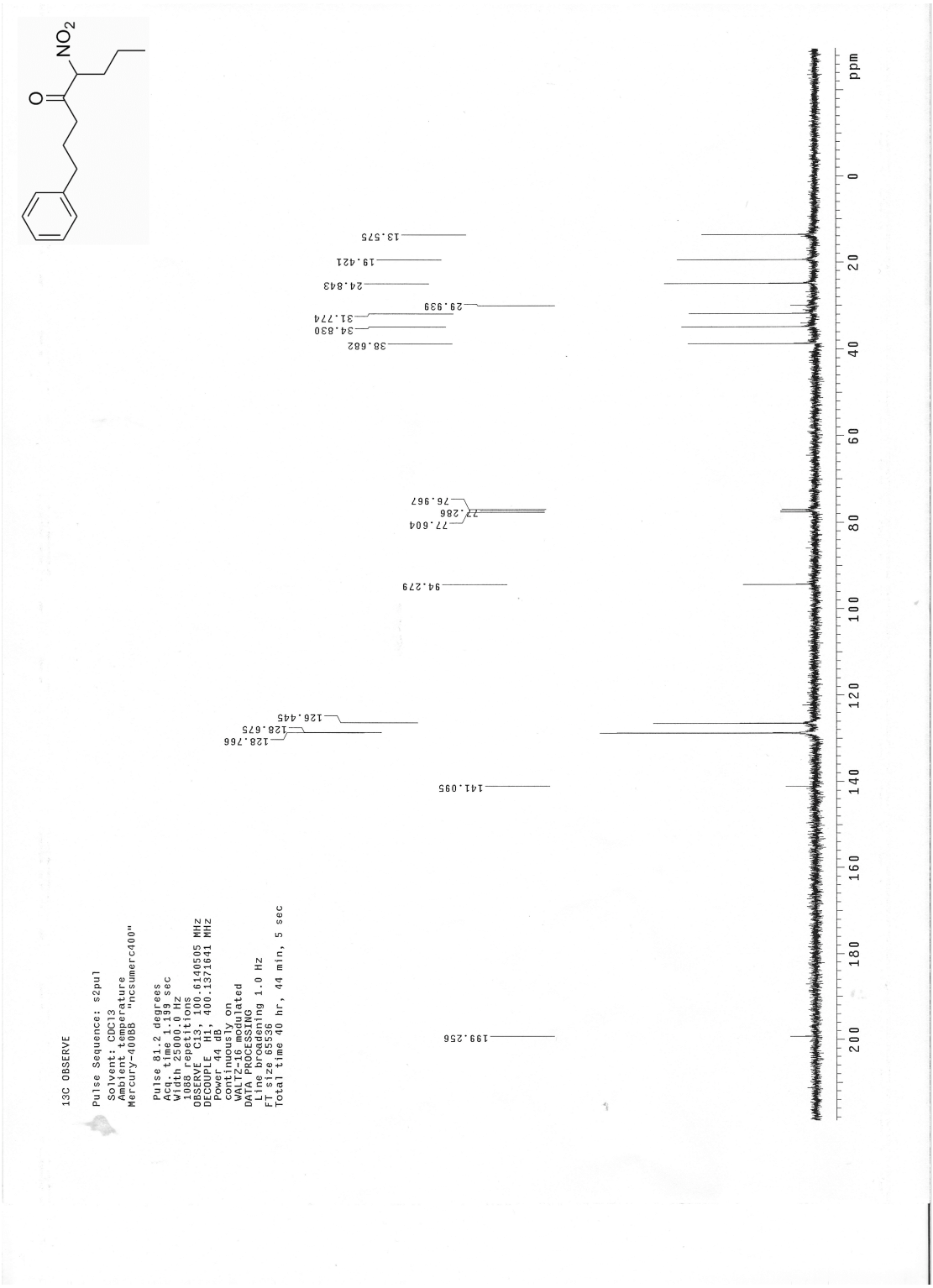
NMR data for α-nitro ketones

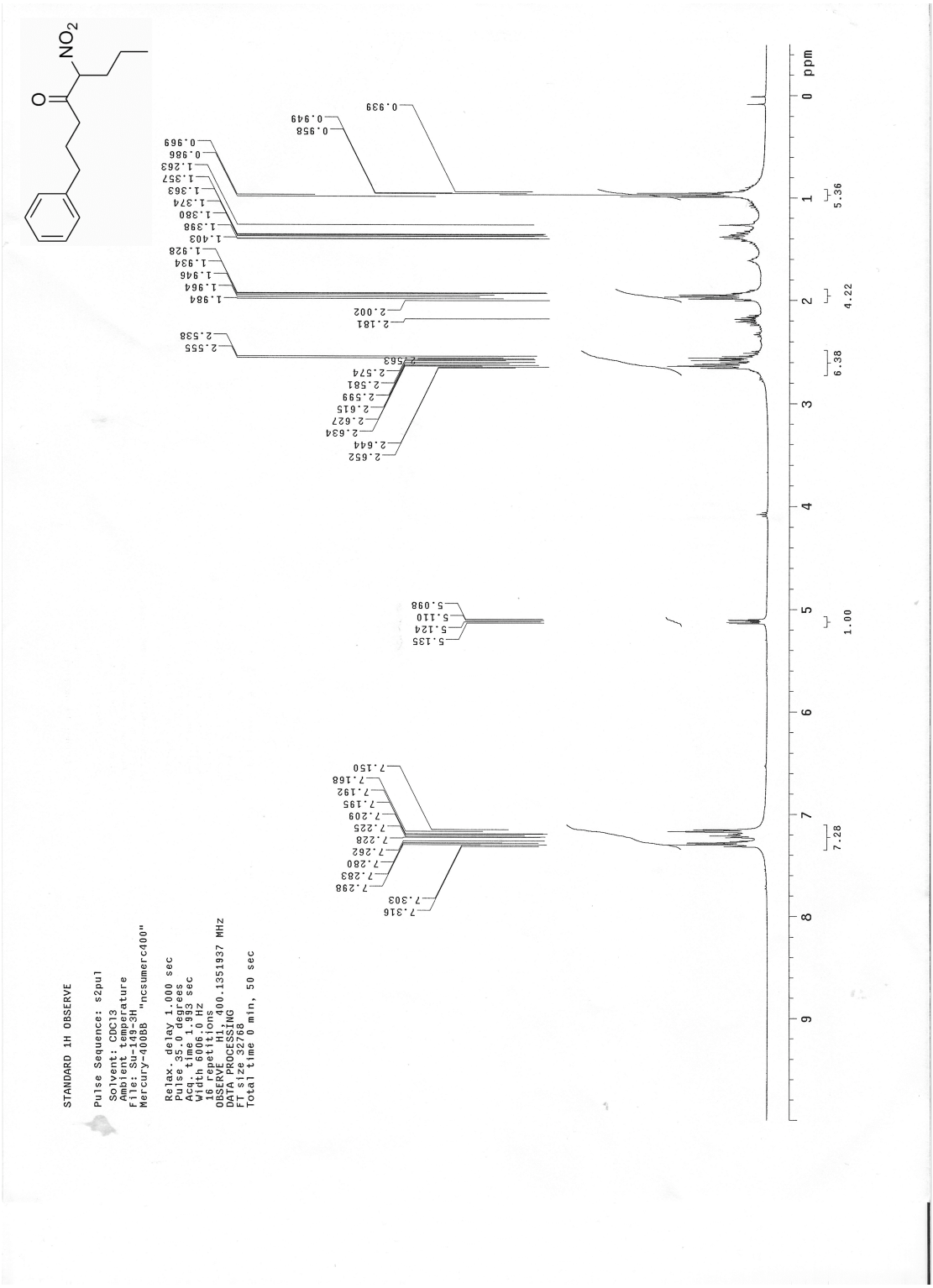


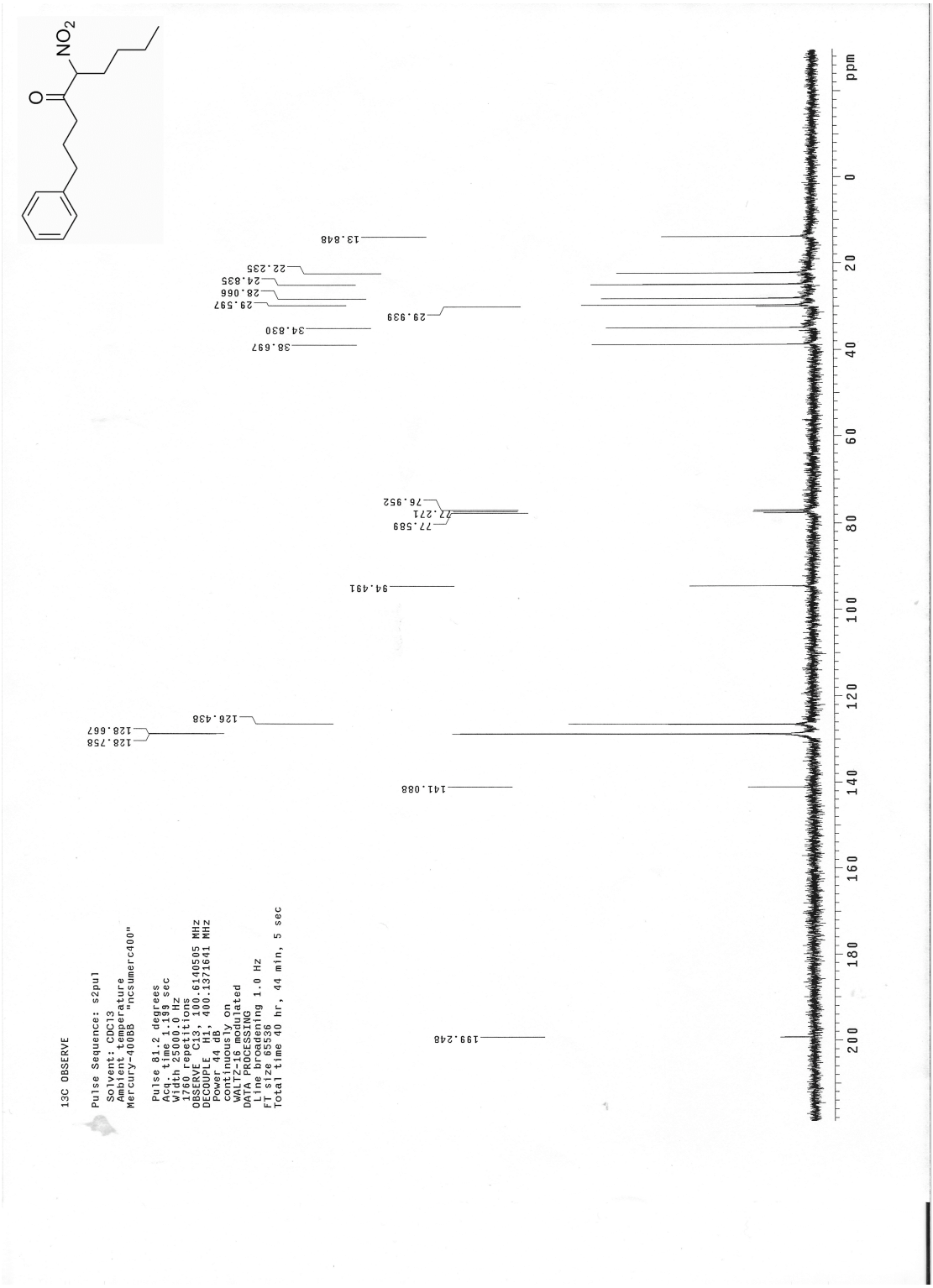

NO2
O
-0.001
0.007
0.068
0.879
1.252
1.531
1.548
1.563
1.614
1.672
1.691
1.847
1.863
1.876
1.938
1.956
1.975
1.994
2.012
2.046
2.061
2.078
2.090
2.191
2.194
2.509
2.526
2.535
2.554
2.568
2.572
2.586
2.590
2.604
2.621
2.640
2.658
5.171
5.189
5.206
5.223
7.145
7.164
7.189
7.208
7.226
7.260
7.276
7.296
7.313
ppm
3.75
3.78
6.19
1.00
10.39
STANDARD 1H OBSERVE
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
Mercury-400BB "ncsumerc400"
Relax. delay 1.000 sec
Pulse 35.0 degrees
Acq. time 1.993 sec
Width 6006.0 Hz
16 repetitions
OBSERVE H1, 400.1351943 MHz
DATA PROCESSING
FT size 32768
Total time 0 min, 0 sec

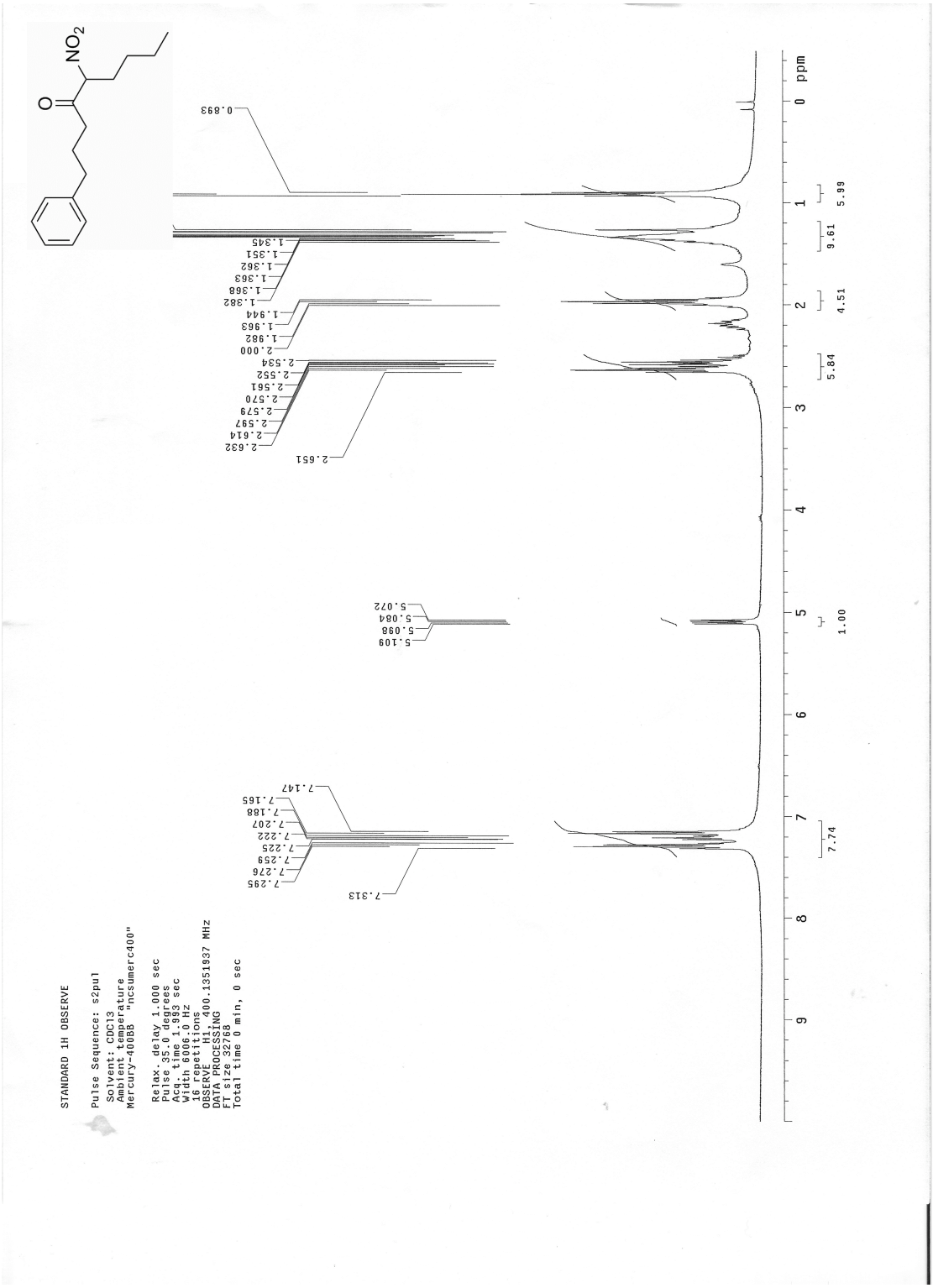

NO2
O
10.587
23.539
24.820
29.939
34.837
38.773
76.945
77.263
77.582
95.773
126.445
128.667
128.766
141.080
200
180
160
140
120
100
80
60
40
20
0
ppm
13C OBSERVE
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
File: Su-149-2C
Mercury-400BB "ncsumerc400"
Pulse 81.2 degrees
Acq. time 1.199 sec
Width 25000.0 Hz
3744 repetitions
OBSERVE C13, 100.6140505 MHz
DECOUPLE H1, 400.1371641 MHz
Power 44 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 65536
Total time 40 hr, 44 min, 5 sec

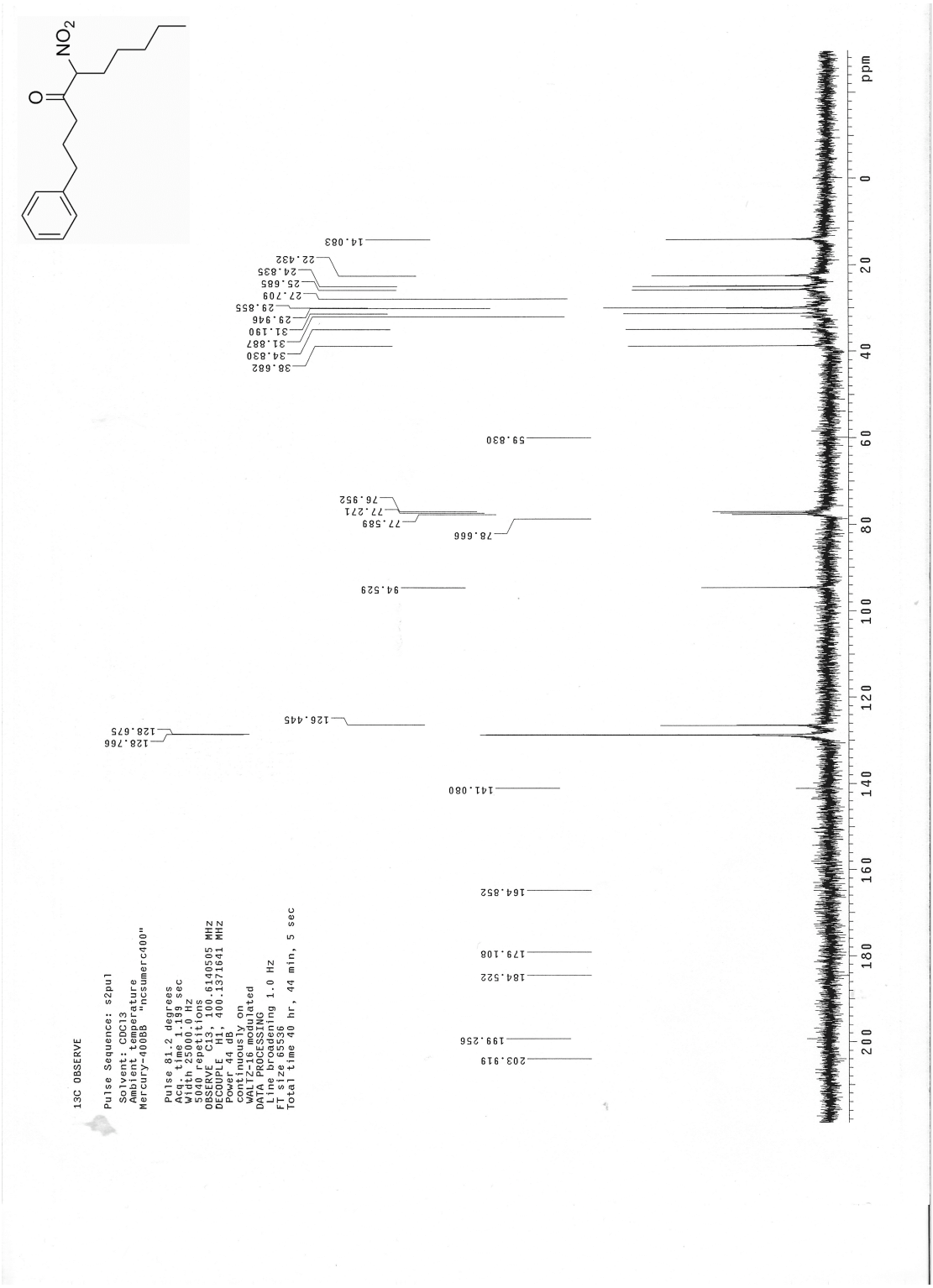

NO2
O
0.076
0.992
1.011
1.029
1.226
1.258
1.576
1.929
1.947
1.965
1.984
2.002
2.194
2.536
2.553
2.566
2.572
2.584
2.602
2.614
2.632
2.651
5.011
5.023
5.036
5.048
7.147
7.165
7.190
7.209
7.228
7.262
7.278
7.297
7.316
ppm
4.58
3.77
6.94
1.00
9.93
STANDARD 1H OBSERVE
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
File: Su-149-2H
Mercury-400BB "ncsumerc400"
Relax. delay 1.000 sec
Pulse 35.0 degrees
Acq. time 1.895 sec
Width 6006.0 Hz
16 repetitions
OBSERVE H1, 400.1351937 MHz
DATA PROCESSING
FT size 32768
Total time 0 min, 50 sec

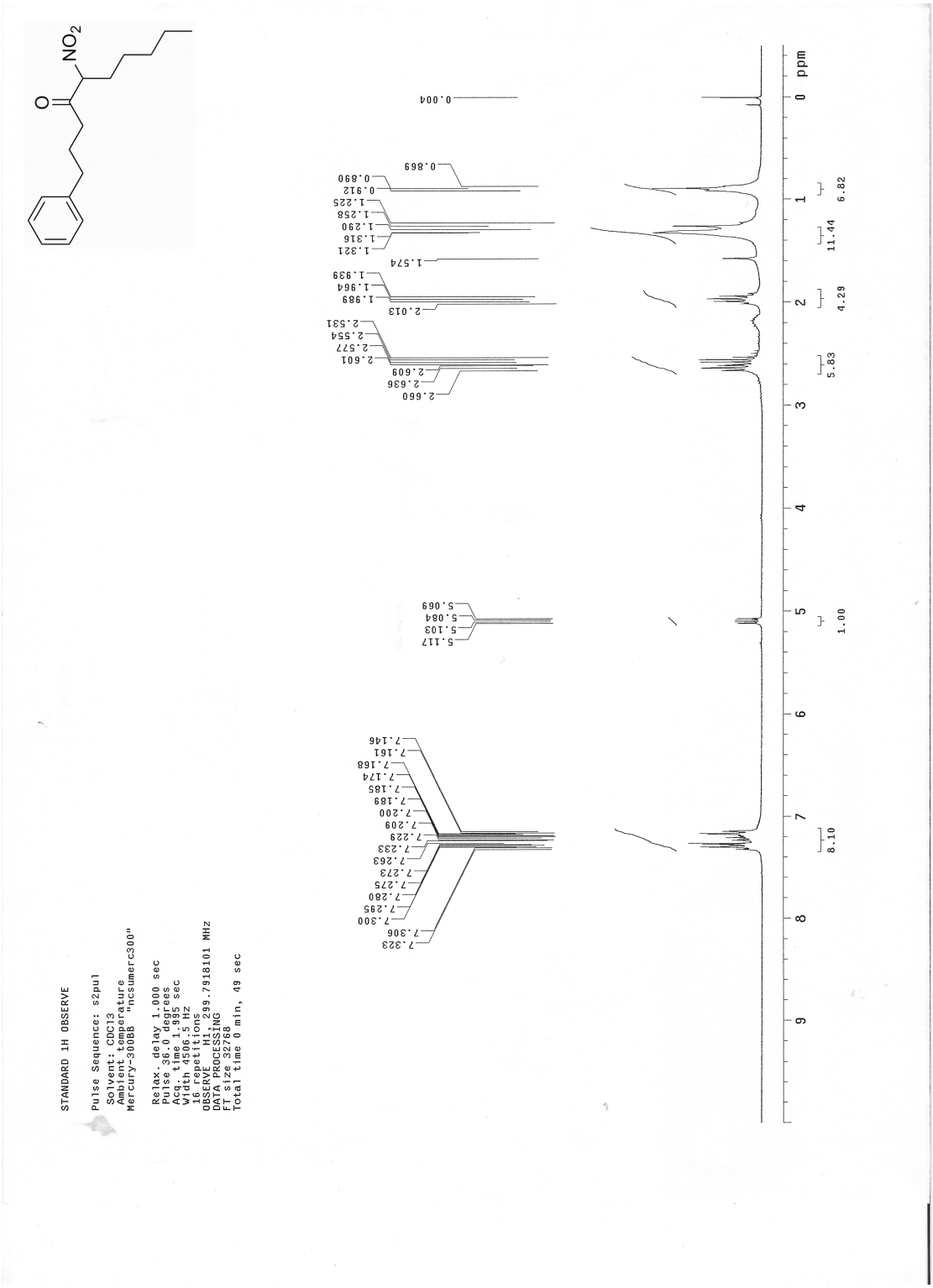

NO2
O
13.575
19.421
24.843
29.939
31.774
34.830
38.682
76.967
77.286
77.604
94.279
126.445
128.675
128.766
141.095
199.256
ppm
0
20
40
60
80
100
120
140
160
180
200
13C OBSERVE
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
Mercury-400BB "ncsumerc400"
Pulse 81.2 degrees
Acq. time 1.199 sec
Width 25001.0 Hz
1008 repetitions
OBSERVE C13, 100.6140505 MHz
DECOUPLE H1, 400.1371641 MHz
Power 44 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 65536
Total time 40 hr, 44 min, 5 sec

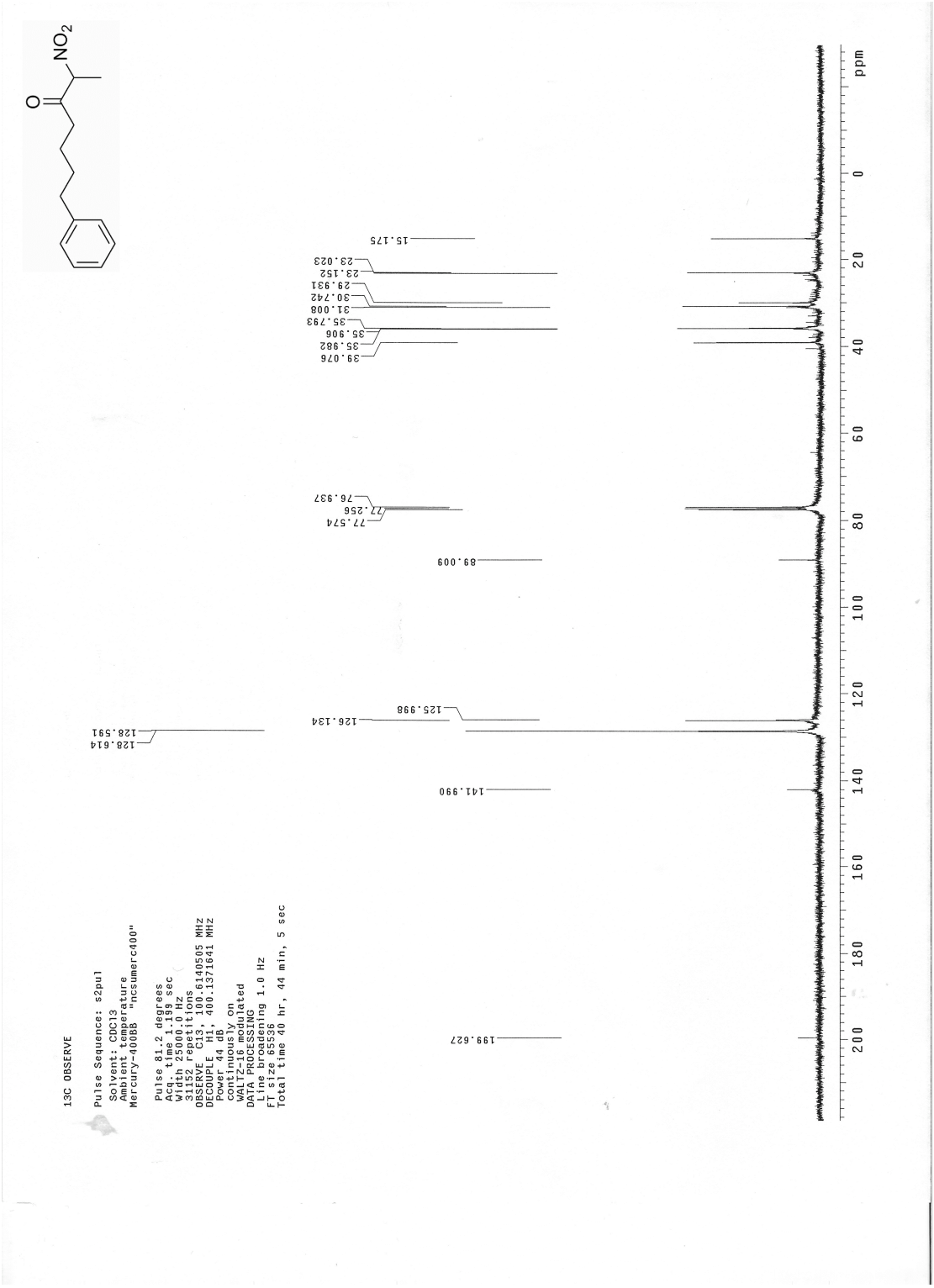

NO2
O
STANDARD 1H OBSERVE
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
File: Su-143-3H
Mercury-400BB "ncsumerc400"
Relax. delay 1.000 sec
Pulse 35.0 degrees
Acq. time 1.993 sec
Width 8065.0 Hz
16 repetitions
OBSERVE H1, 400.1351937 MHz
DATA PROCESSING
FT size 32768
Total time 0 min, 50 sec
0.939
0.958
0.949
0.969
0.986
1.263
1.357
1.363
1.374
1.380
1.398
1.403
1.928
1.934
1.946
1.964
1.984
2.002
2.181
2.538
2.555
2.563
2.574
2.581
2.599
2.615
2.627
2.634
2.644
2.652
5.098
5.110
5.124
5.135
7.150
7.168
7.192
7.195
7.209
7.225
7.228
7.262
7.280
7.283
7.298
7.303
7.316
ppm
5.36
4.22
6.38
1.00
7.28

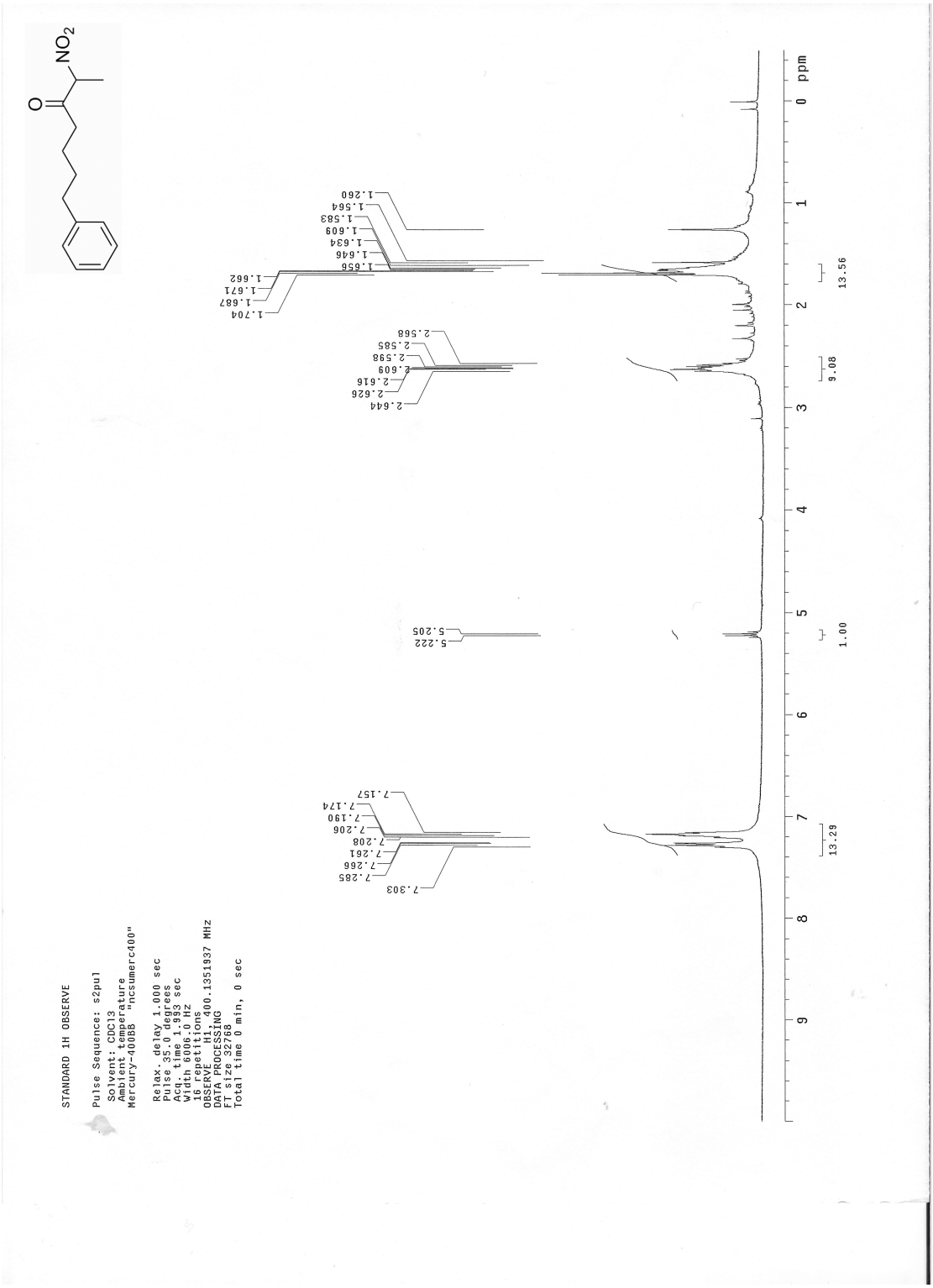

NO2
O
13.848
22.235
24.835
28.066
29.597
29.939
34.830
38.697
76.952
77.271
77.589
94.491
126.438
128.667
128.758
141.088
199.248
ppm
0
20
40
60
80
100
120
140
160
180
200
13C OBSERVE
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
Mercury-400BB "ncsumerc400"
Pulse 81.2 degrees
Acq. time 1.199 sec
Width 25000.0 Hz
1760 repetitions
OBSERVE C13, 100.6140505 MHz
DECOUPLE H1, 400.1371641 MHz
Power 44 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 65536
Total time 40 hr, 44 min, 5 sec

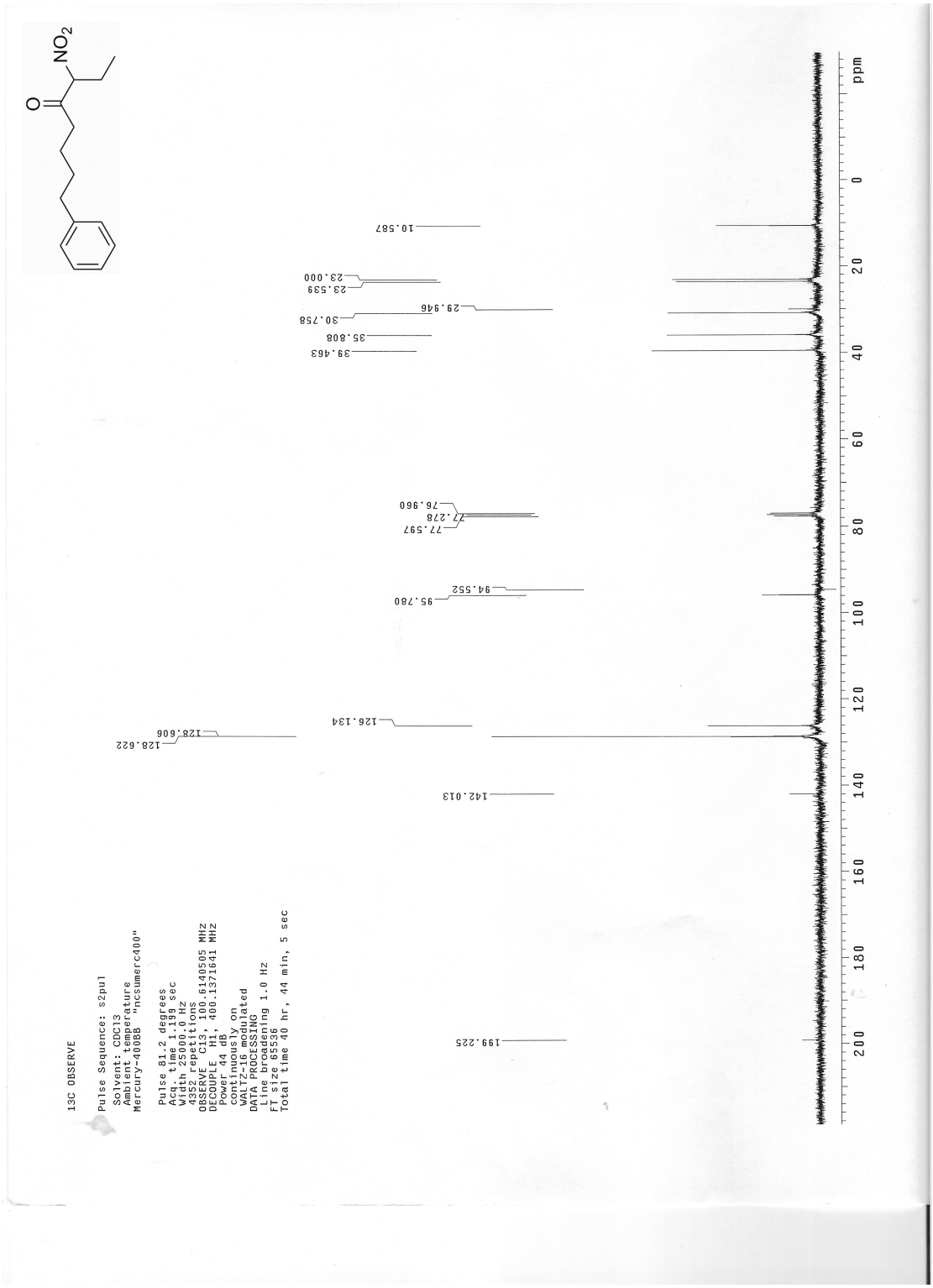

NO2
O
0.893
1.345
1.351
1.362
1.363
1.368
1.382
1.944
1.963
1.982
2.000
2.534
2.552
2.561
2.570
2.579
2.597
2.614
2.632
2.651
5.072
5.084
5.098
5.109
7.147
7.165
7.188
7.207
7.222
7.225
7.259
7.276
7.295
7.313
ppm
5.99
9.61
4.51
5.84
1.00
7.74
STANDARD 1H OBSERVE
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
Mercury-400BB "ncsumerc400"
Relax. delay 1.000 sec
Pulse 85.0 degrees
Acq. time 1.892 sec
Width 6006.0 Hz
16 repetitions
OBSERVE H1, 400.1351937 MHz
DATA PROCESSING
FT size 32768
Total time 0 min, 0 sec

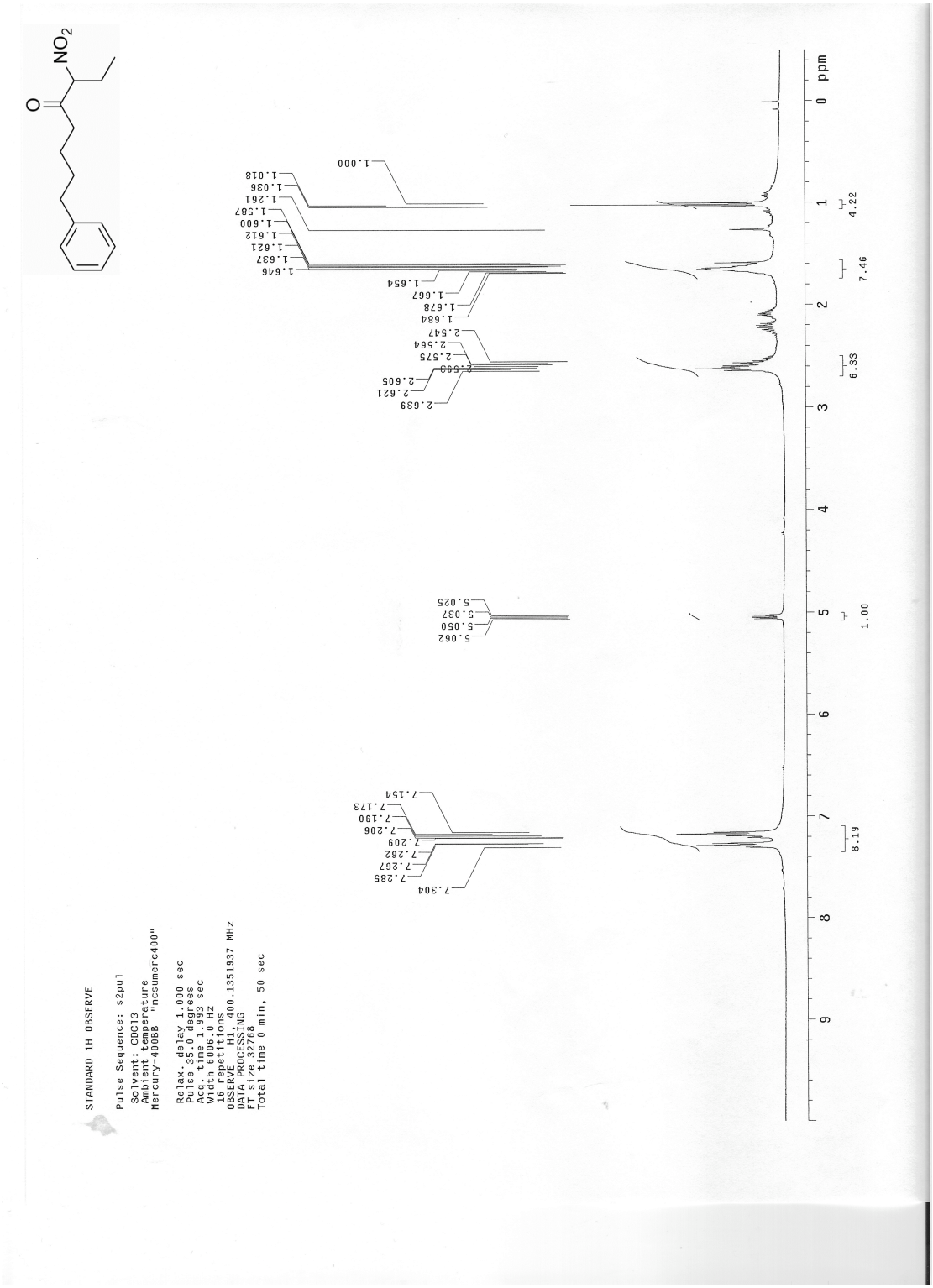

NO2
O
14.083
22.432
24.835
25.685
27.709
29.855
29.946
31.190
31.887
34.830
38.682
59.830
76.952
77.221
77.589
78.666
94.529
126.445
128.675
128.766
141.080
164.852
179.108
184.522
199.256
203.919
13C OBSERVE
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
Mercury-400BB "ncsumerc400"
Pulse 81.2 degrees
Acq. time 1.199 sec
Width 25000.0 Hz
1 repetitions
OBSERVE C13, 100.6140505 MHz
DECOUPLE H1, 400.1371641 MHz
Power 44 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
LB broadening 1.0 Hz
FT size 65536
Total time 40 hr, 44 min, 5 sec
ppm
0
20
40
60
80
100
120
140
160
180
200

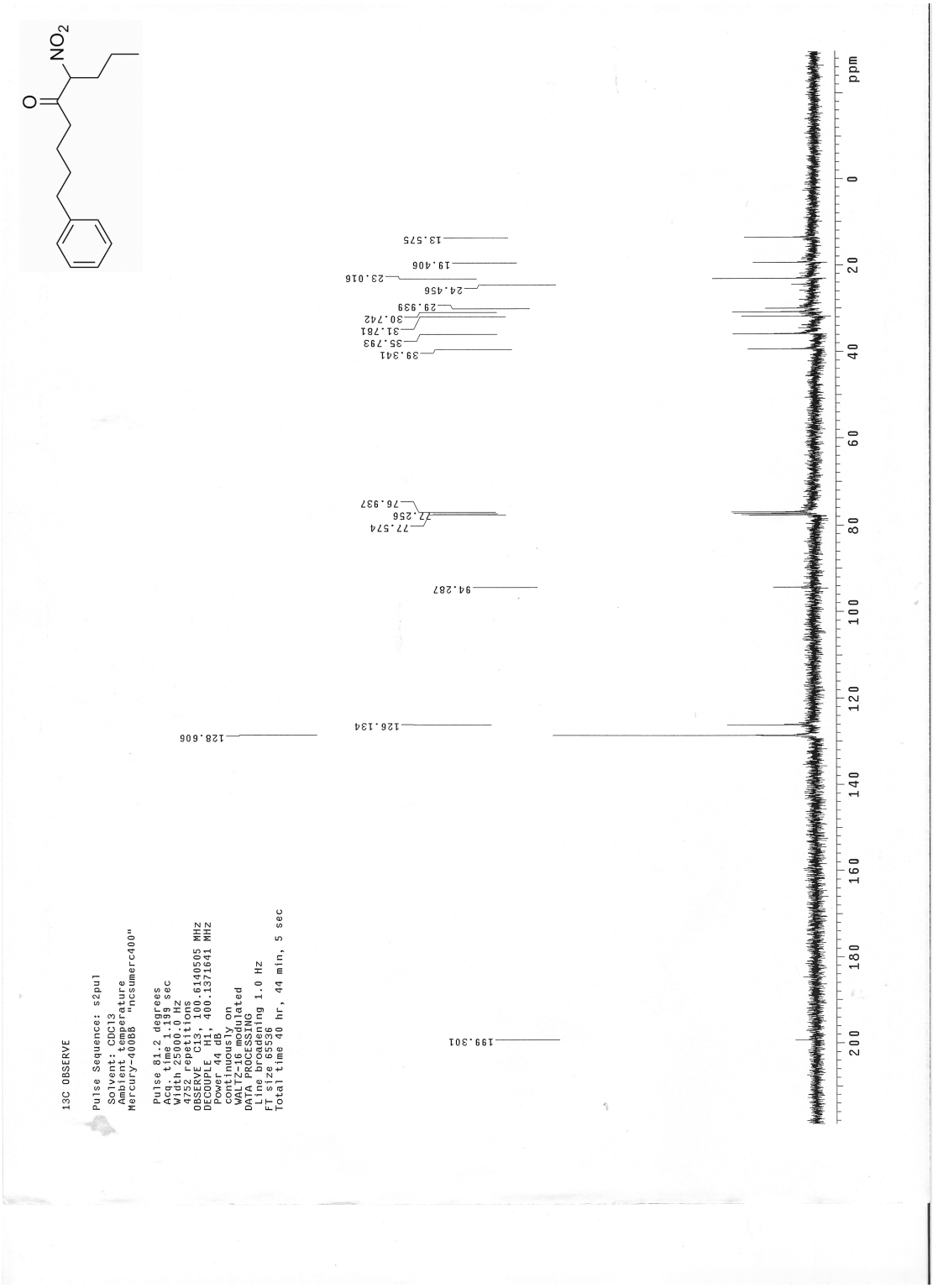

NO2
O
0.004
0.869
0.890
0.912
1.225
1.258
1.290
1.316
1.321
1.574
1.939
1.964
1.989
2.013
2.531
2.554
2.577
2.601
2.609
2.636
2.660
5.069
5.084
5.103
5.117
7.146
7.161
7.168
7.174
7.185
7.189
7.200
7.209
7.229
7.233
7.263
7.273
7.275
7.280
7.295
7.300
7.306
7.323
ppm
6.82
11.44
4.29
5.83
1.00
8.10
STANDARD 1H OBSERVE
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
Mercury-300BB "ncsumerc300"
Relax. delay 1.000 sec
Pulse 30.0 degrees
Acq. time 1.895 sec
Width 4506.5 Hz
16 repetitions
OBSERVE H1, 299.7918101 MHz
DATA PROCESSING
FT size 32768
Total time 0 min, 49 sec

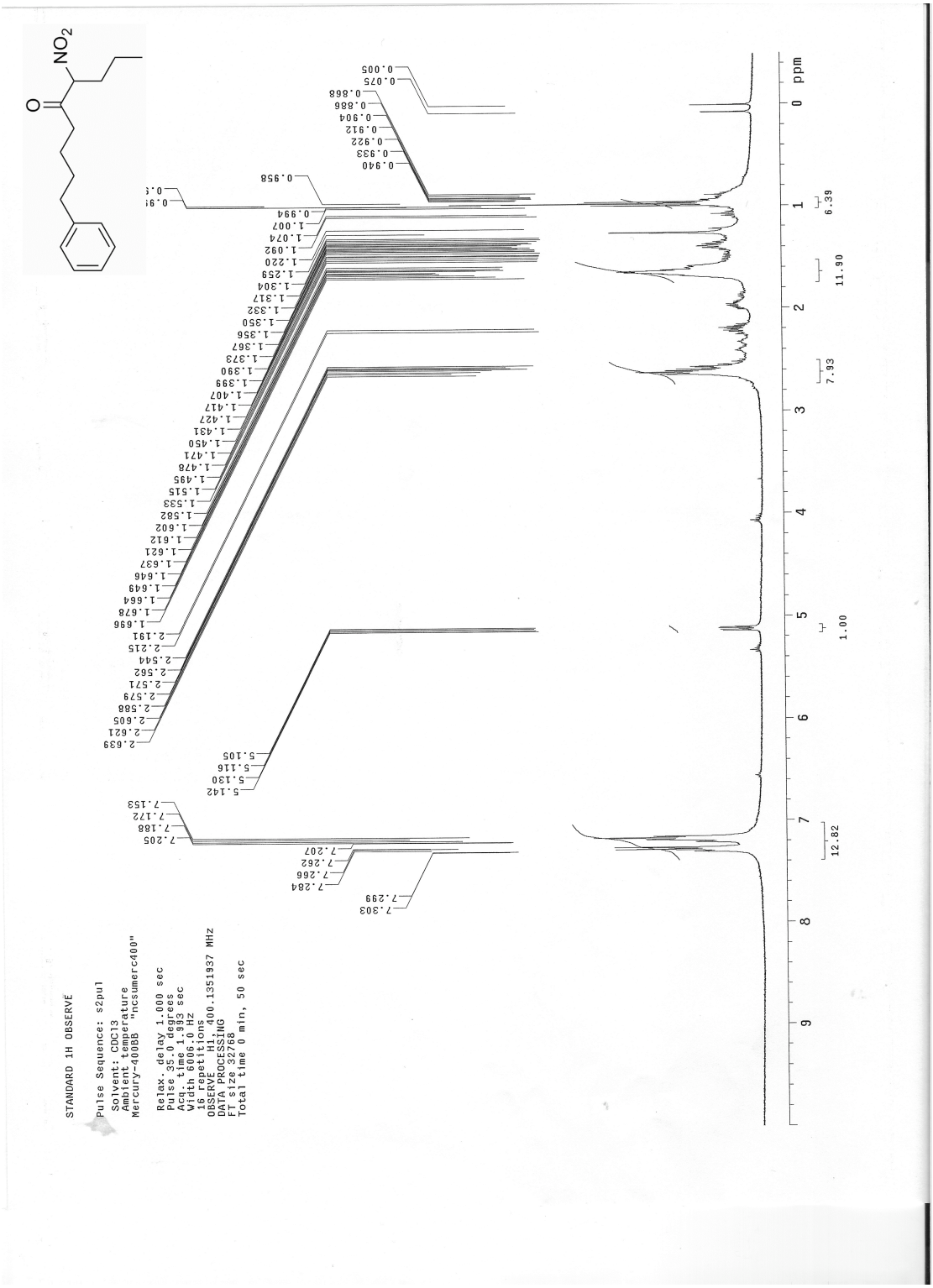

NO2
O
15.175
23.023
23.152
29.931
30.742
31.008
35.793
35.906
35.982
39.076
76.937
77.256
77.574
89.009
125.998
126.134
128.591
128.614
141.990
199.627
ppm
0
20
40
60
80
100
120
140
160
180
200
13C OBSERVE
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
Mercury-400BB "ncsumerc400"
Pulse 81.2 degrees
Acq. time 1.199 sec
Width 25000.0 Hz
2152 repetitions
OBSERVE C13, 100.6140505 MHz
DECOUPLE H1, 400.1371641 MHz
Power 44 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 65536
Total time 40 hr, 44 min, 5 sec

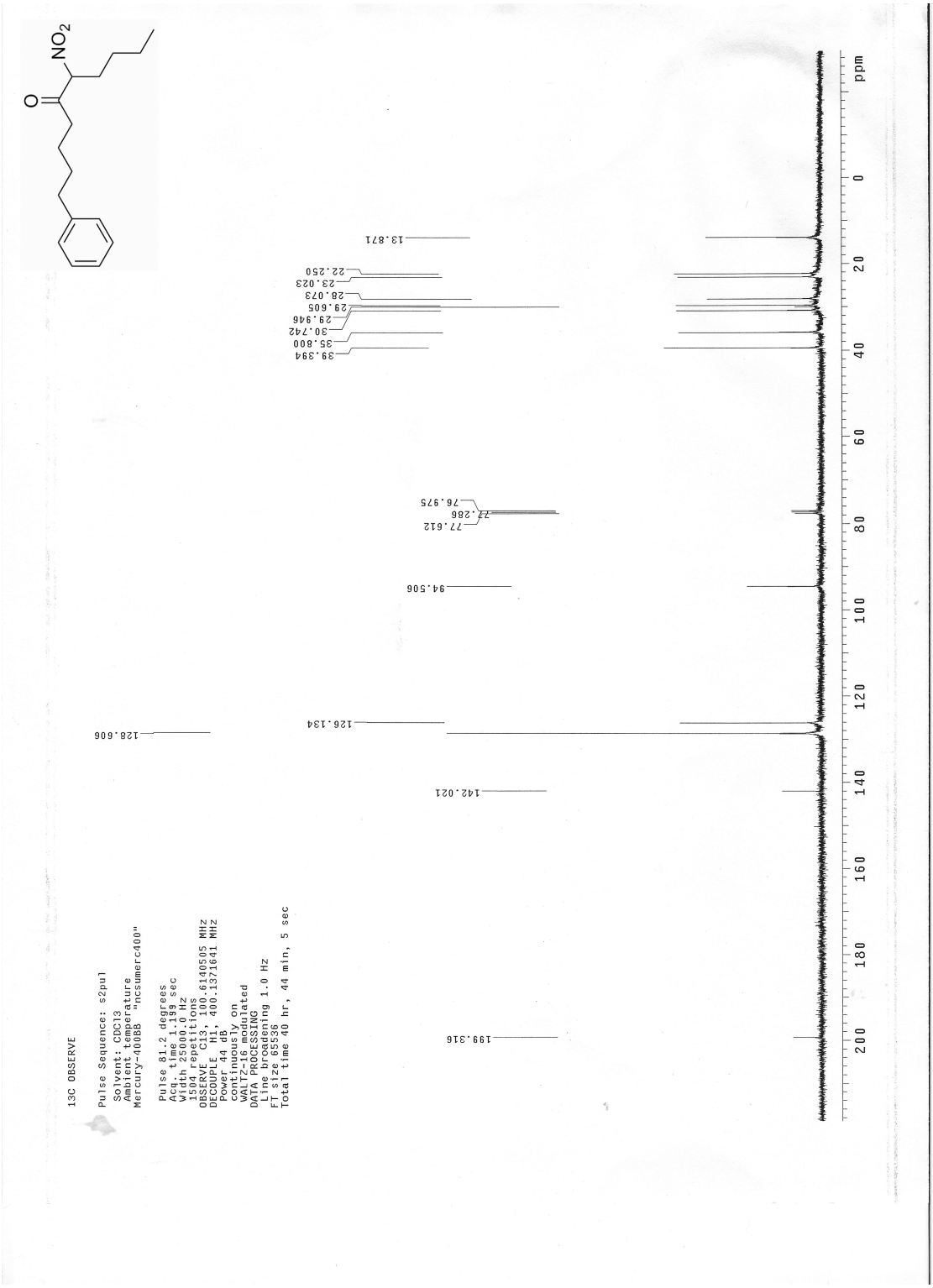

NO2
O
STANDARD 1H OBSERVE
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
Mercury-400BB "ncsumerc400"
Relax. delay 1.000 sec
Pulse 35.0 degrees
Acq. time 1.993 sec
Width 6006.0 HZ
16 repetitions
OBSERVE H1, 400.1351937 MHz
DATA PROCESSING
FT size 32768
Total time 0 min, 0 sec
1.260
1.564
1.583
1.609
1.634
1.646
1.656
1.662
1.671
1.687
1.704
2.568
2.585
2.598
2.609
2.616
2.626
2.644
5.205
5.222
7.157
7.174
7.190
7.206
7.208
7.261
7.266
7.285
7.303
ppm
13.56
9.08
1.00
13.29

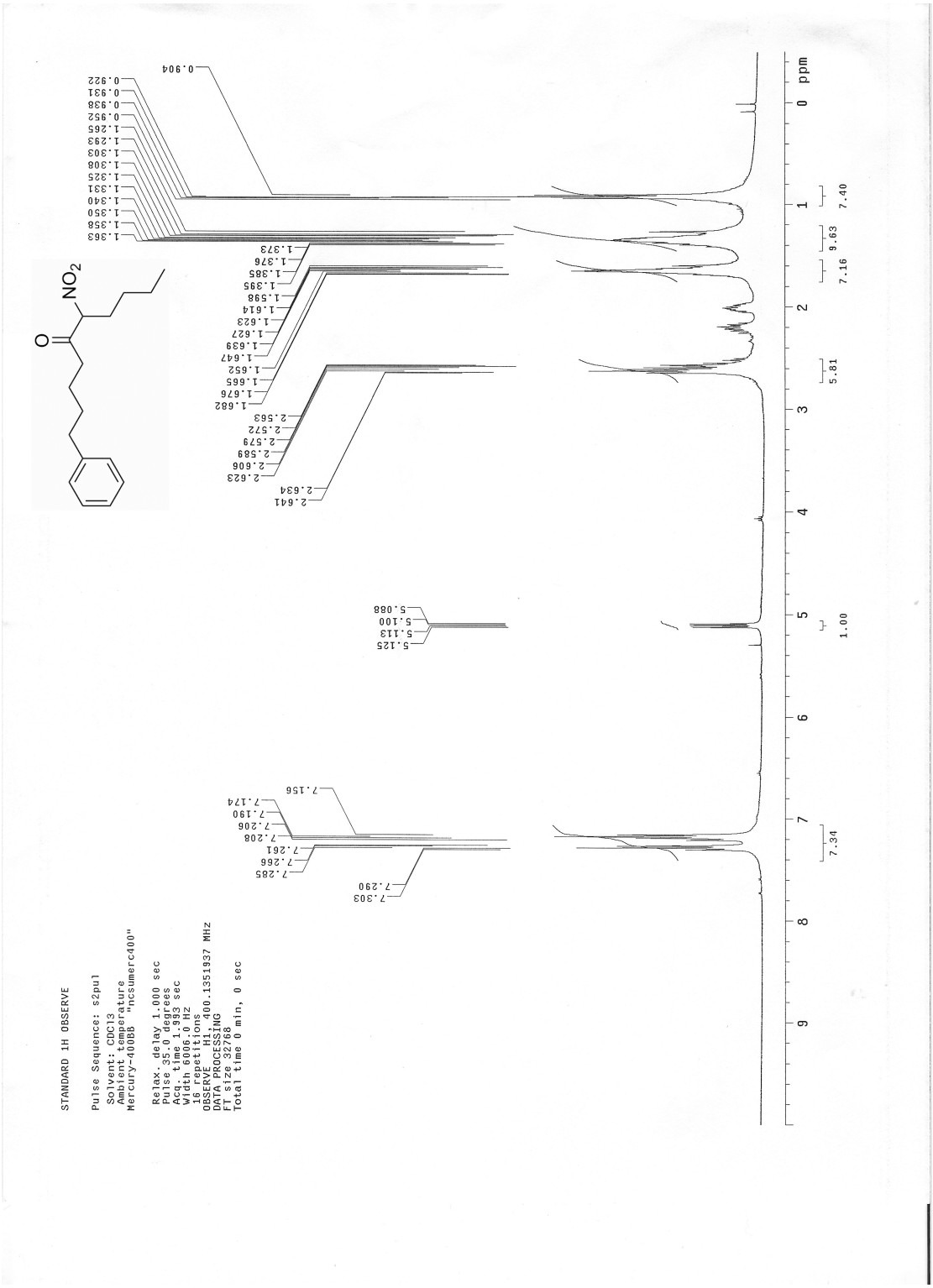

NO2
O
13C OBSERVE
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
Mercury-400BB "ncsumerc400"
Pulse 81.2 degrees
Acq. time 1.199 sec
Width 25000.0 Hz
4352 repetitions
OBSERVE C13, 100.6140505 MHz
DECOUPLE H1, 400.1371641 MHz
Power 44 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 65536
Total time 40 hr, 44 min, 5 sec
10.587
23.000
23.539
29.946
30.758
35.808
39.463
76.960
77.228
77.597
94.552
95.780
126.134
128.606
128.622
142.013
199.225
ppm
0
20
40
60
80
100
120
140
160
180
200

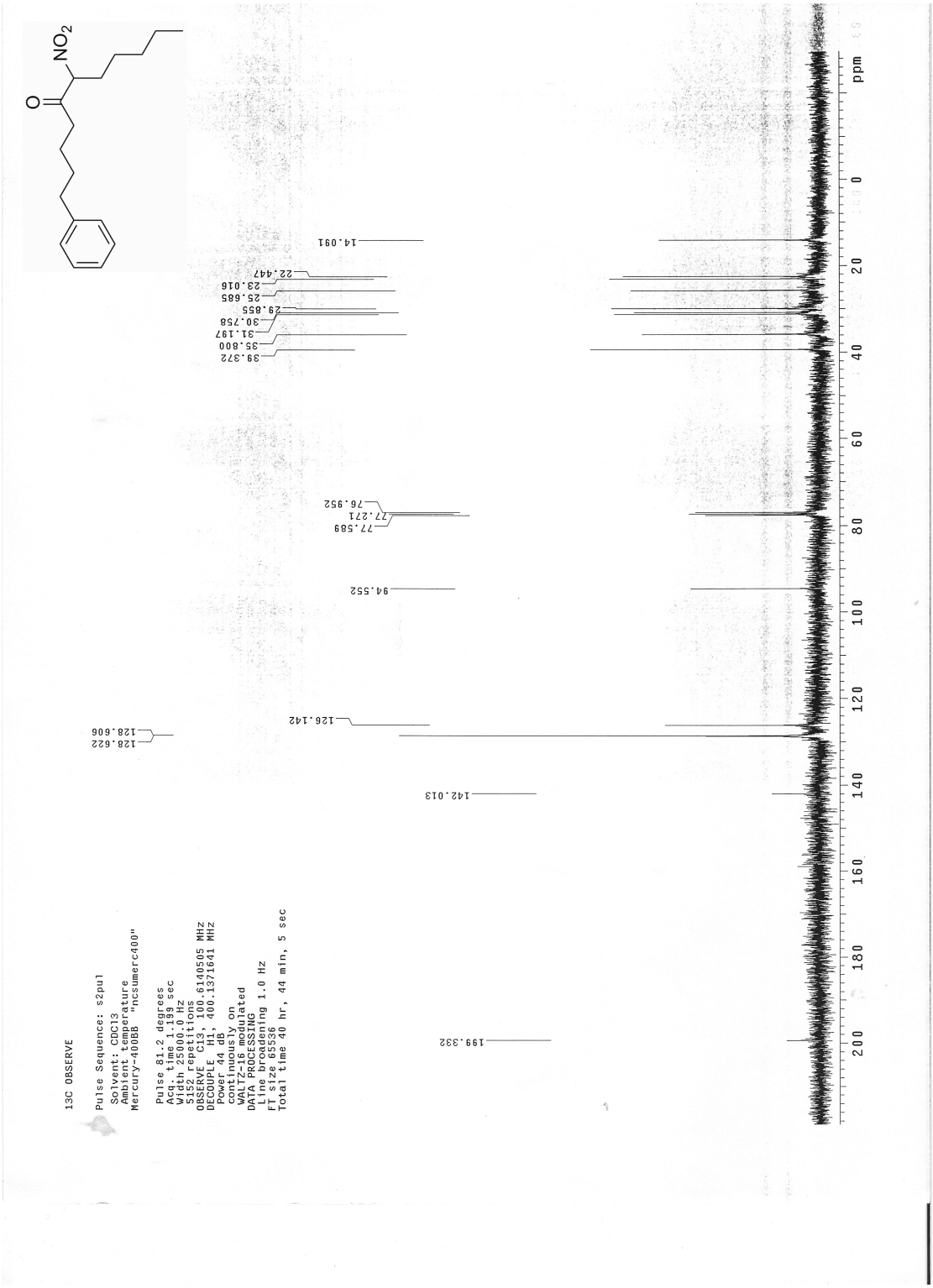

NO2
O
STANDARD 1H OBSERVE
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
Mercury-400BB "ncsumerc400"
Relax. delay 1.000 sec
Pulse 35.0 degrees
Acq. time 1.193 sec
Width 6006.0 HZ
16 repetitions
OBSERVE H1, 400.1351937 MHz
DATA PROCESSING
FT size 32768
Total time 0 min, 50 sec
1.000
1.018
1.036
1.261
1.587
1.600
1.612
1.621
1.637
1.646
1.654
1.667
1.678
1.684
2.547
2.564
2.575
2.583
2.605
2.621
2.639
5.025
5.037
5.050
5.062
7.154
7.173
7.190
7.206
7.209
7.262
7.267
7.285
7.304
ppm
4.22
7.46
6.33
1.00
8.19

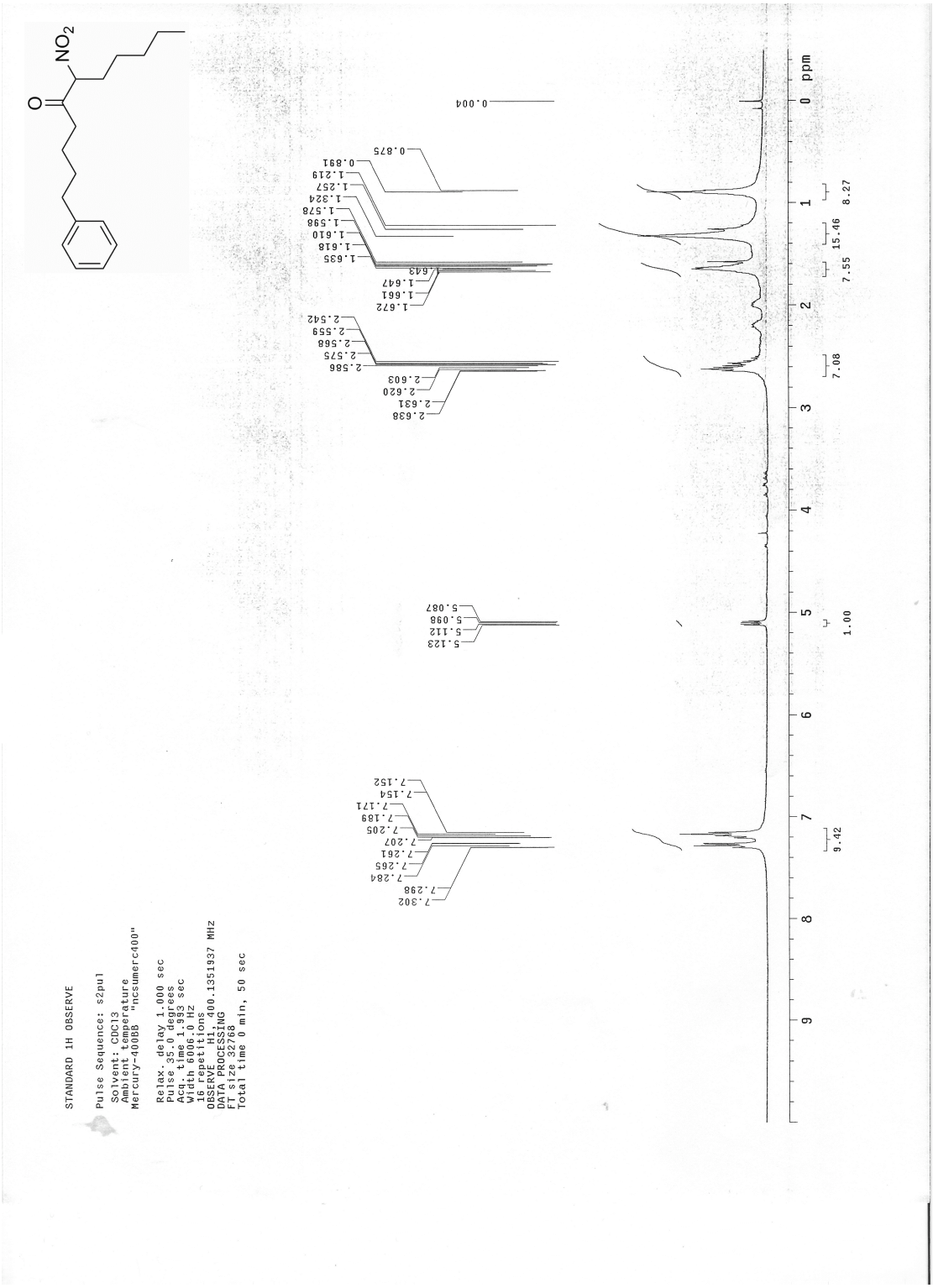

NO2
O
13C OBSERVE
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
Mercury-400BB "ncsumerc400"
Pulse 81.2 degrees
Acq. time 1.199 sec
Width 25000.0 Hz
77575 repetitions
OBSERVE C13, 100.6140505 MHz
DECOUPLE H1, 400.1371641 MHz
Power 44 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 65536
Total time 40 hr, 44 min, 5 sec
13.575
19.406
23.016
24.456
29.939
30.742
31.781
35.793
39.341
76.937
77.256
77.574
94.287
126.134
128.606
199.301
ppm
0
20
40
60
80
100
120
140
160
180
200

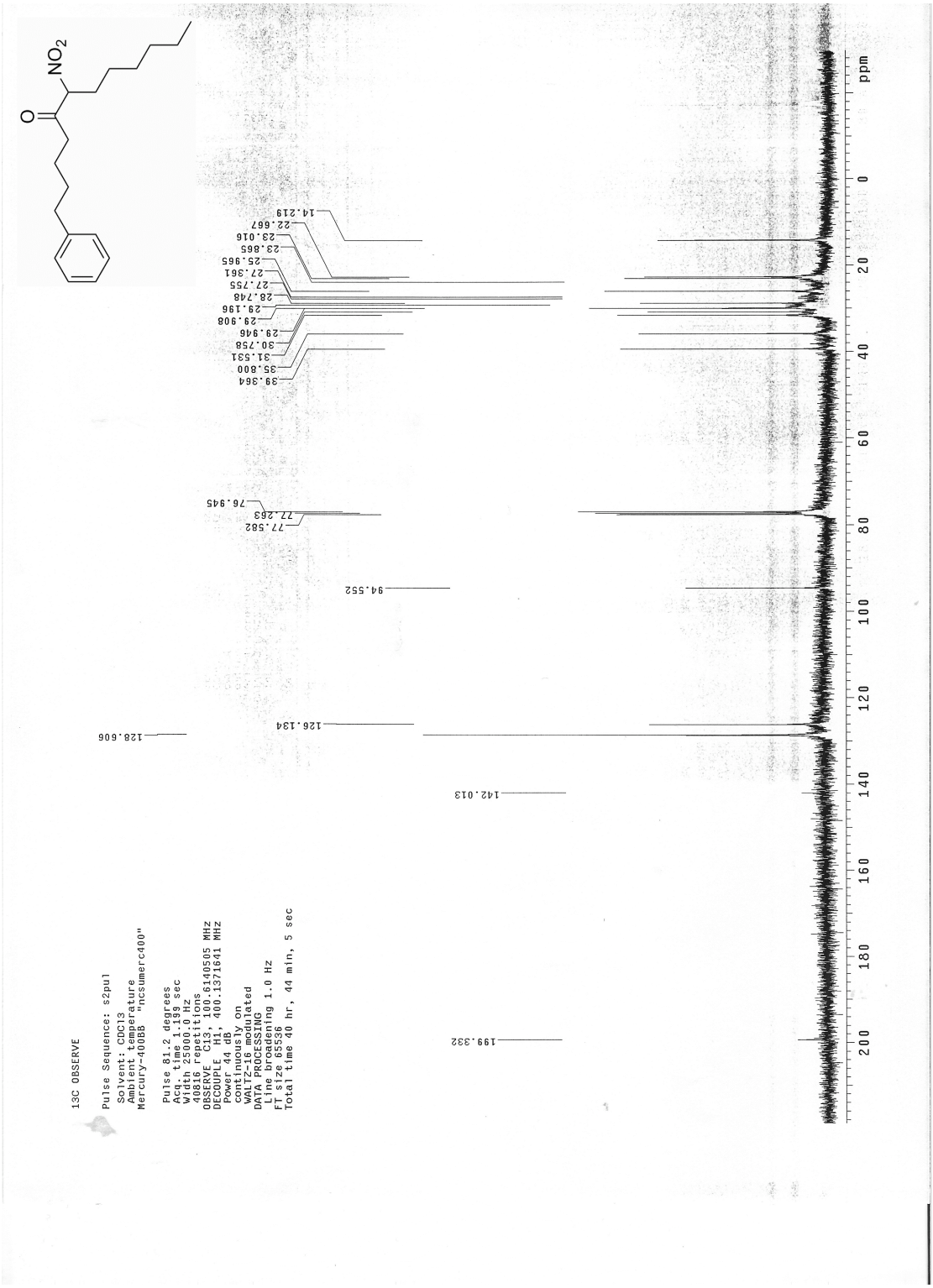

NO2
O
STANDARD 1H OBSERVE
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
Mercury-400BB "ncsumerc400"
Relax. delay 1.000 sec
Pulse 35.0 degrees
Acq. time 1.993 sec
Width 6006.0 Hz
16 repetitions
OBSERVE H1, 400.1351937 MHz
DATA PROCESSING
FT size 32768
Total time 0 min, 50 sec
ppm
6.39
11.90
7.93
1.00
12.82

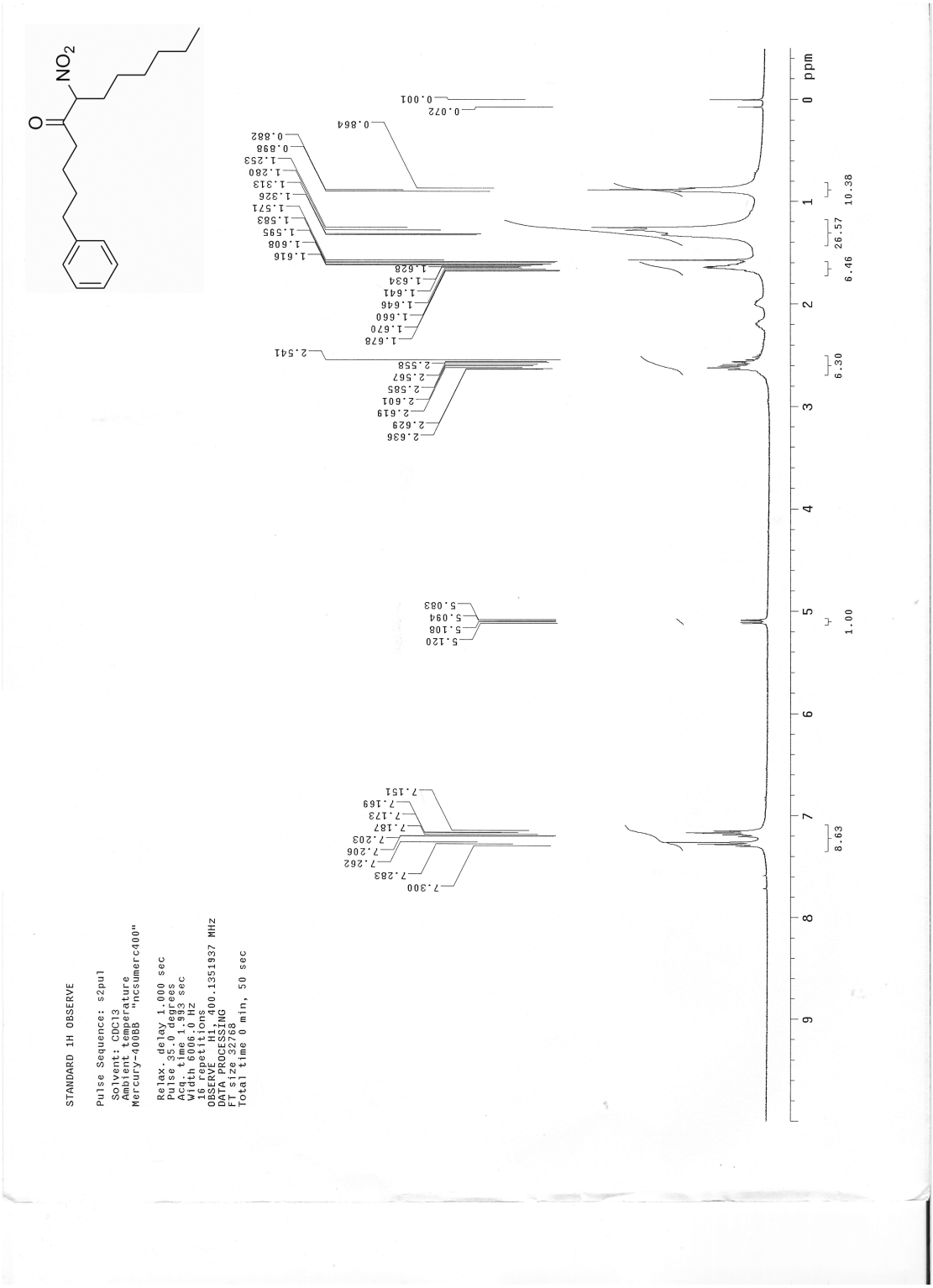


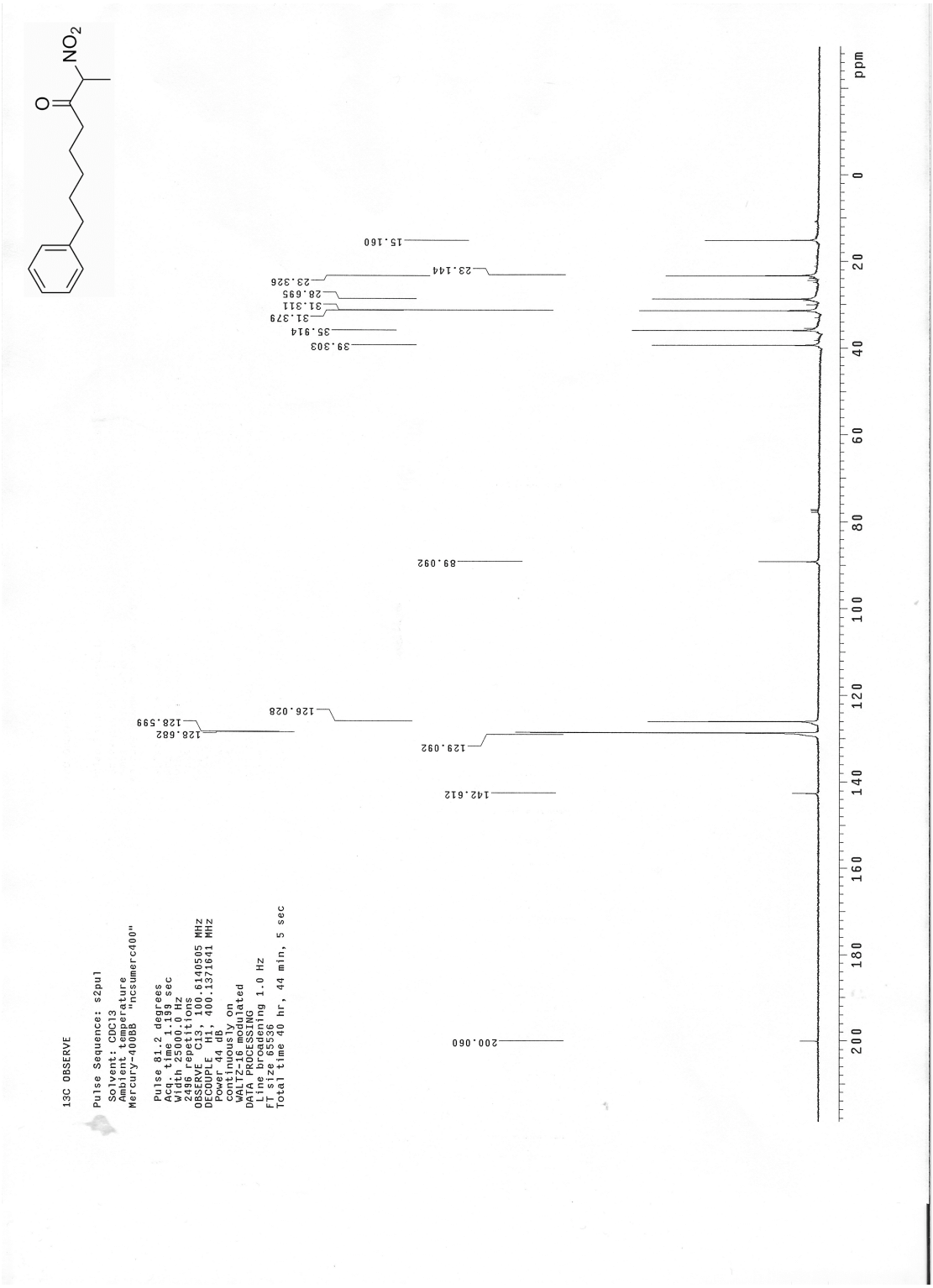

STANDARD 1H OBSERVE
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
Mercury-400BB "ncsumerc400"
Relax. delay 1.000 sec
Pulse 35.0 degrees
Acq. time 1.993 sec
Width 6006.0 HZ
16 repetitions
OBSERVE H1, 400.1351937 MHz
DATA PROCESSING
FT size 32768
Total time 0 min, 0 sec
NO2
O
0.904
0.922
0.931
0.938
0.952
1.265
1.293
1.303
1.308
1.325
1.331
1.340
1.350
1.358
1.363
1.373
1.376
1.385
1.395
1.598
1.614
1.623
1.627
1.639
1.647
1.652
1.665
1.676
1.682
2.563
2.572
2.579
2.589
2.606
2.623
2.634
2.641
5.088
5.100
5.113
5.125
7.156
7.174
7.190
7.206
7.208
7.261
7.266
7.285
7.290
7.303
ppm
7.40
9.63
7.16
5.81
1.00
7.34

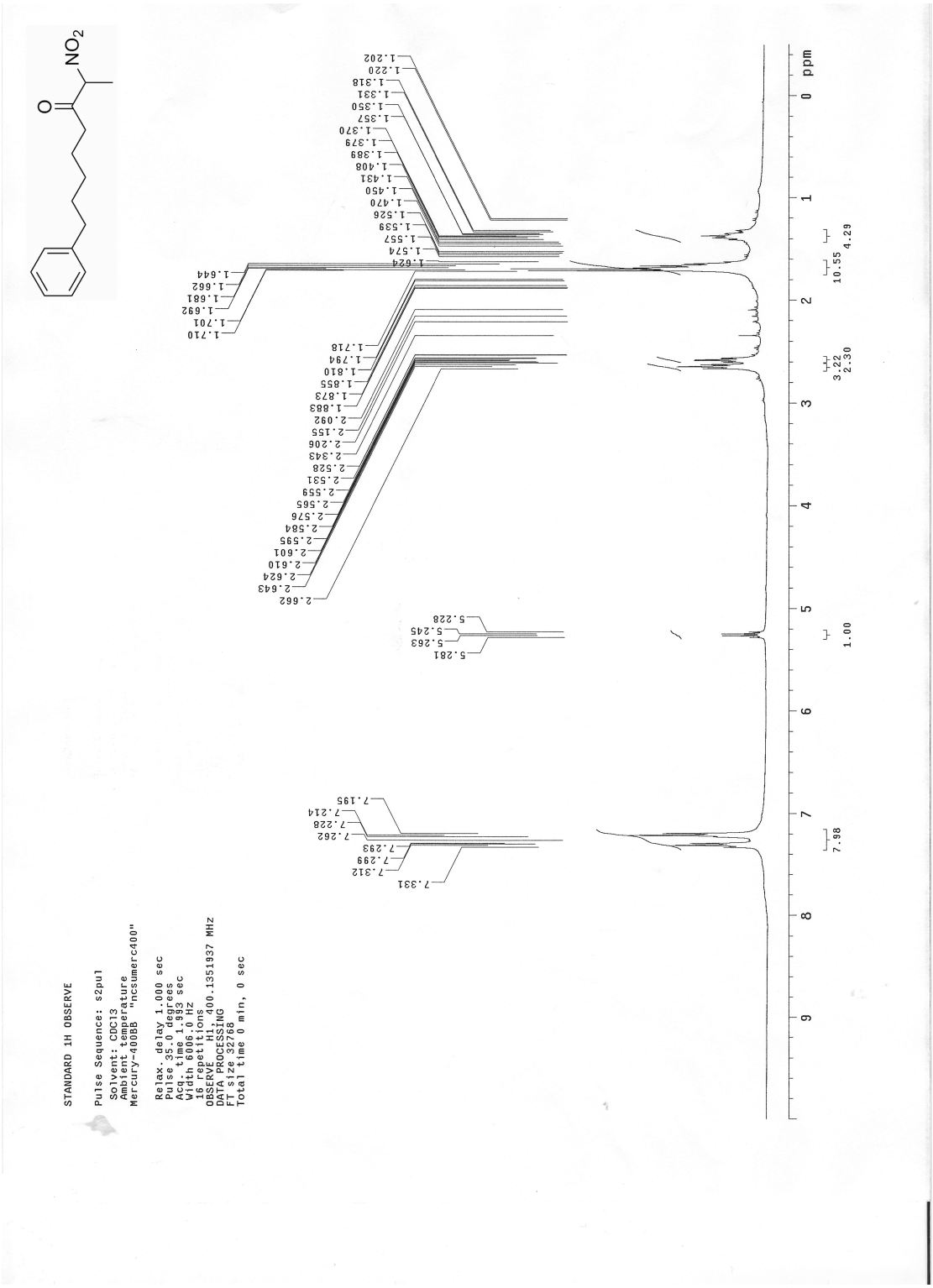

NO2
O
14.091
22.447
23.016
25.685
29.855
30.758
31.197
35.800
39.372
76.952
77.271
77.589
94.552
126.142
128.606
128.622
142.013
199.332
ppm
0
20
40
60
80
100
120
140
160
180
200
13C OBSERVE
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
Mercury-400BB "ncsumerc400"
Pulse 81.2 degrees
Acq. time 1.199 sec
Width 25000.0 Hz
5152 repetitions
OBSERVE C13, 100.6140505 MHz
DECOUPLE H1, 400.1371641 MHz
Power 44 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 65536
Total time 40 hr, 44 min, 5 sec

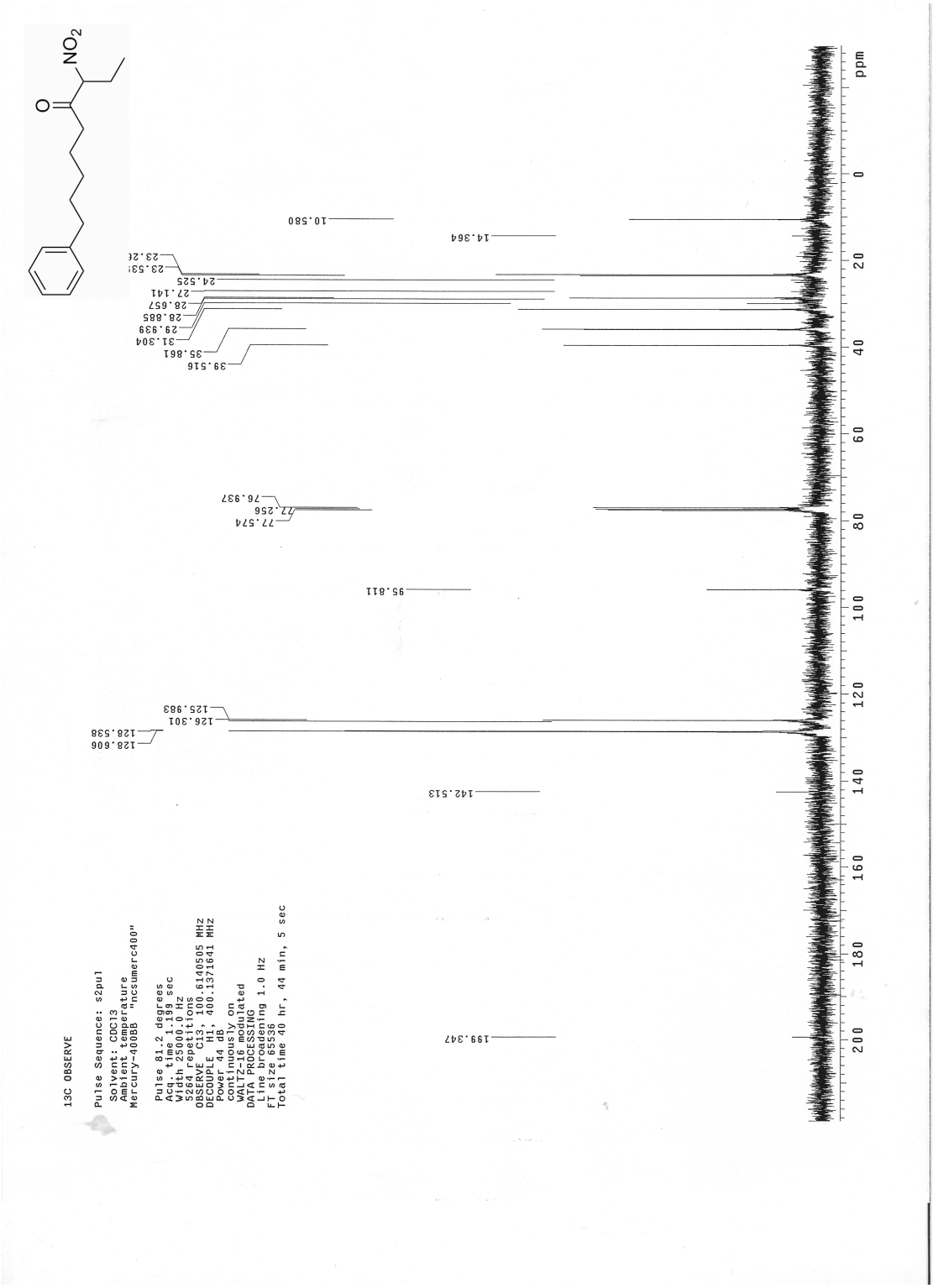

NO2
O
0.004
0.875
0.891
1.219
1.257
1.324
1.578
1.598
1.610
1.618
1.635
1.643
1.647
1.661
1.672
2.542
2.559
2.568
2.575
2.586
2.603
2.620
2.631
2.638
5.087
5.098
5.112
5.123
7.152
7.154
7.171
7.189
7.205
7.207
7.261
7.265
7.284
7.298
7.302
ppm
9.42
1.00
7.08
7.55
15.46
8.27
STANDARD 1H OBSERVE
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
Mercury-400BB "ncsumerc400"
Relax. delay 1.000 sec
Pulse 35.0 degrees
Acq. time 1.993 sec
Width 6006.0 Hz
1 repetitions
OBSERVE H1, 400.1351937 MHz
DATA PROCESSING
FT size 32768
Total time 0 min, 50 sec

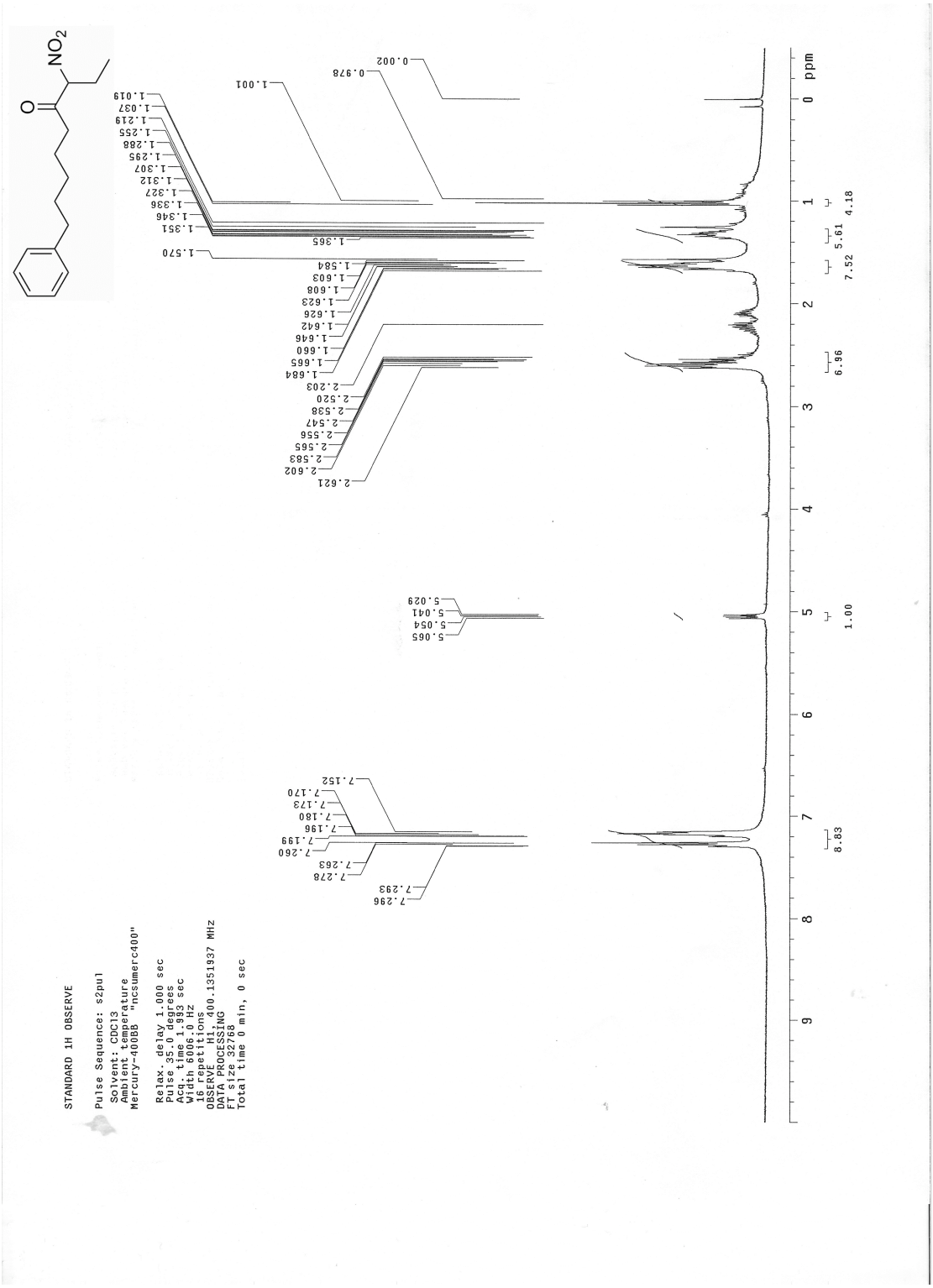

NO2
O
14.219
22.687
23.016
23.865
25.965
27.361
27.755
28.748
29.196
29.908
29.946
30.758
31.531
35.800
39.364
76.945
77.263
77.582
94.552
126.134
128.606
142.013
199.332
ppm
0
20
40
60
80
100
120
140
160
180
200
13C OBSERVE
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
Mercury-400BB "ncsumerc400"
Pulse 81.2 degrees
Acq. time 1.193 sec
Width 25000.0 Hz
40816 repetitions
OBSERVE C13, 100.6140505 MHz
DECOUPLE H1, 400.1371641 MHz
Power 44 dB
continuously on
WALTZ16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 65536
Total time 40 hr, 44 min, 5 sec

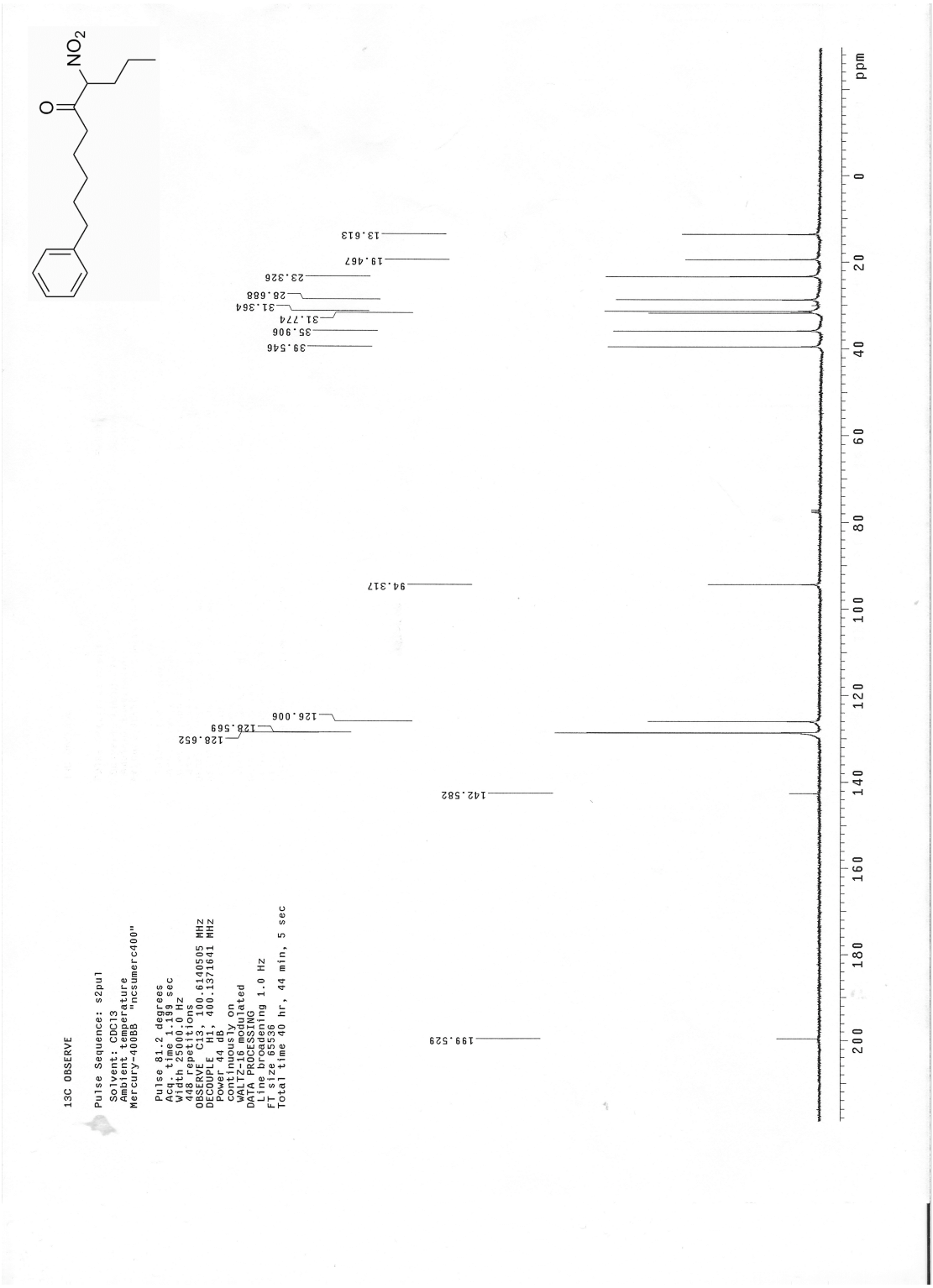

NO2
O
0.001
0.072
0.864
0.882
0.898
1.253
1.280
1.313
1.326
1.571
1.583
1.595
1.608
1.616
1.628
1.634
1.641
1.646
1.660
1.670
1.678
2.541
2.558
2.567
2.585
2.601
2.619
2.629
2.636
5.083
5.094
5.108
5.120
7.151
7.169
7.173
7.187
7.203
7.206
7.262
7.283
7.300
ppm
10.38
26.57
6.46
6.30
1.00
8.63
STANDARD 1H OBSERVE
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
Mercury-400BB "ncsumerc400"
Relax. delay 1.000 sec
Pulse 35.0 degrees
Acq. time 1.993 sec
Width 6006.0 Hz
16 repetitions
OBSERVE H1, 400.1351937 MHz
DATA PROCESSING
FT size 32768
Total time 0 min, 50 sec

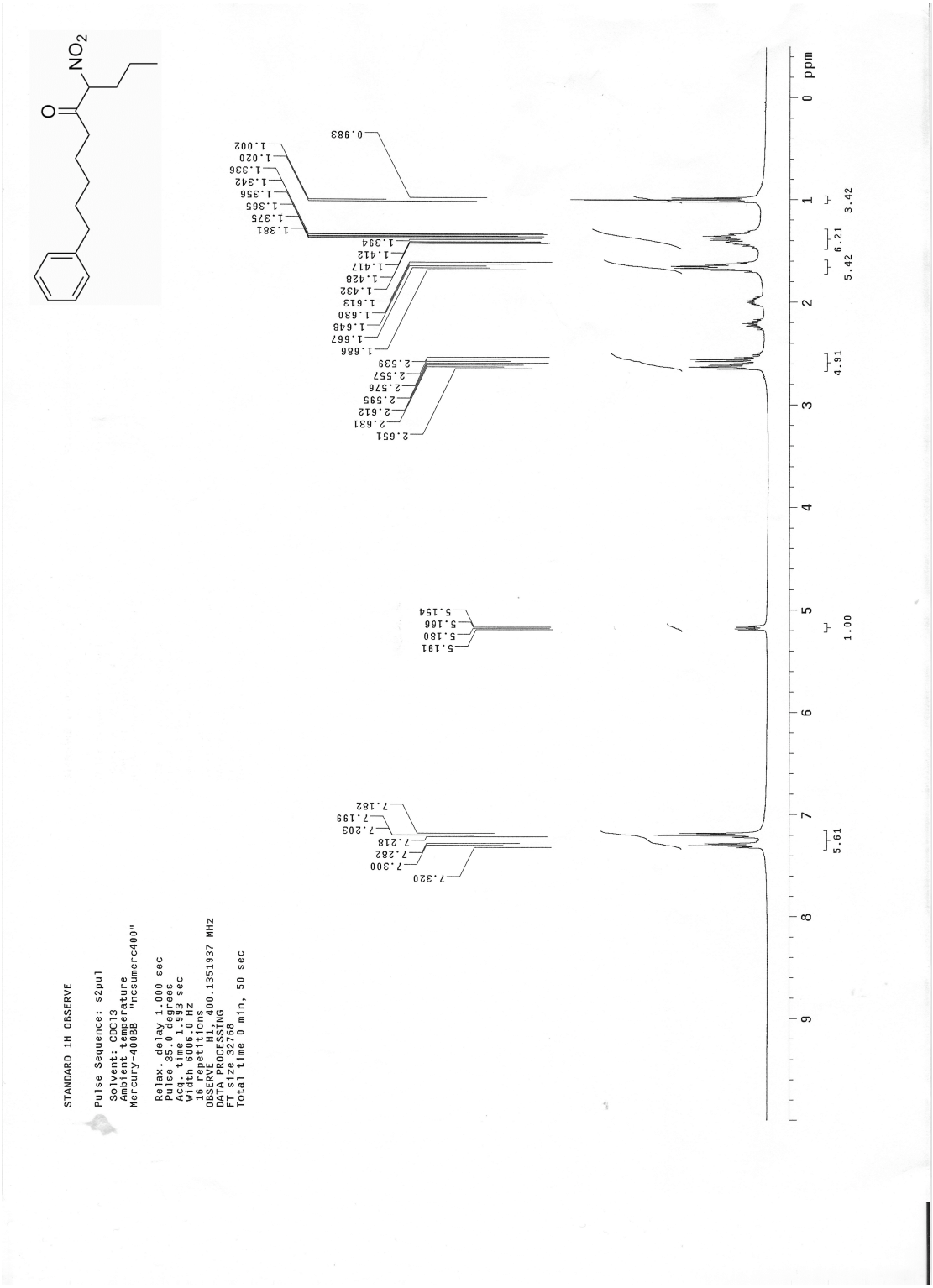

NO2
O
15.160
23.144
23.326
28.695
31.311
31.379
35.914
39.303
89.092
126.028
126.599
126.682
129.092
142.612
200.060
ppm
0
20
40
60
80
100
120
140
160
180
200
13C OBSERVE
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
Mercury-400BB "ncsumerc400"
Pulse 81.2 degrees
Acq. time 1.199 sec
Width 25000.0 Hz
2048 repetitions
OBSERVE C13, 100.6140505 MHz
DECOUPLE H1, 400.1371641 MHz
Power 44 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 65536
Total time 40 hr, 44 min, 5 sec

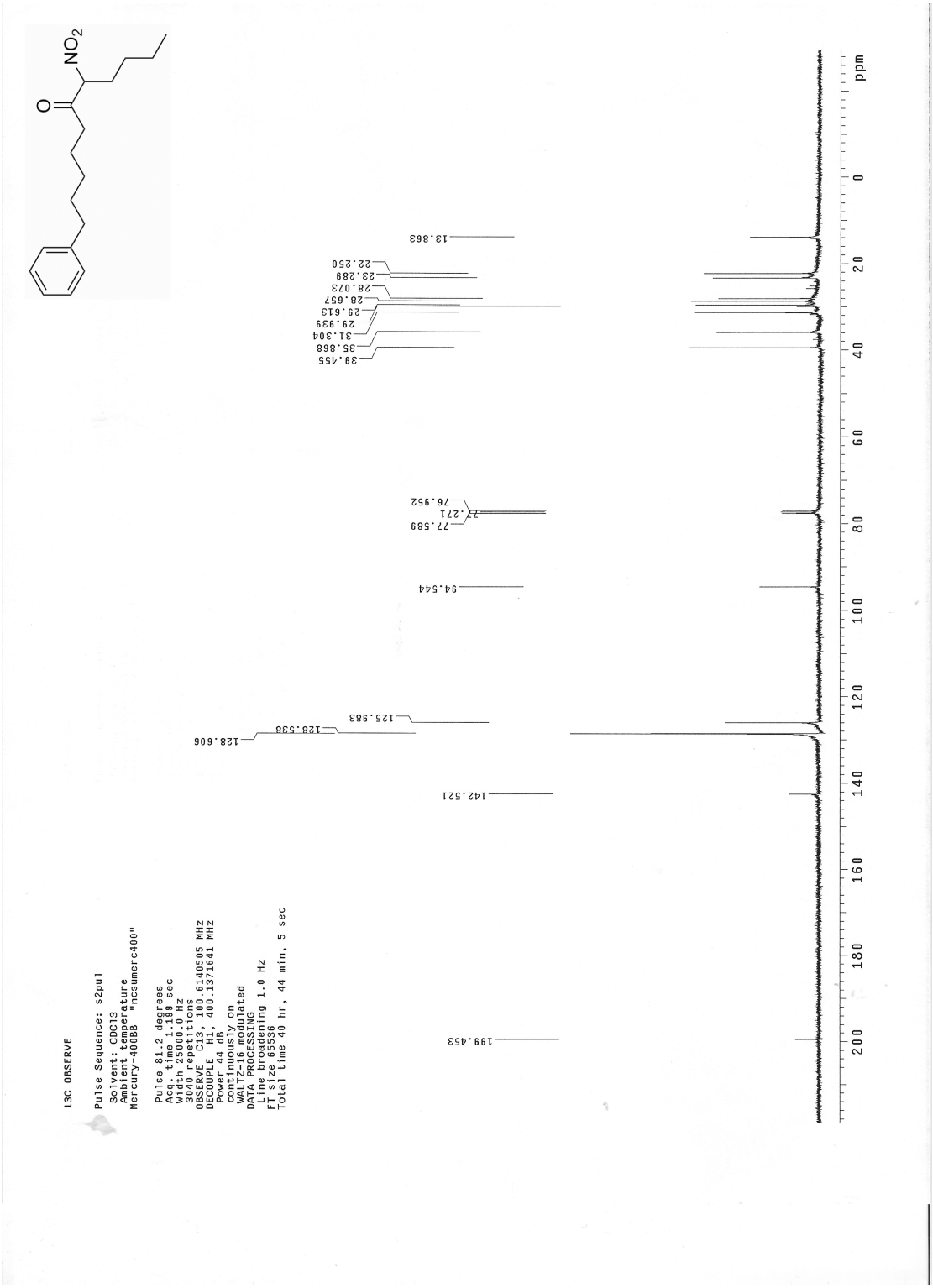

NO2
O
STANDARD 1H OBSERVE
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
Mercury-400BB "ncsumerc400"
Relax. delay 1.000 sec
Pulse 35.0 degrees
Acq. time 1.993 sec
Width 6006.0 Hz
1 repetitions
OBSERVE H1, 400.1351937 MHz
DATA PROCESSING
FT size 32768
Total time 0 min, 0 sec
ppm
10.55
4.29
3.22
2.30
1.00
7.98

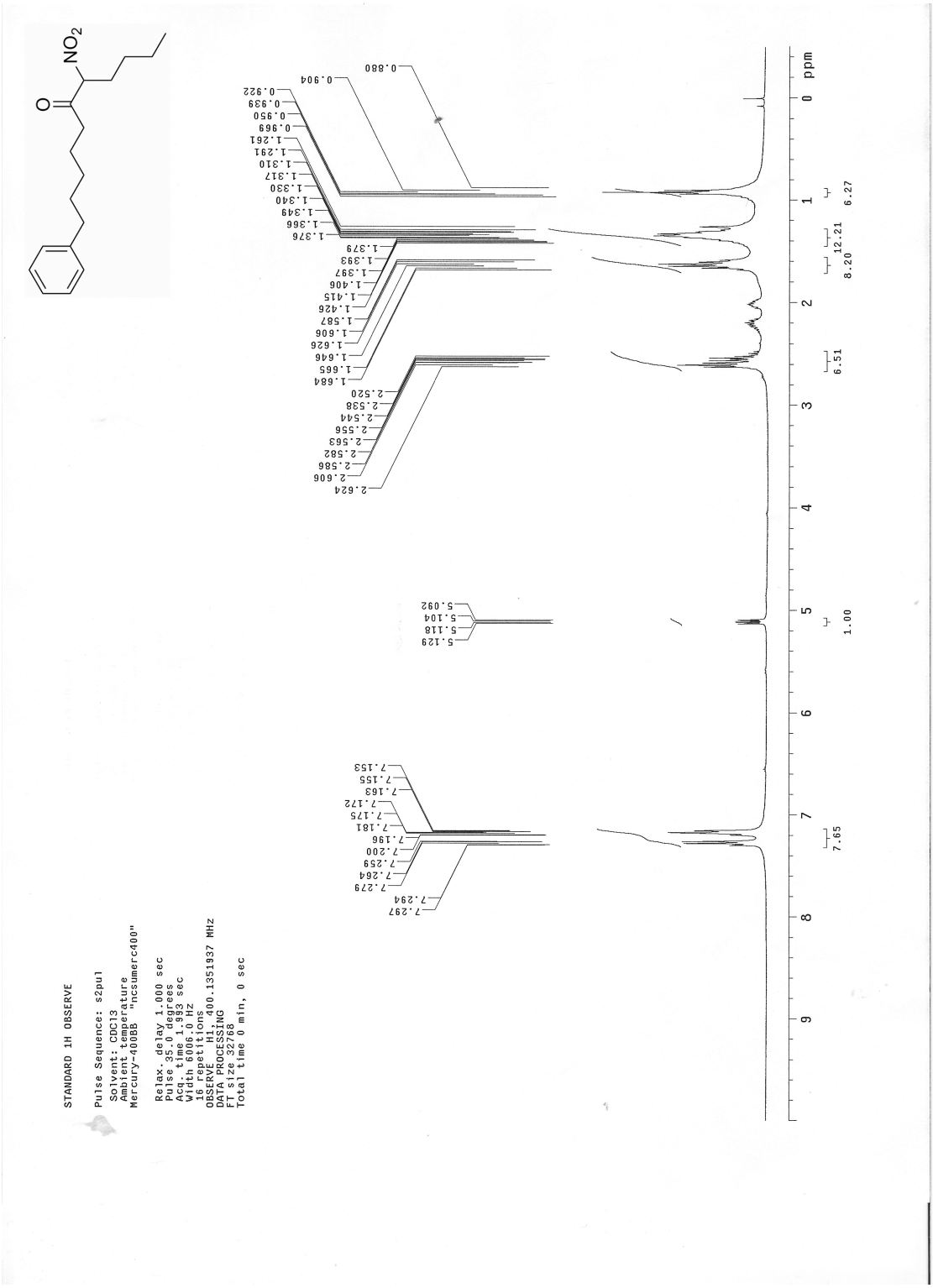

NO2
O
10.580
14.364
23.261
23.539
24.525
27.141
28.657
28.885
29.939
31.304
35.861
39.516
76.937
77.256
77.574
95.811
125.983
126.301
128.538
128.606
142.513
199.347
ppm
0
20
40
60
80
100
120
140
160
180
200
13C OBSERVE
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
Mercury-400BB "ncsumerc400"
Pulse 81.2 degrees
Acq. time 1.199 sec
Width 25000.0 Hz
524 repetitions
OBSERVE C13, 100.6140505 MHz
DECOUPLE H1, 400.1371641 MHz
Power 44 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 65536
Total time 40 hr, 44 min, 5 sec

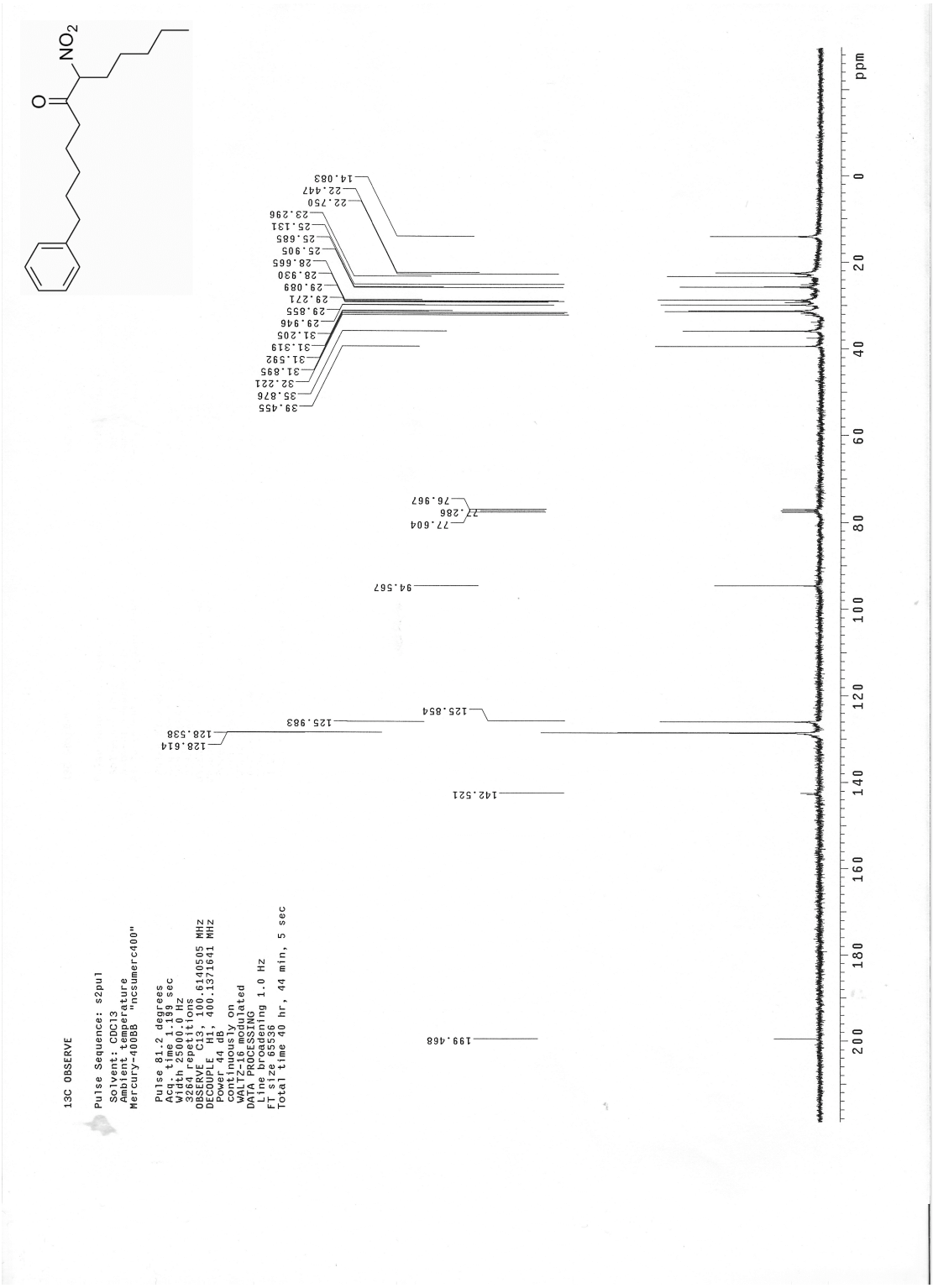

NO2
O
0.002
0.978
1.001
1.019
1.037
1.219
1.255
1.288
1.295
1.307
1.312
1.327
1.336
1.346
1.351
1.365
1.570
1.584
1.603
1.608
1.623
1.626
1.642
1.646
1.660
1.665
1.684
2.203
2.520
2.538
2.547
2.556
2.565
2.583
2.602
2.621
5.029
5.041
5.054
5.065
7.152
7.170
7.173
7.180
7.196
7.199
7.260
7.263
7.278
7.293
7.296
ppm
0
1
2
3
4
5
6
7
8
9
4.18
5.61
7.52
6.96
1.00
8.83
STANDARD 1H OBSERVE
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
Mercury-400BB "ncsumerc400"
Relax. delay 1.000 sec
Pulse 35.0 degrees
Acq. time 1.993 sec
Width 6006.0 Hz
16 repetitions
OBSERVE H1, 400.1351937 MHz
DATA PROCESSING
FT size 32768
Total time 0 min, 0 sec

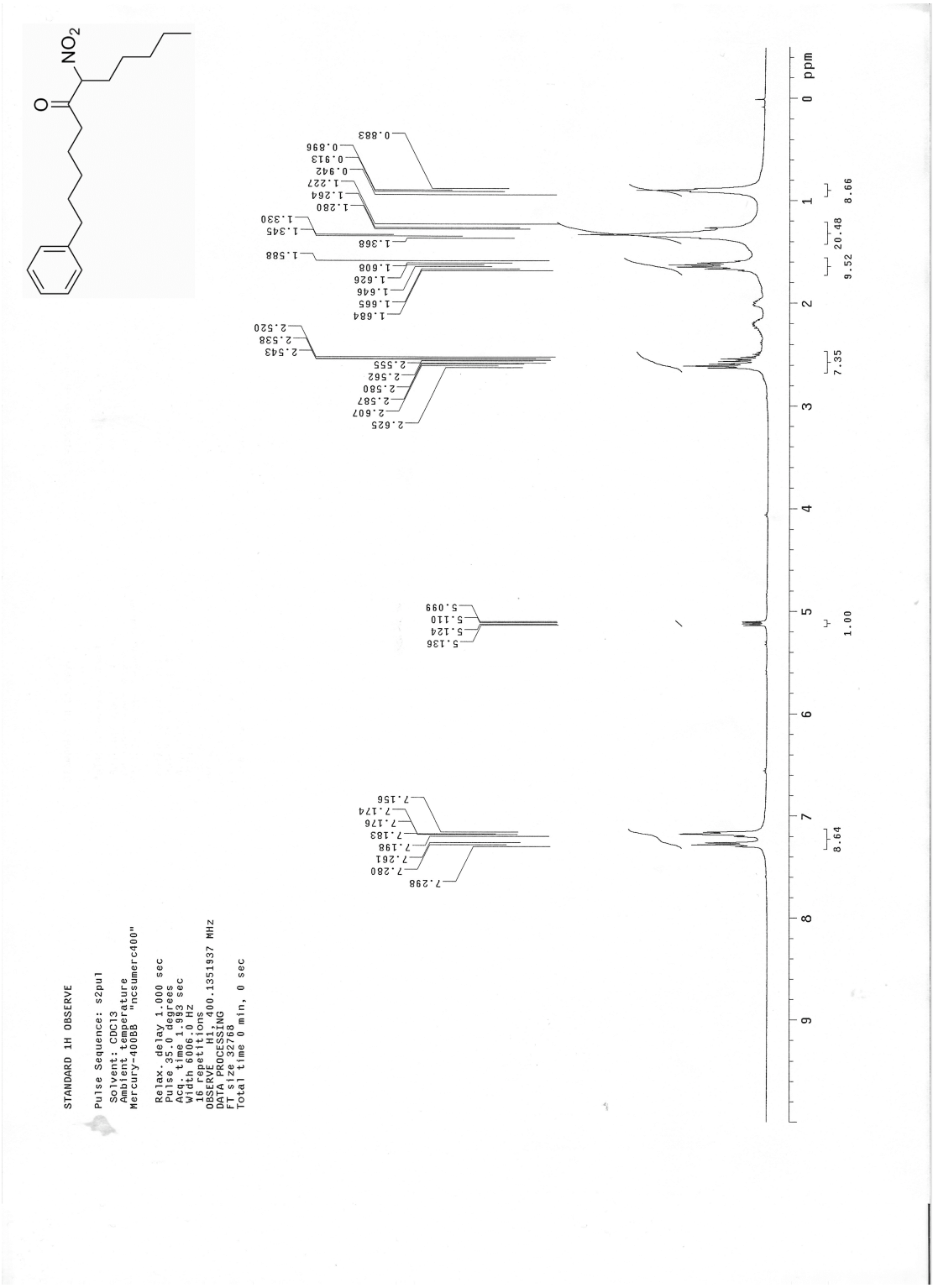

NO2
O
13.613
19.467
23.326
28.688
31.364
31.774
35.906
39.546
94.317
126.006
128.569
128.652
142.582
199.529
ppm
0
20
40
60
80
100
120
140
160
180
200
13C OBSERVE
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
Mercury-400BB "ncsumerc400"
Pulse 81.2 degrees
Acq. time 1.199 sec
Width 25000.0 Hz
448 repetitions
OBSERVE C13, 100.6140505 MHz
DECOUPLE H1, 400.1371641 MHz
Power 44 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 65536
Total time 40 hr, 44 min, 5 sec

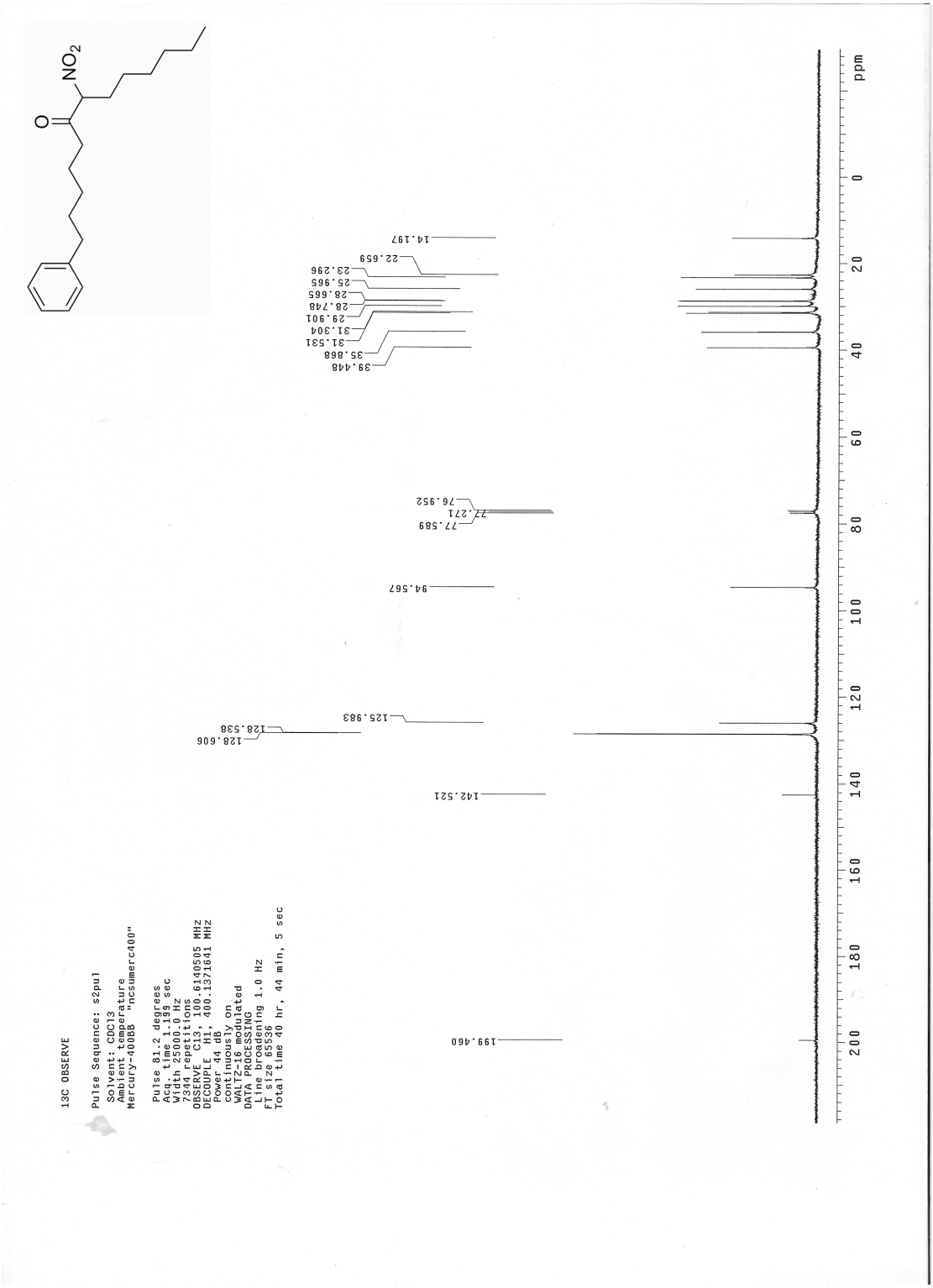

NO2
O
0.983
1.002
1.020
1.336
1.342
1.356
1.365
1.375
1.381
1.394
1.412
1.417
1.428
1.432
1.613
1.630
1.648
1.667
1.686
2.539
2.557
2.576
2.595
2.612
2.631
2.651
5.154
5.166
5.180
5.191
7.182
7.199
7.203
7.218
7.282
7.300
7.320
ppm
3.42
6.21
5.42
4.91
1.00
5.61
STANDARD 1H OBSERVE
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
Mercury-400BB "ncsumerc400"
Relax. delay 1.000 sec
Pulse 35.0 degrees
Acq. time 1.993 sec
Width 6006.0 Hz
16 repetitions
OBSERVE H1, 400.1351937 MHz
DATA PROCESSING
FT size 32768
Total time 0 min, 50 sec

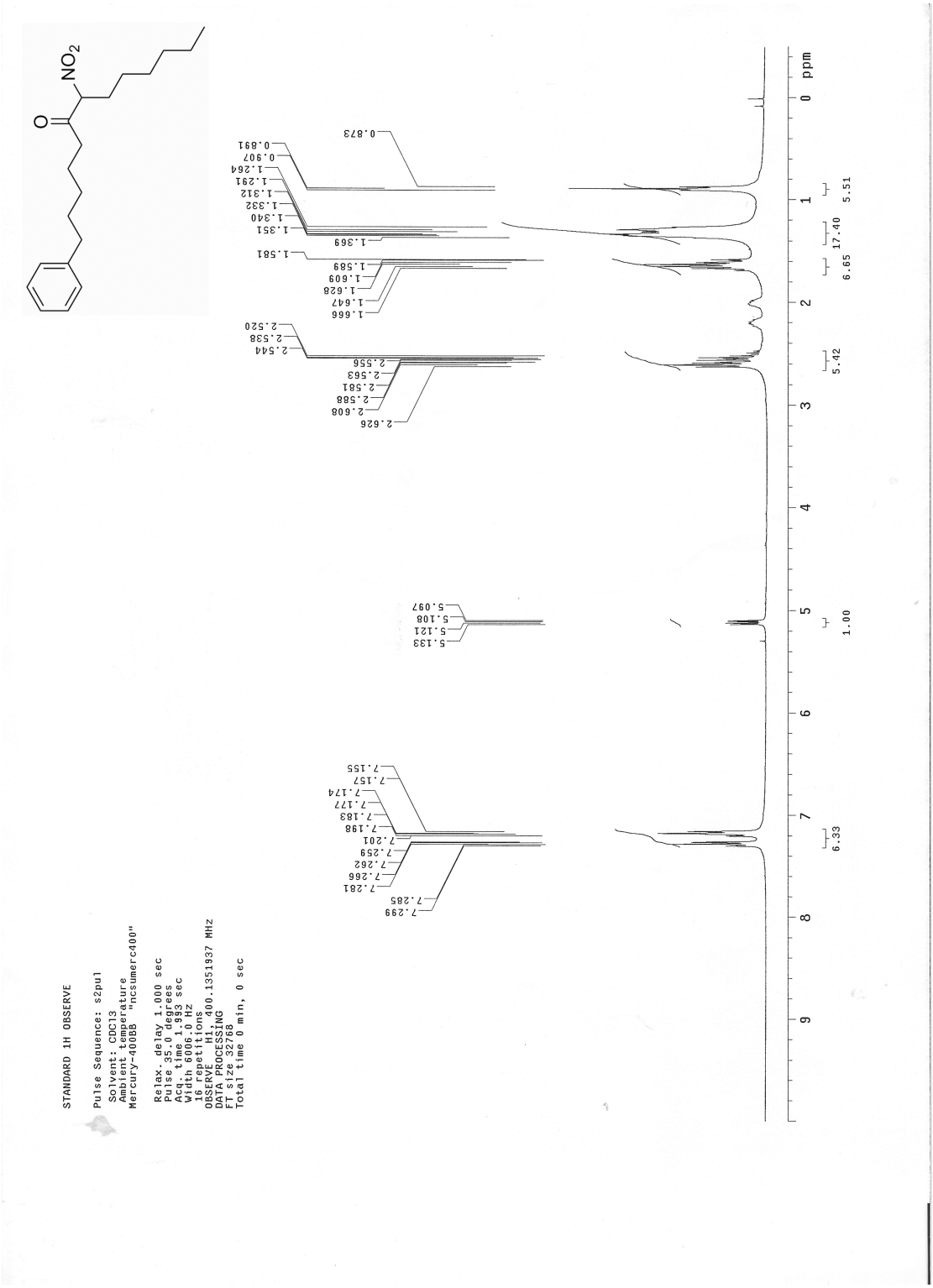

O
NO2
13.863
22.250
23.289
28.073
28.657
29.613
29.939
31.304
35.868
39.455
76.952
77.271
77.589
94.544
125.983
128.538
128.606
142.521
199.453
ppm
0
20
40
60
80
100
120
140
160
180
200
13C OBSERVE
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
Mercury-400BB "ncsumerc400"
Pulse 81.2 degrees
Acq. time 1.199 sec
Width 25000.0 Hz
3040 repetitions
OBSERVE C13, 100.6140505 MHz
DECOUPLE H1, 400.1371641 MHz
Power 44 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 65536
Total time 40 hr, 44 min, 5 sec

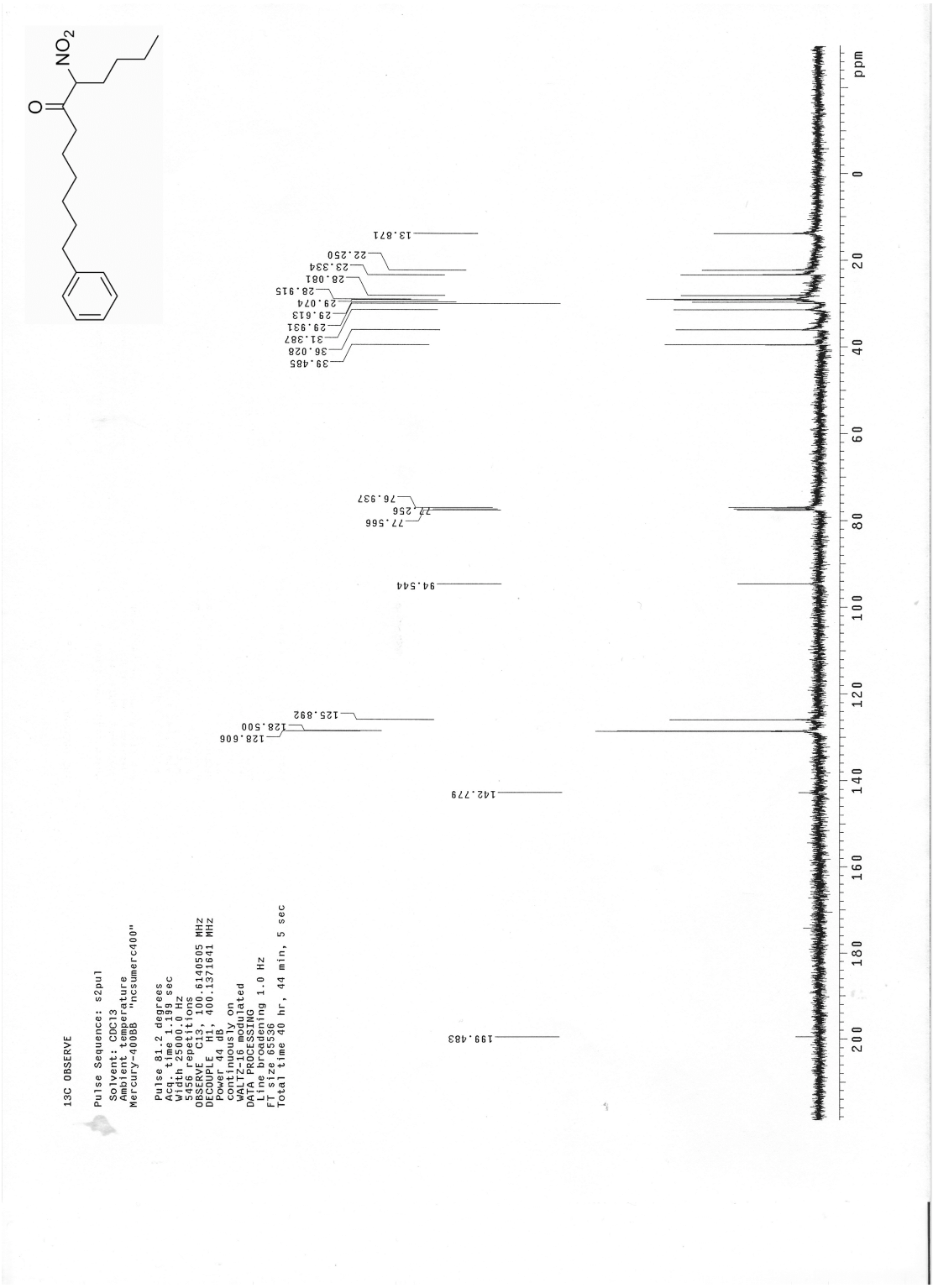

NO2
O
0.860
0.904
0.922
0.939
0.950
0.969
1.261
1.291
1.310
1.317
1.330
1.340
1.349
1.366
1.376
1.379
1.393
1.397
1.406
1.415
1.426
1.587
1.606
1.626
1.646
1.665
1.684
2.520
2.538
2.544
2.556
2.563
2.582
2.586
2.606
2.624
5.092
5.104
5.118
5.129
7.153
7.155
7.163
7.172
7.175
7.181
7.196
7.200
7.259
7.264
7.279
7.294
7.297
ppm
6.27
12.21
8.20
6.51
1.00
7.65
STANDARD 1H OBSERVE
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
Mercury-400BB "ncsumerc400"
Relax. delay 1.000 sec
Pulse 35.0 degrees
Acq. time 1.993 sec
Width 6006.0 Hz
1 repetitions
OBSERVE H1, 400.1351937 MHz
DATA PROCESSING
FT size 32768
Total time 0 min, 0 sec

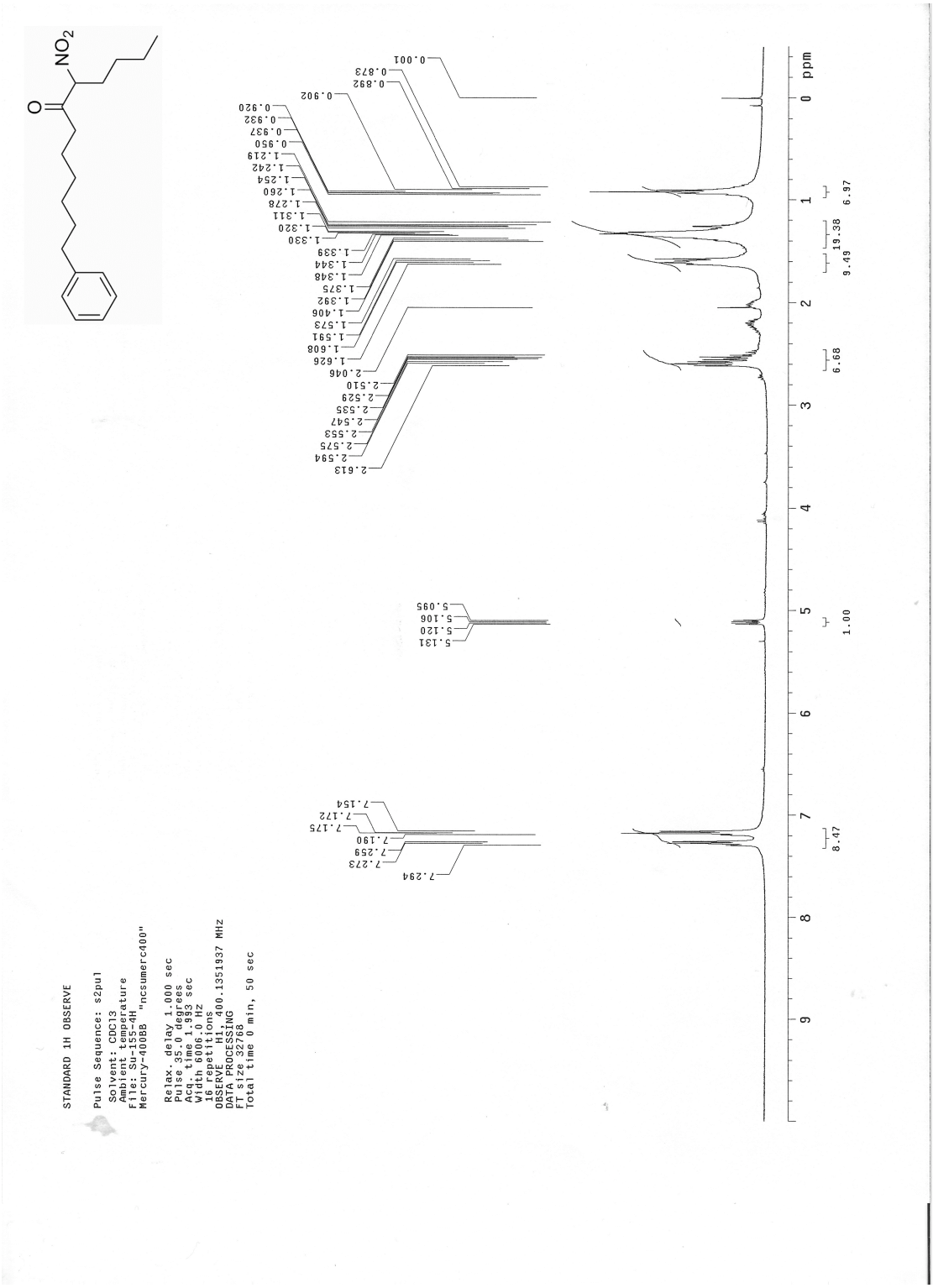

NO2
O
14.083
22.447
22.750
23.296
25.131
25.685
25.905
28.665
28.930
29.089
29.271
29.855
29.946
31.205
31.319
31.592
31.895
32.221
35.876
39.455
76.967
77.286
77.604
94.567
125.854
125.983
128.538
128.614
142.521
199.468
ppm
0
20
40
60
80
100
120
140
160
180
200
13C OBSERVE
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
Mercury-400BB "ncsumerc400"
Pulse 81.2 degrees
Acq. time 1.199 sec
Width 25000.0 Hz
32768 repetitions
OBSERVE C13, 100.6140505 MHz
DECOUPLE H1, 400.1371641 MHz
Power 44 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 65536
Total time 40 hr, 44 min, 5 sec

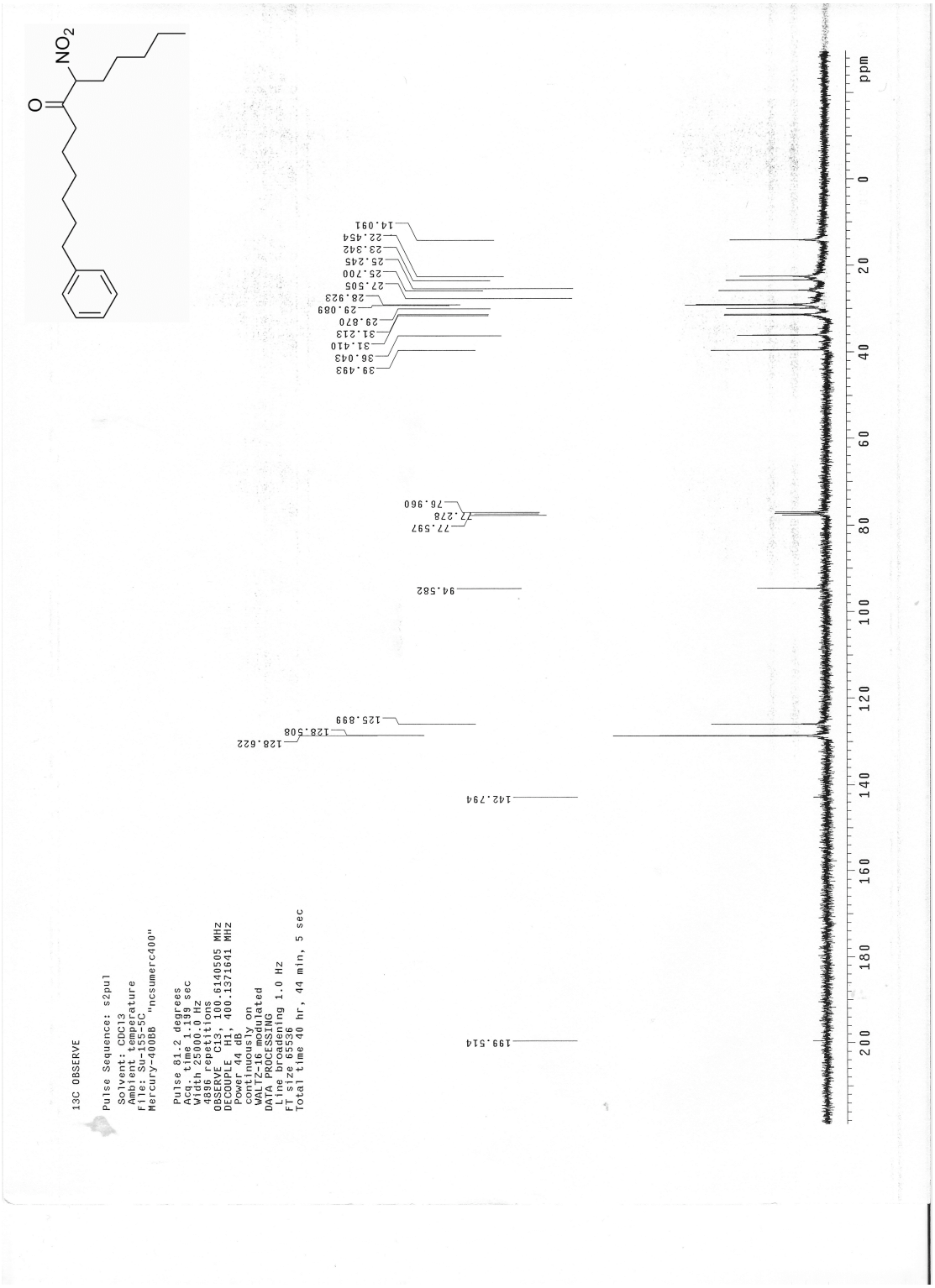

NO2
O
0.883
0.896
0.913
0.942
1.227
1.264
1.280
1.330
1.345
1.368
1.588
1.608
1.626
1.646
1.665
1.684
2.520
2.538
2.543
2.555
2.562
2.580
2.587
2.607
2.625
5.099
5.110
5.124
5.136
7.156
7.174
7.176
7.183
7.198
7.261
7.280
7.298
ppm
8.66
20.48
9.52
7.35
1.00
8.64
STANDARD 1H OBSERVE
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
Mercury-400BB "ncsumerc400"
Relax. delay 1.000 sec
Pulse 35.0 degrees
Acq. time 1.993 sec
Width 6006.0 Hz
16 repetitions
OBSERVE H1, 400.1351937 MHz
DATA PROCESSING
FT size 32768
Total time 0 min, 0 sec

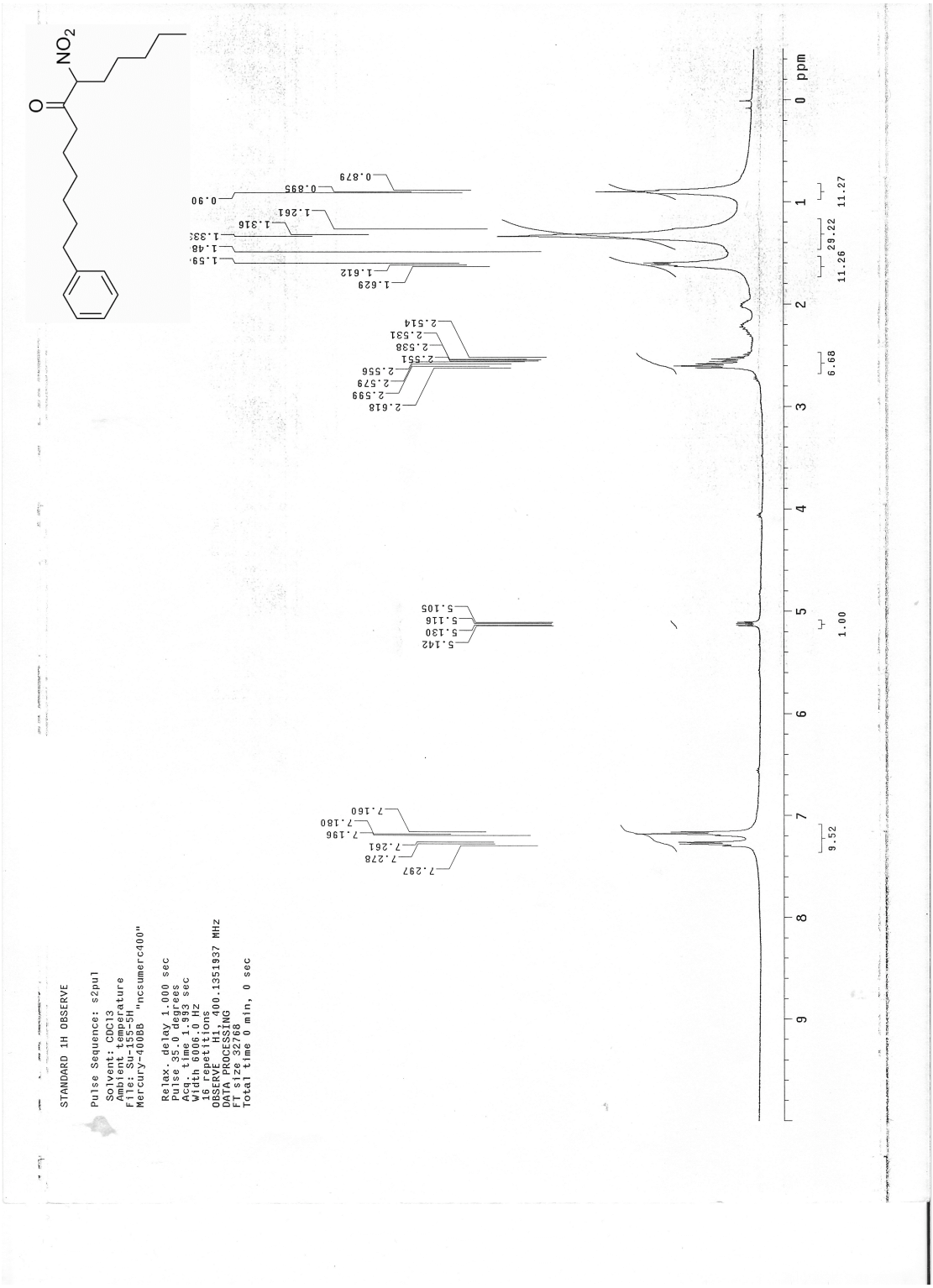



NO2
O
0.873
0.891
0.907
1.264
1.291
1.312
1.332
1.340
1.351
1.369
1.581
1.589
1.609
1.628
1.647
1.666
2.520
2.538
2.544
2.556
2.563
2.581
2.588
2.608
2.626
5.097
5.108
5.121
5.133
7.155
7.157
7.174
7.177
7.183
7.198
7.201
7.259
7.262
7.266
7.281
7.285
7.299
ppm
5.51
17.40
6.65
5.42
1.00
6.33
STANDARD 1H OBSERVE
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
Mercury-400BB "ncsumerc400"
Relax. delay 1.000 sec
Pulse 35.0 degrees
Acq. time 1.993 sec
Width 6016.0 Hz
16 repetitions
OBSERVE H1, 400.1351937 MHz
DATA PROCESSING
FT size 32768
Total time 0 min, 0 sec


NO2
O
13.871
22.250
23.334
28.081
28.915
29.074
29.613
29.931
31.387
36.028
39.485
76.937
77.256
77.566
94.544
125.892
128.500
128.606
142.779
199.483
ppm
0
20
40
60
80
100
120
140
160
180
200
13C OBSERVE
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
Mercury-400BB "ncsumerc400"
Pulse 81.2 degrees
Acq. time 1.199 sec
Width 25000.0 Hz
1 repetitions
OBSERVE C13, 100.6140505 MHz
DECOUPLE H1, 400.1371641 MHz
Power 44 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 65536
Total time 40 hr, 44 min, 5 sec


NO2
O
0.001
0.873
0.892
0.902
0.920
0.932
0.937
0.950
1.219
1.242
1.254
1.260
1.278
1.311
1.320
1.330
1.339
1.344
1.348
1.375
1.392
1.406
1.573
1.591
1.608
1.626
2.046
2.510
2.529
2.535
2.547
2.553
2.575
2.594
2.613
5.095
5.106
5.120
5.131
7.154
7.172
7.175
7.190
7.259
7.273
7.294
STANDARD 1H OBSERVE
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
File: Su-155-4H
Mercury-400BB "ncsumerc400"
Relax. delay 1.000 sec
Pulse 35.0 degrees
Acq. time 1.993 sec
Width 6006.0 HZ
16 repetitions
OBSERVE H1, 400.1351937 MHz
DATA PROCESSING
FT size 32768
Total time 0 min, 50 sec
ppm
6.97
19.38
6.68
1.00
8.47

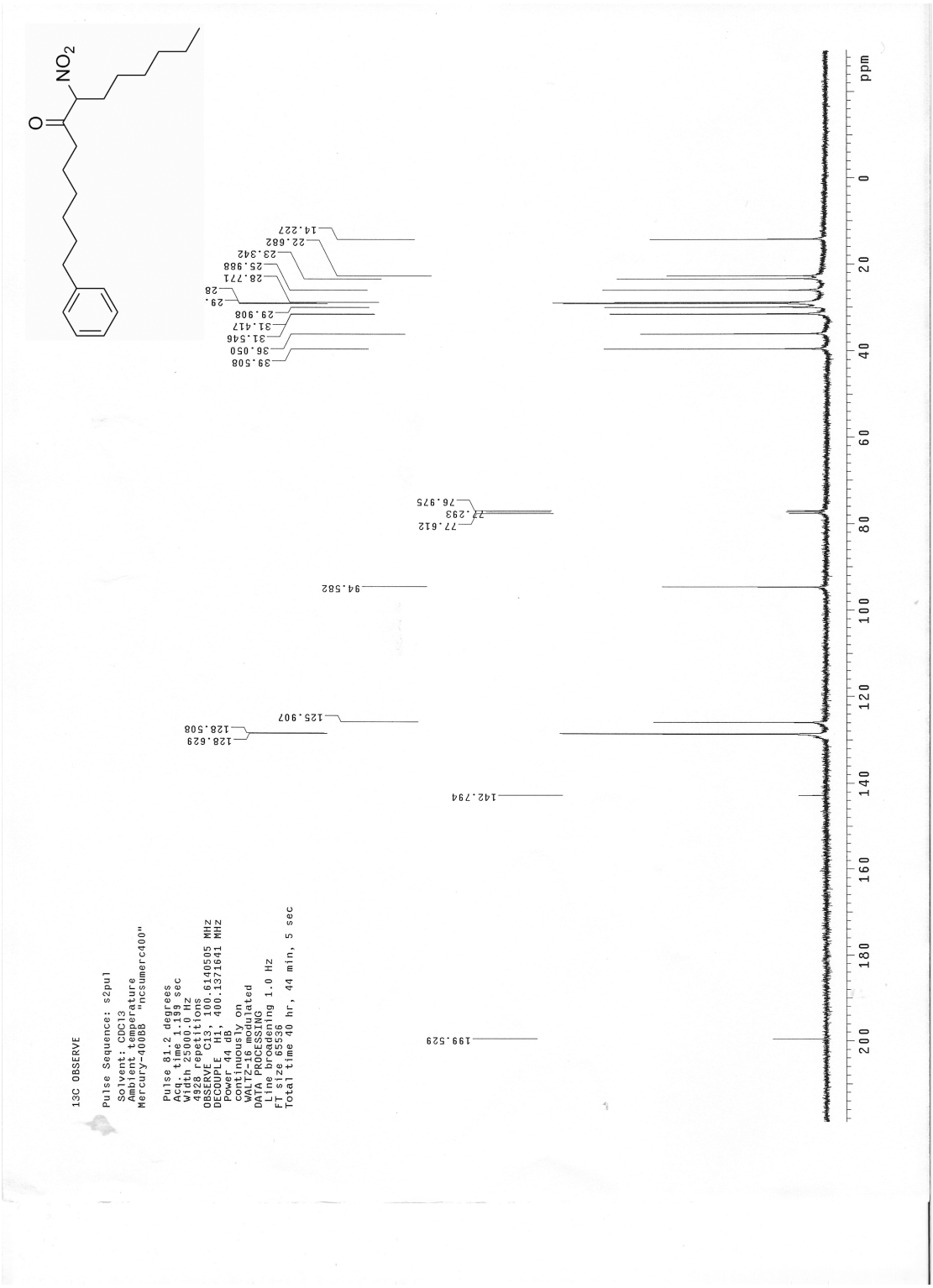

NO2
O
14.091
22.454
23.342
25.245
25.700
27.505
28.923
29.089
29.870
31.213
31.410
36.043
39.493
76.960
77.278
77.597
94.582
125.899
128.508
128.622
142.794
199.514
ppm
13C OBSERVE
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
File: Su-15-5C
Mercury-400B "ncsumerc400"
Pulse 81.2 degrees
Acq. time 1.138 sec
Width 25000.0 Hz
4896 repetitions
OBSERVE C13, 100.6140505 MHz
DECOUPLE H1, 400.1371641 MHz
Power 44 dB
continuously on
WALTZ16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 65536
Total time 40 hr, 44 min, 5 sec

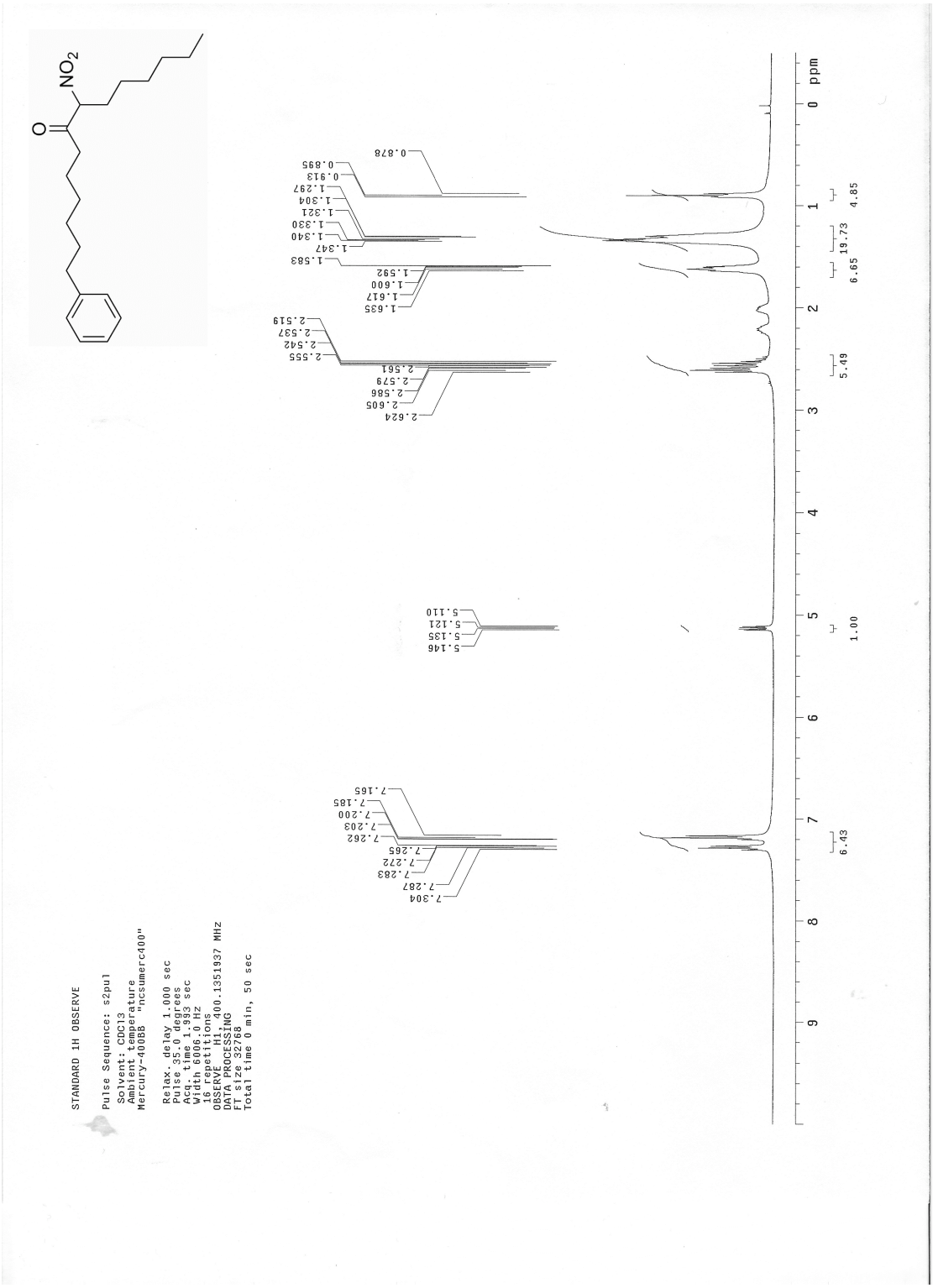


STANDARD 1H OBSERVE

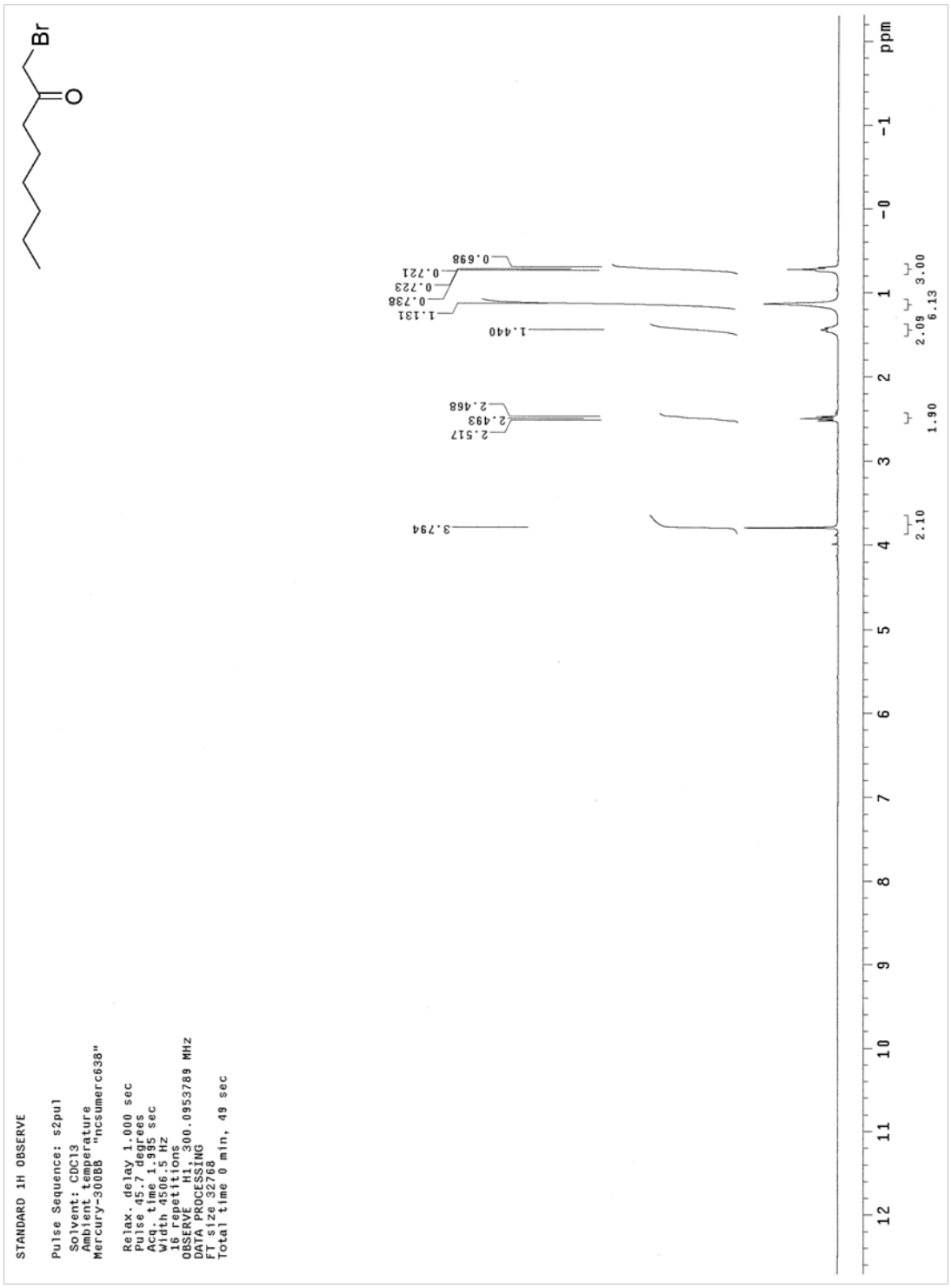
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
File: SU-1-55H
Mercury-400BB "ncsumerc400"

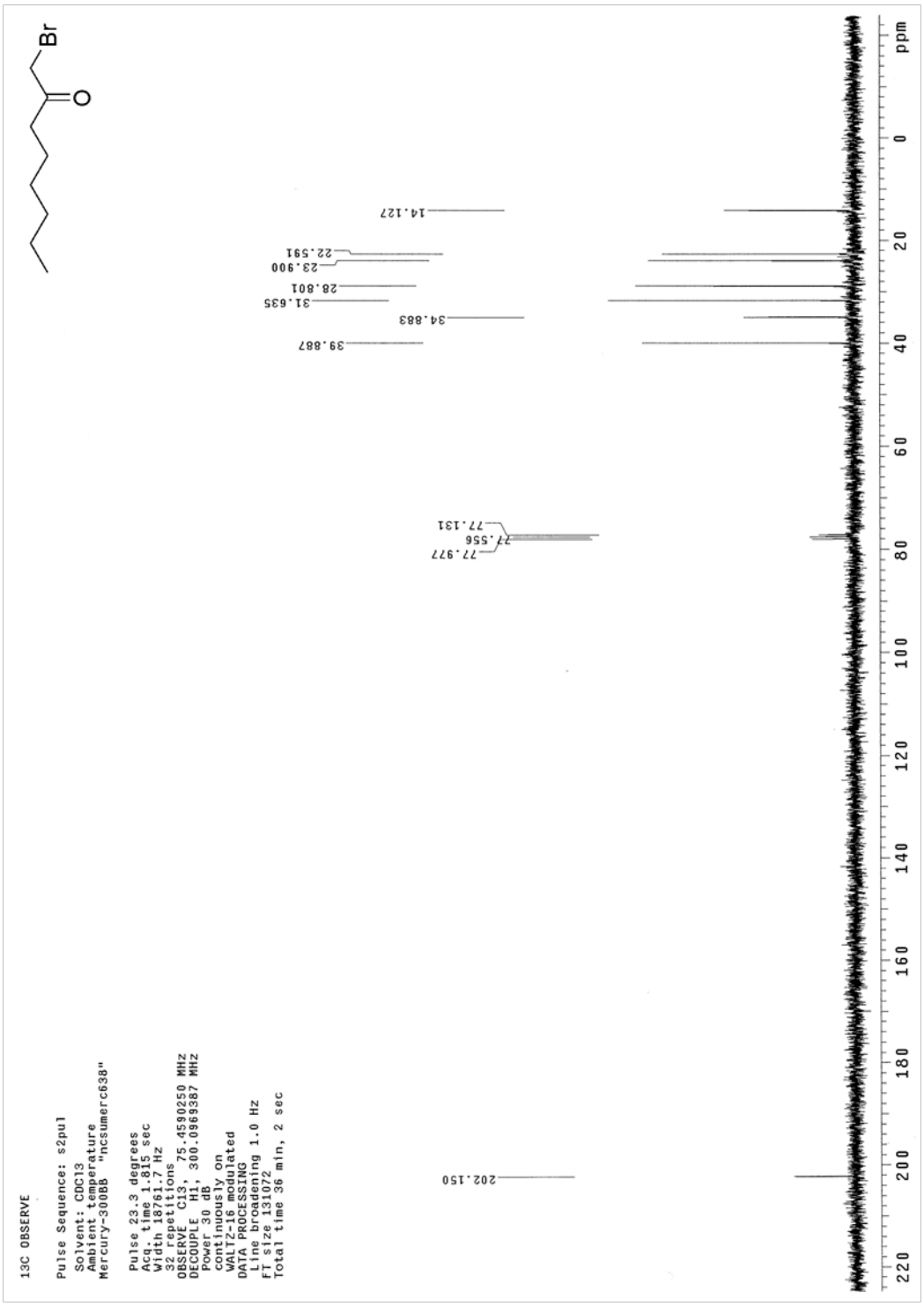
Relax. delay 1.000 sec
Pulse 35.0 degrees
Acq. time 1.993 sec
Width 6006.0 Hz
16 repetitions
OBSERVE H1, 400.1351937 MHz
DATA PROCESSING
FT size 32768
Total time 0 min, 0 sec

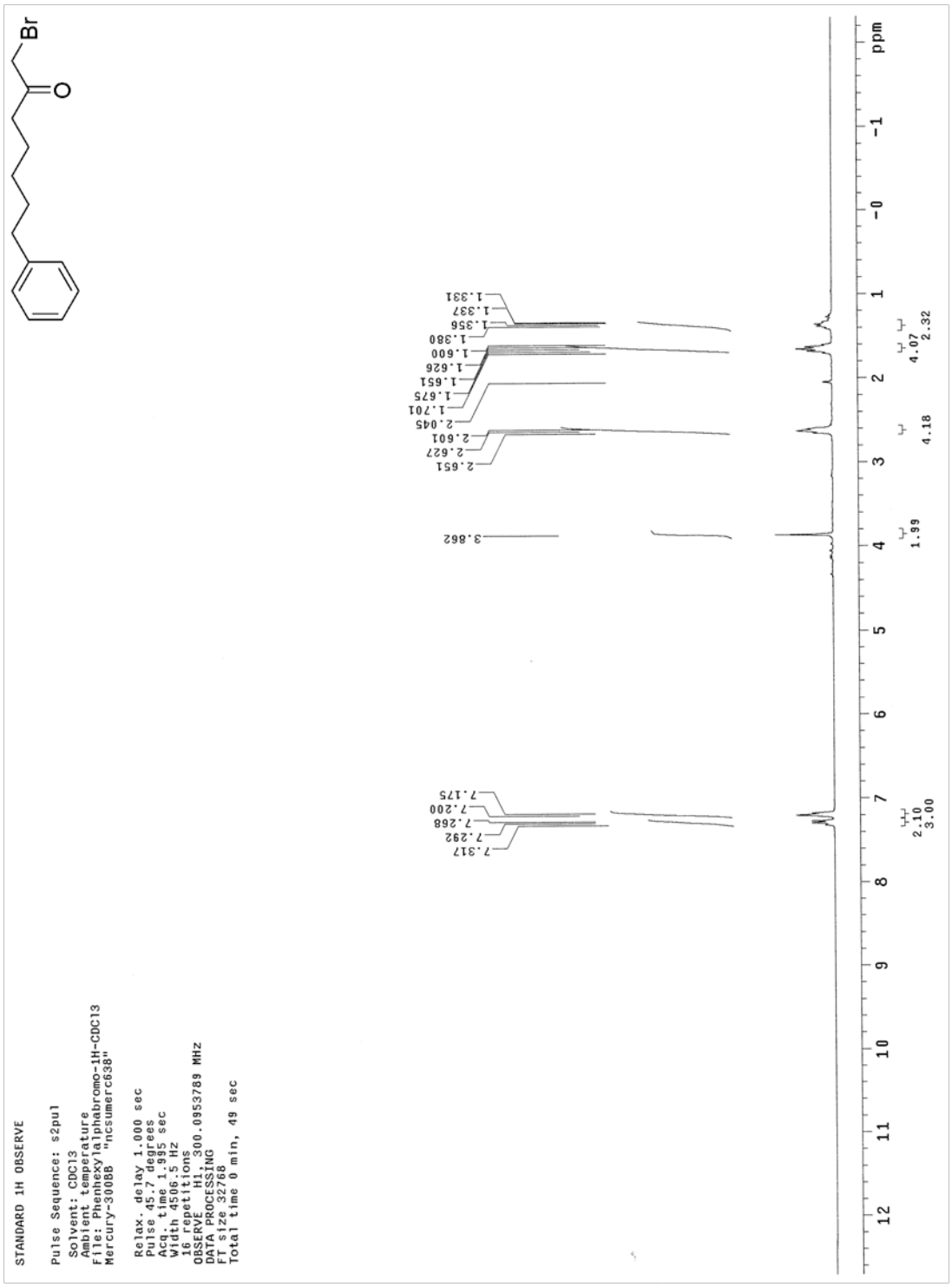


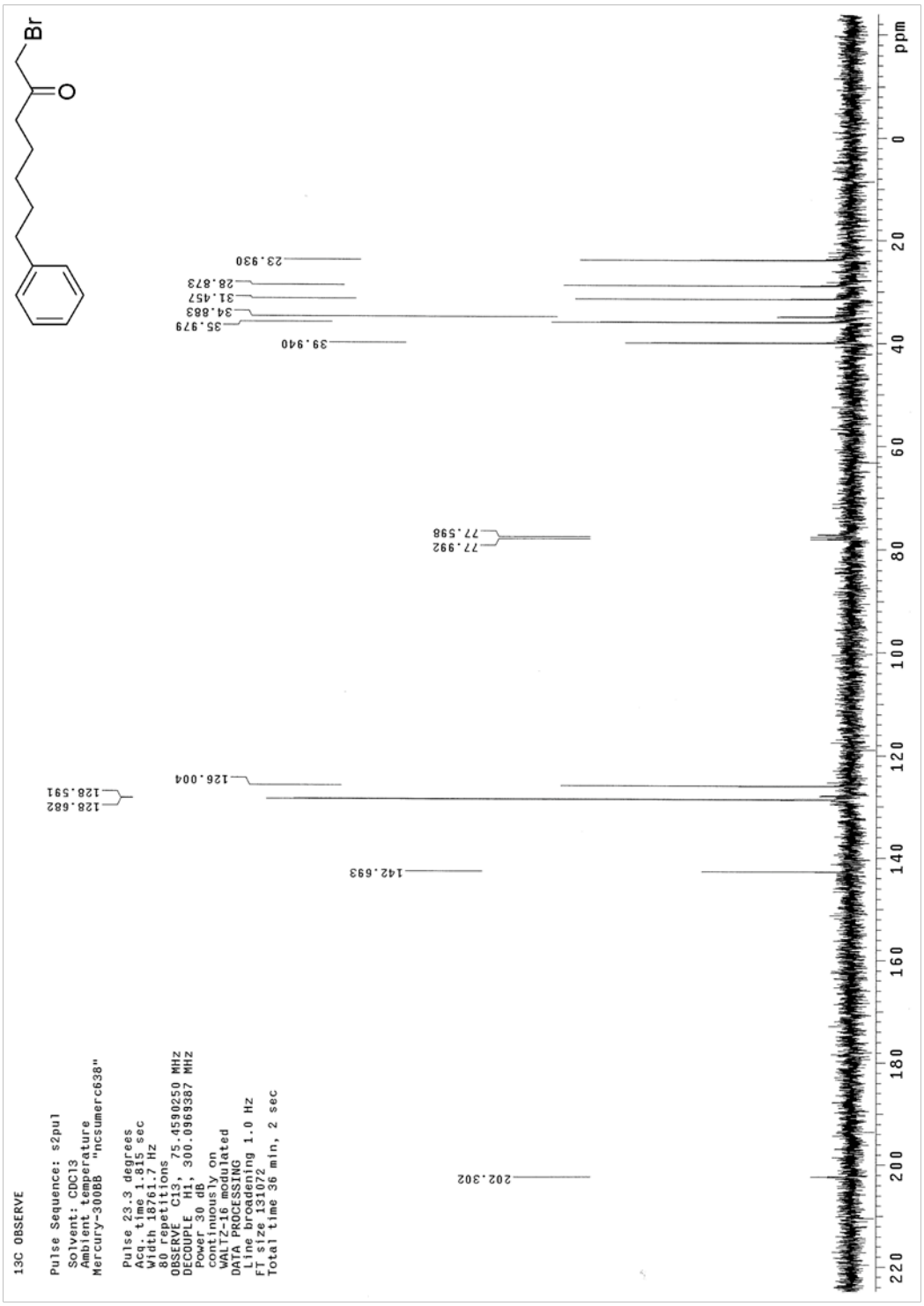

NO2
O
0.878
0.895
0.913
1.297
1.304
1.321
1.330
1.340
1.347
1.583
1.592
1.600
1.617
1.635
2.519
2.537
2.542
2.555
2.561
2.579
2.586
2.605
2.624
5.110
5.121
5.135
5.146
7.165
7.185
7.200
7.203
7.262
7.265
7.272
7.283
7.287
7.304
ppm
4.85
19.73
6.65
5.49
1.00
6.43
STANDARD 1H OBSERVE
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
Mercury-400BB "ncsumerc400"
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.499 sec
Width 6006.0 Hz
16 repetitions
OBSERVE H1, 400.1351937 MHz
DATA PROCESSING
FT size 32768
Total time 0 min, 50 sec

NMR data for α-bromo ketones

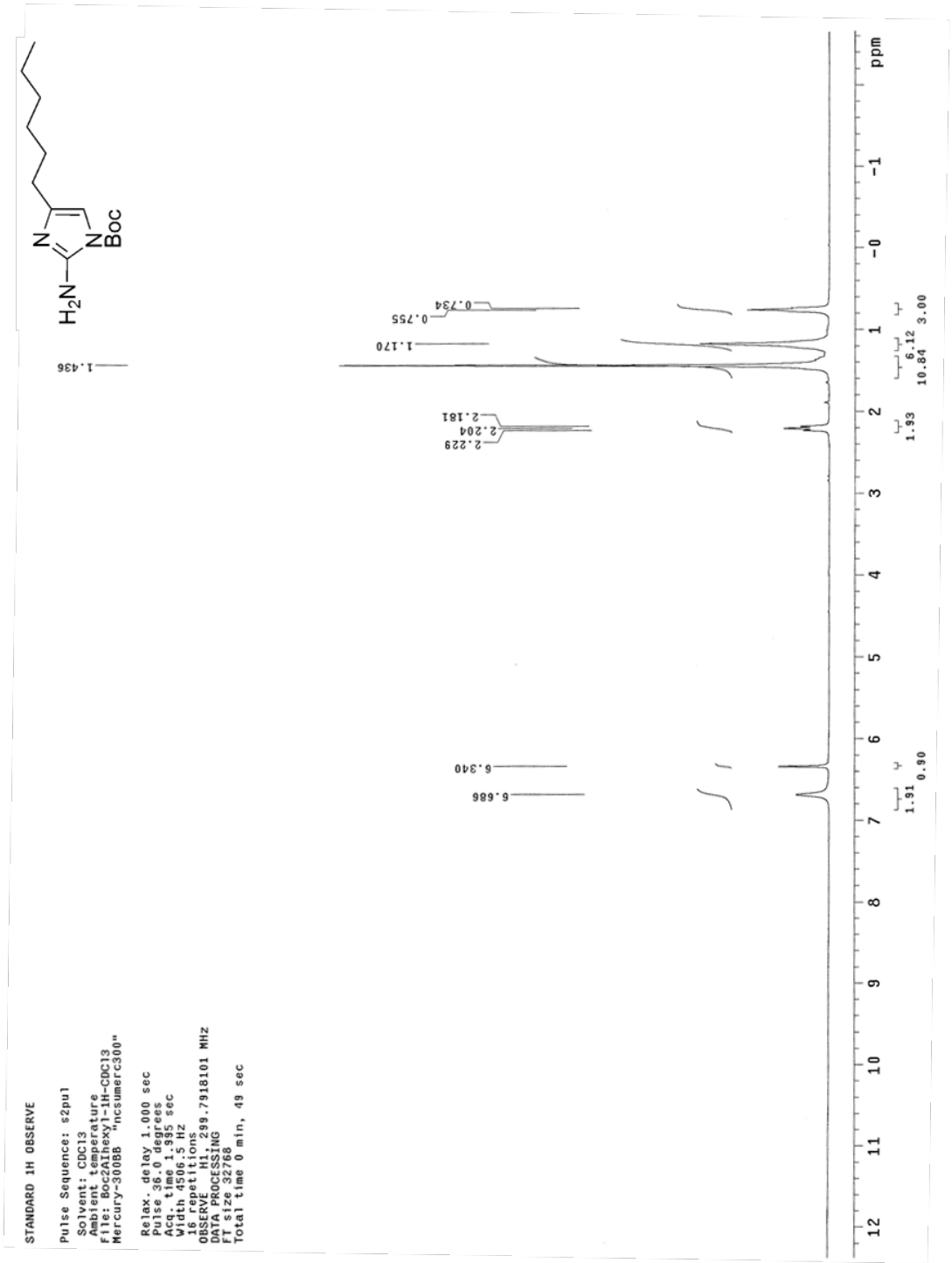


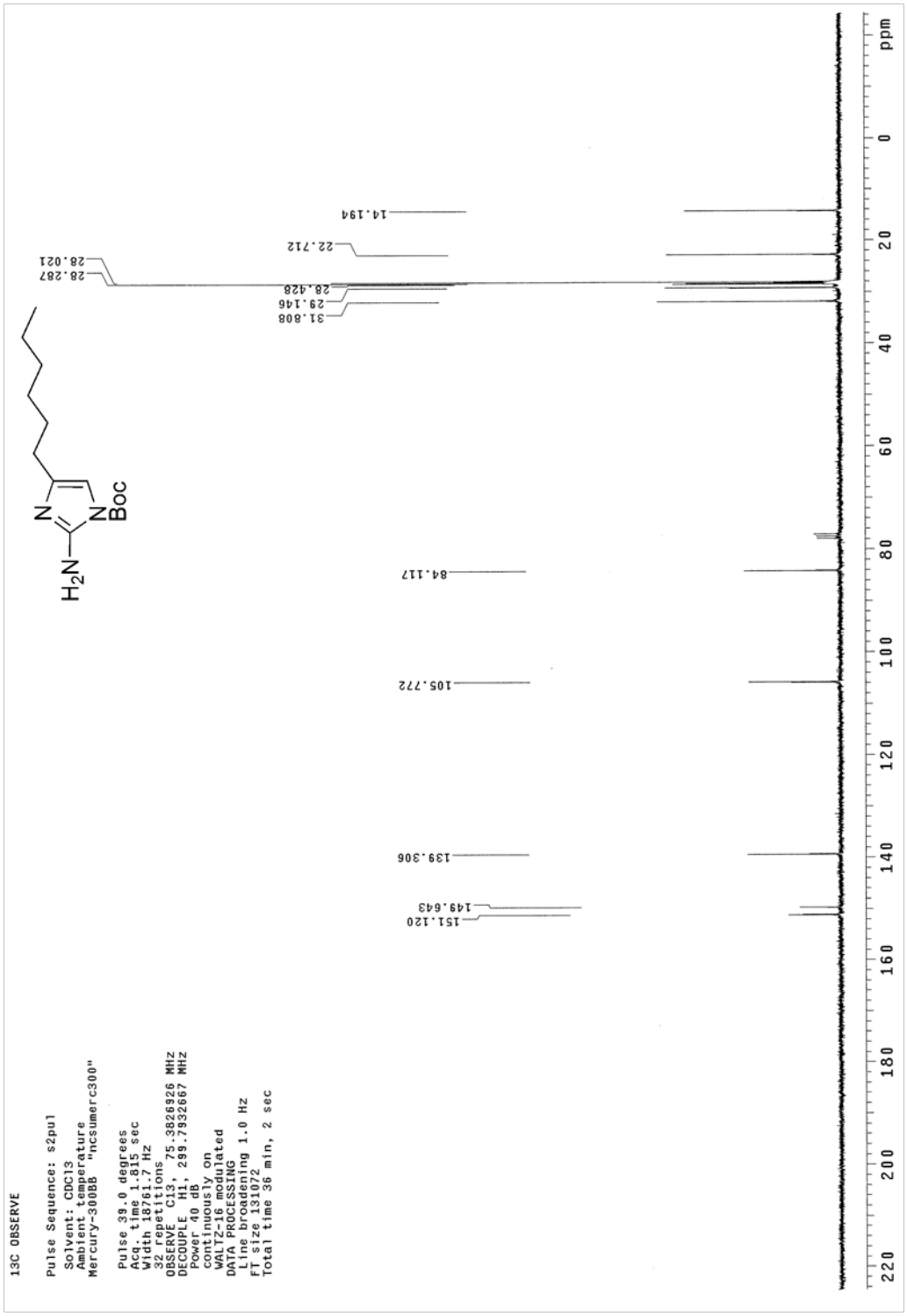

Br
O
14.127
22.591
23.900
28.601
31.635
34.883
39.887
77.131
77.556
77.977
202.150
ppm
0
20
40
60
80
100
120
140
160
180
200
220
13C OBSERVE
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
Mercury-300BB "ncsumerc638"
Pulse 23.3 degrees
Acq. time 1.815 sec
Width 18761.7 Hz
32 repetitions
OBSERVE C13, 75.4590250 MHz
DECOUPLE H1, 300.0969387 MHz
Power 30 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 131072
Total time 36 min, 2 sec

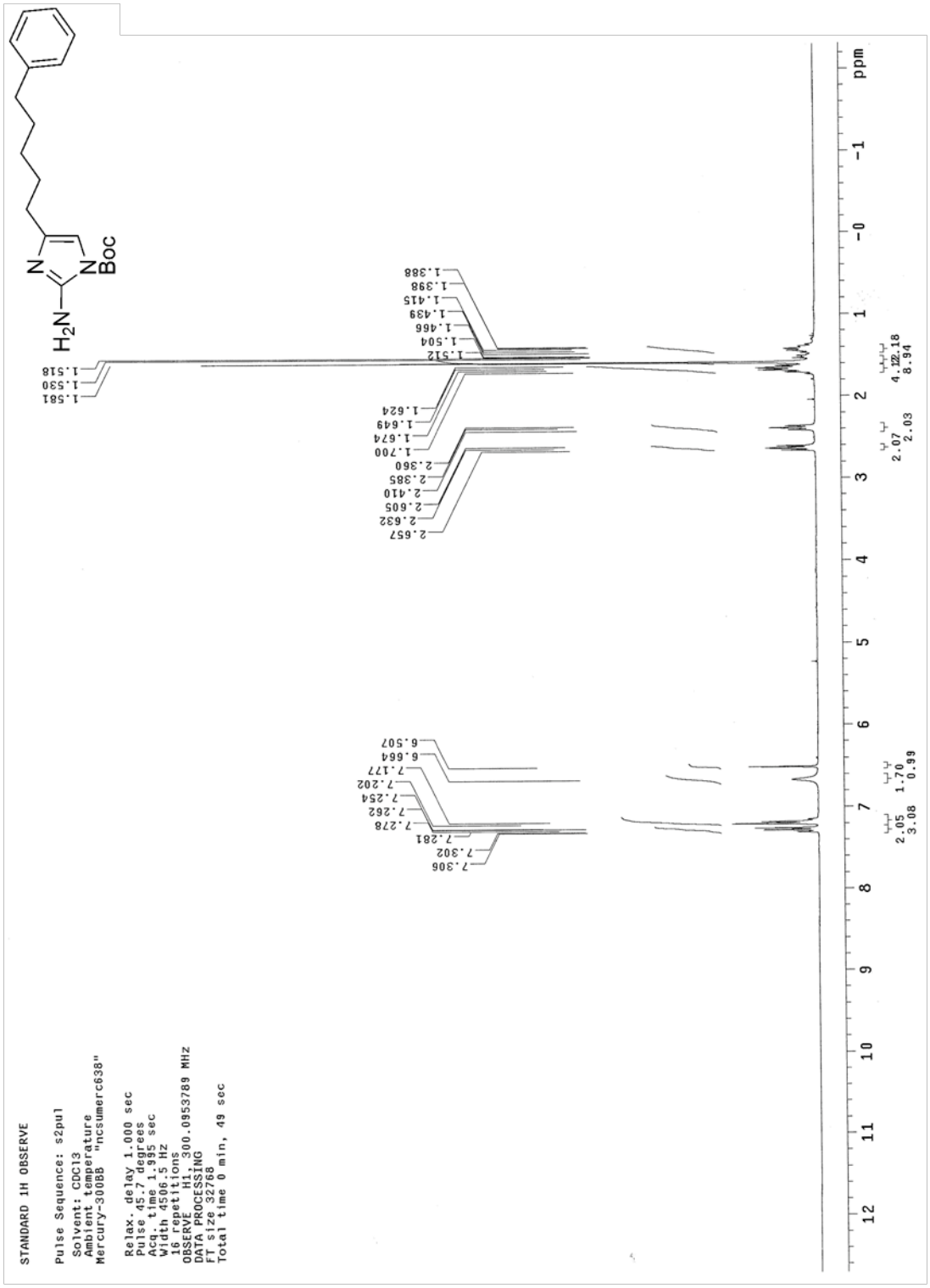

Br
O
STANDARD 1H OBSERVE
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
File: Phenhexylalphabromo-1H-CDCl3
Mercury-300BB "ncsumerc638"
Relax. delay 1.000 sec
Pulse 45.7 degrees
Acq. time 1.995 sec
Width 4506.5 Hz
16 repetitions
OBSERVE H1, 300.0953789 MHz
DATA PROCESSING
FT size 32768
Total time 0 min, 49 sec
1.331
1.337
1.356
1.380
1.600
1.626
1.651
1.675
1.701
2.045
2.601
2.627
2.651
3.862
7.175
7.200
7.268
7.292
7.317
ppm
12
11
10
9
8
7
6
5
4
3
2
1
-0
-1
2.10
3.00
1.99
4.18
4.07
2.32

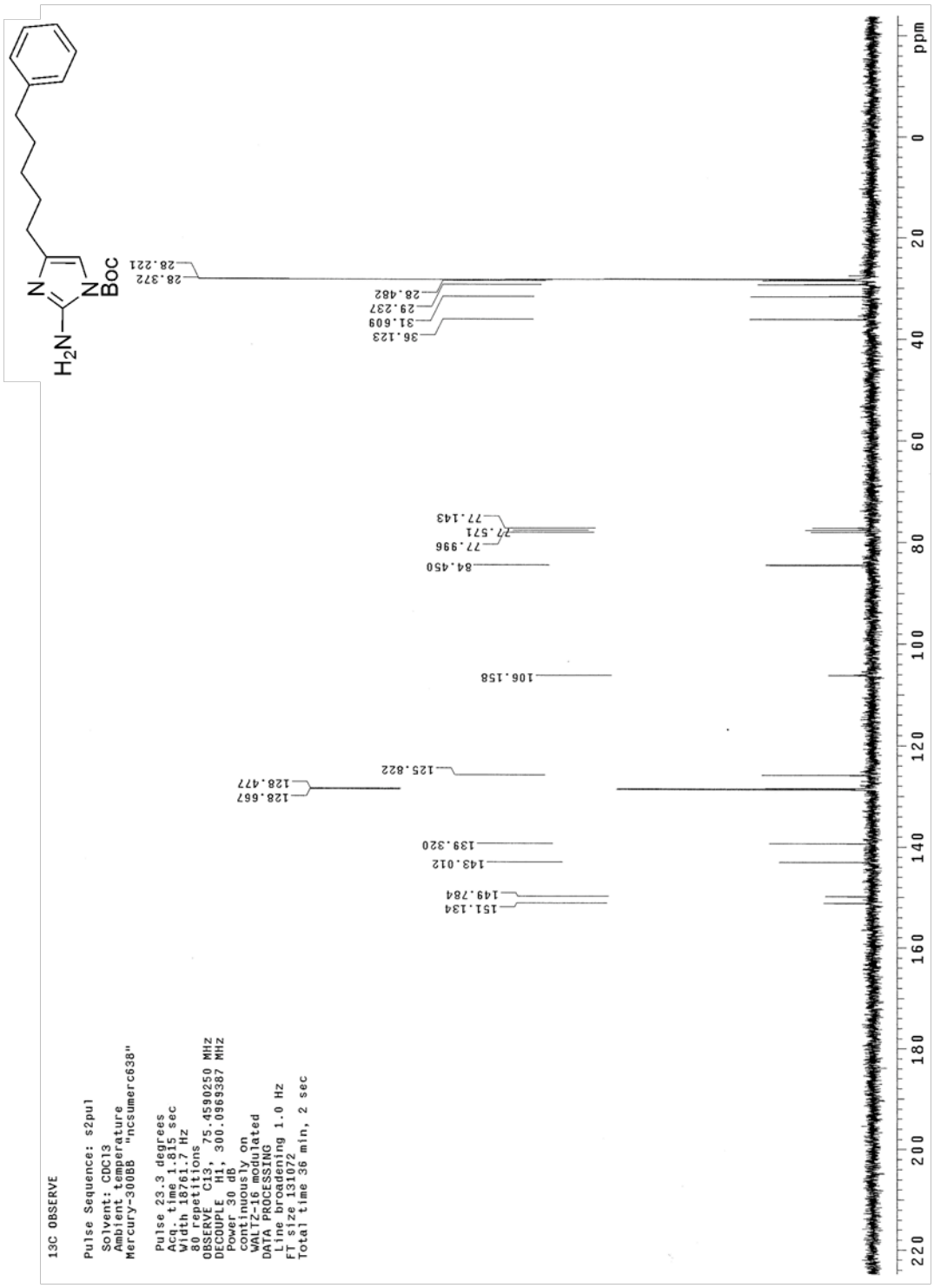

Br
O
23.930
28.873
31.457
34.883
35.979
39.940
77.598
77.992
126.004
128.591
128.682
142.693
202.302
ppm
0
20
40
60
80
100
120
140
160
180
200
220
13C OBSERVE
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
Mercury-300BB "ncsumerc638"
Pulse 23.3 degrees
Acq. time 1.815 sec
Width 18761.7 Hz
80 repetitions
OBSERVE C13, 75.4590250 MHz
DECOUPLE H1, 300.0969387 MHz
Power 30 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 131072
Total time 36 min, 2 sec

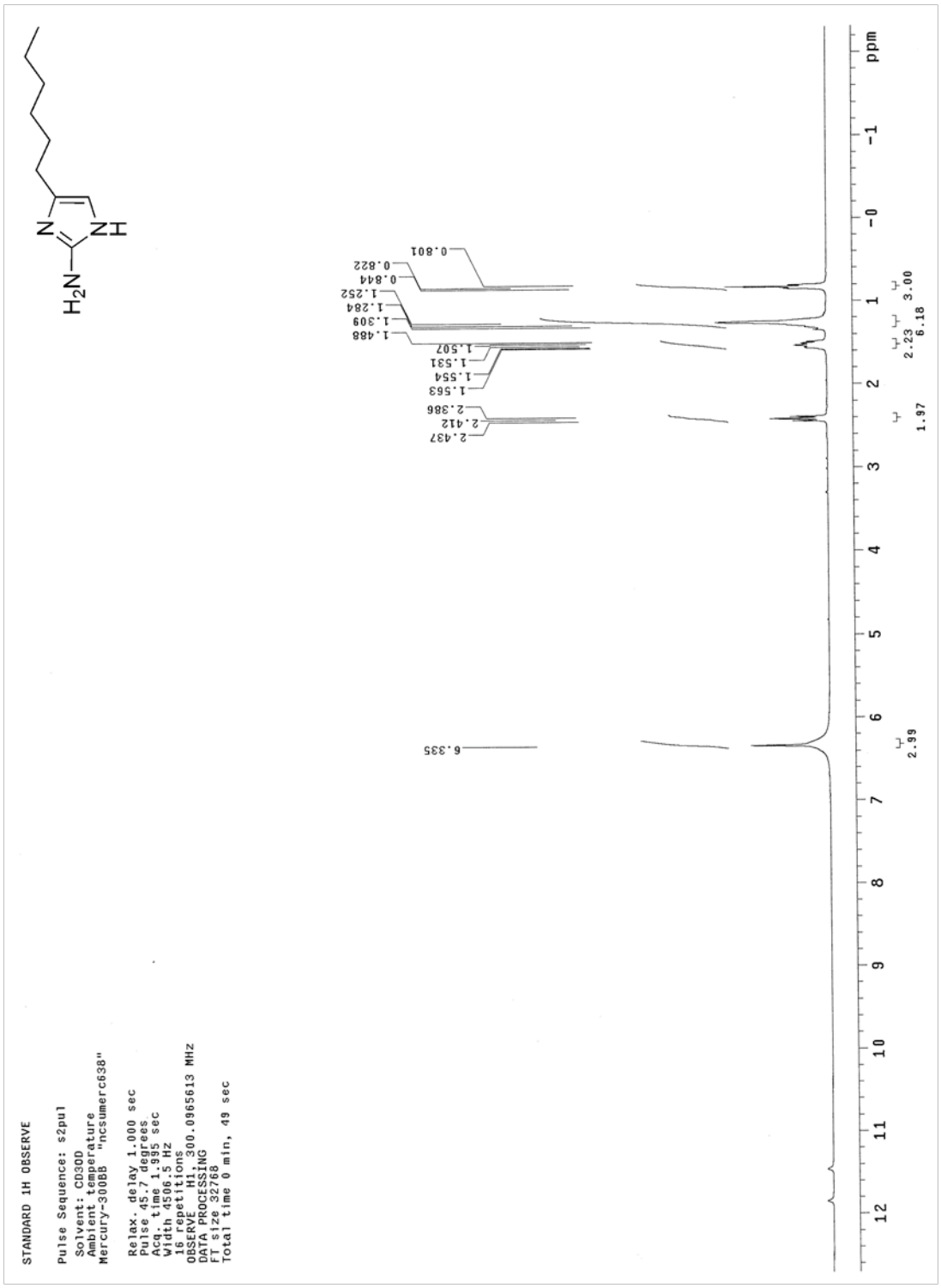
NMR data for monosubstituted-2-aminoimidazole

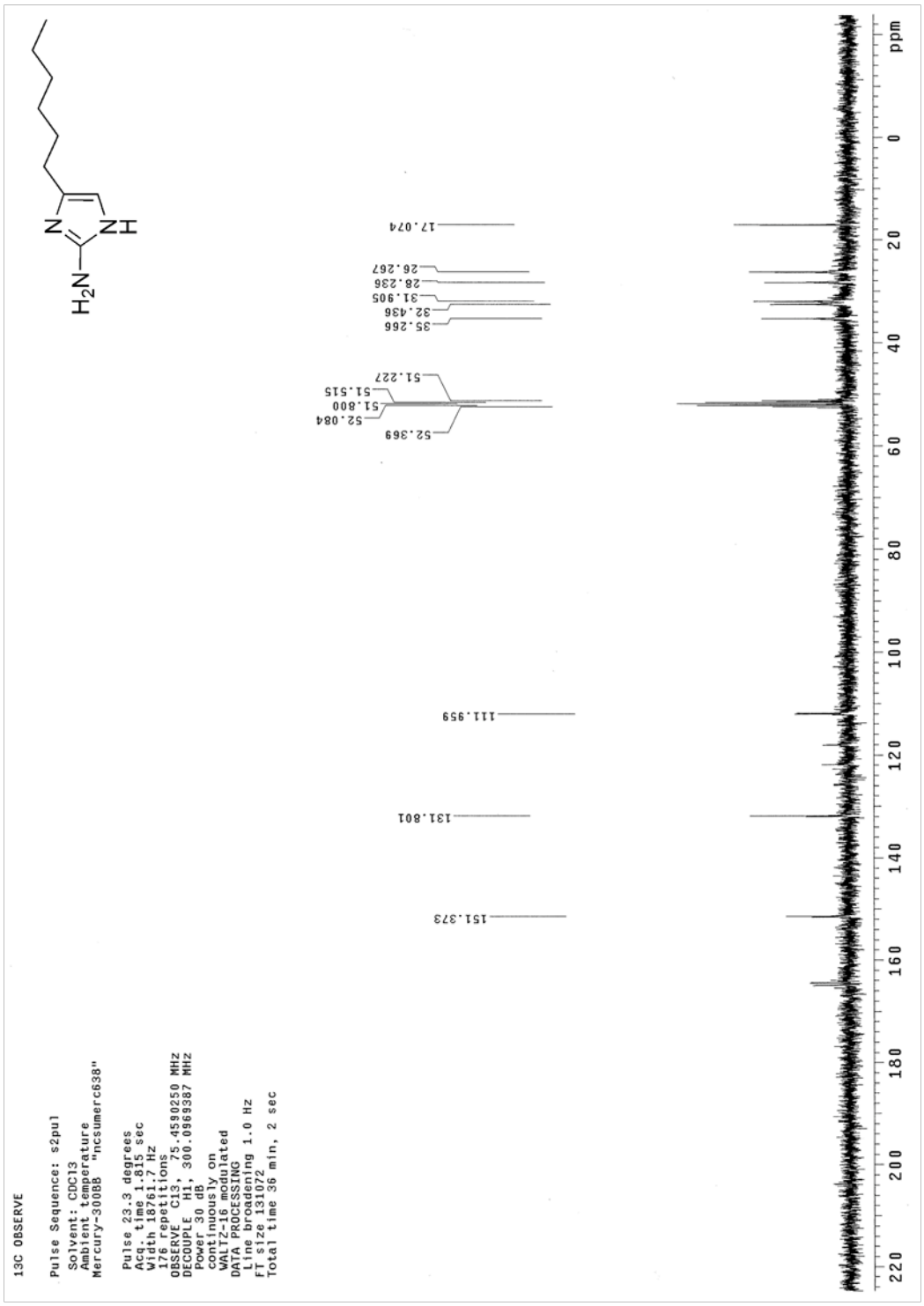


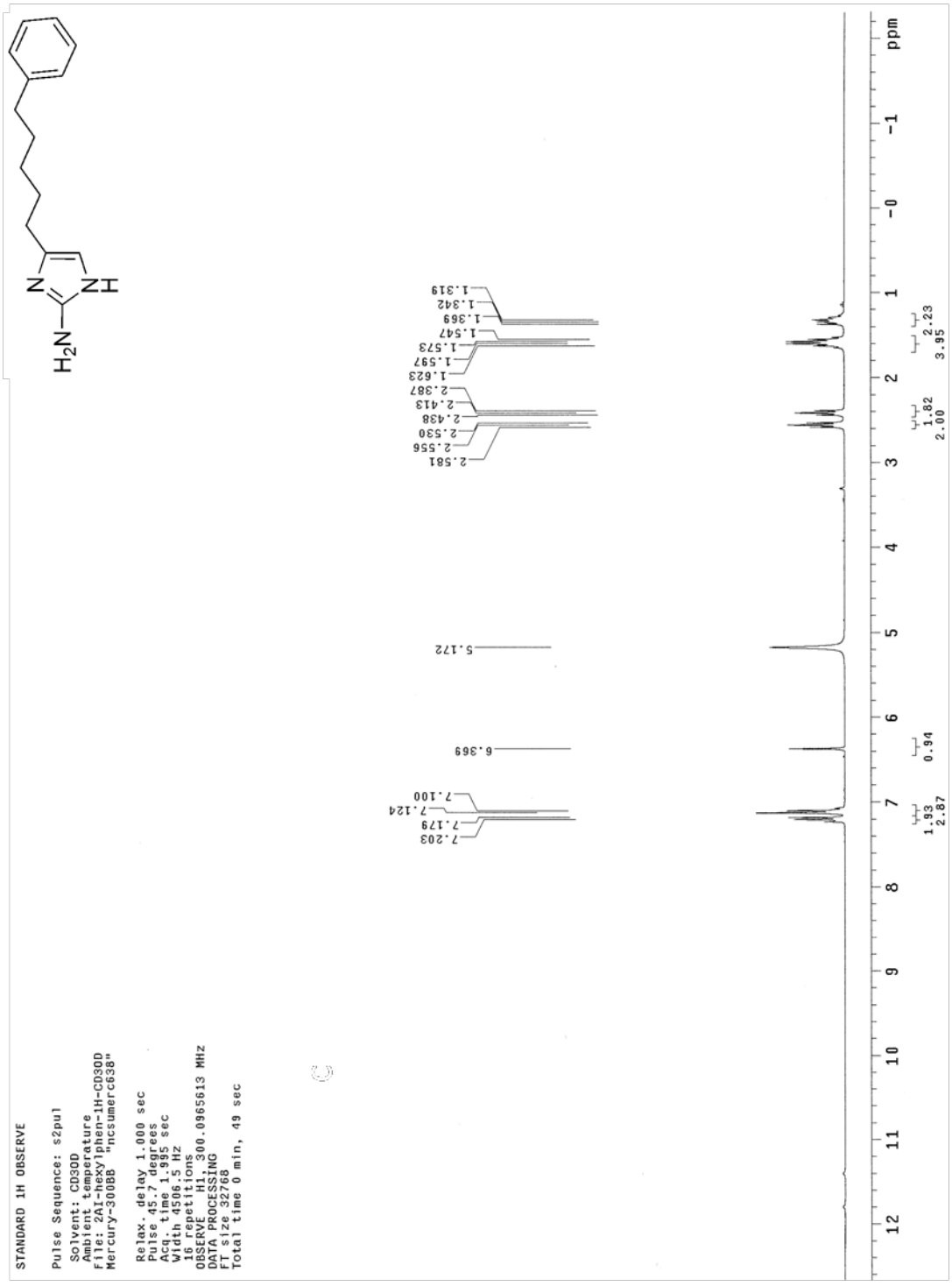

13C OBSERVE
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
Mercury-300BB "ncsumerc300"
Pulse 39.0 degrees
Acq. time 1.815 sec
Width 18761.7 Hz
32 repetitions
OBSERVE C13, 75.3826926 MHz
DECOUPLE H1, 299.7932667 MHz
Power 40 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 131072
Total time 36 min, 2 sec
14.194
22.712
28.021
28.287
28.428
29.146
31.808
84.117
105.772
139.306
149.643
151.120
ppm
220
200
180
160
140
120
100
80
60
40
20
0
N
N
Boc
H2N

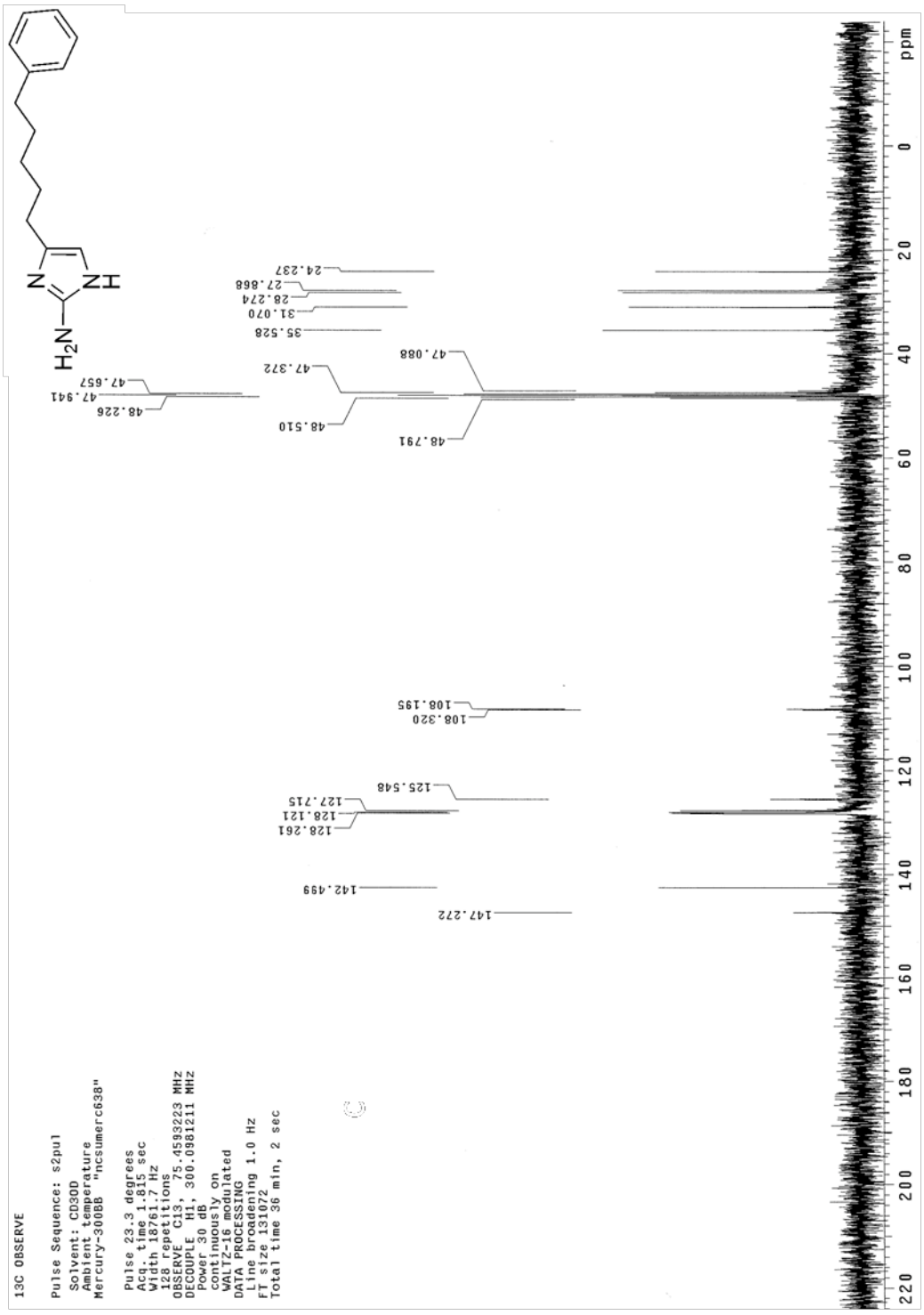

STANDARD 1H OBSERVE
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
Mercury-300BB "ncsumerc638"
Relax. delay 1.000 sec
Pulse 45.7 degrees
Acq. time 1.995 sec
Width 4506.5 Hz
16 repetitions
OBSERVE H1, 300.0953789 MHz
DATA PROCESSING
FT size 32768
Total time 0 min, 49 sec
Boc
N
N
H2N
ppm


13C OBSERVE
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
Mercury-300BB "ncsumerc638"
Pulse 23.3 degrees
Acq. time 1.815 sec
Width 18761.7 Hz
80 repetitions
OBSERVE C13, 75.4590250 MHz
DECOUPLE H1, 300.0969387 MHz
Power 30 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 131072
Total time 36 min, 2 sec
28.221
28.372
28.482
29.237
31.609
36.123
77.143
77.571
77.996
84.450
106.158
125.822
128.477
128.667
139.320
143.012
149.784
151.134
ppm
0
20
40
60
80
100
120
140
160
180
200
220
N
N
Boc
H2N


STANDARD 1H OBSERVE
Pulse Sequence: s2pul
Solvent: CD3OD
Ambient temperature
Mercury-300BB "ncsumerc638"
Relax. delay 1.000 sec
Pulse 45.7 degrees
Acq. time 1.995 sec
Width 4506.5 Hz
16 repetitions
OBSERVE H1, 300.0965613 MHz
DATA PROCESSING
FT size 32768
Total time 0 min, 49 sec
0.801
0.822
0.844
1.252
1.284
1.309
1.488
1.507
1.531
1.554
1.583
2.386
2.412
2.437
6.335
2.99
1.97
2.23
6.18
3.00
ppm


13C OBSERVE
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
Mercury-300BB "ncsumerc638"
Pulse 23.3 degrees
Acq. time 1.815 sec
Width 18761.7 Hz
176 repetitions
OBSERVE C13, 75.4590250 MHz
DECOUPLE H1, 300.0969387 MHz
Power 30 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 131072
Total time 36 min, 2 sec
17.074
26.267
28.236
31.905
32.436
35.266
51.227
51.515
51.800
52.084
52.369
111.959
131.801
151.373
ppm


STANDARD 1H OBSERVE
Pulse Sequence: s2pul
Solvent: CD3OD
Ambient temperature
File: 2AI-hexylphen-1H-CD3OD
Mercury-300BB "ncsumerc638"
Relax. delay 1.000 sec
Pulse 45.7 degrees
Acq. time 1.995 sec
Width 4506.5 Hz
16 repetitions
OBSERVE H1, 300.0965613 MHz
DATA PROCESSING
FT size 32768
Total time 0 min, 49 sec
H2N
N
NH
1.319
1.342
1.369
1.547
1.573
1.597
1.623
2.387
2.413
2.438
2.530
2.556
2.581
5.172
6.369
7.100
7.124
7.179
7.203
1.93
2.87
0.94
1.82
2.00
2.23
3.95
ppm


13C OBSERVE
Pulse Sequence: s2pul
Solvent: CD3OD
Ambient temperature
Mercury-300BB "ncsumerc638"
Pulse 23.3 degrees
Acq. time 1.815 sec
Width 18761.7 Hz
128 repetitions
OBSERVE C13, 75.4593223 MHz
DECOUPLE H1, 300.0981211 MHz
Power 30 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 131072
Total time 36 min, 2 sec
24.237
27.868
28.274
31.070
35.528
47.088
47.372
47.657
47.941
48.226
48.510
48.791
108.195
108.320
125.548
127.715
128.121
128.261
142.499
147.272
ppm
0
20
40
60
80
100
120
140
160
180
200
220