

Supporting Information

A Mild Catalytic Synthesis of 2-Oxazolines via Oxetane Ring-Opening: Rapid Access to A Diverse Family of Natural Products

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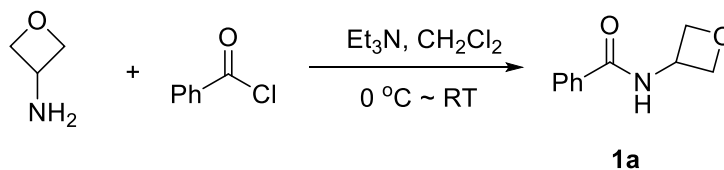
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I. General Information

Flash column chromatography was performed over silica gel (200-300 mesh) purchased from Qindao Puke Co., China. All air or moisture sensitive reactions were conducted in oven-dried glassware under nitrogen atmosphere using anhydrous solvents. Anhydrous toluene, acetonitrile, dichloromethane, chloroform, methanol, and tetrahydrofuran were purified by the Innovative® solvent purification system. ^1H , ^{13}C , and ^{19}F NMR spectra were collected on a Bruker AV 400 MHz NMR spectrometer using residue solvent peaks as an internal standard (^1H NMR: CDCl_3 at 7.26 ppm, $\text{DMSO-}d_6$ at 2.50 ppm, acetone- d_6 at 2.05 ppm; ^{13}C NMR: CDCl_3 at 77.0 ppm, $\text{DMSO-}d_6$ at 39.5 ppm, acetone- d_6 at 29.8 ppm). Mass spectra were collected on an Agilent GC/MS 5975C system, a MALDI Micro MX mass spectrometer, or an API QSTAR XL System. IR spectra were recorded on Bruker TENSOR 27 spectrometer and reported in terms of frequency of absorption (cm^{-1}).

II. Synthesis of the Oxetane Substrates



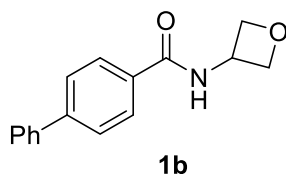
***N*-(Oxetan-3-yl)benzamide (1a).** At 0 °C, to a stirred solution of oxetan-3-amine (731 mg, 10.0 mmol) and trimethylamine (2.8 mL, 20.0 mmol) in anhydrous CH₂Cl₂ (20 mL) was added dropwise a solution of benzoyl chloride (1.69 g, 12.0 mmol) in anhydrous CH₂Cl₂ (10 mL). The mixture was allowed to warm to room temperature spontaneously. After stirring for 6 h, the mixture was quenched with saturated NH₄Cl aqueous solution (20 mL) and diluted with CH₂Cl₂ (60 mL). The organic layer was separated, washed with water (2×20 mL) and brine (20 mL), dried over anhydrous Na₂SO₄, and concentrated under reduced pressure. The residue was purified by simple recrystallization (hexanes and diethyl ether) to afford the pure amide **1a** (95% yield, white solid).

¹H NMR (400 MHz, CDCl₃) δ 7.82–7.77 (m, 2H), 7.53–7.49 (m, 1H), 7.44–7.40 (m, 2H), 6.96 (br s, 1H), 5.25–5.20 (m, 1H), 5.00 (dd, *J*₁ = 6.8 Hz, *J*₂ = 2.8 Hz, 2H), 4.60 (t, *J* = 6.4 Hz, 2H) ppm.

¹³C NMR (100 MHz, CDCl₃) δ 167.1, 133.7, 131.8, 128.6, 127.0, 78.4, 45.3 ppm.

IR (thin film) 3297, 3071, 2961, 2877, 1642, 1547, 1293, 1192, 969, 884, 701 cm⁻¹.

HRMS (CI⁺) Calcd for C₁₀H₁₂NO₂ [M + H]⁺: 178.0868, Found: 178.0875.



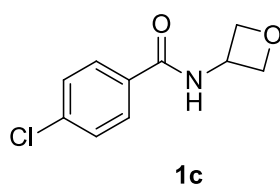
***N*-(oxetan-3-yl)-(1,1'-biphenyl)-4-carboxamide (1b)** was prepared by following the same procedure for the synthesis of **1a** (84% yield, white solid).

$^1\text{H NMR}$ (400 MHz, $\text{DMSO-}d_6$) δ 9.14 (d, $J = 6.4$ Hz, 1H), 7.99 (d, $J = 8.4$ Hz, 2H), 7.79 (d, $J = 8.4$ Hz, 2H), 7.74 (d, $J = 7.2$ Hz, 2H), 7.50 (t, $J = 7.6$ Hz, 2H), 7.43–7.39 (m, 1H), 5.08–5.00 (m, 1H), 4.79 (dd, $J_1 = 7.2$ Hz, $J_2 = 6.4$ Hz, 2H), 4.62 (t, $J = 6.4$ Hz, 2H) ppm.

$^{13}\text{C NMR}$ (100 MHz, $\text{DMSO-}d_6$) δ 165.6, 142.9, 139.1, 132.6, 129.0, 128.1, 128.0, 126.8, 126.5, 76.9, 44.6 ppm.

IR (thin film) 3445, 3277, 2959, 2813, 1632, 1534, 967, 849, 746, 699 cm^{-1} .

HRMS (CI⁺) Calcd for $\text{C}_{16}\text{H}_{16}\text{NO}_2$ [$\text{M} + \text{H}$]⁺: 254.1181, Found: 254.1178.



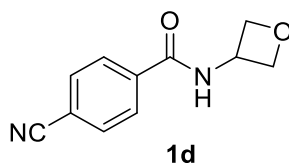
4-Chloro-N-(oxetan-3-yl)benzamide (1c) was prepared by following the same procedure for the synthesis of **1a** (92% yield, white solid).

$^1\text{H NMR}$ (400 MHz, CDCl_3) δ 7.73 (d, $J = 8.0$ Hz, 2H), 7.40 (d, $J = 8.0$ Hz, 2H), 7.01 (br s, 1H), 5.24–5.19 (m, 1H), 5.00 (t, $J = 7.2$ Hz, 2H), 4.60 (t, $J = 6.4$ Hz, 2H) ppm.

$^{13}\text{C NMR}$ (100 MHz, CDCl_3) δ 166.1, 138.2, 132.0, 128.9, 128.4, 78.4, 45.4 ppm.

IR (thin film) 3277, 3075, 2950, 2876, 1637, 1539, 1184, 1084, 967, 715, 674 cm^{-1} .

HRMS (CI⁺) Calcd for $\text{C}_{10}\text{H}_{11}\text{ClNO}_2$ [$\text{M} + \text{H}$]⁺: 212.0478, Found: 212.0470.



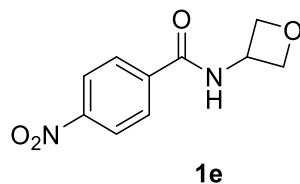
4-Cyano-N-(oxetan-3-yl)benzamide (1d) was prepared by following the same procedure for the synthesis of **1a** (92% yield, white solid).

$^1\text{H NMR}$ (400 MHz, $\text{acetone-}d_6$) δ 8.59 (br s, 1H), 8.10–8.07 (m, 2H), 7.91–7.88 (m, 2H), 5.21–5.12 (m, 1H), 4.85 (t, $J = 7.2$ Hz, 2H), 4.65 (t, $J = 6.4$ Hz, 2H) ppm.

$^{13}\text{C NMR}$ (100 MHz, $\text{acetone-}d_6$) δ 165.7, 139.3, 133.3, 129.1, 118.9, 115.7, 78.2, 46.4, ppm.

IR (thin film) 3440, 2222, 1632, 957, 739, 671 cm^{-1} .

HRMS (CI+) Calcd for $\text{C}_{11}\text{H}_{11}\text{N}_2\text{O}_2$ $[\text{M} + \text{H}]^+$: 203.0821, Found: 203.0818.



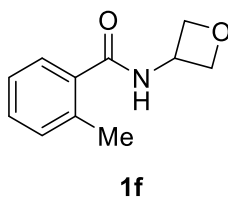
4-Nitro-N-(oxetan-3-yl)benzamide (1e) was prepared by following the same procedure for the synthesis of **1a** (90% yield, pale yellow solid).

^1H NMR (400 MHz, acetone- d_6) δ 8.69 (br s, 1H), 8.31 (dd, $J_1 = 7.2$ Hz, $J_2 = 2.0$ Hz, 2H), 8.15 (dd, $J_1 = 7.2$ Hz, $J_2 = 2.0$ Hz, 2H), 5.22–5.13 (m, 1H), 4.86 (t, $J = 7.2$ Hz, 2H), 4.66 (t, $J = 6.4$ Hz, 2H) ppm.

^{13}C NMR (100 MHz, acetone- d_6) δ 165.5, 150.6, 140.9, 129.7, 124.4, 78.2, 46.4 ppm.

IR (thin film) 3446, 1637, 1515, 1341, 1279, 963, 756, 705 cm^{-1} .

HRMS (CI+) Calcd for $\text{C}_{10}\text{H}_{11}\text{N}_2\text{O}_4$ $[\text{M} + \text{H}]^+$: 223.0719, Found: 223.0716.



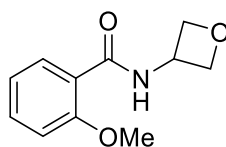
2-Methyl-N-(oxetan-3-yl)benzamide (1f) was prepared by following the same procedure for the synthesis of **1a** (87% yield, white solid).

^1H NMR (400 MHz, CDCl_3) δ 7.36–7.31 (m, 2H), 7.23–7.18 (m, 2H), 6.46 (br s, 1H), 5.24–5.15 (m, 1H), 4.99 (t, $J = 7.2$ Hz, 2H), 4.55 (t, $J = 6.4$ Hz, 2H), 2.42 (s, 3H) ppm.

^{13}C NMR (100 MHz, CDCl_3) δ 169.5, 136.3, 135.4, 131.2, 130.3, 126.6, 125.8, 78.5, 45.0, 19.8 ppm.

IR (thin film) 3453, 3279, 2951, 2879, 1642, 1539, 1290, 1188, 977, 889, 733 cm^{-1} .

HRMS (CI+) Calcd for $\text{C}_{11}\text{H}_{14}\text{NO}_2$ $[\text{M} + \text{H}]^+$: 192.1025, Found: 192.1034.



1g

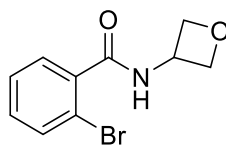
2-Methoxy-N-(oxetan-3-yl)benzamide (1g) was prepared by following the same procedure for the synthesis of **1a** (95% yield, white solid).

¹H NMR (400 MHz, CDCl₃) δ 8.39 (br s, 1H), 8.16 (dd, *J*₁ = 8.0 Hz, *J*₂ = 2.0 Hz, 1H), 7.46 (td, *J*₁ = 4.4 Hz, *J*₂ = 2.0 Hz, 1H), 7.08 (t, *J* = 7.6 Hz, 1H), 6.99 (d, *J* = 8.4 Hz, 1H), 5.28–5.20 (m, 1H), 5.01 (t, *J* = 7.2 Hz, 2H), 4.61 (t, *J* = 6.8 Hz, 2H), 4.00 (s, 3H) ppm.

¹³C NMR (100 MHz, CDCl₃) δ 164.8, 157.5, 133.2, 132.3, 121.4, 120.6, 111.3, 78.8, 56.0, 44.9 ppm.

IR (thin film) 3379, 2963, 2884, 1638, 1537, 1480, 1300, 1246, 1019, 965, 759 cm⁻¹.

HRMS (CI⁺) Calcd for C₁₁H₁₄NO₃ [M + H]⁺: 208.0974, Found: 208.0973.



1h

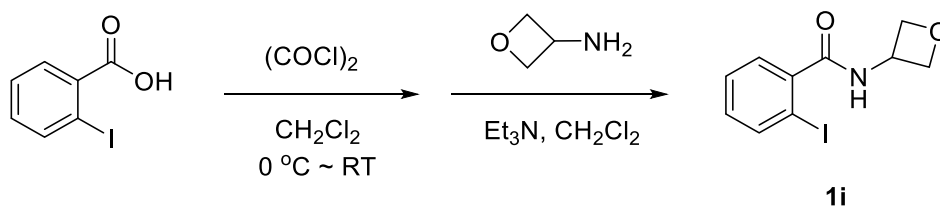
2-Bromo-N-(oxetan-3-yl)benzamide (1h) was prepared by following the same procedure for the synthesis of **1a** (93% yield, white solid).

¹H NMR (400 MHz, CDCl₃) δ 7.58 (dd, *J*₁ = 8.0 Hz, *J*₂ = 1.2 Hz, 1H), 7.49 (dd, *J*₁ = 7.6 Hz, *J*₂ = 2.0 Hz, 1H), 7.35 (td, *J*₁ = 7.6 Hz, *J*₂ = 1.2 Hz, 1H), 7.29 (td, *J*₁ = 7.6 Hz, *J*₂ = 2.0 Hz, 1H), 6.81 (br s, 1H), 5.22–5.15 (m, 1H), 4.97 (t, *J* = 7.2 Hz, 2H), 4.59 (t, *J* = 6.8 Hz, 2H) ppm.

¹³C NMR (100 MHz, CDCl₃) δ 167.0, 136.9, 133.4, 131.6, 129.6, 127.6, 119.2, 78.1, 45.2 ppm.

IR (thin film) 3269, 3068, 2947, 2875, 1648, 1540, 1364, 1540, 1364, 1313, 1023, 979, 891, 735, 685 cm⁻¹.

HRMS (CI⁺) Calcd for C₁₀H₁₁BrNO₂ [M + H]⁺: 255.9973, Found: 255.9970.



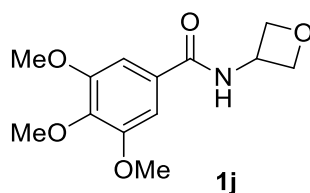
2-Iodo-N-(oxetan-3-yl)benzamide (1i). At 0 °C, to a stirred solution of 2-iodobenzoic acid (1.49 g, 6.0 mmol) and DMF (10 μ L) in anhydrous CH₂Cl₂ (20 mL) was added dropwise oxalyl chloride (767 μ L, 9.0 mmol). After stirring at room temperature overnight, the mixture was concentrated to give the desired crude acyl chloride. Next, at 0 °C, to a stirred solution of oxetan-3-amine (439 mg, 6.0 mmol) and trimethylamine (1.3 mL, 9.0 mmol) in anhydrous CH₂Cl₂ (20 mL) was added dropwise a solution of the crude acyl chloride in anhydrous CH₂Cl₂ (10 mL). The mixture was then allowed to warm to room temperature spontaneously. After stirring for 6 h, the mixture was quenched with saturated NH₄Cl aqueous solution (15 mL) and diluted with CH₂Cl₂ (40 mL). The organic layer was separated, washed with water (2 \times 20 mL) and brine (20 mL), dried over anhydrous Na₂SO₄, and concentrated under reduced pressure. The residue was purified by simple recrystallization (hexanes and diethyl ether) to afford the pure amide **1i** (88% yield, white solid).

¹H NMR (400 MHz, CDCl₃) δ 7.84 (d, J = 8.0 Hz, 1H), 7.38–7.34 (m, 2H), 7.12–7.08 (m, 1H), 6.69 (br s, 1H), 5.21–5.12 (m, 1H), 4.95 (t, J = 7.2 Hz, 2H), 4.61 (t, J = 6.4 Hz, 2H) ppm.

¹³C NMR (100 MHz, CDCl₃) δ 168.8, 141.3, 139.8, 131.4, 128.2, 128.2, 92.3, 78.0, 45.2 ppm.

IR (thin film) 3285, 3063, 2960, 2880, 1642, 1536, 1298, 1016, 967, 885, 747 cm⁻¹.

HRMS (CI⁺) Calcd for C₁₀H₁₁INO₂ [M + H]⁺: 303.9834, Found: 303.9841.



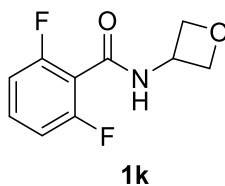
3,4,5-Trimethoxy-N-(oxetan-3-yl)benzamide (1j) was prepared by following the same procedure for the synthesis of **1a** (72% yield, white solid).

$^1\text{H NMR}$ (400 MHz, CDCl_3) δ 7.00 (s, 2H), 6.97 (br s, 1H), 5.22–5.17 (m, 1H), 4.99 (t, $J = 7.2$ Hz, 2H), 4.60 (t, $J = 6.4$ Hz, 2H), 3.86 (s, 9H) ppm.

$^{13}\text{C NMR}$ (100 MHz, CDCl_3) δ 166.8, 153.2, 141.1, 129.0, 104.4, 78.4, 60.9, 56.2, 45.4 ppm.

IR (thin film) 3445, 2954, 2885, 2839, 1638, 1586, 1499, 1339, 1237, 1126, 968, 872 cm^{-1} .

HRMS (CI⁺) Calcd for $\text{C}_{13}\text{H}_{18}\text{NO}_5$ $[\text{M} + \text{H}]^+$: 268.1185, Found: 268.1190.



2,6-Difluoro-N-(oxetan-3-yl)benzamide (1k) was prepared by following the same procedure for the synthesis of **1a** (75% yield, white solid).

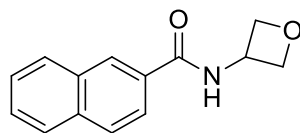
$^1\text{H NMR}$ (400 MHz, CDCl_3) δ 7.41–7.34 (m, 1H), 6.97–6.92 (m, 2H), 6.80 (br s, 1H), 5.26–5.17 (m, 1H), 4.97 (t, $J = 7.2$ Hz, 2H), 4.57 (t, $J = 6.4$ Hz, 2H) ppm.

$^{13}\text{C NMR}$ (100 MHz, CDCl_3) δ 160.0 (dd, $J_1 = 251.0$ Hz, $J_2 = 6.6$ Hz), 159.9, 132.0 (t like, $J = 10.2$ Hz), 113.5 (t like, $J = 19.3$ Hz), 111.9 (dt, $J_1 = 20.1$ Hz, $J_2 = 2.7$ Hz), 78.2, 45.2 ppm.

$^{19}\text{F NMR}$ (376.5 MHz, CDCl_3) δ -112.1 ppm.

IR (thin film) 3260, 3074, 2965, 2875, 1632, 1560, 1470, 1238, 1009, 973, 885, 794 cm^{-1} .

HRMS (CI⁺) Calcd for $\text{C}_{10}\text{H}_{10}\text{F}_2\text{NO}_2$ $[\text{M} + \text{H}]^+$: 214.0680, Found: 214.0686.



1l

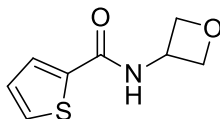
N-(Oxetan-3-yl)-2-naphthamide (1l) was prepared by following the same procedure for the synthesis of **1a** (97% yield, white solid).

¹H NMR (400 MHz, CDCl₃) δ 8.31 (s, 1H), 7.90–7.82 (m, 4H), 7.59–7.52 (m, 2H), 7.06 (br s, 1H), 5.34–5.26 (m, 1H), 5.04 (t, *J* = 7.2 Hz, 2H), 4.67 (t, *J* = 6.8 Hz, 2H) ppm.

¹³C NMR (100 MHz, CDCl₃) δ 167.2, 134.9, 132.5, 130.9, 128.9, 128.6, 127.9, 127.8, 127.6, 126.9, 123.4, 78.6, 45.4 ppm.

IR (thin film) 3446, 3248, 3060, 2965, 2881, 1621, 1545, 1301, 1033, 823, 772, 728 cm⁻¹.

HRMS (CI⁺) Calcd for C₁₄H₁₄NO₂ [M + H]⁺: 228.1025, Found: 228.1026.



1m

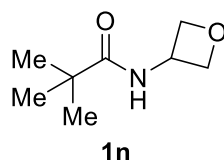
N-(Oxetan-3-yl)thiophene-2-carboxamide (1m) was prepared by following the same procedure for the synthesis of **1a** (90% yield, white solid).

¹H NMR (400 MHz, CDCl₃) δ 7.59 (dd, *J*₁ = 3.6 Hz, *J*₂ = 0.8 Hz, 1H), 7.49 (dd, *J*₁ = 4.8 Hz, *J*₂ = 0.8 Hz, 1H), 7.07 (dd, *J*₁ = 4.8 Hz, *J*₂ = 3.6 Hz, 1H), 7.05 (br s, 1H), 5.24–5.17 (m, 1H), 4.97 (t, *J* = 7.2 Hz, 2H), 4.62 (t, *J* = 6.4 Hz, 2H) ppm.

¹³C NMR (100 MHz, CDCl₃) δ 161.5, 138.1, 130.6, 128.6, 127.7, 78.3, 45.2 ppm.

IR (thin film) 3286, 3083, 2959, 2870, 1626, 1555, 1316, 1184, 958, 868, 723, 673 cm⁻¹.

HRMS (CI⁺) Calcd for C₈H₁₀NO₂S [M + H]⁺: 184.0432, Found: 184.0440.



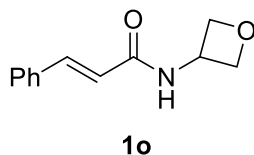
N-(Oxetan-3-yl)pivalamide (1n) was prepared by following the same procedure for the synthesis of **1a** (76% yield, white solid).

¹H NMR (400 MHz, CDCl₃) δ 6.24 (br s, 1H), 5.01–4.89 (m, 3H), 4.45 (t, *J* = 6.4 Hz, 2H), 1.19 (s, 9H) ppm.

¹³C NMR (100 MHz, CDCl₃) δ 178.2, 78.5, 44.9, 38.5, 27.4 ppm.

IR (thin film) 3305, 3051, 2969, 2876, 1633, 1529, 1220, 970, 735, 642 cm⁻¹.

HRMS (CI⁺) Calcd for C₈H₁₆NO₂ [M + H]⁺: 158.1181, Found: 158.1180.



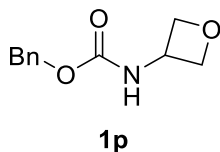
N-(Oxetan-3-yl)cinnamamide (1o) was prepared by following the same procedure for the synthesis of **1a** (89% yield, white solid).

¹H NMR (400 MHz, CDCl₃) δ 7.65 (d, *J* = 14.6 Hz, 1H), 7.50–7.45 (m, 2H), 7.36–7.34 (m, 3H), 6.61 (br s, 1H), 6.45 (d, *J* = 14.6 Hz, 1H), 5.23–5.16 (m, 1H), 4.98 (t, *J* = 7.2 Hz, 2H), 4.58 (t, *J* = 6.8 Hz, 2H) ppm.

¹³C NMR (100 MHz, CDCl₃) δ 165.5, 142.0, 134.5, 129.9, 128.8, 127.8, 119.7, 78.5, 44.9 ppm.

IR (thin film) 3445, 3274, 2954, 2875, 1624, 1561, 1355, 1232, 978, 860, 728, 675 cm⁻¹.

HRMS (CI⁺) Calcd for C₁₂H₁₄NO₂ [M + H]⁺: 204.1025, Found: 204.1024.



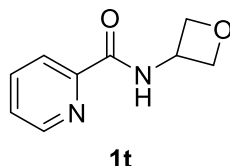
Benzyl oxetan-3-ylcarbamate (1p) was prepared by following the same procedure for the synthesis of **1a** (75% yield, white solid).

$^1\text{H NMR}$ (400 MHz, CDCl_3) δ 7.37–7.31 (m, 5H), 5.58 (br s, 1H), 5.10 (s, 2H), 4.87 (br s, 3H), 4.49 (br s, 2H) ppm.

$^{13}\text{C NMR}$ (100 MHz, CDCl_3) δ 155.3, 136.1, 128.5, 128.2, 128.1, 78.6, 66.9, 46.1 ppm.

IR (thin film) 3516, 3310, 3067, 2960, 2881, 1704, 1541, 1262, 1045, 971, 743, 699 cm^{-1} .

HRMS (CI+) Calcd for $\text{C}_{11}\text{H}_{14}\text{NO}_3$ $[\text{M} + \text{H}]^+$: 208.0974, Found: 208.0976.



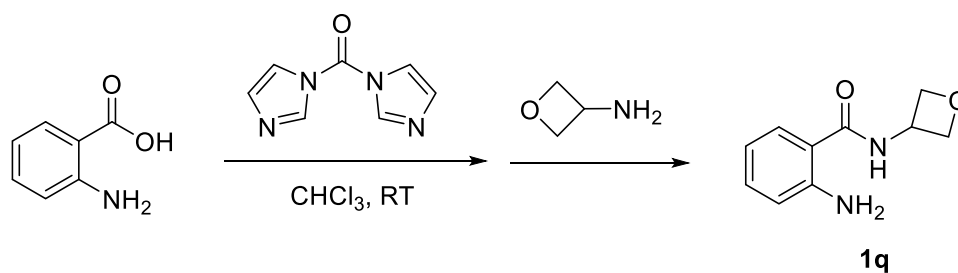
N-(Oxetan-3-yl)picolinamide (1t) was prepared by following the same procedure for the synthesis of **1i** (64% yield, white solid).

$^1\text{H NMR}$ (400 MHz, CDCl_3) δ 8.57 (d, $J = 4.4$ Hz, 2H), 8.17 (d, $J = 7.6$ Hz, 1H), 7.85 (td, $J_1 = 8.0$ Hz, $J_2 = 1.6$ Hz, 1H), 7.47–7.44 (m, 1H), 5.31–5.24 (m, 1H), 5.00 (t, $J = 7.2$ Hz, 2H), 4.68 (t, $J = 6.8$ Hz, 2H) ppm.

$^{13}\text{C NMR}$ (100 MHz, CDCl_3) δ 163.8, 149.2, 148.1, 137.5, 126.5, 122.3, 78.5, 44.5 ppm.

IR (thin film) 3448, 3333, 3056, 2953, 2885, 1658, 1528, 967, 752, 692 cm^{-1} .

HRMS (CI+) Calcd for $\text{C}_9\text{H}_{11}\text{N}_2\text{O}_2$ $[\text{M} + \text{H}]^+$: 179.0821, Found: 179.0815.



2-Amino-N-(oxetan-3-yl)benzamide (1q). A mixture of 2-aminobenzoic acid (823 mg, 6.0 mmol) and 1,1'-carbonyldiimidazole (973 mg, 6.0 mmol) in chloroform (20 mL) was stirred at room temperature for 1 h. Then, a solution of oxetan-3-amine (439 mg, 6.0 mmol) in chloroform (5 mL) was added dropwise. After stirring overnight, the mixture was diluted with CH_2Cl_2 (40 mL), washed with water (2×20 mL) and brine (20 mL), dried over anhydrous Na_2SO_4 , and concentrated under reduced pressure.

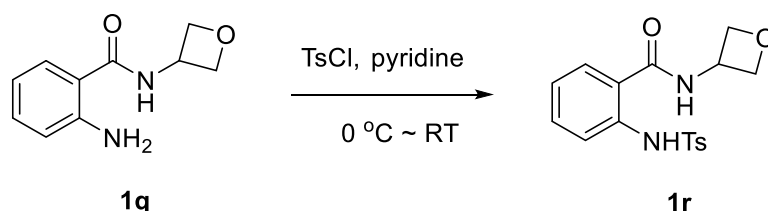
The residue was purified by simple recrystallization (hexanes and diethyl ether) to afford the pure amide **1q** (63% yield, white solid).

¹H NMR (400 MHz, CDCl₃) δ 7.36 (dd, *J*₁ = 7.6 Hz, *J*₂ = 1.2 Hz, 1H), 7.23 (td, *J*₁ = 6.8 Hz, *J*₂ = 1.6 Hz, 1H), 6.69–6.65 (m, 2H), 6.60 (br s, 1H), 5.54 (br s, 2H), 5.22–5.13 (m, 1H), 5.00 (t, *J* = 7.2 Hz, 2H), 4.59 (t, *J* = 6.4 Hz, 2H) ppm.

¹³C NMR (100 MHz, CDCl₃) δ 168.9, 148.9, 132.8, 127.1, 117.5, 116.7, 114.9, 78.6, 45.0 ppm.

IR (thin film) 3453, 3256, 2945, 1625, 1530, 1258, 970, 731, 681 cm⁻¹.

HRMS (CI⁺) Calcd for C₁₀H₁₃N₂O₂ [M + H]⁺: 193.0977, Found: 193.0979.



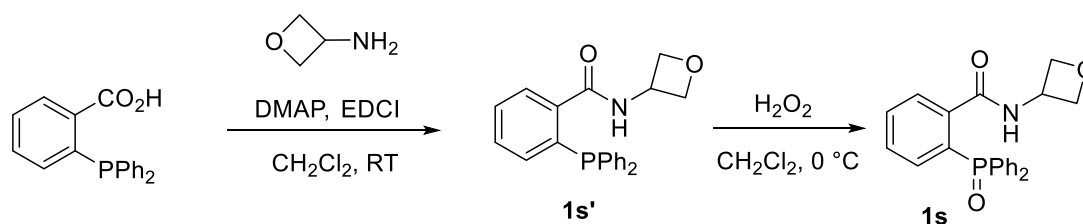
2-(4-Methylphenylsulfonamido)-N-(oxetan-3-yl)benzamide (1r). At 0 °C, to a stirred solution of **1q** (288 mg, 1.5 mmol) in anhydrous pyridine (5 mL) was added *p*-tosyl chloride (343 mg, 1.8 mmol) in three portions. After stirring at room temperature overnight, the mixture was diluted with ethyl acetate (30 mL), and washed with HCl aqueous solution (2 M, 2×15 mL), water (15 mL), and brine (15 mL). The organic layer was dried over anhydrous Na₂SO₄, and concentrated under reduced pressure. The residue was purified by simple recrystallization (hexanes and diethyl ether) to afford the pure amide **1r** (88% yield, white solid).

¹H NMR (400 MHz, acetone-*d*₆) δ 11.16 (s, 1H), 8.51 (br s, 1H), 7.73 (dd, *J*₁ = 8.0 Hz, *J*₂ = 1.2 Hz, 1H), 7.69–7.62 (m, 3H), 7.48 (td, *J*₁ = 7.6 Hz, *J*₂ = 1.6 Hz, 1H), 7.30 (dd, *J*₁ = 8.8 Hz, *J*₂ = 0.8 Hz, 2H), 7.12 (td, *J*₁ = 7.6 Hz, *J*₂ = 0.8 Hz, 1H), 5.08–5.04 (m, 1H), 4.83 (t, *J* = 7.2 Hz, 2H), 4.58 (t, *J* = 6.8 Hz, 2H), 2.34 (s, 3H) ppm.

¹³C NMR (100 MHz, acetone-*d*₆) δ 169.1, 144.8, 140.2, 137.7, 133.6, 130.6, 128.9, 128.0, 124.5, 122.0, 121.8, 77.9, 46.2, 21.5 ppm.

IR (thin film) 3410, 2964, 2883, 1635, 1537, 1332, 1264, 1158, 934, 760 cm⁻¹.

HRMS (CI+) Calcd for C₁₇H₁₉N₂O₄S [M + H]⁺: 347.1066, Found: 347.1042.



2-(Diphenylphosphino)-N-(oxetan-3-yl)benzamide (1s'). To a stirred solution of 2-(diphenylphosphino)benzoic acid (306 mg, 1.0 mmol), EDCI (230 mg, 1.2 mmol), and DMAP (6.1 mg, 5 mol%) in anhydrous CH₂Cl₂ (10 mL) was added a solution of oxetan-3-amine (81 mg, 1.1 mmol) in anhydrous CH₂Cl₂ (2 mL). After stirring at room temperature overnight, the mixture was quenched with saturated NH₄Cl aqueous solution (5 mL) and diluted with CH₂Cl₂ (10 mL). The organic layer was separated, washed with water (2×10 mL) and brine (10 mL), dried over anhydrous Na₂SO₄, and concentrated under reduced pressure. The residue was purified by simple recrystallization (hexanes and diethyl ether) to afford the pure amide **1s'** (78% yield, white solid).

¹H NMR (400 MHz, CDCl₃) δ 7.63–7.60 (m, 1H), 7.39–7.27 (m, 12H), 6.96–6.93 (m, 1H), 6.67 (br s, 1H), 5.06–4.97 (m, 1H), 4.79 (t, *J* = 7.2 Hz, 2H), 4.29 (t, *J* = 6.4 Hz, 2H) ppm.

¹³C NMR (100 MHz, CDCl₃) δ 168.4, 140.3 (d, *J* = 24.3 Hz), 136.4 (d, *J* = 9.9 Hz), 135.8 (d, *J* = 20.1 Hz), 133.88 (d, *J* = 20.0 Hz), 133.93, 130.5, 129.1, 128.8, 128.7 (d, *J* = 7.2 Hz), 128.2, 128.1, 78.0, 45.0 ppm.

IR (thin film) 3265, 3058, 2962, 2877, 1642, 1537, 1298, 971, 744, 696 cm⁻¹.

HRMS (CI+) Calcd for C₂₂H₂₁NO₂P [M + H]⁺: 362.1310, Found: 362.1315.

2-(Diphenylphosphoryl)-N-(oxetan-3-yl)benzamide (1s). At 0 °C, to a stirred solution of 2-(diphenylphosphino)-N-(oxetan-3-yl)benzamide **1s'** (222 mg, 0.62 mmol) in CH₂Cl₂ (5 mL) was added 35% H₂O₂ (0.5 mL). After stirring at 0 °C for 1 hour, the mixture was quenched with saturated Na₂S₂O₃ aqueous solution (2 mL) and diluted with CH₂Cl₂ (10 mL). The organic layer was separated, washed with water (2×10 mL)

and brine (10 mL), dried over anhydrous Na_2SO_4 , and concentrated under reduced pressure. The residue was purified by flash column chromatography (DCM/MeOH = 20:1) to afford **1s** (196 mg, 85% yield, white solid).

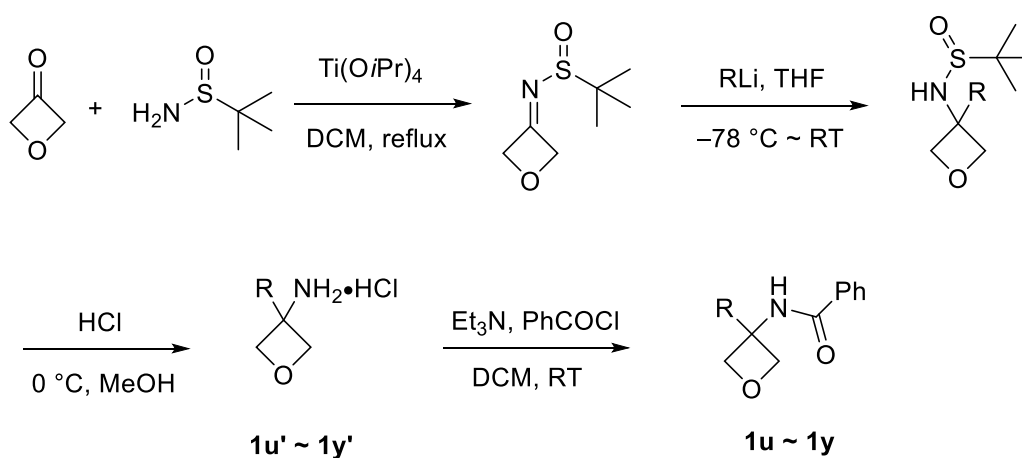
^1H NMR (400 MHz, CDCl_3) δ 9.65 (d, J = 4.8 Hz, 1H), 8.03 (q, J = 4.0 Hz, 1H), 7.69–7.36 (m, 12H), 7.04 (dd, J_1 = 14.4 Hz, J_2 = 7.6 Hz, 1H), 4.69–4.54 (m, 3H), 4.34 (t, J = 6.0 Hz, 2H) ppm.

^{13}C NMR (100 MHz, CDCl_3) δ 166.8 (d, J = 14.8 Hz), 140.2 (d, J = 31.2 Hz), 133.4 (d, J = 47.6 Hz), 132.7 (d, J = 8.4 Hz), 132.6 (d, J = 10.8 Hz), 132.1 (d, J = 37.6 Hz), 131.7 (d, J = 39.2 Hz), 131.4, 130.3 (d, J = 23.2 Hz), 130.1, 129.6, 128.9 (d, J = 49.2 Hz), 128.6, 77.3, 45.3 ppm.

^{31}P NMR (162 MHz, CDCl_3) δ 36.51 ppm.

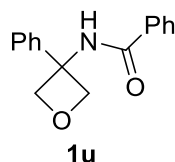
IR (thin film) 3230, 3056, 2960, 2878, 1650, 1543, 1437, 1302, 1118, 722, 693 cm^{-1} .

HRMS (CI+) Calcd for $\text{C}_{22}\text{H}_{21}\text{NO}_3\text{P}$ [$\text{M} + \text{H}$] $^+$: 378.1259, Found: 378.1265.



The precursors **1u'** ~ **1y'** were synthesized according to the reported procedure.^[1] Their spectroscopic data were consistent with those reported in the literature. The starting materials **1u** ~ **1y** were synthesized by following the same procedure for the synthesis of **1i**.

[1] P. J. Hamzik and J. D. Brubaker, *Org. Lett.* **2010**, *12*, 1116–1119.



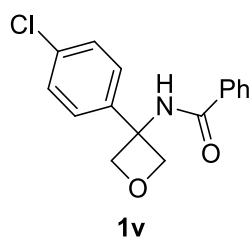
N-(3-Phenyloxetan-3-yl)benzamide (1u) was prepared from **1u'** by following the same procedure for the synthesis of **1a** (65% yield, white solid).

¹H NMR (400 MHz, CDCl₃) δ 7.81 (d, *J* = 7.2 Hz, 2H), 7.57–7.49 (m, 3H), 7.46–7.34 (m, 4H), 7.33–7.24 (m, 1H), 7.17 (s, 1H), 5.10 (d, *J* = 6.8 Hz, 2H), 4.95 (d, *J* = 6.8 Hz, 2H) ppm.

¹³C NMR (100 MHz, CDCl₃) δ 166.6, 141.3, 133.6, 132.0, 128.7 (2C), 127.6, 127.0, 124.8, 83.0, 59.2 ppm.

IR (thin film) 3300, 2960, 1636, 1527, 1489, 1265, 982, 732, 698 cm⁻¹.

HRMS (CI⁺) Calcd for C₁₆H₁₆NO₂ [M + H]⁺: 254.1181, Found: 254.1183.



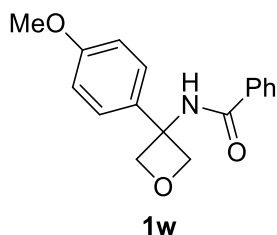
N-(3-(4-Chlorophenyl)oxetan-3-yl)benzamide (1v) was prepared from **1v'** by following the same procedure for the synthesis of **1a** (75% yield, white solid).

¹H NMR (400 MHz, CDCl₃) δ 7.80 (d, *J* = 7.2 Hz, 2H), 7.55 (t, *J* = 7.6 Hz, 1H), 7.50–7.39 (m, 4H), 7.33 (d, *J* = 8.4 Hz, 2H), 7.16 (s, 1H), 5.07 (d, *J* = 6.8 Hz, 2H), 4.90 (d, *J* = 6.8 Hz, 2H) ppm.

¹³C NMR (100 MHz, CDCl₃) δ 166.6, 139.9, 133.5, 133.3, 132.1, 128.8, 128.7, 127.0, 126.3, 82.9, 58.9 ppm

IR (thin film) 3283, 2960, 1633, 1526, 1484, 1310, 1098, 980, 826, 734, 692 cm⁻¹.

HRMS (CI⁺) Calcd for C₁₆H₁₅ClNO₂ [M + H]⁺: 288.0791, Found: 288.0790.



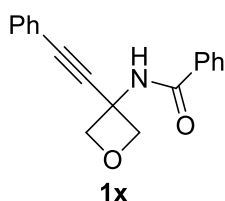
N-(3-(4-Methoxyphenyl)oxetan-3-yl)benzamide (1w) was prepared from **1w'** by following the same procedure for the synthesis of **1a** (82% yield, white solid).

¹H NMR (400 MHz, CDCl₃) δ 7.80 (d, *J* = 7.2 Hz, 2H), 7.53–7.36 (m, 5H), 7.28–7.22 (m, 1H), 6.88 (d, *J* = 6.4 Hz, 2H), 5.08 (d, *J* = 6.4 Hz, 2H), 4.91 (d, *J* = 6.4 Hz, 2H), 3.79 (s, 3H) ppm.

¹³C NMR (100 MHz, CDCl₃) δ 166.6, 158.9, 133.7, 133.5, 131.9, 128.6, 127.0, 126.1, 114.0, 83.0, 58.9, 55.3 ppm.

IR (thin film) 3318, 2956, 1628, 1531, 1478, 1248, 1030, 982, 735, 715 cm⁻¹.

HRMS (CI⁺) Calcd for C₁₇H₁₈NO₃ [M + H]⁺: 284.1287, Found: 284.1276.



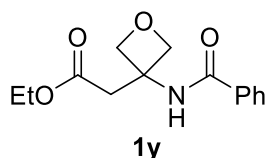
N-(3-(Phenylethynyl)oxetan-3-yl)benzamide (1x) was prepared from **1x'** by following the same procedure for the synthesis of **1a** (78% yield, white solid).

¹H NMR (400 MHz, CDCl₃) δ 7.84 (d, *J* = 7.2 Hz, 2H), 7.55–7.24 (m, 8H), 7.14 (s, 1H), 5.05 (d, *J* = 6.4 Hz, 2H), 5.00 (d, *J* = 6.4 Hz, 2H) ppm.

¹³C NMR (100 MHz, CDCl₃) δ 166.8, 133.4, 132.0, 131.8, 128.6, 128.5, 128.2, 127.1, 122.2, 87.7, 84.4, 81.7, 50.4 ppm.

IR (thin film) 3289, 2957, 1636, 1520, 1487, 1293, 985, 756, 699 cm⁻¹.

HRMS (CI⁺) Calcd for C₁₈H₁₆NO₂ [M + H]⁺: 278.1181, Found: 278.1168.



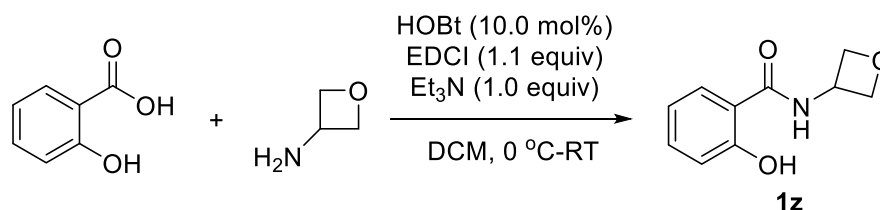
Ethyl 2-(3-Benzamidooxetan-3-yl)acetate (1y) was prepared from **1y'** by following the same procedure for the synthesis of **1a** (74% yield, yellow oil).

¹H NMR (400 MHz, CDCl₃) δ 7.76–7.70 (m, 2H), 7.52–7.43 (m, 1H), 7.42–7.33 (m, 2H), 7.18 (s, 1H), 4.84 (d, *J* = 7.2 Hz, 2H), 4.61 (d, *J* = 7.2 Hz, 2H), 4.08 (q, *J* = 7.2 Hz, 2H), 3.27 (s, 2H), 1.20 (t, *J* = 7.2 Hz, 3H) ppm.

¹³C NMR (100 MHz, CDCl₃) δ 171.2, 166.6, 133.6, 131.7, 128.5, 126.9, 80.2, 60.7, 54.5, 39.7, 14.0 ppm.

IR (thin film) 3305, 2979, 1726, 1638, 1524, 1482, 1196, 1027, 731, 692 cm⁻¹.

HRMS (CI⁺) Calcd for C₁₄H₁₈NO₄ [M + H]⁺: 264.1236, Found: 264.1228.



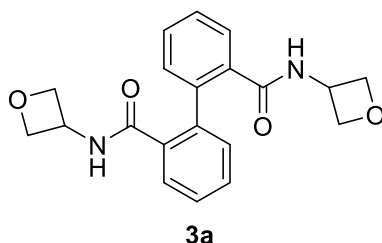
2-Hydroxy-N-(oxetan-3-yl)benzamide (1z). At 0 °C, to a solution of oxetan-3-amine (2.0 mL, 28.6 mmol), salicylic acid (3.60 g, 26 mmol), HOBT (354 mg, 2.6 mmol), and Et₃N (3.6 mL, 26 mmol) in CH₂Cl₂ (75 mL) was added a solution of EDCI (5.48 g, 28.6 mmol) in CH₂Cl₂ (75 mL). After stirring at 6 °C for 12 h, CH₂Cl₂ was removed in vacuo and the residue was dissolved in EtOAc (100 mL). The resulting solution was washed with an aqueous solution of HCl (80 mL, 1 M), a saturated aqueous solution of NaHCO₃ (2 × 100 mL), and brine (100 mL), dried over Na₂SO₄ and concentrated. The residue was purified by simple recrystallization (hexanes and diethyl ether) to afford the pure amide **1z** (4.1 g, 82% yield, white solid).

¹H NMR (400 MHz, CDCl₃) δ 12.0 (s, 1H), 7.46–7.38 (m, 2H), 7.01–6.85 (m, 3H), 5.25–5.15 (m, 1H), 5.03 (t, *J* = 7.2 Hz, 2H), 4.64 (t, *J* = 6.4 Hz, 2H).

^{13}C NMR (100 MHz, CDCl_3) δ 169.7, 161.6, 134.7, 125.5, 118.8, 118.7, 113.6, 78.1, 45.0 ppm.

IR (thin film) 3329, 2960, 2882, 1635, 1593, 1545, 1493, 1378, 1231, 955 cm^{-1} .

HRMS (CI+) Calcd for $\text{C}_{10}\text{H}_{12}\text{NO}_3$ $[\text{M} + \text{H}]^+$: 194.0812, Found: 194.0811.



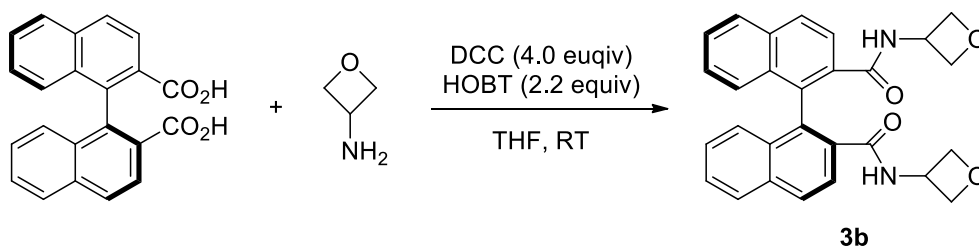
N,N'-Di(oxetan-3-yl)-[1,1'-biphenyl]-2,2'-dicarboxamide (**3a**) was prepared by following the same procedure for the synthesis of **1i** (white solid, 80% yield).

^1H NMR (400 MHz, CDCl_3) δ 8.10-7.98 (m, 2H), 7.58-7.52 (m, 2H), 7.45-7.34 (m, 4H), 7.10-7.01 (m, 2H), 4.97-4.88 (m, 2H), 4.82-4.74 (m, 2H), 4.73-4.66 (m, 2H), 4.34 (t, $J = 6.4$ Hz 2H), 3.98 (t, $J = 6.4$ Hz 2H) ppm.

^{13}C NMR (100 MHz, CDCl_3) δ 169.6, 138.9, 135.5, 129.9, 129.4, 128.1, 126.9, 78.0, 77.9, 44.8 ppm.

IR (thin film) 3490, 3242, 3056, 2960, 2876, 1634, 1545, 1484, 1329, 972, 879, 758, 731 cm^{-1} .

HRMS (CI+) Calcd for $\text{C}_{20}\text{H}_{21}\text{N}_2\text{O}_4$ $[\text{M} + \text{H}]^+$: 353.1501, Found: 353.1495.



(*S*)-*N,N'*-Di(oxetan-3-yl)-[1,1'-binaphthalene]-2,2'-dicarboxamide (**3b**). To a stirred solution of (*S*)-[1,1'-binaphthalene]-2,2'-dicarboxylic acid (513 mg, 1.5 mmol), DCC (810 mg, 6.0 mmol), and HOBT (680 mg, 3.3 mmol) in anhydrous THF (20 mL) was added a solution of oxetan-3-amine (243 mg, 3.3 mmol) in anhydrous THF (4 mL). After stirring at room temperature overnight, the mixture was quenched with

saturated NH₄Cl aqueous solution (10 mL) and diluted with CH₂Cl₂ (20 mL). The layers were separated, and the organic layer was washed with water (2×20 mL) and brine (20 mL), dried over anhydrous Na₂SO₄, and concentrated under reduced pressure. The residue was purified by flash column chromatography (1→3% MeOH in DCM) to afford the pure amide **3b** (500 mg, 73% yield, white solid).

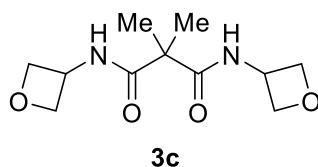
$[\alpha]_{\text{D}}^{25} = -250.0$ (*c* 1.0, CHCl₃).

¹H NMR (400 MHz, CDCl₃) δ 8.03 (d, *J* = 8.4 Hz, 2H), 7.93 (d, *J* = 8.4 Hz, 2H), 7.78 (d, *J* = 8.0 Hz, 2H), 7.69 (d, *J* = 8.4 Hz, 2H), 7.52 (td, *J*₁ = 7.2 Hz, *J*₂ = 0.8 Hz, 2H), 7.32 (td, *J*₁ = 8.4 Hz, *J*₂ = 1.2 Hz, 2H), 7.21 (d, *J* = 8.4 Hz, 2H), 4.53 (t, *J* = 6.8 Hz, 2H), 4.52 (t, *J* = 6.8 Hz, 2H), 3.85 (t, *J* = 6.4 Hz, 2H), 3.76 (t, *J* = 6.4 Hz, 2H) ppm.

¹³C NMR (100 MHz, CDCl₃) δ 169.9, 134.5, 134.0, 133.0, 132.1, 129.2, 128.9, 127.5, 127.4, 126.2, 123.4, 77.8, 44.5 ppm.

IR (thin film) 3238, 3055, 2958, 2875, 1636, 1549, 971 cm⁻¹.

HRMS (CI⁺) Calcd for C₂₈H₂₅N₂O₄ [M + H]⁺: 453.1809, Found: 453.1806.



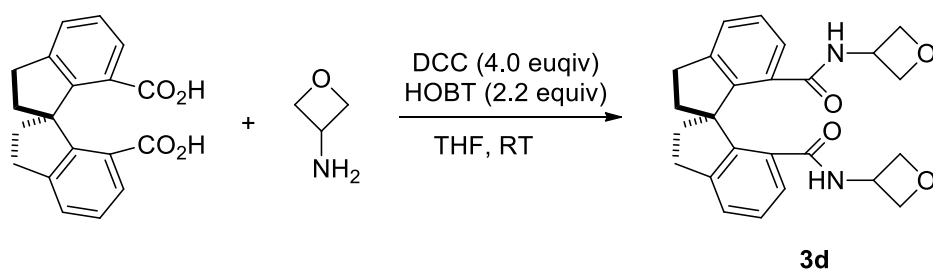
2,2-Dimethyl-N¹,N³-di(oxetan-3-yl)malonamide (3c) was prepared by following the same procedure for the synthesis of **1i** (white solid, 25% yield).

¹H NMR (400 MHz, CDCl₃) δ 7.19 (d, *J* = 4.8 Hz, 2H), 5.01-4.87 (m, 6H), 4.47 (t, *J* = 6.4 Hz, 4H), 1.47 (s, 6H) ppm.

¹³C NMR (100 MHz, CDCl₃) δ 173.1, 78.1, 49.0, 45.1, 23.9 ppm.

IR (thin film) 3292, 3039, 2968, 2873, 1633, 1519, 1274, 1206, 970 cm⁻¹.

HRMS (CI⁺) Calcd for C₁₁H₁₉N₂O₄ [M + H]⁺: 243.1339, Found: 243.1355.



(R)-N',N'-Di(oxetan-3-yl)-2,2',3,3'-tetrahydro-1,1'-spirobi[indene]-7,7'-dicarboxamide (3d). To a stirred solution of (R)-2,2',3,3'-tetrahydro-1,1'-spirobi[indene]-7,7'-dicarboxylic acid (185 mg, 0.6 mmol), DCC (495 mg, 2.4 mmol), and HOBT (270 mg, 1.32 mmol) in anhydrous THF (10 mL) was added oxetan-3-amine (96 mg, 1.32 mmol) in anhydrous THF (2 mL). After stirring at room temperature overnight, the mixture was quenched with saturated NH₄Cl aqueous solution (5 mL) and diluted with CH₂Cl₂ (10 mL). The layers were separated, and the organic layer was washed with water (2×10 mL) and brine (10 mL), dried over anhydrous Na₂SO₄, and concentrated under reduced pressure. The residue was purified by flash column chromatography (1→3% MeOH in DCM) to afford the pure amide **3d** (253 mg, 95% yield, white solid).

$[\alpha]_D^{25} = +73.5$ (*c* 1.0, CHCl₃).

¹H NMR (400 MHz, CDCl₃) δ 7.32–7.19 (m, 6H), 7.08 (d, *J* = 7.2 Hz, 2H), 4.67 (t, *J* = 6.8 Hz, 2H), 4.60–4.46 (m, 4H), 4.19 (t, *J* = 6.0 Hz, 2H), 3.89 (d, *J* = 6.0 Hz, 2H), 3.09–2.94 (m, 4H), 2.50–2.38 (m, 2H), 2.37–2.27 (m, 2H) ppm.

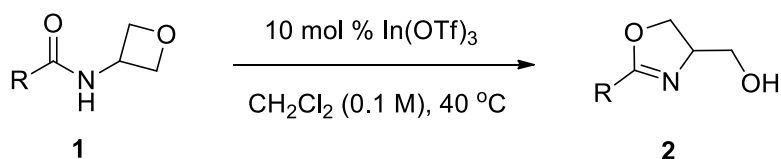
¹³C NMR (100 MHz, CDCl₃) δ 170.0, 144.7, 144.6, 133.7, 127.2, 125.8, 125.7, 77.4, 61.4, 44.6, 40.1, 30.5 ppm.

IR (thin film) 3245, 3058, 2932, 1637, 1538, 1268, 1113, 968 cm⁻¹.

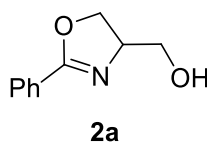
HRMS (CI+) Calcd for C₂₅H₂₇N₂O₄ [M + H]⁺: 419.1965, Found: 419.1979.

III. Catalytic Synthesis of Oxazolines

General Procedure A.



At room temperature under N_2 , to a solution of oxetane **1** (0.50 mmol) in dichloromethane (5.0 mL) was added indium(III) trifluoromethanesulfonate (28.1 mg, 10 mol%). The mixture was heated to 40 °C and kept stirring at the same temperature for a specified period of time before it was quenched with an aqueous solution of NaOH (3 mL, 10% solution) and stirred for 10 min. The mixture was then diluted with water (5 mL), and extracted with dichloromethane (2×15 mL). The combined organic layers were washed with water and brine, dried over anhydrous Na_2SO_4 , and concentrated under reduced pressure. The residue was purified by silica gel column chromatography to afford the desired oxazoline **2**.



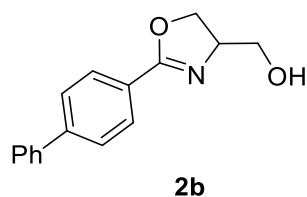
(2-Phenyl-4,5-dihydrooxazol-4-yl)methanol (2a) was prepared from oxetane **1a** (reaction time: 24 h) according to the General Procedure A (purification by flash column chromatography: 50% EtOAc in hexanes→EtOAc, 82.6 mg, white solid, 93% yield).

$^1\text{H NMR}$ (400 MHz, CDCl_3) δ 7.79 (d, $J = 8.4$ Hz, 2H), 7.43–7.38 (m, 1H), 7.30 (t, $J = 7.6$ Hz, 2H), 4.44–4.38 (m, 1H), 3.37–4.30 (m, 2H), 4.08 (br s, 1H), 3.92 (dd, $J_1 = 11.6$ Hz, $J_2 = 3.2$ Hz, 1H), 3.64 (dd, $J_1 = 11.6$ Hz, $J_2 = 3.6$ Hz, 1H) ppm.

$^{13}\text{C NMR}$ (100 MHz, CDCl_3) δ 165.4, 131.4, 128.2, 128.1, 127.0, 69.2, 67.9, 63.5 ppm.

IR (thin film) 3380, 2912, 1645, 1455, 1363, 1100, 1060, 967, 695 cm^{-1} .

HRMS (CI⁺) Calcd for $\text{C}_{10}\text{H}_{12}\text{NO}_2$ [$\text{M} + \text{H}$]⁺: 178.0868, Found: 178.0866.



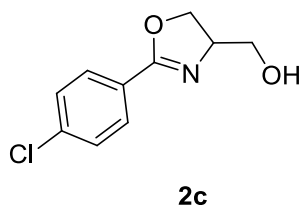
(2-([1,1'-Biphenyl]-4-yl)-4,5-dihydrooxazol-4-yl)methanol (2b) was prepared from oxetane **1k** (reaction time: 36 h) according to the General Procedure A (purification by flash column chromatography: 5% MeOH in dichloromethane, 111.5 mg, white solid, 88% yield).

¹H NMR (400 MHz, CDCl₃) δ 7.92 (d, *J* = 8.4 Hz, 2H), 7.61–7.56 (m, 4H), 7.46 (t, *J* = 7.6 Hz, 2H), 7.38 (t, *J* = 7.2 Hz, 1H), 4.53–4.36 (m, 3H), 4.00 (dd, *J*₁ = 11.6 Hz, *J*₂ = 2.8 Hz, 1H), 3.69 (dd, *J*₁ = 11.6 Hz, *J*₂ = 3.2 Hz, 1H), 3.31 (br s, 1H) ppm.

¹³C NMR (100 MHz, CDCl₃) δ 165.4, 144.2, 140.1, 128.9, 128.8, 127.9, 127.1, 126.9, 126.0, 69.2, 68.1, 63.9 ppm.

IR (thin film) 3419, 1638, 1480, 1400, 1371, 1094, 1068, 979, 848, 737, 690 cm⁻¹.

HRMS (CI⁺) Calcd for C₁₆H₁₆NO₂ [M + H]⁺: 254.1181, Found: 254.1187.



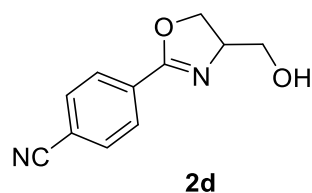
(2-(4-Chlorophenyl)-4,5-dihydrooxazol-4-yl)methanol (2c) was prepared from oxetane **1c** (reaction time: 36 h) according to the General Procedure A (purification by flash column chromatography: 67% EtOAc in hexanes→EtOAc, 97.6 mg, white solid, 92% yield).

¹H NMR (400 MHz, CDCl₃) δ 7.77 (d, *J* = 8.4 Hz, 2H), 7.31 (d, *J* = 8.8 Hz, 2H), 4.49 (dd, *J*₁ = 8.8 Hz, *J*₂ = 6.4 Hz, 1H), 4.44–4.34 (m, 2H), 3.97 (dd, *J*₁ = 11.6 Hz, *J*₂ = 3.2 Hz, 1H), 3.65 (dd, *J*₁ = 11.6 Hz, *J*₂ = 3.6 Hz, 1H), 3.24 (br s, 1H) ppm.

¹³C NMR (100 MHz, CDCl₃) δ 164.7, 137.8, 129.7, 128.6, 125.5, 69.4, 68.0, 63.6 ppm.

IR (thin film) 3428, 3034, 2905, 1639, 1403, 1355, 1266, 1085, 958, 837, 732 cm⁻¹.

HRMS (CI⁺) Calcd for C₁₀H₁₁ClNO₂ [M + H]⁺: 212.0478, Found: 212.0481.



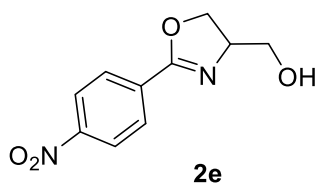
4-(4-(Hydroxymethyl)-4,5-dihydrooxazol-2-yl)benzonitrile (2d) was prepared from oxetane **1f** (reaction time: 36 h) according to the General Procedure A (purification by flash column chromatography: 67% EtOAc in hexanes→EtOAc, 89.4 mg, white solid, 88% yield).

¹H NMR (400 MHz, CDCl₃) δ 7.92 (d, *J* = 8.4 Hz, 2H), 7.62 (d, *J* = 8.4 Hz, 2H), 4.52 (dd, *J*₁ = 8.8 Hz, *J*₂ = 6.4 Hz, 1H), 4.47–4.37 (m, 2H), 3.97 (dd, *J*₁ = 11.6 Hz, *J*₂ = 3.2 Hz, 1H), 3.67 (dd, *J*₁ = 11.6 Hz, *J*₂ = 3.6 Hz, 1H), 3.15 (br s, 1H) ppm.

¹³C NMR (100 MHz, CDCl₃) δ 163.8, 132.0, 131.1, 128.8, 118.0, 114.9, 69.6, 68.2, 63.4 ppm.

IR (thin film) 3429, 2915, 2228, 1641, 1408, 1361, 1091, 963, 852, 675 cm⁻¹.

HRMS (CI⁺) Calcd for C₁₁H₁₁N₂O₂ [M + H]⁺: 203.0821, Found: 203.0820.



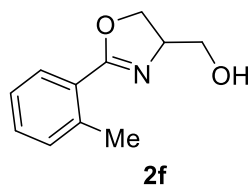
(2-(4-Nitrophenyl)-4,5-dihydrooxazol-4-yl)methanol (2e) was prepared from oxetane **1g** (reaction time: 36 h) according to the General Procedure A (purification by flash column chromatography: 5% MeOH in dichloromethane, 100.1 mg, white solid, 90% yield).

¹H NMR (400 MHz, CDCl₃) δ 8.21 (d, *J* = 8.8 Hz, 2H), 8.05 (d, *J* = 8.8 Hz, 2H), 4.57 (dd, *J*₁ = 9.6 Hz, *J*₂ = 7.2 Hz, 1H), 4.52–4.47 (m, 1H), 4.43 (dd, *J*₁ = 11.6 Hz, *J*₂ = 3.2 Hz, 1H), 3.99 (dd, *J*₁ = 11.6 Hz, *J*₂ = 3.6 Hz, 1H), 3.70 (dd, *J*₁ = 11.6 Hz, *J*₂ = 4.0 Hz, 1H), 2.79 (br s, 1H) ppm.

¹³C NMR (100 MHz, CDCl₃) δ 163.7, 149.6, 132.8, 129.4, 123.5, 69.7, 68.3, 63.6 ppm.

IR (thin film) 3406, 3236, 2924, 1649, 1600, 1522, 1346, 1265, 1093, 860, 693 cm⁻¹.

HRMS (CI+) Calcd for C₁₀H₁₁N₂O₄ [M + H]⁺: 223.0719, Found: 223.0716.



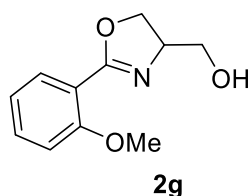
(2-(*o*-Tolyl)-4,5-dihydrooxazol-4-yl)methanol (**2f**) was prepared from oxetane **1h** (reaction time: 36 h) according to the General Procedure A (purification by flash column chromatography: 50% EtOAc in hexanes→EtOAc, 86.4 mg, colorless oil, 90% yield).

¹H NMR (400 MHz, CDCl₃) δ 7.71 (d, *J* = 8.0 Hz, 1H), 7.33–7.29 (m, 1H), 7.20–7.16 (m, 2H), 4.40–4.34 (m, 2H), 4.25–4.18 (m, 1H), 3.78 (dd, *J*₁ = 11.6 Hz, *J*₂ = 4.0 Hz, 1H), 3.61 (dd, *J*₁ = 11.6 Hz, *J*₂ = 4.0 Hz, 1H), 3.56 (br s, 1H), 2.49 (s, 3H) ppm.

¹³C NMR (100 MHz, CDCl₃) δ 166.2, 138.4, 131.0, 130.6, 129.7, 126.8, 125.5, 68.9, 68.1, 63.9, 21.4 ppm.

IR (thin film) 3411, 2926, 1728, 1641, 1456, 1356, 1255, 1047, 965, 732 cm⁻¹.

HRMS (CI+) Calcd for C₁₁H₁₄NO₂ [M + H]⁺: 192.1025, Found: 192.1033.



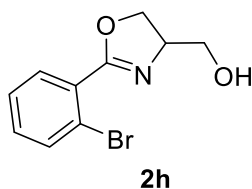
(2-(2-Methoxyphenyl)-4,5-dihydrooxazol-4-yl)methanol (**2g**) was prepared from oxetane **1i** (reaction time: 36 h) according to the General Procedure A (purification by flash column chromatography: 67% EtOAc in hexanes→EtOAc, 86.1 mg, colorless oil, 83% yield).

¹H NMR (400 MHz, CDCl₃) δ 7.71 (d, *J* = 8.0 Hz, 1H), 7.42–7.37 (m, 1H), 6.95–6.92 (m, 2H), 4.44–4.38 (m, 2H), 4.23 (t, *J* = 6.4 Hz, 1H), 3.89–3.84 (m, 4H), 3.63 (dd, *J*₁ = 11.6 Hz, *J*₂ = 4.0 Hz, 1H), 3.56 (br s, 1H) ppm.

^{13}C NMR (100 MHz, CDCl_3) δ 164.0, 158.3, 132.5, 131.1, 120.2, 116.4, 111.5, 68.7, 68.3, 64.0, 55.8 ppm.

IR (thin film) 3455, 2939, 2844, 1720, 1641, 1538, 1490, 1360, 1249, 1050, 968 cm^{-1} .

HRMS (CI+) Calcd for $\text{C}_{11}\text{H}_{14}\text{NO}_3$ $[\text{M} + \text{H}]^+$: 208.0974, Found: 208.0976.



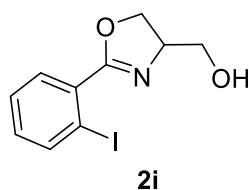
(2-(2-Bromophenyl)-4,5-dihydrooxazol-4-yl)methanol (2h) was prepared from oxetane **1d** (reaction time: 30 h) according to the General Procedure A (purification by flash column chromatography: 67% EtOAc in hexanes \rightarrow EtOAc, 108.9 mg, white solid, 85% yield).

^1H NMR (400 MHz, CDCl_3) δ 7.61–7.59 (m, 2H), 7.33–7.23 (m, 2H), 4.47–4.37 (m, 2H), 4.28 (t, $J = 6.0$ Hz, 1H), 3.81 (dd, $J_1 = 11.6$ Hz, $J_2 = 4.0$ Hz, 1H), 3.62 (dd, $J_1 = 11.6$ Hz, $J_2 = 4.0$ Hz, 1H), 3.32 (br s, 1H) ppm.

^{13}C NMR (100 MHz, CDCl_3) δ 164.8, 133.6, 131.8, 131.1, 129.4, 127.1, 121.6, 69.7, 68.2, 63.7 ppm.

IR (thin film) 3392, 2928, 1653, 1472, 1433, 1360, 1106, 1035, 956, 762 cm^{-1} .

HRMS (CI+) Calcd for $\text{C}_{10}\text{H}_{11}\text{BrNO}_2$ $[\text{M} + \text{H}]^+$: 255.9973, Found: 255.9976.



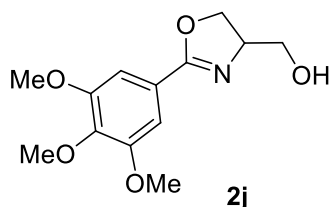
(2-(2-Iodophenyl)-4,5-dihydrooxazol-4-yl)methanol (2i) was prepared from oxetane **1e** (reaction time: 48 h) according to the General Procedure A (purification by flash column chromatography: 67% EtOAc in hexanes \rightarrow EtOAc, 122.6 mg, white solid, 81% yield).

$^1\text{H NMR}$ (400 MHz, CDCl_3) δ 7.92 (d, $J = 7.6$ Hz, 1H), 7.59 (dd, $J_1 = 7.6$ Hz, $J_2 = 1.6$ Hz, 1H), 7.37 (td, $J_1 = 7.6$ Hz, $J_2 = 1.2$ Hz, 1H), 7.12 (td, $J_1 = 7.6$ Hz, $J_2 = 1.6$ Hz, 1H), 4.52–4.45 (m, 2H), 4.35–4.32 (m, 1H), 3.92 (dd, $J_1 = 11.6$ Hz, $J_2 = 3.6$ Hz, 1H), 3.67 (dd, $J_1 = 11.6$ Hz, $J_2 = 4.4$ Hz, 1H), 2.61 (br s, 1H) ppm.

$^{13}\text{C NMR}$ (100 MHz, CDCl_3) δ 166.0, 140.3, 133.2, 131.8, 130.5, 127.9, 94.8, 69.7, 68.3, 64.0 ppm.

IR (thin film) 3378, 2927, 1729, 1653, 1469, 1429, 1359, 1246, 1103, 1045, 955, 760 cm^{-1} .

HRMS (CI+) Calcd for $\text{C}_{10}\text{H}_{11}\text{INO}_2$ [$\text{M} + \text{H}$] $^+$: 303.9834, Found: 303.9832.



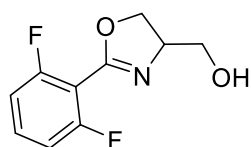
(2-(3,4,5-Trimethoxyphenyl)-4,5-dihydrooxazol-4-yl)methanol (2j) was prepared from oxetane **1j** (reaction time: 16 h) according to the General Procedure A (purification by flash column chromatography: 5% MeOH in dichloromethane, 115.0 mg, white solid, 86% yield).

$^1\text{H NMR}$ (400 MHz, CDCl_3) δ 7.03 (s, 2H), 4.46–4.43 (m, 1H), 4.41–4.33 (m, 2H), 4.24 (br s, 1H), 4.00 (dd, $J_1 = 11.6$ Hz, $J_2 = 2.8$ Hz, 1H), 3.83 (s, 9H), 3.63 (dd, $J_1 = 11.6$ Hz, $J_2 = 3.2$ Hz, 1H) ppm.

$^{13}\text{C NMR}$ (100 MHz, CDCl_3) δ 165.3, 152.7, 140.7, 121.9, 105.4, 69.2, 67.8, 63.3, 60.8, 56.0 ppm.

IR (thin film) 3382, 2941, 2842, 1643, 1588, 1505, 1463, 1371, 1234, 1123, 989, 855 cm^{-1} .

HRMS (CI+) Calcd for $\text{C}_{13}\text{H}_{18}\text{NO}_5$ [$\text{M} + \text{H}$] $^+$: 268.1185, Found: 268.1178.



2k

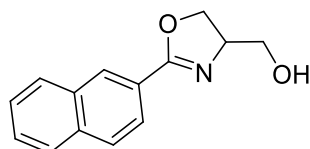
(2-(2,6-Difluorophenyl)-4,5-dihydrooxazol-4-yl)methanol (2k) was prepared from oxetane **1b** (reaction time: 36 h) according to the General Procedure A (purification by flash column chromatography: 67% EtOAc in hexanes→EtOAc, 93.2 mg, white solid, 87% yield).

¹H NMR (400 MHz, CDCl₃) δ 7.40–7.35 (m, 1H), 6.93 (td, *J*₁ = 11.6 Hz, *J*₂ = 3.6 Hz, 2H), 4.51–4.43 (m, 2H), 4.36–4.31 (m, 1H), 3.86 (dd, *J*₁ = 11.6 Hz, *J*₂ = 3.6 Hz, 1H), 3.66 (dd, *J*₁ = 11.6 Hz, *J*₂ = 4.0 Hz, 1H), 2.95 (br s, 1H) ppm.

¹³C NMR (100 MHz, CDCl₃) δ 161.0 (dd, *J*₁ = 254.6 Hz, *J*₂ = 5.8 Hz), 158.1, 132.4 (t like, *J* = 10.4 Hz), 111.9 (dt, *J*₁ = 20.2 Hz, *J*₂ = 2.5 Hz), 106.9 (t like, *J* = 17.4 Hz), 69.5, 68.2, 63.7 ppm.

IR (thin film) 3407, 2913, 1663, 1473, 1358, 1247, 1106, 1055, 1011, 795 cm⁻¹.

HRMS (CI⁺) Calcd for C₁₀H₁₀F₂NO₂ [M + H]⁺: 214.0680, Found: 214.0675.



2l

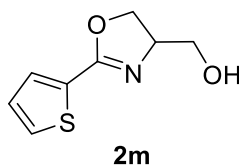
(2-(Naphthalen-2-yl)-4,5-dihydrooxazol-4-yl)methanol (2l) was prepared from oxetane **1l** (reaction time: 36 h) according to the General Procedure A (purification by flash column chromatography: 67% EtOAc in hexanes→EtOAc, 102.3 mg, white solid, 90% yield).

¹H NMR (400 MHz, CDCl₃) δ 8.16 (s, 1H), 7.87 (dd, *J*₁ = 8.4 Hz, *J*₂ = 1.2 Hz, 1H), 7.79 (d, *J* = 8.0 Hz, 1H), 7.69 (t, *J* = 8.4 Hz, 2H), 7.52 (t, *J* = 7.2 Hz, 1H), 7.42 (t, *J* = 7.6 Hz, 1H), 4.53–4.43 (m, 3H), 4.06 (dd, *J*₁ = 12.0 Hz, *J*₂ = 2.0 Hz, 1H), 3.87 (br s, 1H), 3.72 (dd, *J*₁ = 12.0 Hz, *J*₂ = 2.8 Hz, 1H) ppm.

¹³C NMR (100 MHz, CDCl₃) δ 165.7, 134.6, 132.4, 129.0, 128.9, 127.9, 127.6 (2C), 126.4, 124.5, 124.1, 69.3, 68.0, 63.6 ppm.

IR (thin film) 3446, 2866, 1640, 1472, 1375, 1103, 1067, 966, 750 cm⁻¹.

HRMS (CI⁺) Calcd for C₁₄H₁₄NO₂ [M + H]⁺: 228.1025, Found: 228.1022.



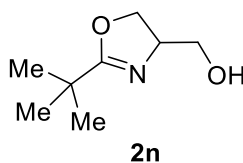
(2-(Thiophen-2-yl)-4,5-dihydrooxazol-4-yl)methanol (2m) was prepared from oxetane **1m** (reaction time: 36 h) according to the General Procedure A (purification by flash column chromatography: 50% EtOAc in hexanes → EtOAc, 82.4 mg, colorless oil, 90% yield).

¹H NMR (400 MHz, CDCl₃) δ 7.58 (dd, *J*₁ = 3.6 Hz, *J*₂ = 1.2 Hz, 1H), 7.43 (dd, *J*₁ = 5.2 Hz, *J*₂ = 1.2 Hz, 1H), 7.03 (dd, *J*₁ = 5.2 Hz, *J*₂ = 3.6 Hz, 1H), 4.48 (dd, *J*₁ = 8.8 Hz, *J*₂ = 6.4 Hz, 1H), 4.43–4.34 (m, 2H), 3.94 (dd, *J*₁ = 11.6 Hz, *J*₂ = 3.2 Hz, 1H), 3.66 (dd, *J*₁ = 11.6 Hz, *J*₂ = 3.6 Hz, 1H), 3.01 (br s, 1H) ppm.

¹³C NMR (100 MHz, CDCl₃) δ 161.1, 130.8, 130.1, 129.6, 127.5, 69.7, 68.1, 63.5 ppm.

IR (thin film) 3375, 3104, 2919, 1642, 1525, 1430, 1372, 1061, 1032, 954, 851, 721 cm⁻¹.

HRMS (CI⁺) Calcd for C₈H₁₀NO₂S [M + H]⁺: 184.0432, Found: 184.0440.



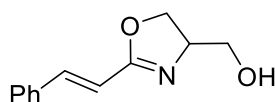
(2-(*tert*-Butyl)-4,5-dihydrooxazol-4-yl)methanol (2n) was prepared from oxetane **1o** (reaction time: 24 h) according to the General Procedure A (purification by flash column chromatography: 50% EtOAc in hexanes → EtOAc, 73.9 mg, colorless oil, 94% yield).

$^1\text{H NMR}$ (400 MHz, CDCl_3) δ 4.26 (dd, $J_1 = 9.6$ Hz, $J_2 = 7.6$ Hz, 1H), 4.19–4.13 (m, 1H), 4.05 (t like, $J = 7.6$ Hz, 1H), 3.69 (dd, $J_1 = 11.2$ Hz, $J_2 = 4.4$ Hz, 1H), 3.54 (dd, $J_1 = 11.2$ Hz, $J_2 = 4.8$ Hz, 1H), 3.38 (br s, 1H), 1.18 (s, 9H) ppm.

$^{13}\text{C NMR}$ (100 MHz, CDCl_3) δ 176.2, 69.5, 67.4, 64.1, 33.3, 27.8 ppm.

IR (thin film) 3383, 2972, 2919, 1645, 1473, 1358, 1153, 1052, 977 cm^{-1} .

HRMS (CI+) Calcd for $\text{C}_8\text{H}_{16}\text{NO}_2$ $[\text{M} + \text{H}]^+$: 158.1181, Found: 158.1186.



2o

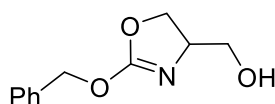
(E)-(2-Styryl-4,5-dihydrooxazol-4-yl)methanol (2o) was prepared from oxetane **1n** in DCE with 20 mol% of $\text{In}(\text{OTf})_3$ at 60 °C according to the General Procedure A (reaction time: 24 h, purification by flash column chromatography: 67% EtOAc in hexanes \rightarrow EtOAc, 100.4 mg, white solid, 99% yield).

$^1\text{H NMR}$ (400 MHz, CDCl_3) δ 7.35–7.29 (m, 5H), 7.24 (d, $J = 16.4$ Hz, 1H), 6.54 (d, $J = 16.0$ Hz, 1H), 4.47 (br s, 1H), 4.43–4.29 (m, 3H), 3.92 (d, $J = 10.0$ Hz, 1H), 3.62 (d, $J_1 = 9.6$ Hz, $J_2 = 2.0$ Hz, 1H) ppm.

$^{13}\text{C NMR}$ (100 MHz, CDCl_3) δ 165.2, 140.6, 134.9, 129.5, 128.7, 127.5, 114.3, 68.9, 67.8, 63.3 ppm.

IR (thin film) 3410, 2909, 1653, 1607, 1370, 1264, 1053, 984, 760, 690 cm^{-1} .

HRMS (CI+) Calcd for $\text{C}_{12}\text{H}_{14}\text{NO}_2$ $[\text{M} + \text{H}]^+$: 204.1025, Found: 204.1031.



2p

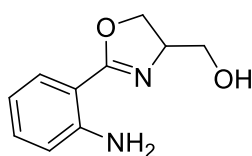
(2-(Benzyloxy)-4,5-dihydrooxazol-4-yl)methanol (2p) was prepared from oxetane **1p** (reaction time: 24 h) according to the General Procedure A (purification by flash column chromatography: 50% EtOAc in hexanes, 85.2 mg, colorless oil, 82% yield). The reaction was quenched with Et_3N (0.5 mL) instead of aqueous solution of NaOH.

$^1\text{H NMR}$ (400 MHz, CDCl_3) δ 7.36–7.28 (m, 5H), 6.61 (br s, 1H), 4.51 (s, 2H), 4.39 (t, J = 8.8 Hz, 1H), 4.12 (dd, J_1 = 8.8 Hz, J_2 = 4.8 Hz, 1H), 4.01–3.95 (m, 1H), 3.44 (dd, J_1 = 6.4 Hz, J_2 = 1.2 Hz, 2H) ppm.

$^{13}\text{C NMR}$ (100 MHz, CDCl_3) δ 159.9, 137.3, 128.3, 127.8, 127.6, 73.3, 71.3, 67.2, 51.7 ppm.

IR (thin film) 3291, 2916, 2864, 1753, 1411, 1233, 1108, 1031, 939, 745, 703 cm^{-1} .

HRMS (CI+) Calcd for $\text{C}_{11}\text{H}_{14}\text{NO}_3$ [$\text{M} + \text{H}$] $^+$: 208.0974, Found: 208.0971.



2q

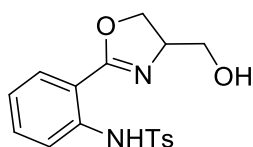
(2-(2-Aminophenyl)-4,5-dihydrooxazol-4-yl)methanol (2q) was prepared from oxetane **1q** (reaction time: 18 h) according to the General Procedure A (purification by flash column chromatography: 50% EtOAc in hexanes \rightarrow EtOAc, 86.3 mg, pale yellow oil, 90% yield).

$^1\text{H NMR}$ (400 MHz, CDCl_3) δ 7.70 (d, J = 8.4 Hz, 1H), 7.20 (td, J_1 = 7.6 Hz, J_2 = 1.6 Hz, 1H), 6.69–6.65 (m, 2H), 4.85 (br s, 3H), 4.46–4.40 (m, 1H), 4.33 (dd, J_1 = 8.0 Hz, J_2 = 4.0 Hz, 1H), 4.18 (t, J = 8.0 Hz, 1H), 3.82 (dd, J_1 = 11.6 Hz, J_2 = 4.0 Hz, 1H), 3.61 (dd, J_1 = 11.2 Hz, J_2 = 4.4 Hz, 1H) ppm.

$^{13}\text{C NMR}$ (100 MHz, CDCl_3) δ 165.4, 148.4, 132.3, 129.7, 116.3, 115.8, 108.9, 68.0, 67.5, 64.2 ppm.

IR (thin film) 3376, 2934, 1633, 1524, 1257, 1160, 1100, 1047, 971, 749, 693 cm^{-1} .

HRMS (CI+) Calcd for $\text{C}_{10}\text{H}_{13}\text{N}_2\text{O}_2$ [$\text{M} + \text{H}$] $^+$: 193.0977, Found: 193.0976.



2r

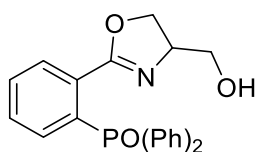
N-(2-(4-(Hydroxymethyl)-4,5-dihydrooxazol-2-yl)phenyl)-4-methylbenzenesulfonamide (2r) was prepared from oxetane **1r** (reaction time: 24 h) according to the General Procedure A (purification by flash column chromatography: 67% EtOAc in hexanes→EtOAc, 161.3 mg, white solid, 93% yield). The reaction was quenched with Et₃N (0.5 mL) instead of aqueous solution of NaOH.

¹H NMR (400 MHz, CDCl₃) δ 12.1 (br s, 1H), 7.74–7.71 (m, 3H), 7.65 (d, *J* = 8.4 Hz, 1H), 7.35 (td, *J*₁ = 8.4 Hz, *J*₂ = 1.6 Hz, 1H), 7.19 (d, *J* = 8.4 Hz, 2H), 7.01 (td, *J*₁ = 8.0 Hz, *J*₂ = 0.8 Hz, 1H), 4.53–4.48 (m, 1H), 4.40 (dd, *J*₁ = 9.6 Hz, *J*₂ = 8.0 Hz, 1H), 4.28 (t, *J* = 8.0 Hz, 1H), 3.87 (dd, *J*₁ = 11.6 Hz, *J*₂ = 4.4 Hz, 1H), 3.73 (dd, *J*₁ = 11.2 Hz, *J*₂ = 4.0 Hz, 1H), 2.35 (s, 3H), 2.15 (br s, 1H) ppm.

¹³C NMR (100 MHz, CDCl₃) δ 165.1, 143.7, 139.1, 136.7, 132.6, 129.5 (2C), 127.0, 122.6, 118.3, 113.5, 68.3, 67.7, 63.9, 21.4 ppm.

IR (thin film) 3527, 2916, 1634, 1593, 1502, 1335, 1269, 1159, 1058, 952, 762 cm⁻¹.

HRMS (CI⁺) Calcd for C₁₇H₁₉N₂O₄S [M + H]⁺: 347.1066, Found: 347.1076.



2s

(2-(4-(Hydroxymethyl)-4,5-dihydrooxazol-2-yl)phenyl)diphenylphosphine oxide (2s) was prepared from oxetane **1s** (0.3 mmol scale) in DCE with 10 mol% of In(OTf)₃ at 60 °C according to the General Procedure A (reaction time: 48 h, purification by flash column chromatography: DCM/MeOH = 25/1, 79 mg, white solid, 70% yield).

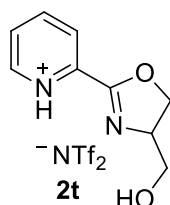
$^1\text{H NMR}$ (400 MHz, CDCl_3) δ 7.82-7.75 (m, 1H), 7.70-7.34 (m, 12H), 7.09 (dd, $J_1 = 14.0$ Hz, $J_2 = 7.6$ Hz, 1H), 5.53 (brs, 1H), 4.60-4.53 (m, 1H), 4.34-4.25 (m, 1H), 4.21-4.13 (m, 1H), 3.89-3.82 (m, 1H), 3.47-3.40 (m, 1H) ppm.

$^{13}\text{C NMR}$ (100 MHz, CDCl_3) δ 163.8, 133.4 (d, $J = 48.4$ Hz), 133.8 (d, $J = 139.6$ Hz), 133.2 (d, $J = 20.8$ Hz), 132.7 (d, $J = 134.8$ Hz), 132.2 (d, $J = 38.0$ Hz), 132.0, 131.8 (dd, $J_1 = 16.8$, $J_2 = 11.2$ Hz), 131.5 (d, $J = 10.4$ Hz), 130.9 (d, $J = 40.4$ Hz), 130.6 (d, $J = 34.0$ Hz), 129.5 (d, $J = 50.4$ Hz), 128.5 (d, $J = 9.2$ Hz), 128.4 (d, $J = 12.8$ Hz), 69.4, 69.0, 63.5 ppm.

IR (thin film) 3290, 2926, 1663, 1588, 1482, 1437, 1354, 1177, 1111, 1043, 721, 694 cm^{-1} .

$^{31}\text{P NMR}$ (162 MHz, CDCl_3) δ 33.54 ppm.

HRMS (CI+) Calcd for $\text{C}_{22}\text{H}_{21}\text{N}_2\text{O}_3\text{P}$ [$\text{M} + \text{H}$] $^+$: 378.1259, Found: 378.1242.



2-(4-(Hydroxymethyl)-4,5-dihydrooxazol-2-yl)pyridin-1-ium bis((trifluoromethyl)sulfonyl)amide (2t) was prepared from oxetane **1t** in DCM with one equivalent of HNTf_2 at 40 °C according to the General Procedure A (reaction time: 12 h, purification by flash column chromatography: DCM/MeOH = 10:1, 115 mg, oil, 50% yield).

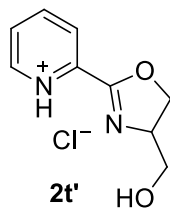
$^1\text{H NMR}$ (400 MHz, CDCl_3) δ 8.67-8.61 (m, 1H), 7.96-7.90 (m, 1H), 7.77-7.69 (m, 1H), 7.39-7.32 (m, 1H), 4.60-4.38 (m, 3H), 3.97 (dd, $J_1 = 11.6$ Hz, $J_2 = 3.6$ Hz 1H), 3.70 (dd, $J_1 = 11.6$ Hz, $J_2 = 3.6$ Hz 1H) ppm.

$^{13}\text{C NMR}$ (100 MHz, CDCl_3) δ 164.3, 149.7, 146.1, 136.7, 125.7, 123.9, 69.9, 68.4, 63.9 ppm.

$^{19}\text{F NMR}$ (376 MHz, CDCl_3) δ -78.88 ppm.

IR (thin film) 3314, 2906, 1734, 1642, 1583, 1470, 1362, 1105, 1043, 959, 800, 724, 678 cm^{-1} .

HRMS (CI+) Calcd for $\text{C}_9\text{H}_{11}\text{N}_2\text{O}_2$ [$\text{M} - \text{NTf}_2$] $^+$: 179.0821, Found: 179.0831.



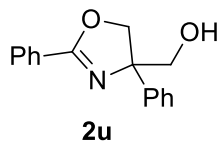
2-(4-(Hydroxymethyl)-4,5-dihydrooxazol-2-yl)pyridin-1-ium chloride (2t') was prepared from oxetane **1t** in DCE with 2.5 equivalents of HCl (4 M in MeOH) in place of In(OTf)₃ at 60 °C according to the General Procedure A (reaction time: 72 h, purification by flash column chromatography: 67% EtOAc in hexanes→EtOAc, 43 mg, oil, 48% yield).

¹H NMR (400 MHz, CDCl₃) δ 8.57-8.45 (m, 2H), 8.16 (d, *J* = 7.6 Hz 1H), 7.88-7.80 (m, 1H), 7.47-7.40 (m, 1H), 4.48-4.38 (m, 1H), 4.02-3.93 (m, 1H), 3.92-3.76 (m, 3H) ppm.

¹³C NMR (100 MHz, CDCl₃) δ 164.6, 149.2, 148.2, 137.4, 126.5, 122.4, 61.8, 51.8, 43.9 ppm.

IR (thin film) 3368, 2954, 1662, 1580, 1517, 1464, 1045, 906, 725, 698 cm⁻¹.

HRMS (CI⁺) Calcd for C₉H₁₂ClN₂O₂ [M + H]⁺: 215.0593, Found: 215.0596.



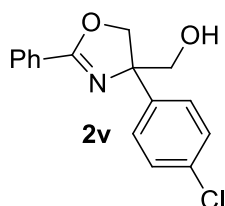
(2,4-Diphenyl-4,5-dihydrooxazol-4-yl)methanol (2u) was prepared from oxetane **1u** (reaction time: 22 h) according to the General Procedure A (purification by flash column chromatography: 67% EtOAc in hexanes→EtOAc, 117 mg, white solid, 92% yield).

¹H NMR (400 MHz, CDCl₃) δ 8.06-7.97 (m, 2H), 7.52 (t, *J* = 7.2 Hz, 1H), 7.49-7.34 (m, 6H), 7.32-7.26 (m, 1H), 4.87 (d, *J* = 8.0 Hz 1H), 4.54 (d, *J* = 8.0 Hz, 1H), 3.94 (d, *J* = 11.6 Hz, 1H), 3.76 (d, *J* = 11.6 Hz, 1H) ppm.

¹³C NMR (100 MHz, CDCl₃) δ 165.1, 143.6, 131.7, 128.6, 128.5, 128.3, 127.4, 127.0, 125.7, 80.0, 75.3, 68.8 ppm.

IR (thin film) 3179, 2896, 1645, 1579, 1493, 1083, 978, 764, 693 cm⁻¹.

HRMS (CI⁺) Calcd for C₁₆H₁₆NO₂ [M + H]⁺: 254.1181, Found: 254.1187.



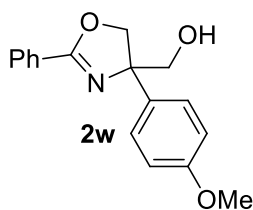
(4-(4-Chlorophenyl)-2-phenyl-4,5-dihydrooxazol-4-yl)methanol (2v) was prepared from oxetane **1v** (reaction time: 22 h) according to the General Procedure A (purification by flash column chromatography: 67% EtOAc in hexanes→EtOAc, 138 mg, white solid, 96% yield).

¹H NMR (400 MHz, CDCl₃) δ 7.94-7.88 (m, 2H), 7.47 (t, *J* = 7.2 Hz, 1H), 7.42-7.28 (m, 6H), 4.86 (d, *J* = 8.0 Hz 1H), 4.46 (d, *J* = 8.0 Hz, 1H), 3.89 (d, *J* = 11.6 Hz, 1H), 3.70 (d, *J* = 11.6 Hz, 1H) ppm.

¹³C NMR (100 MHz, CDCl₃) δ 165.2, 142.2, 133.3, 131.7, 128.7, 128.5, 128.3, 127.2, 126.9, 77.7, 75.1, 68.7 ppm.

IR (thin film) 3211, 2896, 1649, 1571, 1493, 1400, 1067, 977, 689 cm⁻¹.

HRMS (CI⁺) Calcd for C₁₆H₁₅ClNO₂ [M + H]⁺: 288.0791, Found: 288.0785.



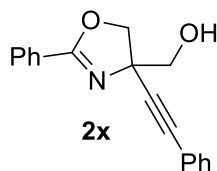
(4-(4-Methoxyphenyl)-2-phenyl-4,5-dihydrooxazol-4-yl)methanol (2w) was prepared from oxetane **1w** (reaction time: 22 h) according to the General Procedure A (purification by flash column chromatography: 67% EtOAc in hexanes→EtOAc, 151 mg, white solid, 95% yield).

¹H NMR (400 MHz, CDCl₃) δ 7.97-7.90 (m, 2H), 7.48 (t, *J* = 7.2 Hz, 1H), 7.41-7.28 (m, 4H), 6.92-6.86 (m, 2H), 4.86 (d, *J* = 8.0 Hz 1H), 4.50 (d, *J* = 8.0 Hz, 1H), 3.93 (d, *J* = 12.0 Hz, 1H), 3.79 (s, 3H), 3.72 (d, *J* = 12.0 Hz, 1H) ppm.

^{13}C NMR (100 MHz, CDCl_3) δ 165.0, 158.8, 135.7, 131.6, 128.5, 128.3, 127.0, 126.8, 114.0, 77.5, 75.5, 68.8, 55.3 ppm.

IR (thin film) 3196, 2957, 1642, 1579, 1510, 1450, 1244, 1025, 734, 692 cm^{-1} .

HRMS (CI+) Calcd for $\text{C}_{17}\text{H}_{18}\text{NO}_3$ $[\text{M} + \text{H}]^+$: 284.1287, Found: 284.1284.



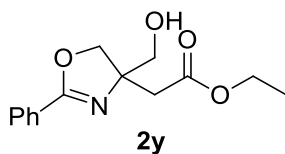
(2-Phenyl-4-(phenylethynyl)-4,5-dihydrooxazol-4-yl)methanol (2x) was prepared from oxetane **1x** (reaction time: 22 h) according to the General Procedure A (purification by flash column chromatography: 67% EtOAc in hexanes \rightarrow EtOAc, 134 mg, white solid, 97% yield).

^1H NMR (400 MHz, CDCl_3) δ 8.03-7.95 (m, 2H), 7.52-7.36 (m, 5H), 7.34-7.26 (m, 3H), 4.69 (d, $J = 8.0$ Hz 1H), 4.62 (d, $J = 8.0$ Hz, 1H), 4.03 (d, $J = 11.6$ Hz, 1H), 3.79 (d, $J = 11.6$ Hz, 1H) ppm.

^{13}C NMR (100 MHz, CDCl_3) δ 166.3, 131.9, 131.8, 128.6, 128.5, 128.3, 128.2, 126.7, 122.2, 88.1, 85.7, 74.8, 70.2, 67.2 ppm.

IR (thin film) 3237, 2902, 1642, 1578, 1490, 1449, 1062, 755, 687 cm^{-1} .

HRMS (CI+) Calcd for $\text{C}_{18}\text{H}_{16}\text{NO}_2$ $[\text{M} + \text{H}]^+$: 278.1181, Found: 278.1178.



Ethyl 2-(4-(hydroxymethyl)-2-phenyl-4,5-dihydrooxazol-4-yl)acetate (2y) was prepared from oxetane **1y** (reaction time: 22 h) according to the General Procedure A (purification by flash column chromatography: 67% EtOAc in hexanes \rightarrow EtOAc, 103 mg, yellow oil, 79% yield).

^1H NMR (400 MHz, CDCl_3) δ 7.85-7.80 (m, 2H), 7.44 (t, $J = 7.2$ Hz, 1H), 7.37-7.30 (m, 2H), 4.48 (dd, $J_1 = 13.6$ Hz, $J_2 = 8.8$ Hz 2H), 4.10 (q, $J = 7.2$ Hz, 2H), 3.82 (d, $J = 11.6$ Hz,

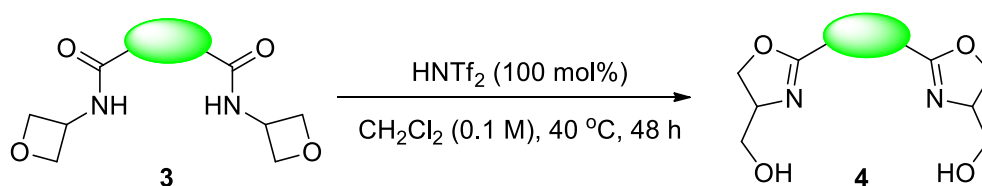
1H), 3.65 (d, $J = 11.6$ Hz, 1H), 2.81 (d, $J = 15.6$ Hz, 1H), 2.66 (d, $J = 15.6$ Hz, 1H), 1.20 (t, $J = 7.2$ Hz, 3H) ppm.

^{13}C NMR (100 MHz, CDCl_3) δ 170.6, 165.1, 131.6, 128.4, 128.2, 127.0, 73.20, 73.1, 67.0, 60.7, 40.9, 14.1 ppm.

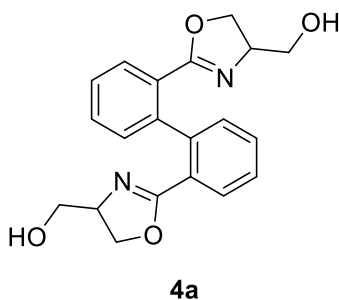
IR (thin film) 3300, 2982, 1727, 1643, 1580, 1497, 1466, 1450, 1026, 974, 732, 697 cm^{-1} .

HRMS (CI+) Calcd for $\text{C}_{14}\text{H}_{18}\text{NO}_4$ [$\text{M} + \text{H}$] $^+$: 264.1236, Found: 264.1225.

General Procedure B.



To a solution of oxetane **3** (0.50 mmol) in dichloromethane (5.0 mL) was added triflimide (141 mg, 100 mol%). After stirring at 40 °C for 48 h, the reaction was quenched with an aqueous solution of NaOH (3 mL, 10%) followed by stirring for 10 min. The mixture was then diluted with water (5 mL) and extracted with dichloromethane (2×15 mL). The combined extracts were washed with water and brine, dried over anhydrous Na_2SO_4 , and concentrated under reduced pressure. The residue was purified by silica gel column chromatography to afford the desired oxazoline **4**.



[1,1'-Biphenyl]-2,2'-diylbis(4,5-dihydrooxazole-2,4-diy)dimethanol (4a) was prepared from oxetane **3a** (reaction time: 72 h) according to the General Procedure A (purification by flash column chromatography: DCM/MeOH = 30:1, 89 mg, white solid, 50% yield, > 20:1 *dr*).

¹H NMR (400 MHz, CDCl₃) δ 7.58-7.48 (m, 4H), 7.46-7.36 (m, 4H), 4.23-4.01 (m, 6H), 3.90 (t, *J* = 8.0 Hz, 2H), 3.60 (dd, *J*₁ = 12.8 Hz, *J*₂ = 2.8 Hz, 2H) ppm.

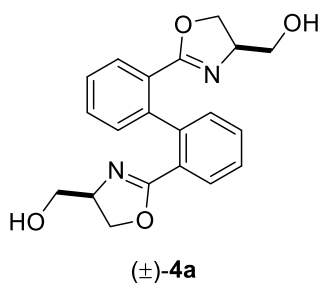
¹³C NMR (100 MHz, CDCl₃) δ 168.3, 140.1, 130.3, 129.3 (2C), 128.5, 127.8, 68.7, 67.8, 61.4 ppm.

IR (thin film) 3216, 2902, 1653, 1598, 1497, 1468, 1444, 1356, 1110, 1038, 953, 771, 732, 698 cm⁻¹.

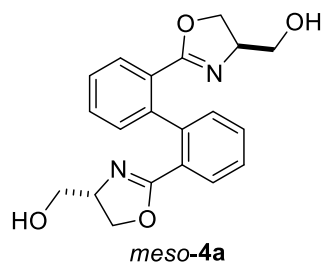
HRMS (CI⁺) Calcd for C₂₀H₂₁N₂O₄ [M + H]⁺: 353.1501, Found: 353.1495.

Notes to determination of the relative stereochemistry:

The following two possible isomers regarding relative stereochemistry are possible. (±)-**4a** and *meso*-**4a** both have symmetry and thus degeneracy are expected for both structures. Therefore, both structures are possible for this product.

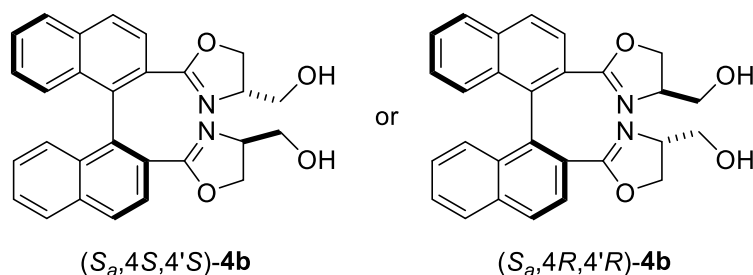


C₂ symmetry



plane symmetry

Degeneracy expected for NMR spectra for both structures



((4S,4'S)/(4R,4'R)-((S)-[1,1'-Binaphthalene]-2,2'-diyl)bis(4,5-dihydrooxazole-2,4-diyl)dimethanol (4b) was prepared from oxetane **3b** according to the general procedure B (purification by flash column chromatography: DCM/MeOH = 100:1 → 50:1, 99.6 mg, white solid, 44% yield, single isomer).^[2]

$[\alpha]_{\text{D}}^{25} = +63.0$ (c 1.0, CHCl₃).

¹H NMR (400 MHz, acetone-*d*₆) δ 8.08 (t, *J* = 8.8 Hz 4H), 7.69 (d, *J* = 8.4 Hz 2H), 7.63-7.56 (m, 2H), 7.41-7.35 (m, 2H), 7.24 (d, *J* = 8.4 Hz 2H), 4.17-4.10 (m, 2H), 3.95 (dd, *J*₁ = 10.0 Hz, *J*₂ = 8.0 Hz 2H), 3.85 (dd, *J*₁ = 12.4 Hz, *J*₂ = 2.0 Hz 2H), 3.54 (t, *J* = 8.0 Hz 2H), 3.21 (dd, *J*₁ = 12.4 Hz, *J*₂ = 3.2 Hz 2H) ppm.

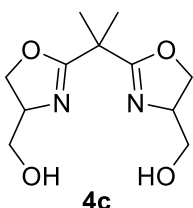
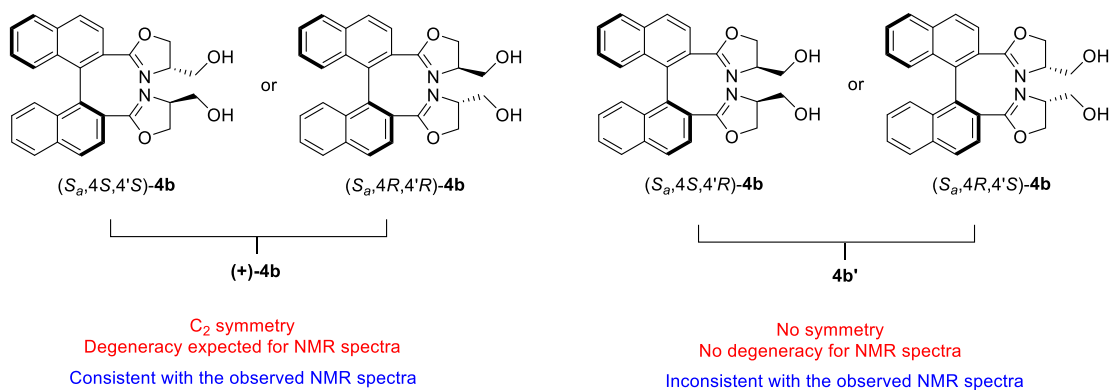
¹³C NMR (100 MHz, acetone-*d*₆) δ 168.3, 136.4, 134.3, 133.1, 128.8, 128.5, 127.8, 127.6, 127.5, 127.2, 126.5, 69.0, 68.4, 61.5 ppm.

IR (thin film) 3181, 2929, 2863, 1653, 1328, 1193, 1134, 1055, 975 cm⁻¹.

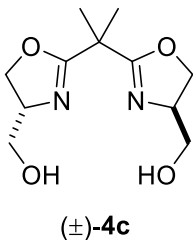
HRMS (CI⁺) Calcd for C₂₈H₂₅N₂O₄ [M + H]⁺: 453.1814, Found: 453.1809.

Notes to determination of the relative stereochemistry:

There are four possible diastereomers for **4b**: (*S*_a, 4*S*, 4'*S*), (*S*_a, 4*R*, 4'*R*), (*S*_a, 4*S*, 4'*R*) and (*S*_a, 4*S*, 4'*R*). The former two structures have C₂-symmetry and thus degeneracy should be expected from the NMR spectra, particularly ¹³C NMR spectra. For the latter two, there is no symmetry and their NMR spectra should have more peaks.



(2,2'-(Propane-2,2-diyl)bis(4,5-dihydrooxazole-4,2-diyl))dimethanol (4c) was prepared from oxetane **3c** according to the general procedure B (purification by flash column chromatography: DCM/MeOH = 20:1 → 12:1, 115 mg, white solid, 95% yield, 1:1 *dr*). The two diastereomers can be separated on silica gel.

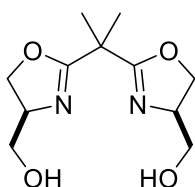


¹H NMR (400 MHz, acetone-*d*₆) δ 4.36-4.28 (m, 2H), 4.18-4.16 (m, 4H), 3.67-3.60 (m, 2H), 3.53 (dd, *J*₁ = 10.8 Hz, *J*₂ = 4.4 Hz, 2H), 1.46 (s, 6H) ppm.

¹³C NMR (100 MHz, acetone-*d*₆) δ 170.9, 70.4, 68.1, 64.3, 39.4, 24.0 ppm.

IR (thin film) 3282, 2986, 2938, 1651, 1470, 1352, 1265, 1192, 1120, 1059, 976 cm⁻¹.

HRMS (CI⁺) Calcd for C₁₁H₁₉N₂O₄ [M + H]⁺: 243.1345, Found: 243.1350.



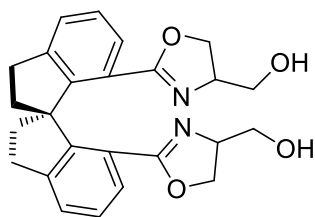
meso-**4c**

$^1\text{H NMR}$ (400 MHz, acetone- d_6) δ 4.34-4.26 (m, 2H), 4.24-4.14 (m, 4H), 3.58 (dd, $J_1 = 10.8$ Hz, $J_2 = 4.0$ Hz, 2H), 3.52 (dd, $J_1 = 11.2$ Hz, $J_2 = 4.0$ Hz, 2H), 1.48 (s, 3H), 1.42 (s, 3H) ppm.

$^{13}\text{C NMR}$ (100 MHz, acetone- d_6) δ 170.7, 70.4, 67.9, 64.3, 39.2, 24.6, 23.0 ppm.

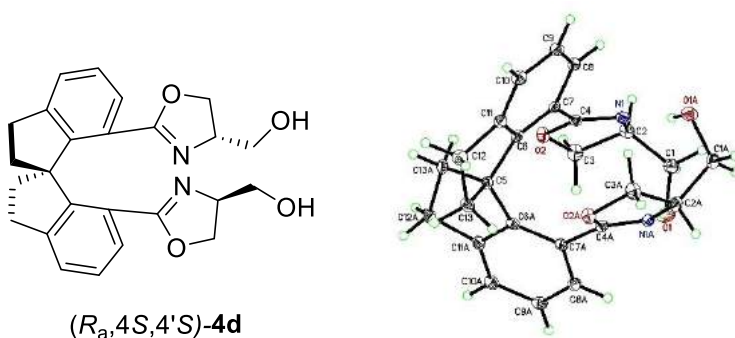
IR (thin film) 3279, 2989, 2941, 1651, 1470, 1348, 1266, 1190, 1130, 1056, 977 cm^{-1} .

HRMS (CI+) Calcd for $\text{C}_{11}\text{H}_{19}\text{N}_2\text{O}_4$ $[\text{M} + \text{H}]^+$: 243.1345, Found: 243.1350.



4d

(2,2'-((*R*)-2,2',3,3'-Tetrahydro-1,1'-spirobi[indene]-7,7'-diyl)bis(4,5-dihydrooxazole-4,2-diyl))dimethanol (**4d**) was prepared from oxetane **3d** in DCM with one equivalent of HNTf₂ at 40 °C according to the general procedure B (reaction time: 48 h, purification by flash column chromatography: DCM/MeOH = 30:1 → 20:1, 183 mg, white solid, 89% yield, 1:1 *dr*). The two diastereomers can be separated on silica gel.



(*R*_a,4*S*,4'*S*)-**4d**

(*R_a,4S,4'S*)-((2,2',3,3'-Tetrahydro-1,1'-spirobi[indene]-7,7'-diyl)bis(4,5-dihydrooxazole-2,4-diyl))dimethanol.

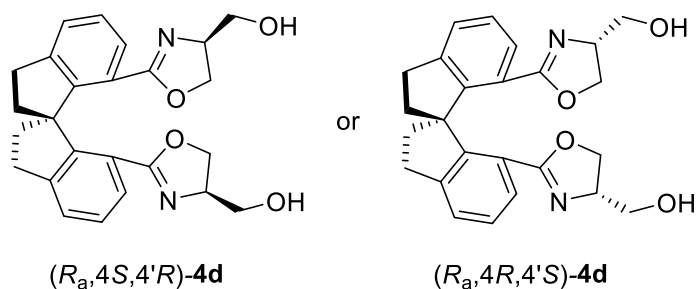
$[\alpha]_{\text{D}}^{25} = +215.0$ (*c* 1.0, CHCl₃).

¹H NMR (400 MHz, CDCl₃) δ 7.55 (d, *J* = 7.6 Hz, 2H), 7.41 (d, *J* = 7.6 Hz, 2H), 7.25 (t, *J* = 7.6 Hz, 2H), 5.83 (br s, 2H), 4.09 (d, *J* = 13.6 Hz, 2H), 4.06-3.96 (m, 4H), 3.31 (dd, *J*₁ = 12.4 Hz, *J*₂ = 2.8 Hz, 2H), 3.13-2.92 (m, 6H), 2.47-2.36 (m, 2H), 2.27 (dd, *J*₁ = 11.6 Hz, *J*₂ = 6.8 Hz, 2H) ppm.

¹³C NMR (100 MHz, CDCl₃) δ 168.7, 148.1, 144.7, 130.5, 127.7, 126.3, 122.2, 68.4, 67.1, 62.6, 60.9, 38.5, 30.4 ppm.

IR (thin film) 3221, 2931, 2851, 1641, 1447, 1353, 1271, 1113, 1062, 952 cm⁻¹.

HRMS (CI⁺) Calcd for C₂₅H₂₇N₂O₄ [M + H]⁺: 419.1971, Found: 419.1955.



(*R_a,4S,4'R*)/(*R_a,4R,4'S*)-((2,2',3,3'-tetrahydro-1,1'-spirobi[indene]-7,7'-diyl)bis(4,5-dihydrooxazole-2,4-diyl))dimethanol.^[2]

$[\alpha]_{\text{D}}^{25} = +177.6$ (*c* 1.0, CHCl₃).

¹H NMR (400 MHz, CDCl₃) δ 7.64 (d, *J* = 7.6 Hz, 1H), 7.51 (d, *J* = 7.6 Hz, 1H), 7.38 (t like, *J* = 6.8 Hz, 2H), 7.64 (td, *J*₁ = 7.6 Hz, *J*₂ = 2.0 Hz, 2H), 4.06-3.99 (m, 1H), 3.97-3.85 (m, 4H), 3.40-3.30 (m, 2H), 3.27 (dd, *J*₁ = 12.0 Hz, *J*₂ = 4.0 Hz, 1H), 3.15-2.87 (m, 6H), 2.54-2.41 (m, 2H), 2.32-2.20 (m, 2H) ppm.

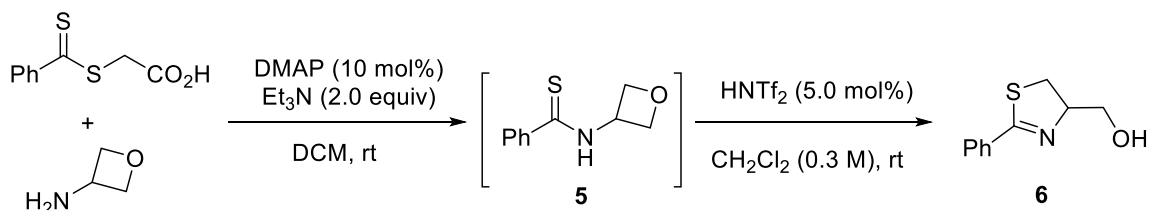
¹³C NMR (100 MHz, CDCl₃) δ 167.0, 166.0, 148.5, 148.3, 145.3, 144.6, 128.9, 128.7, 127.3, 127.2, 126.2, 126.1, 123.4, 122.7, 68.8, 68.3, 67.3, 66.9, 63.7, 62.9, 62.3, 38.3, 38.2, 30.5, 30.4 ppm.

IR (thin film) 3256, 2939, 1643, 1363, 1267, 1113, 1055, 978 cm⁻¹.

HRMS (CI⁺) Calcd for C₂₅H₂₇N₂O₄ [M + H]⁺: 419.1971, Found: 419.1973.

Notes to determination of the relative stereochemistry:

X-Ray crystallography confirmed the relative stereochemistry of one diastereomer. For the other diastereomer, similar to the case of **4b**, the absence of degeneracy in ^{13}C NMR indicated that both ($R_a,4S,4'R$) and ($R_a,4R,4'S$) are possible.



(2-Phenyl-4,5-dihydrothiazol-4-yl)methanol (6). At 0 °C, to a solution of oxetan-3-amine (0.23 mL, 3.3 mmol), DMAP (36.4 mg, 0.3 mmol), and Et₃N (0.83 mL, 6.0 mmol) in CH₂Cl₂ (10 mL) was added 2-((phenylcarbonothioyl)thio)acetic acid (636 mg, 3.0 mmol). After stirring at room temperature for 12 h, the resulting solution was washed with a saturated aqueous solution of NH₄Cl (20 mL). The layers were separated. Then the organic layer was treated with triflimide (42 mg, 5.0 mol%). After stirring for another 12 h, the reaction was quenched with an aqueous solution of NaHCO₃ (20 mL, 10%). The mixture was stirred for 10 min and then diluted with water (30 mL). The layers were separated, and the organic layer was extracted with dichloromethane (2×30 mL). The combined organic layers were washed with water and brine, dried over anhydrous Na₂SO₄, and concentrated under reduced pressure. The residue was purified by simple recrystallization (hexanes and diethyl ether) to afford the pure amide **1a** (422 mg, 73% yield, yellow solid).

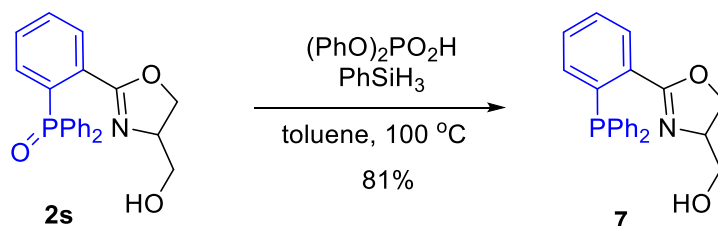
^1H NMR (400 MHz, CDCl₃) δ 7.80 (d, J = 7.2 Hz, 2H), 7.50-7.44 (m, 1H), 7.39 (t, J = 8.0 Hz, 2H), 4.84-4.73 (m, 1H), 4.03 (dd, J_1 = 11.2 Hz, J_2 = 4.8 Hz, 1H), 3.79 (dd, J_1 = 11.2 Hz, J_2 = 45.6 Hz, 1H), 3.43 (dd, J_1 = 10.8 Hz, J_2 = 0.8 Hz, 1H), 3.32 (dd, J_1 = 10.8 Hz, J_2 = 1.2 Hz, 1H), 3.09 (br s, 1H) ppm.

¹³C NMR (100 MHz, CDCl₃) δ 170.3, 132.6, 131.6, 128.5, 128.4, 79.0, 64.3, 34.3 ppm.

IR (thin film) 3351, 2935, 2869, 1600, 1488, 1444, 1317, 1260, 1054, 947 cm⁻¹.

HRMS (CI+) Calcd for C₁₀H₁₂NOS [M + H]⁺: 194.0634, Found: 194.0644.

IV. Product Derivatizations and Utility



(2-(2-(Diphenylphosphino)phenyl)-4,5-dihydrooxazol-4-yl)methanol (7). Under Ar, to an oven-dried 5-mL charged with $(\text{PhO})_2\text{PO}_2\text{H}$ (5.1 mg, 0.02 mmol) and **2s** (75.5 mg, 0.2 mmol) were added dry toluene (1 mL) and PhSiH_3 (75 μL , 0.6 mmol). The mixture was stirred at $100\text{ }^\circ\text{C}$ for overnight before it was cooled to $0\text{ }^\circ\text{C}$. Methanolic KOH (2 mL, 3N) was added slowly, and then the mixture was stirred vigorously for 3 h at room temperature. Next, water (3 mL) was added and the mixture was extracted by ethyl acetate. The organic layer was washed by an aqueous solution of HCl (1 M, 5 mL) followed by a saturated aqueous NaHCO_3 solution (5 mL). The organic layer was then dried over Na_2SO_4 and concentrated. The residue was purified by silica gel column chromatography (hexanes/EtOAc = 2:1) to give phosphine **7** as a white solid (61.0 mg, 81% yield).

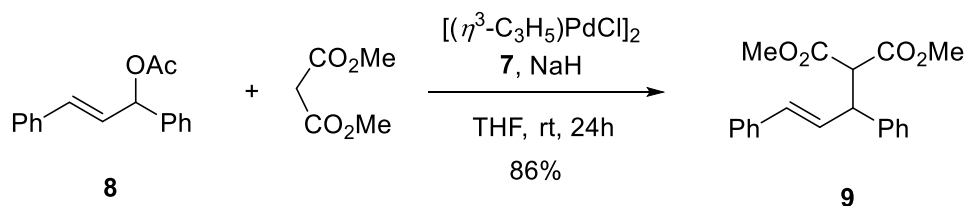
$^1\text{H NMR}$ (400 MHz, CDCl_3) δ 7.93-7.87 (m, 1H), 7.42-7.24 (m, 12H), 6.97-6.92 (m, 1H), 4.38-4.28 (m, 2H), 4.17 (t, $J = 6.4\text{ Hz}$, 1H), 3.67 (dd, $J_1 = 11.6\text{ Hz}$, $J_2 = 2.8\text{ Hz}$, 1H), 3.30 (dd, $J_1 = 11.6\text{ Hz}$, $J_2 = 3.6\text{ Hz}$, 1H), 1.82 (br s, 1H) ppm.

$^{13}\text{C NMR}$ (100 MHz, CDCl_3) δ 164.4 (d, $J = 2.0\text{ Hz}$), 138.8 (d, $J = 22.0\text{ Hz}$), 138.3 (d, $J = 7.0\text{ Hz}$), 137.4 (d, $J = 9.0\text{ Hz}$), 134.3 (d, $J = 21.0\text{ Hz}$), 133.3 (d, $J = 20.0\text{ Hz}$), 131.4 (d, $J = 20.0\text{ Hz}$), 130.7, 129.6 (d, $J = 3.0\text{ Hz}$), 128.7 (d, $J = 12.6\text{ Hz}$), 128.5 (d, $J = 7.4\text{ Hz}$), 128.3, 68.8, 68.4, 64.0 ppm.

$^{31}\text{P NMR}$ (162 MHz, CDCl_3) δ -6.59 ppm.

IR (thin film) 3350, 3056, 2928, 1648, 1472, 1433, 1354, 1263, 1099, 1040 cm^{-1} .

HRMS (CI+) Calcd for $\text{C}_{22}\text{H}_{21}\text{NO}_2\text{P}$ $[\text{M} + \text{H}]^+$: 362.1310, Found: 362.1310.



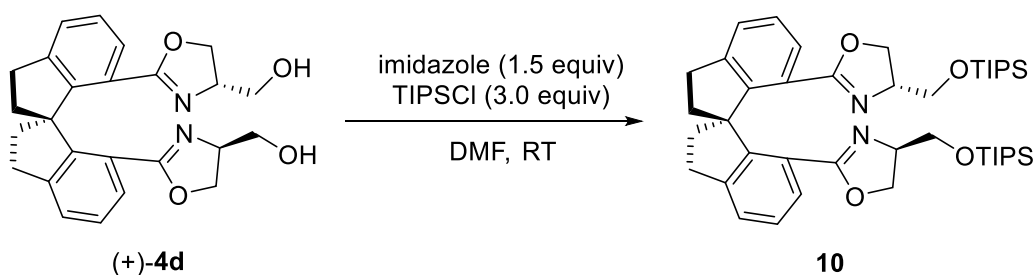
(E)-Dimethyl 2-(1,3-diphenylallyl)malonate (9). This procedure was based on literature.^[2] Ligand **7** (3.7 mg, 0.01 mmol), $[(\eta^3\text{-C}_3\text{H}_5)\text{-PdCl}]_2$ (1.9 mg, 0.005 mmol), and (*E*)-1,3-diphenylallyl acetate **8** (51.0 mg, 0.20 mmol) were dissolved in THF (1 mL), and stirred for 1 h at room temperature. In a separate flask, dimethyl malonate (55 μL , 0.48 mmol) was added dropwise to a suspension of NaH (19.0 mg, 0.48 mmol, 60% in mineral oil) in THF (2 mL). This suspension was cooled to 0 $^\circ\text{C}$, and the above-prepared solution of electrophile was added slowly. The mixture was stirred at room temperature for 24 h and filtered through a pad of silica, which was washed with EtOAc. The filtrate was concentrated and then purified by flash chromatography on silica gel (hexanes/EtOAc = 20:1 to 15:1) to give product **9** as a colorless oil (55.9 mg, 86% yield).

$^1\text{H NMR}$ (400 MHz, CDCl_3) δ 7.35-7.18 (m, 10H), 7.49 (d, $J = 15.6$ Hz, 1H), 6.34 (dd, $J_1 = 16.0$ Hz, $J_2 = 8.8$ Hz, 1H), 4.28 (dd, $J_1 = 10.8$ Hz, $J_2 = 8.4$ Hz, 1H), 3.97 (d, $J = 10.8$ Hz, 1H), 3.71 (s, 3H), 3.53 (s, 3H) ppm.

$^{13}\text{C NMR}$ (100 MHz, CDCl_3) δ 168.2, 167.7, 140.1, 136.8, 131.8, 129.1, 128.7, 128.4, 127.8, 127.5, 127.1, 126.4, 57.6, 52.6, 52.4, 29.2 ppm.

This product is a known compound. The characterization data match the literature.^[2]

[2]. H. Aït-Haddou, O. Hoarau, D. Cramailÿe, F. Pezet, J. C. Daran and G. G. A. Balavoine, *Chem. Eur. J.* **2004**, *10*, 699–707.



(R)-7,7'-Bis((S)-4-(((triisopropylsilyl)oxy)methyl)-4,5-dihydro

oxazol-2-yl)-2,2',3,3'-tetrahydro-1,1'-spirobi[indene] (10). To a solution of **4d** (70.5 mg, 0.17 mmol, 1.0 equiv) in DMF (2.0 mL) were sequentially added imidazole (47.3 mg, 0.68 mmol, 4.0 equiv) and TIPSCl (150 μ L, 0.68 mmol, 4.0 equiv). The reaction mixture was stirred at room temperature overnight. Then, water (5 mL) and Et₂O (10 mL) were added. The layers were separated and the aqueous layer was extracted with Et₂O (2 \times 10 mL). The combined organic layers were washed with brine, dried over Na₂SO₄, and concentrated under reduced pressure. The residue was purified by flash column chromatography (5% ether in hexanes) to give the desired **10** (87.0 mg, 70% yield).

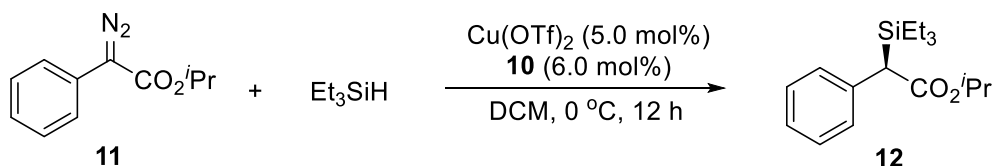
$[\alpha]_{\text{D}}^{25} = +77.3$ (*c* 1.0, CHCl₃).

¹H NMR (400MHz, CDCl₃) δ 7.51 (d, *J* = 6.8 Hz, 2H), 7.32 (d, *J* = 7.6 Hz, 2H), 7.16-7.10 (m, 2H), 4.02-3.92 (m, 2H), 3.81 (dd, *J*₁ = 9.6 Hz, *J*₂ = 4.0 Hz, 2H), 3.77-3.66 (m, 2H), 3.36-3.20 (m, 4H), 3.12-2.92 (m, 4H), 2.65 (dd, *J*₁ = 20.4 Hz, *J*₂ = 10.8 Hz, 2H), 2.24 (dd, *J*₁ = 11.6 Hz, *J*₂ = 7.2 Hz, 2H), 1.07-0.95 (m, 42H).

¹³C NMR (101MHz, CDCl₃) δ 164.4, 149.0, 145.3, 127.9, 126.5, 126.4, 125.8, 70.9, 68.3, 66.0, 63.0, 38.6, 30.7, 17.9, 11.9 ppm.

IR (thin film) 2937, 2863, 1649, 1461, 1355, 1284, 1250, 1102, 985 cm⁻¹.

HRMS (CI+) Calcd for C₄₃H₆₆N₂O₄Si₂ [M]⁺: 730.4561, Found: 730.4573.



Isopropyl (*R*)-2-phenyl-2-(triethylsilyl)acetate (12). This procedure was based on literature.^[3] Under N₂, Cu(OTf)₂ (1.8 mg, 5.0 μmol) and **10** (4.4 mg, 6.0 μmol) were dissolved in CH₂Cl₂ (1.5 mL) in a 2-dram vial. The mixture was stirred at 0 °C for 10 min. Next, a solution of 2-diazo-2-phenyl acetates **11** (20.5 mg, 0.1 mmol) and triethylsilane (64 μL, 0.4 mmol) in CH₂Cl₂ (0.5 mL) was injected into the reaction mixture. The reaction mixture was stirred at 40 °C for 12 h and then cooled to room temperature and concentrated under reduced pressure. The residue was purified by flash chromatography on silica gel (hexanes/ether = 50:1) to afford the pure product **12** (24.2 mg, 83% yield, 84:16 er, colorless oil).

$[\alpha]_{\text{D}}^{25} = +8.8$ (*c* 1.0, CHCl₃).

HPLC analysis of the product: Daicel CHIRALPAK OD-H column; 0.05% *i*-PrOH in hexanes; 1.0 mL/min; retention times: 7.0 min (major), 20.0 min (minor).

¹H NMR (400 MHz, CDCl₃) δ 7.38-7.33 (m, 2H), 7.30-7.24 (m, 2H), 7.16 (t like, *J* = 7.2 Hz, 1H), 5.07-4.96 (m, 1H), 3.48 (s, 1H), 1.27 (d, *J* = 6.0 Hz, 3H), 1.23 (d, *J* = 6.4 Hz, 3H), 0.91 (t, *J* = 8.0 Hz, 9H), 0.67-0.52 (m, 6H).

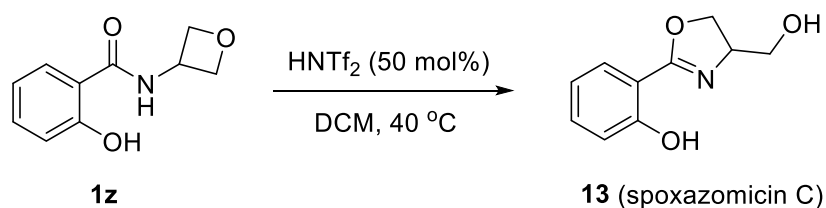
¹³C NMR (100 MHz, CDCl₃) δ 172.7, 136.8, 128.5, 128.0, 125.4, 67.6, 43.0, 22.1, 21.9, 7.1, 2.7 ppm.

IR (thin film) 2955, 2807, 1711, 1265, 1152, 1105 cm⁻¹.

HRMS (CI⁺) Calcd for C₁₇H₂₈O₂Si [M]⁺: 292.1859, Found: 292.1859.

[3]. Y.-Z. Zhang, S.-F. Zhu, L.-X. Wang and Q.-L. Zhou, *Angew. Chem. Int. Ed.* **2008**, *47*, 8496–8498.

V. Synthesis of Diverse Natural Products.



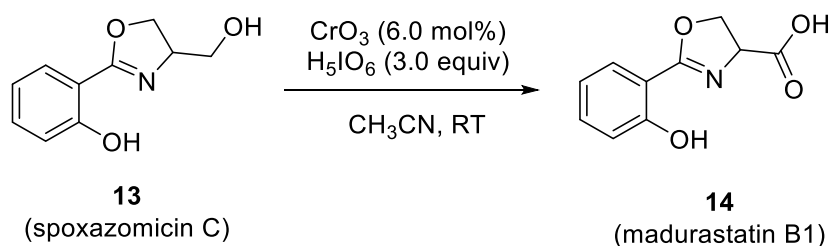
Spoxazomicin C (13). To a solution of oxetane **1z** (1.93 g, 10.0 mmol) in dichloromethane (50 mL) was added triflimide (1.47 g, 50 mol%). After stirring at 40 °C for 48 h, the reaction was quenched with an aqueous solution of NaHCO₃ (30 mL, 10%) followed by stirring for 10 min. The mixture was then diluted with water (50 mL). The layers were separated and the organic layer was extracted with dichloromethane (2×50 mL). The combined organic layers were washed with water and brine, dried over anhydrous Na₂SO₄, and concentrated under reduced pressure. The residue was purified by simple recrystallization (hexanes and diethyl ether) to afford the pure amide **1a** (1.63 g, 85% yield, white solid).

¹H NMR (400 MHz, CDCl₃) δ 7.65 (dd, *J*₁ = 8.0 Hz, *J*₂ = 4.0 Hz, 1H), 7.40-7.34 (m, 1H), 7.00 (dd, *J*₁ = 12.0 Hz, *J*₂ = 4.0 Hz, 1H), 6.87 (t, *J* = 8.0 Hz, 1H), 4.52-4.43 (m, 2H), 4.38-4.29 (m, 1H), 3.91-3.82 (m, 1H), 3.73-3.64 (m, 1H) ppm.

¹³C NMR (100 MHz, CDCl₃) δ 166.8, 159.7, 133.6, 128.2, 118.8, 116.7, 110.4, 68.5, 66.8, 63.9 ppm.

IR (thin film) 3409, 2935, 1638, 1490, 1367, 1259, 1063, 958 cm⁻¹.

HRMS (CI⁺) Calcd for C₁₀H₁₁NO₃ [M]⁺: 193.0739, Found: 193.0748.



Madurastatin B1 (14). At room temperature, to a solution of alcohol **13** (96.3 mg, 0.5 mmol) in CH₃CN (2 mL) was added a solution of H₅IO₆ (351.6 mg, 1.5 mmol) and CrO₃ (3.3 mg, 0.03 mmol) in CH₃CN (4.0 mL) over a period of 15 min, and the mixture was allowed to stir for 30 min. It was diluted with water (2 mL) and extracted with ethyl acetate (3 × 5 mL). The combined organic layers were washed with brine, dried over MgSO₄, and concentrated to give pure product **14** (72.6 mg, 75% yield, yellow solid).

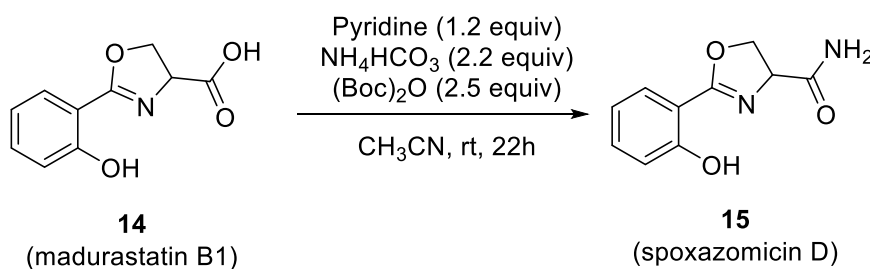
This product is a known compound. The characterization data match the literature.^[4]

¹H NMR (400 MHz, MeOD-*d*₄) δ 7.67 (d, *J* = 7.6 Hz, 1H), 7.40 (t, *J* = 7.6 Hz, 1H), 6.95 (d, *J* = 8.0 Hz, 1H), 6.88 (d, *J* = 7.6 Hz, 1H), 5.02-4.85 (1H, covered with H₂O peak), 4.64 (d, *J* = 4.4 Hz, 2H) ppm.

¹³C NMR (100 MHz, MeOD-*d*₄) δ 173.8, 168.8, 161.1, 135.2, 129.5, 120.0, 117.7, 111.2, 70.7, 68.1 ppm.

IR (thin film) 2955, 1729, 1632, 1487, 1446, 1369, 1258, 1084 cm⁻¹.

HRMS (CI⁺) Calcd for C₁₀H₉NO₄ [M]⁺: 207.0532, Found: 207.0533.



Sproxazomicin D (15). At room temperature, to a solution of acid **14** (31.7 mg, 0.15 mmol), NH₄HCO₃ (26.3 mg, 0.33 mmol) and (Boc)₂O (81.8 mg, 0.375 mmol) in

[4] K. A. Shaaban, M. A. Saunders, Y. Zhang, T. Tran, S. I. Elshahawi, L. V. Ponomareva, X. Wang, J. Zhang, G. C. Copley, M. Sunkara, M. K. Kharel, A. J. Morris, J. C. Hower, M. S. Tremblay, M. A. Prendergast and J. S. Thorson, *J. Nat. Prod.* **2017**, *80*, 2–11.

CH₃CN (1 mL) was added pyridine (14.5 μ L, 0.18 mmol). The mixture was allowed to stir at room temperature for 22 h before it was diluted with water (2 mL). The mixture was extracted with ethyl acetate (3 \times 5 mL). The combined organic layers were washed with brine, dried over MgSO₄, and concentrated. The residue was purified by flash column chromatography (hexanes and ethyl acetate) to afford the amide **15** (25.6 mg, 83% yield, white solid).

This product is a known compound. The characterization data match the literature.^[5]

¹H NMR (400 MHz, CDCl₃) δ 11.46 (br s, 1H), 7.68 (dd, $J_1 = 8.0$ Hz, $J_2 = 1.6$ Hz, 1H), 7.43 (td, $J_1 = 8.4$ Hz, $J_2 = 1.6$ Hz, 1H), 7.02 (d, $J_1 = 8.4$ Hz, 1H), 6.91 (t, $J = 7.6$ Hz, 1H), 6.48 (br s, 1H), 6.03 (br s, 1H), 4.94 (dd, $J_1 = 10.4$ Hz, $J_2 = 8.4$ Hz, 1H), 4.68 (dd, $J_1 = 10.0$ Hz, $J_2 = 8.8$ Hz, 2H), ppm.

¹³C NMR (100 MHz, CDCl₃) δ 173.2, 168.0, 159.7, 134.4, 128.6, 119.2, 116.9, 109.8, 69.6, 67.6 ppm.

IR (thin film) 3323, 3183, 1674, 1637, 1488, 1366, 1254, 1156, 1074, 958 cm⁻¹.

HRMS (CI+) Calcd for C₁₀H₁₁N₂O₃ [M + H]⁺: 207.0764, Found: 207.0778.

[5] K. M. Nelson, C. E. Salomon and C. C. Aldrich, *J. Nat. Prod.* **2012**, *75*, 1037–1043.

VI. Product Structure Determination

The structure and stereochemistry of products **2s** and **4d** were determined by X-ray diffraction. The X-ray data of **2s** (CCDC 1908430) and **4d** (CCDC 1908431) have been deposited at the Cambridge Crystallographic Data Center.

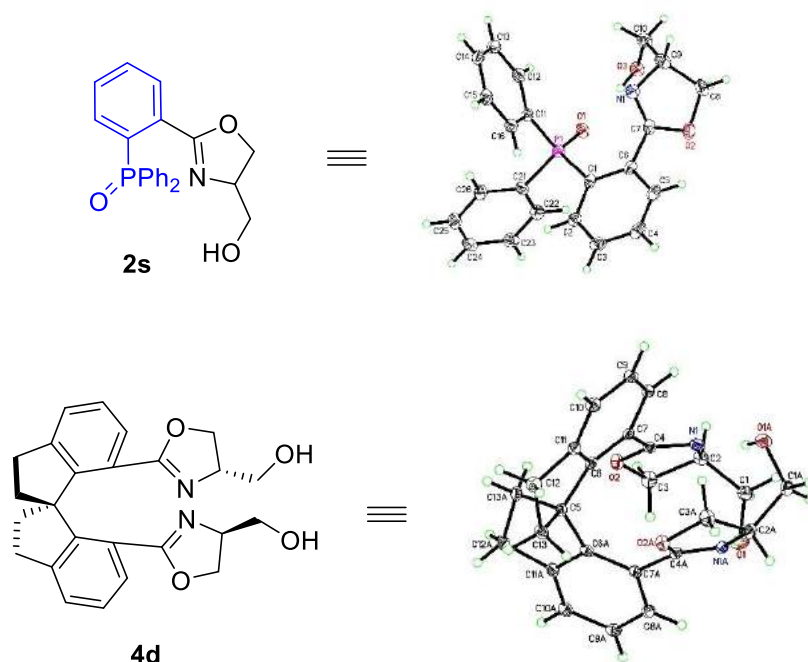


Table S1. Crystal data and structure refinement for 2s.

Identification code	2s
Empirical formula	C ₂₂ H ₂₀ NO ₃ P
Formula weight	377.36
Temperature/K	100.01(10)
Crystal system	monoclinic
Space group	P2 ₁
a/Å	9.5956(3)
b/Å	9.7344(4)
c/Å	10.4231(4)
α/°	90
β/°	93.158(3)
γ/°	90
Volume/Å ³	972.12(6)
Z	2

$\rho_{\text{calc}}/\text{cm}^3$	1.289
μ/mm^{-1}	1.431
F(000)	396.0
Crystal size/ mm^3	$0.2 \times 0.03 \times 0.02$
Radiation	CuK α ($\lambda = 1.54184$)
2 Θ range for data collection/ $^\circ$	8.496 to 134.976
Index ranges	$-11 \leq h \leq 11, -9 \leq k \leq 11, -12 \leq l \leq 12$
Reflections collected	5136
Independent reflections	2411 [$R_{\text{int}} = 0.0327, R_{\text{sigma}} = 0.0434$]
Data/restraints/parameters	2411/1/245
Completeness to $\theta = 66.5^\circ$	99.1%
Goodness-of-fit on F^2	1.002
Final R indexes [$I \geq 2\sigma(I)$]	$R_1 = 0.0327, wR_2 = 0.0757$
Final R indexes [all data]	$R_1 = 0.0366, wR_2 = 0.0770$
Largest diff. peak/hole / $e \text{ \AA}^{-3}$	0.34/-0.19
Flack parameter	0.01(3)

Table S2. Fractional Atomic Coordinates ($\times 10^4$) and Equivalent Isotropic Displacement Parameters ($\text{\AA}^2 \times 10^3$) for 2s. U_{eq} is defined as 1/3 of the trace of the orthogonalised U_{H} tensor.

Atom	x	y	z	$U(\text{eq})$
P1	2647.5 (6)	3212.1 (7)	3460.4 (6)	19.29 (16)
O1	2186 (2)	1857 (2)	2933 (2)	24.9 (5)
O2	5752 (2)	617 (2)	1995 (2)	30.5 (5)
O3	2331 (2)	163 (2)	917 (2)	26.3 (5)
N1	4471 (2)	2329 (3)	1050 (2)	24.1 (5)
C1	4495 (3)	3320 (3)	3934 (2)	20.8 (5)
C2	4925 (3)	4041 (3)	5039 (3)	25.0 (6)
C3	6325 (3)	4140 (3)	5443 (3)	29.9 (7)
C4	7320 (3)	3476 (4)	4747 (3)	32.8 (8)
C5	6915 (3)	2735 (3)	3659 (3)	28.3 (7)
C6	5507 (3)	2658 (3)	3227 (3)	21.4 (6)
C7	5180 (3)	1892 (3)	2021 (3)	21.5 (6)
C8	5370 (3)	83 (4)	715 (3)	31.1 (7)
C9	4426 (3)	1203 (4)	101 (3)	28.8 (7)
C10	2918 (3)	738 (4)	-180 (3)	30.4 (7)
C11	2269 (3)	4632 (3)	2382 (3)	21.9 (6)

C12	1263 (3)	4435 (3)	1374 (3)	26.1 (6)
C13	922 (3)	5520 (4)	548 (3)	32.3 (7)
C14	1572 (3)	6779 (4)	706 (3)	30.1 (7)
C15	2563 (3)	6975 (4)	1722 (3)	27.7 (6)
C16	2916 (3)	5905 (3)	2542 (3)	23.8 (6)
C21	1747 (3)	3561 (3)	4913 (3)	23.2 (7)
C22	1603 (3)	2459 (4)	5747 (3)	28.3 (7)
C23	875 (3)	2622 (4)	6855 (3)	30.7 (7)
C24	310 (3)	3901 (4)	7127 (3)	27.6 (7)
C25	460 (3)	4988 (4)	6307 (3)	28.1 (7)
C26	1176 (3)	4825 (3)	5187 (3)	25.0 (6)

Table S3. Anisotropic Displacement Parameters ($\text{\AA}^2 \times 10^3$) for 2s. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^*U_{11}+2hka^*b^*U_{12}+\dots]$.

Atom	U ₁₁	U ₂₂	U ₃₃	U ₂₃	U ₁₃	U ₁₂
P1	14.9 (3)	21.0 (3)	22.2 (3)	-1.3 (3)	2.6 (2)	-0.6 (3)
O1	19.2 (9)	27.8 (11)	28.2 (11)	-3.6 (9)	6.0 (8)	-2.7 (8)
O2	27.4 (11)	26.0 (12)	38.0 (12)	-4.6 (10)	0.2 (9)	7.4 (9)
O3	23.0 (9)	27.8 (12)	28.5 (11)	-3.7 (9)	3.7 (8)	-3.1 (8)
N1	20.7 (11)	26.5 (14)	25.4 (12)	1.7 (10)	4.3 (9)	-2.1 (9)
C1	20.4 (12)	16.8 (13)	25.2 (12)	4.3 (13)	1.4 (10)	1.8 (12)
C2	24.9 (14)	22.1 (16)	27.7 (14)	1.9 (13)	-0.3 (11)	2.2 (12)
C3	29.8 (15)	29.6 (17)	29.2 (15)	-0.9 (13)	-7.9 (12)	-4.6 (13)
C4	19.8 (13)	36 (2)	41.3 (17)	2.7 (14)	-8.5 (12)	-0.3 (12)
C5	17.1 (13)	30.0 (17)	37.4 (17)	3.4 (13)	-1.2 (12)	1.7 (12)
C6	18.5 (12)	18.5 (13)	27.1 (15)	4.7 (12)	1.0 (11)	-1.3 (11)
C7	14.7 (12)	21.3 (15)	29.3 (14)	2.7 (12)	7.2 (10)	-0.6 (11)
C8	25.2 (14)	33.0 (18)	36.0 (16)	-9.9 (14)	9.7 (12)	-0.4 (13)
C9	28.4 (15)	34.2 (18)	24.4 (14)	-2.0 (14)	7.4 (12)	-7.4 (13)
C10	28.8 (15)	36.3 (19)	25.7 (14)	-5.5 (13)	-0.8 (12)	-4.2 (14)
C11	17.2 (12)	26.0 (15)	22.8 (13)	0.8 (12)	3.2 (10)	4.3 (11)
C12	17.9 (13)	30.6 (17)	29.8 (15)	-6.4 (13)	1.7 (11)	-0.4 (11)
C13	22.7 (14)	47 (2)	26.5 (15)	-6.4 (14)	-0.9 (11)	10.7 (14)
C14	27.8 (14)	37.3 (19)	25.5 (14)	4.9 (14)	4.9 (12)	13.3 (14)
C15	22.9 (13)	29.0 (17)	31.9 (16)	2.6 (14)	8.7 (12)	2.7 (13)
C16	17.6 (12)	28.5 (17)	25.4 (14)	-2.5 (12)	2.9 (11)	-0.4 (11)
C21	15.2 (11)	32.2 (19)	22.3 (13)	-6.0 (11)	3.2 (10)	-1.5 (10)
C22	27.3 (14)	28.6 (17)	29.1 (16)	-0.3 (13)	2.2 (12)	1.6 (12)
C23	29.5 (15)	37.7 (18)	25.0 (16)	2.0 (14)	2.2 (12)	-2.5 (14)

C24	18.3 (13)	39.9 (19)	24.8 (14)	-8.6 (14)	3.9 (11)	-6.2 (13)
C25	14.8 (12)	33.4 (17)	36.3 (16)	-7.4 (14)	3.6 (11)	1.5 (12)
C26	18.0 (12)	25.2 (15)	32.1 (15)	-1.2 (13)	3.4 (11)	-1.6 (11)

Table S4. Bond Lengths for 2s.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
P1	O1	1.487 (2)	C6	C7	1.481 (4)
P1	C1	1.817 (3)	C8	C9	1.535 (5)
P1	C11	1.806 (3)	C9	C10	1.529 (4)
P1	C21	1.816 (3)	C11	C12	1.400 (4)
O2	C7	1.358 (4)	C11	C16	1.392 (4)
O2	C8	1.460 (4)	C12	C13	1.390 (5)
O3	C10	1.418 (4)	C13	C14	1.382 (5)
N1	C7	1.261 (4)	C14	C15	1.396 (5)
N1	C9	1.475 (4)	C15	C16	1.378 (5)
C1	C2	1.392 (4)	C21	C22	1.392 (5)
C1	C6	1.406 (4)	C21	C26	1.383 (4)
C2	C3	1.389 (4)	C22	C23	1.391 (5)
C3	C4	1.390 (5)	C23	C24	1.393 (5)
C4	C5	1.382 (5)	C24	C25	1.373 (5)
C5	C6	1.402 (4)	C25	C26	1.396 (4)

Table S5. Bond Angles for 2s.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
O1	P1	C1	114.69 (13)	O2	C8	C9	103.9 (2)
O1	P1	C11	113.78 (13)	N1	C9	C8	104.7 (2)
O1	P1	C21	109.17 (13)	N1	C9	C10	109.9 (2)
C11	P1	C1	106.54 (13)	C10	C9	C8	113.6 (3)
C11	P1	C21	106.70 (13)	O3	C10	C9	112.1 (2)
C21	P1	C1	105.36 (12)	C12	C11	P1	118.0 (2)
C7	O2	C8	105.2 (2)	C16	C11	P1	122.2 (2)
C7	N1	C9	106.4 (3)	C16	C11	C12	119.8 (3)
C2	C1	P1	119.6 (2)	C13	C12	C11	119.3 (3)
C2	C1	C6	118.9 (2)	C14	C13	C12	120.7 (3)
C6	C1	P1	121.5 (2)	C13	C14	C15	119.7 (3)
C3	C2	C1	121.6 (3)	C16	C15	C14	120.1 (3)
C2	C3	C4	119.4 (3)	C15	C16	C11	120.4 (3)

C5	C4	C3	120.0(3)	C22	C21	P1	116.4(2)
C4	C5	C6	120.9(3)	C26	C21	P1	123.4(2)
C1	C6	C7	123.7(2)	C26	C21	C22	120.1(3)
C5	C6	C1	119.2(3)	C23	C22	C21	120.2(3)
C5	C6	C7	117.0(3)	C22	C23	C24	119.3(3)
O2	C7	C6	114.2(2)	C25	C24	C23	120.4(3)
N1	C7	O2	119.6(3)	C24	C25	C26	120.4(3)
N1	C7	C6	126.2(3)	C21	C26	C25	119.6(3)

Table S6. Hydrogen Bonds for 2s.

D	H	A	d(D-H)/Å	d(H-A)/Å	d(D-A)/Å	D-H-A/°
O3	H3	O1	0.84	1.85	2.681(3)	170.6

Table S7. Torsion Angles for 2s.

A	B	C	D	Angle/°	A	B	C	D	Angle/°
P1	C1	C2	C3	179.4(2)	C5	C6	C7	N1	-127.5(3)
P1	C1	C6	C5	-177.9(2)	C6	C1	C2	C3	1.2(5)
P1	C1	C6	C7	3.4(4)	C7	O2	C8	C9	-4.1(3)
P1	C11	C12	C13	178.3(2)	C7	N1	C9	C8	-4.6(3)
P1	C11	C16	C15	-177.8(2)	C7	N1	C9	C10	117.8(3)
P1	C21	C22	C23	-177.3(2)	C8	O2	C7	N1	1.4(3)
P1	C21	C26	C25	177.8(2)	C8	O2	C7	C6	-177.0(2)
O1	P1	C1	C2	-141.2(2)	C8	C9	C10	O3	52.6(4)
O1	P1	C1	C6	37.0(3)	C9	N1	C7	O2	2.2(3)
O1	P1	C11	C12	18.4(3)	C9	N1	C7	C6	-179.7(3)
O1	P1	C11	C16	-163.1(2)	C11	P1	C1	C2	92.0(3)
O1	P1	C21	C22	41.2(2)	C11	P1	C1	C6	-89.8(3)
O1	P1	C21	C26	-136.4(2)	C11	P1	C21	C22	164.6(2)
O2	C8	C9	N1	5.2(3)	C11	P1	C21	C26	-13.1(3)
O2	C8	C9	C10	-114.7(3)	C11	C12	C13	C14	0.6(5)
N1	C9	C10	O3	-64.3(3)	C12	C11	C16	C15	0.7(4)
C1	P1	C11	C12	145.8(2)	C12	C13	C14	C15	-1.3(5)
C1	P1	C11	C16	-35.7(3)	C13	C14	C15	C16	1.7(5)
C1	P1	C21	C22	-82.4(2)	C14	C15	C16	C11	-1.4(4)
C1	P1	C21	C26	99.9(2)	C16	C11	C12	C13	-0.3(4)
C1	C2	C3	C4	-1.6(5)	C21	P1	C1	C2	-21.1(3)
C1	C6	C7	O2	-130.5(3)	C21	P1	C1	C6	157.1(2)

C1 C6 C7 N1	51.2 (4)	C21 P1 C11 C12	-102.1 (2)
C2 C1 C6 C5	0.4 (4)	C21 P1 C11 C16	76.4 (3)
C2 C1 C6 C7	-178.4 (3)	C21 C22 C23 C24	-0.8 (5)
C2 C3 C4 C5	0.5 (5)	C22 C21 C26 C25	0.3 (4)
C3 C4 C5 C6	1.0 (5)	C22 C23 C24 C25	0.5 (5)
C4 C5 C6 C1	-1.4 (5)	C23 C24 C25 C26	0.3 (4)
C4 C5 C6 C7	177.4 (3)	C24 C25 C26 C21	-0.6 (4)
C5 C6 C7 O2	50.7 (4)	C26 C21 C22 C23	0.5 (4)

Table S8. Hydrogen Atom Coordinates ($\text{\AA}\times 10^4$) and Isotropic Displacement Parameters ($\text{\AA}^2\times 10^3$) for 2s.

Atom	x	y	z	U(eq)
H3	2359	744	1514	40
H2	4245	4476	5528	30
H3A	6600	4656	6187	36
H4	8280	3531	5020	39
H5	7599	2272	3196	34
H8A	4862	-799	768	37
H8B	6208	-58	218	37
H9	4825	1529	-711	35
H10A	2349	1535	-481	36
H10B	2891	47	-878	36
H12	819	3569	1255	31
H13	233	5393	-133	39
H14	1346	7509	126	36
H15	2993	7848	1847	33
H16	3606	6037	3220	29
H22	2003	1594	5560	34
H23	765	1869	7421	37
H24	-183	4021	7885	33
H25	74	5857	6503	34
H26	1270	5576	4617	30

Table S9. Crystal data and structure refinement for 4d.

Identification code	4d
Empirical formula	$\text{C}_{25}\text{H}_{26}\text{N}_2\text{O}_4$
Formula weight	418.48

Temperature/K	100.00(10)
Crystal system	monoclinic
Space group	C2
a/Å	12.1435(3)
b/Å	10.3089(2)
c/Å	8.5206(2)
α /°	90
β /°	106.293(3)
γ /°	90
Volume/Å ³	1023.82(5)
Z	2
ρ_{calc} /cm ³	1.357
μ /mm ⁻¹	0.747
F(000)	444.0
Crystal size/mm ³	0.2 × 0.2 × 0.18
Radiation	CuK α (λ = 1.54184)
2 Θ range for data collection/°	11.46 to 134.992
Index ranges	-9 ≤ h ≤ 14, -12 ≤ k ≤ 7, -9 ≤ l ≤ 10
Reflections collected	1521
Independent reflections	1226 [R_{int} = 0.0055, R_{sigma} = 0.0103]
Data/restraints/parameters	1226/1/142
Goodness-of-fit on F ²	1.026
Final R indexes [$I \geq 2\sigma(I)$]	R_1 = 0.0230, wR_2 = 0.0610
Final R indexes [all data]	R_1 = 0.0233, wR_2 = 0.0612
Largest diff. peak/hole / e Å ⁻³	0.15/-0.15
Flack parameter	0.11(7)

Table S10. Fractional Atomic Coordinates ($\times 10^4$) and Equivalent Isotropic Displacement Parameters ($\text{\AA}^2 \times 10^3$) for 4d. U_{eq} is defined as 1/3 of the trace of the orthogonalised U_{ij} tensor.

Atom	x	y	z	U(eq)
O1	4171.3 (10)	-1283.0 (14)	2385.4 (14)	23.8 (3)
O2	6252.3 (10)	1689.4 (12)	3399.9 (13)	18.0 (3)
N1	6294.0 (11)	-158.0 (15)	4838.4 (16)	15.0 (3)
C1	5323.6 (14)	-1663.7 (19)	2600 (2)	21.1 (4)
C2	6196.5 (15)	-586.0 (19)	3145 (2)	18.1 (4)
C3	5928.0 (16)	671 (2)	2162 (2)	21.0 (4)
C4	6332.5 (13)	1073.4 (18)	4834.9 (19)	13.2 (4)
C5	5000	3754 (3)	5000	14.3 (5)
C6	5866.0 (14)	3025.8 (17)	6354.3 (19)	13.8 (4)

C7	6483.8 (13)	1891.5 (17)	6311.4 (19)	13.7 (4)
C8	7271.1 (14)	1456.8 (17)	7752 (2)	15.5 (4)
C9	7457.7 (14)	2150.4 (18)	9193 (2)	17.4 (4)
C10	6845.0 (14)	3281.8 (18)	9242 (2)	18.3 (4)
C11	6043.6 (13)	3703.9 (18)	7831 (2)	16.6 (4)
C12	5298.5 (15)	4892.8 (19)	7607 (2)	20.7 (4)
C13	4374.1 (14)	4614.3 (18)	5984.7 (19)	17.6 (4)

Table S11. Anisotropic Displacement Parameters ($\text{\AA}^2 \times 10^3$) for 4d. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^*2U_{11}+2hka^*b^*U_{12}+\dots]$.

Atom	U ₁₁	U ₂₂	U ₃₃	U ₂₃	U ₁₃	U ₁₂
O1	19.5 (6)	30.4 (8)	20.1 (6)	-9.8 (6)	3.0 (5)	-0.7 (6)
O2	24.8 (7)	16.2 (7)	13.2 (5)	0.4 (5)	5.9 (5)	-0.8 (5)
N1	14.0 (7)	15.1 (7)	15.2 (7)	-1.2 (5)	2.8 (5)	1.8 (6)
C1	21.2 (8)	18.6 (9)	22.5 (8)	-5.8 (8)	4.2 (7)	2.3 (7)
C2	18.8 (8)	20 (1)	16.2 (7)	-3.5 (7)	6.2 (6)	3.2 (7)
C3	27.3 (9)	22.3 (10)	14.2 (8)	-2.5 (7)	7.2 (7)	-1.3 (8)
C4	11.1 (8)	14.8 (9)	13.9 (8)	1.9 (7)	4.0 (6)	0.9 (6)
C5	15.5 (10)	11.7 (12)	14.9 (10)	0	3.0 (9)	0
C6	13.7 (7)	14.4 (9)	13.0 (7)	0.3 (6)	3.2 (6)	-4.1 (6)
C7	12.7 (7)	13.7 (9)	14.9 (7)	0.9 (7)	4.2 (6)	-3.3 (7)
C8	14.7 (7)	14.9 (9)	17.1 (7)	2.4 (6)	4.8 (6)	-0.3 (6)
C9	16.7 (8)	20.3 (9)	13.5 (7)	4.2 (6)	1.2 (6)	-1.5 (7)
C10	19.9 (8)	20.7 (10)	13.2 (7)	-1.8 (7)	2.8 (7)	-2.2 (7)
C11	16.0 (8)	16.0 (9)	17.8 (8)	-1.1 (7)	4.5 (6)	-2.0 (7)
C12	23.6 (8)	18.6 (10)	16.9 (8)	-6.3 (7)	0.7 (7)	1.3 (7)
C13	19.8 (8)	14.2 (9)	16.7 (8)	-2.3 (7)	1.8 (7)	3.1 (7)

Table S12. Bond Lengths for 4d.

Atom Atom	Length/\AA	Atom Atom	Length/\AA
O1 C1	1.415 (2)	C5 C13	1.558 (2)
O2 C3	1.462 (2)	C5 C13 ¹	1.558 (2)
O2 C4	1.357 (2)	C6 C7	1.395 (3)
N1 C2	1.482 (2)	C6 C11	1.402 (2)
N1 C4	1.270 (2)	C7 C8	1.401 (2)
C1 C2	1.516 (3)	C8 C9	1.384 (2)
C2 C3	1.527 (3)	C9 C10	1.390 (3)

C4	C7	1.483 (2)	C10	C11	1.388 (2)
C5	C6 ¹	1.523 (2)	C11	C12	1.503 (3)
C5	C6	1.523 (2)	C12	C13	1.543 (2)

¹1-X,+Y,1-Z

Table S13. Bond Angles for 4d.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
C4	O2	C3	104.51 (13)	C13	C5	C13 ¹	110.6 (2)
C4	N1	C2	106.75 (15)	C7	C6	C5	130.93 (15)
O1	C1	C2	114.69 (15)	C7	C6	C11	119.53 (15)
N1	C2	C1	111.98 (14)	C11	C6	C5	109.50 (15)
N1	C2	C3	103.16 (14)	C6	C7	C4	124.02 (15)
C1	C2	C3	115.50 (15)	C6	C7	C8	119.00 (15)
O2	C3	C2	103.95 (12)	C8	C7	C4	116.95 (15)
O2	C4	C7	117.32 (15)	C9	C8	C7	120.92 (15)
N1	C4	O2	118.45 (15)	C8	C9	C10	120.28 (15)
N1	C4	C7	124.22 (15)	C11	C10	C9	119.23 (15)
C6 ¹	C5	C6	121.0 (2)	C6	C11	C12	110.92 (14)
C6 ¹	C5	C13	110.56 (8)	C10	C11	C6	121.00 (16)
C6	C5	C13	102.13 (9)	C10	C11	C12	128.05 (15)
C6 ¹	C5	C13 ¹	102.13 (9)	C11	C12	C13	102.86 (14)
C6	C5	C13 ¹	110.56 (8)	C12	C13	C5	104.24 (12)

¹1-X,+Y,1-Z

Table S14. Hydrogen Bonds for 4d.

D	H	A	d(D-H)/Å	d(H-A)/Å	d(D-A)/Å	D-H-A/°
O1	H1	N1 ¹	0.84	2.00	2.8302 (19)	169.9

¹1-X,+Y,1-Z

Table S15. Torsion Angles for 4d.

A	B	C	D	Angle/°	A	B	C	D	Angle/°
O1	C1	C2	N1	68.64 (19)	C6 ¹	C5	C6	C11	-143.94 (13)
O1	C1	C2	C3	-49.1 (2)	C6	C5	C13	C12	30.96 (18)

O2 C4C7 C6	44.1(2)	C6 ¹ C5 C13C12	160.95(15)
O2 C4C7 C8	-138.17(15)	C6 C7 C8 C9	-1.4(2)
N1 C2C3 O2	17.12(15)	C6 C11C12C13	18.04(19)
N1 C4C7 C6	-137.13(17)	C7 C6 C11C10	1.6(2)
N1 C4C7 C8	40.6(2)	C7 C6 C11C12	179.84(15)
C1 C2C3 O2	139.63(14)	C7 C8 C9 C10	1.4(2)
C2 N1C4 O2	1.6(2)	C8 C9 C10C11	0.2(2)
C2 N1C4 C7	-177.10(14)	C9 C10C11C6	-1.7(2)
C3 O2C4 N1	10.01(19)	C9 C10C11C12	-179.58(17)
C3 O2C4 C7	-171.19(14)	C10 C11C12C13	-163.86(17)
C4 O2C3 C2	-16.31(15)	C11 C6 C7 C4	177.60(15)
C4 N1C2 C1	-136.77(16)	C11 C6 C7 C8	0.0(2)
C4 N1C2 C3	-11.93(17)	C11 C12C13C5	-30.05(18)
C4 C7C8 C9	-179.25(15)	C13 C5 C6 C7	161.61(17)
C5 C6C7 C4	-4.9(3)	C13 ¹ C5 C6 C7	-80.7(2)
C5 C6C7 C8	177.41(15)	C13 C5 C6 C11	-20.73(18)
C5 C6C11C10	-176.37(14)	C13 ¹ C5 C6 C11	96.94(16)
C5 C6C11C12	1.88(18)	C13 ¹ C5 C13C12	-86.70(13)
C6 ¹ C5C6 C7	38.40(15)		

¹1-X,+Y,I-Z

Table S16. Hydrogen Atom Coordinates ($\text{\AA}\times 10^4$) and Isotropic Displacement Parameters ($\text{\AA}^2\times 10^3$) for 4d.

Atom	x	y	z	U(eq)
H1	4093	-1014	3278	36
H1A	5394	-2021	1555	25
H1B	5512	-2369	3422	25
H2	6962	-911	3096	22
H3A	6382	734	1366	25
H3B	5102	725	1568	25
H8	7682	675	7739	19
H9	8007	1852	10154	21
H10	6973	3760	10230	22
H12A	5741	5684	7523	25
H12B	4952	4996	8521	25
H13A	4096	5430	5392	21
H13B	3714	4147	6185	21



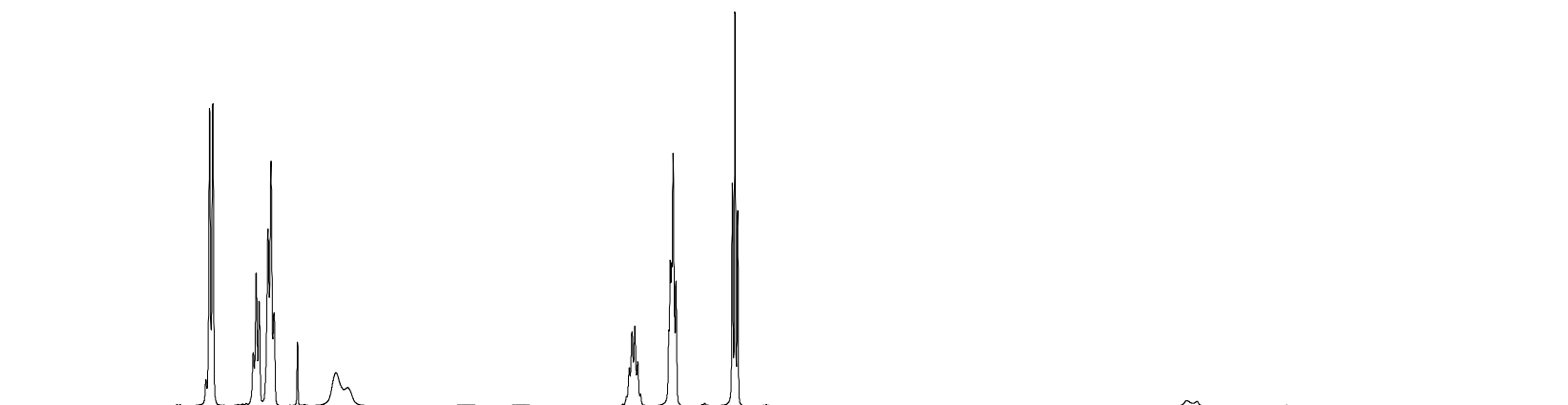
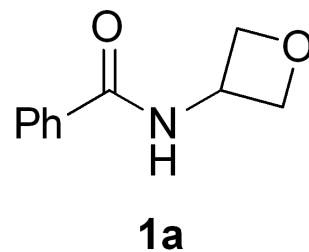
Current Data Parameters
NAME YW-1543
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20160120
Time 20.05
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 4
DS 0
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 82.92
DW 62.400 usec
DE 6.50 usec
TE 301.8 K
D1 1.00000000 sec
TD0 1

==== CHANNEL f1 =====
SFO1 400.1324710 MHz
NUC1 1H
P1 14.50 usec
PLW1 11.99499989 W

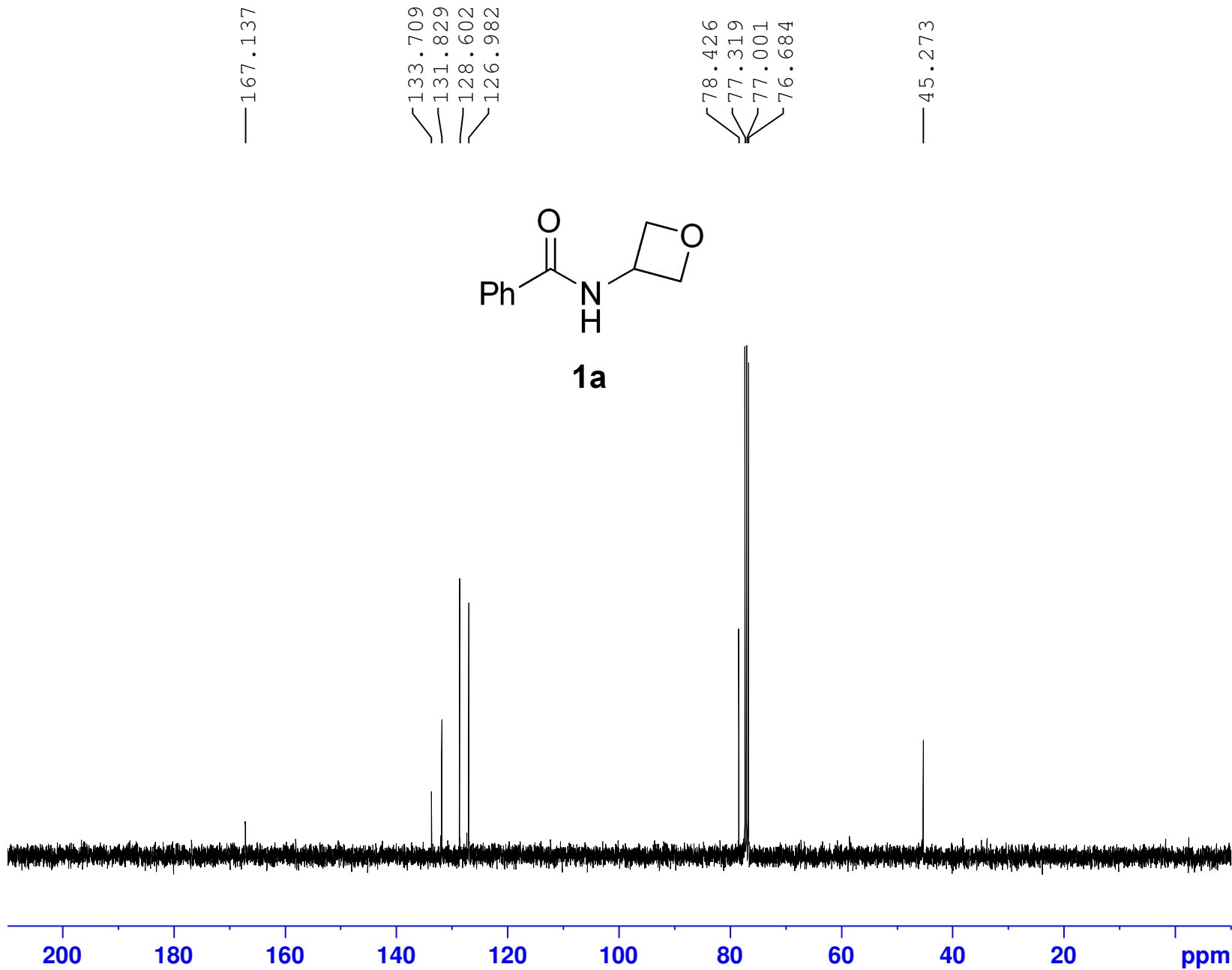
F2 - Processing parameters
SI 65536
SF 400.1300090 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

7.817
7.794
7.774
7.530
7.527
7.511
7.493
7.440
7.421
7.402
7.260
7.025
6.956
5.246
5.229
5.212
5.195
5.005
4.998
4.988
4.981
4.963
4.620
4.604
4.588



8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 ppm

2.11
1.07
2.13
0.90
1.00
2.02
2.01



Current Data Parameters
NAME YW-1543-carbon
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20160120
Time 20.08
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 28
DS 0
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 196.92
DW 20.800 usec
DE 6.50 usec
TE 302.2 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

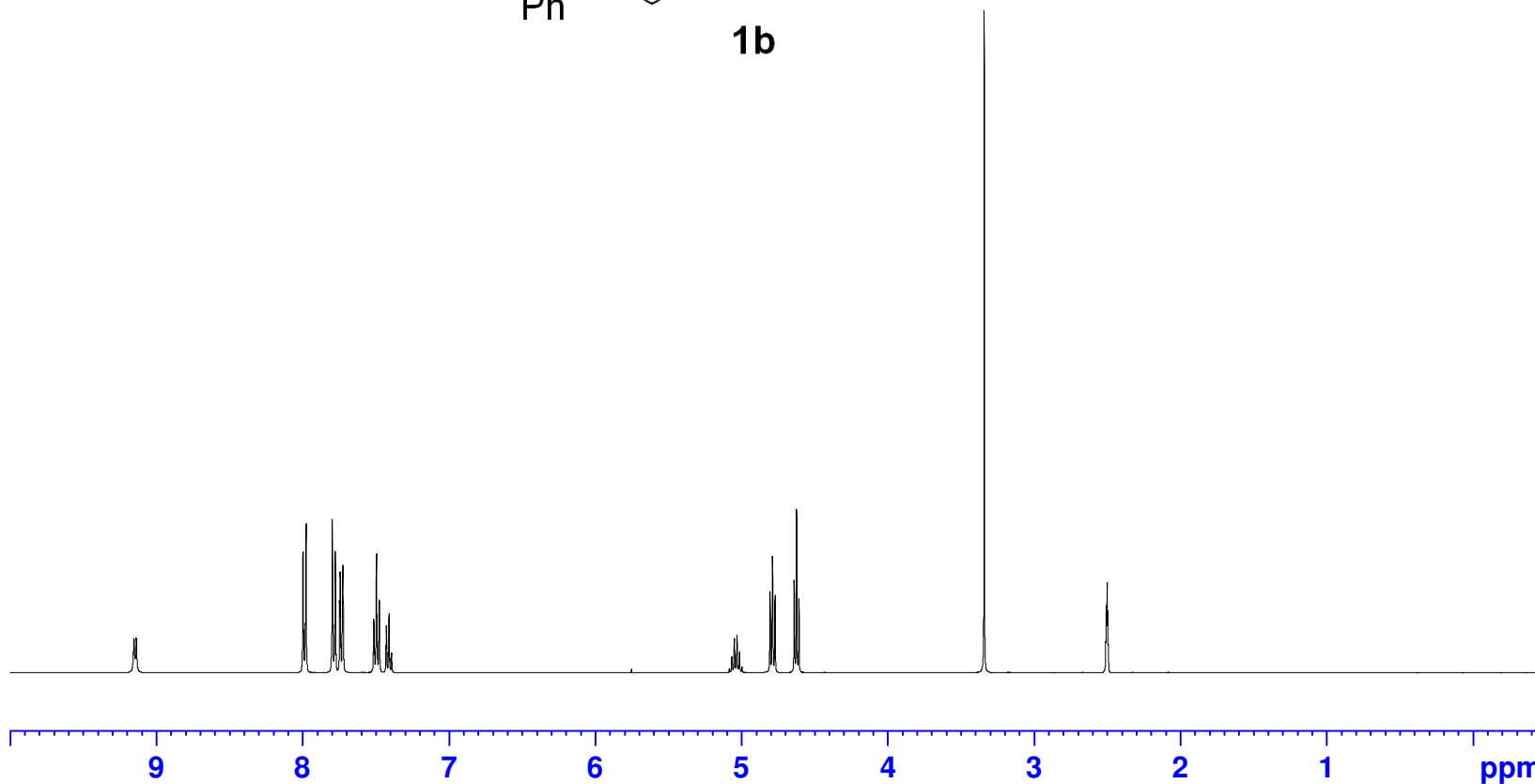
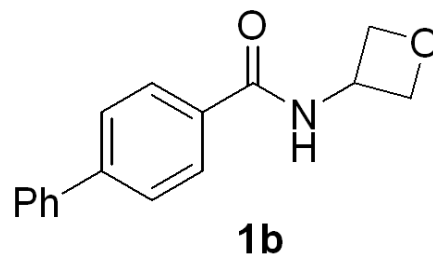
==== CHANNEL f1 =====
SFO1 100.6228298 MHz
NUC1 13C
P1 9.70 usec
PLW1 46.98899841 W

==== CHANNEL f2 =====
SFO2 400.1316005 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 90.00 usec
PLW2 11.99499989 W
PLW12 0.34213999 W
PLW13 0.27713001 W

F2 - Processing parameters
SI 32768
SF 100.6127736 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



9.137
7.997
7.976
7.797
7.776
7.743
7.725
7.513
7.495
7.475
7.430
7.427
7.424
7.414
7.409
7.404
7.394
7.391
7.388
5.082
5.066
5.047
5.031
5.012
4.996
4.805
4.788
4.786
4.770
4.639
4.623
4.607
3.340
2.509
2.505
2.500
2.496
2.491

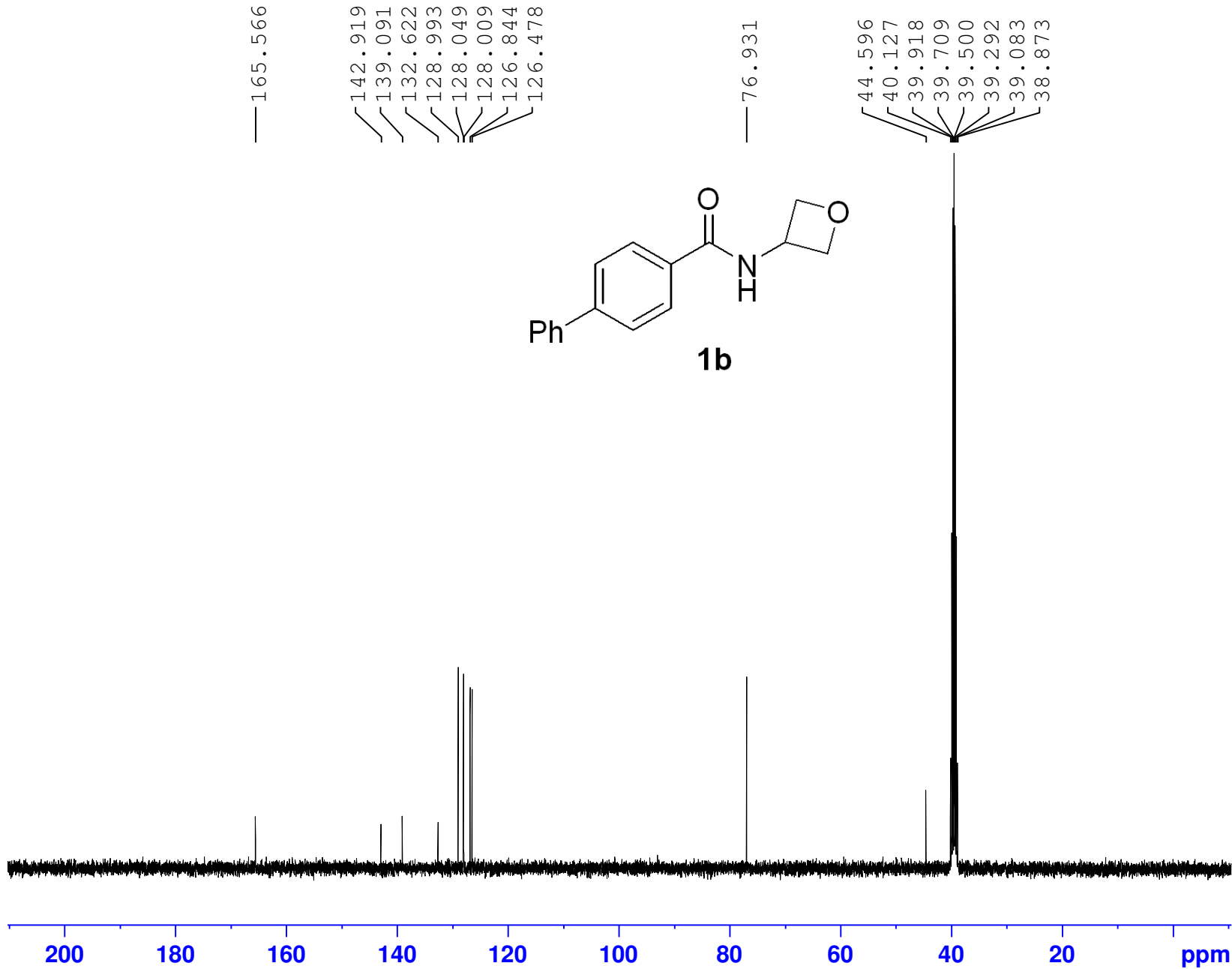


Current Data Parameters
NAME YW-1724
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20160812
Time 22.20
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 6
DS 0
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 112.31
DW 62.400 usec
DE 6.50 usec
TE 299.7 K
D1 1.00000000 sec
TD0 1

==== CHANNEL f1 =====
SFO1 400.1324710 MHz
NUC1 1H
P1 14.50 usec
PLW1 11.99499989 W

F2 - Processing parameters
SI 65536
SF 400.1300027 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



Current Data Parameters
NAME YW-1724-carbon
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20160812
Time 22.25
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 82
DS 0
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 196.92
DW 20.800 usec
DE 6.50 usec
TE 300.7 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

==== CHANNEL f1 =====
SFO1 100.6228298 MHz
NUC1 13C
P1 9.70 usec
PLW1 46.98899841 W

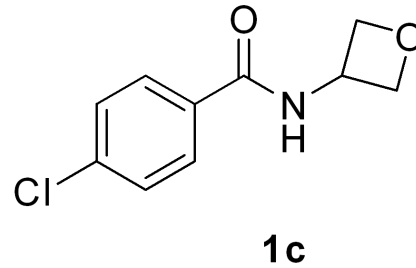
==== CHANNEL f2 =====
SFO2 400.1316005 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 90.00 usec
PLW2 11.99499989 W
PLW12 0.34213999 W
PLW13 0.27713001 W

F2 - Processing parameters
SI 32768
SF 100.6128192 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



7.735
7.715
7.410
7.390
7.262
7.011

5.235
5.219
5.202
5.186
5.018
5.001
4.983
4.618
4.603
4.587

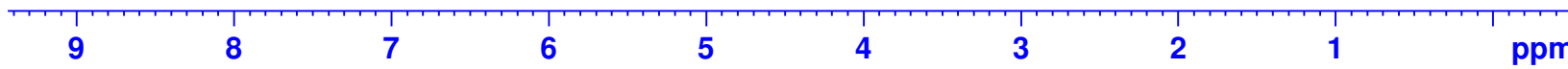
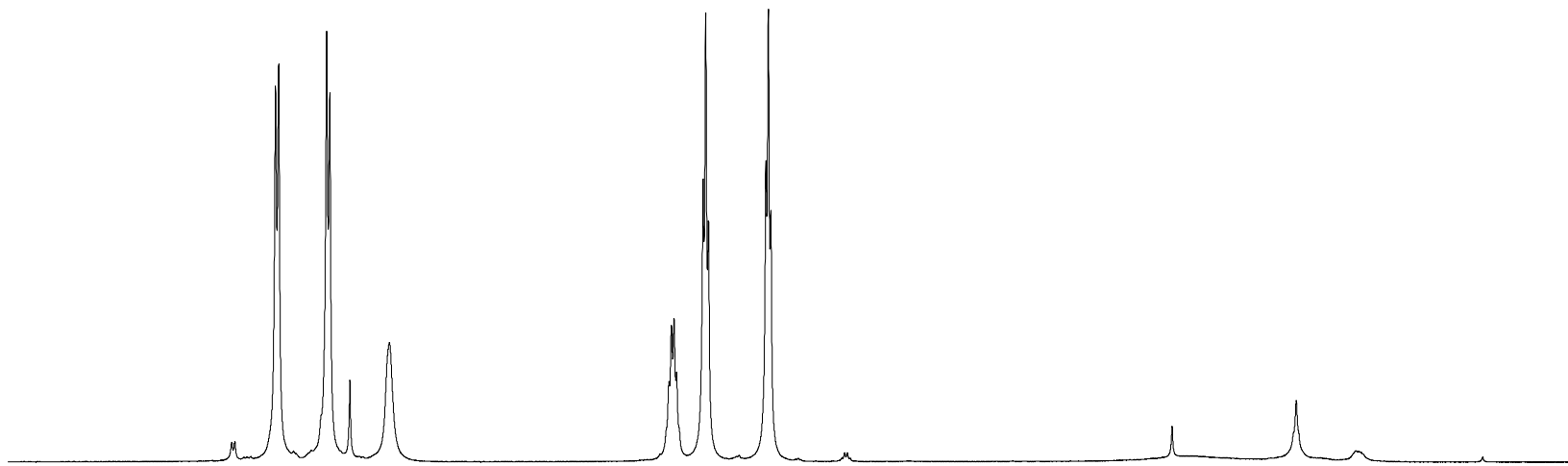


Current Data Parameters
NAME lzw2079-H
EXPNO 1
PROCNO 1

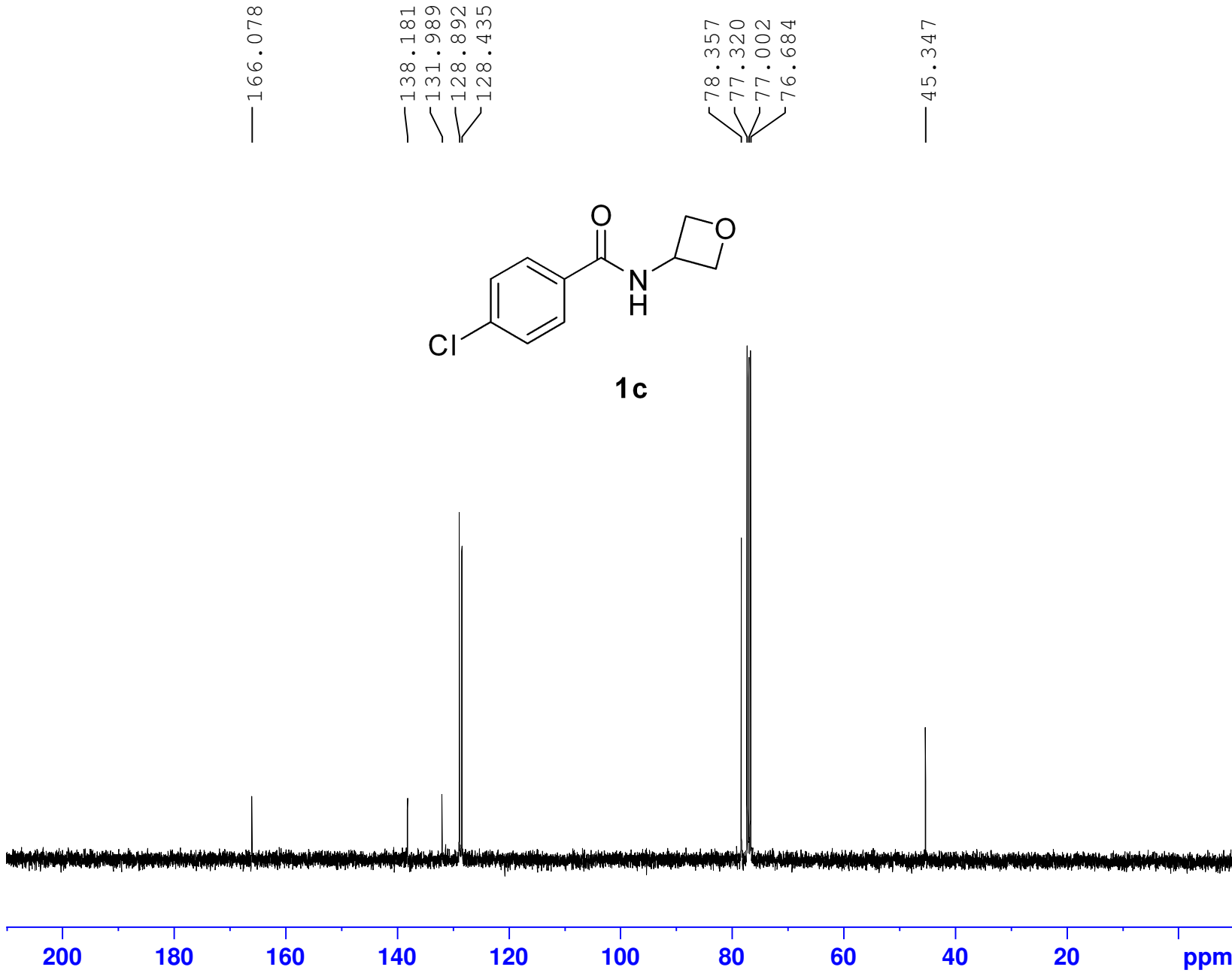
F2 - Acquisition Parameters
Date_ 20150319
Time 15.26
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT CDC13
NS 9
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 103.52
DW 62.400 usec
DE 6.50 usec
TE 295.9 K
D1 1.00000000 sec
TD0 1

==== CHANNEL f1 =====
SFO1 400.1324710 MHz
NUC1 1H
P1 14.50 usec
PLW1 11.99499989 W

F2 - Processing parameters
SI 65536
SF 400.1300082 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



1.91
2.02
0.95
1.00
1.96
1.98



Current Data Parameters
NAME lzw2079-C
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20150319
Time 15.32
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 82
DS 2
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 196.92
DW 20.800 usec
DE 6.50 usec
TE 297.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

==== CHANNEL f1 =====
SFO1 100.6228298 MHz
NUC1 13C
P1 9.70 usec
PLW1 46.98899841 W

==== CHANNEL f2 =====
SFO2 400.1316005 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 90.00 usec
PLW2 11.99499989 W
PLW12 0.34213999 W
PLW13 0.27713001 W

F2 - Processing parameters
SI 32768
SF 100.6127737 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



Current Data Parameters
NAME YW-(LZW2068B)
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20160813
Time 9.39
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT Acetone
NS 16
DS 0
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 112.31
DW 62.400 usec
DE 6.50 usec
TE 300.4 K
D1 1.00000000 sec
TD0 1

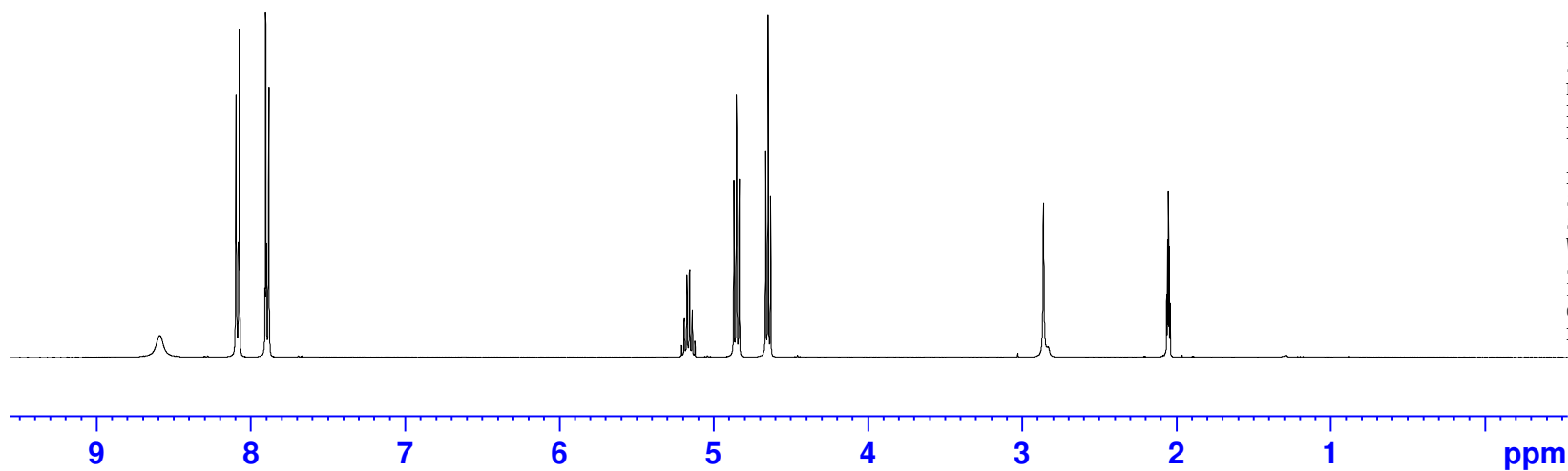
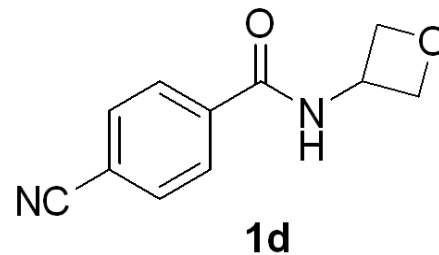
==== CHANNEL f1 =====
SFO1 400.1324710 MHz
NUC1 1H
P1 14.50 usec
PLW1 11.99499989 W

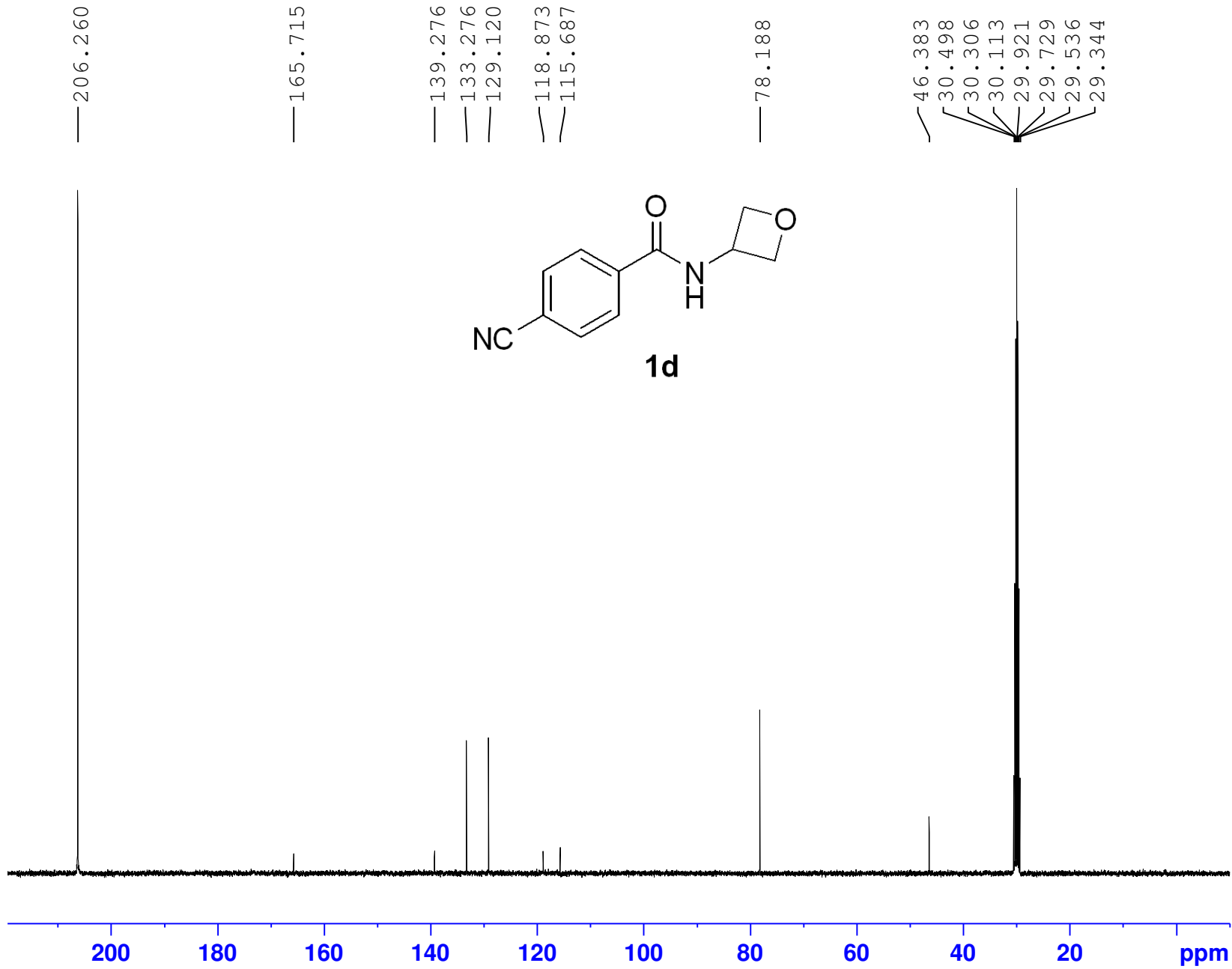
F2 - Processing parameters
SI 65536
SF 400.1300067 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

8.590
8.100
8.096
8.091
8.079
8.074
8.071
7.907
7.903
7.898
7.887
7.882
7.878

5.206
5.190
5.171
5.155
5.136
5.120
4.868
4.851
4.833
4.662
4.645
4.629

— 2.860
2.061
2.056
2.050
2.045
2.039





Current Data Parameters
NAME YW-(LZW2068B)-carbon
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20160813
Time 9.47
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT Acetone
NS 129
DS 0
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 196.92
DW 20.800 usec
DE 6.50 usec
TE 301.2 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

==== CHANNEL f1 =====
SFO1 100.6228298 MHz
NUC1 13C
P1 9.70 usec
PLW1 46.98899841 W

==== CHANNEL f2 =====
SFO2 400.1316005 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 90.00 usec
PLW2 11.99499989 W
PLW12 0.34213999 W
PLW13 0.27713001 W

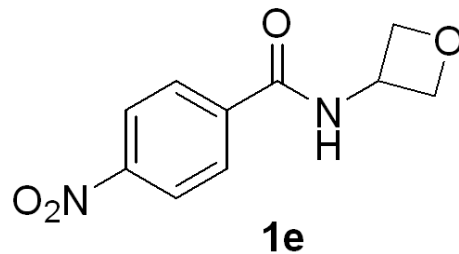
F2 - Processing parameters
SI 32768
SF 100.6126695 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



8.685
8.322
8.317
8.304
8.300
8.161
8.156
8.143
8.139

5.218
5.202
5.184
5.167
5.149
5.132
4.877
4.860
4.842
4.675
4.659
4.642

2.921
2.061
2.055
2.050
2.045
2.039

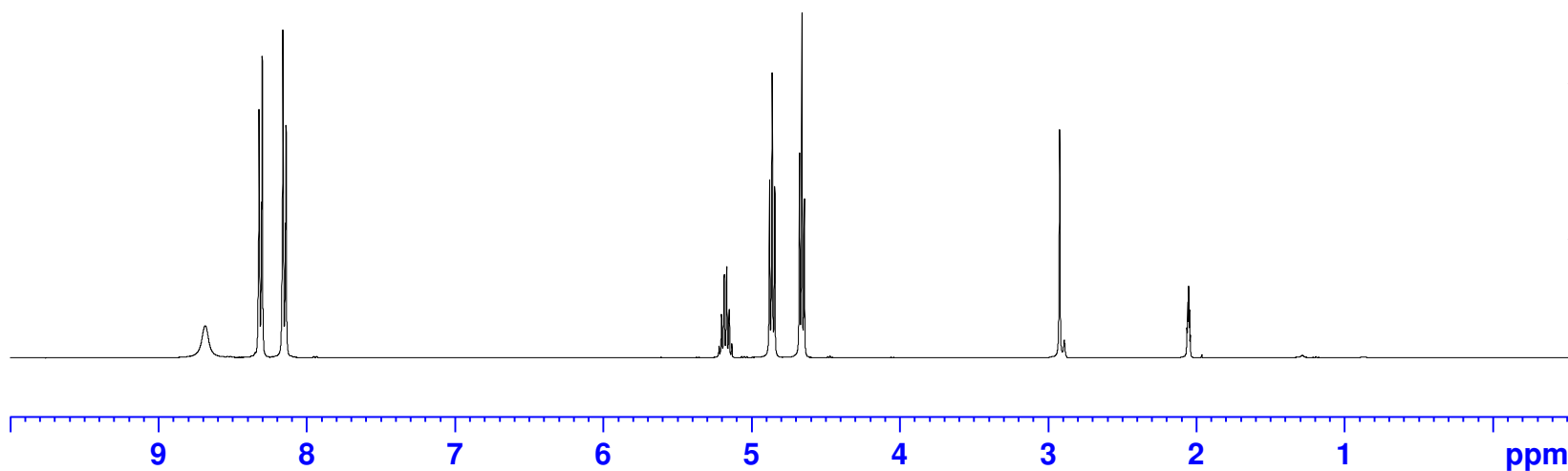


Current Data Parameters
NAME YW-(LZW2068A)
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20160813
Time 9.50
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT Acetone
NS 5
DS 0
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 62.93
DW 62.400 usec
DE 6.50 usec
TE 300.3 K
D1 1.00000000 sec
TD0 1

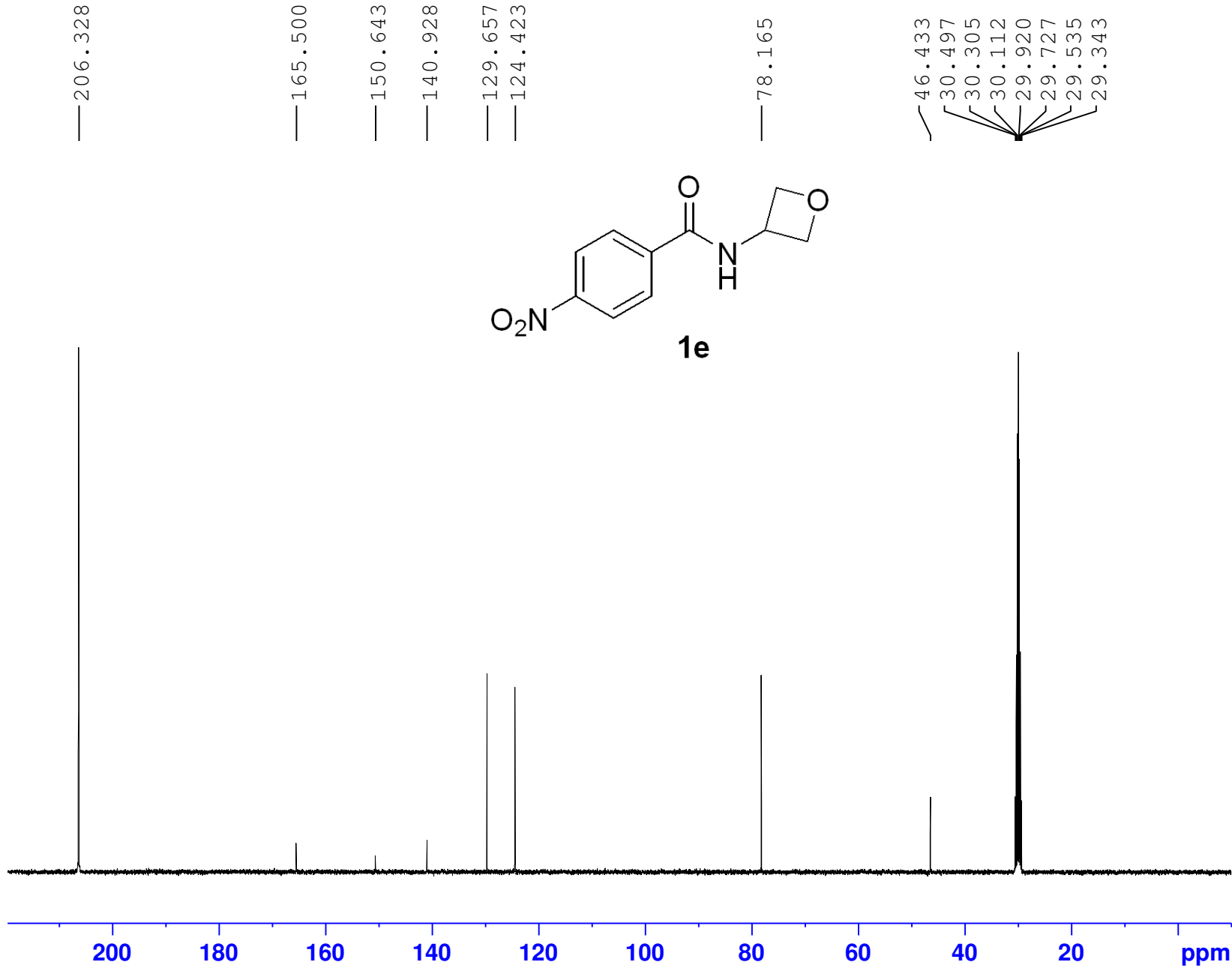
==== CHANNEL f1 =====
SFO1 400.1324710 MHz
NUC1 1H
P1 14.50 usec
PLW1 11.99499989 W

F2 - Processing parameters
SI 65536
SF 400.1300065 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



0.98
2.00
2.04

1.00
2.10
2.10



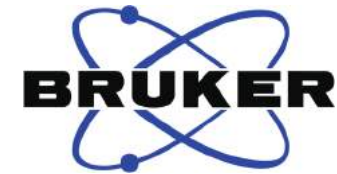
Current Data Parameters
NAME YW-(LZW2068A)-carbon
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20160813
Time 9.59
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT Acetone
NS 137
DS 0
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 196.92
DW 20.800 usec
DE 6.50 usec
TE 300.9 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

==== CHANNEL f1 =====
SFO1 100.6228298 MHz
NUC1 13C
P1 9.70 usec
PLW1 46.98899841 W

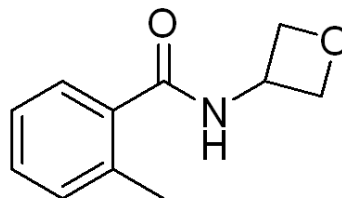
==== CHANNEL f2 =====
SFO2 400.1316005 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 90.00 usec
PLW2 11.99499989 W
PLW12 0.34213999 W
PLW13 0.27713001 W

F2 - Processing parameters
SI 32768
SF 100.6126702 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

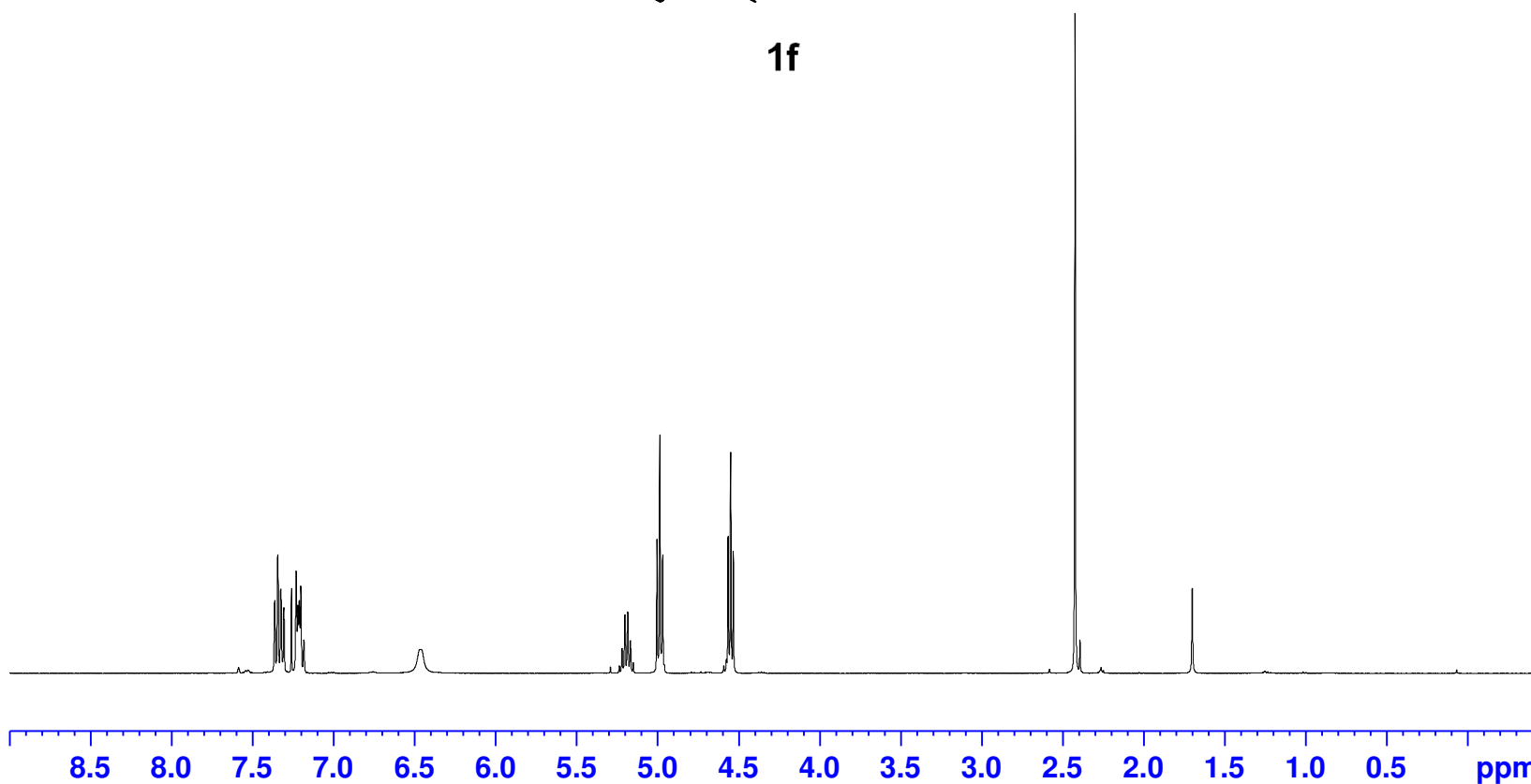


7.363
7.344
7.326
7.308
7.259
7.230
7.221
7.211
7.202
7.183
6.458
5.235
5.220
5.217
5.202
5.183
5.168
5.150
5.003
4.985
4.968
4.564
4.548
4.532

— 2.422



1f

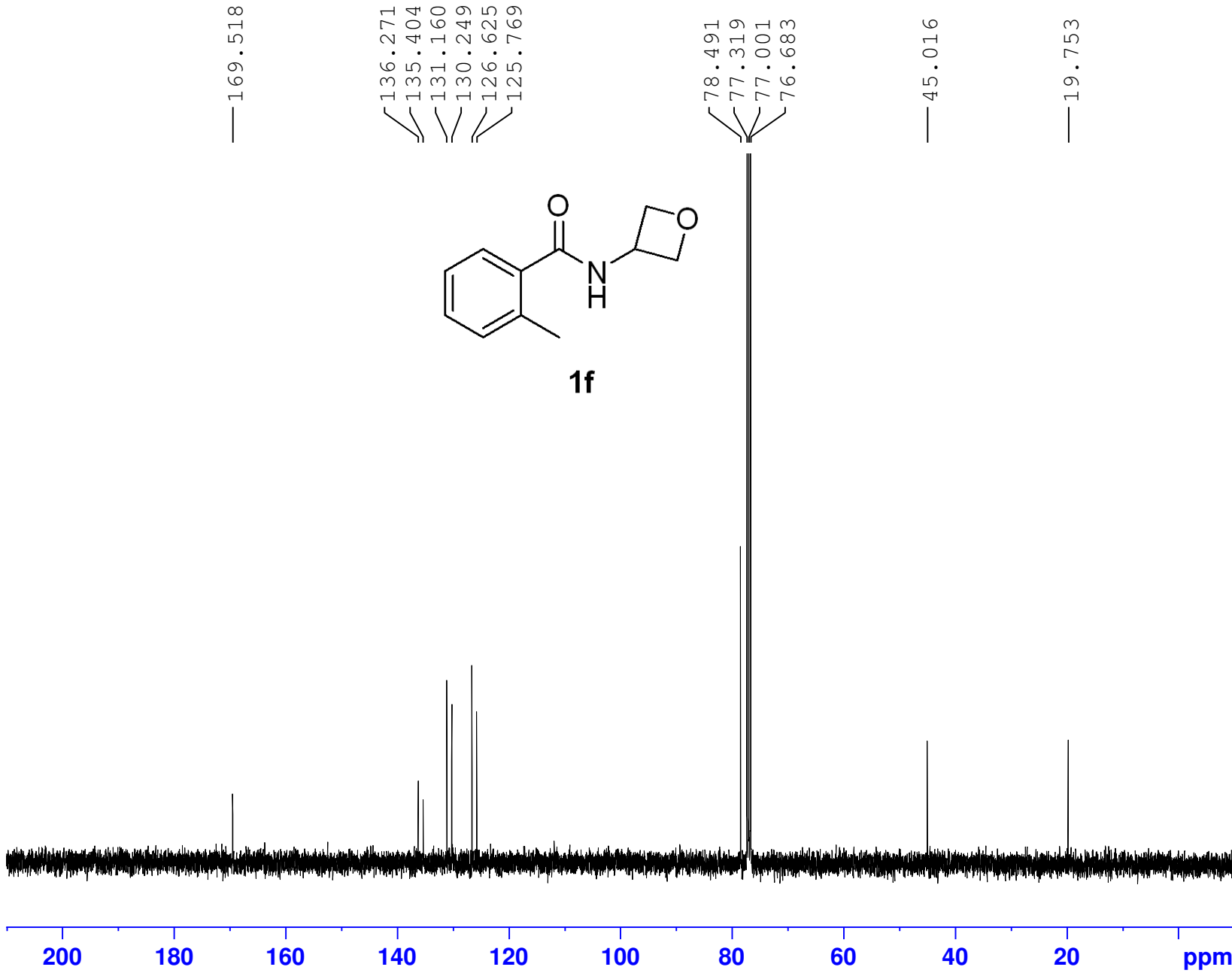


Current Data Parameters
NAME lzw2058-h
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20150310
Time 20.57
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT CDC13
NS 5
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 112.31
DW 62.400 usec
DE 6.50 usec
TE 298.0 K
D1 1.00000000 sec
TD0 1

==== CHANNEL f1 =====
SFO1 400.1324710 MHz
NUC1 1H
P1 14.50 usec
PLW1 11.99499989 W

F2 - Processing parameters
SI 65536
SF 400.1300095 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



Current Data Parameters
NAME lzw2058-c
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20150310
Time 21.00
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 34
DS 2
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 196.92
DW 20.800 usec
DE 6.50 usec
TE 298.7 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

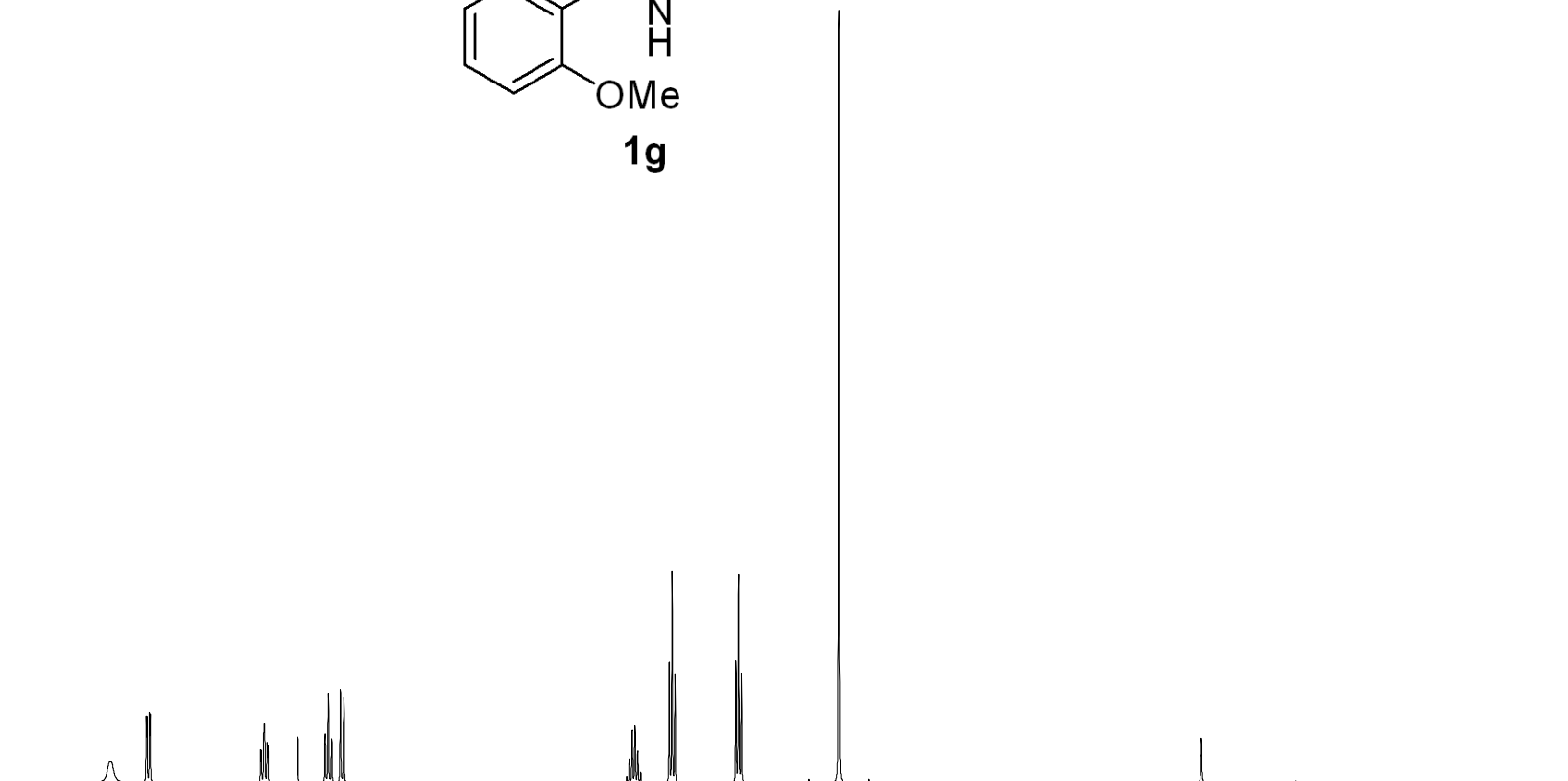
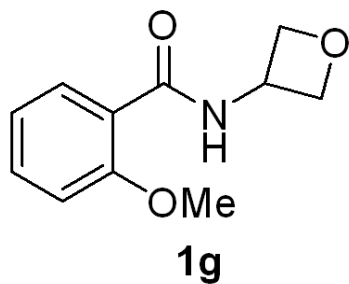
==== CHANNEL f1 =====
SFO1 100.6228298 MHz
NUC1 13C
P1 9.70 usec
PLW1 46.98899841 W

==== CHANNEL f2 =====
SFO2 400.1316005 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 90.00 usec
PLW2 11.99499989 W
PLW12 0.34213999 W
PLW13 0.27713001 W

F2 - Processing parameters
SI 32768
SF 100.6127729 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



8.156
8.152
7.486
7.481
7.465
7.464
7.447
7.442
7.260
7.096
7.095
7.077
7.058
7.005
6.984
5.280
5.263
5.246
5.228
5.212
5.195
5.024
5.006
4.989
4.621
4.605
4.588
4.002



8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 ppm

0.96 0.98 0.99 1.00 1.01 1.00 2.05 2.05 3.09

Current Data Parameters
NAME lzw2052
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20150307
Time 20.55
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT CDC13
NS 11
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 82.92
DW 62.400 usec
DE 6.50 usec
TE 297.5 K
D1 1.00000000 sec
TD0 1

==== CHANNEL f1 =====
SFO1 400.1324710 MHz
NUC1 1H
P1 14.50 usec
PLW1 11.99499989 W

F2 - Processing parameters
SI 65536
SF 400.1300092 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

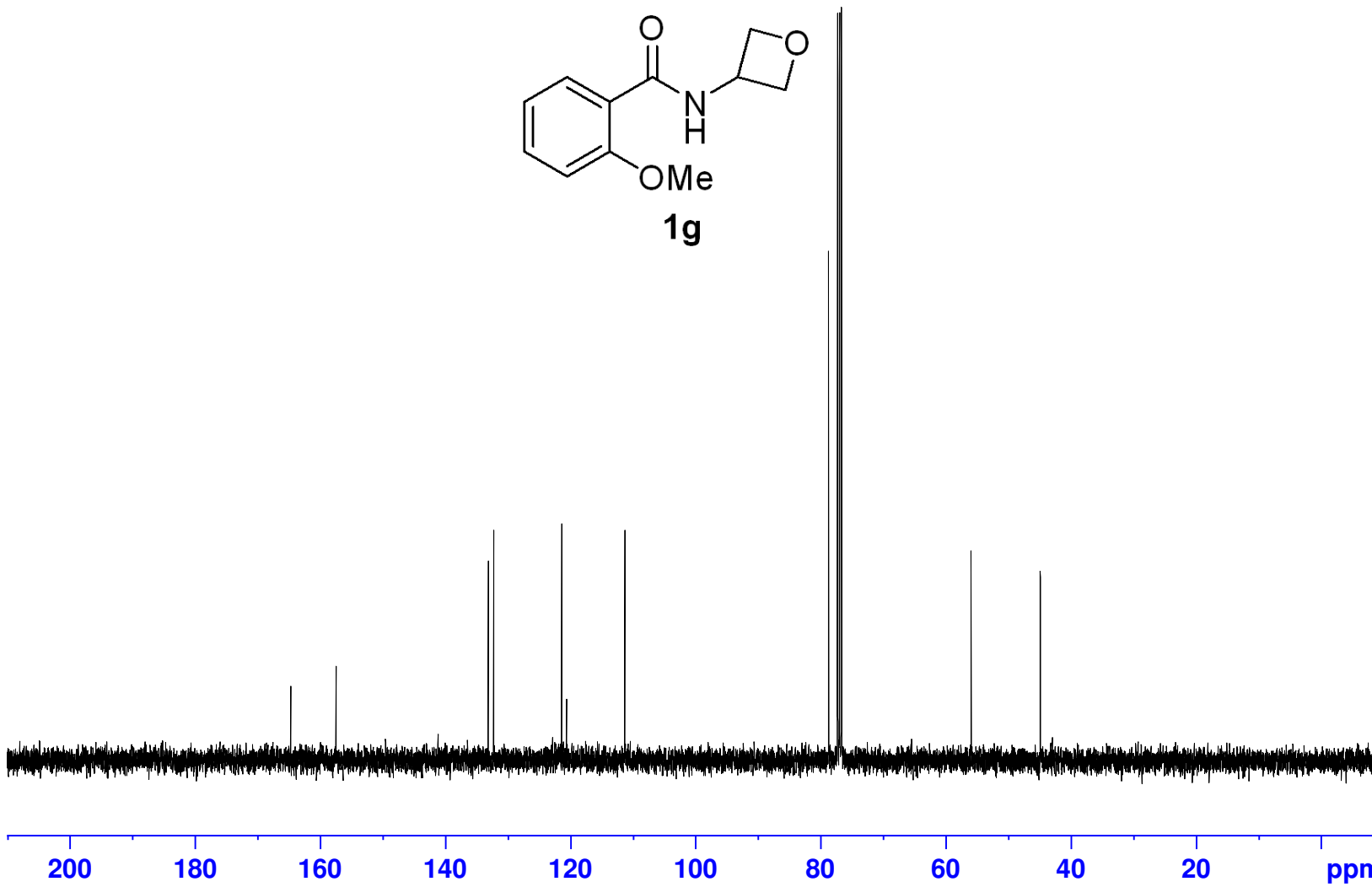
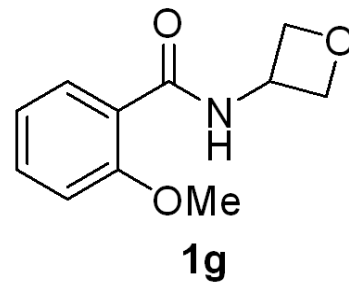


— 164.747
— 157.486

133.158
132.282
121.402
120.640
— 111.312

78.769
77.319
77.001
76.684

— 55.968
— 44.899



Current Data Parameters
NAME lzw2052-c
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20150307
Time 20.57
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 17
DS 2
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 196.92
DW 20.800 usec
DE 6.50 usec
TE 298.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

==== CHANNEL f1 =====
SFO1 100.6228298 MHz
NUC1 13C
P1 9.70 usec
PLW1 46.98899841 W

==== CHANNEL f2 =====
SFO2 400.1316005 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 90.00 usec
PLW2 11.99499989 W
PLW12 0.34213999 W
PLW13 0.27713001 W

F2 - Processing parameters
SI 32768
SF 100.6127753 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

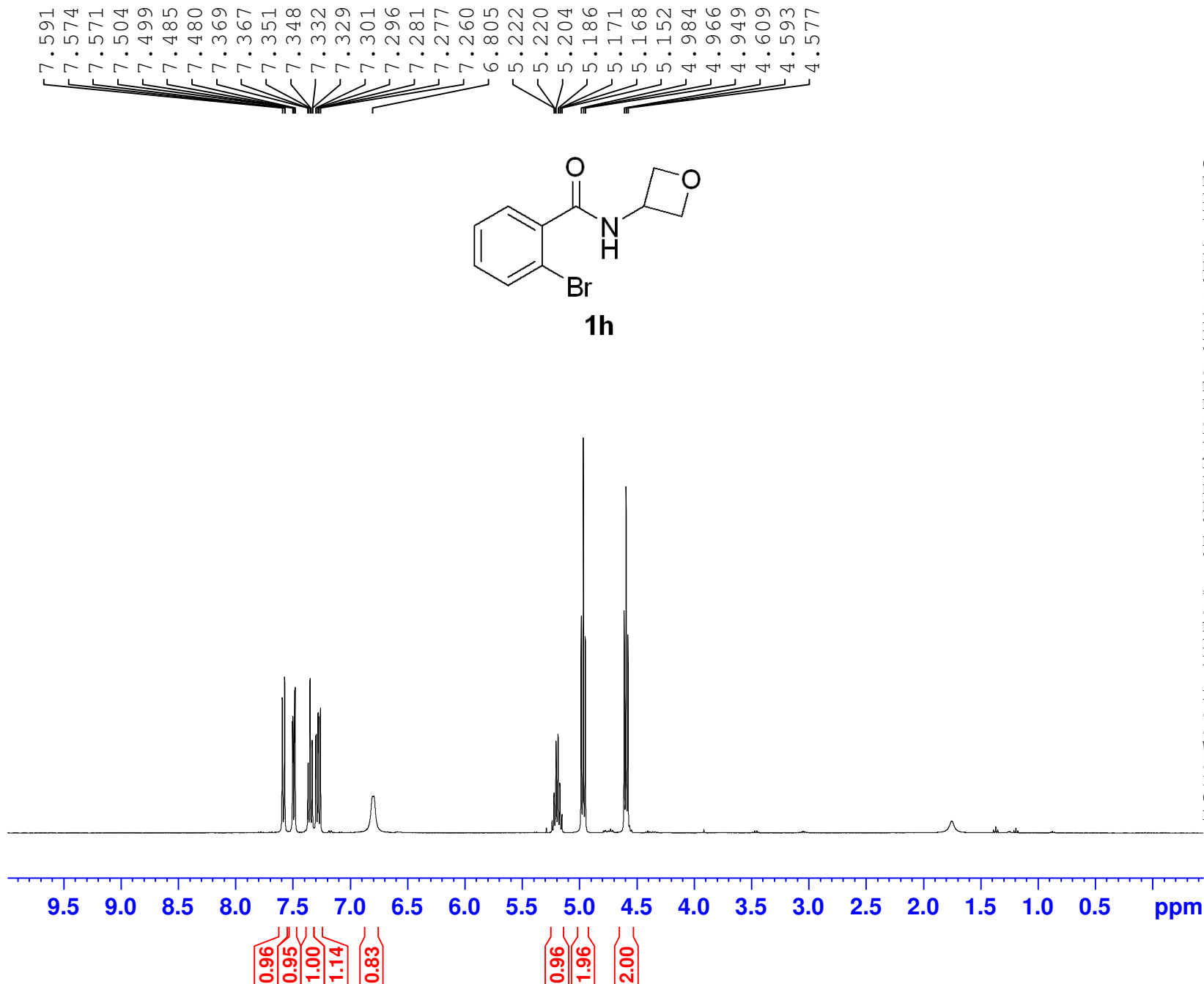


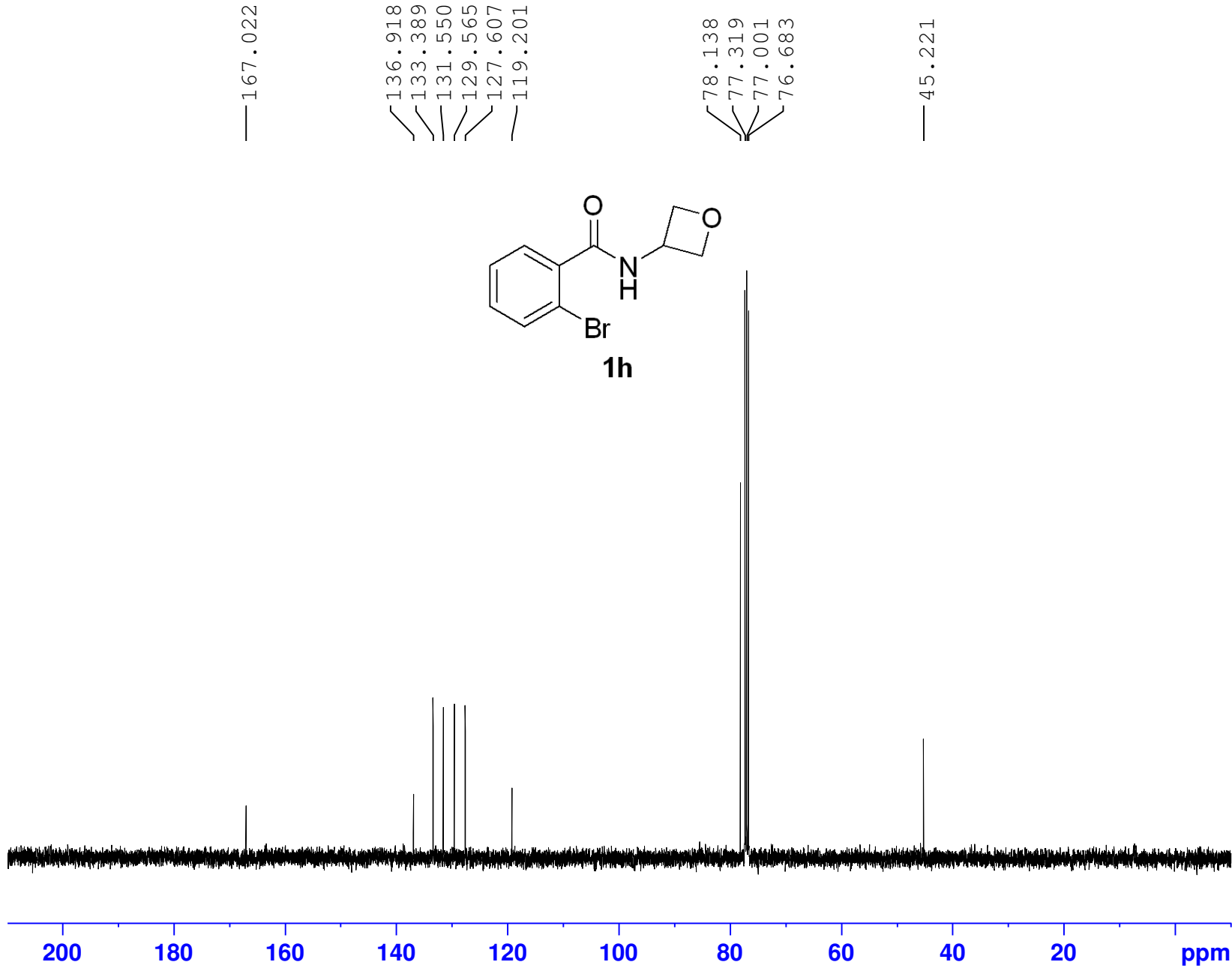
Current Data Parameters
NAME YW-1691
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20160319
Time 20.02
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT CDC13
NS 14
DS 0
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 88.84
DW 62.400 usec
DE 6.50 usec
TE 297.8 K
D1 1.00000000 sec
TD0 1

==== CHANNEL f1 =====
SFO1 400.1324710 MHz
NUC1 1H
P1 14.50 usec
PLW1 11.99499989 W

F2 - Processing parameters
SI 65536
SF 400.1300093 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00





Current Data Parameters
NAME YW-1691-carbon
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20160319
Time 20.04
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 30
DS 0
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 196.92
DW 20.800 usec
DE 6.50 usec
TE 298.6 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

==== CHANNEL f1 =====
SFO1 100.6228298 MHz
NUC1 13C
P1 9.70 usec
PLW1 46.98899841 W

==== CHANNEL f2 =====
SFO2 400.1316005 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 90.00 usec
PLW2 11.99499989 W
PLW12 0.34213999 W
PLW13 0.27713001 W

F2 - Processing parameters
SI 32768
SF 100.6127744 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



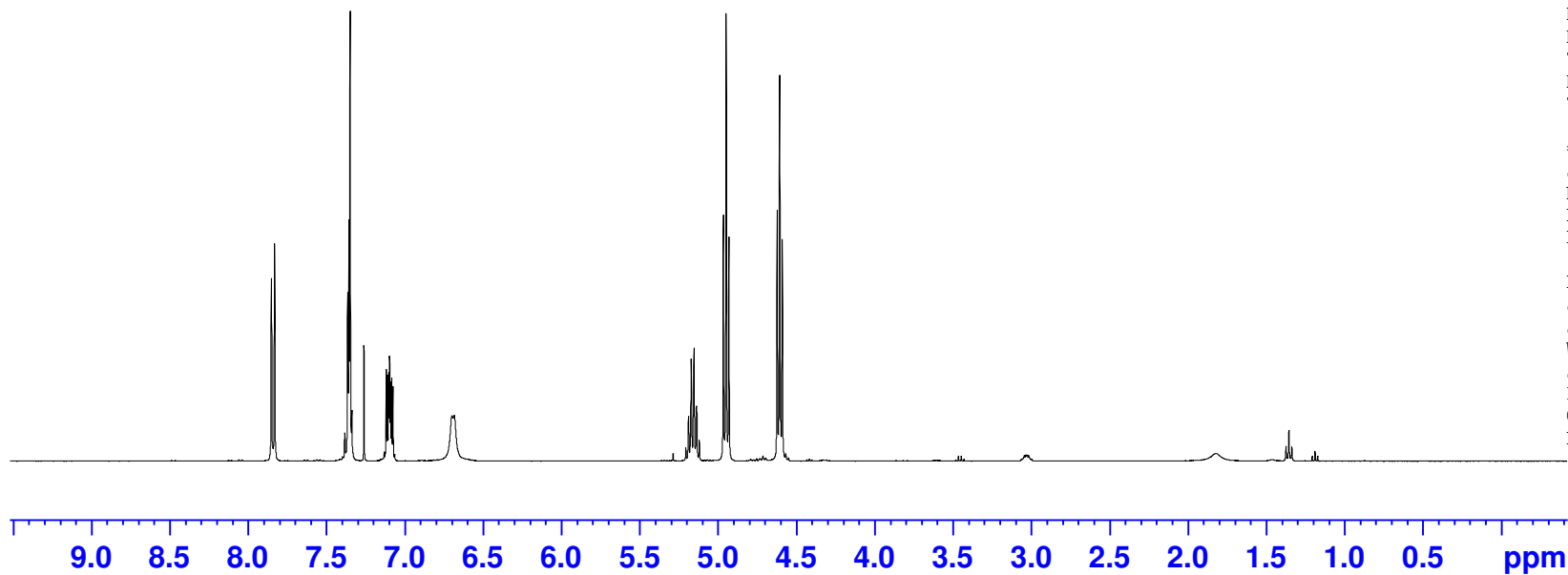
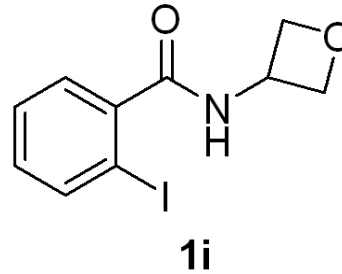
Current Data Parameters
NAME YW-1693
EXPNO 1
PROCNO 1

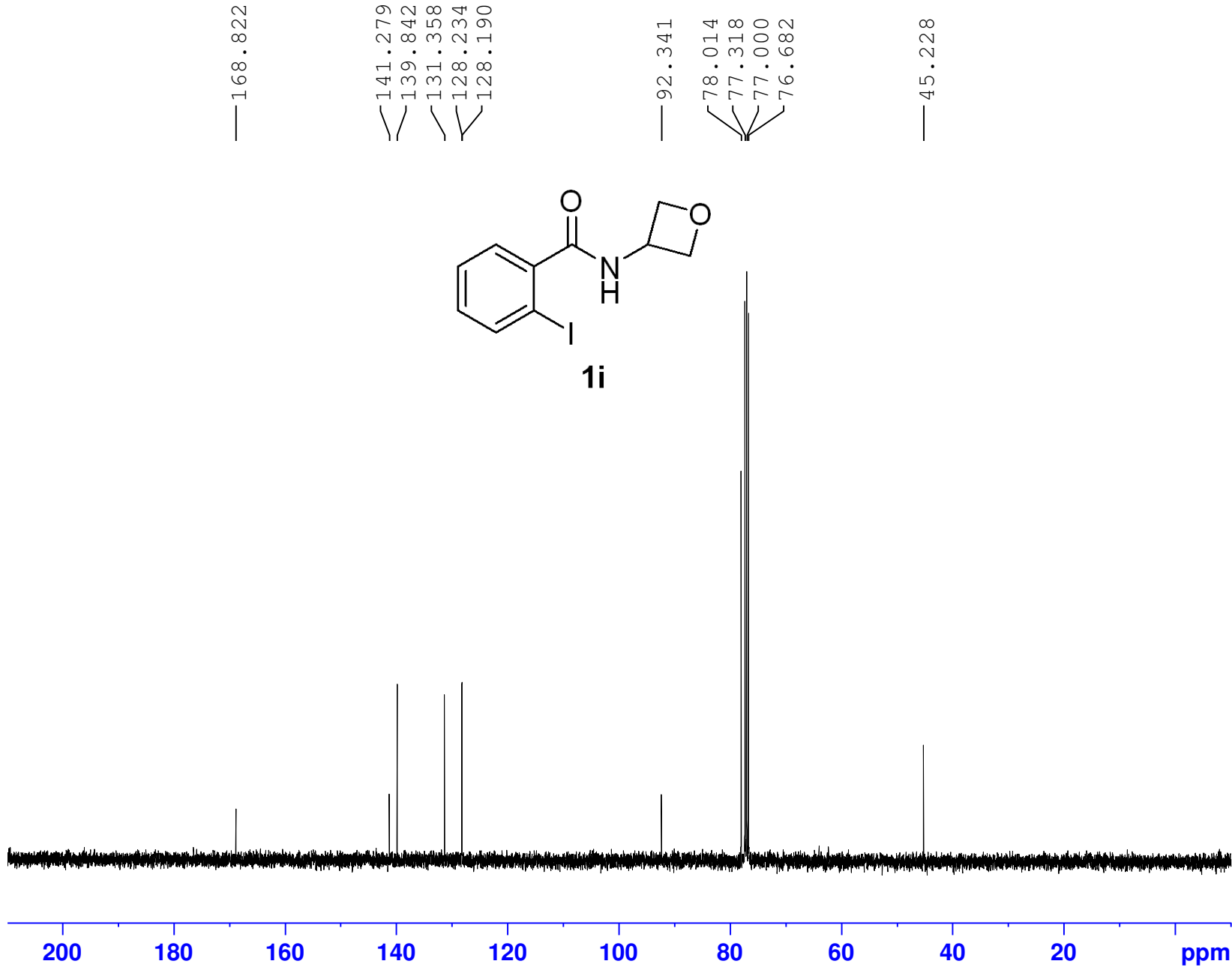
F2 - Acquisition Parameters
Date_ 20160323
Time 20.22
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT CDC13
NS 4
DS 0
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 88.84
DW 62.400 usec
DE 6.50 usec
TE 297.4 K
D1 1.00000000 sec
TD0 1

==== CHANNEL f1 =====
SFO1 400.1324710 MHz
NUC1 1H
P1 14.50 usec
PLW1 11.99499989 W

F2 - Processing parameters
SI 65536
SF 400.130094 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

7.384
7.382
7.365
7.363
7.356
7.348
7.337
7.260
7.118
7.110
7.103
7.098
7.095
7.090
7.083
7.075
6.699
6.684
5.205
5.190
5.187
5.171
5.153
5.138
5.135
5.119
4.966
4.948
4.930
4.622
4.606
4.590





Current Data Parameters
NAME YW-1693-carbon
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20160323
Time 20.24
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 34
DS 0
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 196.92
DW 20.800 usec
DE 6.50 usec
TE 298.2 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

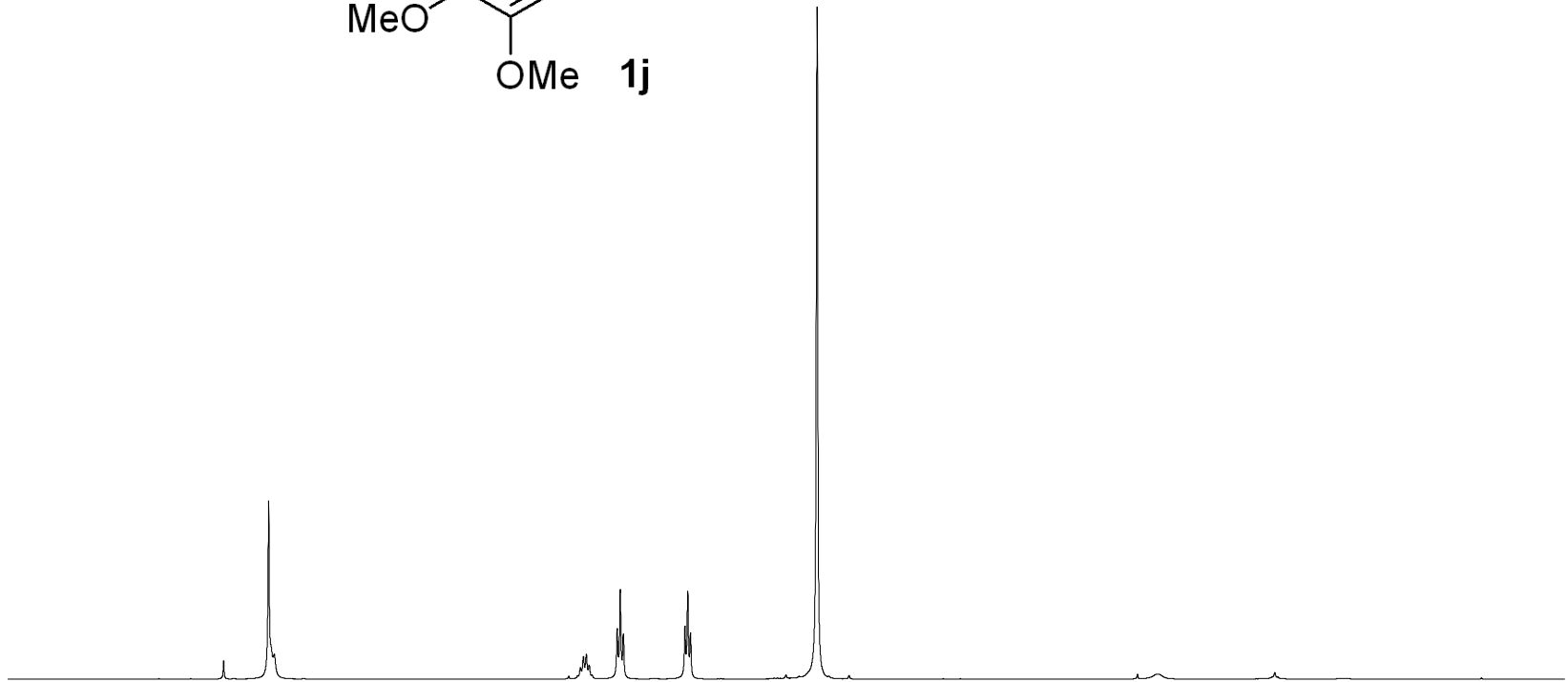
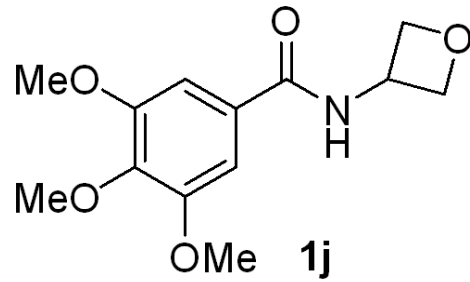
==== CHANNEL f1 =====
SFO1 100.6228298 MHz
NUC1 13C
P1 9.70 usec
PLW1 46.98899841 W

==== CHANNEL f2 =====
SFO2 400.1316005 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 90.00 usec
PLW2 11.99499989 W
PLW12 0.34213999 W
PLW13 0.27713001 W

F2 - Processing parameters
SI 32768
SF 100.6127758 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



7.260
7.003
6.971
5.216
5.199
5.182
5.166
5.005
4.988
4.970
4.617
4.601
4.585
3.859

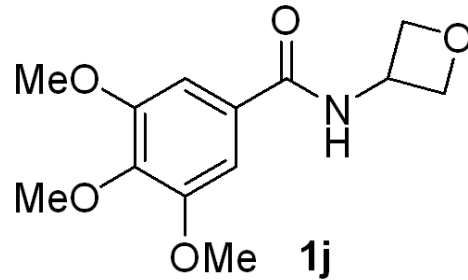
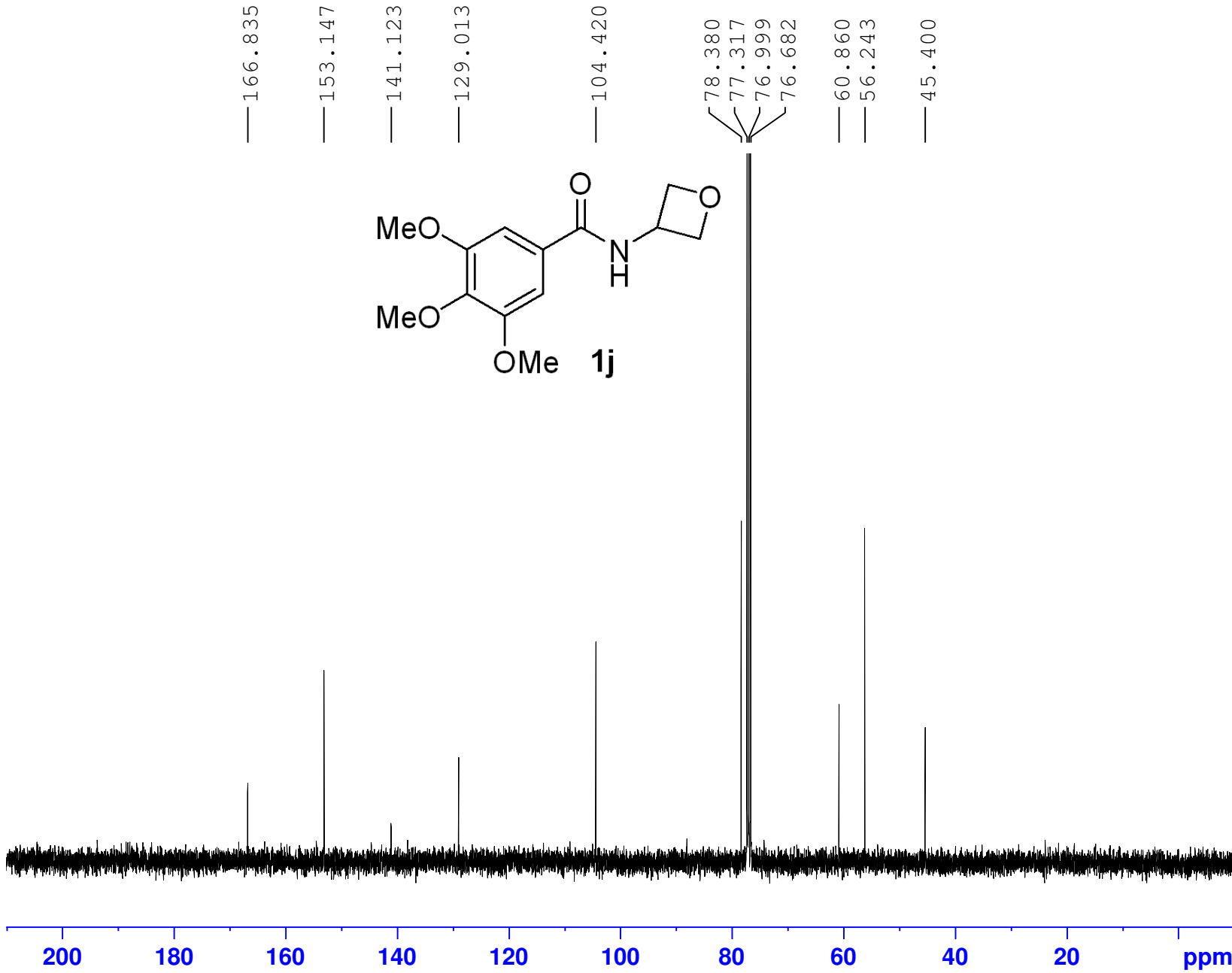


Current Data Parameters
NAME lzw2051-h
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20150307
Time 14.31
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT CDC13
NS 8
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 70.97
DW 62.400 usec
DE 6.50 usec
TE 296.4 K
D1 1.00000000 sec
TD0 1

==== CHANNEL f1 =====
SFO1 400.1324710 MHz
NUC1 1H
P1 14.50 usec
PLW1 11.99499989 W

F2 - Processing parameters
SI 65536
SF 400.1300089 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



Current Data Parameters
NAME lzw2051-c
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20150307
Time 14.34
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 29
DS 2
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 196.92
DW 20.800 usec
DE 6.50 usec
TE 297.1 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

==== CHANNEL f1 =====
SFO1 100.6228298 MHz
NUC1 13C
P1 9.70 usec
PLW1 46.98899841 W

==== CHANNEL f2 =====
SFO2 400.1316005 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 90.00 usec
PLW2 11.99499989 W
PLW12 0.34213999 W
PLW13 0.27713001 W

F2 - Processing parameters
SI 32768
SF 100.6127754 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



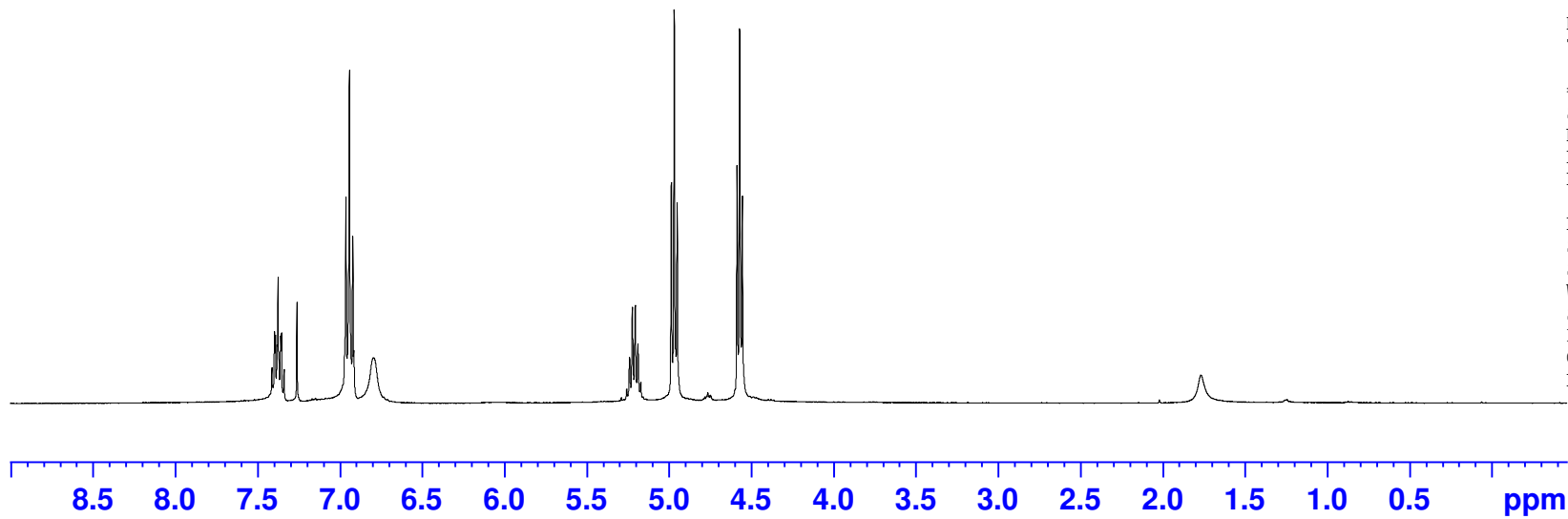
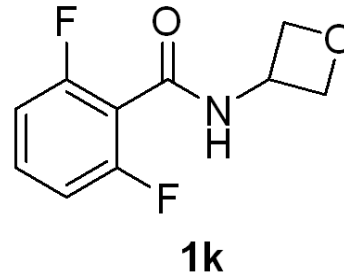
Current Data Parameters
NAME YW-(LZW2019)
EXPNO 2
PROCNO 1

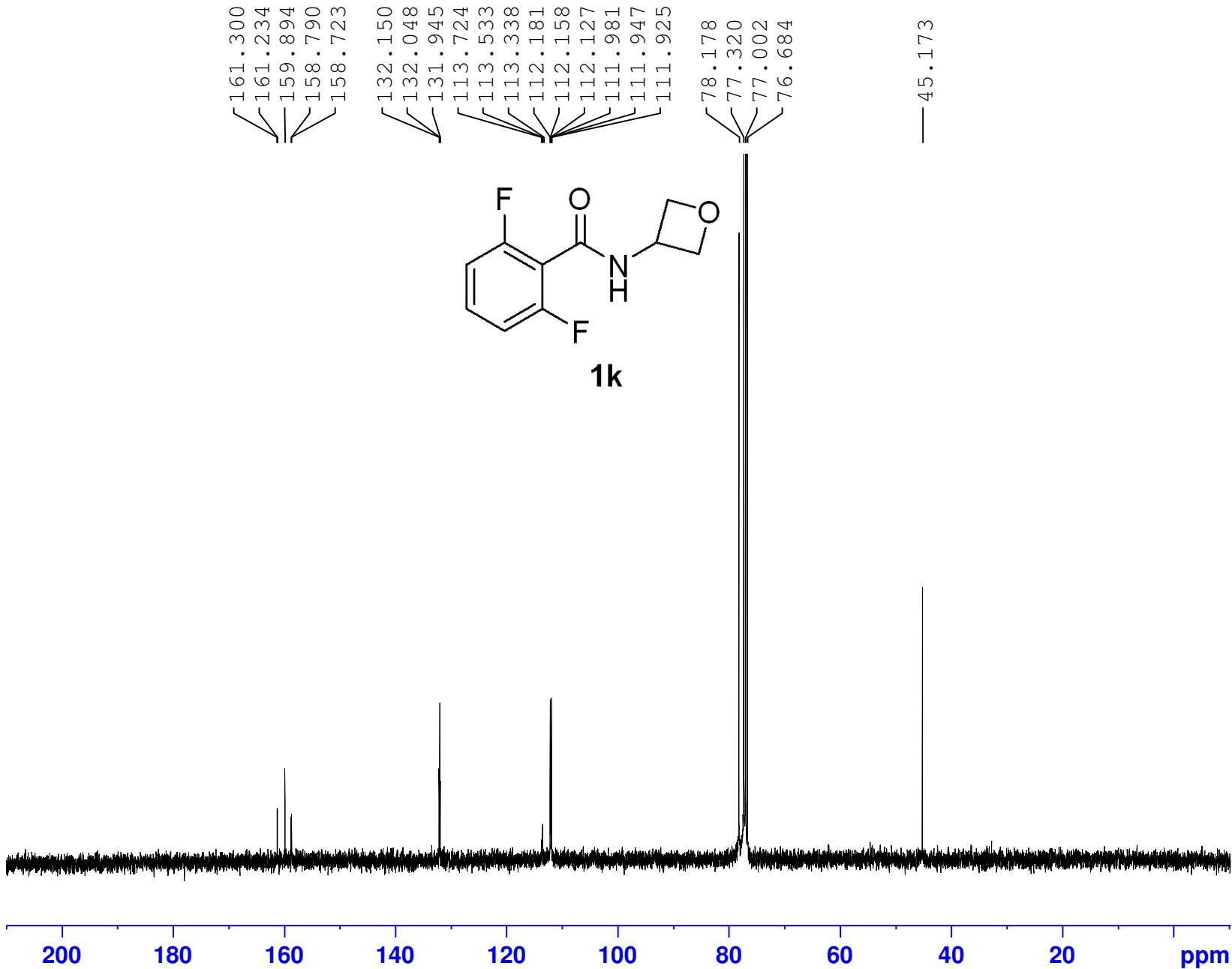
F2 - Acquisition Parameters
Date_ 20160813
Time 9.09
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT CDC13
NS 5
DS 0
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 88.84
DW 62.400 usec
DE 6.50 usec
TE 301.7 K
D1 1.00000000 sec
TD0 1

==== CHANNEL f1 =====
SFO1 400.1324710 MHz
NUC1 1H
P1 14.50 usec
PLW1 11.99499989 W

F2 - Processing parameters
SI 65536
SF 400.1300089 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

7.392
7.381
7.376
7.371
7.360
7.355
7.339
7.260
6.971
6.962
6.950
6.942
6.937
6.922
6.915
6.795
5.257
5.240
5.223
5.205
5.189
5.171
4.986
4.968
4.951
4.587
4.571
4.554





Current Data Parameters
NAME YW-(LZW2019)-carbon
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20160813
Time 9.26
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 240
DS 0
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 196.92
DW 20.800 usec
DE 6.50 usec
TE 301.9 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

==== CHANNEL f1 =====
SFO1 100.6228298 MHz
NUC1 13C
P1 9.70 usec
PLW1 46.98899841 W

==== CHANNEL f2 =====
SFO2 400.1316005 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 90.00 usec
PLW2 11.99499989 W
PLW12 0.34213999 W
PLW13 0.27713001 W

F2 - Processing parameters
SI 32768
SF 100.6127716 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

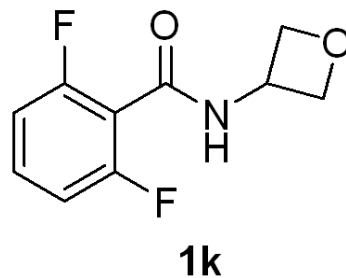


Current Data Parameters
NAME YW-(LZW2019)-19F
EXPNO 1
PROCNO 1

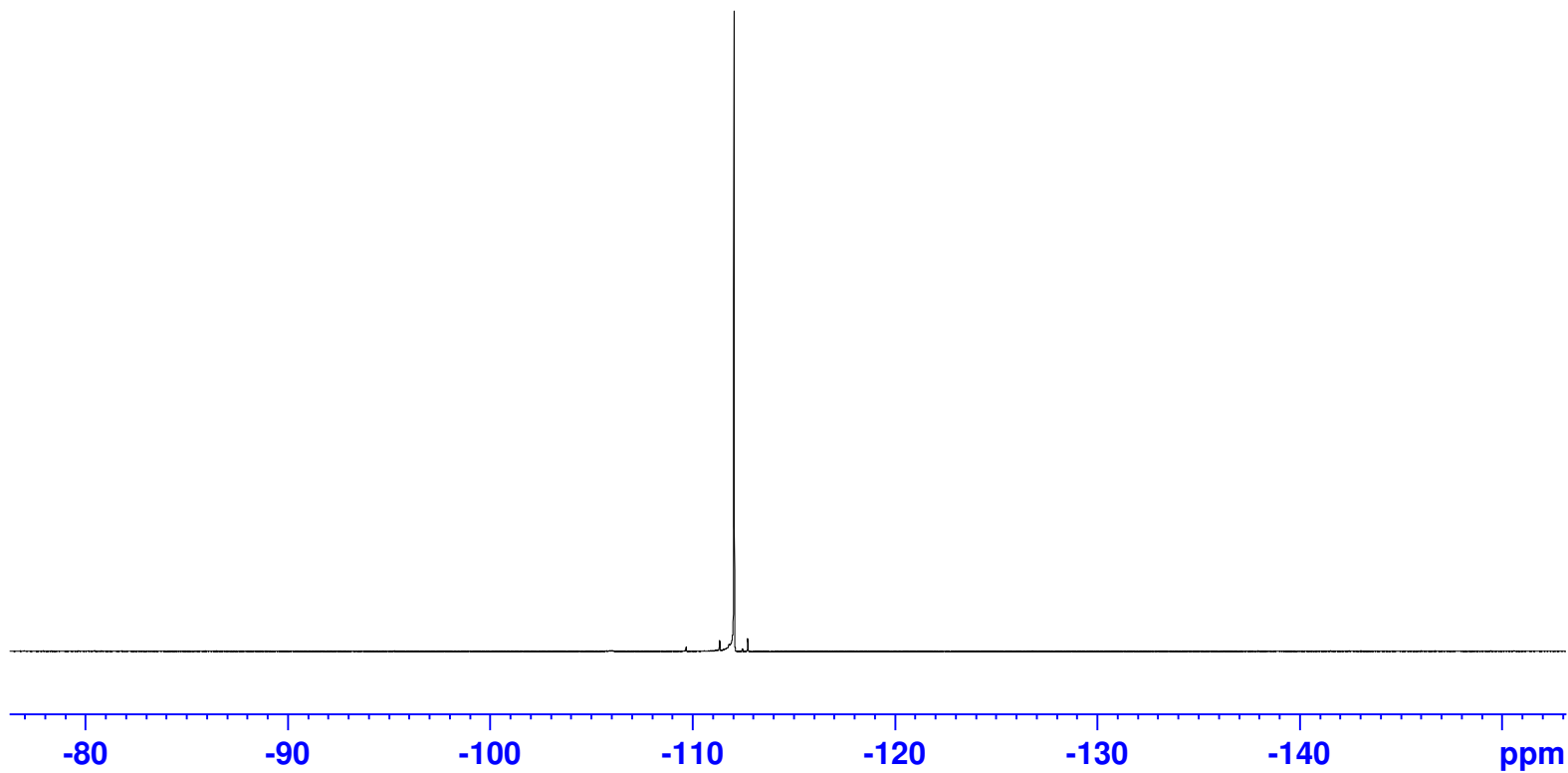
F2 - Acquisition Parameters
Date_ 20160813
Time 10.05
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgflqn
TD 131072
SOLVENT CDCl3
NS 16
DS 0
SWH 89285.711 Hz
FIDRES 0.681196 Hz
AQ 0.7340032 sec
RG 196.92
DW 5.600 usec
DE 6.50 usec
TE 299.8 K
D1 1.00000000 sec
TD0 1

==== CHANNEL f1 =====
SFO1 376.4607164 MHz
NUC1 19F
P1 14.70 usec
PLW1 15.99600029 W

F2 - Processing parameters
SI 65536
SF 376.4983660 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



-112.06





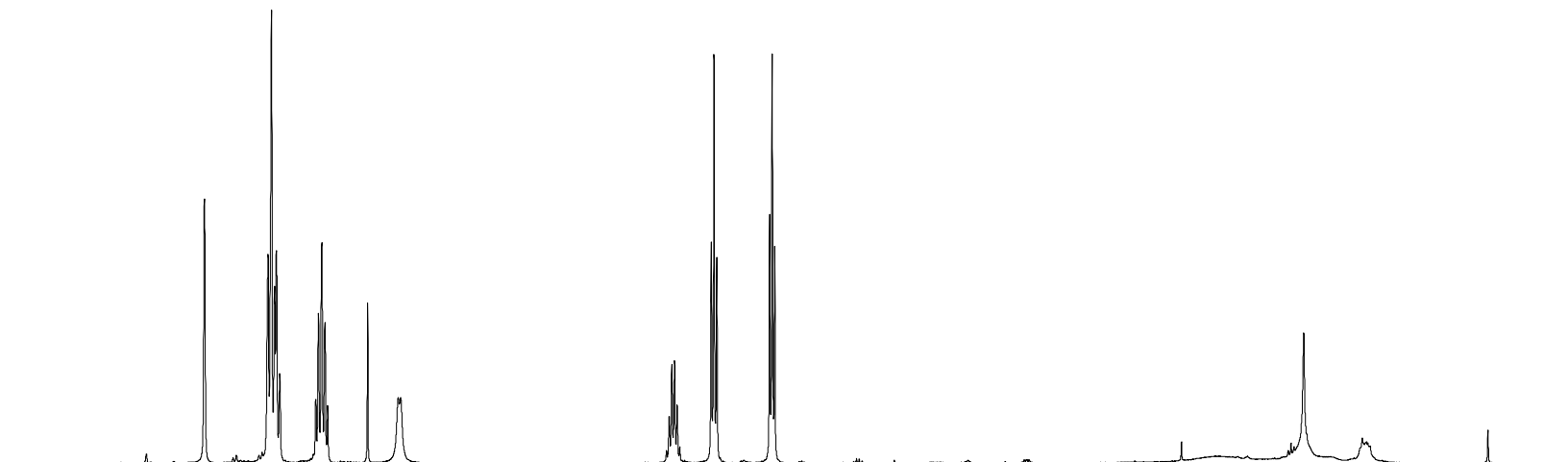
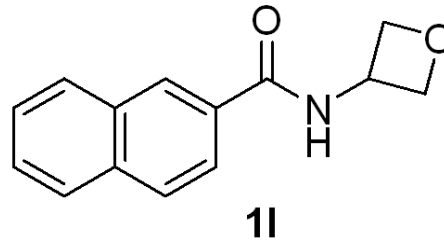
Current Data Parameters
NAME lzw2060-h
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20150310
Time 21.06
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 6
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 112.31
DW 62.400 usec
DE 6.50 usec
TE 297.7 K
D1 1.00000000 sec
TD0 1

==== CHANNEL f1 =====
SFO1 400.1324710 MHz
NUC1 1H
P1 14.50 usec
PLW1 11.99499989 W

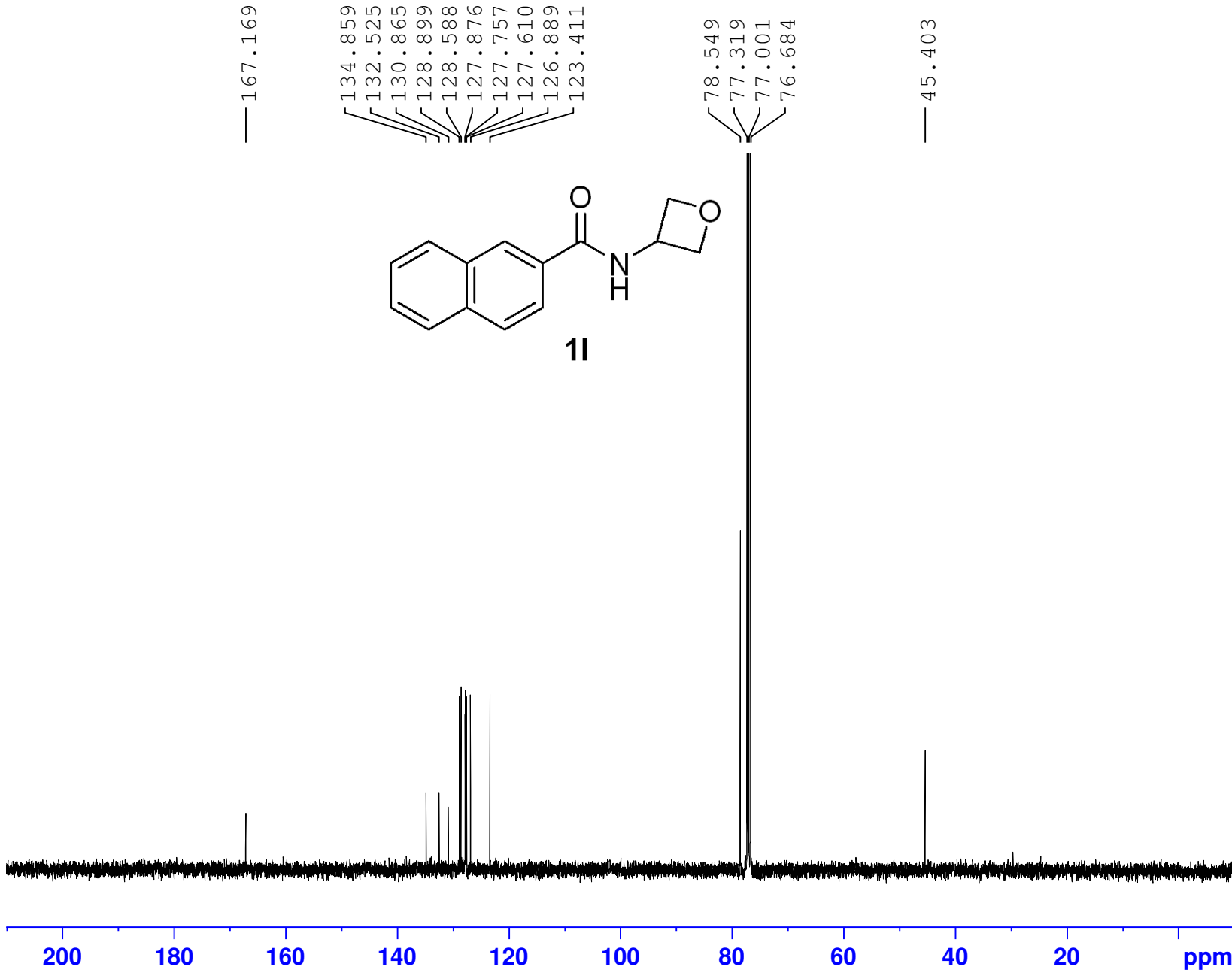
F2 - Processing parameters
SI 65536
SF 400.1300095 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

8.307
7.898
7.876
7.856
7.846
7.824
7.593
7.591
7.576
7.554
7.534
7.517
7.259
7.063
7.048
5.342
5.325
5.308
5.291
5.274
5.257
5.055
5.037
5.020
4.681
4.665
4.648



9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 ppm

1.02
4.16
2.09
0.98
1.00
2.05
2.05



Current Data Parameters
NAME lzw2060-c
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20150310
Time 21.15
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 122
DS 2
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 196.92
DW 20.800 usec
DE 6.50 usec
TE 298.5 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

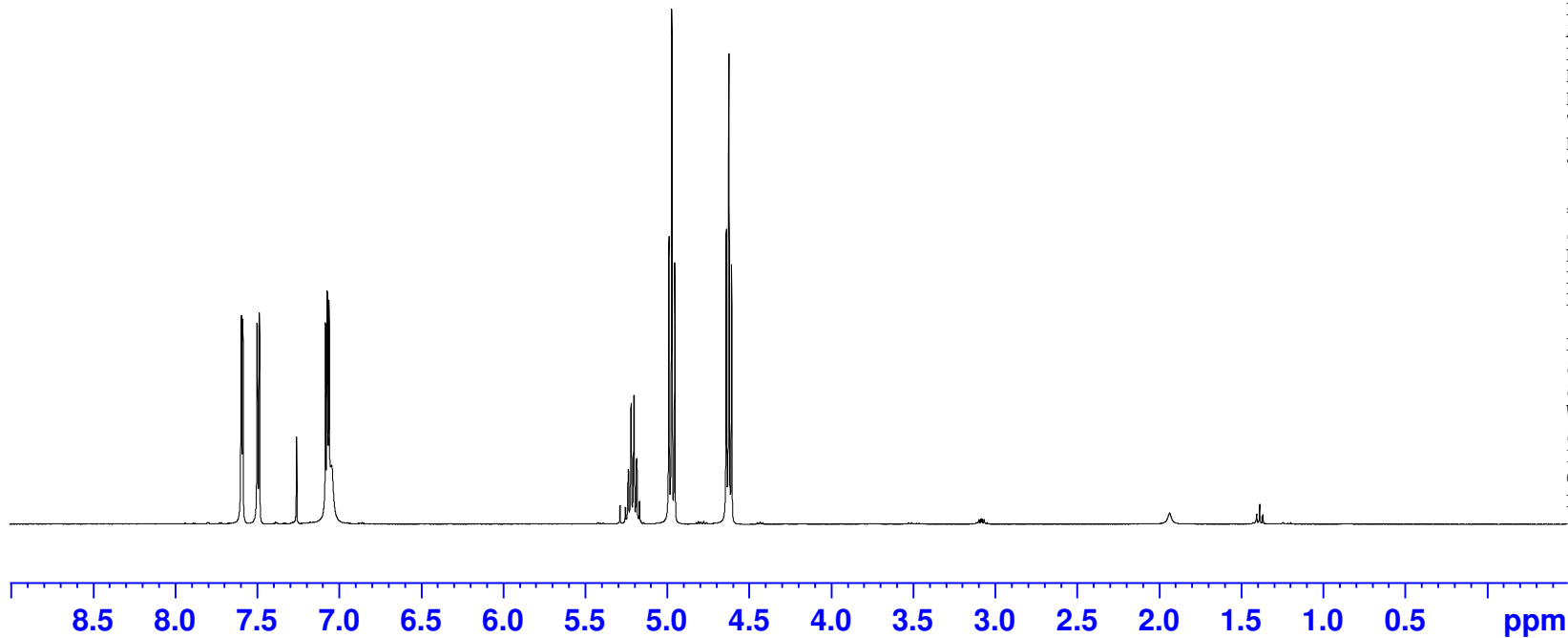
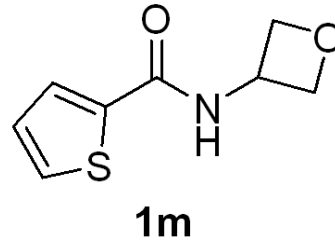
==== CHANNEL f1 =====
SFO1 100.6228298 MHz
NUC1 13C
P1 9.70 usec
PLW1 46.98899841 W

==== CHANNEL f2 =====
SFO2 400.1316005 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 90.00 usec
PLW2 11.99499989 W
PLW12 0.34213999 W
PLW13 0.27713001 W

F2 - Processing parameters
SI 32768
SF 100.6127728 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



7.598
7.596
7.589
7.587
7.500
7.498
7.488
7.486
7.260
7.083
7.074
7.071
7.062
7.046
5.236
5.220
5.202
5.186
5.168
4.989
4.971
4.954
4.639
4.623
4.607

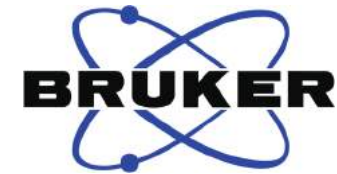


Current Data Parameters
NAME YW-1777
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20160512
Time 18.35
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT CDC13
NS 7
DS 0
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 103.52
DW 62.400 usec
DE 6.50 usec
TE 296.5 K
D1 1.00000000 sec
TD0 1

==== CHANNEL f1 =====
SFO1 400.1324710 MHz
NUC1 1H
P1 14.50 usec
PLW1 11.99499989 W

F2 - Processing parameters
SI 65536
SF 400.1300093 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

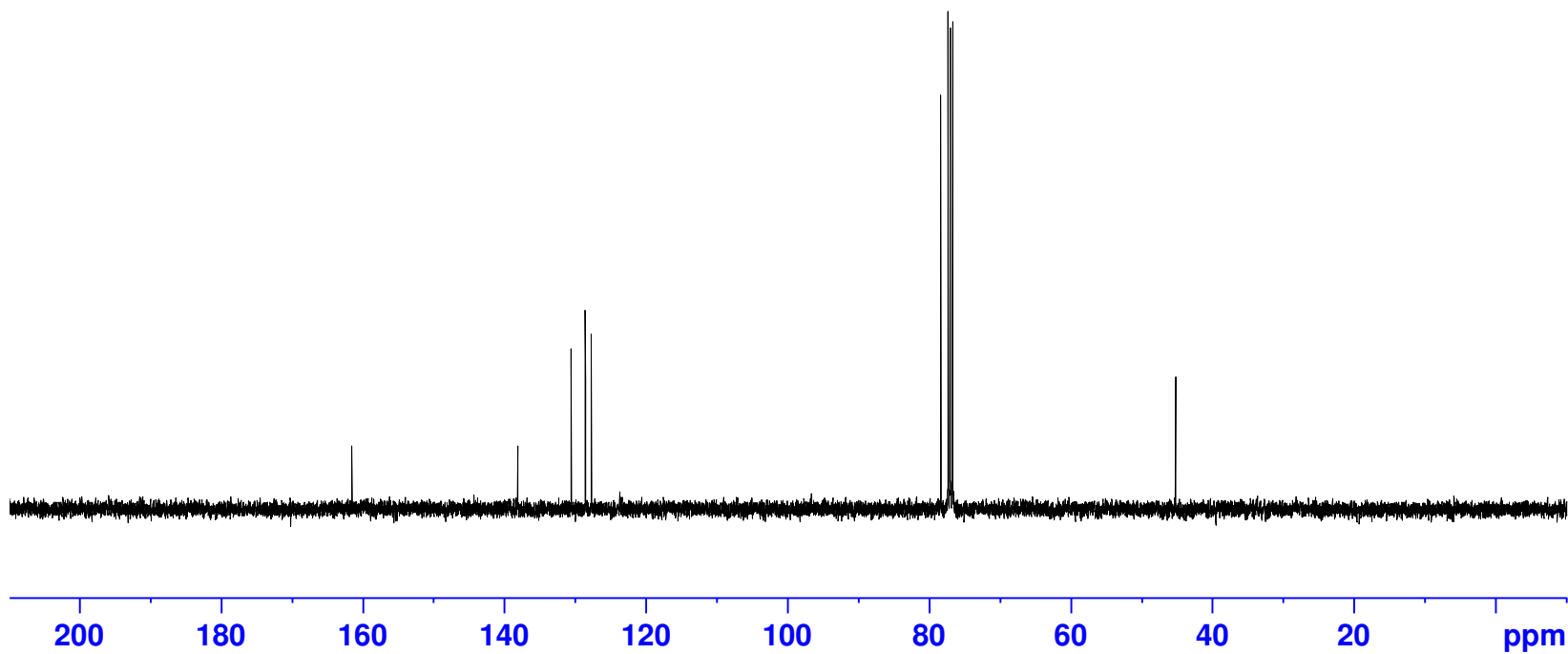
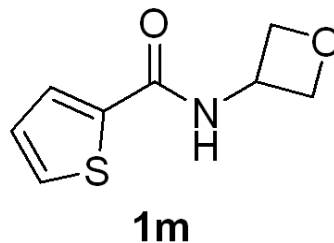


— 161.532

— 138.093
— 130.569
— 128.556
— 127.714

— 78.342
— 77.321
— 77.003
— 76.686

— 45.155



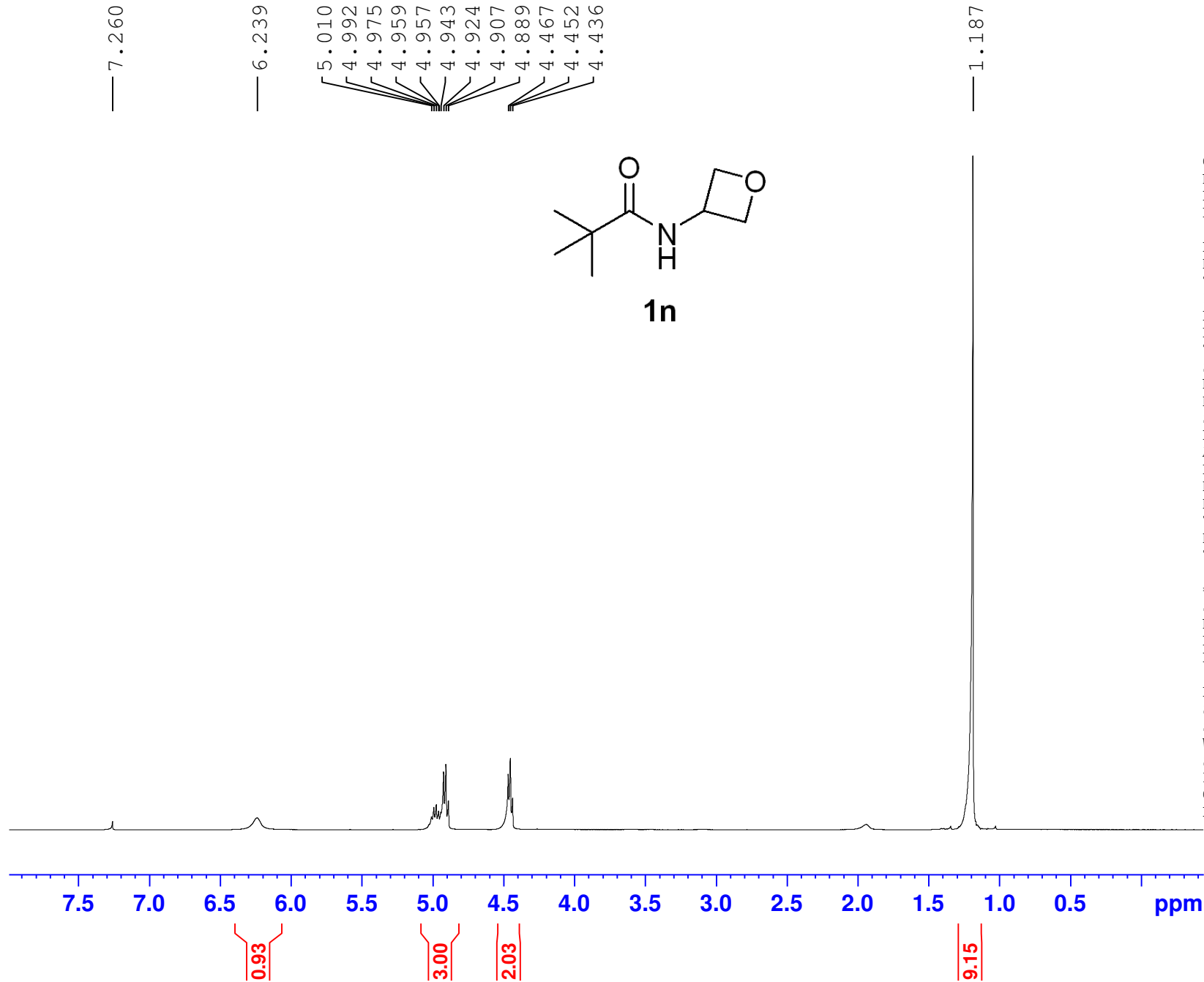
Current Data Parameters
NAME YW-1777-carbon
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20160512
Time 18.37
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 22
DS 0
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 196.92
DW 20.800 usec
DE 6.50 usec
TE 297.1 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

==== CHANNEL f1 =====
SFO1 100.6228298 MHz
NUC1 13C
P1 9.70 usec
PLW1 46.98899841 W

==== CHANNEL f2 =====
SFO2 400.1316005 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 90.00 usec
PLW2 11.99499989 W
PLW12 0.34213999 W
PLW13 0.27713001 W

F2 - Processing parameters
SI 32768
SF 100.6127758 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

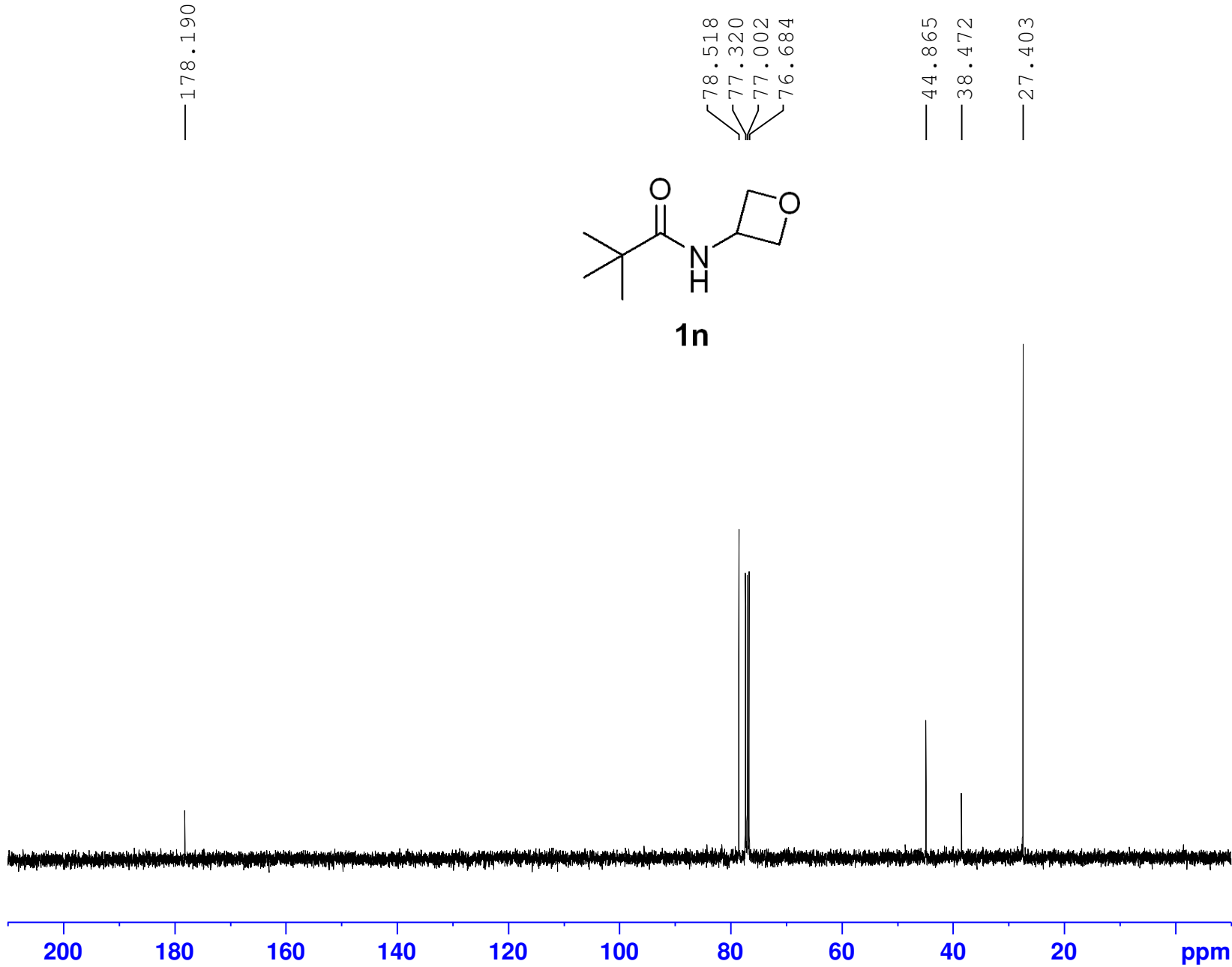
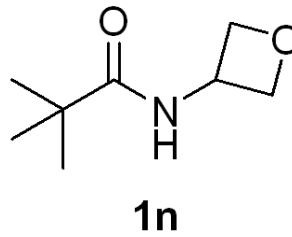


Current Data Parameters
NAME YW-1780
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20160813
Time 8.49
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT CDC13
NS 3
DS 0
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 62.93
DW 62.400 usec
DE 6.50 usec
TE 302.8 K
D1 1.00000000 sec
TD0 1

==== CHANNEL f1 =====
SFO1 400.1324710 MHz
NUC1 1H
P1 14.50 usec
PLW1 11.99499989 W

F2 - Processing parameters
SI 65536
SF 400.1300079 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



Current Data Parameters
NAME YW-1780-carbon
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20160813
Time 8.52
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 39
DS 0
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 196.92
DW 20.800 usec
DE 6.50 usec
TE 303.3 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

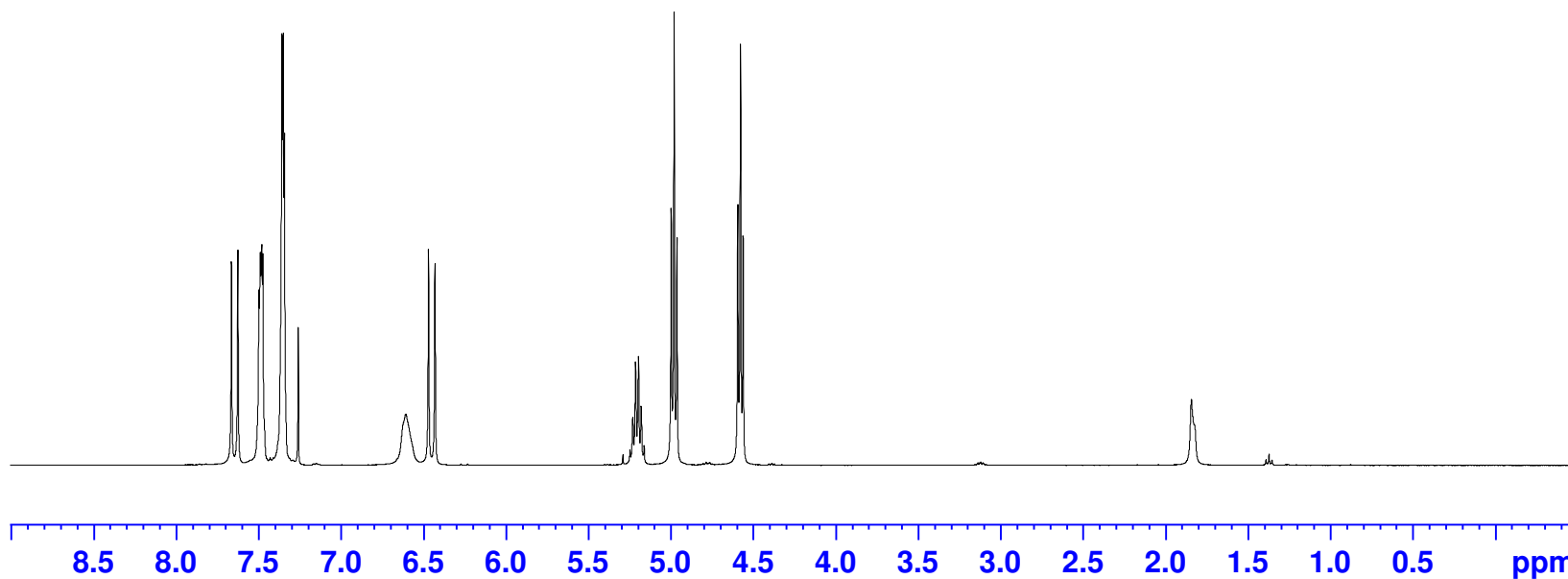
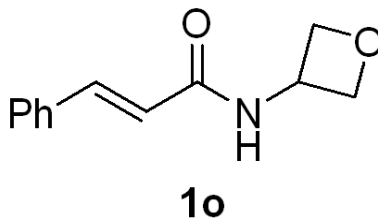
=====
CHANNEL f1
SFO1 100.6228298 MHz
NUC1 13C
P1 9.70 usec
PLW1 46.98899841 W

=====
CHANNEL f2
SFO2 400.1316005 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 90.00 usec
PLW2 11.99499989 W
PLW12 0.34213999 W
PLW13 0.27713001 W

F2 - Processing parameters
SI 32768
SF 100.6127737 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

7.665
7.626
7.498
7.489
7.485
7.481
7.475
7.359
7.351
7.344
7.260
6.608
6.470
6.431
5.230
5.214
5.196
5.180
5.162
4.998
4.980
4.962
4.594
4.578
4.561

— 1.843



Current Data Parameters
NAME YW-1905
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20160809
Time 15.16
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT CDC13
NS 16
DS 0
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 88.84
DW 62.400 usec
DE 6.50 usec
TE 298.7 K
D1 1.00000000 sec
TD0 1

==== CHANNEL f1 =====
SFO1 400.1324710 MHz
NUC1 1H
P1 14.50 usec
PLW1 11.99499989 W

F2 - Processing parameters
SI 65536
SF 400.1300093 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

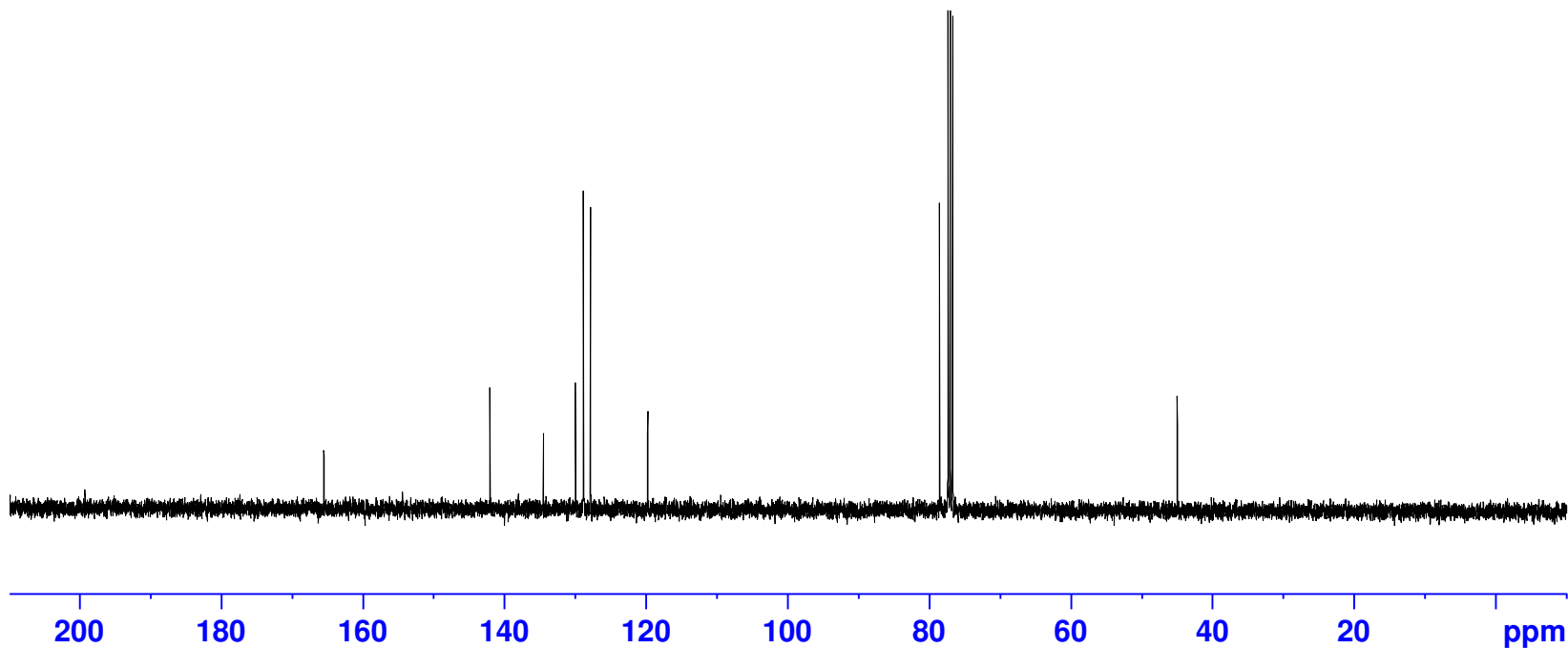
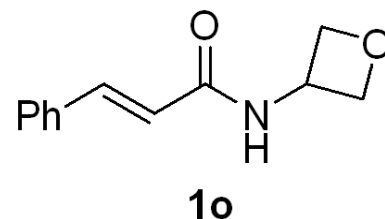


— 165.485

— 142.046
— 134.483
— 129.942
— 128.847
— 127.821
— 119.744

78.531
77.320
77.002
76.685

— 44.941



Current Data Parameters
NAME YW-1905-carbon
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20160809
Time 15.19
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 52
DS 0
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 196.92
DW 20.800 usec
DE 6.50 usec
TE 299.6 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

==== CHANNEL f1 =====
SFO1 100.6228298 MHz
NUC1 13C
P1 9.70 usec
PLW1 46.98899841 W

==== CHANNEL f2 =====
SFO2 400.1316005 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 90.00 usec
PLW2 11.99499989 W
PLW12 0.34213999 W
PLW13 0.27713001 W

F2 - Processing parameters
SI 32768
SF 100.6127736 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

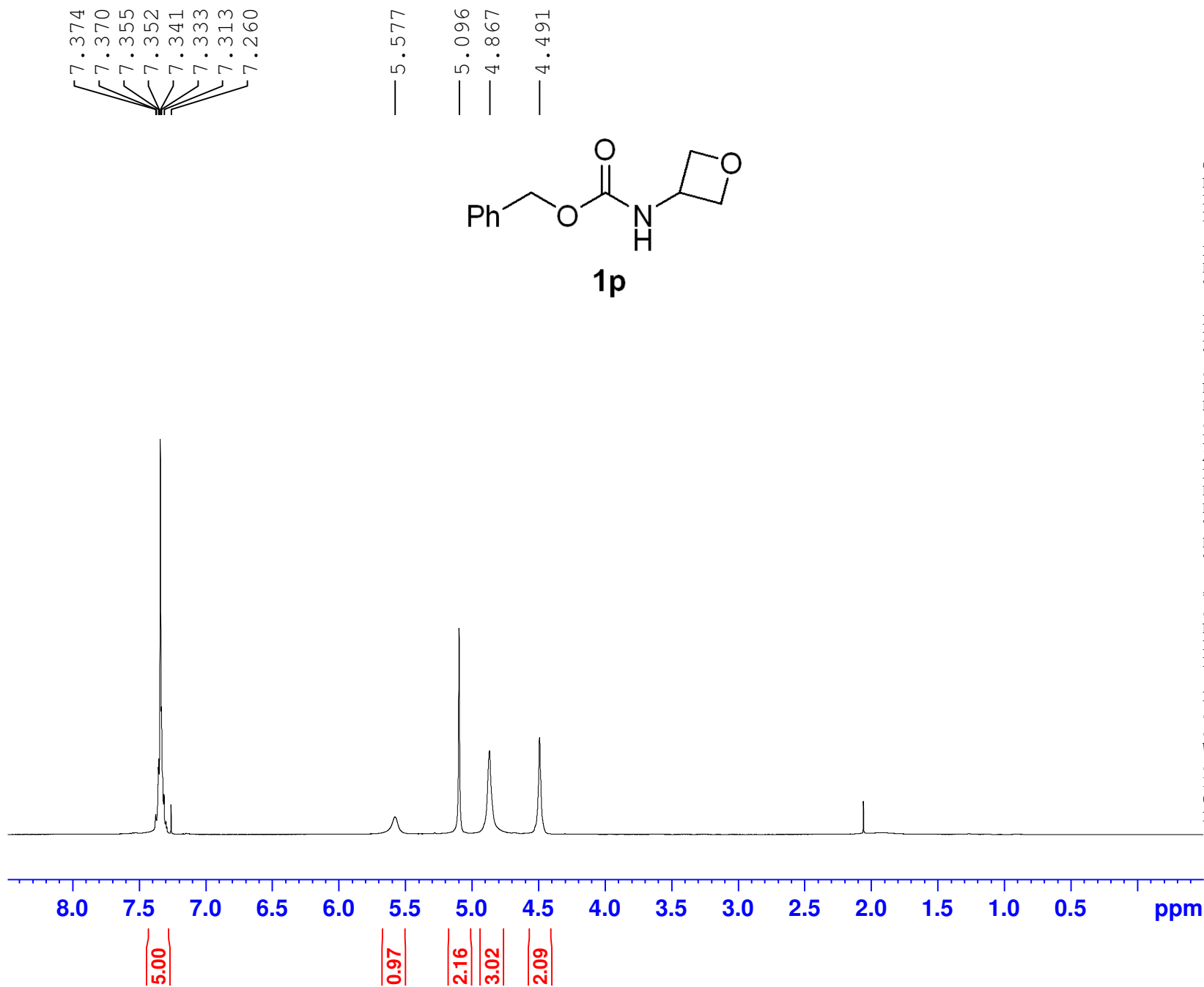
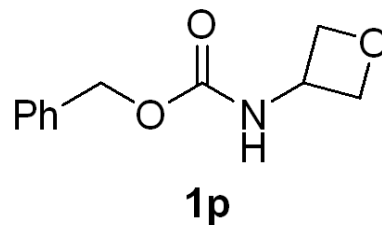


Current Data Parameters
NAME YW-1750
EXPNO 3
PROCNO 1

F2 - Acquisition Parameters
Date_ 20160813
Time 8.56
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 4
DS 0
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 54.81
DW 62.400 usec
DE 6.50 usec
TE 302.3 K
D1 1.00000000 sec
TD0 1

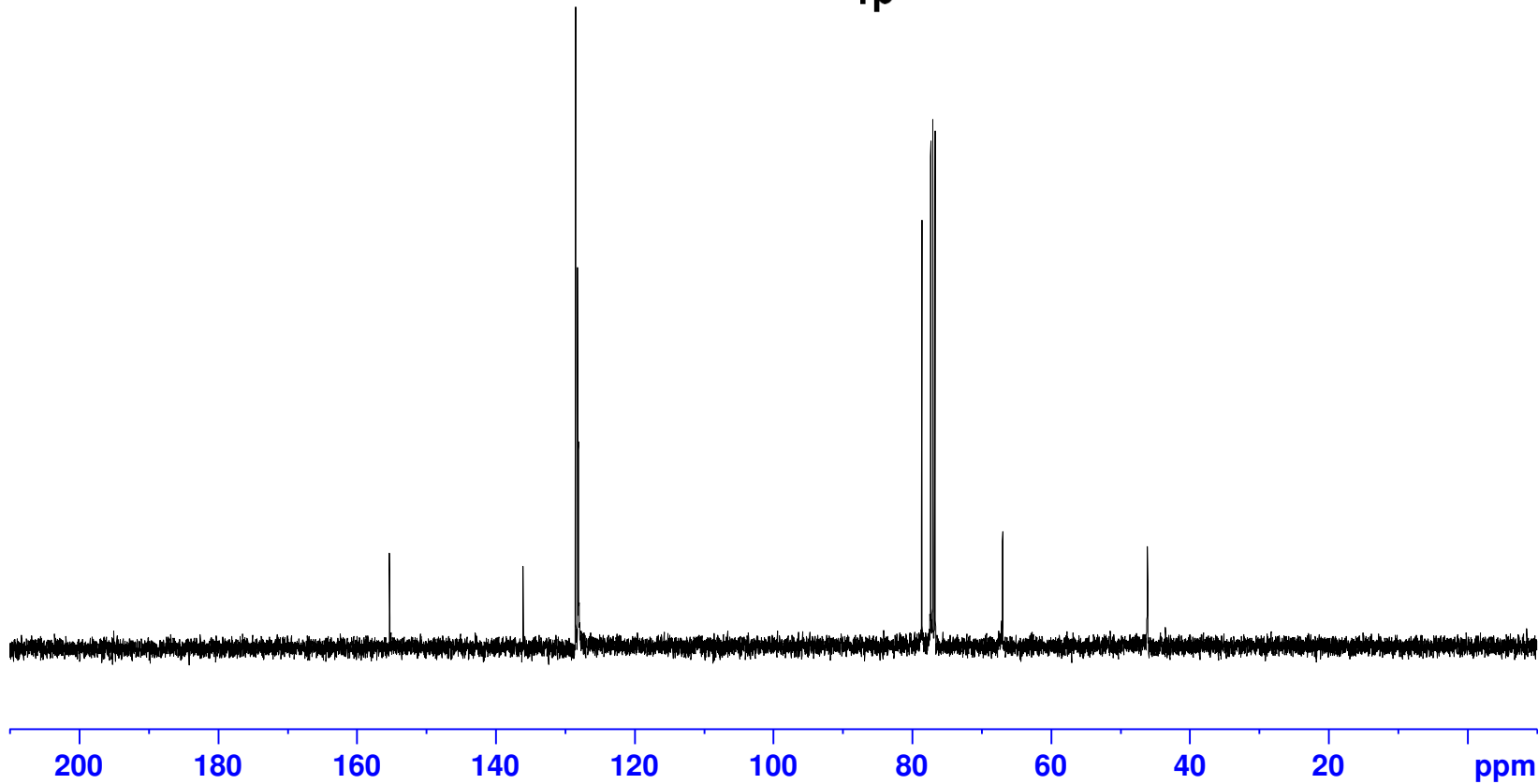
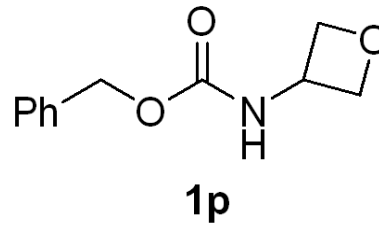
==== CHANNEL f1 =====
SFO1 400.1324710 MHz
NUC1 1H
P1 14.50 usec
PLW1 11.99499989 W

F2 - Processing parameters
SI 65536
SF 400.1300093 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00





— 155.303
— 136.062
— 128.501
— 128.222
— 128.084
— 78.590
— 77.317
— 76.999
— 76.681
— 66.949
— 46.077



Current Data Parameters
NAME YW-1750-carbon
EXPNO 3
PROCNO 1

F2 - Acquisition Parameters
Date_ 20160813
Time 9.01
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 45
DS 0
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 196.92
DW 20.800 usec
DE 6.50 usec
TE 302.8 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

==== CHANNEL f1 =====
SFO1 100.6228298 MHz
NUC1 13C
P1 9.70 usec
PLW1 46.98899841 W

==== CHANNEL f2 =====
SFO2 400.1316005 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 90.00 usec
PLW2 11.99499989 W
PLW12 0.34213999 W
PLW13 0.27713001 W

F2 - Processing parameters
SI 32768
SF 100.6127773 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



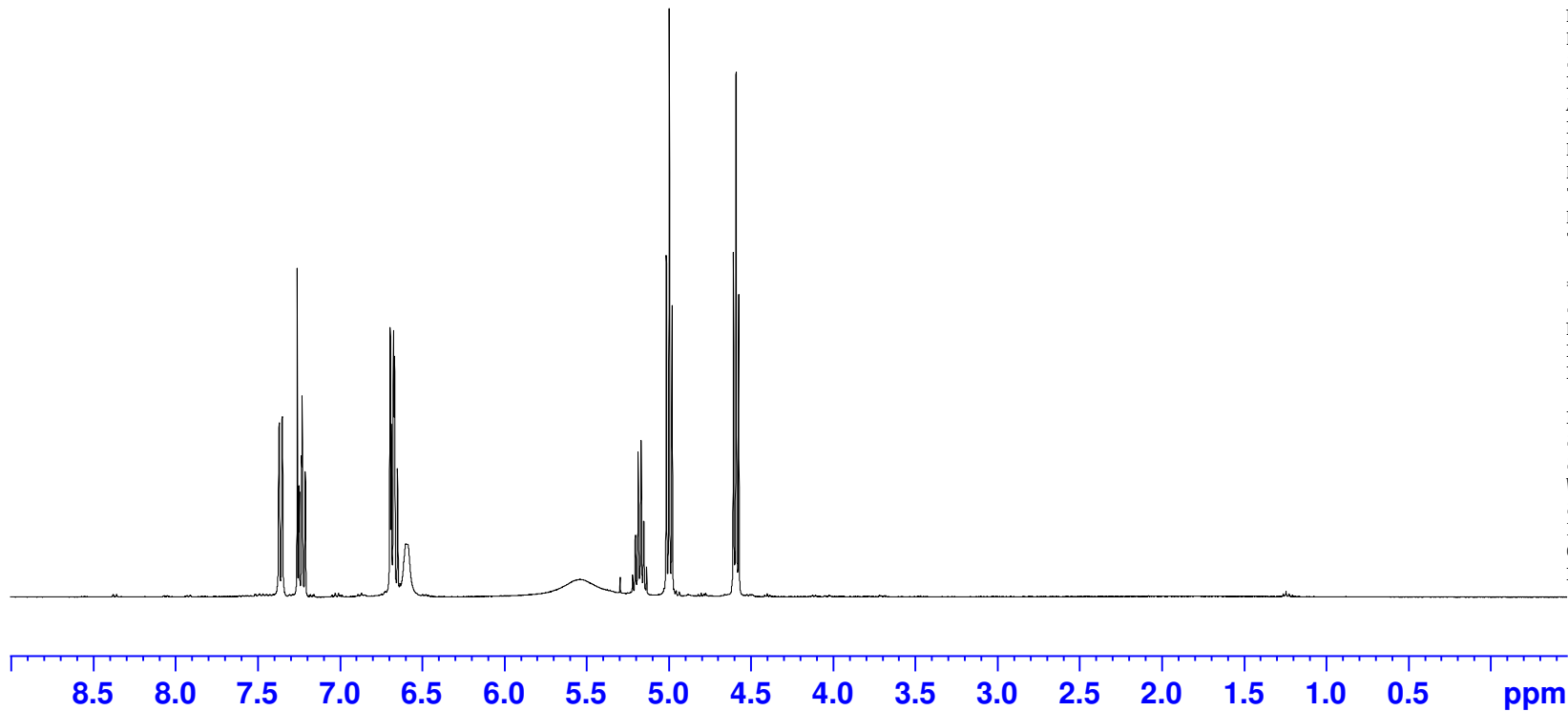
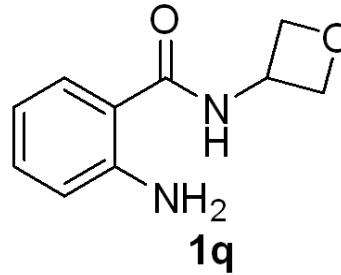
Current Data Parameters
NAME YW-1688
EXPNO 1
PROCNO 1

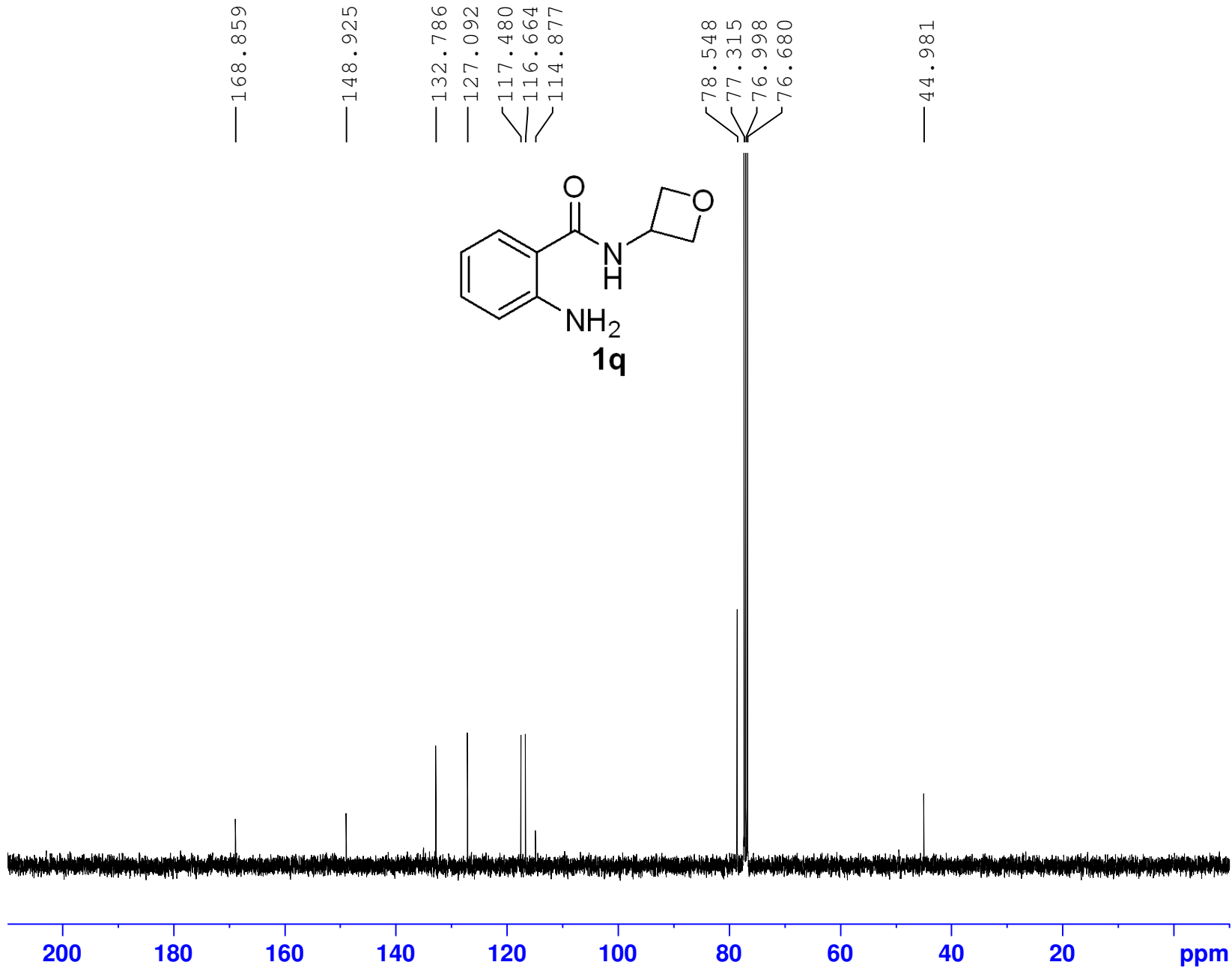
F2 - Acquisition Parameters
Date_ 20160319
Time 20.16
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 11
DS 0
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 112.31
DW 62.400 usec
DE 6.50 usec
TE 298.0 K
D1 1.00000000 sec
TD0 1

==== CHANNEL f1 =====
SFO1 400.1324710 MHz
NUC1 1H
P1 14.50 usec
PLW1 11.99499989 W

F2 - Processing parameters
SI 65536
SF 400.1300095 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

7.260
7.251
7.247
7.233
7.230
7.227
7.213
7.209
6.694
6.688
6.685
6.673
6.669
6.668
6.650
6.647
6.600
5.542
5.219
5.204
5.202
5.186
5.168
5.152
5.134
5.014
4.997
4.979
4.606
4.590
4.574





Current Data Parameters
NAME YW-1688-carbon
EXPNO 1
PROCNO 1

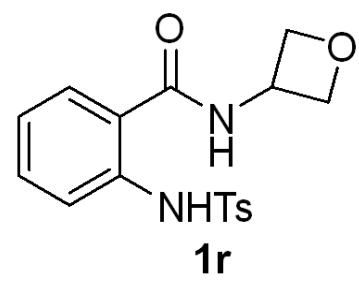
F2 - Acquisition Parameters
Date_ 20160319
Time 20.20
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 63
DS 0
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 196.92
DW 20.800 usec
DE 6.50 usec
TE 298.8 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

==== CHANNEL f1 =====
SFO1 100.6228298 MHz
NUC1 13C
P1 9.70 usec
PLW1 46.98899841 W

==== CHANNEL f2 =====
SFO2 400.1316005 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 90.00 usec
PLW2 11.99499989 W
PLW12 0.34213999 W
PLW13 0.27713001 W

F2 - Processing parameters
SI 32768
SF 100.6127721 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

11.159
7.746
7.743
7.726
7.723
7.685
7.683
7.664
7.662
7.641
7.637
7.625
7.621
7.616
7.501
7.497
7.482
7.479
7.462
7.458
7.308
7.306
7.286
7.285
7.139
7.136
7.120
7.119
7.118
7.117
7.101
7.098
5.078
5.076
5.059
5.057
5.041
4.847
4.829
4.811
4.592
4.575
4.559
2.875
2.342
2.056
2.050
2.045

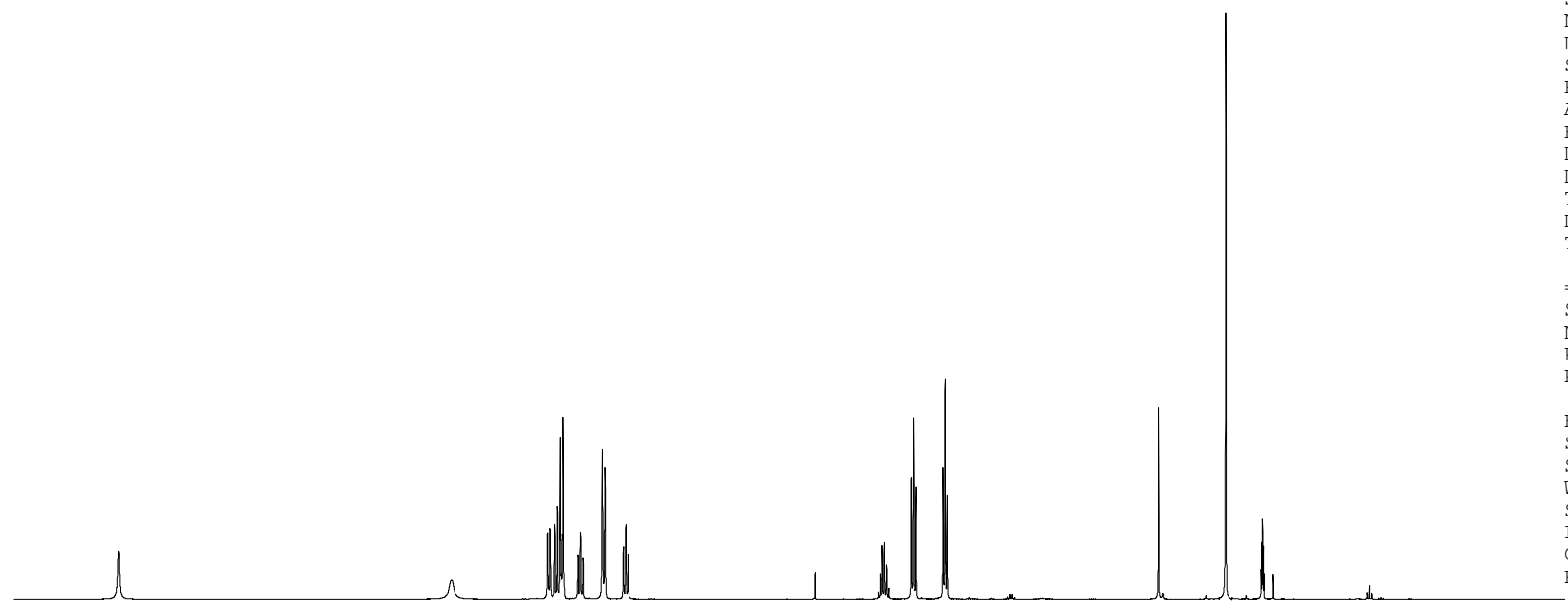


Current Data Parameters
NAME YW-1701
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20160813
Time 9.31
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT Acetone
NS 4
DS 0
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 49.32
DW 62.400 usec
DE 6.50 usec
TE 300.7 K
D1 1.00000000 sec
TD0 1

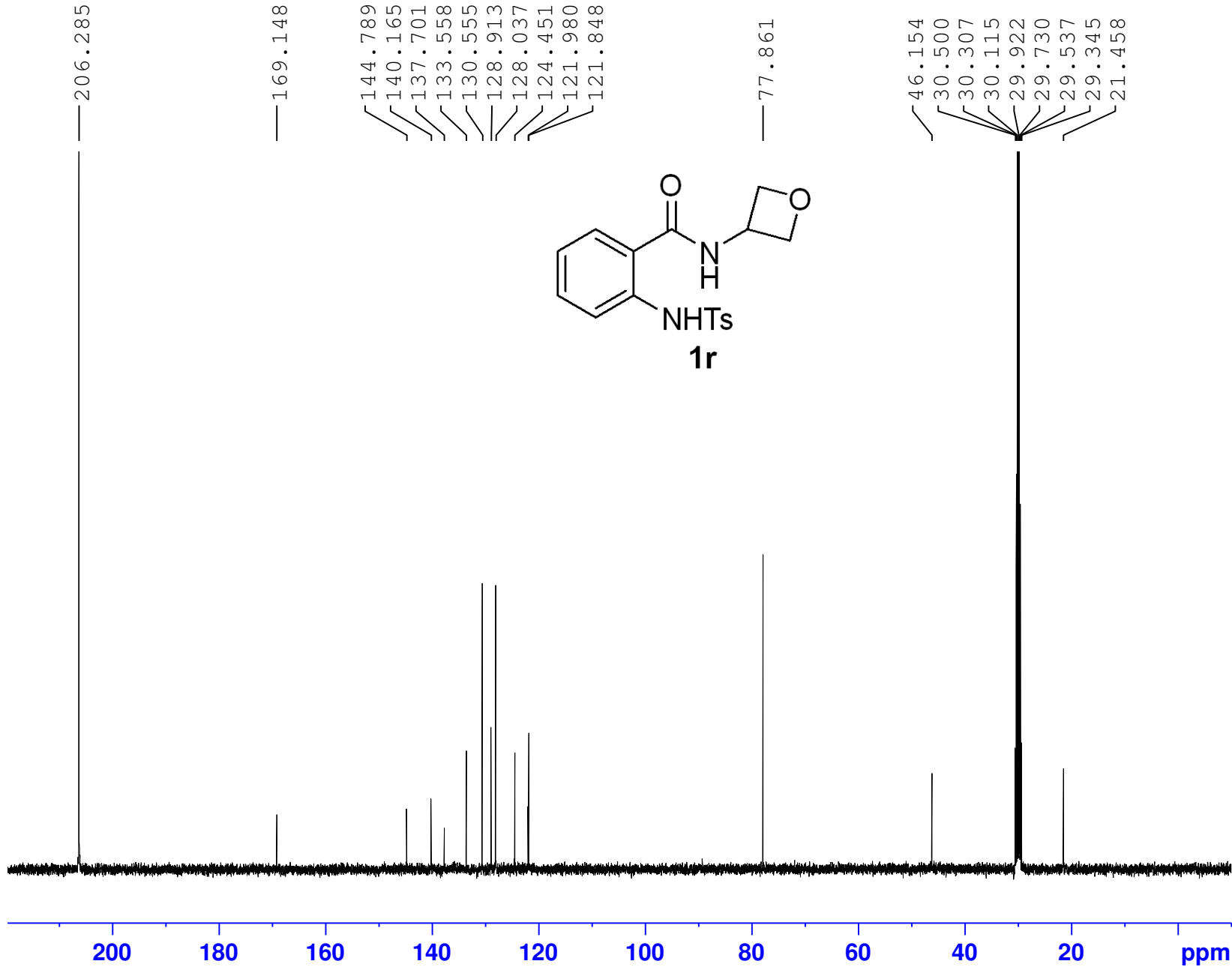
==== CHANNEL f1 =====
SFO1 400.1324710 MHz
NUC1 1H
P1 14.50 usec
PLW1 11.99499989 W

F2 - Processing parameters
SI 65536
SF 400.1300067 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



11 10 9 8 7 6 5 4 3 2 1 ppm

0.89 0.98 1.05 2.97 1.02 1.99 1.02 1.00 2.06 2.06 3.08



Current Data Parameters
NAME YW-1701-carbon
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20160813
Time 9.35
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT Acetone
NS 58
DS 0
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 196.92
DW 20.800 usec
DE 6.50 usec
TE 301.4 K
D1 2.0000000 sec
D11 0.0300000 sec
TD0 1

==== CHANNEL f1 =====
SFO1 100.6228298 MHz
NUC1 13C
P1 9.70 usec
PLW1 46.98899841 W

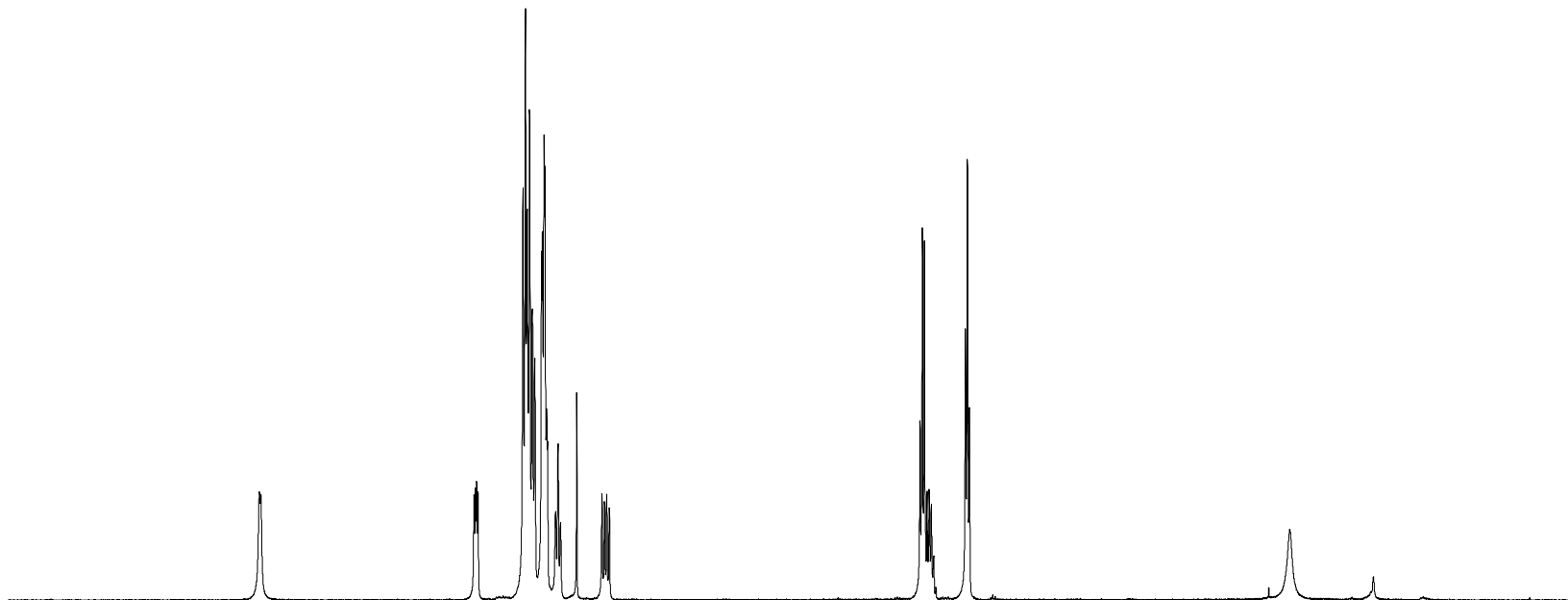
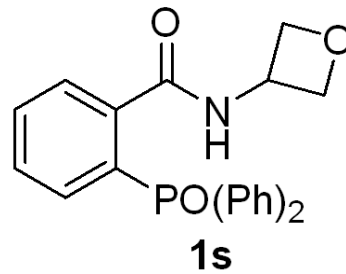
==== CHANNEL f2 =====
SFO2 400.1316005 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 90.00 usec
PLW2 11.99499989 W
PLW12 0.34213999 W
PLW13 0.27713001 W

F2 - Processing parameters
SI 32768
SF 100.6126725 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



9.658
9.646
8.036
8.026
8.017
8.007
7.666
7.648
7.635
7.617
7.597
7.578
7.526
7.519
7.507
7.500
7.489
7.481
7.420
7.401
7.382
7.260
7.070
7.051
7.034
7.015
4.667
4.649
4.634
4.614
4.599
4.582
4.564
4.325
4.310
4.295

— 1.874



11 10 9 8 7 6 5 4 3 2 1 ppm

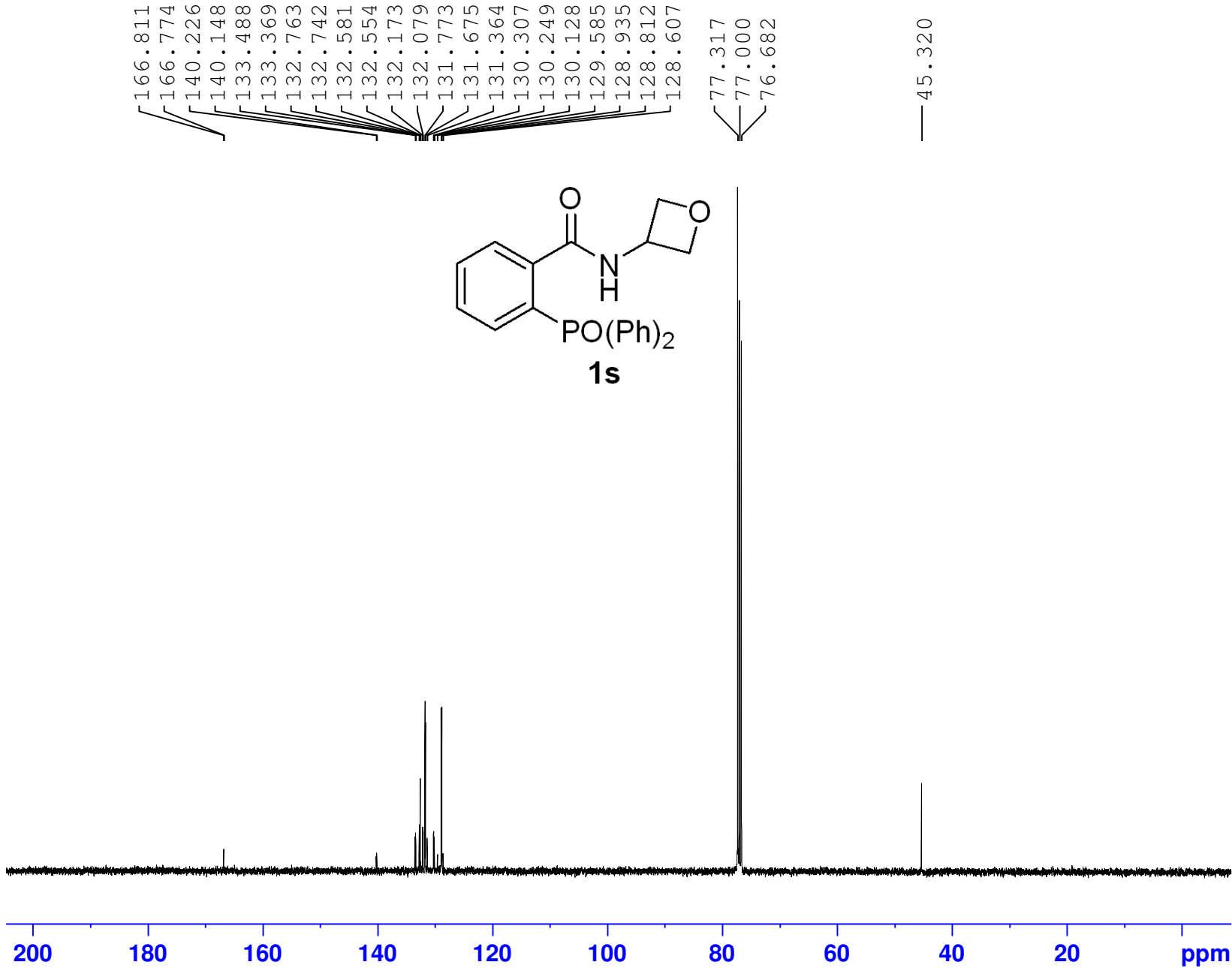
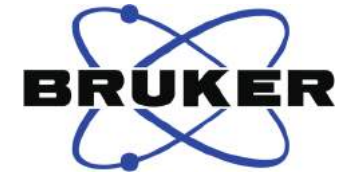
1.00
1.00
7.24
4.12
1.08
1.03
3.09
2.06
S-98

Current Data Parameters
NAME cz1-2-6
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20170822
Time 16.00
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT CDC13
NS 4
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 187.77
DW 62.400 usec
DE 6.50 usec
TE 296.4 K
D1 1.00000000 sec
TD0 1

==== CHANNEL f1 =====
SFO1 400.1324710 MHz
NUC1 1H
P1 14.50 usec
PLW1 11.99499989 W

F2 - Processing parameters
SI 65536
SF 400.1300101 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



Current Data Parameters
NAME czl-2-6
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20170822
Time 16.06
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 200
DS 2
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 196.92
DW 20.800 usec
DE 6.50 usec
TE 297.4 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

==== CHANNEL f1 =====
SFO1 100.6228298 MHz
NUC1 13C
P1 9.70 usec
PLW1 46.98899841 W

==== CHANNEL f2 =====
SFO2 400.1316005 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 90.00 usec
PLW2 11.99499989 W
PLW12 0.34213999 W
PLW13 0.27713001 W

F2 - Processing parameters
SI 32768
SF 100.6127736 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



Current Data Parameters
NAME cz1-2-6
EXPNO 3
PROCNO 1

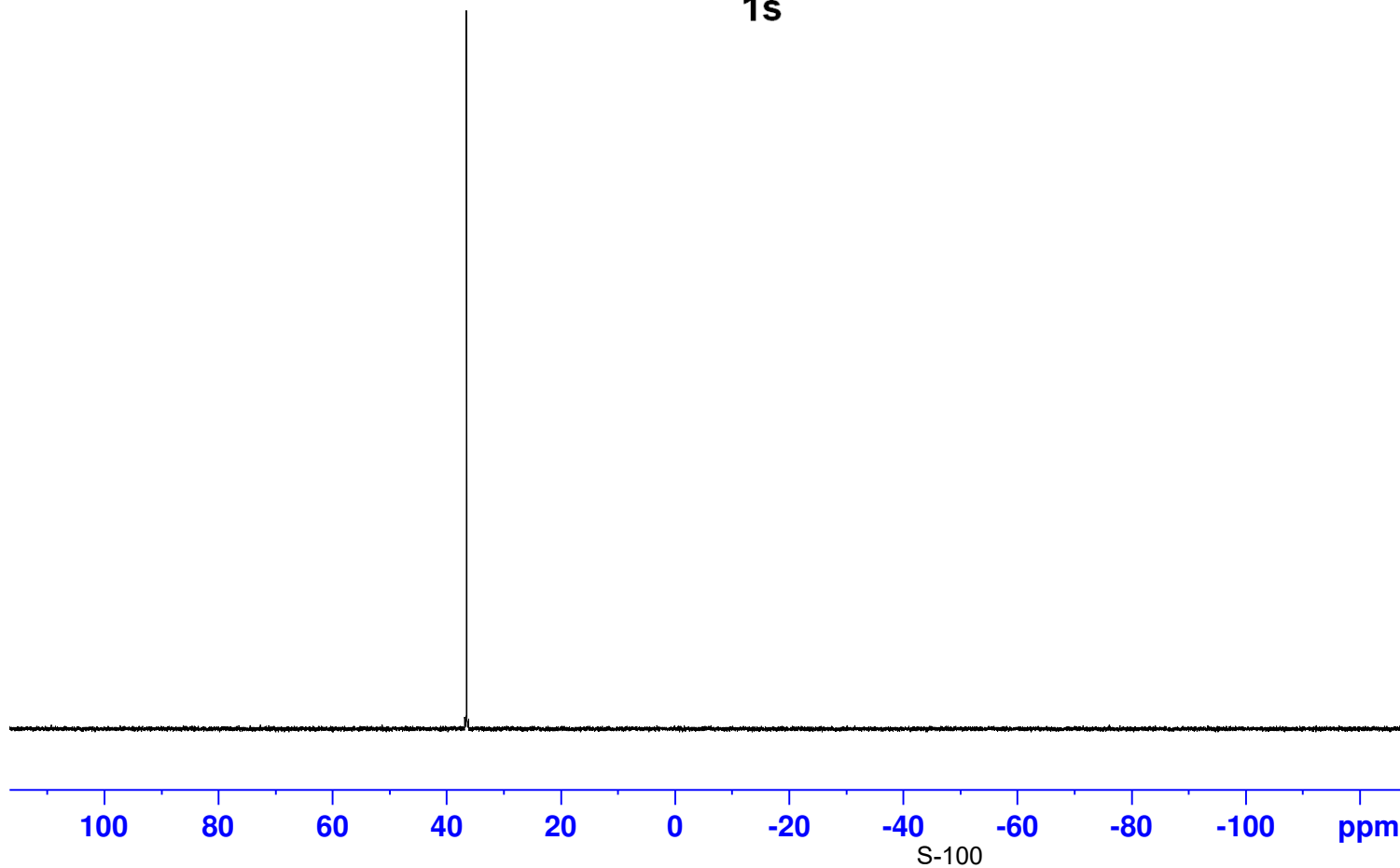
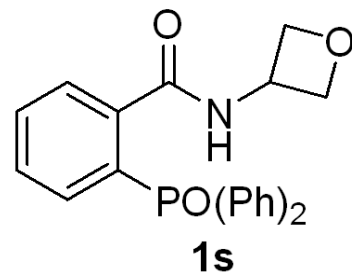
F2 - Acquisition Parameters
Date_ 20170822
Time 16.15
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 32
DS 4
SWH 64102.563 Hz
FIDRES 0.978127 Hz
AQ 0.5111808 sec
RG 196.92
DW 7.800 usec
DE 6.50 usec
TE 297.1 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

=====
CHANNEL f1
SFO1 161.9674942 MHz
NUC1 31P
P1 14.70 usec
PLW1 11.99499989 W

=====
CHANNEL f2
SFO2 400.1316005 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 90.00 usec
PLW2 11.99499989 W
PLW12 0.34213999 W
PLW13 0.27713001 W

F2 - Processing parameters
SI 32768
SF 161.9755930 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

36.51



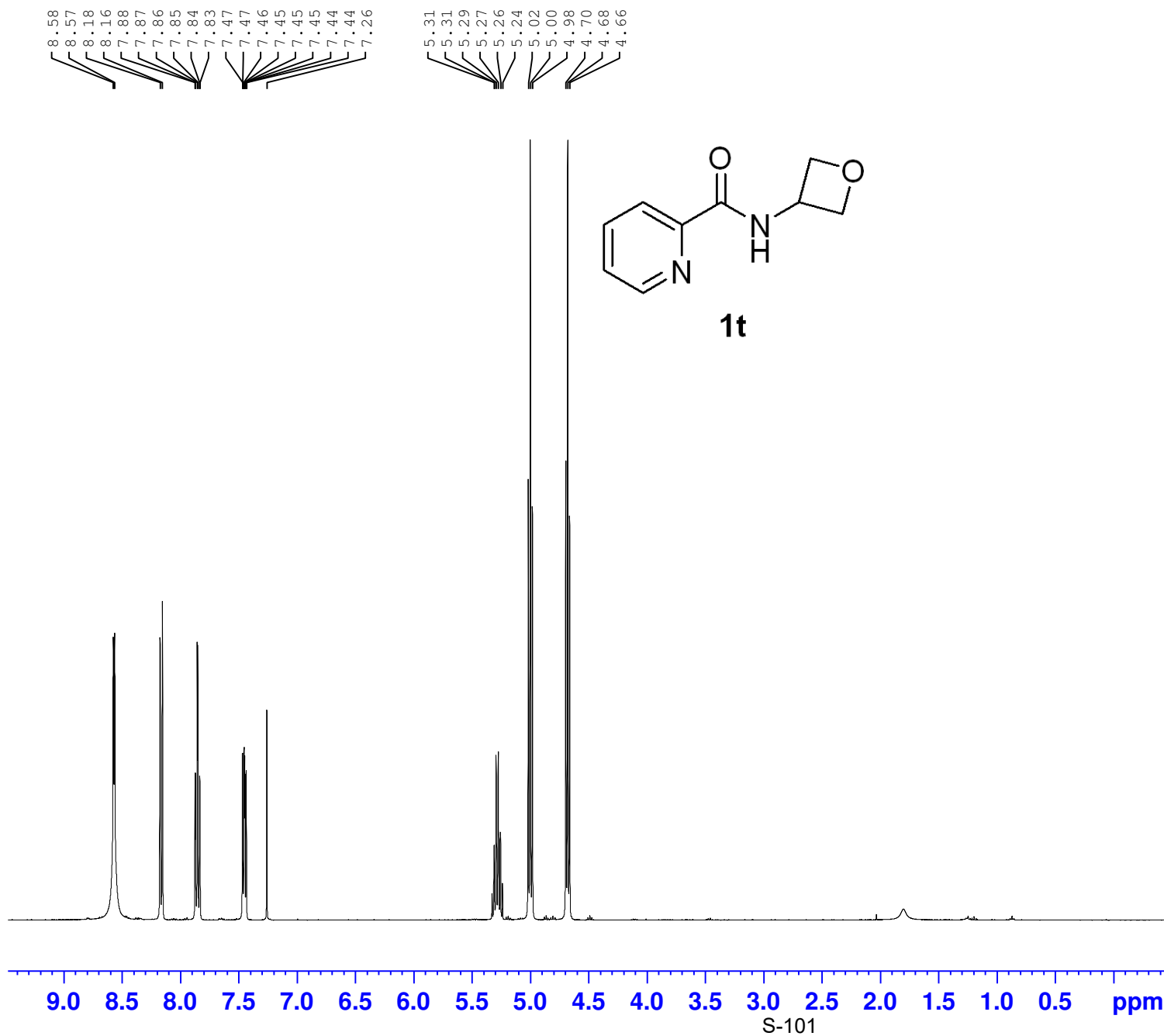


Current Data Parameters
NAME YW-1668
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20160319
Time 20.07
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 8
DS 0
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 103.52
DW 62.400 usec
DE 6.50 usec
TE 297.9 K
D1 1.00000000 sec
TD0 1

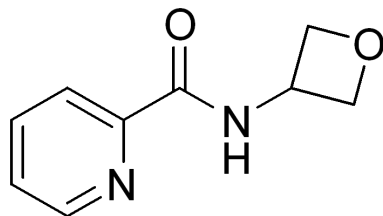
==== CHANNEL f1 =====
SFO1 400.1324710 MHz
NUC1 1H
P1 14.50 usec
PLW1 11.99499989 W

F2 - Processing parameters
SI 65536
SF 400.1300094 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

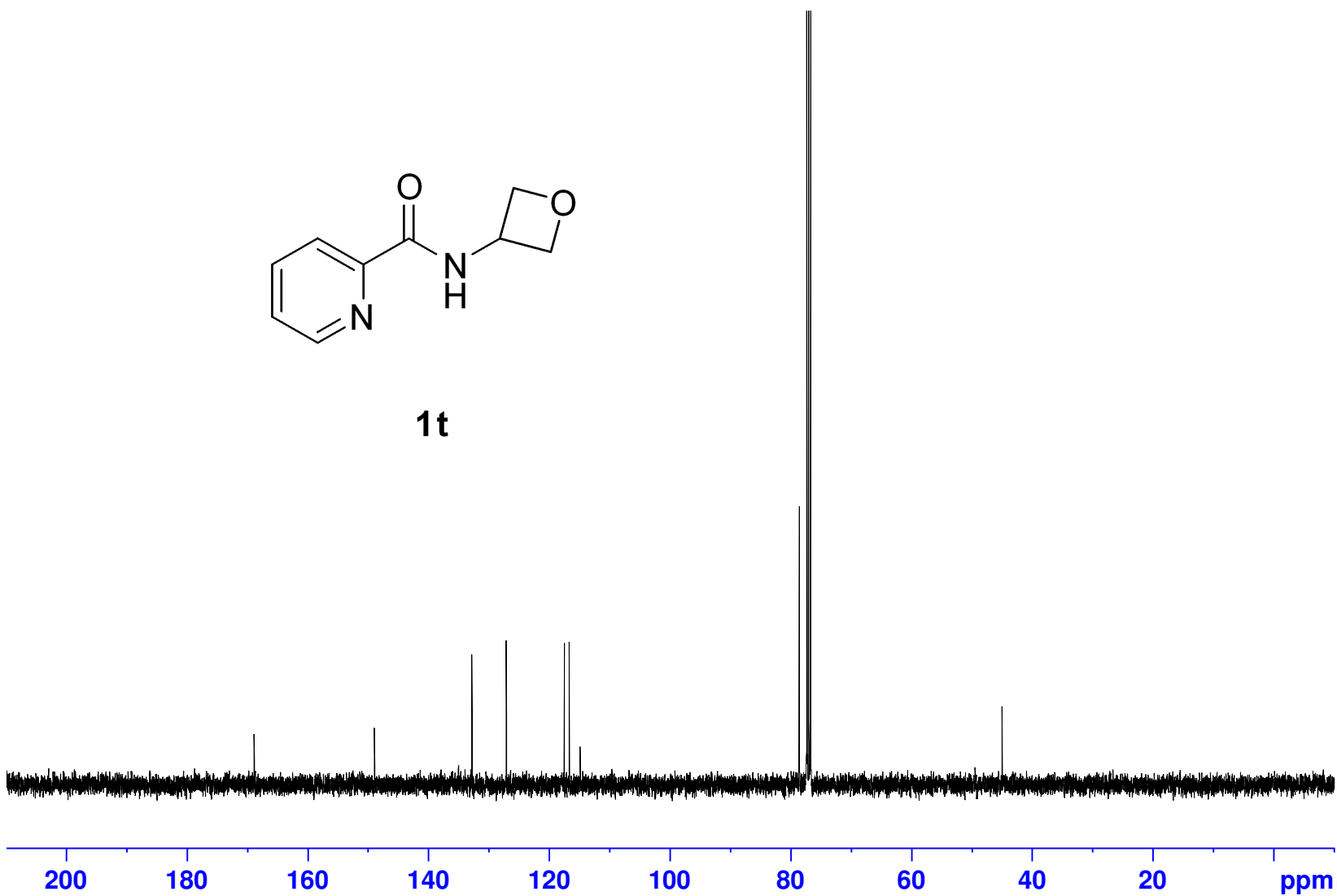




—168.859
—148.925
—132.786
—127.092
117.480
116.664
114.877
78.548
77.315
76.998
76.680
—44.981



1t



Current Data Parameters
NAME YW-1688-carbon
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20160319
Time 20.20
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 63
DS 0
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 196.92
DW 20.800 usec
DE 6.50 usec
TE 298.8 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

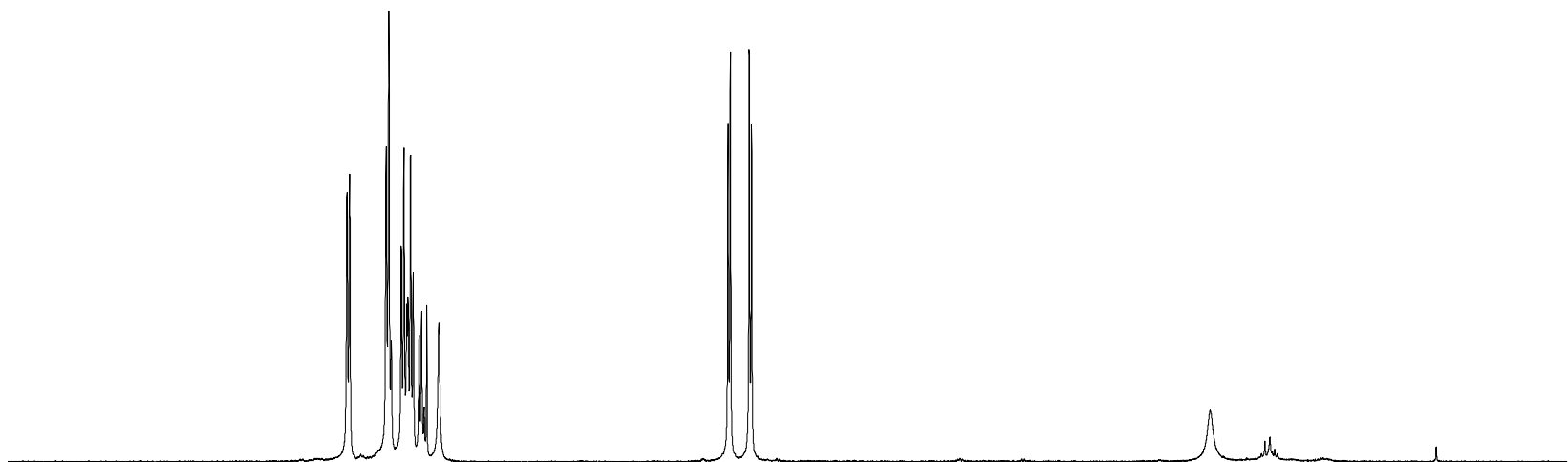
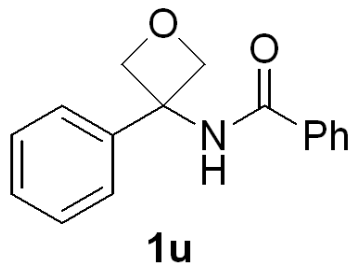
==== CHANNEL f1 =====
SFO1 100.6228298 MHz
NUC1 13C
P1 9.70 usec
PLW1 46.98899841 W

==== CHANNEL f2 =====
SFO2 400.1316005 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 90.00 usec
PLW2 11.99499989 W
PLW12 0.34213999 W
PLW13 0.27713001 W

F2 - Processing parameters
SI 32768
SF 100.6127721 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



7.827
7.809
7.548
7.529
7.512
7.441
7.421
7.402
7.393
7.375
7.355
7.314
7.295
7.277
7.259
7.172
5.114
5.097
4.963
4.946

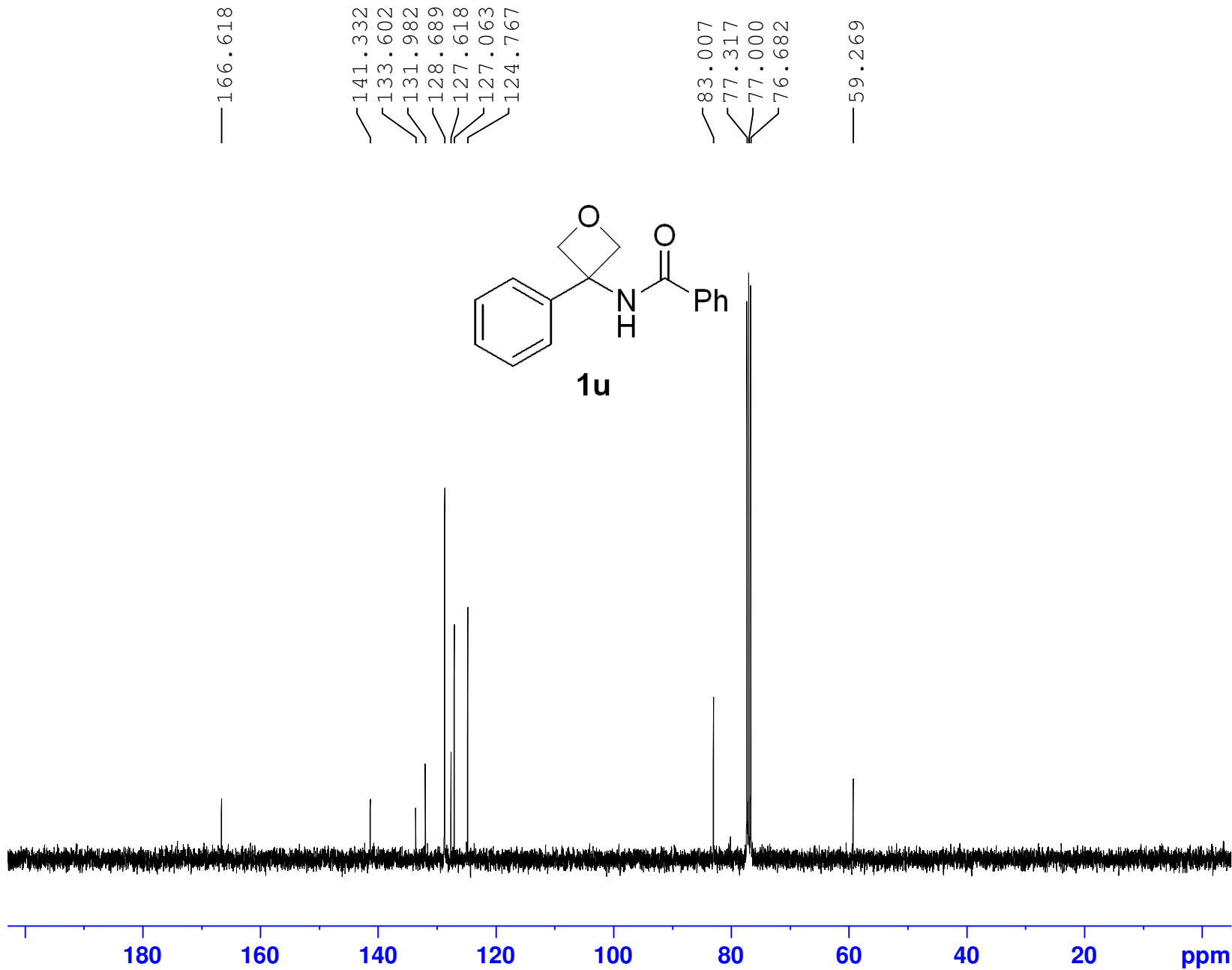
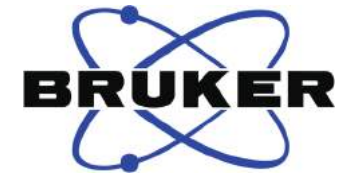


Current Data Parameters
NAME czl-1-180
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20170731
Time 13.01
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT CDC13
NS 4
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 187.77
DW 62.400 usec
DE 6.50 usec
TE 297.4 K
D1 1.00000000 sec
TD0 1

==== CHANNEL f1 =====
SFO1 400.1324710 MHz
NUC1 1H
P1 14.50 usec
PLW1 11.99499989 W

F2 - Processing parameters
SI 65536
SF 400.1300105 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



Current Data Parameters
NAME czl-1-180
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20170731
Time 13.17
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 80
DS 2
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 196.92
DW 20.800 usec
DE 6.50 usec
TE 297.9 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

==== CHANNEL f1 =====
SFO1 100.6228298 MHz
NUC1 13C
P1 9.70 usec
PLW1 46.98899841 W

==== CHANNEL f2 =====
SFO2 400.1316005 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 90.00 usec
PLW2 11.99499989 W
PLW12 0.34213999 W
PLW13 0.27713001 W

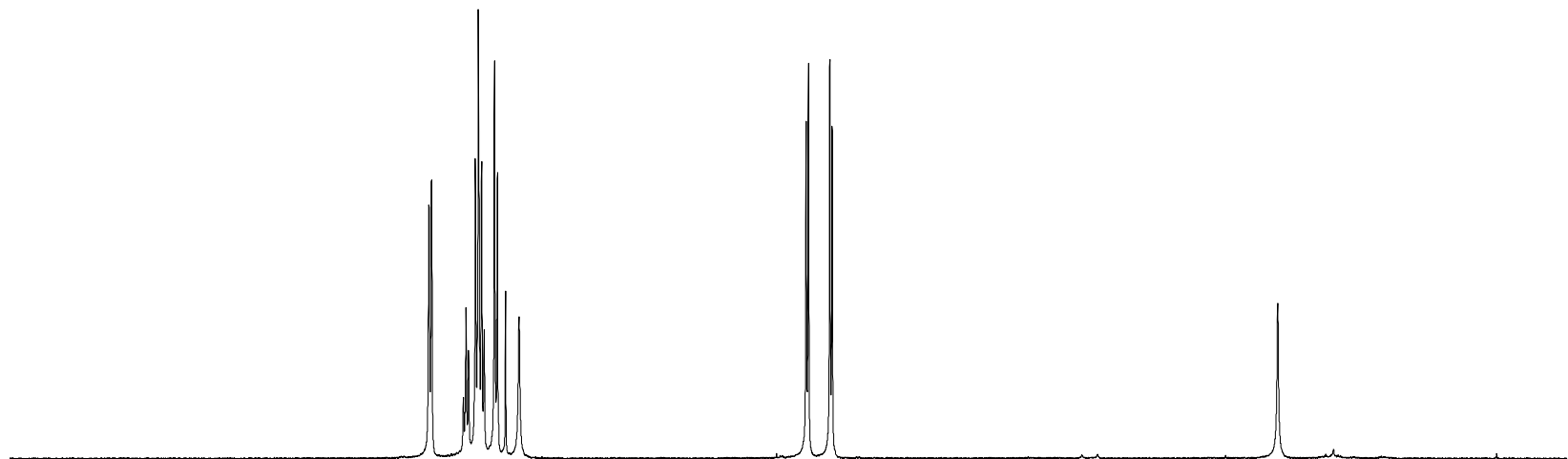
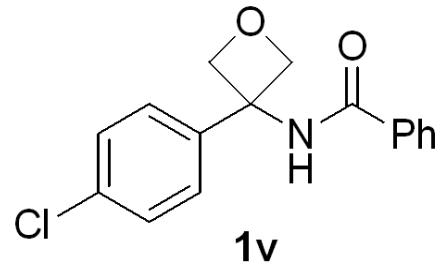
F2 - Processing parameters
SI 32768
SF 100.6127736 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



7.815
7.797
7.566
7.547
7.528
7.479
7.458
7.453
7.433
7.414
7.340
7.319
7.260
7.162

5.080
5.062
4.908
4.891

—1.658



10 9 8 7 6 5 4 3 2 1 ppm

2.04
1.14
4.09
2.10
1.00

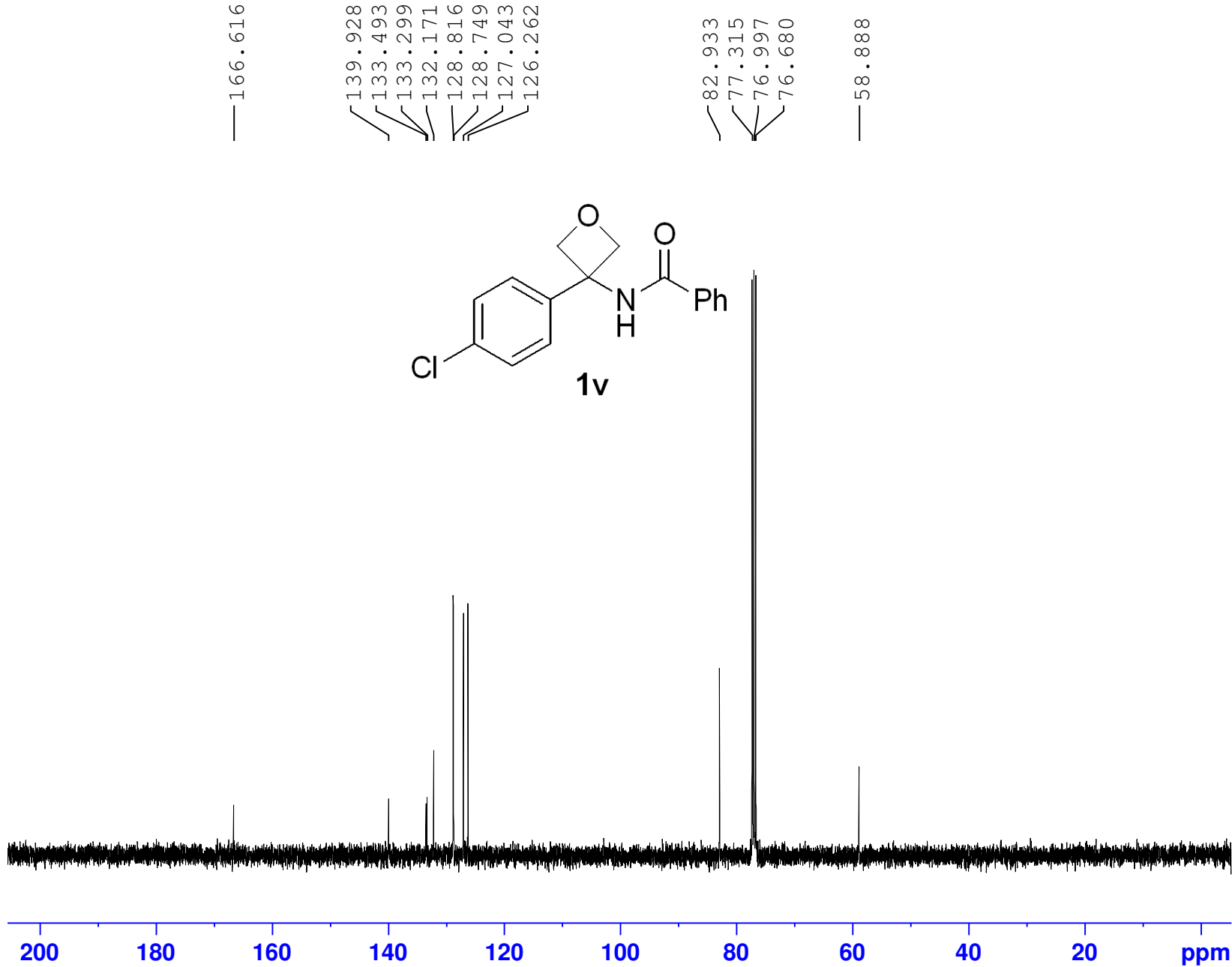
2.09
2.04

Current Data Parameters
NAME czl-1-181
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20170731
Time 13.03
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 4
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 187.77
DW 62.400 usec
DE 6.50 usec
TE 297.3 K
D1 1.00000000 sec
TD0 1

==== CHANNEL f1 =====
SFO1 400.1324710 MHz
NUC1 1H
P1 14.50 usec
PLW1 11.99499989 W

F2 - Processing parameters
SI 65536
SF 400.1300104 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



Current Data Parameters
NAME czl-1-181
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20170731
Time 13.22
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 100
DS 2
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 196.92
DW 20.800 usec
DE 6.50 usec
TE 298.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

==== CHANNEL f1 =====
SFO1 100.6228298 MHz
NUC1 13C
P1 9.70 usec
PLW1 46.98899841 W

==== CHANNEL f2 =====
SFO2 400.1316005 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 90.00 usec
PLW2 11.99499989 W
PLW12 0.34213999 W
PLW13 0.27713001 W

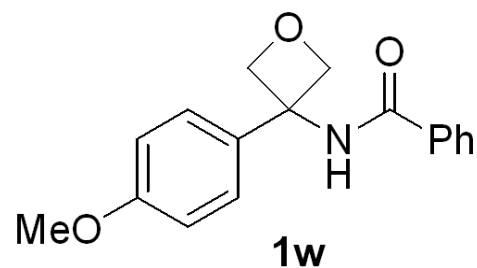
F2 - Processing parameters
SI 32768
SF 100.6127734 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



7.805
7.787
7.514
7.495
7.439
7.417
7.398
7.379
7.260
7.248
6.890
6.869

5.088
5.072
4.920
4.904

— 3.789

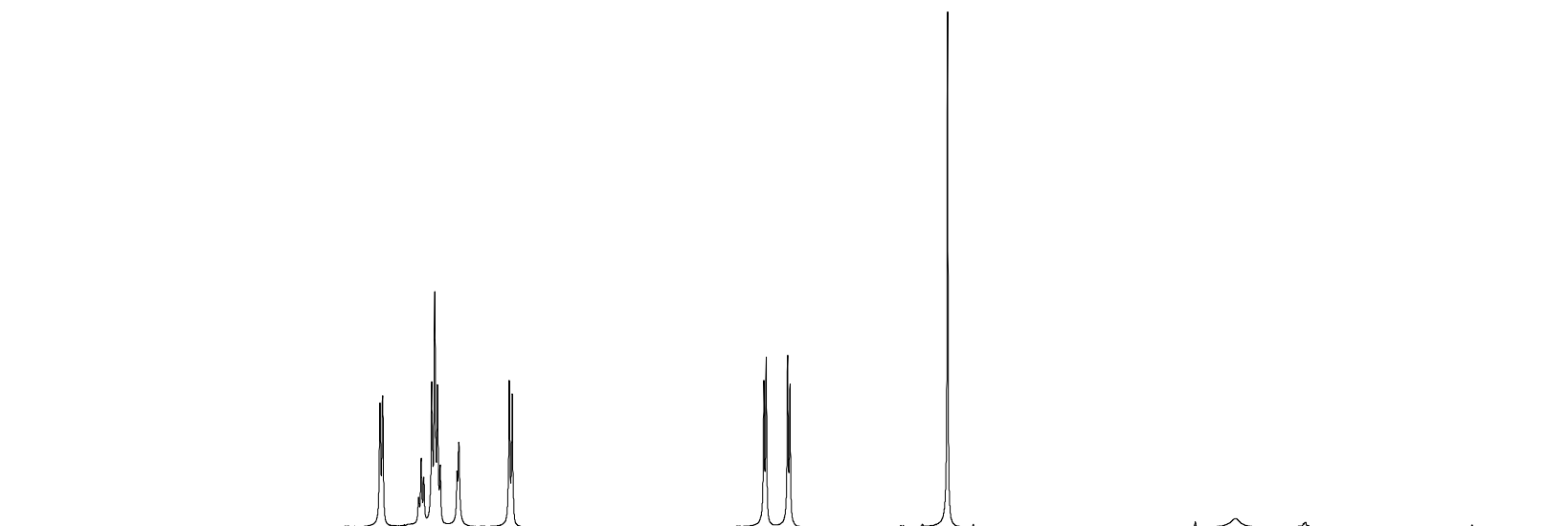


Current Data Parameters
NAME czl-1-183
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20170801
Time 20.01
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT CDC13
NS 4
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 88.84
DW 62.400 usec
DE 6.50 usec
TE 297.3 K
D1 1.00000000 sec
TD0 1

==== CHANNEL f1 =====
SFO1 400.1324710 MHz
NUC1 1H
P1 14.50 usec
PLW1 11.99499989 W

F2 - Processing parameters
SI 65536
SF 400.1300102 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



10 9 8 7 6 5 4 3 2 1 ppm

2.00
1.08
4.00
1.16
2.01

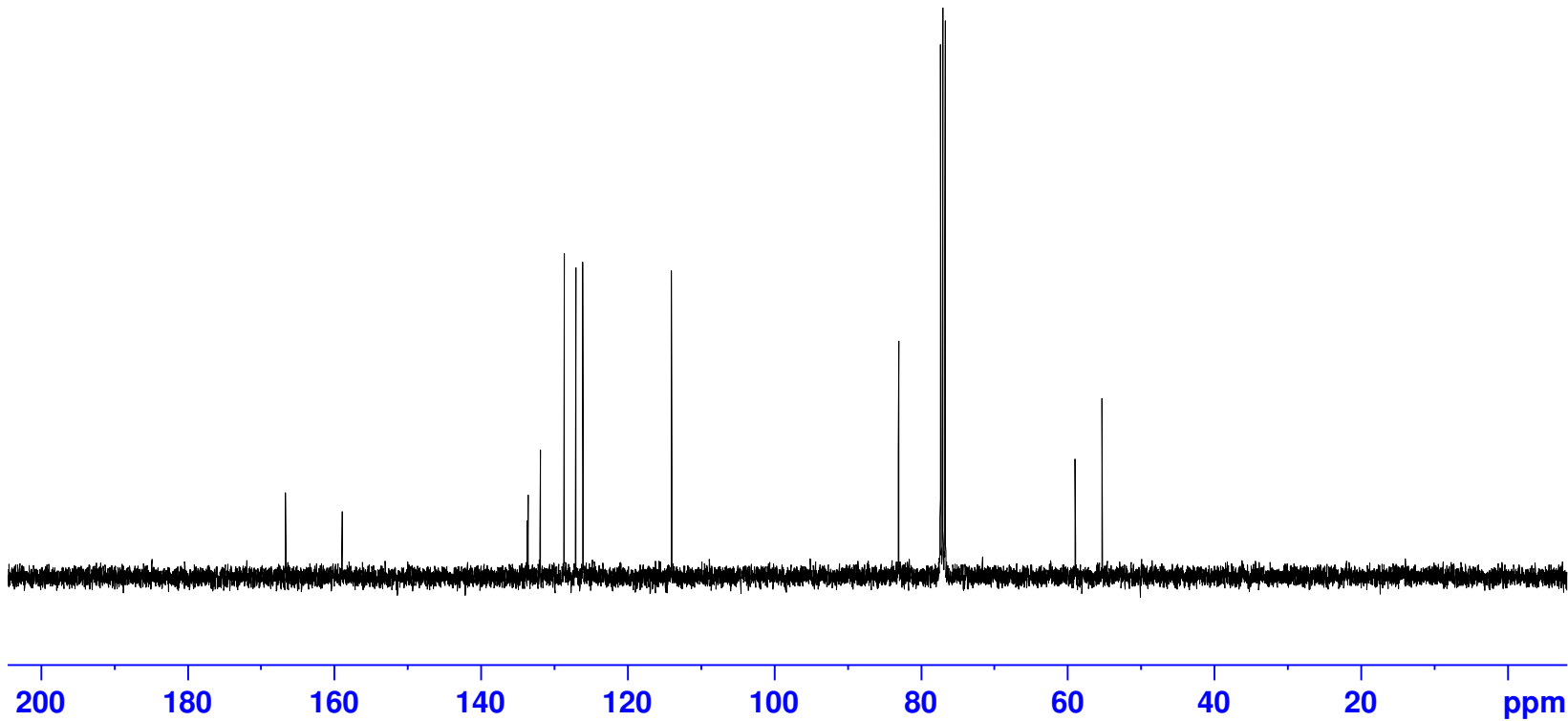
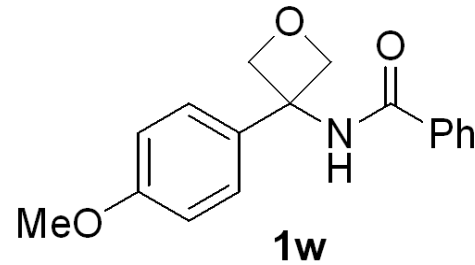
2.05
2.06

3.04

S-107



— 166.625
— 158.919
└─ 133.664
└─ 133.549
└─ 131.899
└─ 128.623
└─ 127.043
└─ 126.084
— 113.987
└─ 83.025
└─ 77.318
└─ 77.000
└─ 76.682
└─ 58.944
└─ 55.279



Current Data Parameters
NAME czl-1-183
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20170801
Time 20.04
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 40
DS 2
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 196.92
DW 20.800 usec
DE 6.50 usec
TE 298.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

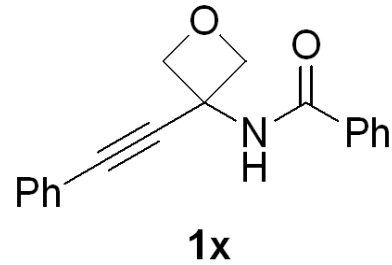
==== CHANNEL f1 =====
SFO1 100.6228298 MHz
NUC1 13C
P1 9.70 usec
PLW1 46.98899841 W

==== CHANNEL f2 =====
SFO2 400.1316005 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 90.00 usec
PLW2 11.99499989 W
PLW12 0.34213999 W
PLW13 0.27713001 W

F2 - Processing parameters
SI 32768
SF 100.6127751 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



7.849
7.830
7.527
7.509
7.490
7.448
7.444
7.435
7.432
7.425
7.416
7.398
7.360
7.309
7.297
7.280
7.266
7.259
7.143
5.058
5.042
5.010
4.994

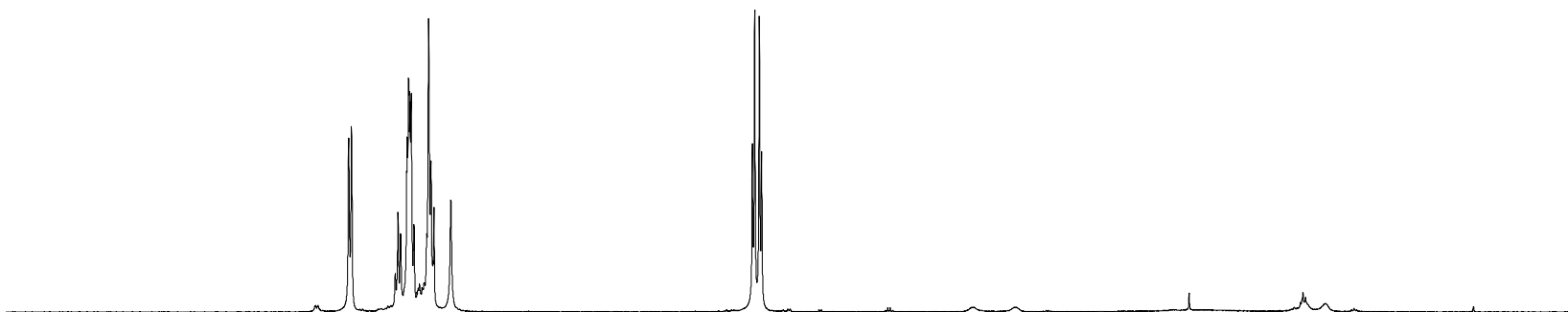


Current Data Parameters
NAME czi-1-182
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20170731
Time 13.06
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 4
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 187.77
DW 62.400 usec
DE 6.50 usec
TE 297.4 K
D1 1.00000000 sec
TD0 1

==== CHANNEL f1 =====
SFO1 400.1324710 MHz
NUC1 1H
P1 14.50 usec
PLW1 11.99499989 W

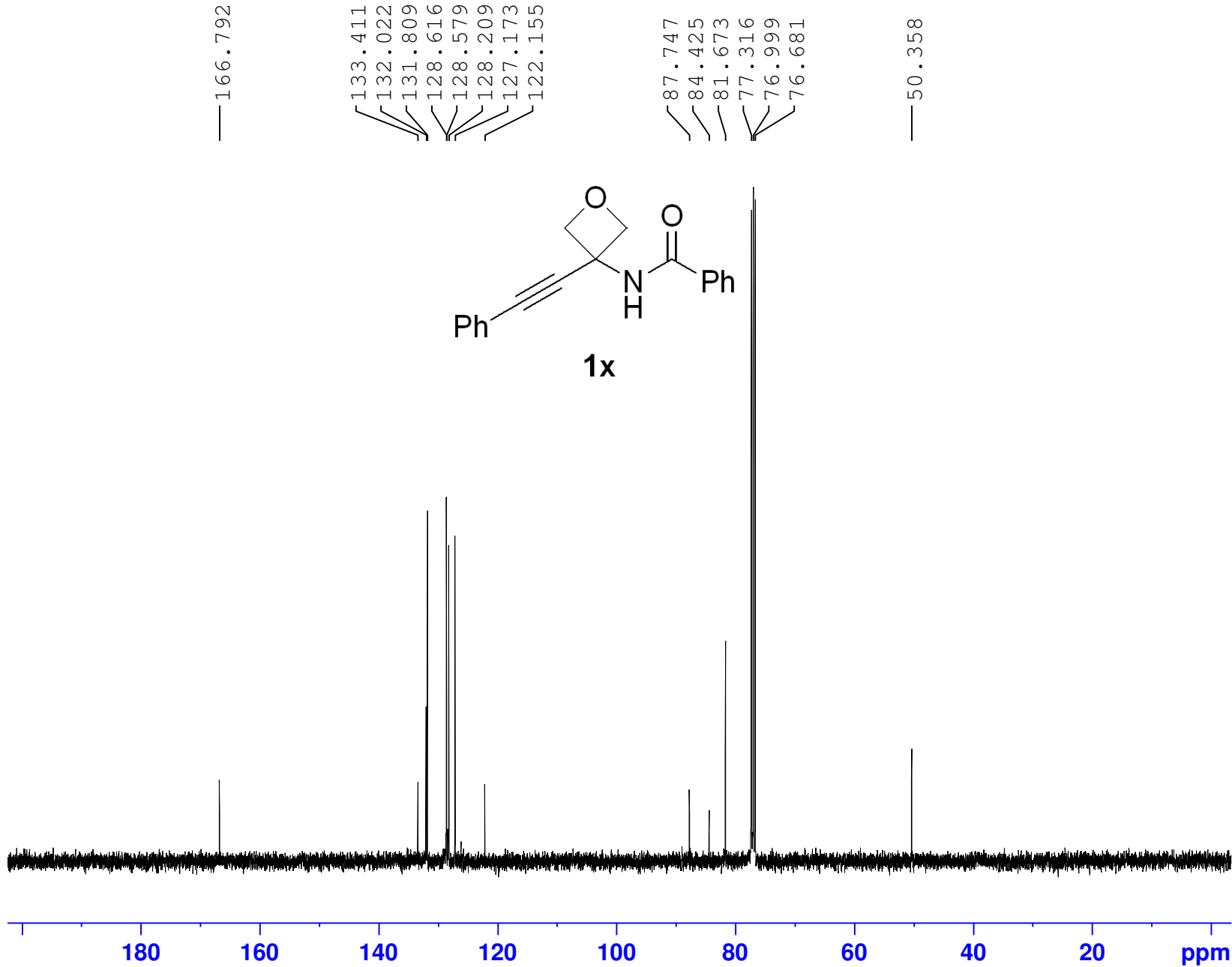
F2 - Processing parameters
SI 65536
SF 400.1300105 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



10 9 8 7 6 5 4 3 2 1 ppm

2.00
1.15
4.13
3.15
1.00

2.05
2.01



Current Data Parameters
NAME czi-1-182
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20170731
Time 13.13
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 100
DS 2
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 196.92
DW 20.800 usec
DE 6.50 usec
TE 297.9 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

==== CHANNEL f1 =====
SFO1 100.6228298 MHz
NUC1 13C
P1 9.70 usec
PLW1 46.98899841 W

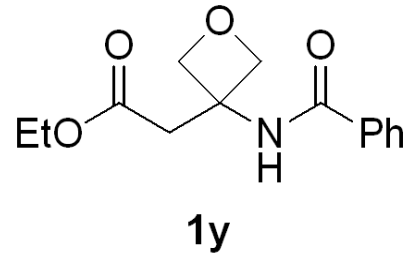
==== CHANNEL f2 =====
SFO2 400.1316005 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 90.00 usec
PLW2 11.99499989 W
PLW12 0.34213999 W
PLW13 0.27713001 W

F2 - Processing parameters
SI 32768
SF 100.6127743 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



7.747
7.734
7.729
7.726
7.496
7.493
7.489
7.479
7.474
7.469
7.459
7.456
7.452
7.404
7.401
7.388
7.385
7.371
7.367
7.260
7.185
4.852
4.834
4.625
4.607
4.108
4.090
4.072
4.055
3.273

1.213
1.195
1.178

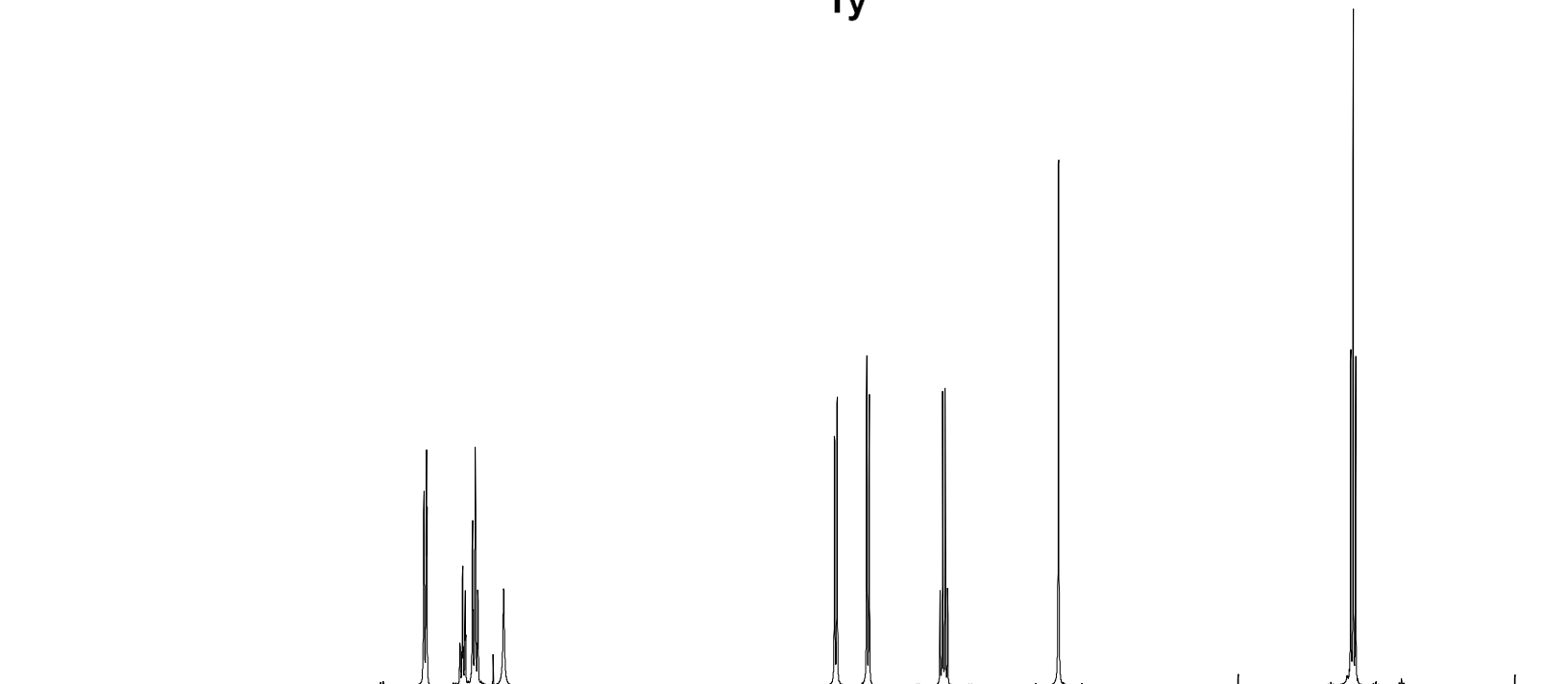


Current Data Parameters
NAME czl-1-186
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20170802
Time 13.44
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT CDC13
NS 4
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 54.81
DW 62.400 usec
DE 6.50 usec
TE 299.0 K
D1 1.00000000 sec
TD0 1

==== CHANNEL f1 =====
SFO1 400.1324710 MHz
NUC1 1H
P1 14.50 usec
PLW1 11.99499989 W

F2 - Processing parameters
SI 65536
SF 400.1300100 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



10 9 8 7 6 5 4 3 2 1 ppm

2.00
1.00
2.03
0.98

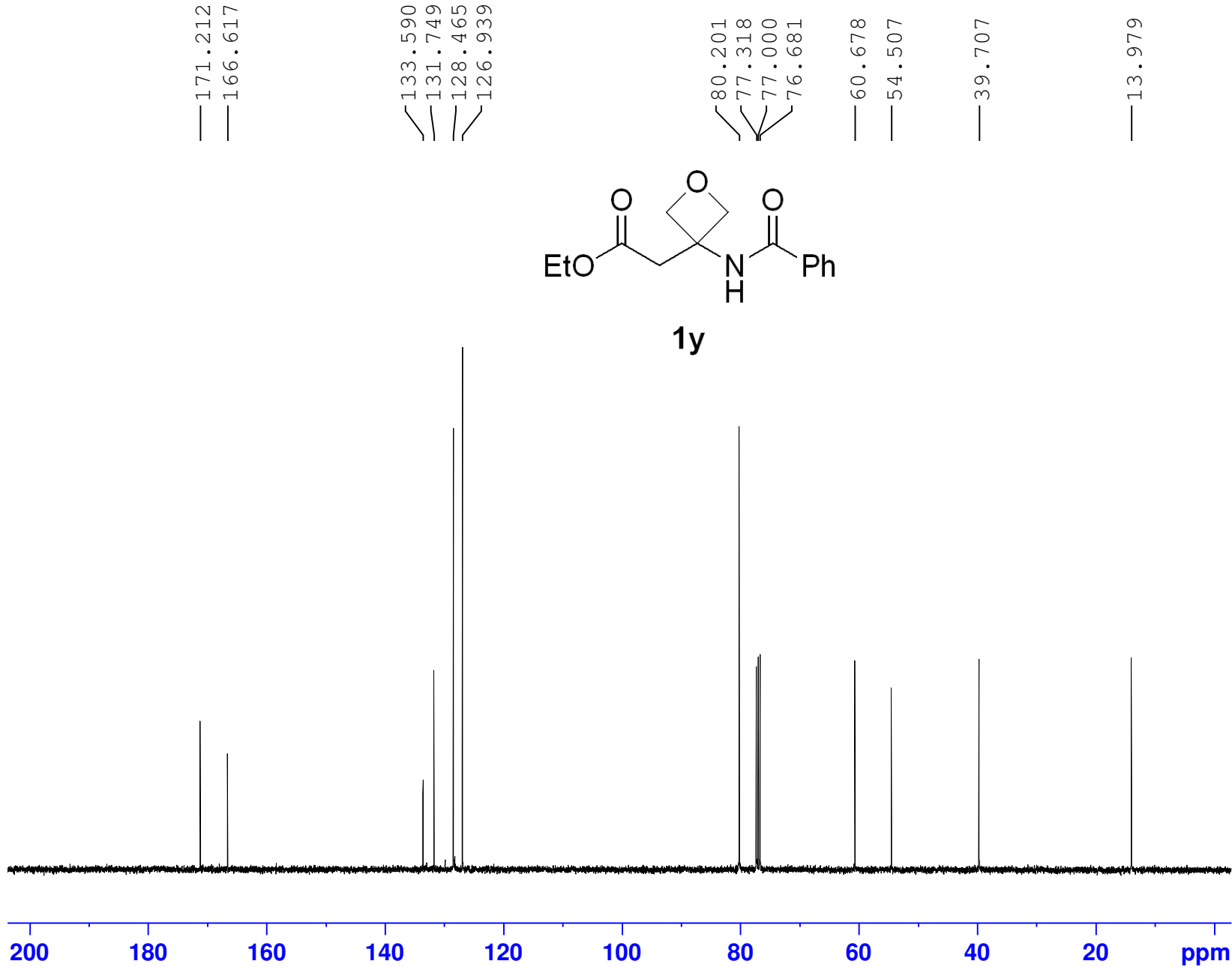
2.00
2.00

S-111

2.01

2.00

3.11



Current Data Parameters
NAME czi-1-186
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20170802
Time 13.49
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 400
DS 2
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 196.92
DW 20.800 usec
DE 6.50 usec
TE 299.1 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

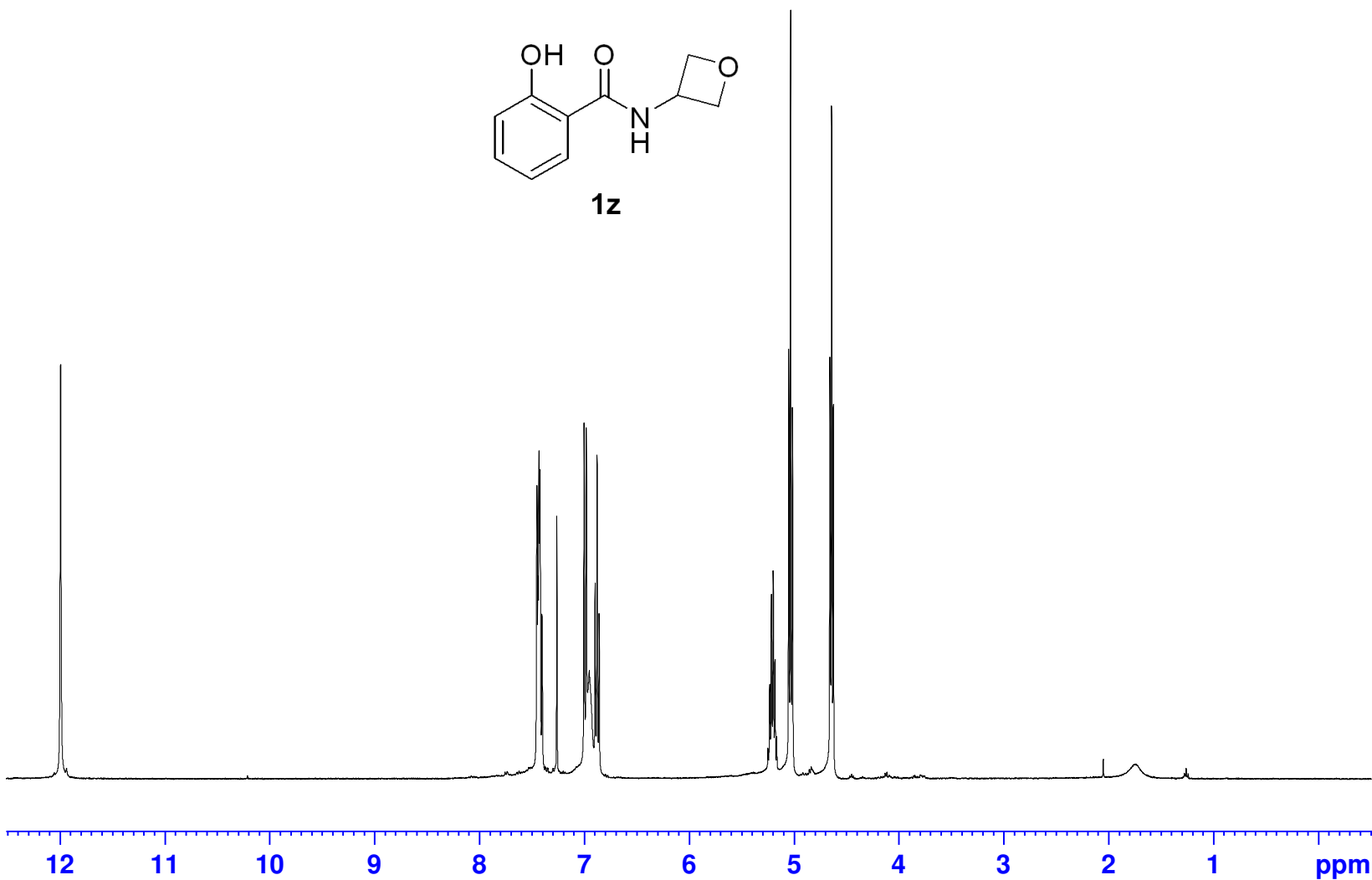
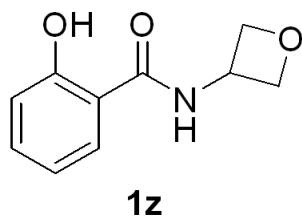
==== CHANNEL f1 =====
SFO1 100.6228298 MHz
NUC1 13C
P1 9.70 usec
PLW1 46.98899841 W

==== CHANNEL f2 =====
SFO2 400.1316005 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 90.00 usec
PLW2 11.99499989 W
PLW12 0.34213999 W
PLW13 0.27713001 W

F2 - Processing parameters
SI 32768
SF 100.6127808 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

—11.993

7.449
7.441
7.429
7.421
7.402
7.399
7.260
7.000
6.979
6.950
6.894
6.876
6.856
5.229
5.213
5.196
5.179
5.048
5.030
5.012
4.655
4.639
4.623

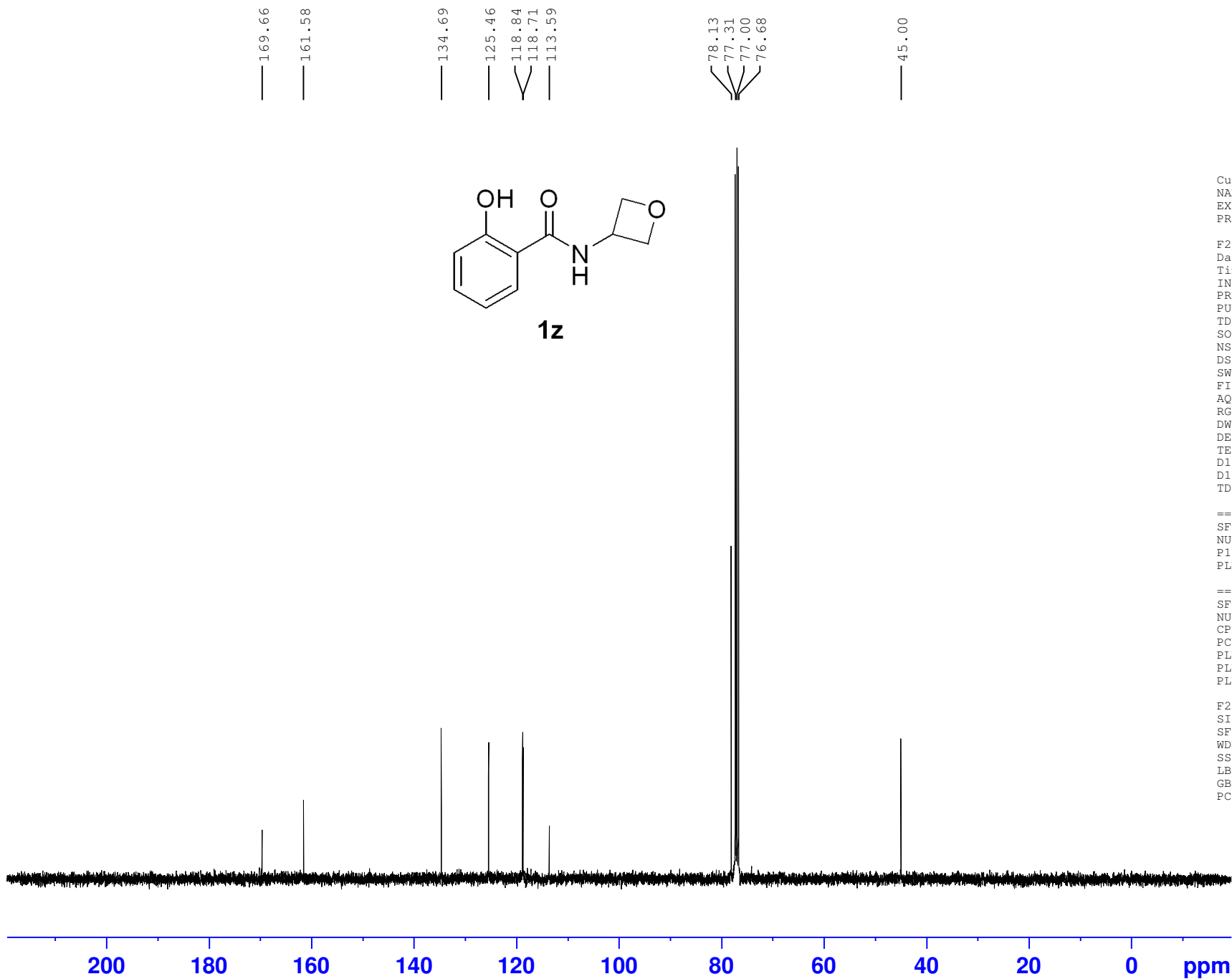


Current Data Parameters
NAME hh-3-140-h-crude
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20190701
Time 13.53
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 6
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 103.52
DW 62.400 usec
DE 6.50 usec
TE 294.5 K
D1 1.00000000 sec
TD0 1

==== CHANNEL f1 =====
SFO1 400.1324710 MHz
NUC1 1H
P1 14.50 usec
PLW1 11.99499989 W

F2 - Processing parameters
SI 65536
SF 400.1300103 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



Current Data Parameters
NAME hh-3-140-c-crude
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20190701
Time 14.11
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 166
DS 0
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 196.92
DW 20.800 usec
DE 6.50 usec
TE 295.7 K
D1 2.0000000 sec
D11 0.0300000 sec
TD0 1

==== CHANNEL f1 =====
SFO1 100.6228298 MHz
NUC1 13C
P1 9.70 usec
PLW1 46.98899841 W

==== CHANNEL f2 =====
SFO2 400.1316005 MHz
NUC2 1H
PCPD2 waltz16
PLW2 90.00 usec
PLW12 11.99499989 W
PLW13 0.34213999 W
PLW13 0.27713001 W

F2 - Processing parameters
SI 32768
SF 100.6127739 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

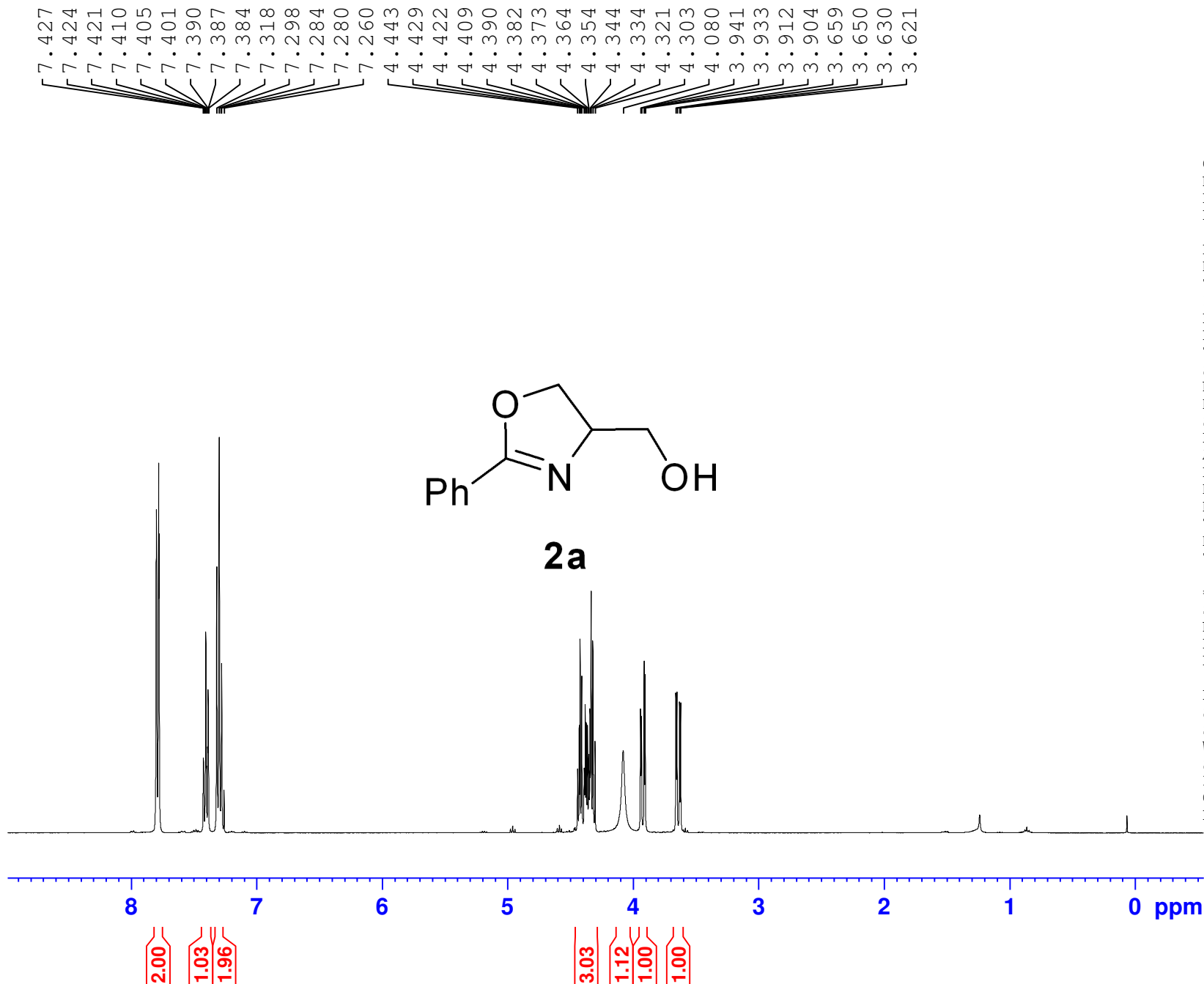


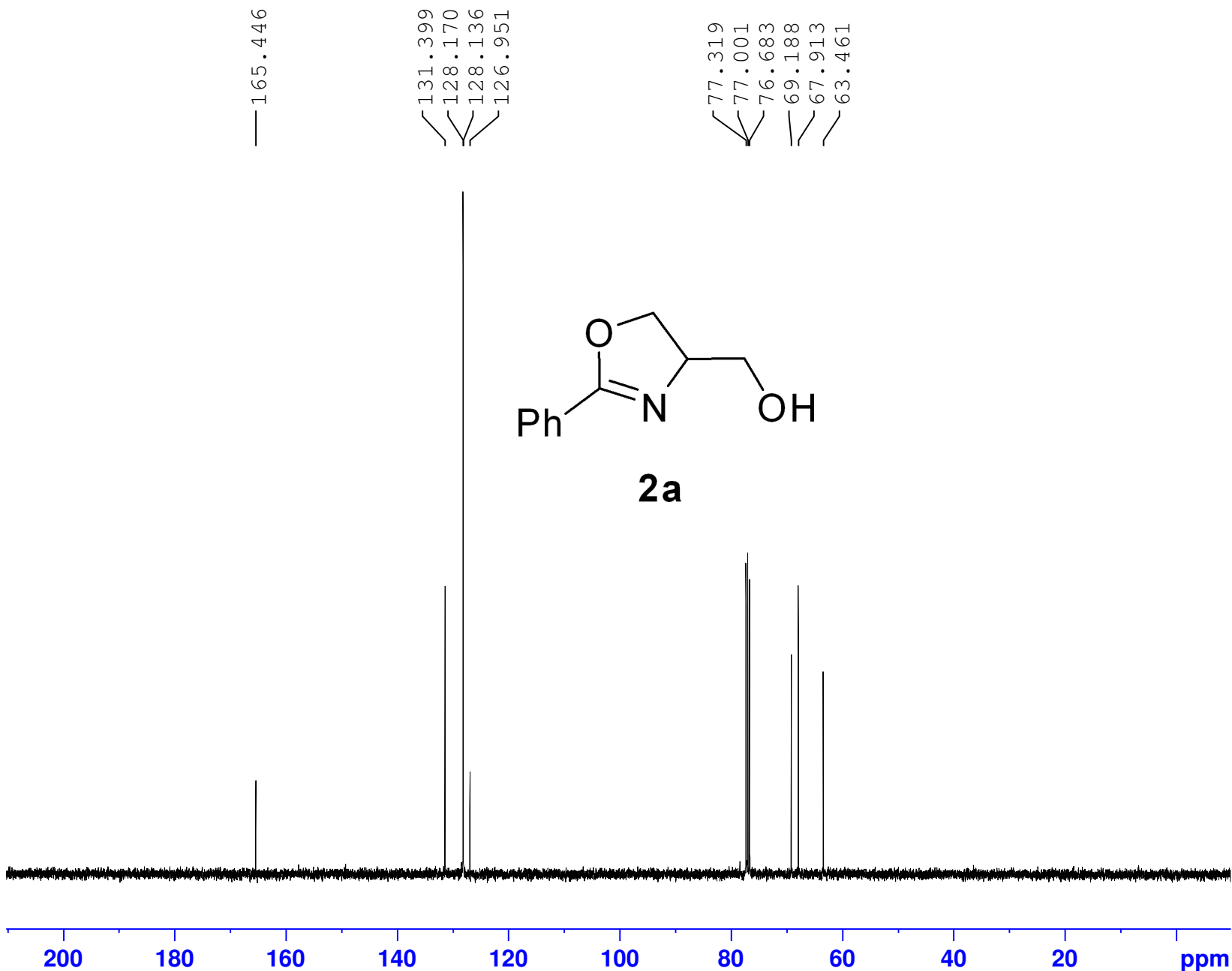
Current Data Parameters
NAME YW-1722
EXPNO 1
PROCNO 2

F2 - Acquisition Parameters
Date_ 20160413
Time 14.34
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT CDC13
NS 4
DS 0
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 34.77
DW 62.400 usec
DE 6.50 usec
TE 296.6 K
D1 1.00000000 sec
TD0 1

==== CHANNEL f1 =====
SFO1 400.1324710 MHz
NUC1 1H
P1 14.50 usec
PLW1 11.99499989 W

F2 - Processing parameters
SI 65536
SF 400.1300091 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00





Current Data Parameters
NAME YW-1722-carbon
EXPNO 2
PROCNO 2

F2 - Acquisition Parameters
Date_ 20160413
Time 14.40
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 21
DS 0
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 196.92
DW 20.800 usec
DE 6.50 usec
TE 297.3 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

==== CHANNEL f1 =====
SFO1 100.6228298 MHz
NUC1 13C
P1 9.70 usec
PLW1 46.98899841 W

==== CHANNEL f2 =====
SFO2 400.1316005 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 90.00 usec
PLW2 11.99499989 W
PLW12 0.34213999 W
PLW13 0.27713001 W

F2 - Processing parameters
SI 32768
SF 100.6127795 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



7.930
7.909
7.609
7.589
7.585
7.563
7.476
7.458
7.439
7.399
7.381
7.363
7.260

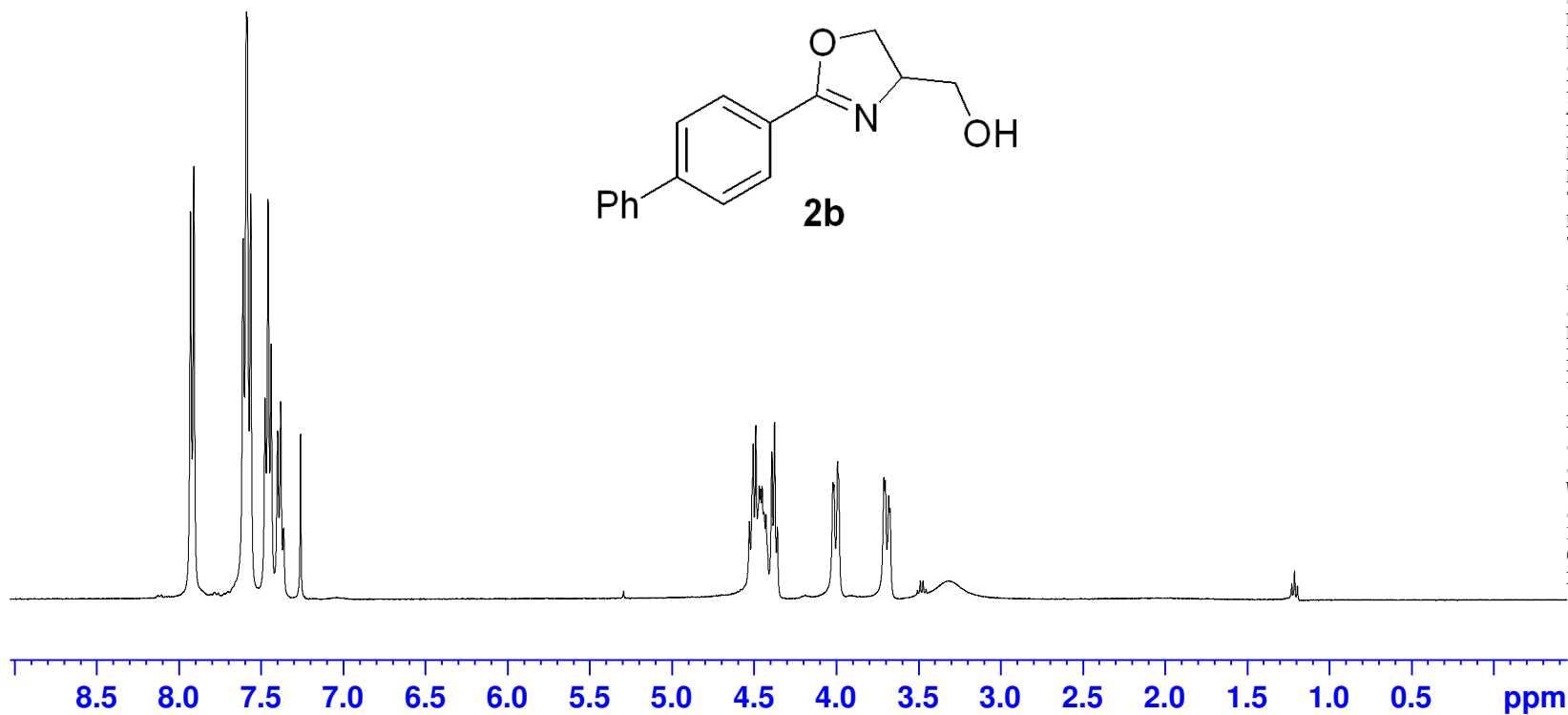
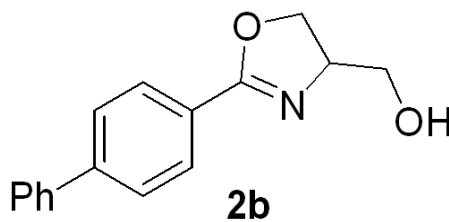
4.528
4.505
4.489
4.468
4.460
4.451
4.441
4.427
4.392
4.375
4.358
4.020
4.013
3.991
3.709
3.701
3.680
3.672
3.311

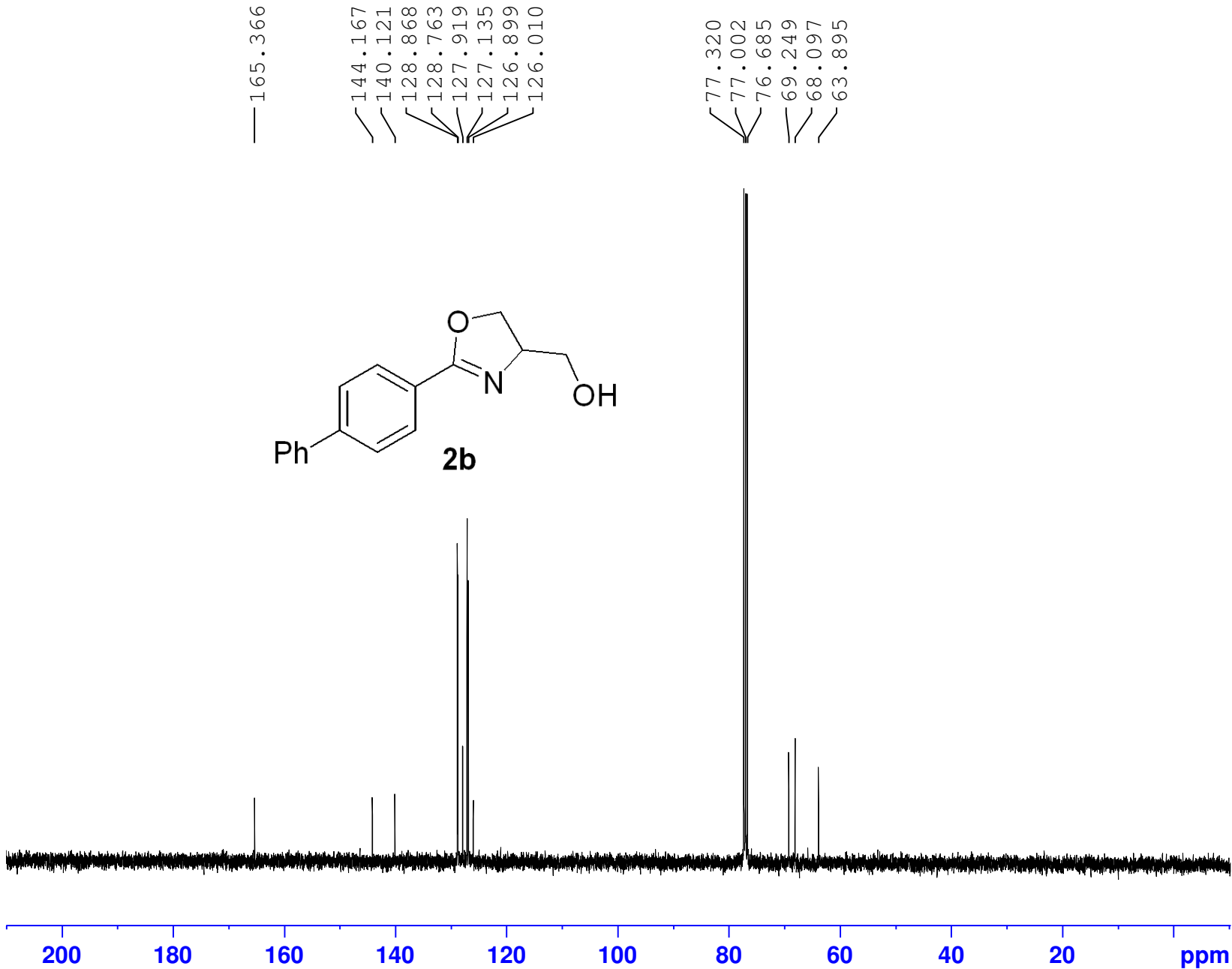
Current Data Parameters
NAME YW-1735D-carbon
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20160415
Time 19.39
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT CDC13
NS 6
DS 0
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 103.52
DW 62.400 usec
DE 6.50 usec
TE 296.7 K
D1 1.00000000 sec
TD0 1

==== CHANNEL f1 =====
SFO1 400.1324710 MHz
NUC1 1H
P1 14.50 usec
PLW1 11.99499989 W

F2 - Processing parameters
SI 65536
SF 400.1300092 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00





Current Data Parameters
NAME YW-1735D-carbon
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20160415
Time 19.49
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 162
DS 0
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 196.92
DW 20.800 usec
DE 6.50 usec
TE 297.8 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

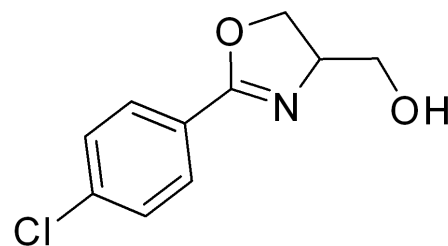
==== CHANNEL f1 =====
SFO1 100.6228298 MHz
NUC1 13C
P1 9.70 usec
PLW1 46.98899841 W

==== CHANNEL f2 =====
SFO2 400.1316005 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 90.00 usec
PLW2 11.99499989 W
PLW12 0.34213999 W
PLW13 0.27713001 W

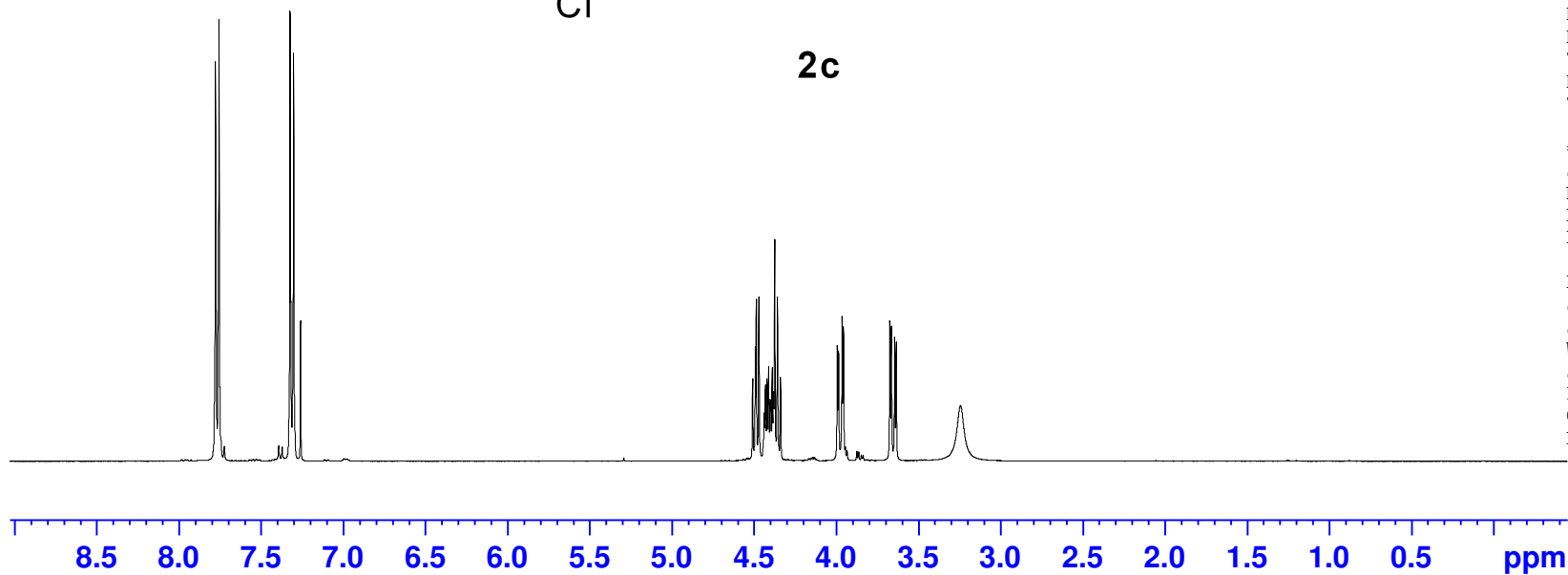
F2 - Processing parameters
SI 32768
SF 100.6127722 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



7.778
7.761
7.757
7.324
7.319
7.306
7.302
7.260
4.508
4.492
4.486
4.470
4.439
4.430
4.421
4.411
4.402
4.398
4.389
4.381
4.374
4.358
4.339
3.993
3.985
3.964
3.956
3.673
3.664
3.644
3.635
3.244



2c

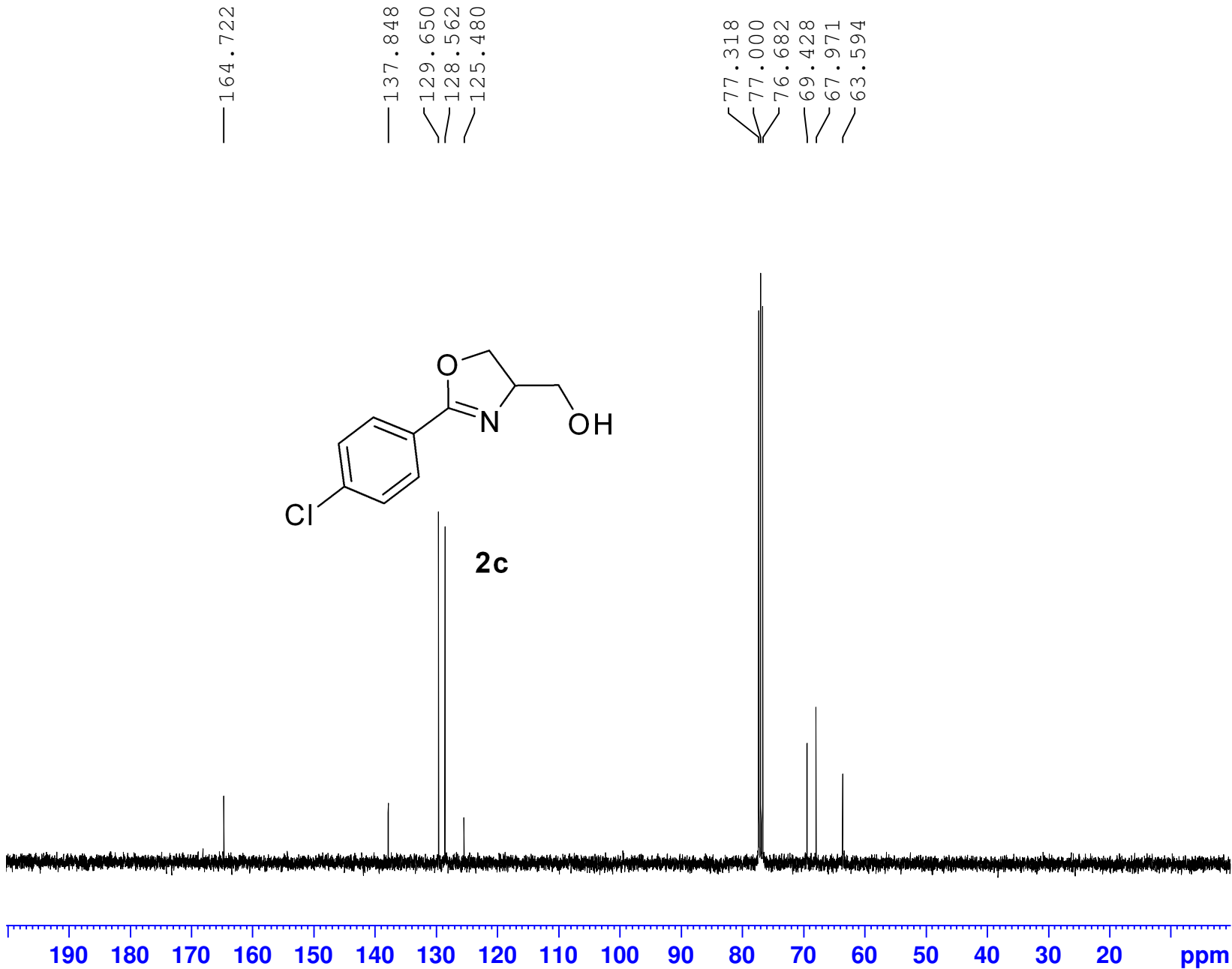


Current Data Parameters
NAME YW-1736A
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20160416
Time 10.11
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT CDC13
NS 16
DS 0
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 112.31
DW 62.400 usec
DE 6.50 usec
TE 298.3 K
D1 1.00000000 sec
TD0 1

==== CHANNEL f1 =====
SFO1 400.1324710 MHz
NUC1 1H
P1 14.50 usec
PLW1 11.99499989 W

F2 - Processing parameters
SI 65536
SF 400.1300094 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



Current Data Parameters
NAME YW-1736A-carbon
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20160416
Time 10.17
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 75
DS 0
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 196.92
DW 20.800 usec
DE 6.50 usec
TE 299.1 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

==== CHANNEL f1 =====
SFO1 100.6228298 MHz
NUC1 13C
P1 9.70 usec
PLW1 46.98899841 W

==== CHANNEL f2 =====
SFO2 400.1316005 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 90.00 usec
PLW2 11.99499989 W
PLW12 0.34213999 W
PLW13 0.27713001 W

F2 - Processing parameters
SI 32768
SF 100.6127714 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



7.934
7.913
7.633
7.612
— 7.260

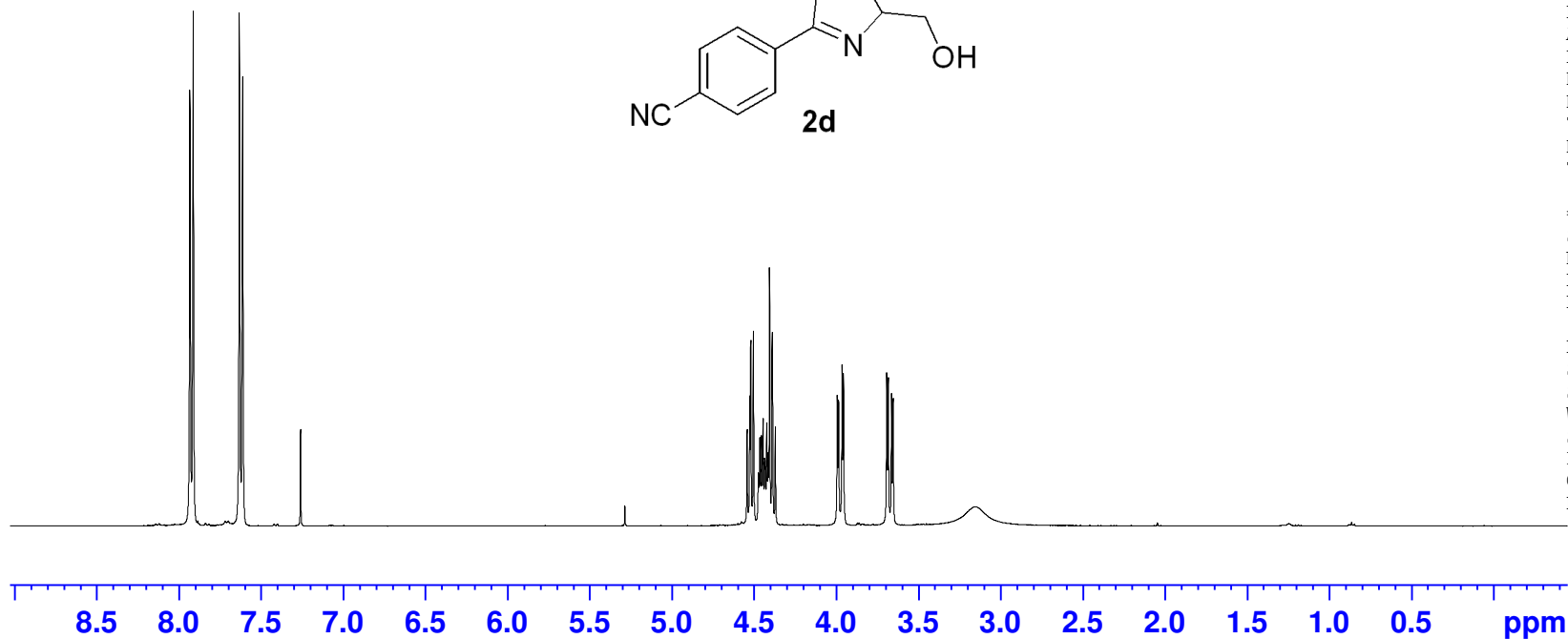
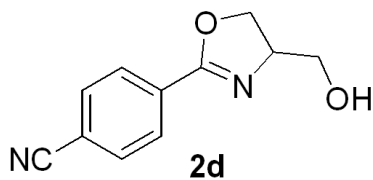
4.542
4.526
4.520
4.504
4.473
4.464
4.455
4.445
4.435
4.431
4.422
4.414
4.406
4.390
4.370
3.993
3.985
3.964
3.956
3.692
3.683
3.663
3.654
3.152

Current Data Parameters
NAME YW-1736B
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20160416
Time 10.19
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT CDC13
NS 3
DS 0
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 103.52
DW 62.400 usec
DE 6.50 usec
TE 298.3 K
D1 1.00000000 sec
TD0 1

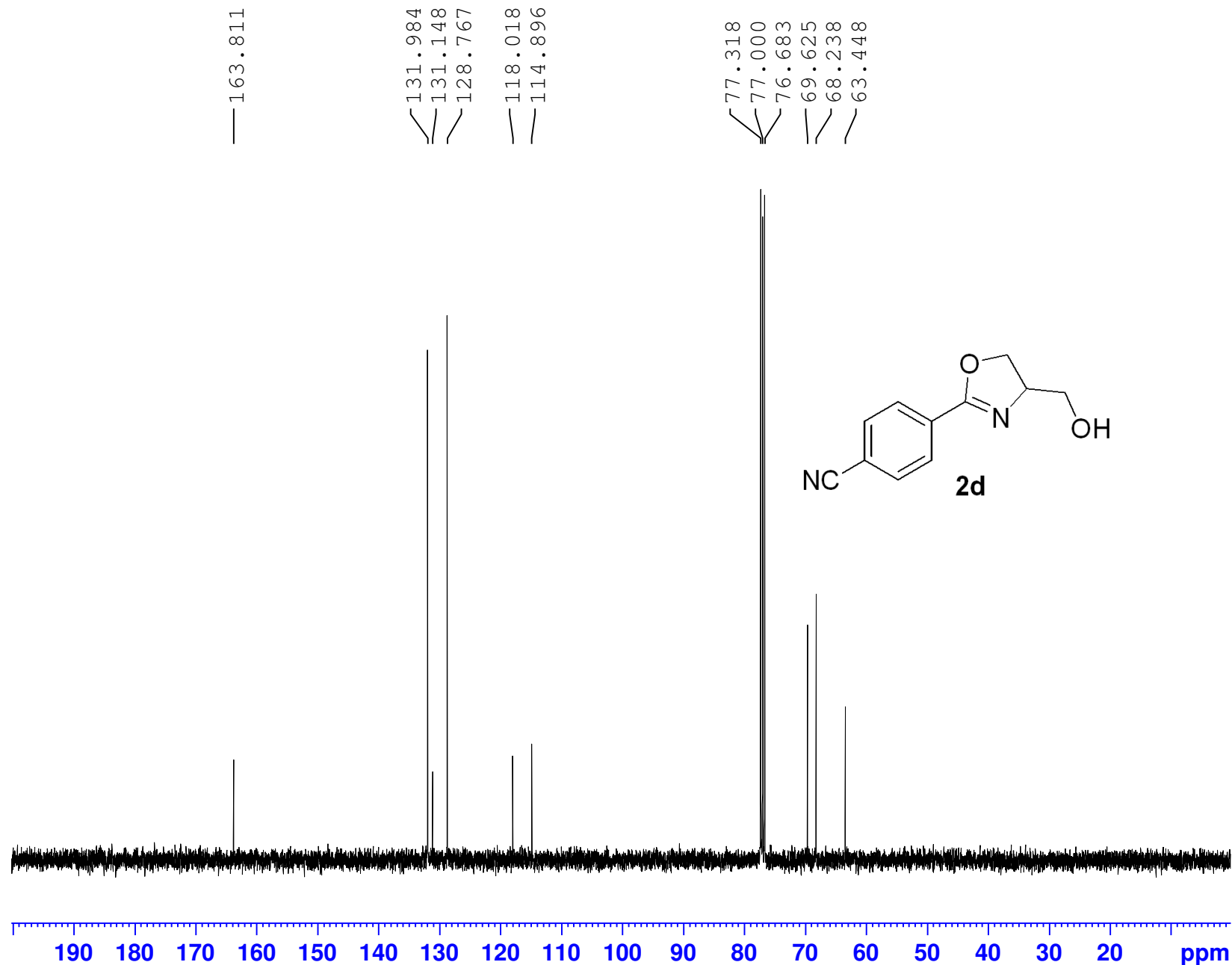
==== CHANNEL f1 =====
SFO1 400.1324710 MHz
NUC1 1H
P1 14.50 usec
PLW1 11.99499989 W

F2 - Processing parameters
SI 65536
SF 400.1300094 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



1.96
1.93

0.95
2.03
1.01
1.00
0.91



Current Data Parameters
NAME YW-1736B-carbon
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20160416
Time 10.22
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 37
DS 0
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 196.92
DW 20.800 usec
DE 6.50 usec
TE 299.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

==== CHANNEL f1 =====
SFO1 100.6228298 MHz
NUC1 13C
P1 9.70 usec
PLW1 46.98899841 W

==== CHANNEL f2 =====
SFO2 400.1316005 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 90.00 usec
PLW2 11.99499989 W
PLW12 0.34213999 W
PLW13 0.27713001 W

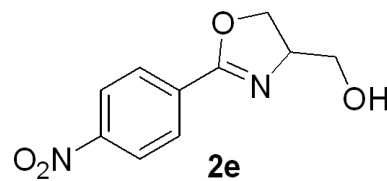
F2 - Processing parameters
SI 32768
SF 100.6127747 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



8.219
8.197
8.062
8.040

7.260

4.588
4.570
4.564
4.547
4.519
4.509
4.500
4.490
4.480
4.477
4.467
4.457
4.435
4.417
4.398
4.007
3.998
3.978
3.969
3.720
3.710
3.691
3.681
2.785

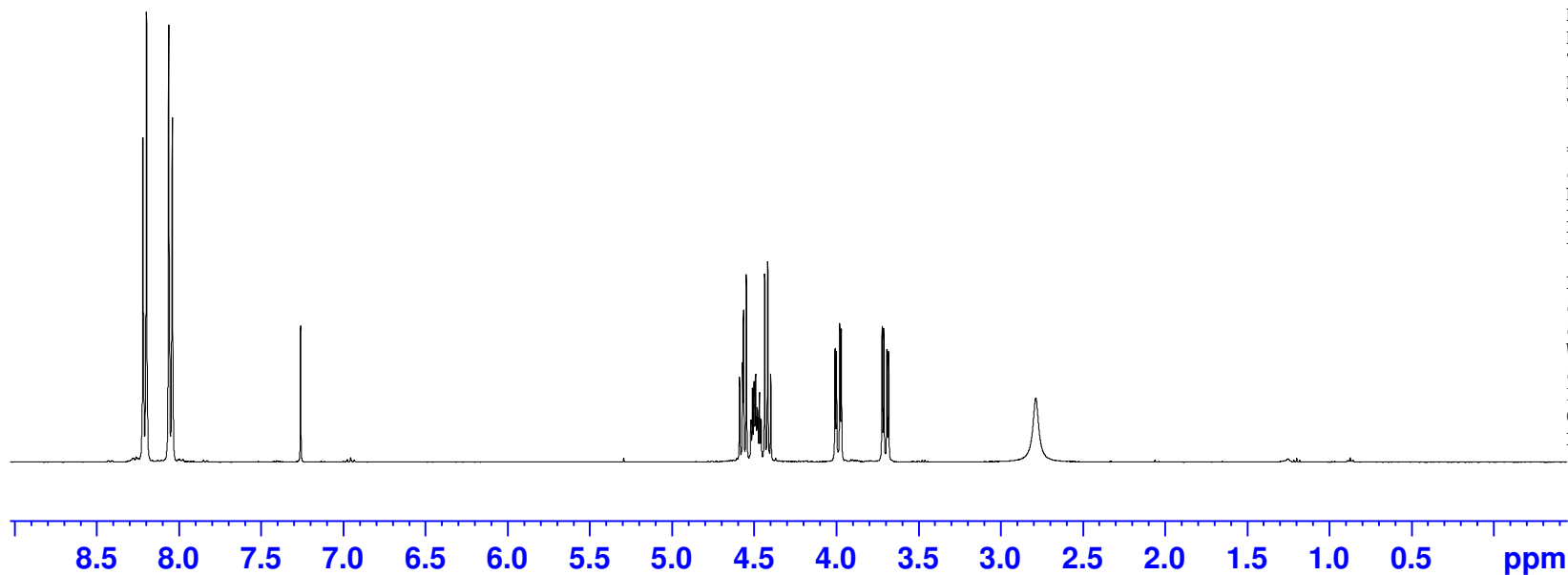


Current Data Parameters
NAME YW-1738B
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20160418
Time 21.06
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT CDC13
NS 7
DS 0
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 112.31
DW 62.400 usec
DE 6.50 usec
TE 296.6 K
D1 1.00000000 sec
TD0 1

==== CHANNEL f1 =====
SFO1 400.1324710 MHz
NUC1 1H
P1 14.50 usec
PLW1 11.99499989 W

F2 - Processing parameters
SI 65536
SF 400.1300095 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



1.94
1.94

0.97
1.06
0.98

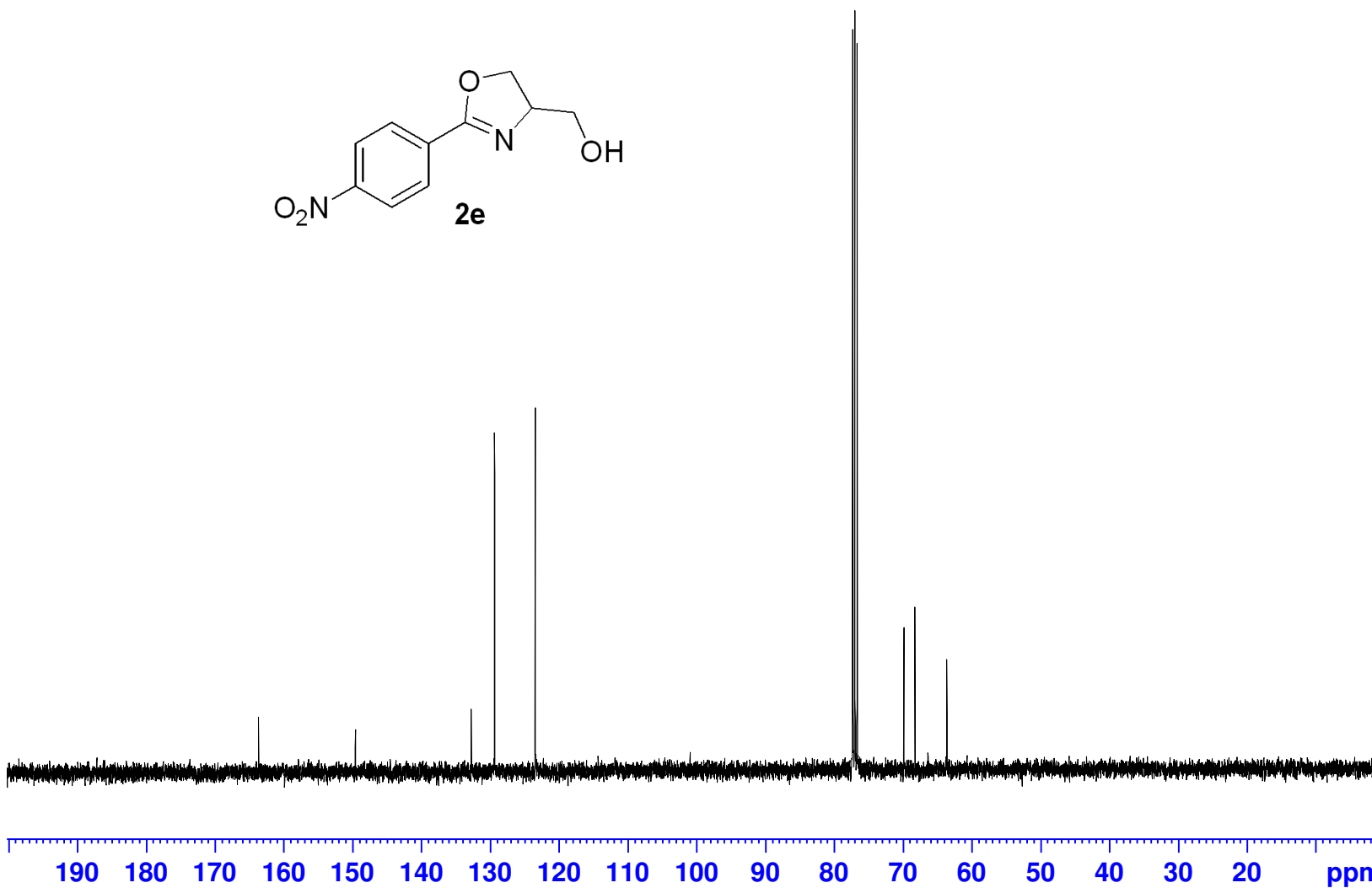
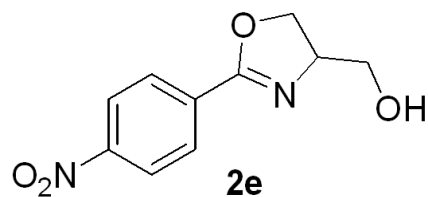
1.01
1.00

1.13



— 163.696
— 149.610
— 132.798
— 129.378
— 123.469

77.319
77.001
76.684
69.866
68.274
63.636



Current Data Parameters
NAME YW-1738B-carbon
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20160418
Time 21.10
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 65
DS 0
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 196.92
DW 20.800 usec
DE 6.50 usec
TE 297.6 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

==== CHANNEL f1 =====
SFO1 100.6228298 MHz
NUC1 13C
P1 9.70 usec
PLW1 46.98899841 W

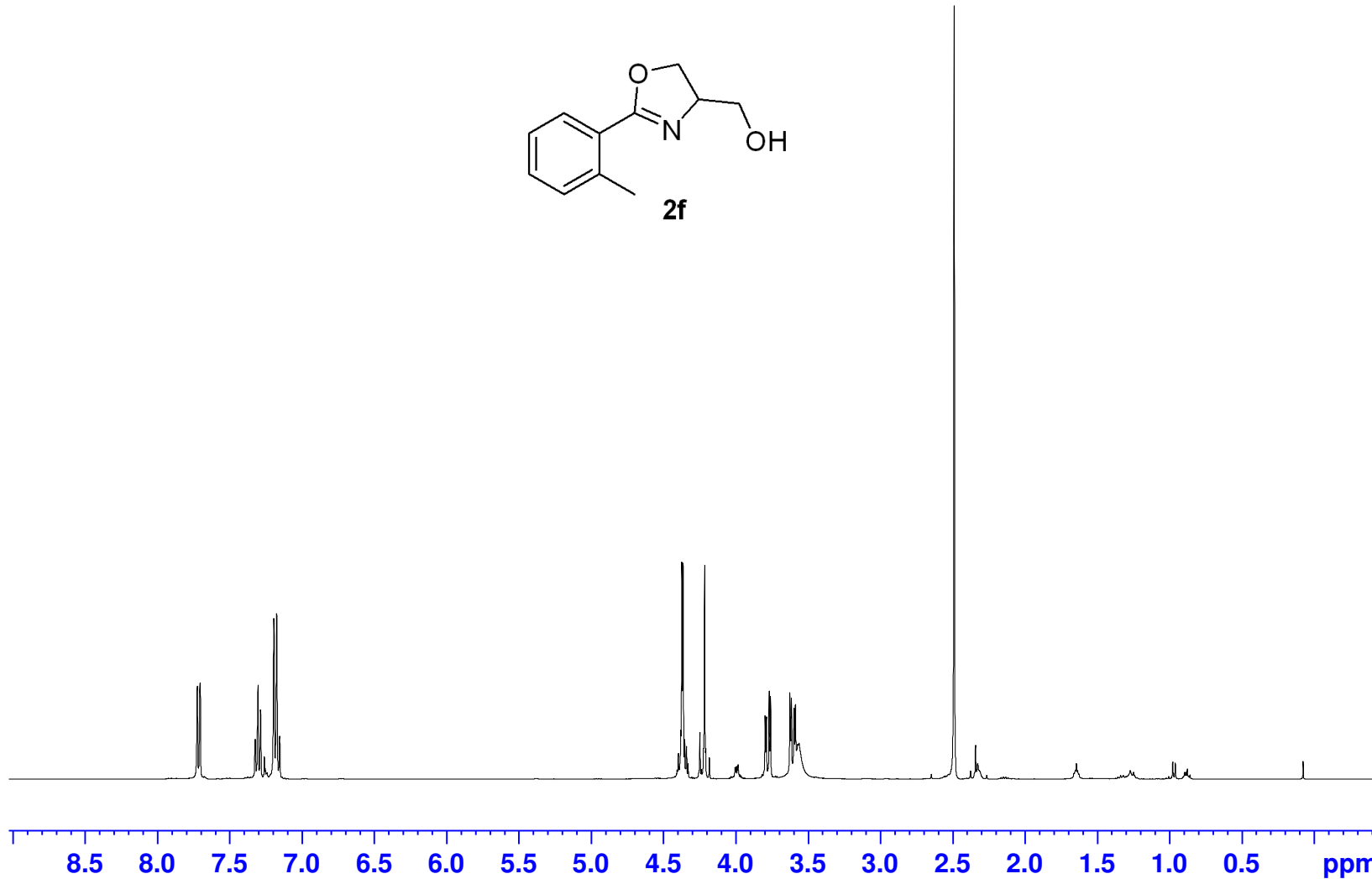
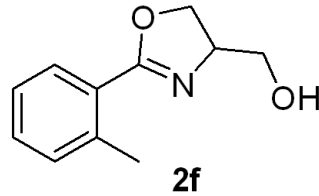
==== CHANNEL f2 =====
SFO2 400.1316005 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 90.00 usec
PLW2 11.99499989 W
PLW12 0.34213999 W
PLW13 0.27713001 W

F2 - Processing parameters
SI 32768
SF 100.6127722 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



7.724
7.704
7.325
7.322
7.303
7.288
7.285
7.195
7.175
7.155

4.397
4.380
4.372
4.364
4.354
4.340
4.247
4.215
4.208
4.182
3.797
3.787
3.768
3.759
3.625
3.615
3.596
3.587
3.561
2.489



Current Data Parameters
NAME YW-1735A
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20160416
Time 20.10
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT CDC13
NS 3
DS 0
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 27.78
DW 62.400 usec
DE 6.50 usec
TE 298.6 K
D1 1.00000000 sec
TD0 1

==== CHANNEL f1 =====
SFO1 400.1324710 MHz
NUC1 1H
P1 14.50 usec
PLW1 11.99499989 W

F2 - Processing parameters
SI 65536
SF 400.1300091 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

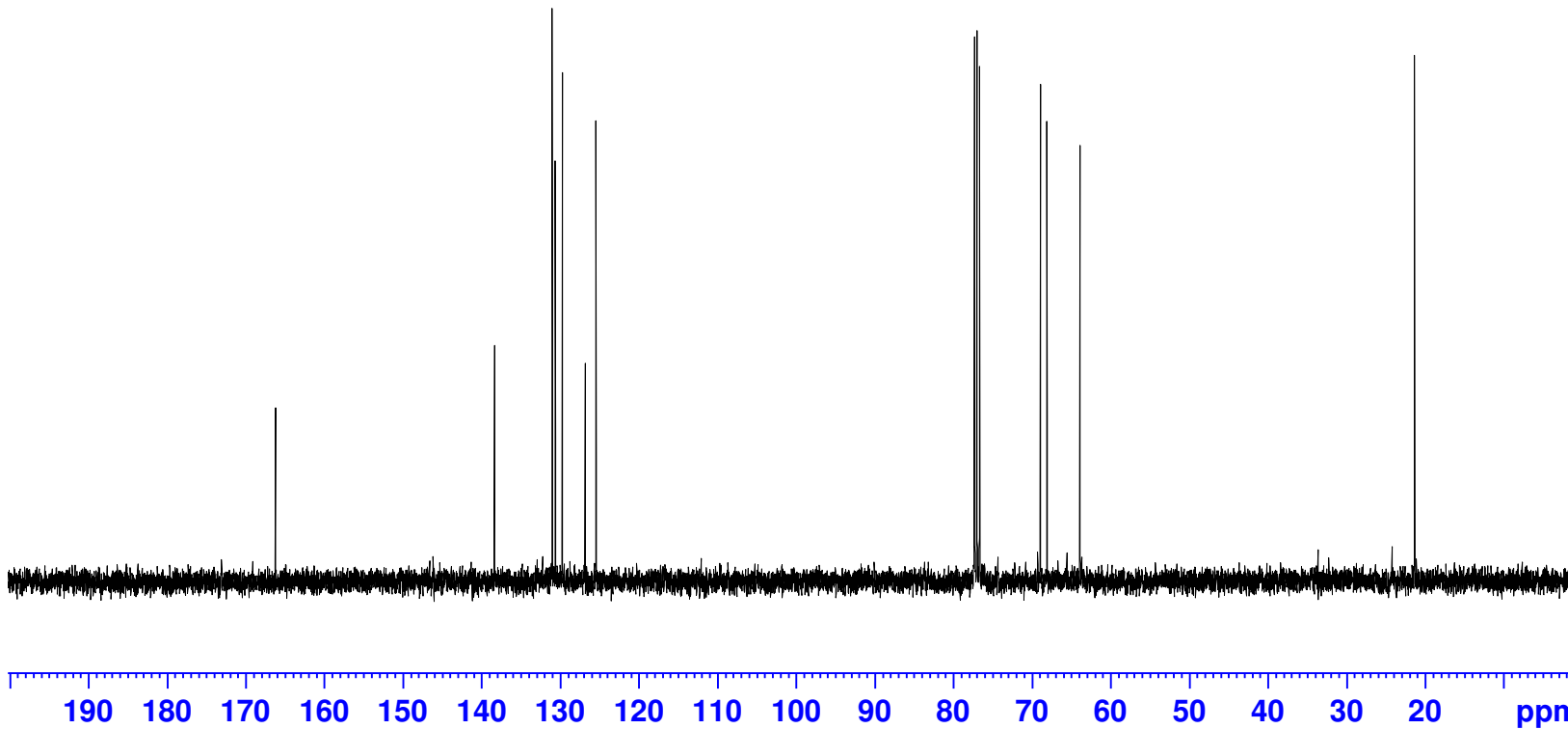
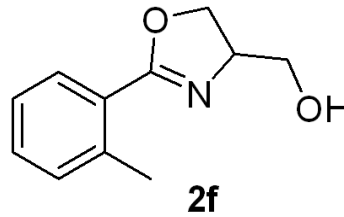


—166.210

138.380
131.029
130.639
129.732
126.843
125.456

77.321
77.002
76.684
68.936
68.100
63.901

—21.376



Current Data Parameters
NAME YW-1735A-carbon
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20160416
Time 20.12
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 9
DS 0
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 196.92
DW 20.800 usec
DE 6.50 usec
TE 298.9 K
D1 2.0000000 sec
D11 0.0300000 sec
TD0 1

==== CHANNEL f1 =====
SFO1 100.6228298 MHz
NUC1 13C
P1 9.70 usec
PLW1 46.98899841 W

==== CHANNEL f2 =====
SFO2 400.1316005 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 90.00 usec
PLW2 11.99499989 W
PLW12 0.34213999 W
PLW13 0.27713001 W

F2 - Processing parameters
SI 32768
SF 100.6127831 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

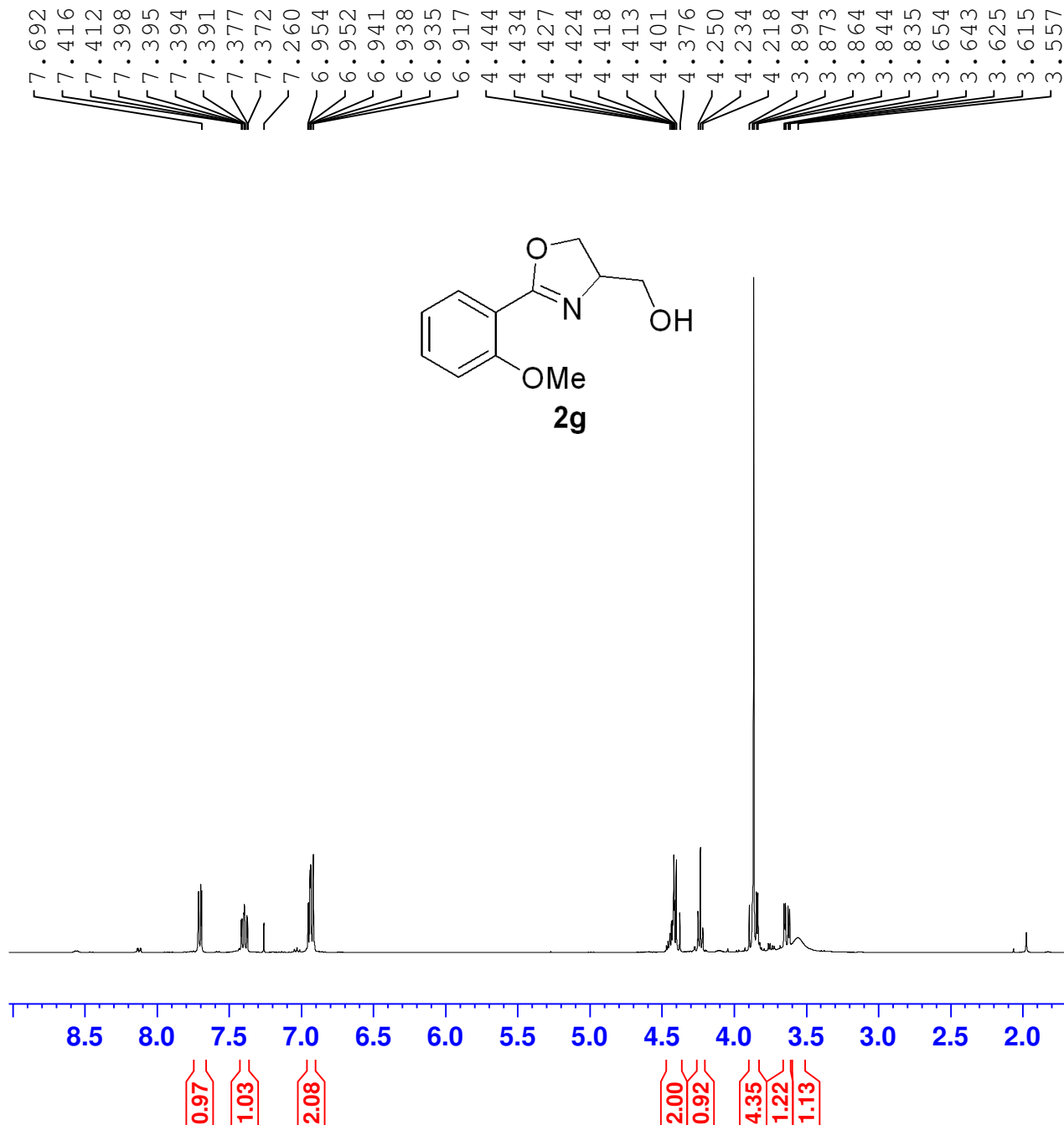


Current Data Parameters
NAME YW-1735B
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20160416
Time 10.04
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT CDC13
NS 4
DS 0
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 49.32
DW 62.400 usec
DE 6.50 usec
TE 298.5 K
D1 1.00000000 sec
TD0 1

==== CHANNEL f1 =====
SFO1 400.1324710 MHz
NUC1 1H
P1 14.50 usec
PLW1 11.99499989 W

F2 - Processing parameters
SI 65536
SF 400.1300093 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

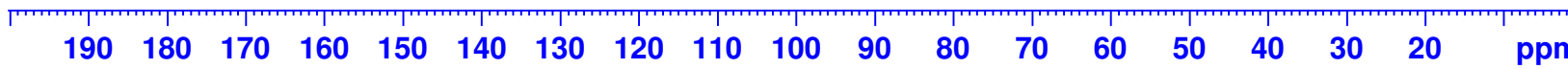
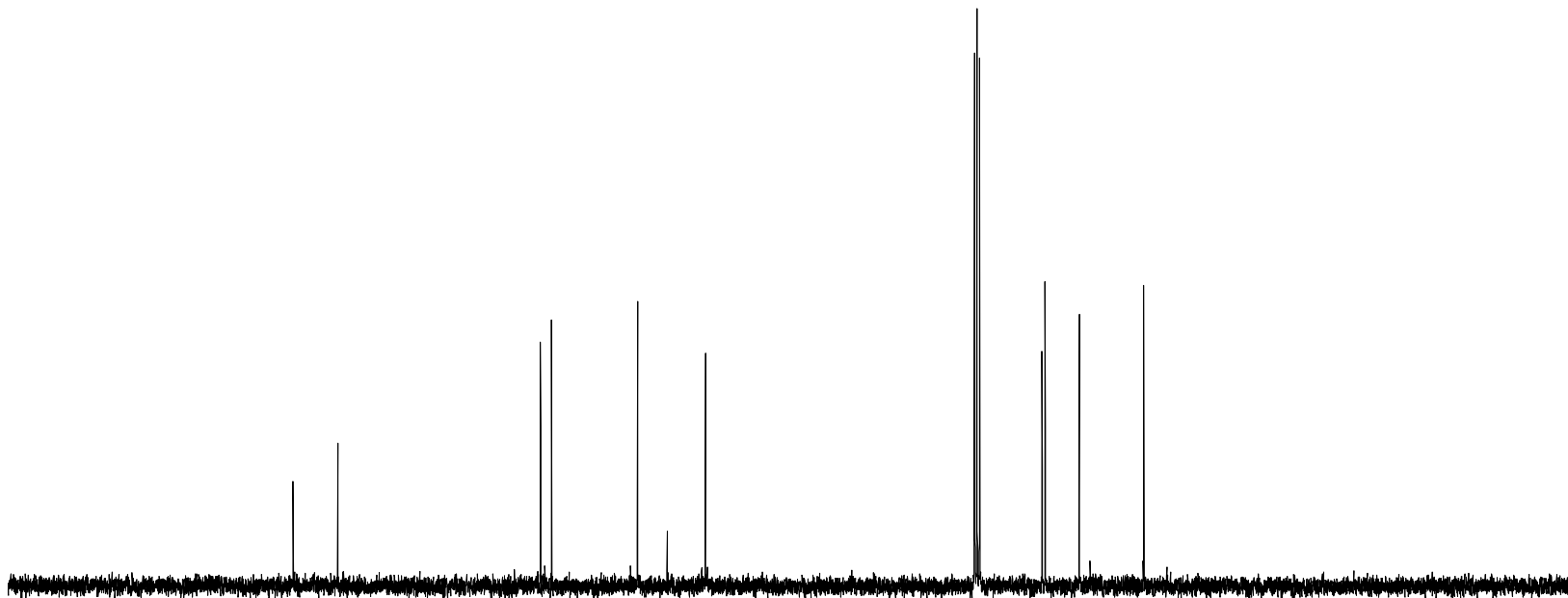
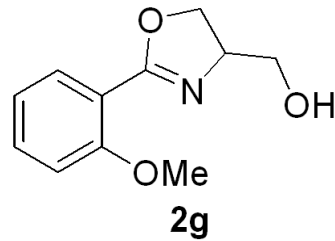




— 163.985
— 158.291

— 132.516
— 131.126
— 120.178
— 116.414
— 111.526

— 77.318
— 77.000
— 76.682
— 68.726
— 68.330
— 63.999
— 55.791



Current Data Parameters
NAME YW-1735B-carbon
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20160416
Time 10.06
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 26
DS 0
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 196.92
DW 20.800 usec
DE 6.50 usec
TE 299.1 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

==== CHANNEL f1 =====
SFO1 100.6228298 MHz
NUC1 13C
P1 9.70 usec
PLW1 46.98899841 W

==== CHANNEL f2 =====
SFO2 400.1316005 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 90.00 usec
PLW2 11.99499989 W
PLW12 0.34213999 W
PLW13 0.27713001 W

F2 - Processing parameters
SI 32768
SF 100.6127780 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



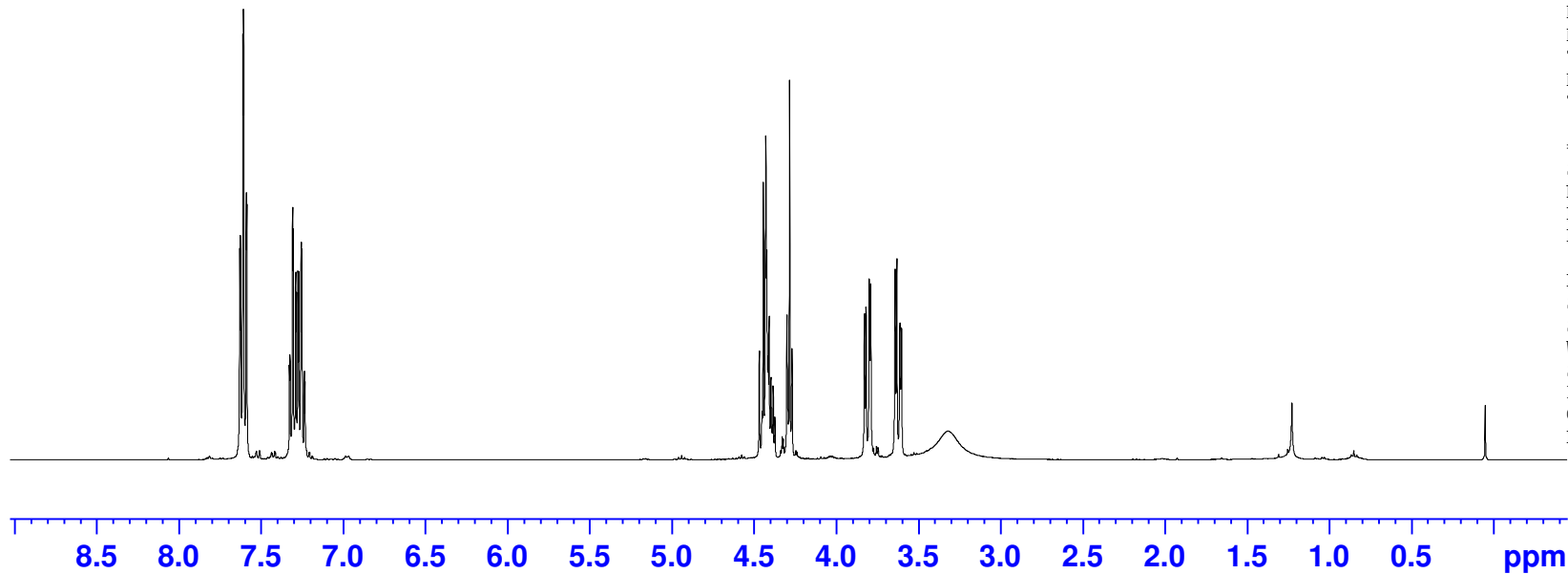
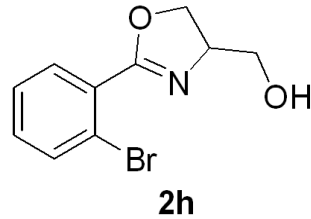
Current Data Parameters
NAME YW-1726A
EXPNO 1
PROCNO 2

F2 - Acquisition Parameters
Date_ 20160413
Time 14.43
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT CDC13
NS 3
DS 0
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 39.46
DW 62.400 usec
DE 6.50 usec
TE 296.7 K
D1 1.00000000 sec
TD0 1

==== CHANNEL f1 =====
SFO1 400.1324710 MHz
NUC1 1H
P1 14.50 usec
PLW1 11.99499989 W

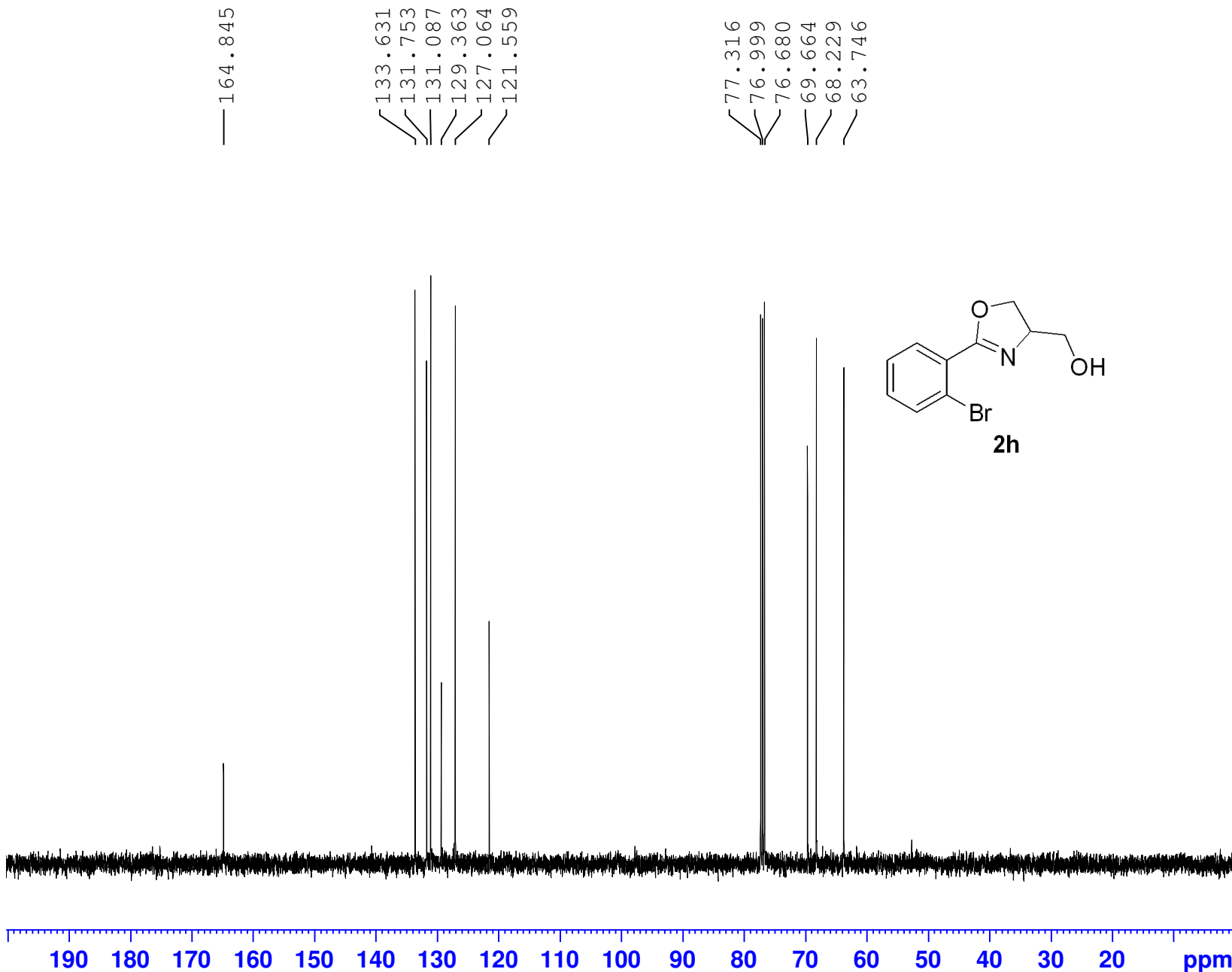
F2 - Processing parameters
SI 65536
SF 400.1300092 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

7.590
7.587
7.327
7.324
7.308
7.305
7.290
7.286
7.275
7.270
7.260
7.256
7.251
7.237
7.232
4.468
4.451
4.443
4.428
4.423
4.414
4.408
4.397
4.384
4.373
4.299
4.284
4.269
3.828
3.818
3.799
3.789
3.641
3.631
3.613
3.609
3.602
3.317



2.00
2.16

2.05
0.96
1.05
1.13
1.36



Current Data Parameters
NAME YW-1726A-carbon
EXPNO 1
PROCNO 2

F2 - Acquisition Parameters
Date_ 20160413
Time 14.44
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 22
DS 0
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 196.92
DW 20.800 usec
DE 6.50 usec
TE 297.3 K
D1 2.0000000 sec
D11 0.0300000 sec
TD0 1

==== CHANNEL f1 =====
SFO1 100.6228298 MHz
NUC1 13C
P1 9.70 usec
PLW1 46.98899841 W

==== CHANNEL f2 =====
SFO2 400.1316005 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 90.00 usec
PLW2 11.99499989 W
PLW12 0.34213999 W
PLW13 0.27713001 W

F2 - Processing parameters
SI 32768
SF 100.6127830 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



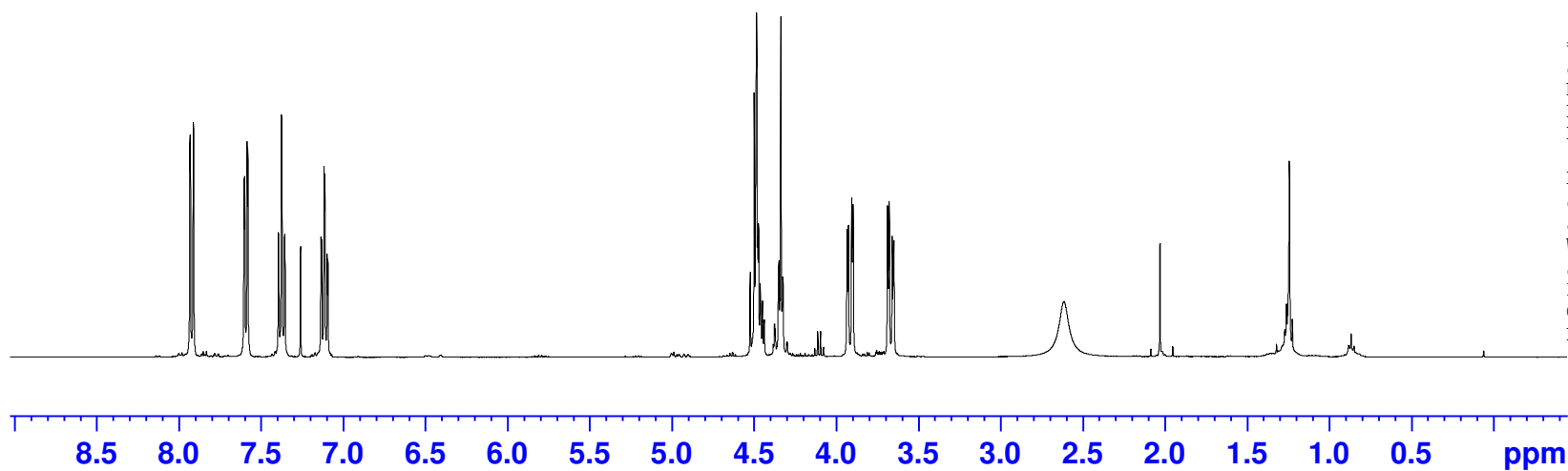
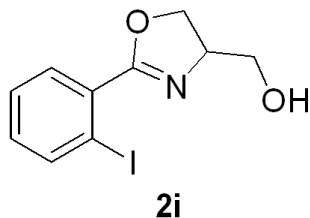
Current Data Parameters
NAME YW-1726B
EXPNO 3
PROCNO 1

F2 - Acquisition Parameters
Date_ 20160414
Time 20.05
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT CDC13
NS 11
DS 0
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 70.97
DW 62.400 usec
DE 6.50 usec
TE 296.5 K
D1 1.00000000 sec
TD0 1

==== CHANNEL f1 =====
SFO1 400.1324710 MHz
NUC1 1H
P1 14.50 usec
PLW1 11.99499989 W

F2 - Processing parameters
SI 65536
SF 400.1300094 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

7.585
7.581
7.395
7.392
7.376
7.373
7.357
7.354
7.260
7.136
7.132
7.117
7.113
7.097
7.093
4.523
4.499
4.485
4.477
4.472
4.462
4.448
4.349
4.343
4.337
4.329
4.324
3.934
3.926
3.906
3.901
3.897
3.688
3.677
3.659
3.653
3.648
2.614



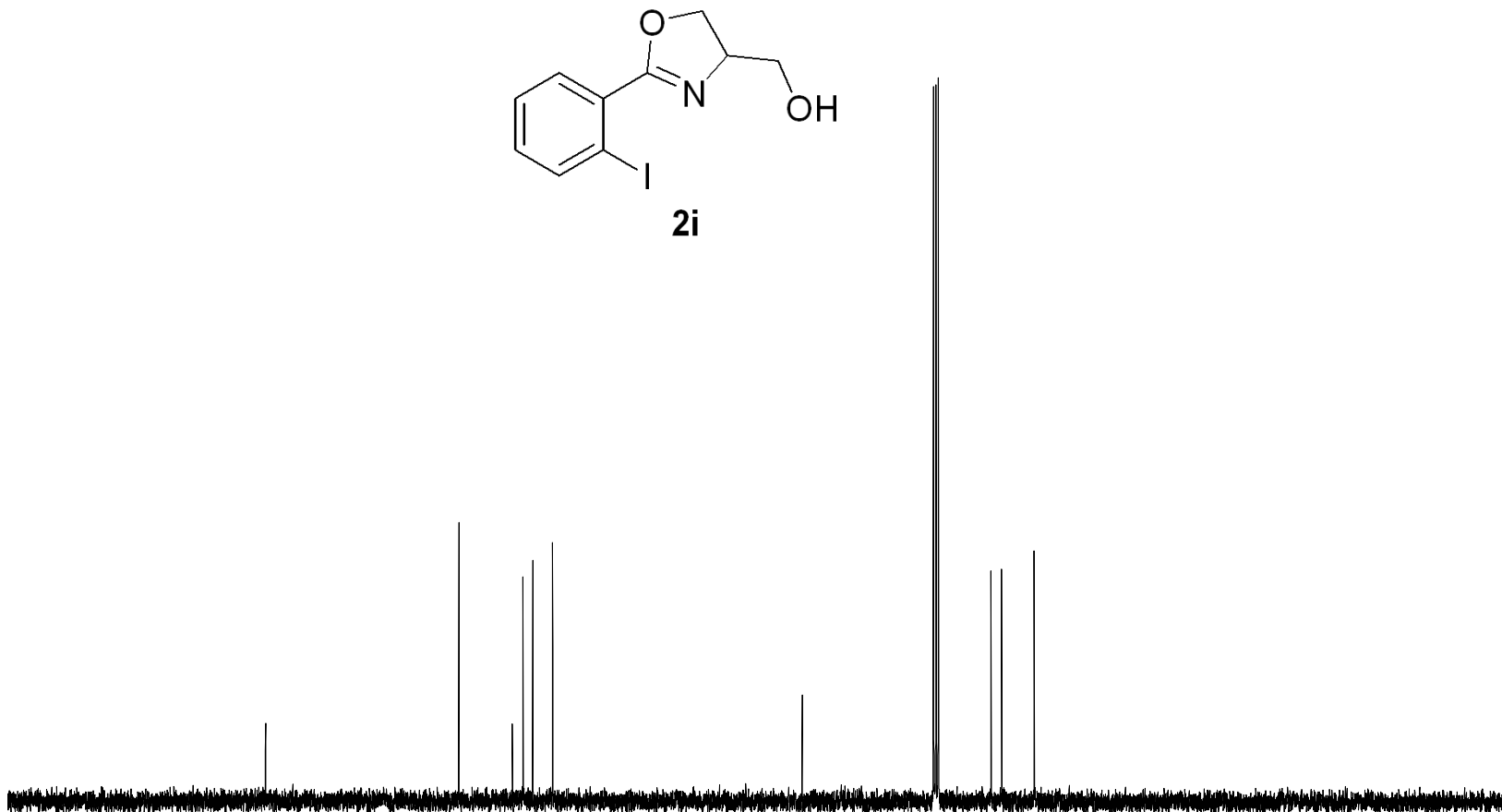
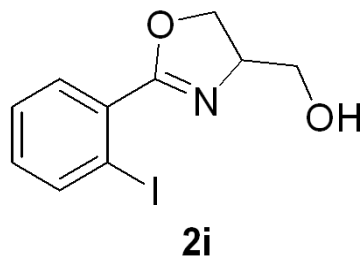


— 166.011

— 140.338
— 133.240
— 131.825
— 130.513
— 127.886

— 94.761

— 77.315
— 76.998
— 76.680
— 69.678
— 68.273
— 63.957



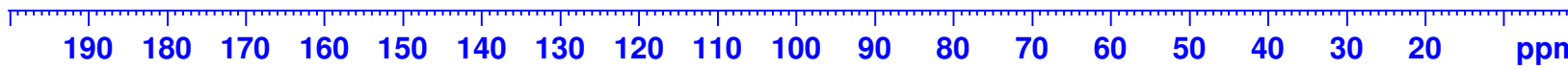
Current Data Parameters
NAME YW-1726B-carbon
EXPNO 4
PROCNO 1

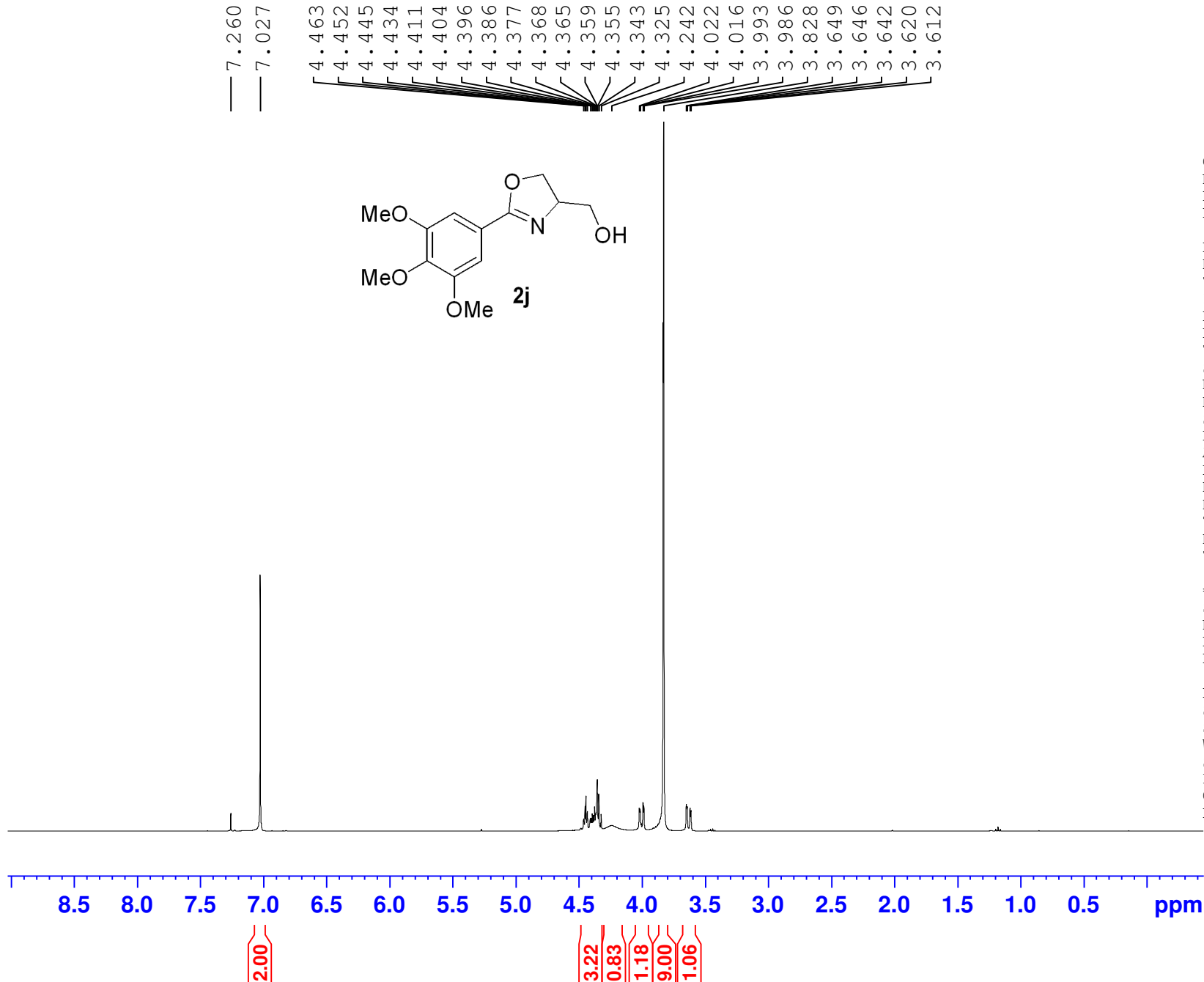
F2 - Acquisition Parameters
Date_ 20160414
Time 20.09
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 29
DS 0
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 196.92
DW 20.800 usec
DE 6.50 usec
TE 297.2 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

==== CHANNEL f1 =====
SFO1 100.6228298 MHz
NUC1 13C
P1 9.70 usec
PLW1 46.98899841 W

==== CHANNEL f2 =====
SFO2 400.1316005 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 90.00 usec
PLW2 11.99499989 W
PLW12 0.34213999 W
PLW13 0.27713001 W

F2 - Processing parameters
SI 32768
SF 100.6127766 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40





Current Data Parameters
NAME YW-1735C
EXPNO 3
PROCNO 1

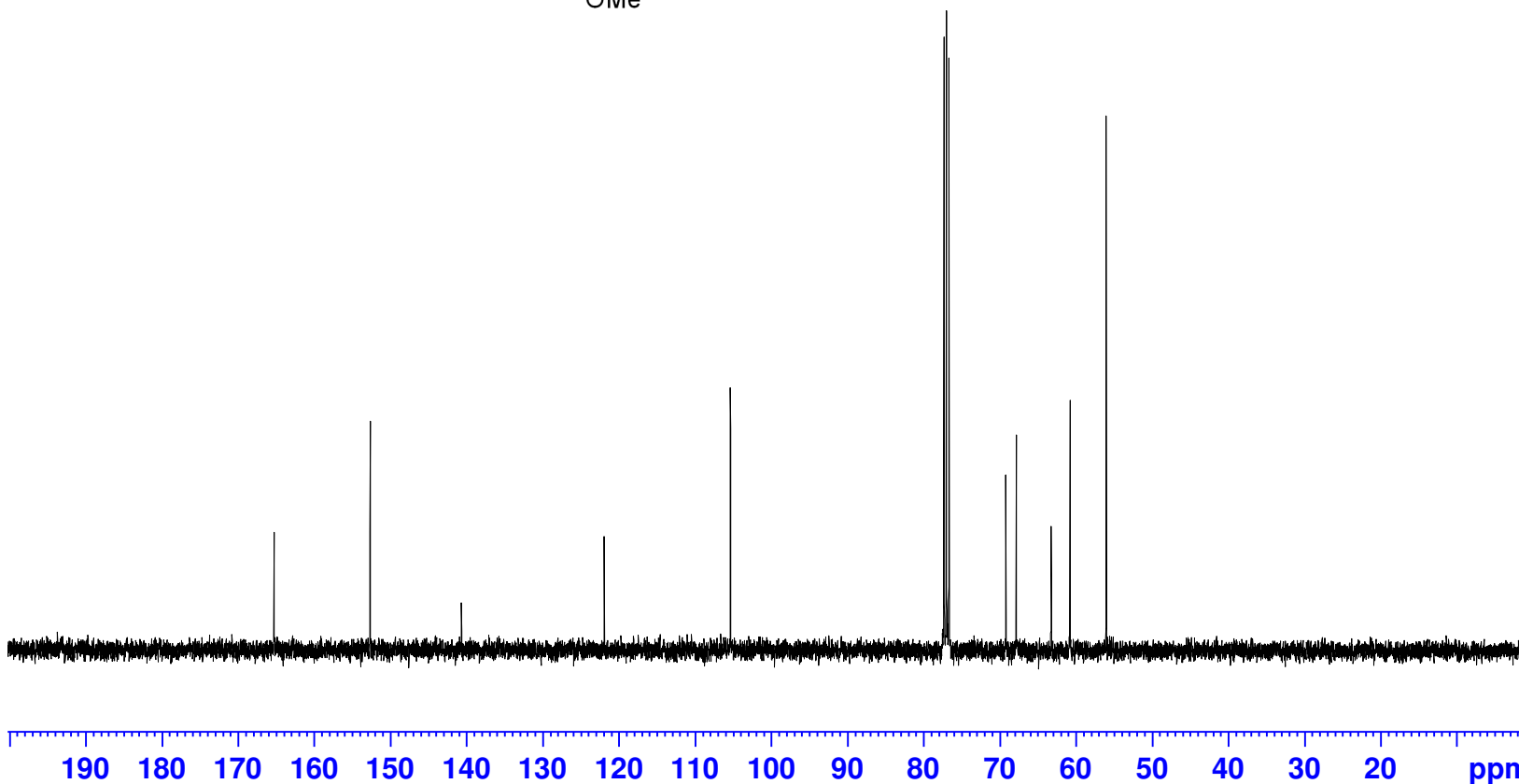
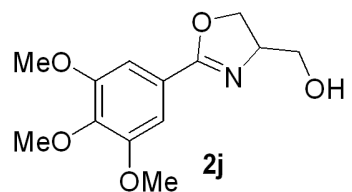
F2 - Acquisition Parameters
Date_ 20160415
Time 14.45
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT CDC13
NS 4
DS 0
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 49.32
DW 62.400 usec
DE 6.50 usec
TE 296.8 K
D1 1.00000000 sec
TD0 1

==== CHANNEL f1 =====
SFO1 400.1324710 MHz
NUC1 1H
P1 14.50 usec
PLW1 11.99499989 W

F2 - Processing parameters
SI 65536
SF 400.1300092 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



— 165.288
— 152.674
— 140.706
— 121.943
— 105.376
77.319
77.001
76.683
69.210
67.829
63.263
60.761
56.030



Current Data Parameters
NAME YW-1735C-carbon
EXPNO 3
PROCNO 1

F2 - Acquisition Parameters
Date_ 20160415
Time 14.48
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 37
DS 0
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 196.92
DW 20.800 usec
DE 6.50 usec
TE 297.6 K
D1 2.0000000 sec
D11 0.0300000 sec
TD0 1

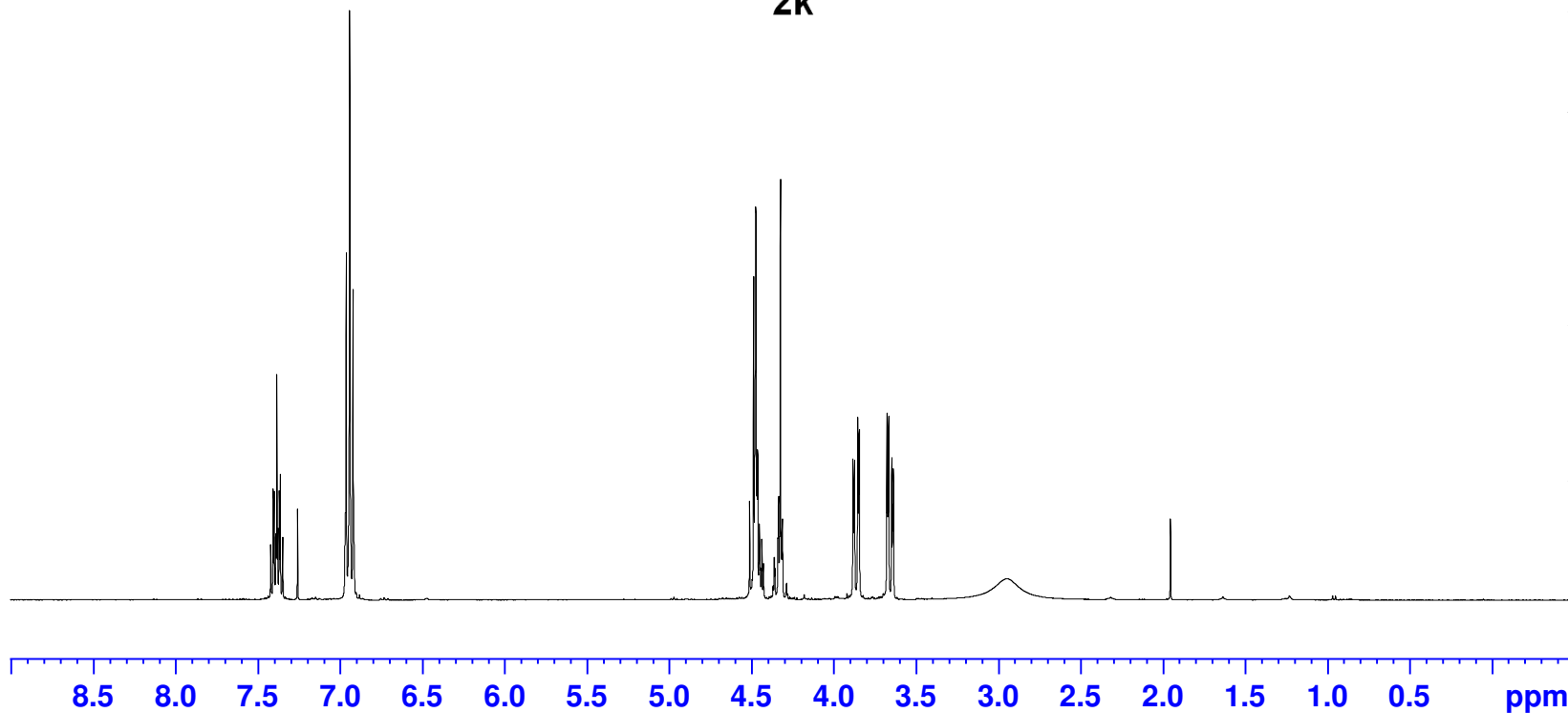
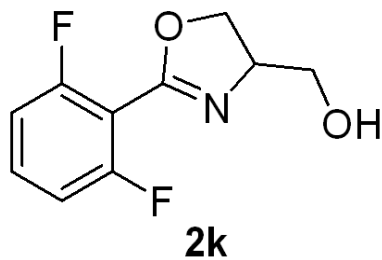
==== CHANNEL f1 =====
SFO1 100.6228298 MHz
NUC1 13C
P1 9.70 usec
PLW1 46.98899841 W

==== CHANNEL f2 =====
SFO2 400.1316005 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 90.00 usec
PLW2 11.99499989 W
PLW12 0.34213999 W
PLW13 0.27713001 W

F2 - Processing parameters
SI 32768
SF 100.6127758 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



7.392
7.386
7.381
7.371
7.365
7.350
7.260
6.972
6.964
6.943
6.923
6.918
4.512
4.487
4.474
4.467
4.463
4.453
4.448
4.438
4.428
4.362
4.358
4.340
4.336
4.329
4.325
4.318
4.313
3.883
3.880
3.874
3.854
3.849
3.845
3.677
3.673
3.667
3.648
3.642
3.638
2.947



Current Data Parameters
NAME YW-1738
EXPNO 3
PROCNO 1

F2 - Acquisition Parameters
Date_ 20160419
Time 14.39
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT CDC13
NS 4
DS 0
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 62.93
DW 62.400 usec
DE 6.50 usec
TE 296.5 K
D1 1.00000000 sec
TD0 1

==== CHANNEL f1 =====
SFO1 400.1324710 MHz
NUC1 1H
P1 14.50 usec
PLW1 11.99499989 W

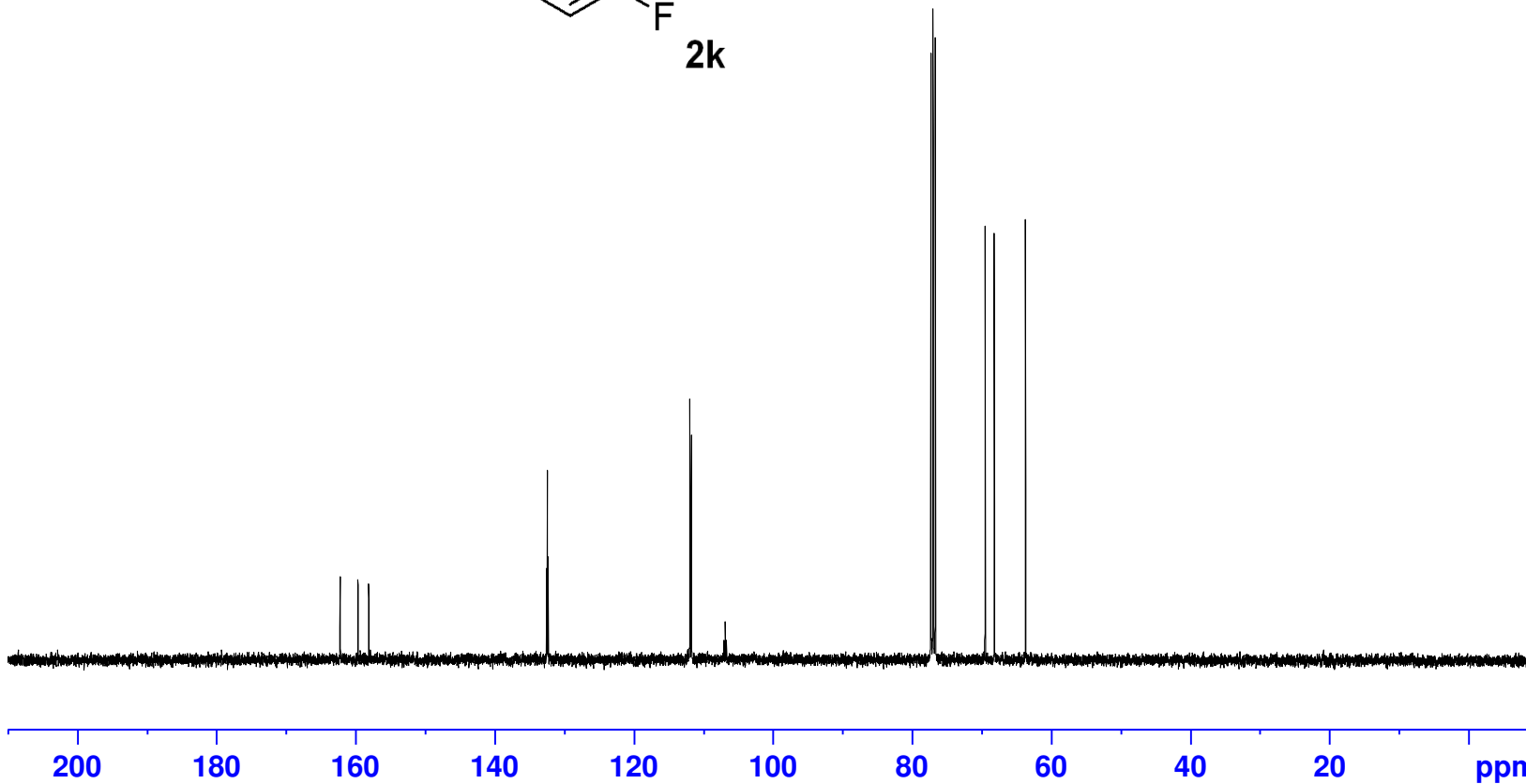
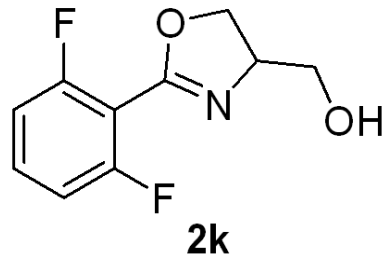
F2 - Processing parameters
SI 65536
SF 400.1300094 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



162.270
162.211
159.724
159.664
158.138

132.548
132.444
132.341
111.999
111.972
111.948
111.794
111.772
111.746
107.059
106.885
106.711

77.318
77.000
76.681
69.527
68.199
63.708



Current Data Parameters
NAME YW-1738-carbon
EXPNO 3
PROCNO 1

F2 - Acquisition Parameters
Date_ 20160419
Time 14.48
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 144
DS 0
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 196.92
DW 20.800 usec
DE 6.50 usec
TE 297.7 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

==== CHANNEL f1 =====
SFO1 100.6228298 MHz
NUC1 13C
P1 9.70 usec
PLW1 46.98899841 W

==== CHANNEL f2 =====
SFO2 400.1316005 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 90.00 usec
PLW2 11.99499989 W
PLW12 0.34213999 W
PLW13 0.27713001 W

F2 - Processing parameters
SI 32768
SF 100.6127758 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



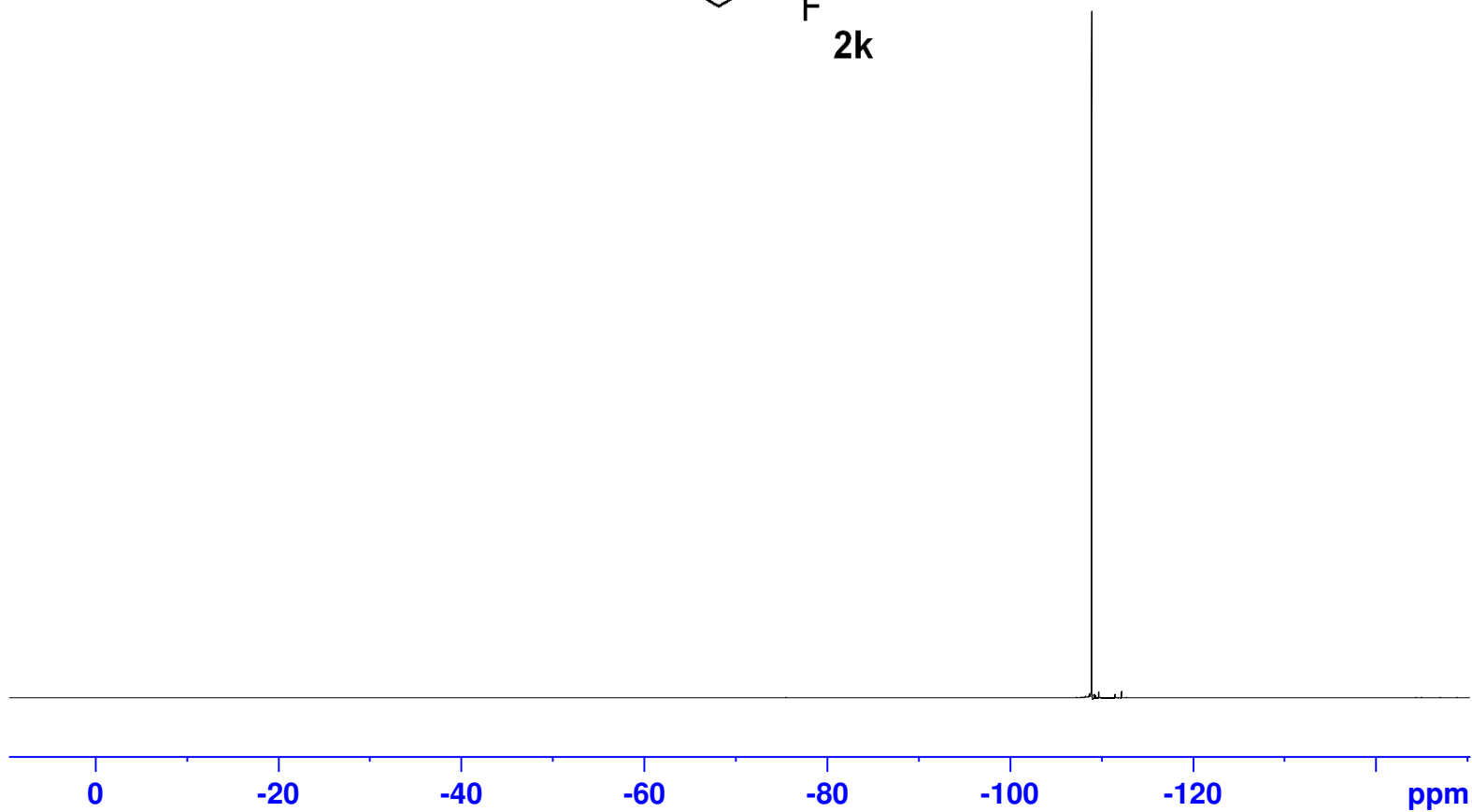
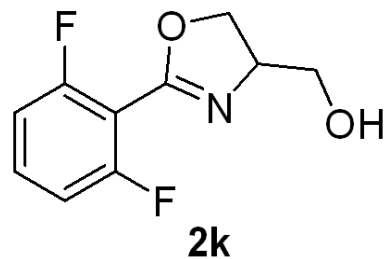
Current Data Parameters
NAME YW-1738-19F
EXPNO 3
PROCNO 1

F2 - Acquisition Parameters
Date_ 20160419
Time 14.52
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgflqn
TD 131072
SOLVENT CDC13
NS 11
DS 0
SWH 89285.711 Hz
FIDRES 0.681196 Hz
AQ 0.7340032 sec
RG 196.92
DW 5.600 usec
DE 6.50 usec
TE 296.7 K
D1 1.00000000 sec
TD0 1

==== CHANNEL f1 =====
SFO1 376.4607164 MHz
NUC1 19F
P1 14.70 usec
PLW1 15.99600029 W

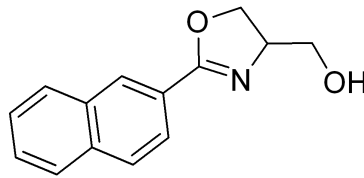
F2 - Processing parameters
SI 65536
SF 376.4983660 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

↙
-108.92
-108.94
↘

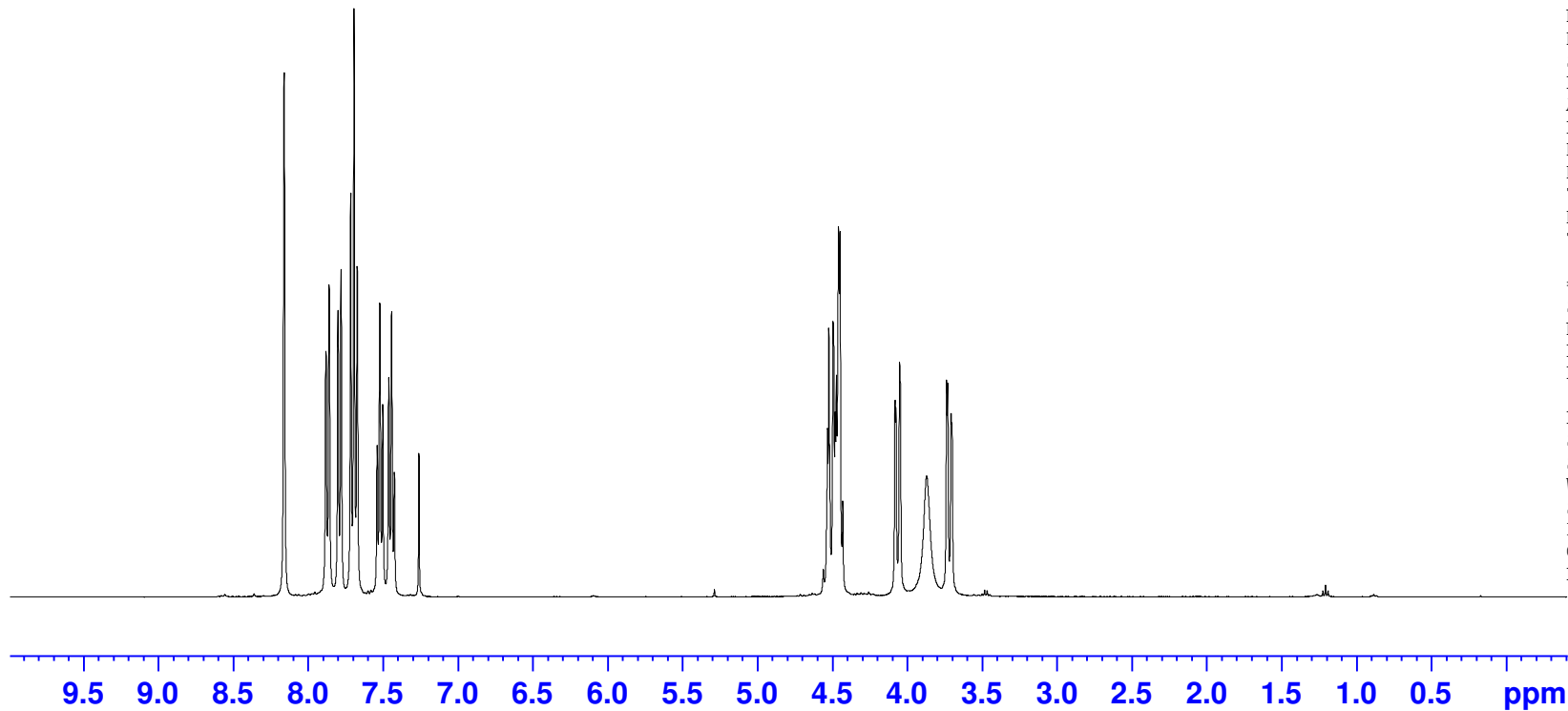




8.160
7.882
7.880
7.861
7.858
7.800
7.780
7.715
7.693
7.672
7.538
7.521
7.502
7.461
7.442
7.424
7.260
4.531
4.523
4.494
4.480
4.471
4.458
4.447
4.429
4.080
4.075
4.050
3.869
3.736
3.729
3.706
3.699



2I



1.00
1.05
1.03
2.02
1.03
1.02

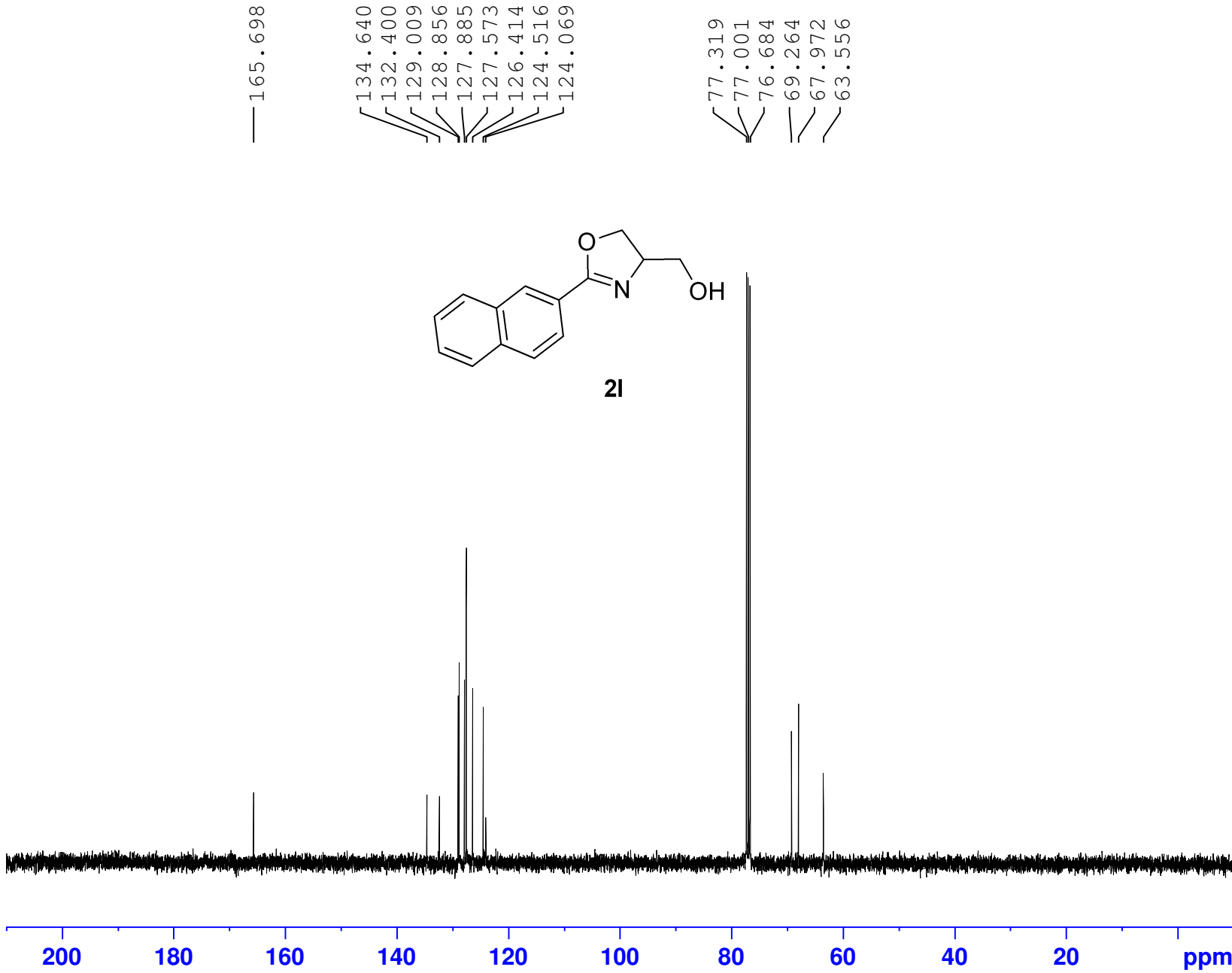
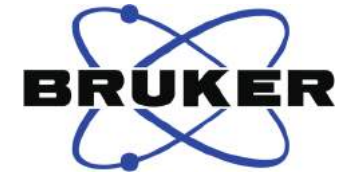
3.07
1.03
1.09
1.07

Current Data Parameters
NAME YW-1728
EXPNO 3
PROCNO 1

F2 - Acquisition Parameters
Date_ 20160414
Time 20.12
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT CDC13
NS 16
DS 0
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 82.92
DW 62.400 usec
DE 6.50 usec
TE 296.5 K
D1 1.00000000 sec
TD0 1

==== CHANNEL f1 =====
SFO1 400.1324710 MHz
NUC1 1H
P1 14.50 usec
PLW1 11.99499989 W

F2 - Processing parameters
SI 65536
SF 400.1300094 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



— 165.698

134.640
132.400
129.009
128.856
127.885
127.573
126.414
124.516
124.069

77.319
77.001
76.684
69.264
67.972
63.556

Current Data Parameters
NAME YW-1728-carbon
EXPNO 3
PROCNO 1

F2 - Acquisition Parameters
Date_ 20160414
Time 20.16
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 36
DS 0
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 196.92
DW 20.800 usec
DE 6.50 usec
TE 297.3 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

==== CHANNEL f1 =====
SFO1 100.6228298 MHz
NUC1 13C
P1 9.70 usec
PLW1 46.98899841 W

==== CHANNEL f2 =====
SFO2 400.1316005 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 90.00 usec
PLW2 11.99499989 W
PLW12 0.34213999 W
PLW13 0.27713001 W

F2 - Processing parameters
SI 32768
SF 100.6127744 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

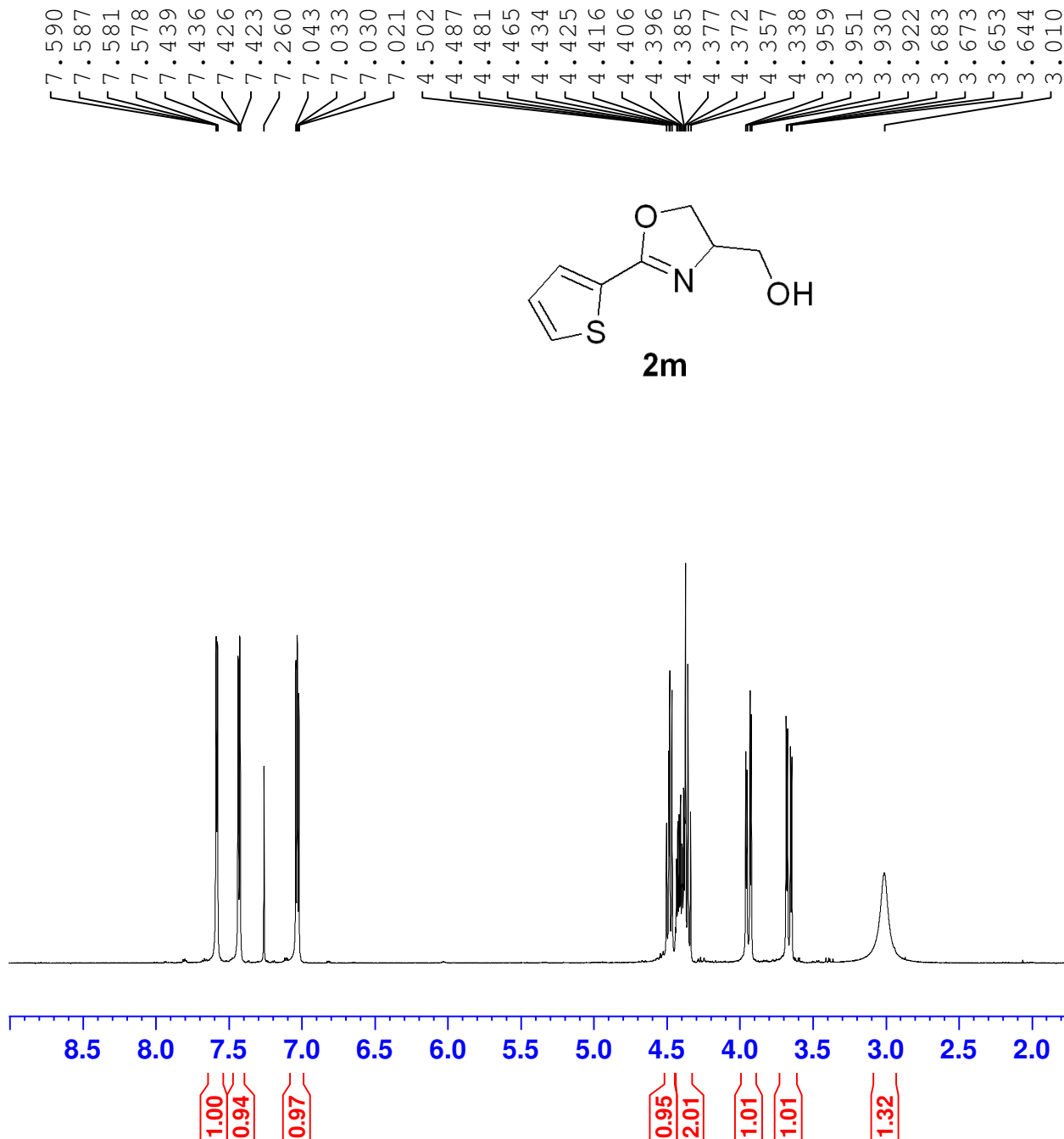
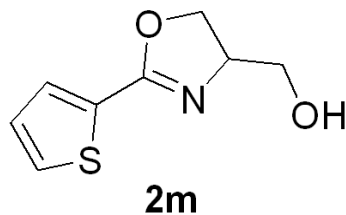


Current Data Parameters
NAME YW-1782
EXPNO 4
PROCNO 1

F2 - Acquisition Parameters
Date_ 20160801
Time 20.10
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT CDC13
NS 3
DS 0
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 126.97
DW 62.400 usec
DE 6.50 usec
TE 299.0 K
D1 1.00000000 sec
TD0 1

==== CHANNEL f1 =====
SFO1 400.1324710 MHz
NUC1 1H
P1 14.50 usec
PLW1 11.99499989 W

F2 - Processing parameters
SI 65536
SF 400.1300094 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

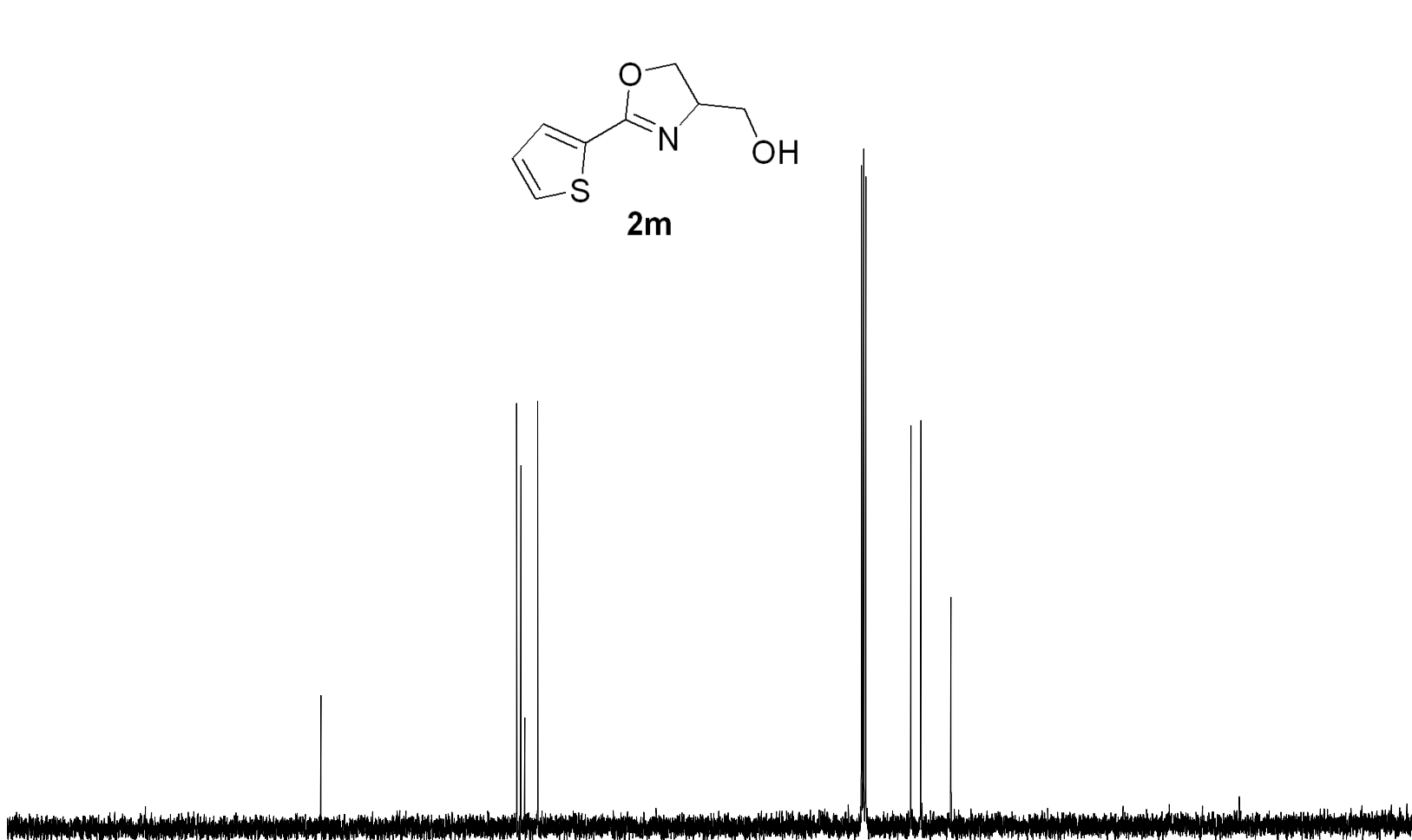
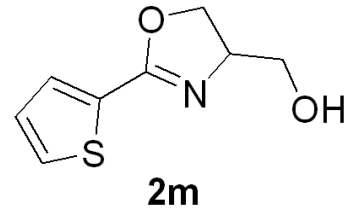




— 161.140

130.802
130.146
129.554
127.545

77.320
77.001
76.684
69.673
68.125
63.487



Current Data Parameters
NAME YW-1782-carbon
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20160730
Time 20.52
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 48
DS 0
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 196.92
DW 20.800 usec
DE 6.50 usec
TE 300.7 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

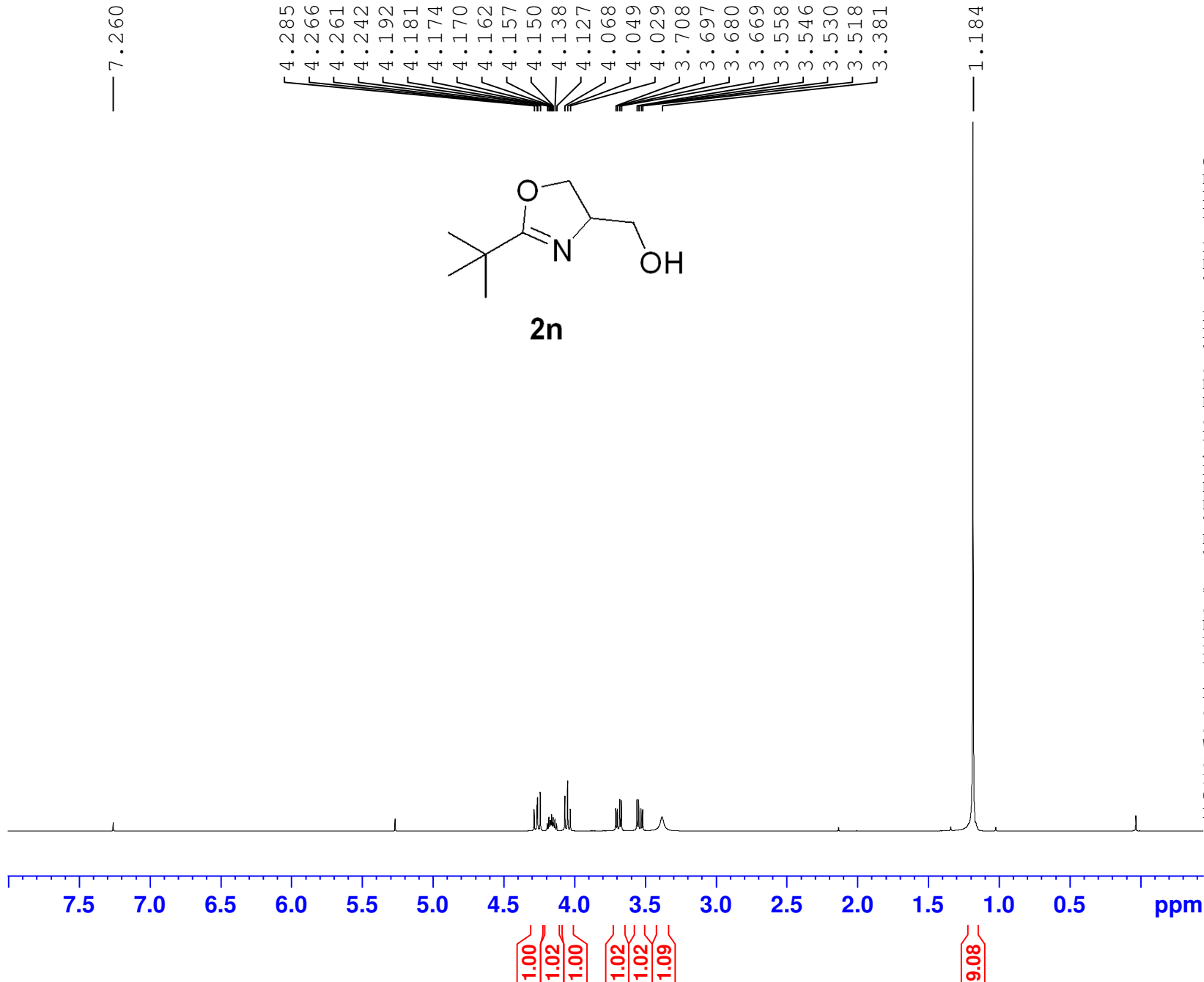
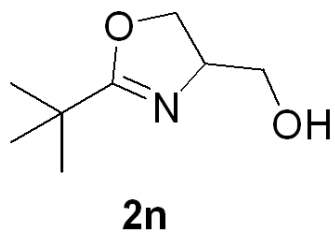
==== CHANNEL f1 =====
SFO1 100.6228298 MHz
NUC1 13C
P1 9.70 usec
PLW1 46.98899841 W

==== CHANNEL f2 =====
SFO2 400.1316005 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 90.00 usec
PLW2 11.99499989 W
PLW12 0.34213999 W
PLW13 0.27713001 W

F2 - Processing parameters
SI 32768
SF 100.6127751 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

— 7.260

4.285
4.266
4.261
4.242
4.192
4.181
4.174
4.170
4.162
4.157
4.150
4.138
4.127
4.068
4.049
4.029
3.708
3.697
3.680
3.669
3.558
3.546
3.530
3.518
3.381

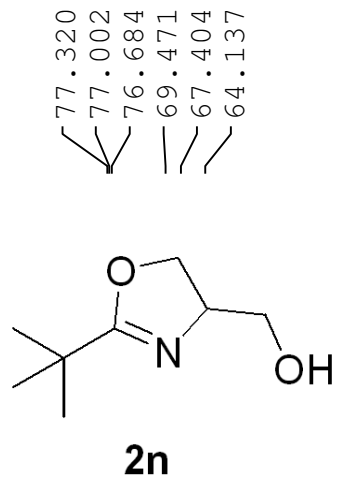
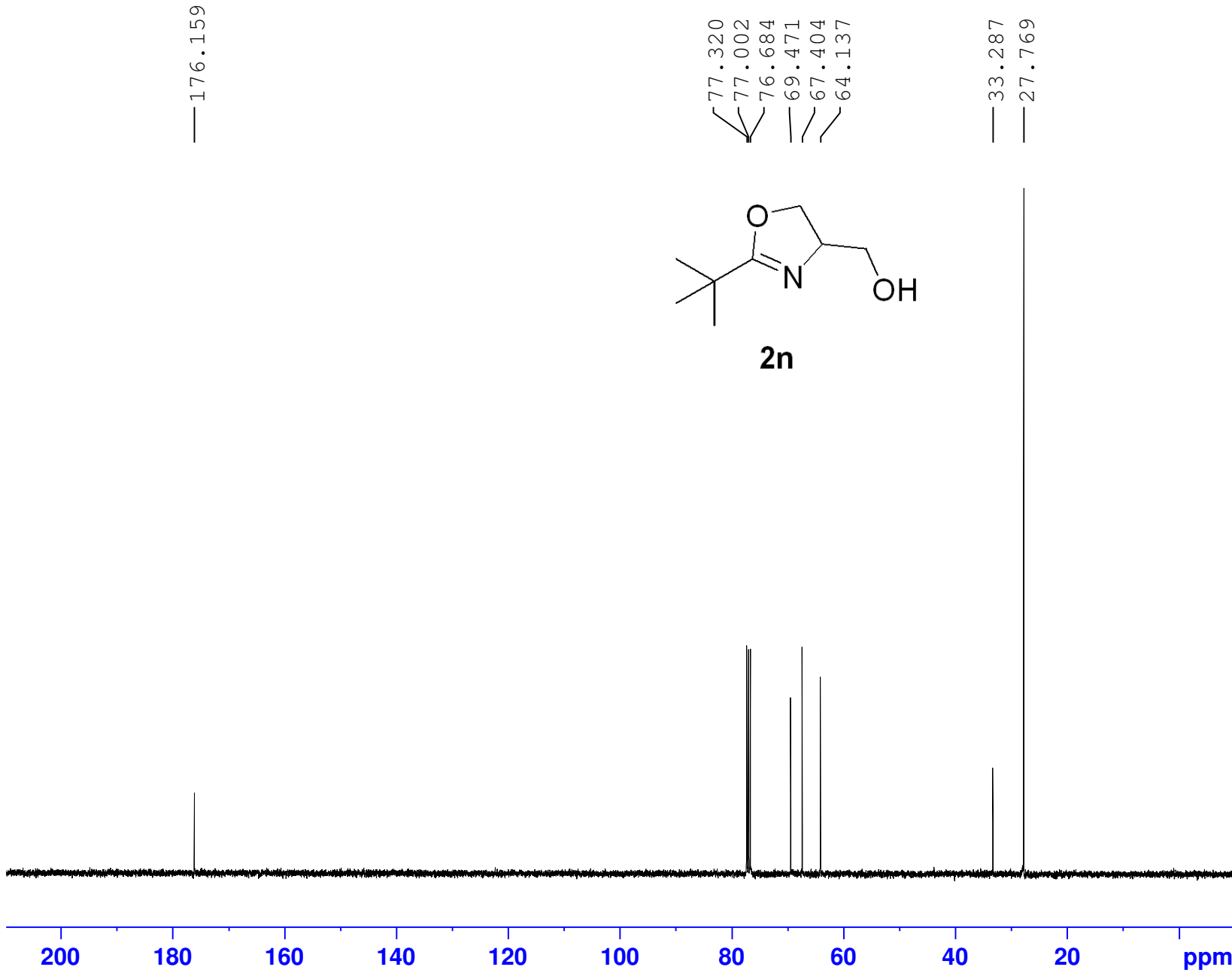
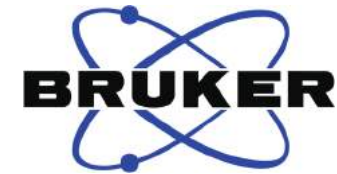


Current Data Parameters
NAME YW-1783
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20160802
Time 15.54
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT CDC13
NS 10
DS 0
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 34.77
DW 62.400 usec
DE 6.50 usec
TE 298.8 K
D1 1.00000000 sec
TD0 1

==== CHANNEL f1 =====
SFO1 400.1324710 MHz
NUC1 1H
P1 14.50 usec
PLW1 11.99499989 W

F2 - Processing parameters
SI 65536
SF 400.1300094 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



Current Data Parameters
NAME YW-1783-carbon
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20160802
Time 15.56
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 34
DS 0
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 196.92
DW 20.800 usec
DE 6.50 usec
TE 299.6 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

==== CHANNEL f1 =====
SFO1 100.6228298 MHz
NUC1 13C
P1 9.70 usec
PLW1 46.98899841 W

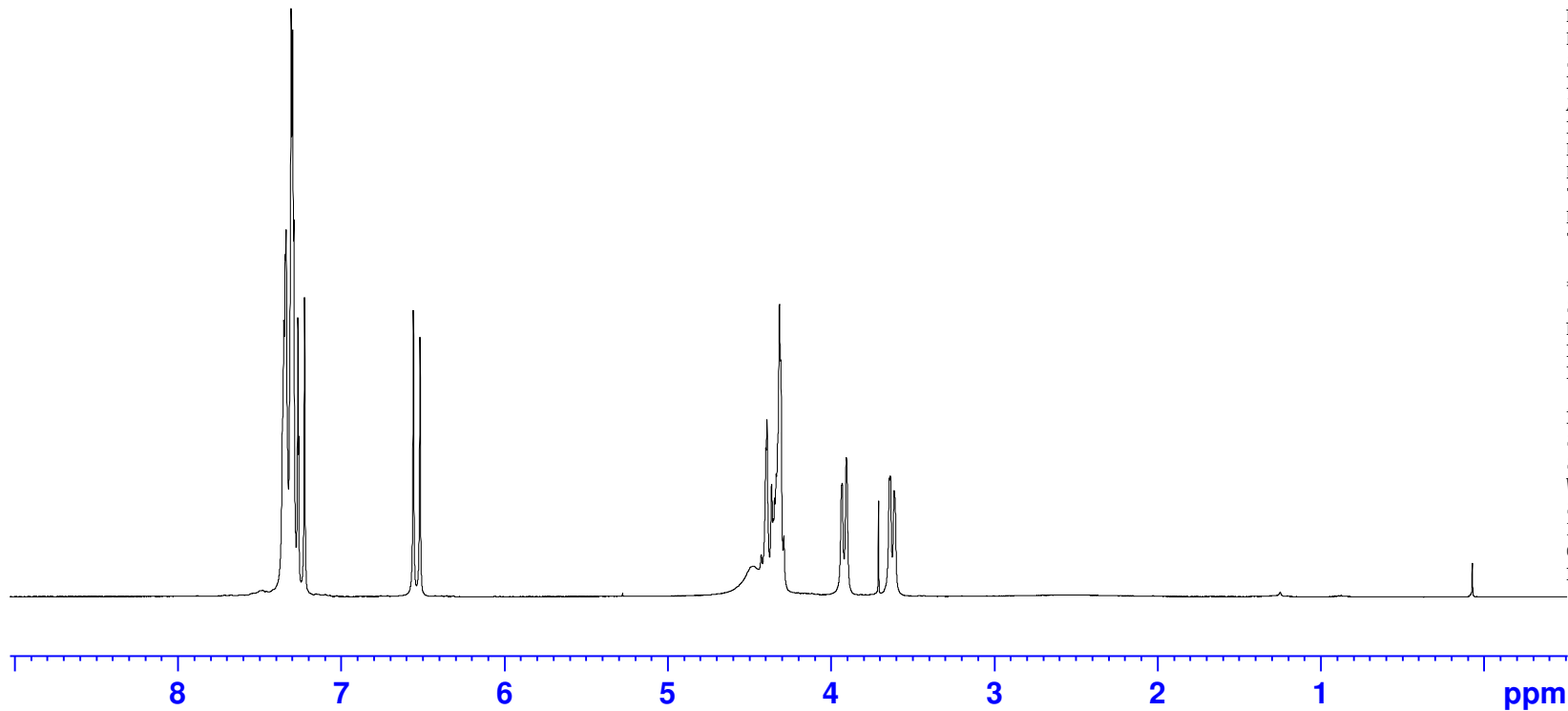
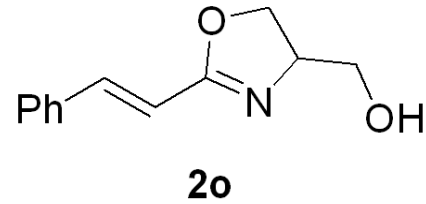
==== CHANNEL f2 =====
SFO2 400.1316005 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 90.00 usec
PLW2 11.99499989 W
PLW12 0.34213999 W
PLW13 0.27713001 W

F2 - Processing parameters
SI 32768
SF 100.6127737 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



7.351
7.342
7.336
7.306
7.298
7.290
7.265
7.260
7.224
6.557
6.517

4.474
4.426
4.398
4.392
4.363
4.352
4.344
4.334
4.315
4.307
4.288
3.931
3.906
3.708
3.641
3.636
3.612



Current Data Parameters
NAME YW-1907B
EXPNO 1
PROCNO 1

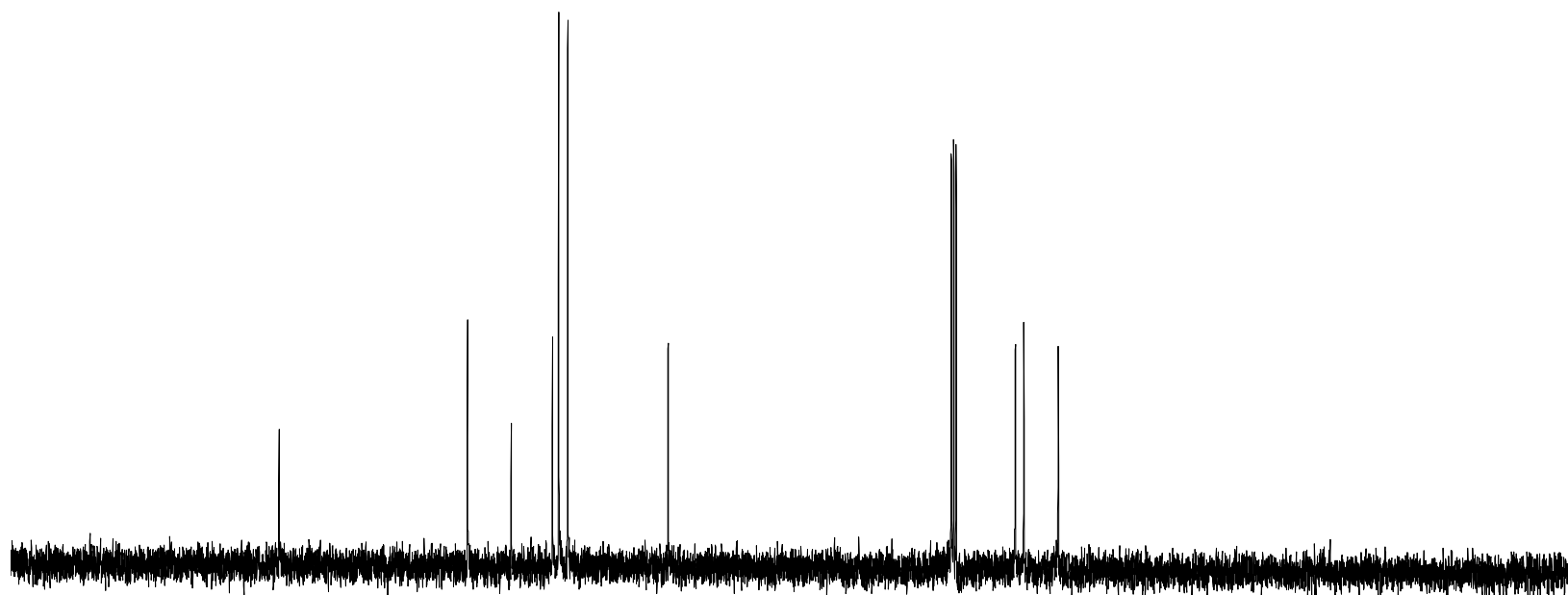
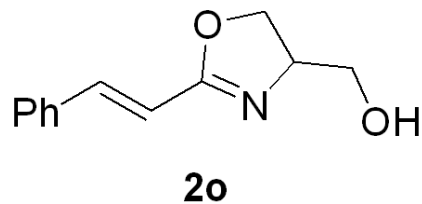
F2 - Acquisition Parameters
Date_ 20160811
Time 10.52
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT CDC13
NS 3
DS 0
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 49.32
DW 62.400 usec
DE 6.50 usec
TE 299.3 K
D1 1.00000000 sec
TD0 1

==== CHANNEL f1 =====
SFO1 400.1324710 MHz
NUC1 1H
P1 14.50 usec
PLW1 11.99499989 W

F2 - Processing parameters
SI 65536
SF 400.1300095 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



— 165.206
— 140.568
— 134.854
— 129.459
— 128.653
— 127.462
— 114.343
77.317
77.000
76.681
68.945
67.842
63.345



Current Data Parameters
NAME YW-1907B-carbon
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20160811
Time 13.00
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 31
DS 0
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 196.92
DW 20.800 usec
DE 6.50 usec
TE 299.5 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

==== CHANNEL f1 =====
SFO1 100.6228298 MHz
NUC1 13C
P1 9.70 usec
PLW1 46.98899841 W

==== CHANNEL f2 =====
SFO2 400.1316005 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 90.00 usec
PLW2 11.99499989 W
PLW12 0.34213999 W
PLW13 0.27713001 W

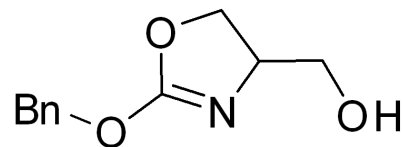
F2 - Processing parameters
SI 32768
SF 100.6127767 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

180 160 140 120 100 80 60 40 20 ppm

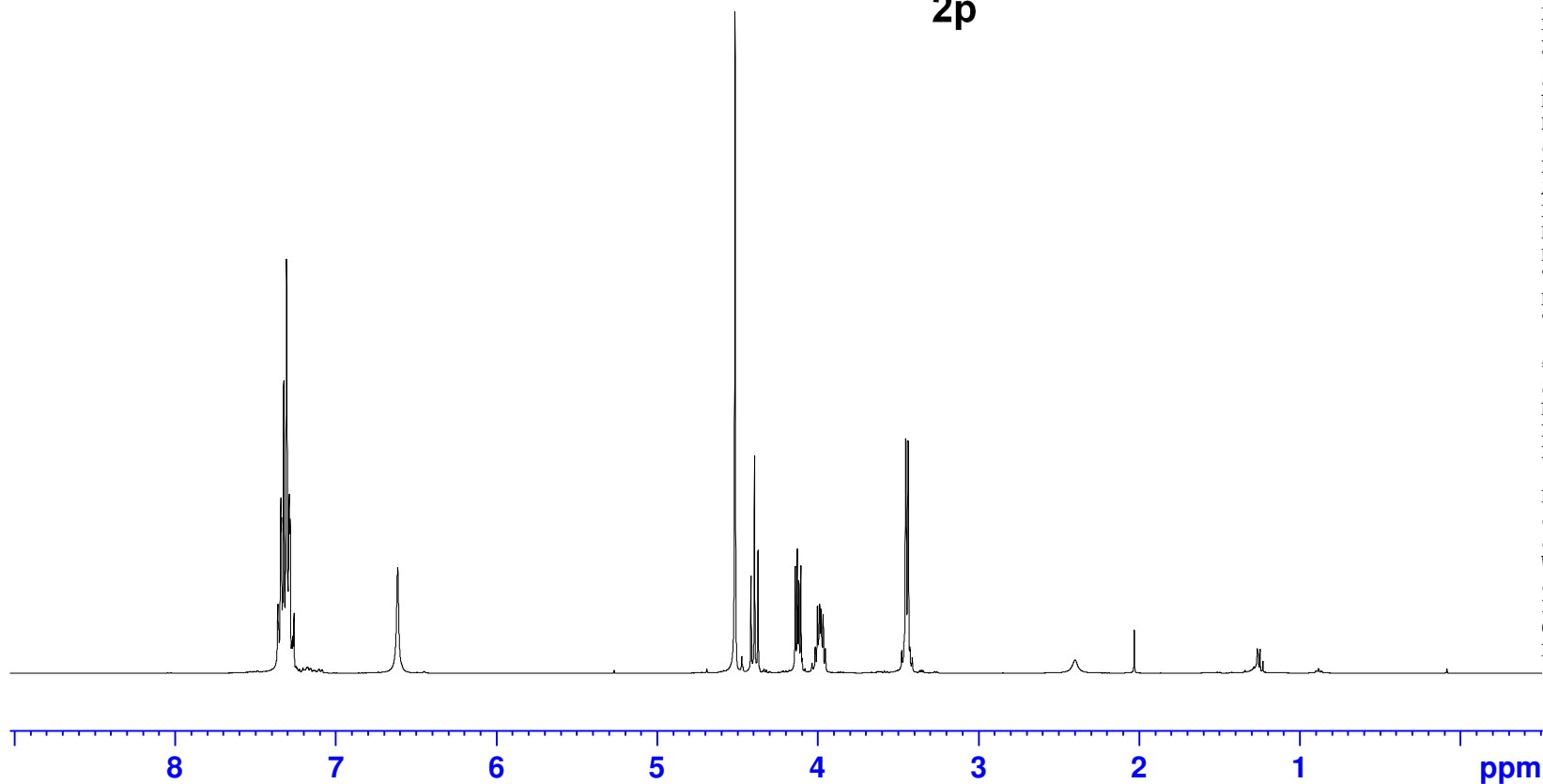


7.359
7.355
7.342
7.338
7.331
7.324
7.306
7.289
7.284
7.260
6.614

4.514
4.415
4.393
4.371
4.139
4.127
4.117
4.105
4.014
4.001
3.987
3.979
3.965
3.952
3.453
3.449
3.438
3.436



2p

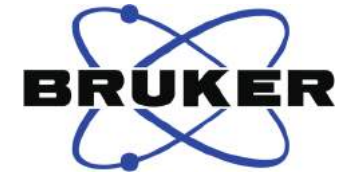


Current Data Parameters
NAME YW-1761A
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20160504
Time 18.41
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT CDC13
NS 8
DS 0
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 25.32
DW 62.400 usec
DE 6.50 usec
TE 296.0 K
D1 1.00000000 sec
TD0 1

==== CHANNEL f1 =====
SFO1 400.1324710 MHz
NUC1 1H
P1 14.50 usec
PLW1 11.99499989 W

F2 - Processing parameters
SI 65536
SF 400.1300091 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



—159.913

—137.255

128.330

127.762

127.561

77.317

76.999

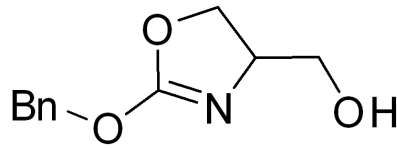
76.680

73.285

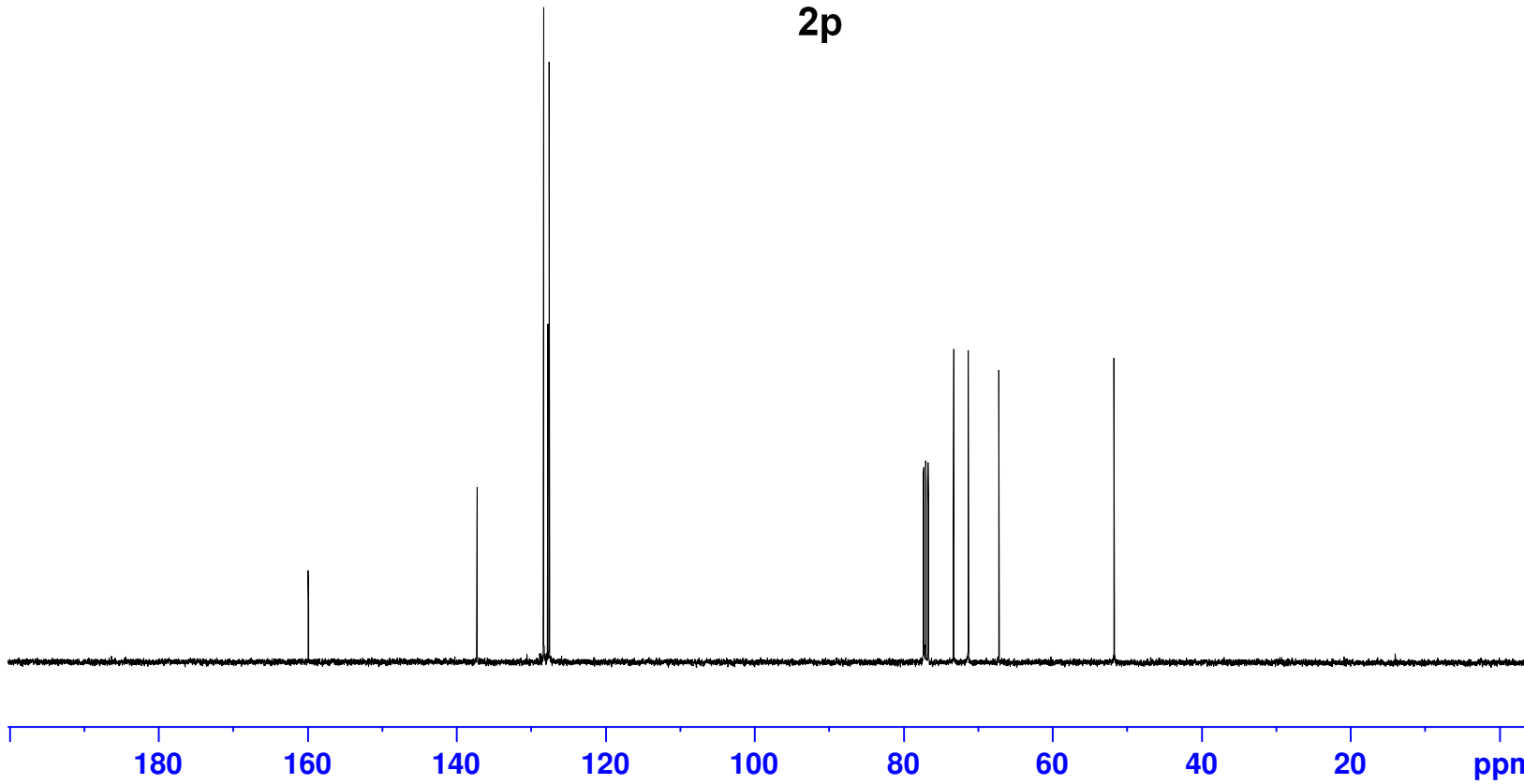
71.315

67.203

—51.739



2p



Current Data Parameters
NAME YW-1761A-carbon
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20160504
Time 18.45
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 48
DS 0
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 196.92
DW 20.800 usec
DE 6.50 usec
TE 296.9 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

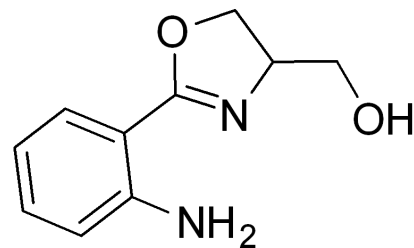
==== CHANNEL f1 =====
SFO1 100.6228298 MHz
NUC1 13C
P1 9.70 usec
PLW1 46.98899841 W

==== CHANNEL f2 =====
SFO2 400.1316005 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 90.00 usec
PLW2 11.99499989 W
PLW12 0.34213999 W
PLW13 0.27713001 W

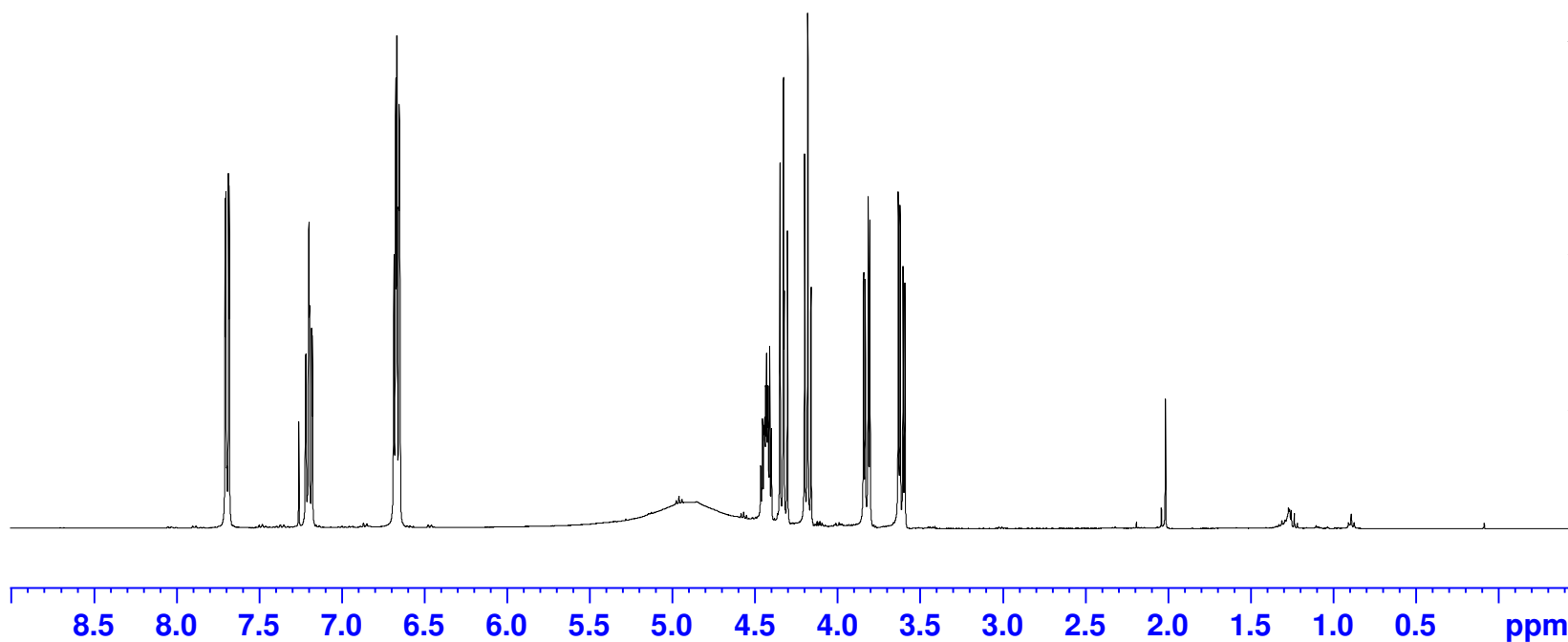
F2 - Processing parameters
SI 32768
SF 100.6127912 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



7.220
7.216
7.202
7.199
7.196
7.182
7.178
6.686
6.684
6.675
6.672
6.666
6.655
6.652
6.649
4.851
4.464
4.453
4.444
4.439
4.434
4.429
4.424
4.420
4.410
4.399
4.347
4.327
4.323
4.302
4.199
4.179
4.160
3.842
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3.813
3.803
3.631
3.620
3.603
3.592



2q

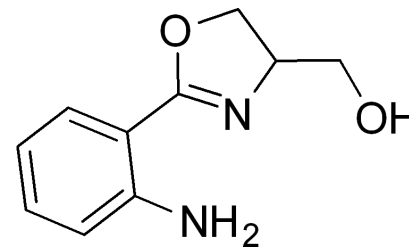


Current Data Parameters
NAME YW-1742A
EXPNO 4
PROCNO 1

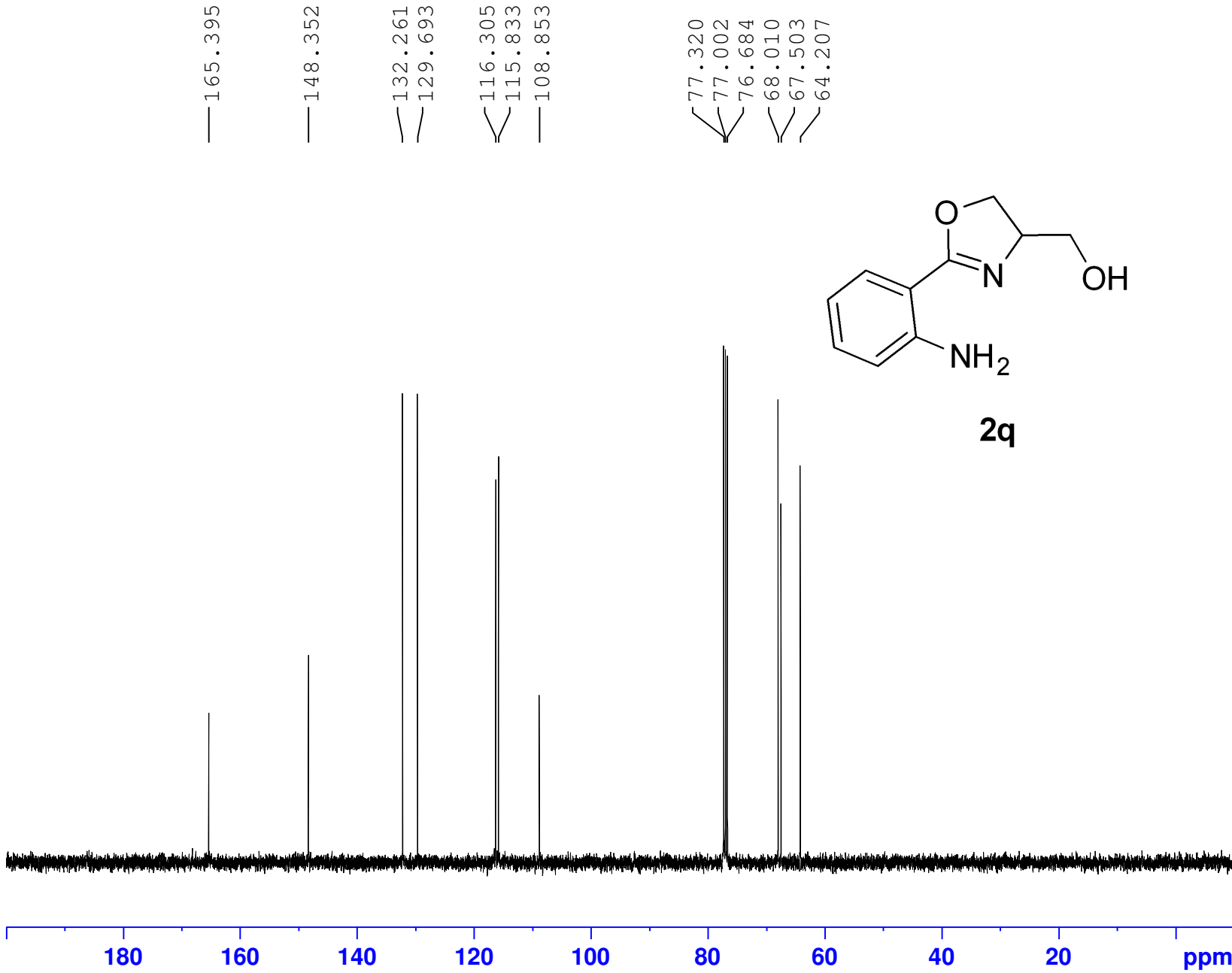
F2 - Acquisition Parameters
Date_ 20160420
Time 20.02
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT CDC13
NS 5
DS 0
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 45.67
DW 62.400 usec
DE 6.50 usec
TE 297.3 K
D1 1.00000000 sec
TD0 1

==== CHANNEL f1 =====
SFO1 400.1324710 MHz
NUC1 1H
P1 14.50 usec
PLW1 11.99499989 W

F2 - Processing parameters
SI 65536
SF 400.1300093 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



2q



Current Data Parameters
NAME YW-1742A-carbon
EXPNO 4
PROCNO 1

F2 - Acquisition Parameters
Date_ 20160420
Time 20.05
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 32
DS 0
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 196.92
DW 20.800 usec
DE 6.50 usec
TE 298.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

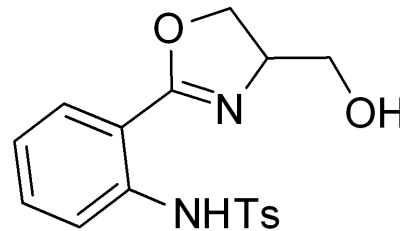
==== CHANNEL f1 =====
SFO1 100.6228298 MHz
NUC1 13C
P1 9.70 usec
PLW1 46.98899841 W

==== CHANNEL f2 =====
SFO2 400.1316005 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 90.00 usec
PLW2 11.99499989 W
PLW12 0.34213999 W
PLW13 0.27713001 W

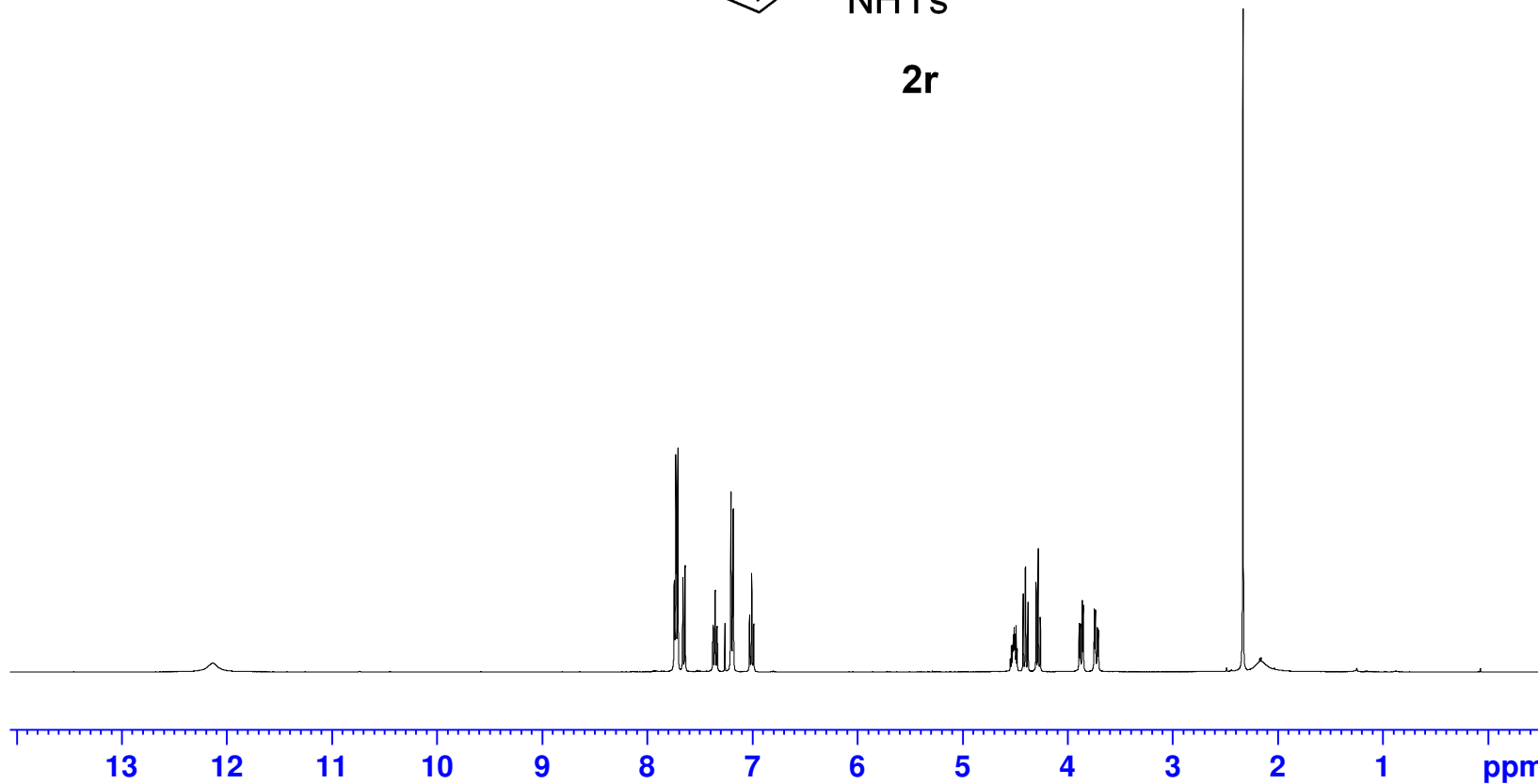
F2 - Processing parameters
SI 32768
SF 100.6127810 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



12.137
7.744
7.740
7.729
7.724
7.720
7.708
7.660
7.639
7.375
7.371
7.353
7.336
7.332
7.260
7.202
7.181
7.026
7.024
7.006
6.988
6.986
4.533
4.524
4.520
4.514
4.509
4.499
4.490
4.479
4.421
4.401
4.397
4.376
4.298
4.278
4.258
3.889
3.878
3.860
3.850
3.744
3.734



2r



0.87

2.95
0.99
1.01
1.98
1.00

1.01
1.00
1.00
1.02
1.01

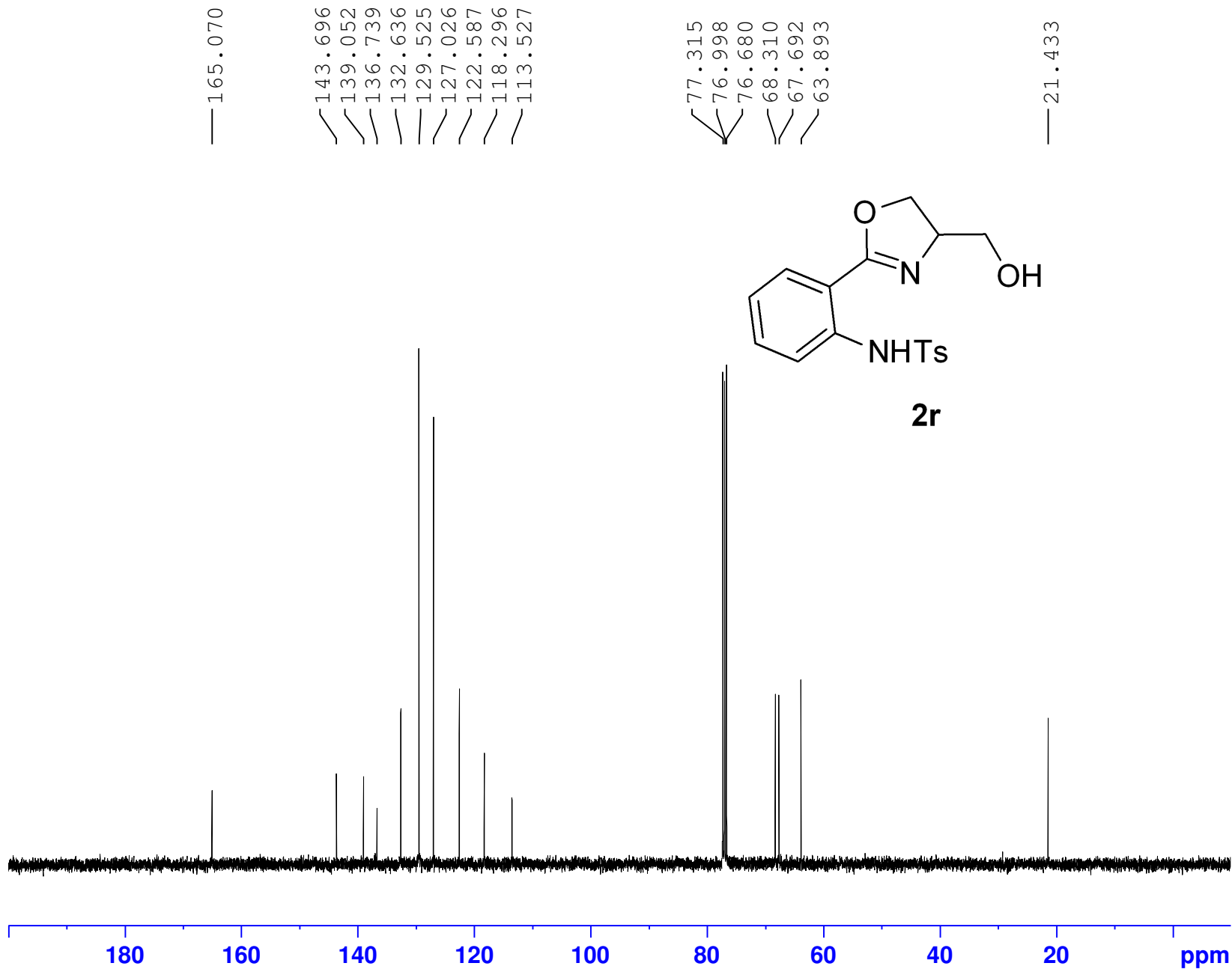
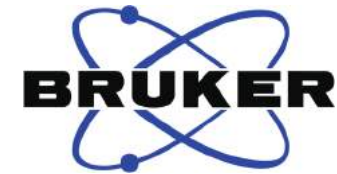
3.07
0.93

Current Data Parameters
NAME YW-1742B
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20160422
Time 20.23
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT CDC13
NS 3
DS 0
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 54.81
DW 62.400 usec
DE 6.50 usec
TE 296.4 K
D1 1.00000000 sec
TD0 1

==== CHANNEL f1 =====
SFO1 400.1324710 MHz
NUC1 1H
P1 14.50 usec
PLW1 11.99499989 W

F2 - Processing parameters
SI 65536
SF 400.1300094 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



Current Data Parameters
NAME YW-1742B-carbon
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20160422
Time 20.27
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 50
DS 0
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 196.92
DW 20.800 usec
DE 6.50 usec
TE 297.4 K
D1 2.0000000 sec
D11 0.0300000 sec
TD0 1

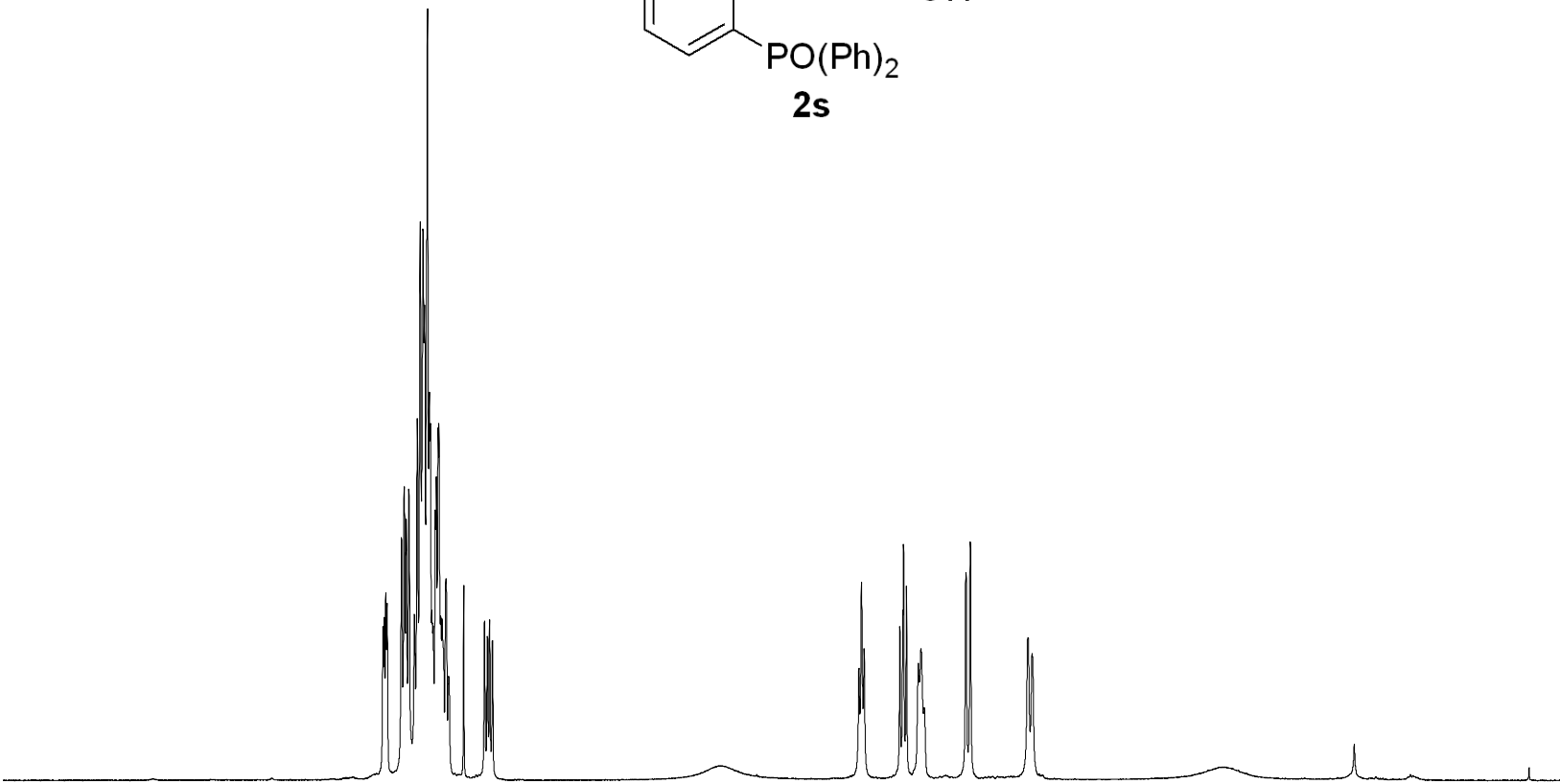
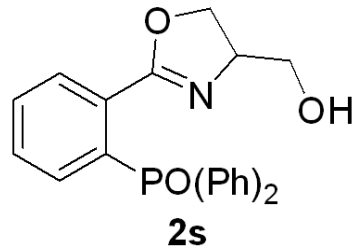
==== CHANNEL f1 =====
SFO1 100.6228298 MHz
NUC1 13C
P1 9.70 usec
PLW1 46.98899841 W

==== CHANNEL f2 =====
SFO2 400.1316005 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 90.00 usec
PLW2 11.99499989 W
PLW12 0.34213999 W
PLW13 0.27713001 W

F2 - Processing parameters
SI 32768
SF 100.6127765 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



7.804
7.795
7.785
7.777
7.679
7.662
7.647
7.630
7.592
7.573
7.553
7.534
7.523
7.504
7.491
7.484
7.474
7.471
7.466
7.451
7.444
7.432
7.427
7.414
7.406
7.379
7.361
7.259
7.119
7.100
7.084
7.065
5.526
4.591
4.573
4.556
4.315
4.295
4.290
4.270
4.190
4.172
4.150
3.870
3.867
3.840
3.448
3.422



1.02
2.19
10.48
1.02
0.81
1.00
1.03
1.02
1.02
1.03

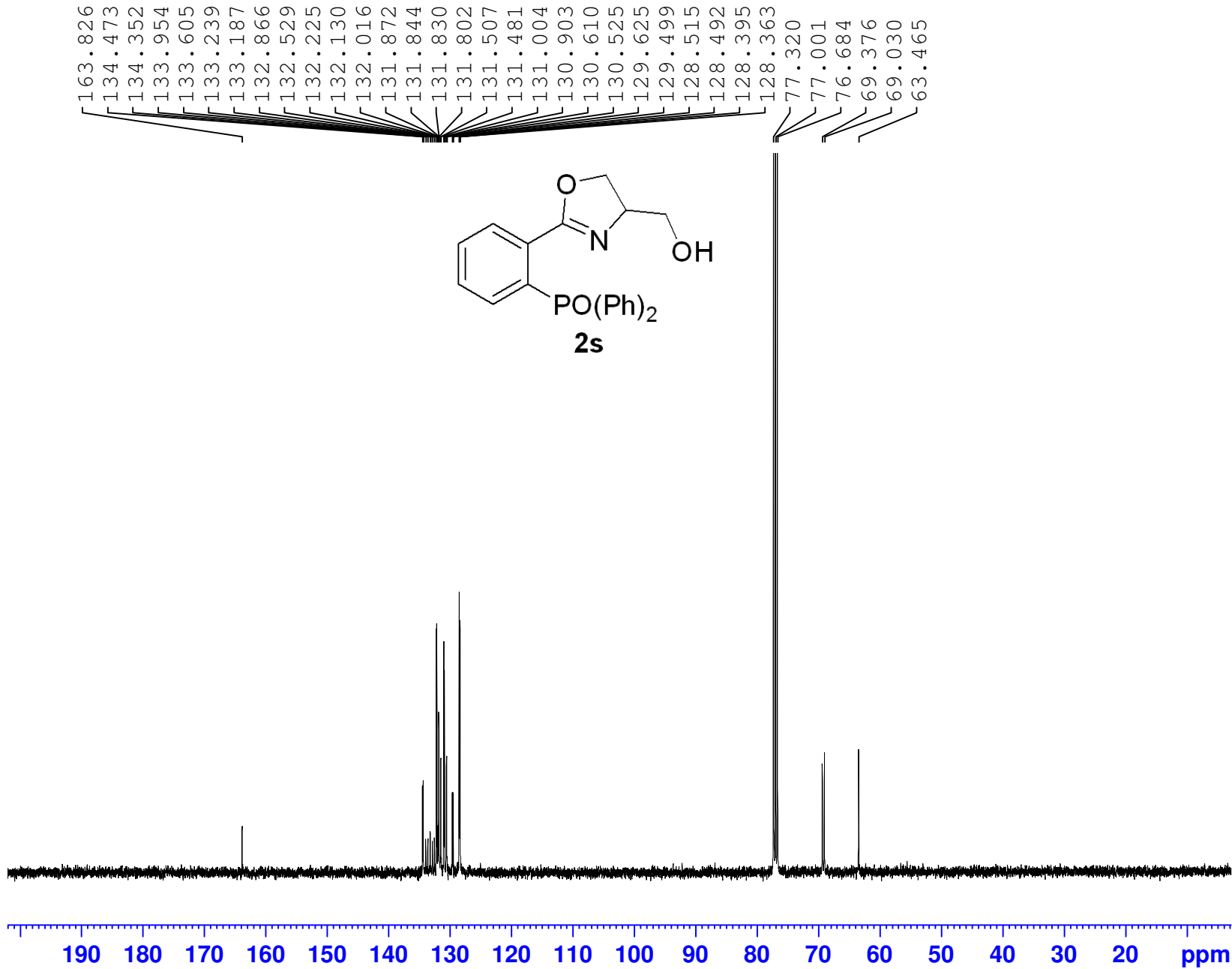
Current Data Parameters
NAME czl-2-8-HNMR
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20170825
Time 14.03
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT CDC13
NS 4
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 70.97
DW 62.400 usec
DE 6.50 usec
TE 295.7 K
D1 1.00000000 sec
TD0 1

==== CHANNEL f1 =====
SFO1 400.1324710 MHz
NUC1 1H
P1 14.50 usec
PLW1 11.99499989 W

F2 - Processing parameters
SI 65536
SF 400.1300107 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

10 9 8 7 6 5 4 3 2 1 ppm



Current Data Parameters
NAME czl-2-8-CNMR
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20170825
Time 14.11
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 415
DS 2
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 196.92
DW 20.800 usec
DE 6.50 usec
TE 296.2 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

==== CHANNEL f1 =====
SFO1 100.6228298 MHz
NUC1 13C
P1 9.70 usec
PLW1 46.98899841 W

==== CHANNEL f2 =====
SFO2 400.1316005 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 90.00 usec
PLW2 11.99499989 W
PLW12 0.34213999 W
PLW13 0.27713001 W

F2 - Processing parameters
SI 32768
SF 100.6127773 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



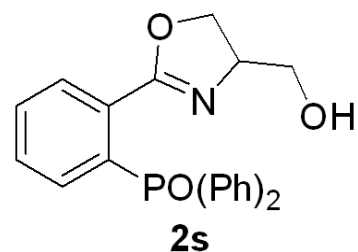
Current Data Parameters
NAME czl-2-8-PNMR
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20170825
Time 14.33
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 32
DS 4
SWH 64102.563 Hz
FIDRES 0.978127 Hz
AQ 0.5111808 sec
RG 196.92
DW 7.800 usec
DE 6.50 usec
TE 296.5 K
D1 2.0000000 sec
D11 0.0300000 sec
TD0 1

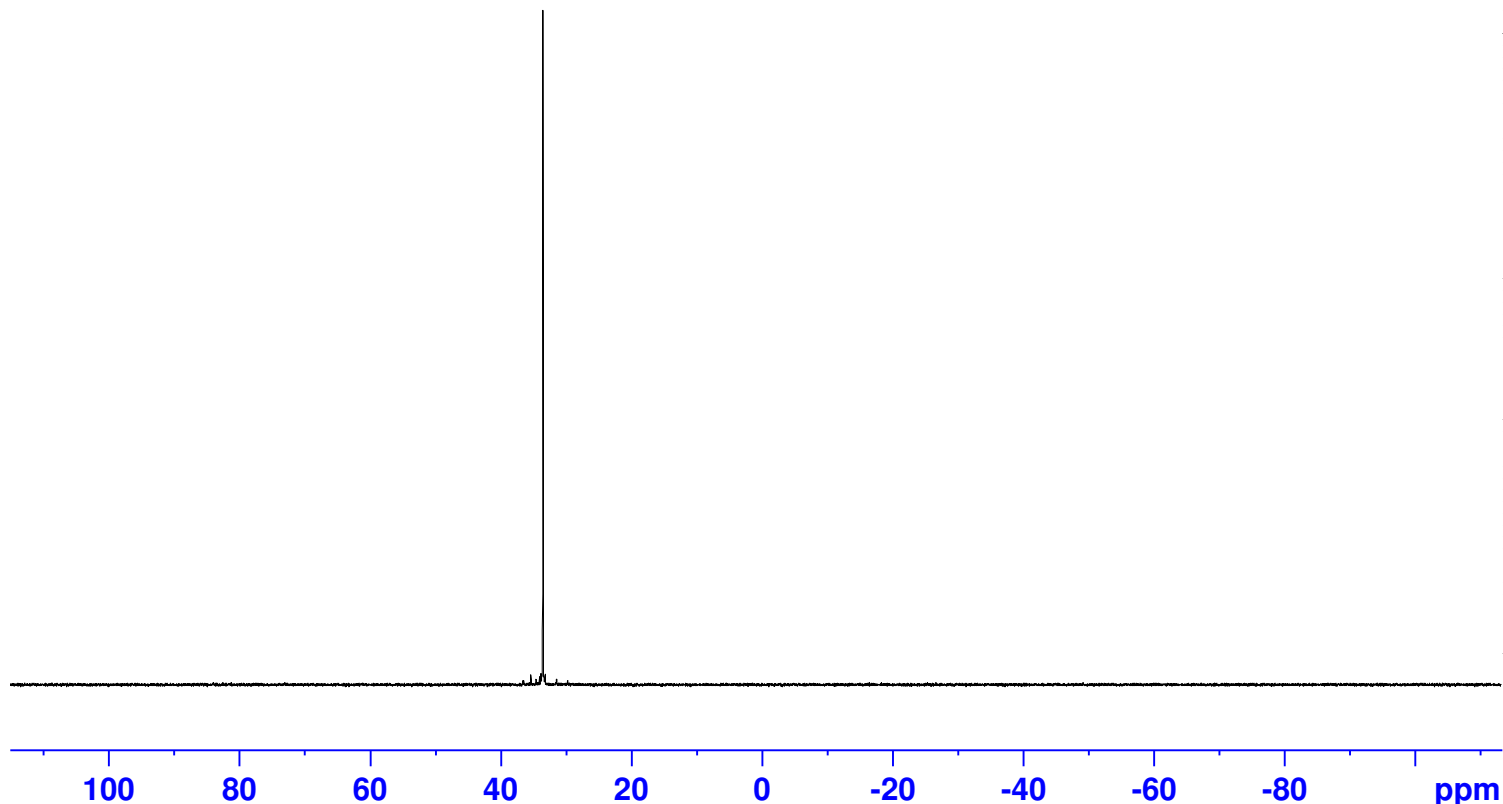
=====
CHANNEL f1
SFO1 161.9674942 MHz
NUC1 31P
P1 14.70 usec
PLW1 11.99499989 W

=====
CHANNEL f2
SFO2 400.1316005 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 90.00 usec
PLW2 11.99499989 W
PLW12 0.34213999 W
PLW13 0.27713001 W

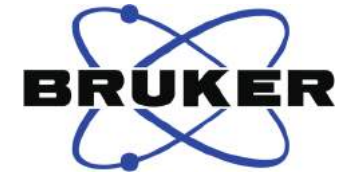
F2 - Processing parameters
SI 32768
SF 161.9755930 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



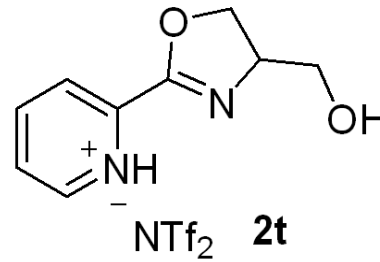
33.54



S-154



8.650
8.648
8.646
8.644
8.638
8.636
8.634
8.632
7.942
7.924
7.922
7.752
7.748
7.733
7.728
7.713
7.709
7.373
7.370
7.361
7.358
7.354
7.351
7.342
7.339
7.260
4.580
4.564
4.557
4.540
4.520
4.511
4.502
4.492
4.482
4.479
4.469
4.440
4.423
4.405
3.989
3.980
3.960
3.951
3.718
3.708
3.689
3.679

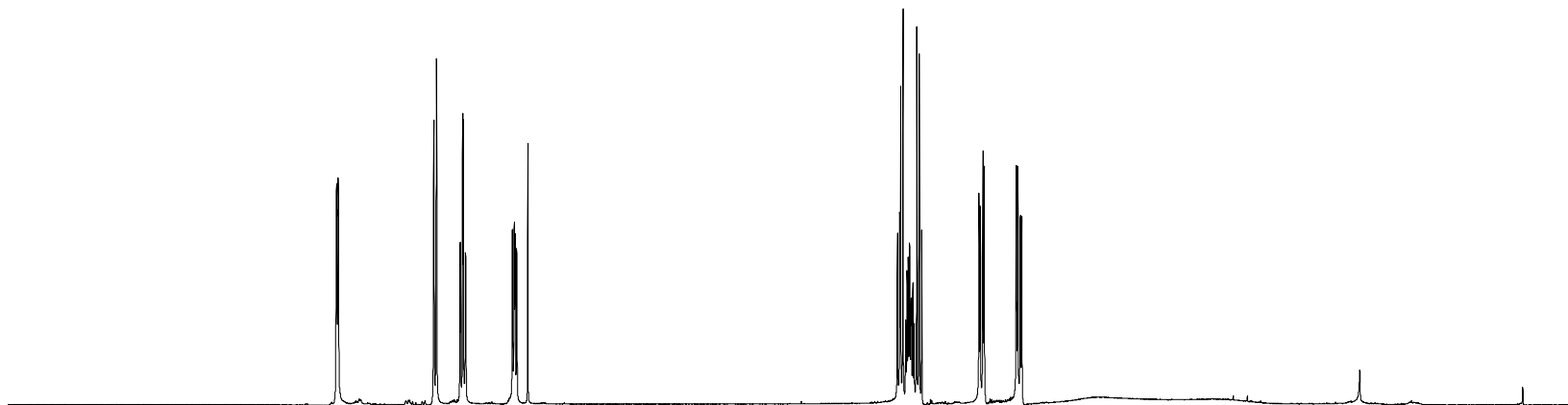


Current Data Parameters
NAME cz1-2-7-second
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20170823
Time 16.41
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT CDC13
NS 4
DS 0
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 88.84
DW 62.400 usec
DE 6.50 usec
TE 296.2 K
D1 1.00000000 sec
TD0 1

==== CHANNEL f1 =====
SFO1 400.1324710 MHz
NUC1 1H
P1 14.50 usec
PLW1 11.99499989 W

F2 - Processing parameters
SI 65536
SF 400.1300102 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



10 9 8 7 6 5 4 3 2 1 ppm

1.01

1.00

1.05

1.05

3.16

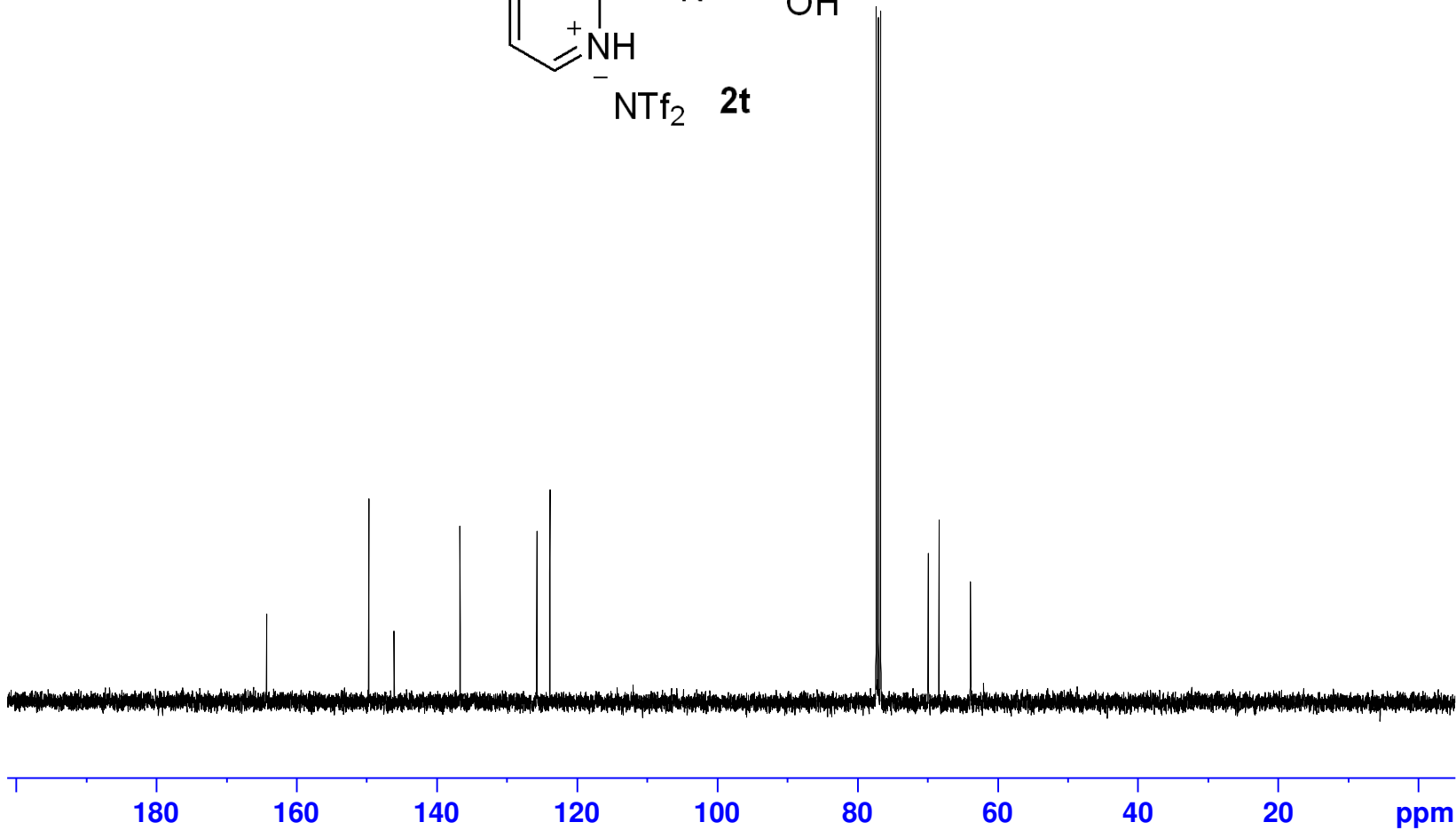
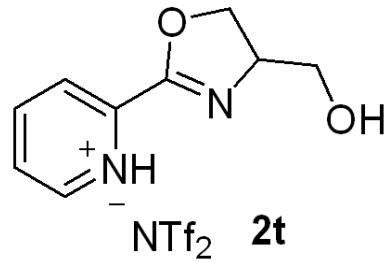
1.07

1.10

S-155



— 164.270
— 149.695
— 146.086
— 136.678
— 125.721
— 123.870
— 77.321
— 77.003
— 76.685
— 69.869
— 68.352
— 63.866



Current Data Parameters
NAME czl-2-7-second
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20170823
Time 16.44
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 62
DS 2
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 196.92
DW 20.800 usec
DE 6.50 usec
TE 296.7 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

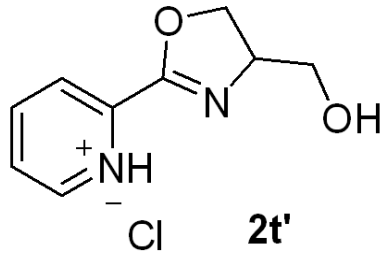
==== CHANNEL f1 =====
SFO1 100.6228298 MHz
NUC1 13C
P1 9.70 usec
PLW1 46.98899841 W

==== CHANNEL f2 =====
SFO2 400.1316005 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 90.00 usec
PLW2 11.99499989 W
PLW12 0.34213999 W
PLW13 0.27713001 W

F2 - Processing parameters
SI 32768
SF 100.6127751 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



8.549
8.548
8.491
8.472
8.170
8.151
7.866
7.862
7.847
7.843
7.828
7.823
7.453
7.451
7.441
7.439
7.434
7.432
7.423
7.420
7.260
4.456
4.443
4.434
4.431
4.422
4.409
4.006
3.992
3.980
3.964
3.952
3.901
3.889
3.873
3.861
3.847
3.834
3.823
3.809
3.795
3.781

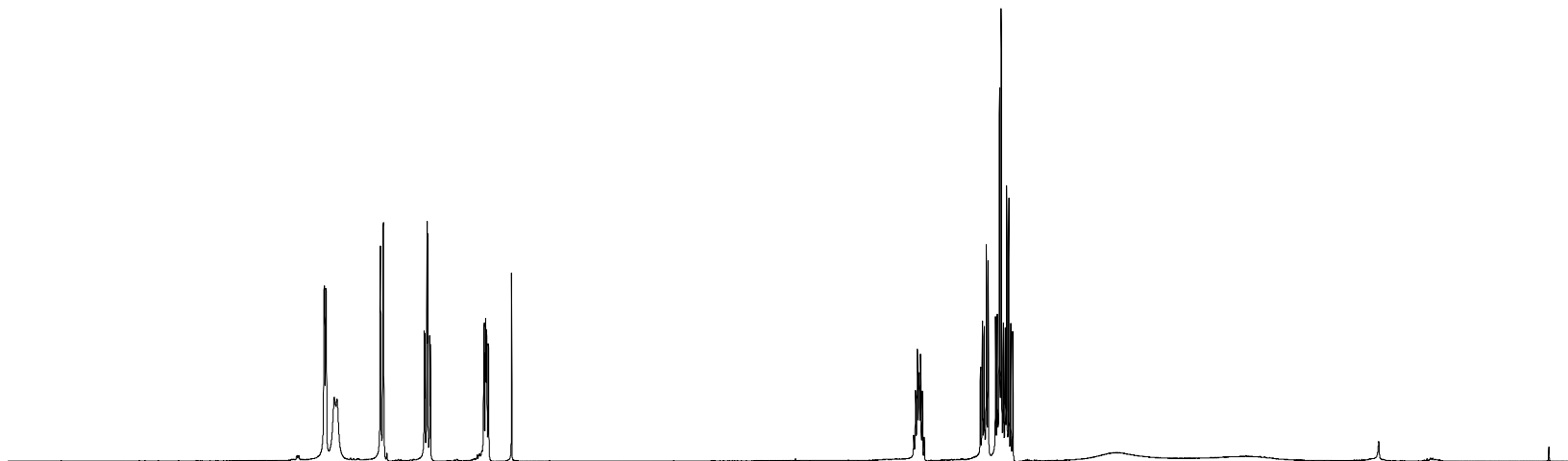


Current Data Parameters
NAME czl-2-4-second
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20170823
Time 16.35
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT CDC13
NS 4
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 103.52
DW 62.400 usec
DE 6.50 usec
TE 296.3 K
D1 1.00000000 sec
TD0 1

==== CHANNEL f1 =====
SFO1 400.1324710 MHz
NUC1 1H
P1 14.50 usec
PLW1 11.99499989 W

F2 - Processing parameters
SI 65536
SF 400.1300102 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



10 9 8 7 6 5 4 3 2 1 ppm

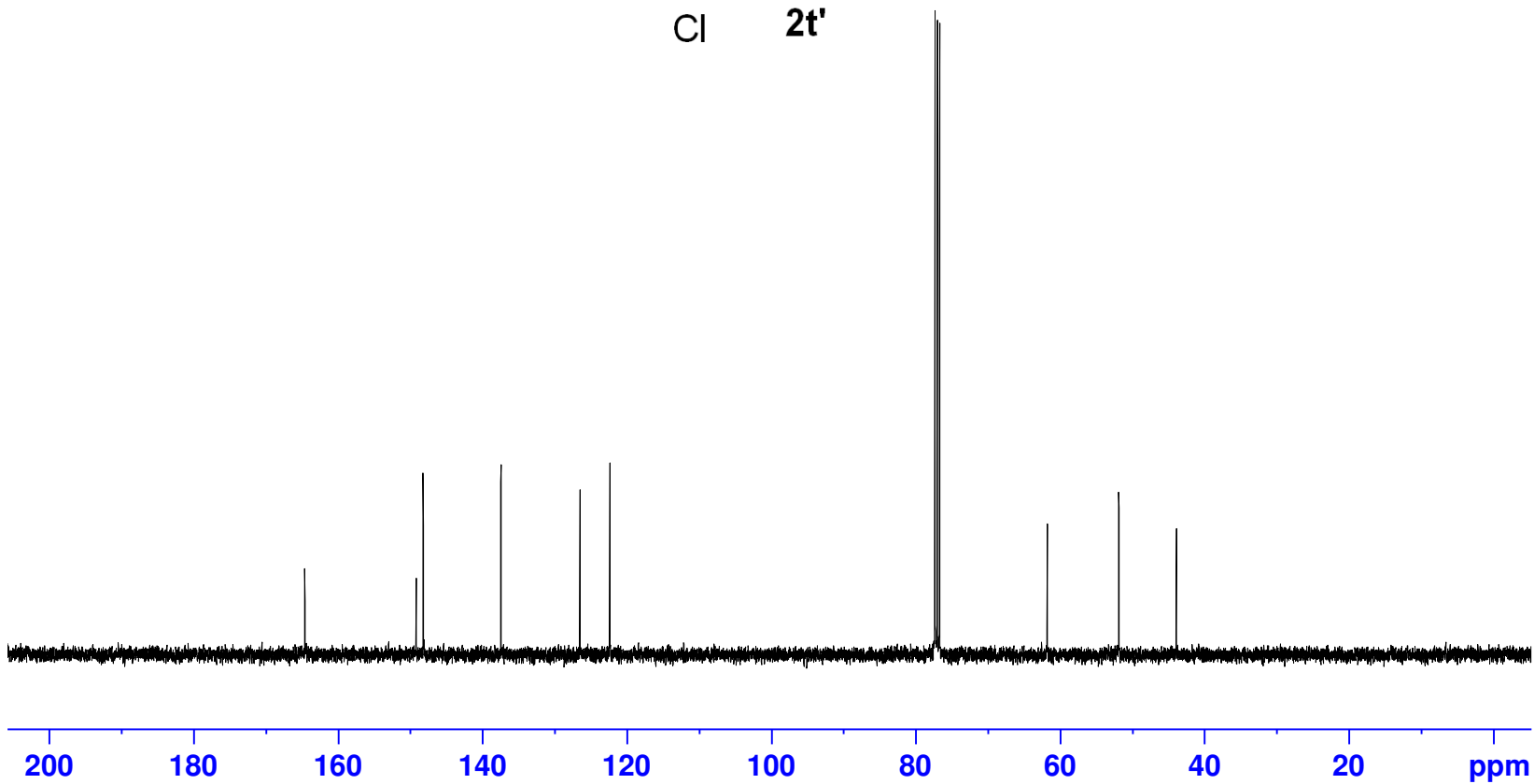
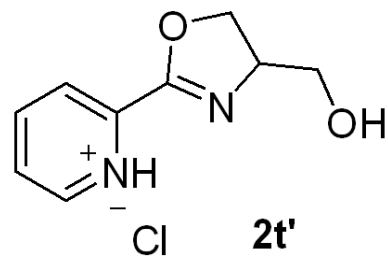
1.04
0.90
1.02
1.03
1.02

1.00
1.13
3.02

S-157



— 164.611
— 149.175
— 148.219
— 137.447
— 126.502
— 122.360
— 77.320
— 77.002
— 76.684
— 61.757
— 51.849
— 43.875



Current Data Parameters
NAME czl-2-4-second
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20170823
Time 16.54
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 87
DS 2
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 196.92
DW 20.800 usec
DE 6.50 usec
TE 296.4 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

==== CHANNEL f1 =====
SFO1 100.6228298 MHz
NUC1 13C
P1 9.70 usec
PLW1 46.98899841 W

==== CHANNEL f2 =====
SFO2 400.1316005 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 90.00 usec
PLW2 11.99499989 W
PLW12 0.34213999 W
PLW13 0.27713001 W

F2 - Processing parameters
SI 32768
SF 100.6127737 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

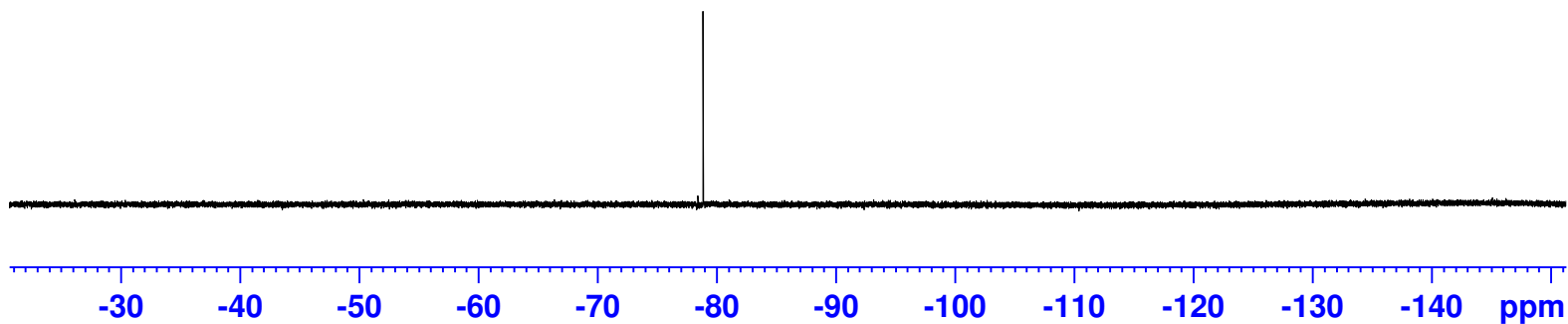
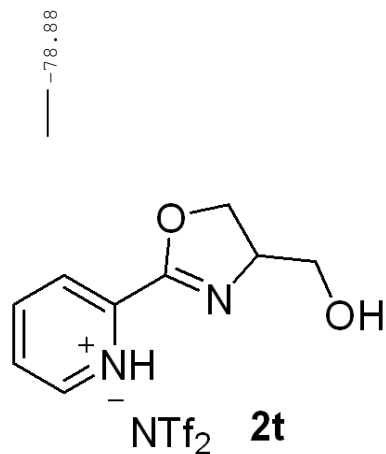


Current Data Parameters
NAME cz1-2-7-second
EXPNO 3
PROCNO 1

F2 - Acquisition Parameters
Date_ 20170823
Time 16.47
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgflqn
TD 131072
SOLVENT CDCl3
NS 16
DS 4
SWH 89285.711 Hz
FIDRES 0.681196 Hz
AQ 0.7340032 sec
RG 196.92
DW 5.600 usec
DE 6.50 usec
TE 296.3 K
D1 1.00000000 sec
TD0 1

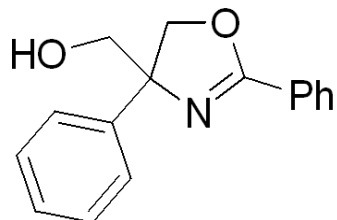
==== CHANNEL f1 =====
SFO1 376.4607164 MHz
NUC1 19F
P1 14.70 usec
PLW1 15.99600029 W

F2 - Processing parameters
SI 65536
SF 376.4983660 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

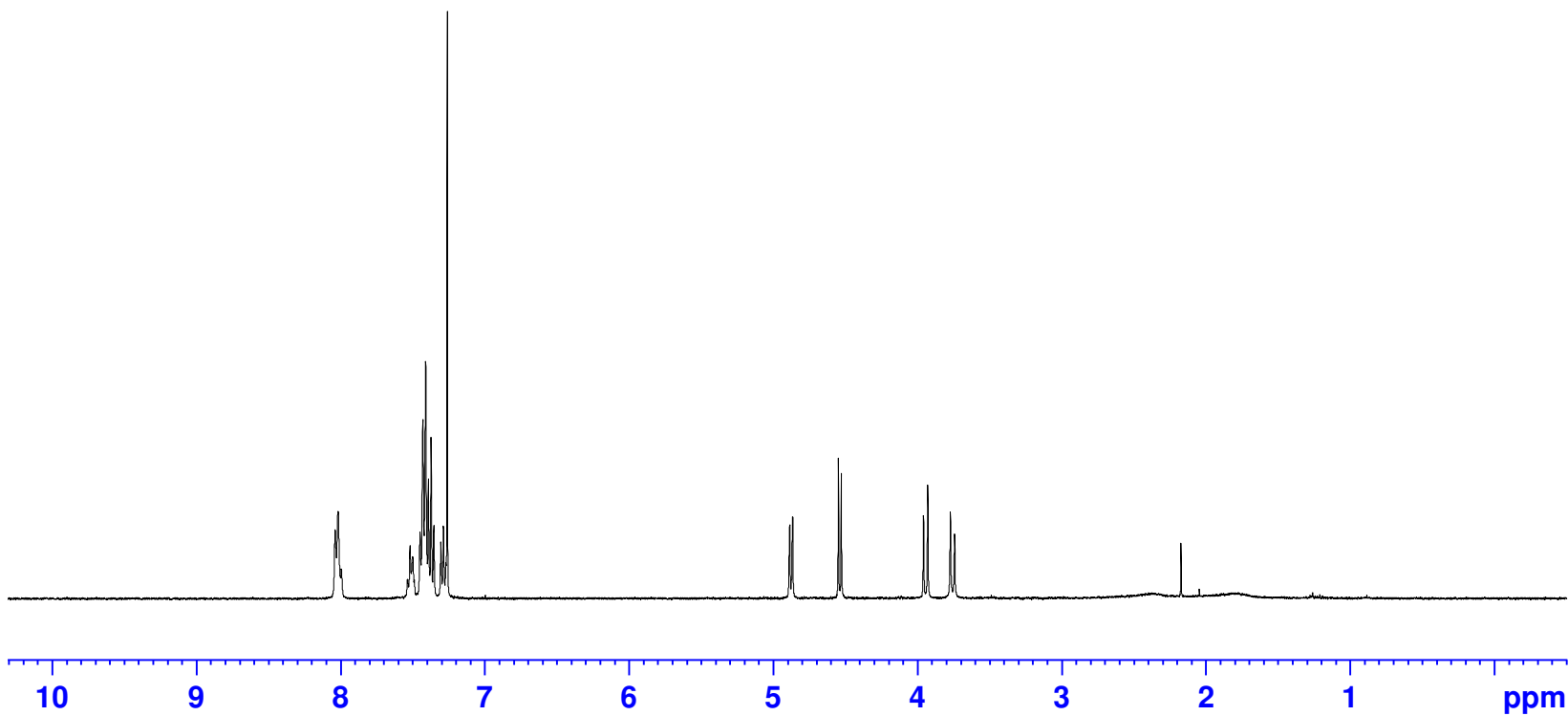




8.037
8.016
7.995
7.535
7.517
7.499
7.488
7.449
7.428
7.410
7.390
7.372
7.352
7.304
7.286
7.269
7.259
4.884
4.864
4.547
4.527
3.957
3.928
3.771
3.742



2u



2.01
1.08
6.00
1.03

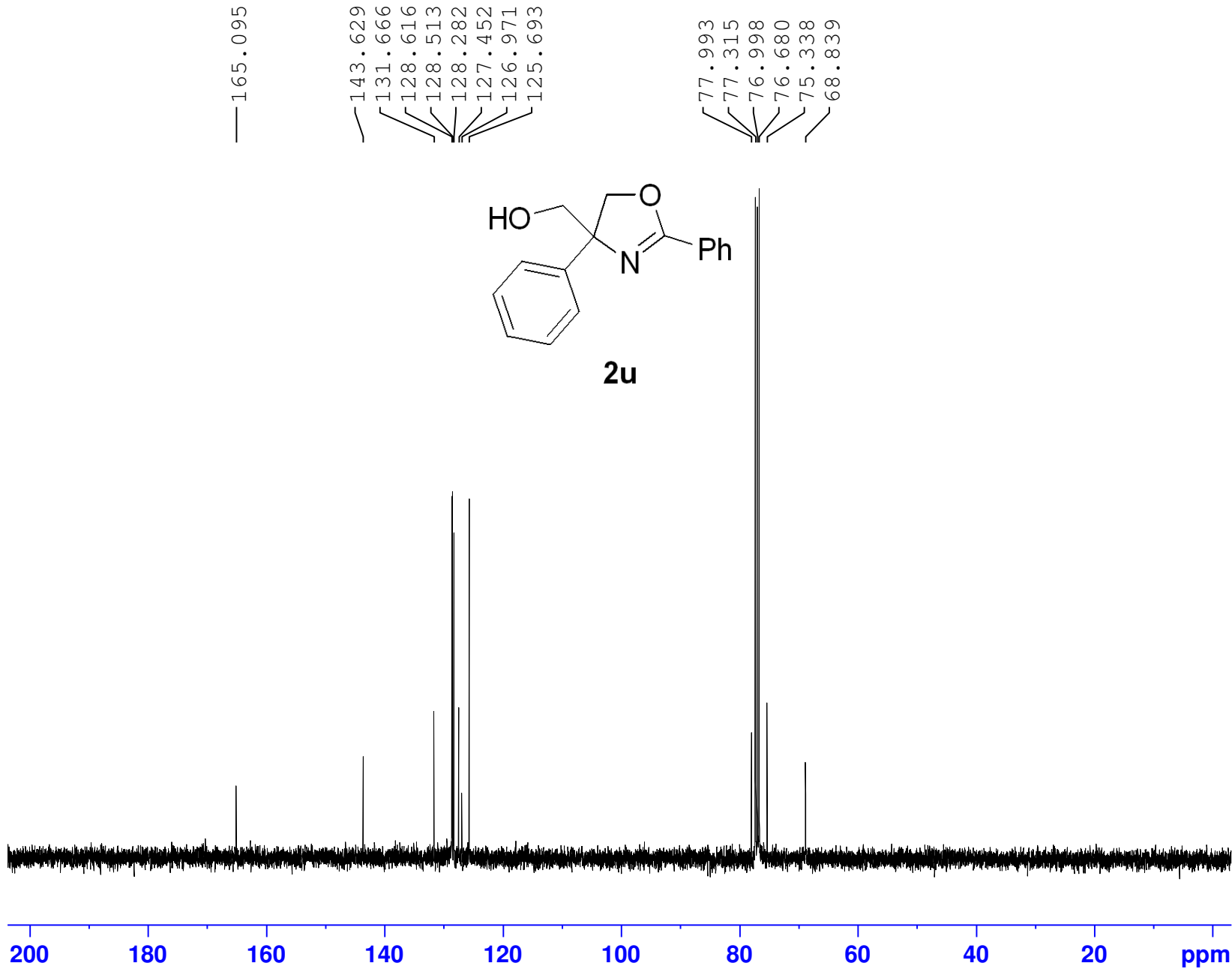
1.06
1.07
1.09
1.07
S-160

Current Data Parameters
NAME czl-1-188-A H
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20170805
Time 16.17
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 4
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 196.92
DW 62.400 usec
DE 6.50 usec
TE 296.1 K
D1 1.00000000 sec
TD0 1

==== CHANNEL f1 =====
SFO1 400.1324710 MHz
NUC1 1H
P1 14.50 usec
PLW1 11.99499989 W

F2 - Processing parameters
SI 65536
SF 400.1300104 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



Current Data Parameters
NAME czl-1-188A- C
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20170805
Time 12.36
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 18
DS 2
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 196.92
DW 20.800 usec
DE 6.50 usec
TE 298.3 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

==== CHANNEL f1 =====
SFO1 100.6228298 MHz
NUC1 13C
P1 9.70 usec
PLW1 46.98899841 W

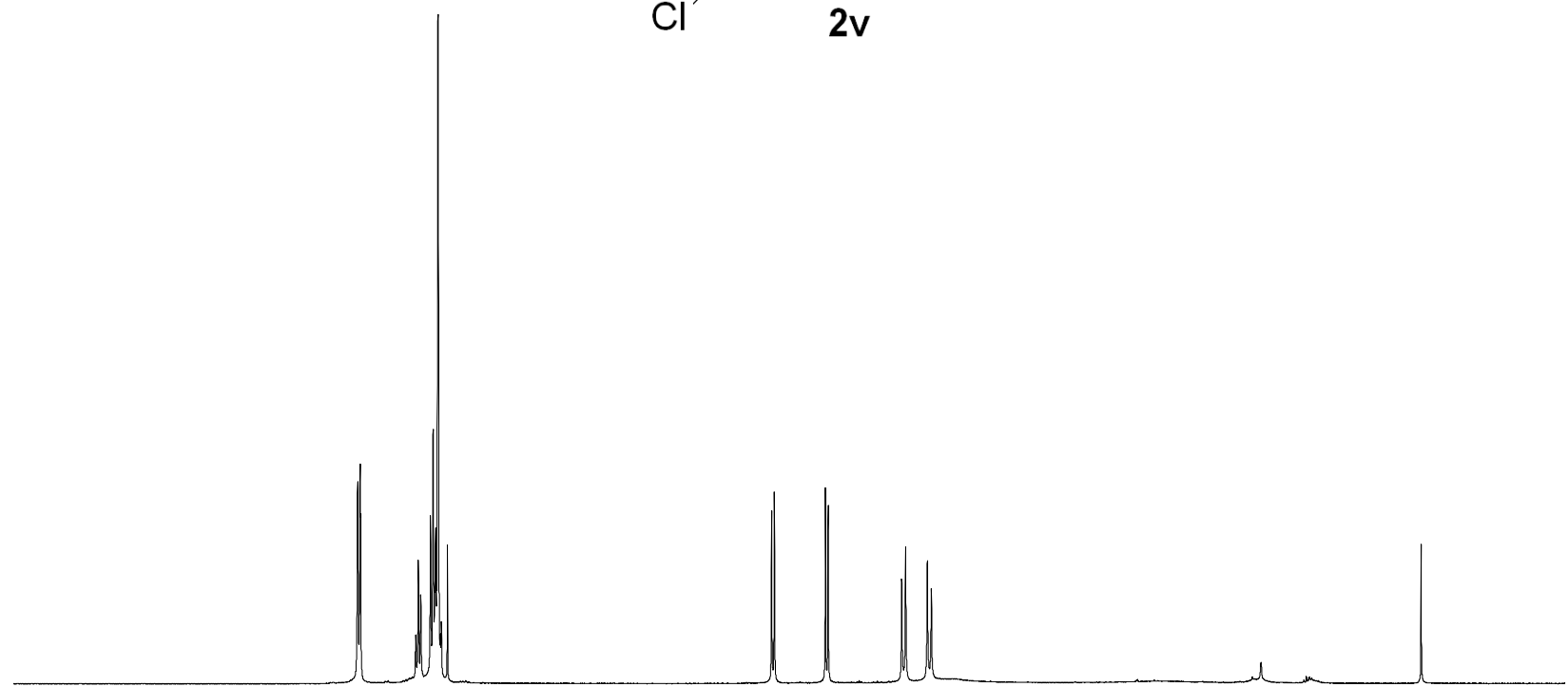
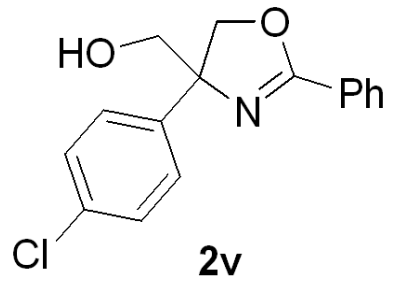
==== CHANNEL f2 =====
SFO2 400.1316005 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 90.00 usec
PLW2 11.99499989 W
PLW12 0.34213999 W
PLW13 0.27713001 W

F2 - Processing parameters
SI 32768
SF 100.6127736 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

7.921
7.903
7.900
7.492
7.474
7.455
7.384
7.364
7.353
7.351
7.346
7.331
7.326
7.311
7.303
7.259

4.866
4.846
4.470
4.449
3.907
3.877
3.717
3.688

— 0.073

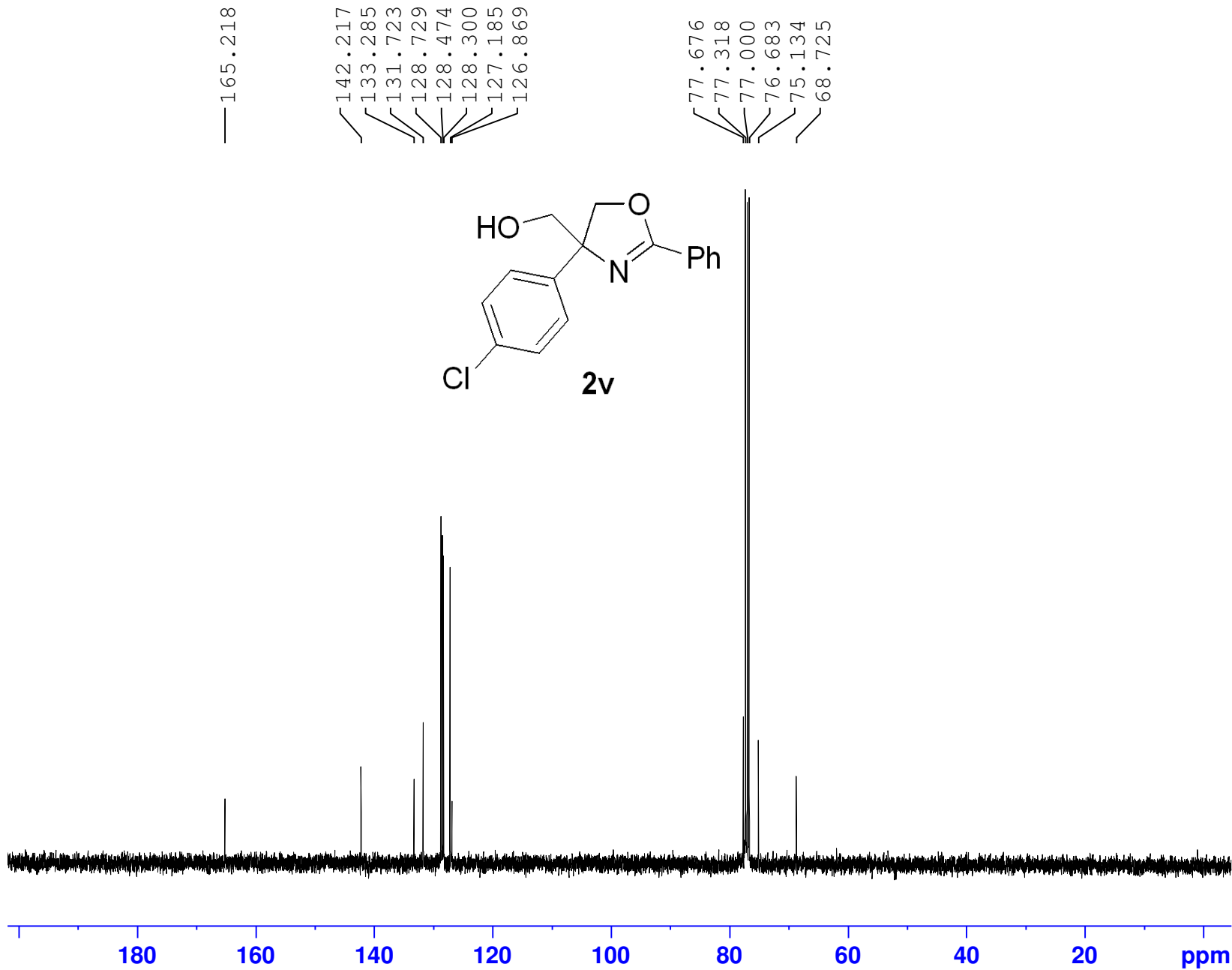


Current Data Parameters
 NAME czl-1-188-B H
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20170805
 Time 16.21
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 4
 DS 2
 SWH 8012.820 Hz
 FIDRES 0.122266 Hz
 AQ 4.0894465 sec
 RG 187.77
 DW 62.400 usec
 DE 6.50 usec
 TE 296.1 K
 D1 1.00000000 sec
 TD0 1

==== CHANNEL f1 =====
 SFO1 400.1324710 MHz
 NUC1 1H
 P1 14.50 usec
 PLW1 11.99499989 W

F2 - Processing parameters
 SI 65536
 SF 400.1300107 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00



Current Data Parameters
NAME czl-1-188B- C
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20170805
Time 10.44
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 62
DS 2
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 196.92
DW 20.800 usec
DE 6.50 usec
TE 297.3 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

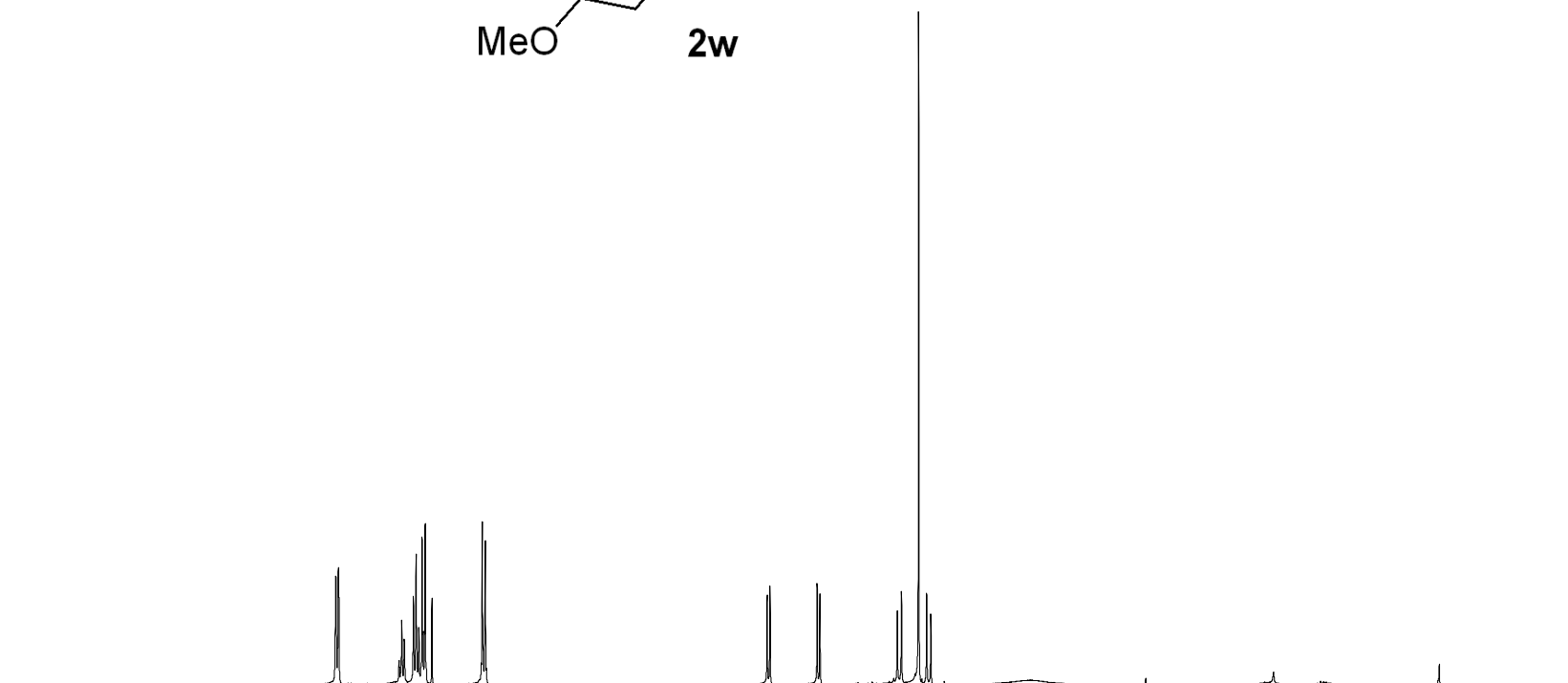
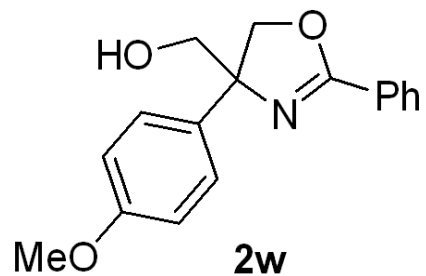
==== CHANNEL f1 =====
SFO1 100.6228298 MHz
NUC1 13C
P1 9.70 usec
PLW1 46.98899841 W

==== CHANNEL f2 =====
SFO2 400.1316005 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 90.00 usec
PLW2 11.99499989 W
PLW12 0.34213999 W
PLW13 0.27713001 W

F2 - Processing parameters
SI 32768
SF 100.6127732 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



7.945
7.927
7.924
7.494
7.476
7.457
7.392
7.373
7.354
7.338
7.330
7.325
7.313
7.308
7.301
7.260
6.901
6.879
4.870
4.849
4.513
4.493
3.941
3.911
3.789
3.732
3.702



Current Data Parameters
NAME czl-1-188-C H
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20170805
Time 16.24
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT CDC13
NS 4
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 187.77
DW 62.400 usec
DE 6.50 usec
TE 296.1 K
D1 1.00000000 sec
TD0 1

==== CHANNEL f1 =====
SFO1 400.1324710 MHz
NUC1 1H
P1 14.50 usec
PLW1 11.99499989 W

F2 - Processing parameters
SI 65536
SF 400.1300102 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

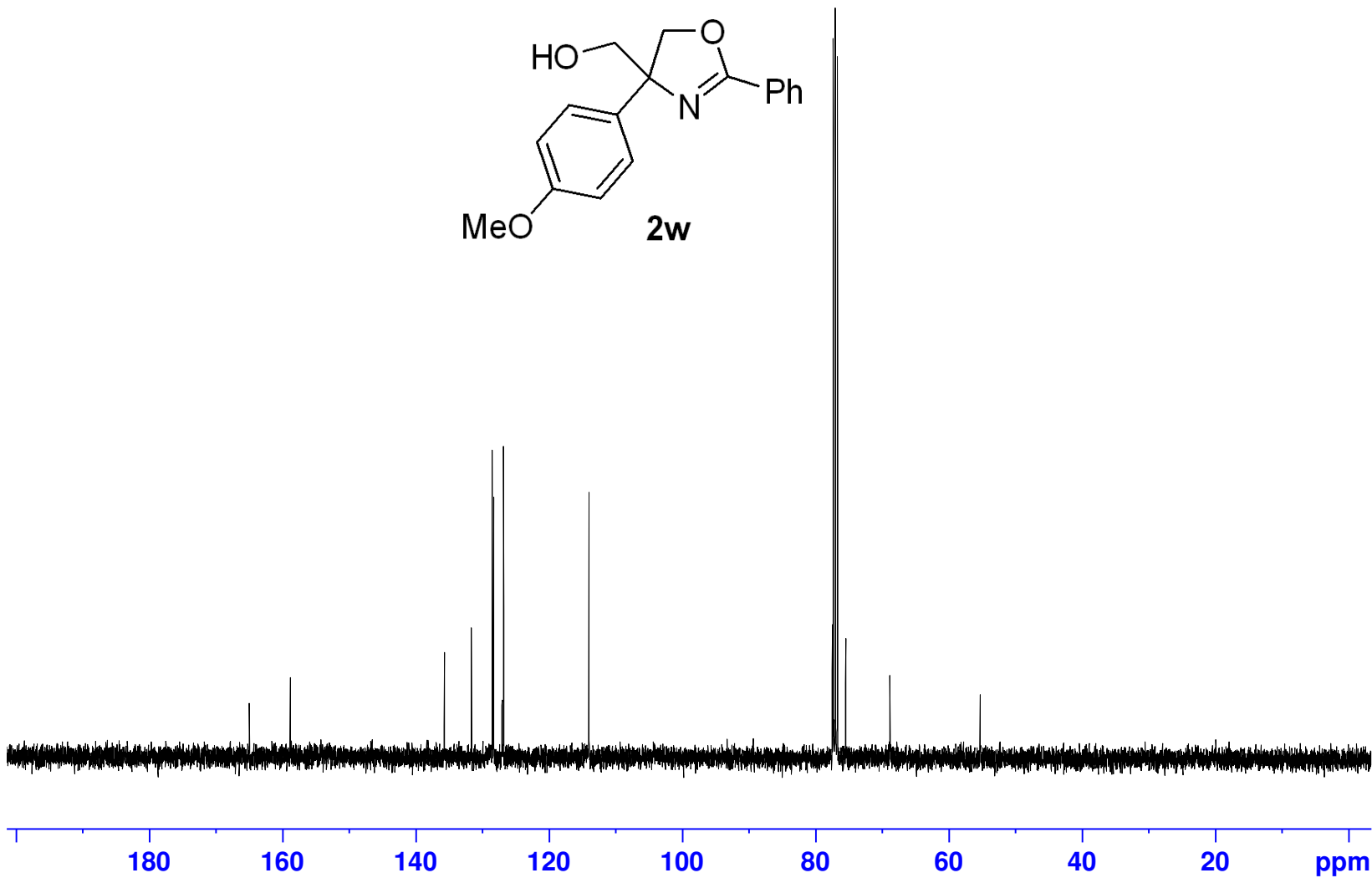
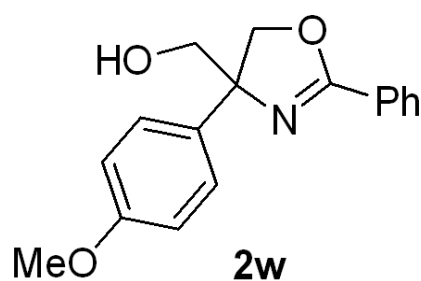
10 9 8 7 6 5 4 3 2 1 0 ppm

2.00
1.09
2.08
2.01
2.02
1.03
1.03
1.10
3.14
0.97

S-164



—164.973
—158.836
135.702
131.646
128.506
128.284
127.035
126.800
—113.980
77.475
77.319
77.001
76.684
75.468
68.828
—55.258



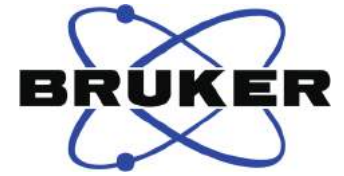
Current Data Parameters
NAME czl-1-188C- C
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20170805
Time 10.34
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 51
DS 2
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 196.92
DW 20.800 usec
DE 6.50 usec
TE 297.4 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

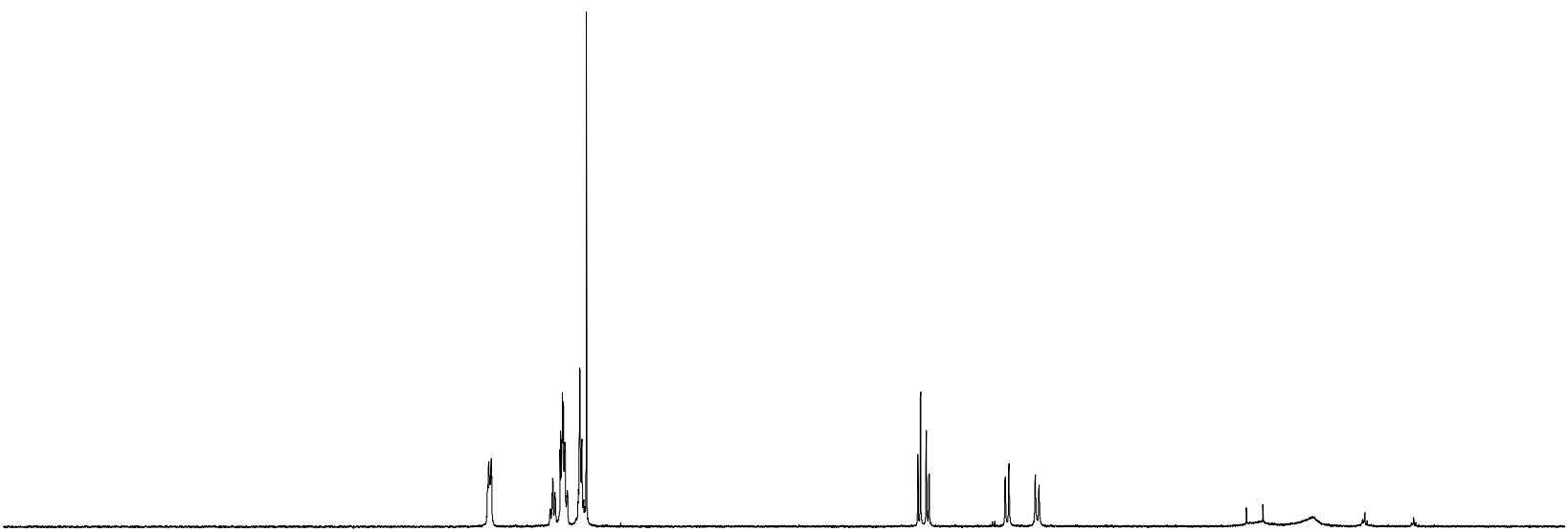
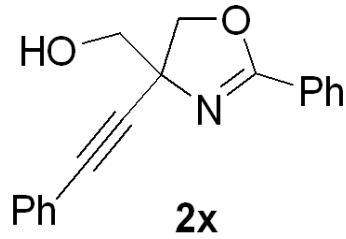
==== CHANNEL f1 =====
SFO1 100.6228298 MHz
NUC1 13C
P1 9.70 usec
PLW1 46.98899841 W

==== CHANNEL f2 =====
SFO2 400.1316005 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 90.00 usec
PLW2 11.99499989 W
PLW12 0.34213999 W
PLW13 0.27713001 W

F2 - Processing parameters
SI 32768
SF 100.6127729 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



8.022
8.012
8.004
8.000
7.994
7.990
7.537
7.524
7.519
7.503
7.500
7.462
7.458
7.450
7.445
7.438
7.425
7.410
7.406
7.326
7.321
7.313
7.309
7.294
7.286
7.281
7.272
7.260
4.704
4.684
4.638
4.617
4.031
4.003
3.799
3.771



Current Data Parameters
NAME czl-1-188-D H
EXPNO 1
PROCNO 1

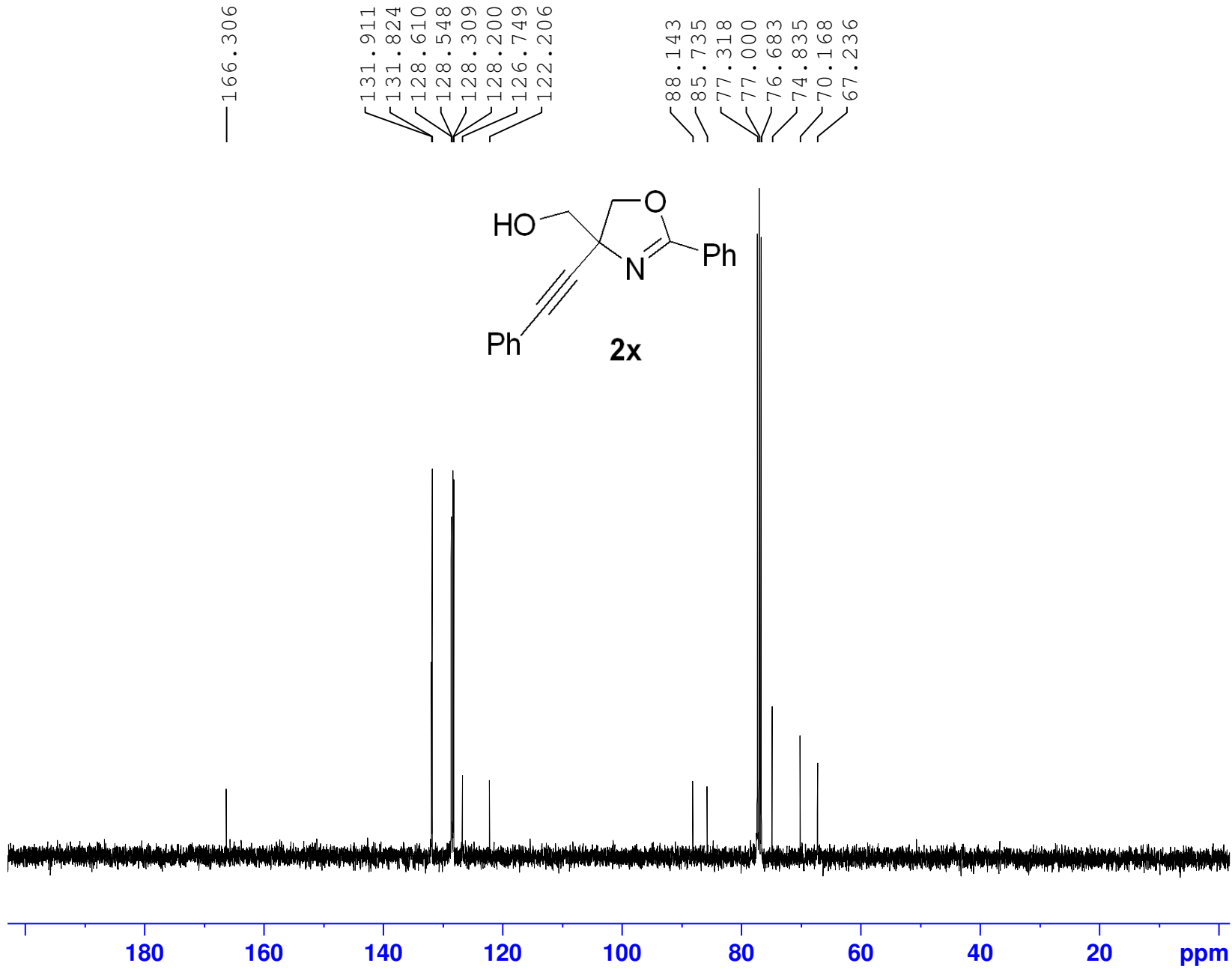
F2 - Acquisition Parameters
Date_ 20170805
Time 16.27
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 4
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 196.92
DW 62.400 usec
DE 6.50 usec
TE 296.1 K
D1 1.00000000 sec
TD0 1

==== CHANNEL f1 =====
SFO1 400.1324710 MHz
NUC1 1H
P1 14.50 usec
PLW1 11.99499989 W

F2 - Processing parameters
SI 65536
SF 400.1300102 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

11 10 9 8 7 6 5 4 3 2 1 ppm

2.04
1.07
4.03
3.00
1.05
1.09
1.04
1.07



Current Data Parameters
NAME czl-1-188D C
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20170805
Time 10.29
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 50
DS 2
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 196.92
DW 20.800 usec
DE 6.50 usec
TE 297.4 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

==== CHANNEL f1 =====
SFO1 100.6228298 MHz
NUC1 13C
P1 9.70 usec
PLW1 46.98899841 W

==== CHANNEL f2 =====
SFO2 400.1316005 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 90.00 usec
PLW2 11.99499989 W
PLW12 0.34213999 W
PLW13 0.27713001 W

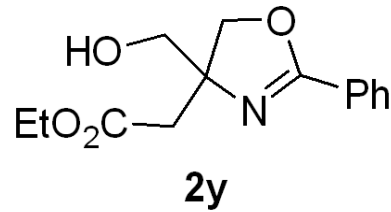
F2 - Processing parameters
SI 32768
SF 100.6127743 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



7.833
7.817
7.815
7.460
7.441
7.423
7.353
7.334
7.316
7.260

4.507
4.485
4.473
4.451
4.128
4.110
4.092
4.075
3.831
3.803
3.665
3.636
2.828
2.789
2.682
2.643

1.216
1.198
1.181

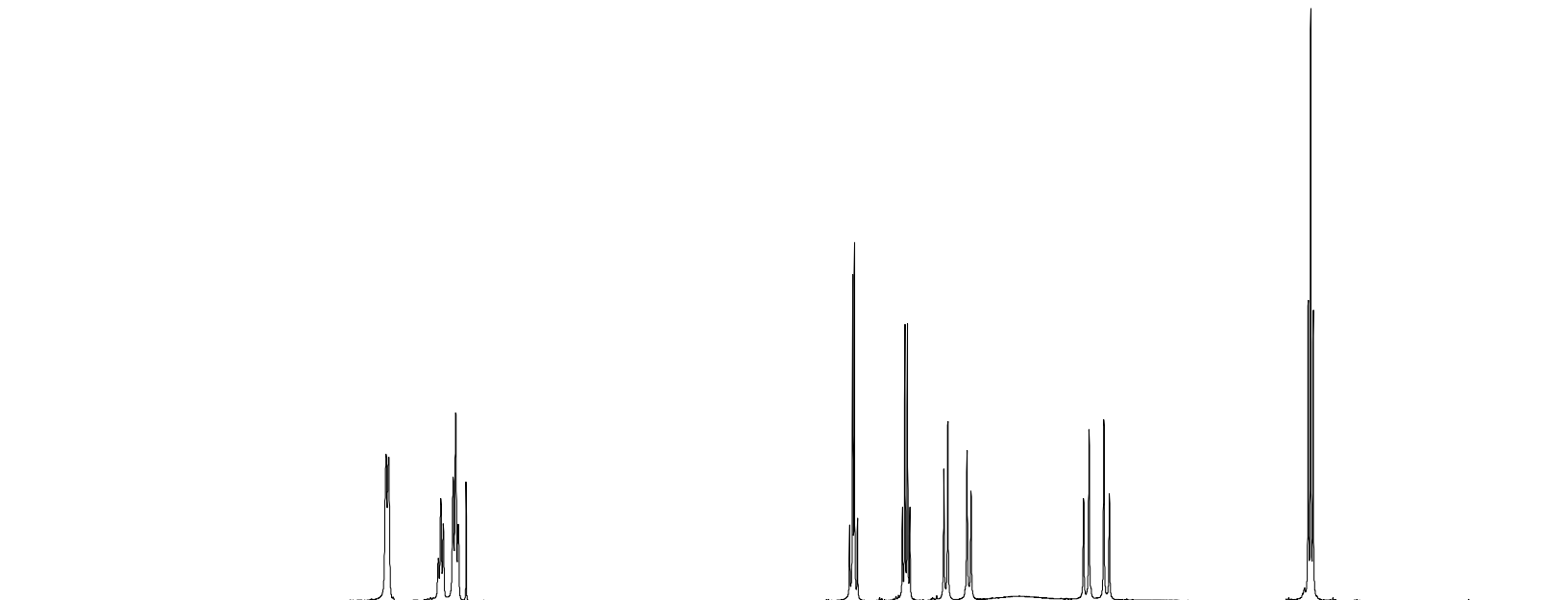


Current Data Parameters
NAME czl-1-188-E H
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20170805
Time 16.31
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT CDC13
NS 4
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 187.77
DW 62.400 usec
DE 6.50 usec
TE 296.1 K
D1 1.00000000 sec
TD0 1

==== CHANNEL f1 =====
SFO1 400.1324710 MHz
NUC1 1H
P1 14.50 usec
PLW1 11.99499989 W

F2 - Processing parameters
SI 65536
SF 400.1300103 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



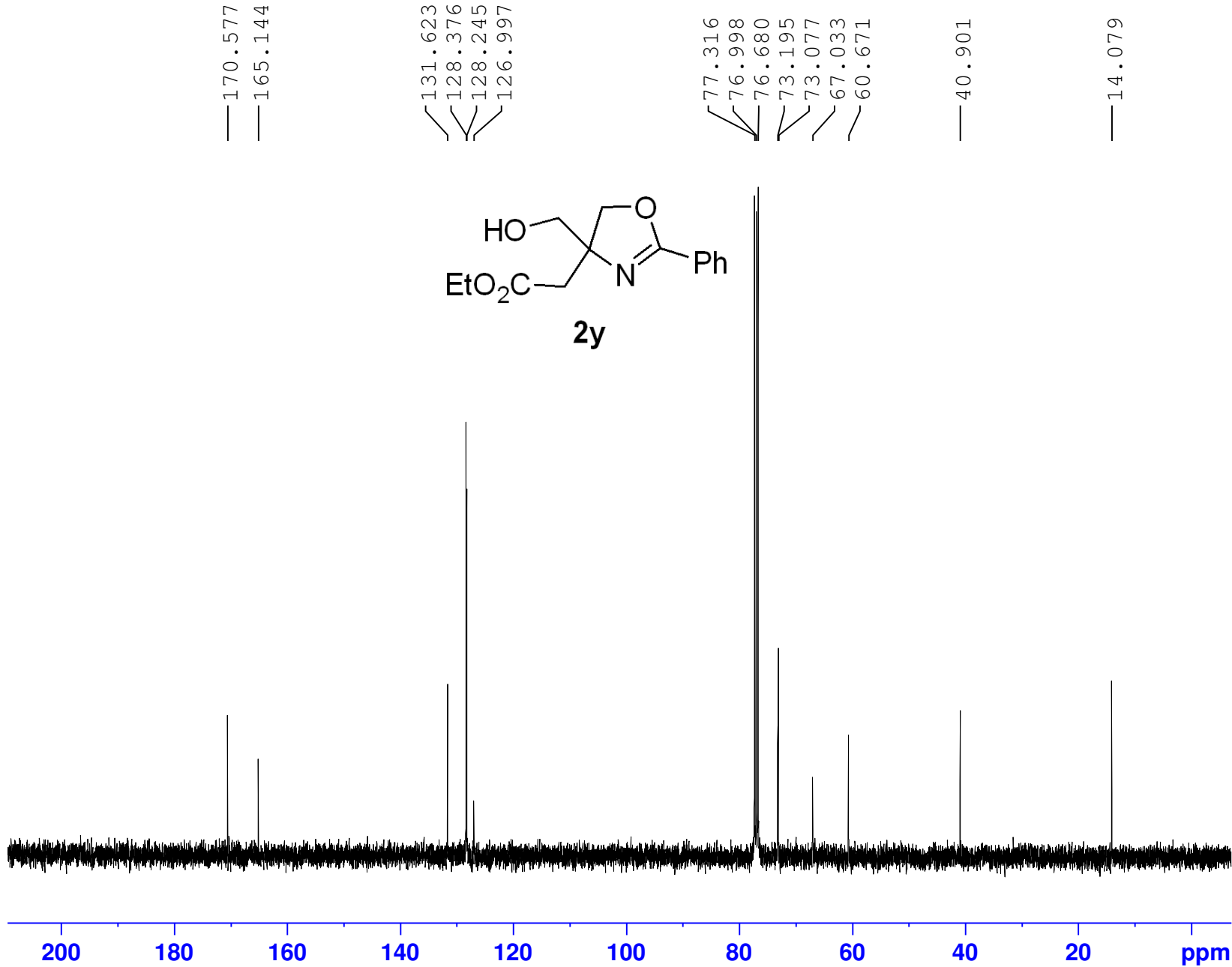
10 9 8 7 6 5 4 3 2 1 0 ppm

2.03
1.05
2.00

2.01
2.02
1.06
1.07
S-168

1.08
1.06

3.08



Current Data Parameters
NAME czl-1-188E C
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20170805
Time 10.16
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 60
DS 2
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 196.92
DW 20.800 usec
DE 6.50 usec
TE 297.5 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

==== CHANNEL f1 =====
SFO1 100.6228298 MHz
NUC1 13C
P1 9.70 usec
PLW1 46.98899841 W

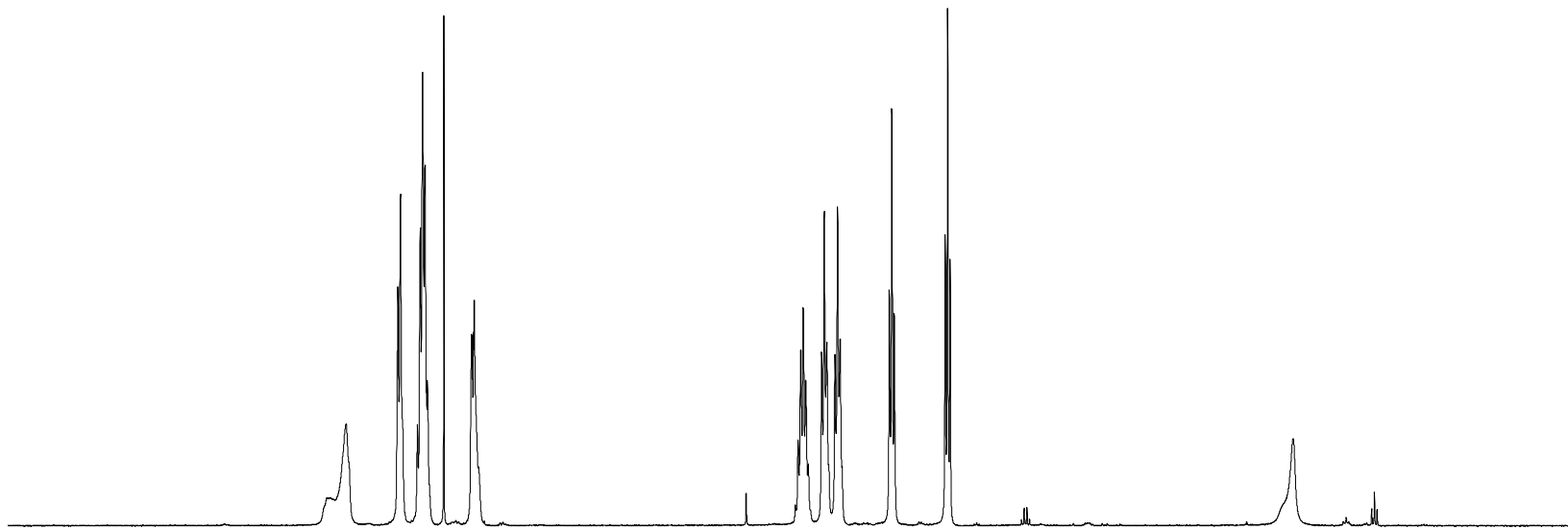
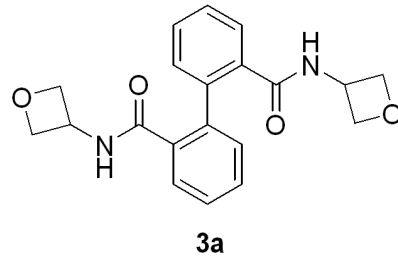
==== CHANNEL f2 =====
SFO2 400.1316005 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 90.00 usec
PLW2 11.99499989 W
PLW12 0.34213999 W
PLW13 0.27713001 W

F2 - Processing parameters
SI 32768
SF 100.6127735 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



8.018
8.000
7.896
7.560
7.542
7.433
7.414
7.399
7.385
7.382
7.367
7.260
7.078
7.067
7.062
7.033
4.953
4.936
4.919
4.904
4.800
4.783
4.765
4.713
4.696
4.679
4.359
4.343
4.327
3.995
3.979
3.963

— 1.729



2.01
2.06
4.09
2.02

2.10
2.04
2.04
2.01
2.00

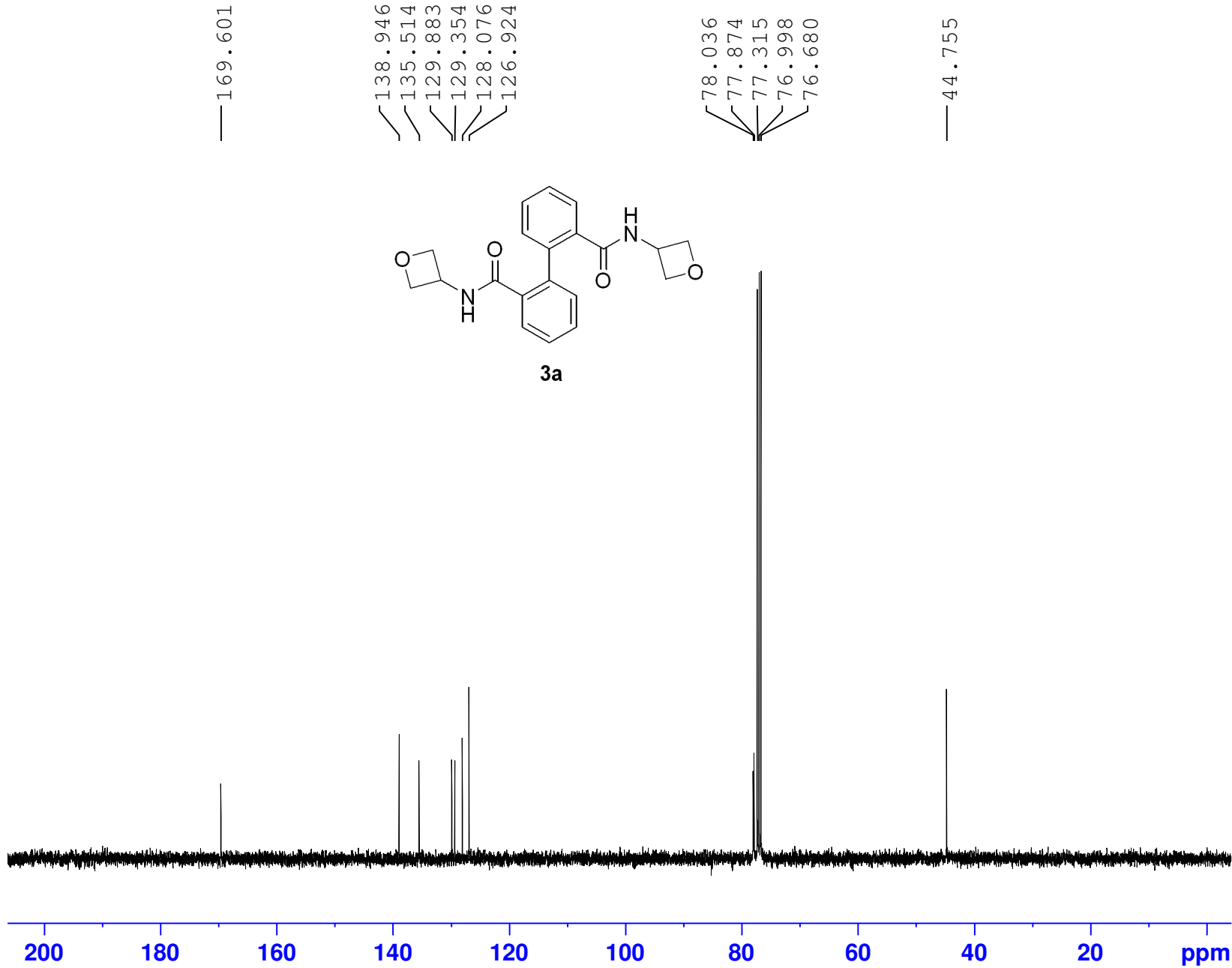
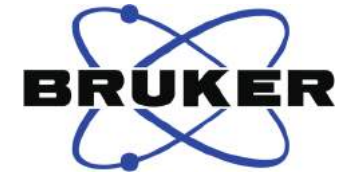
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Current Data Parameters
NAME czl-2-5-SM
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20170826
Time 10.11
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 4
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 112.31
DW 62.400 usec
DE 6.50 usec
TE 297.2 K
D1 1.00000000 sec
TD0 1

==== CHANNEL f1 =====
SF01 400.1324710 MHz
NUC1 1H
P1 14.50 usec
PLW1 11.99499989 W

F2 - Processing parameters
SI 65536
SF 400.1300102 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



Current Data Parameters
NAME czl-2-5-SM
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20170826
Time 10.20
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 107
DS 2
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 196.92
DW 20.800 usec
DE 6.50 usec
TE 297.5 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

==== CHANNEL f1 =====
SFO1 100.6228298 MHz
NUC1 13C
P1 9.70 usec
PLW1 46.98899841 W

==== CHANNEL f2 =====
SFO2 400.1316005 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 90.00 usec
PLW2 11.99499989 W
PLW12 0.34213999 W
PLW13 0.27713001 W

F2 - Processing parameters
SI 32768
SF 100.6127737 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

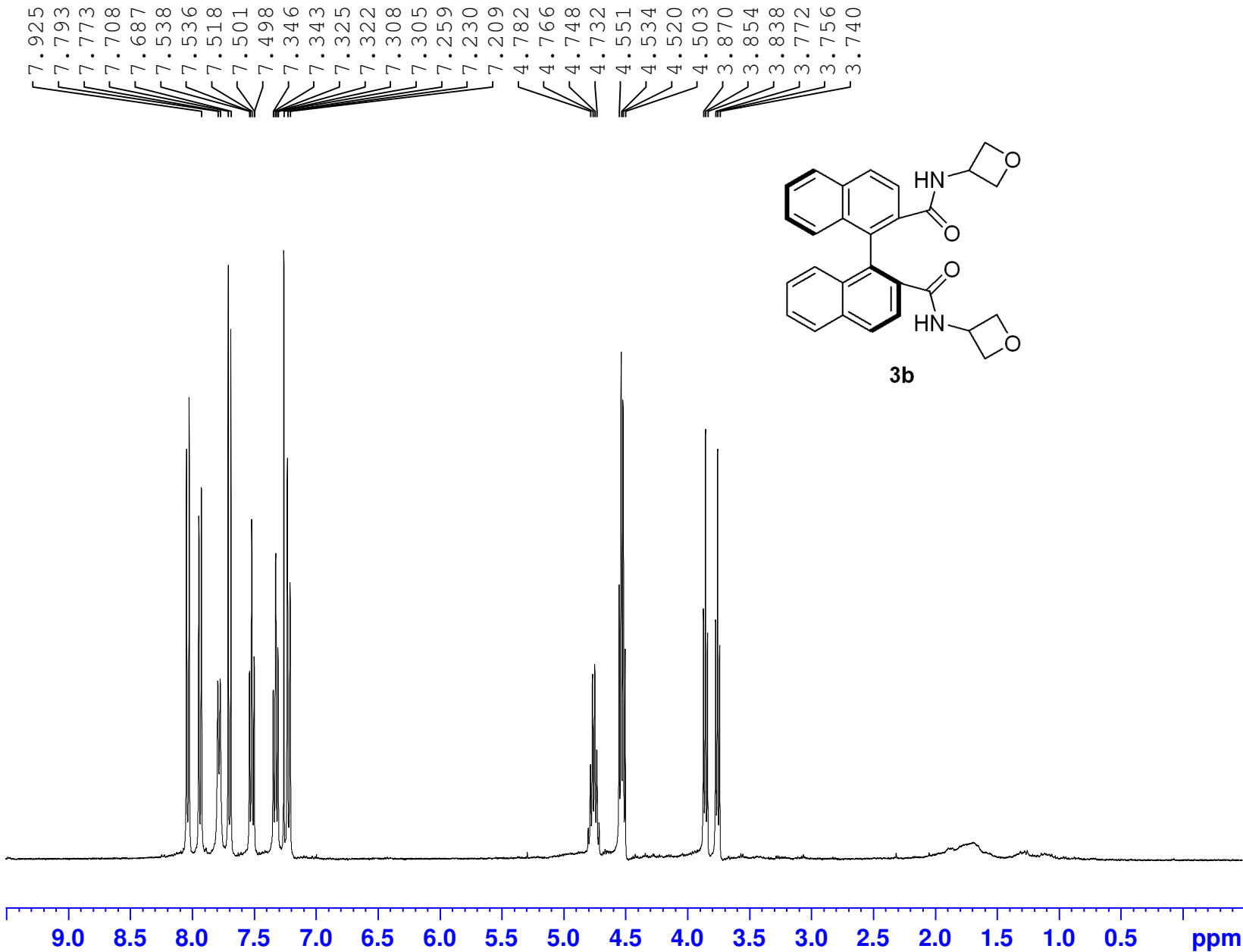
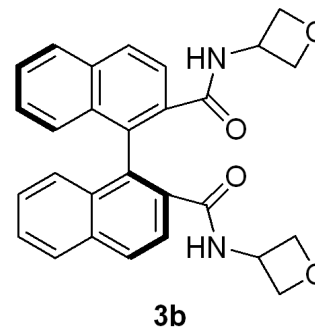


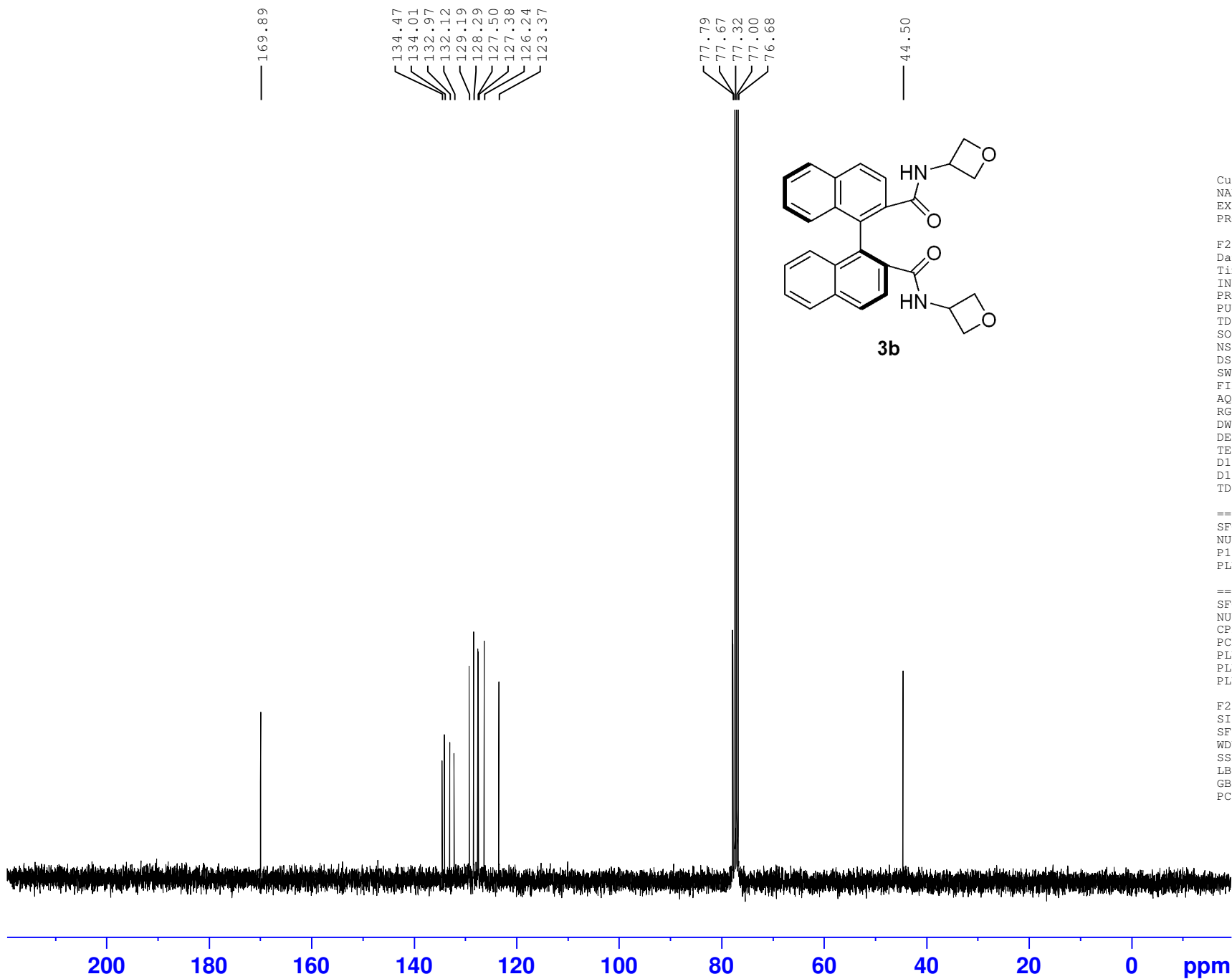
Current Data Parameters
NAME hh-3-410b-h-fr1
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20190411
Time 13.31
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT CDC13
NS 4
DS 0
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 142.88
DW 62.400 usec
DE 6.50 usec
TE 297.9 K
D1 1.00000000 sec
TD0 1

==== CHANNEL f1 =====
SFO1 400.1324710 MHz
NUC1 1H
P1 14.50 usec
PLW1 11.99499989 W

F2 - Processing parameters
SI 65536
SF 400.1300106 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00





Current Data Parameters
NAME hh-3-410c-c-fr1
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20190411
Time 10.13
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 135
DS 0
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 196.92
DW 20.800 usec
DE 6.50 usec
TE 299.4 K
D1 2.0000000 sec
D11 0.03000000 sec
TD0 1

==== CHANNEL f1 =====
SFO1 100.6228298 MHz
NUC1 13C
P1 9.70 usec
PLW1 46.98899841 W

==== CHANNEL f2 =====
SFO2 400.1316005 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 90.00 usec
PLW2 11.99499989 W
PLW12 0.34213999 W
PLW13 0.27713001 W

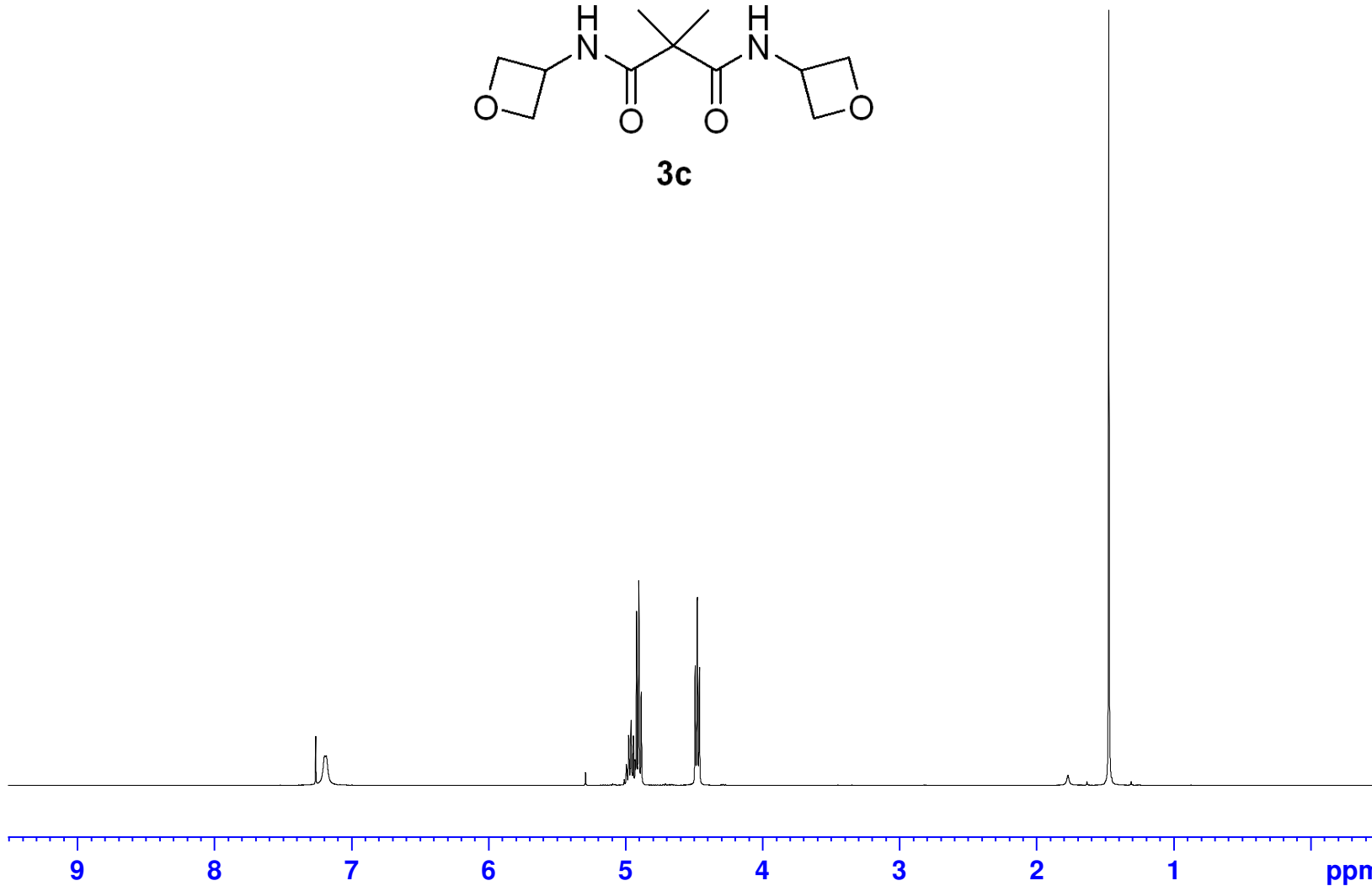
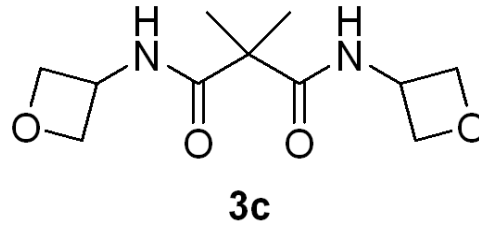
F2 - Processing parameters
SI 32768
SF 100.6127729 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



7.260
7.195
7.183

4.976
4.958
4.941
4.928
4.918
4.902
4.884
4.490
4.474
4.459

1.471



1.87

5.99

4.00

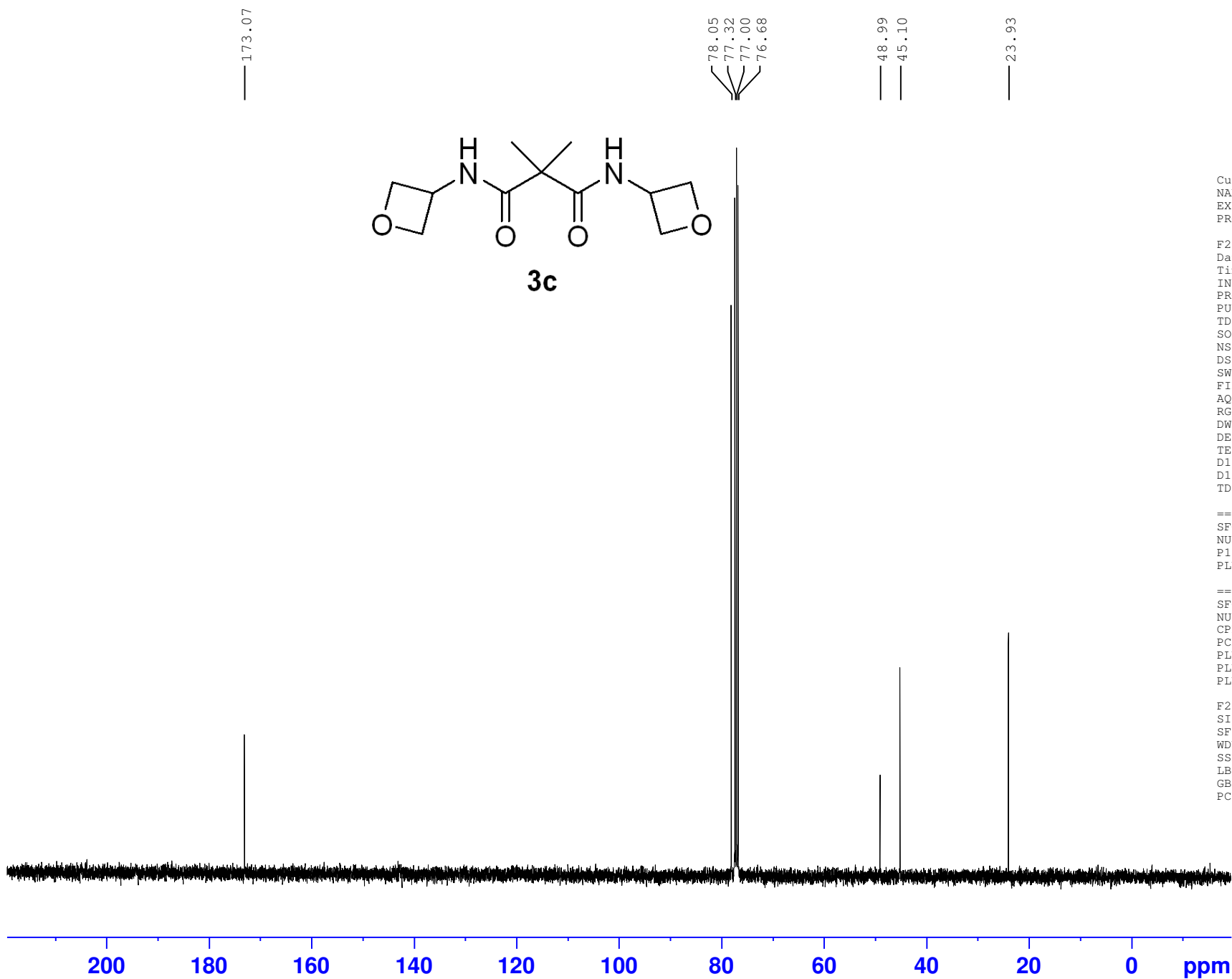
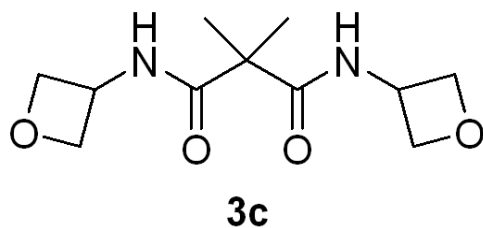
6.02

Current Data Parameters
NAME hh-3-410a-h-fr1
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20190411
Time 9.57
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT CDC13
NS 6
DS 0
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 112.31
DW 62.400 usec
DE 6.50 usec
TE 298.4 K
D1 1.00000000 sec
TD0 1

==== CHANNEL f1 =====
SFO1 400.1324710 MHz
NUC1 1H
P1 14.50 usec
PLW1 11.99499989 W

F2 - Processing parameters
SI 65536
SF 400.1300103 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



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Current Data Parameters
NAME hh-3-410a-c-fr1
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20190411
Time 10.01
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 75
DS 0
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 196.92
DW 20.800 usec
DE 6.50 usec
TE 299.4 K
D1 2.0000000 sec
D11 0.0300000 sec
TD0 1

==== CHANNEL f1 =====
SFO1 100.6228298 MHz
NUC1 13C
P1 9.70 usec
PLW1 46.98899841 W

==== CHANNEL f2 =====
SFO2 400.1316005 MHz
NUC2 1H
PCPD2 waltz16
PLW2 90.00 usec
PLW12 11.99499989 W
PLW13 0.34213999 W
PLW13 0.27713001 W

F2 - Processing parameters
SI 32768
SF 100.6127728 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



Current Data Parameters
NAME 20181025-WJL-1-35 (H)
EXPNO 1
PROCNO 1

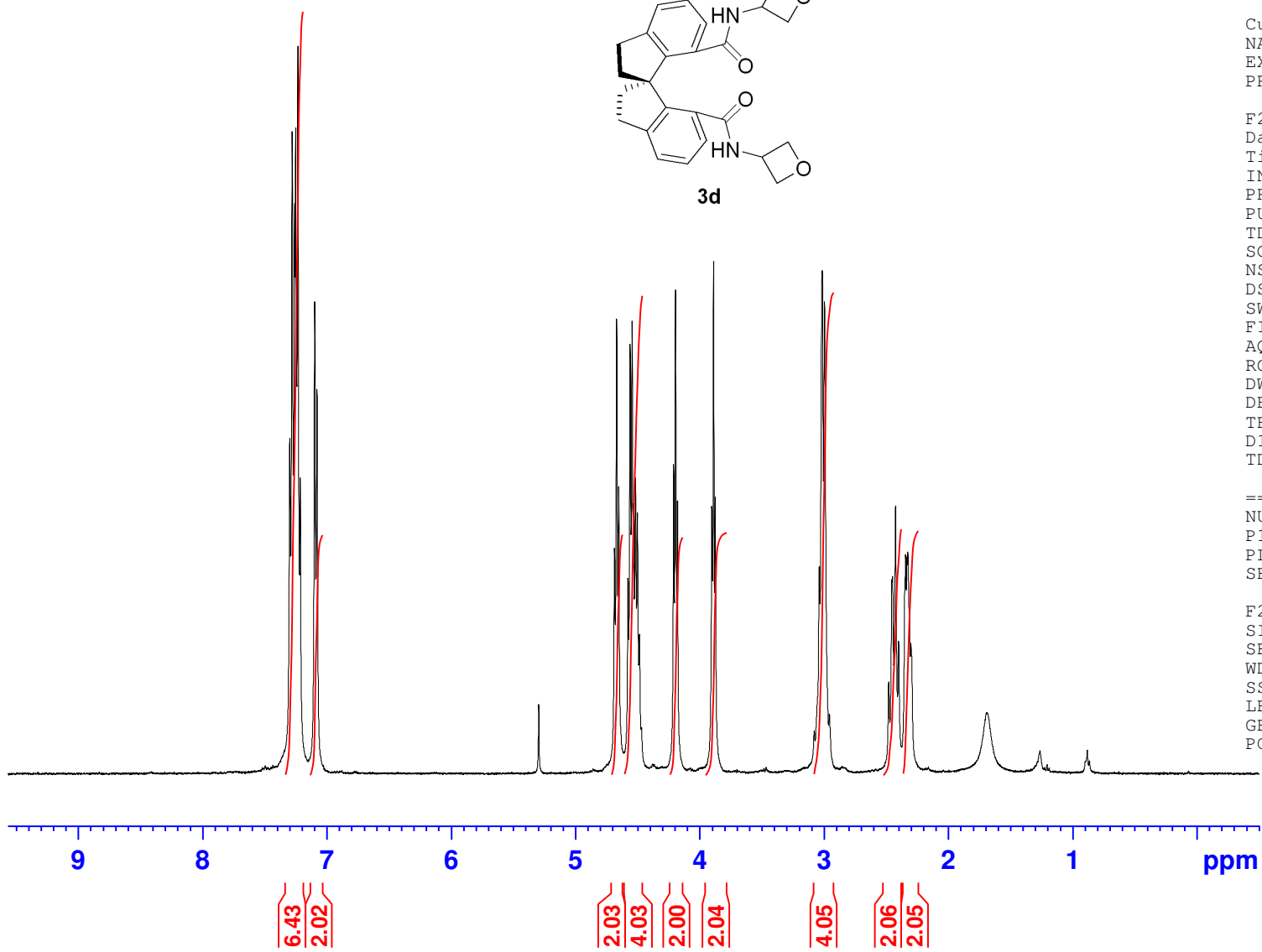
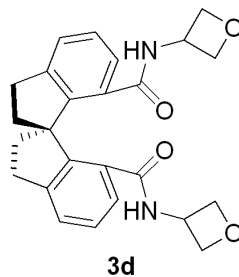
F2 - Acquisition Parameters
Date_ 20181025
Time 22.39
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 8
DS 0
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9845889 sec
RG 406
DW 60.800 usec
DE 6.00 usec
TE 295.3 K
D1 1.0000000 sec
TD0 1

==== CHANNEL f1 =====
NUC1 1H
P1 15.80 usec
PL1 -1.00 dB
SFO1 400.1324710 MHz

F2 - Processing parameters
SI 32768
SF 400.1300095 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

7.30
7.28
7.26
7.25
7.23
7.21
7.10
7.08

4.68
4.67
4.65
4.58
4.56
4.54
4.53
4.52
4.50
4.48
4.48
4.21
4.19
4.18
3.90
3.89
3.87
3.04
3.01
2.99
2.48
2.45
2.45
2.42
2.40
2.34
2.33
2.32
2.31
2.30





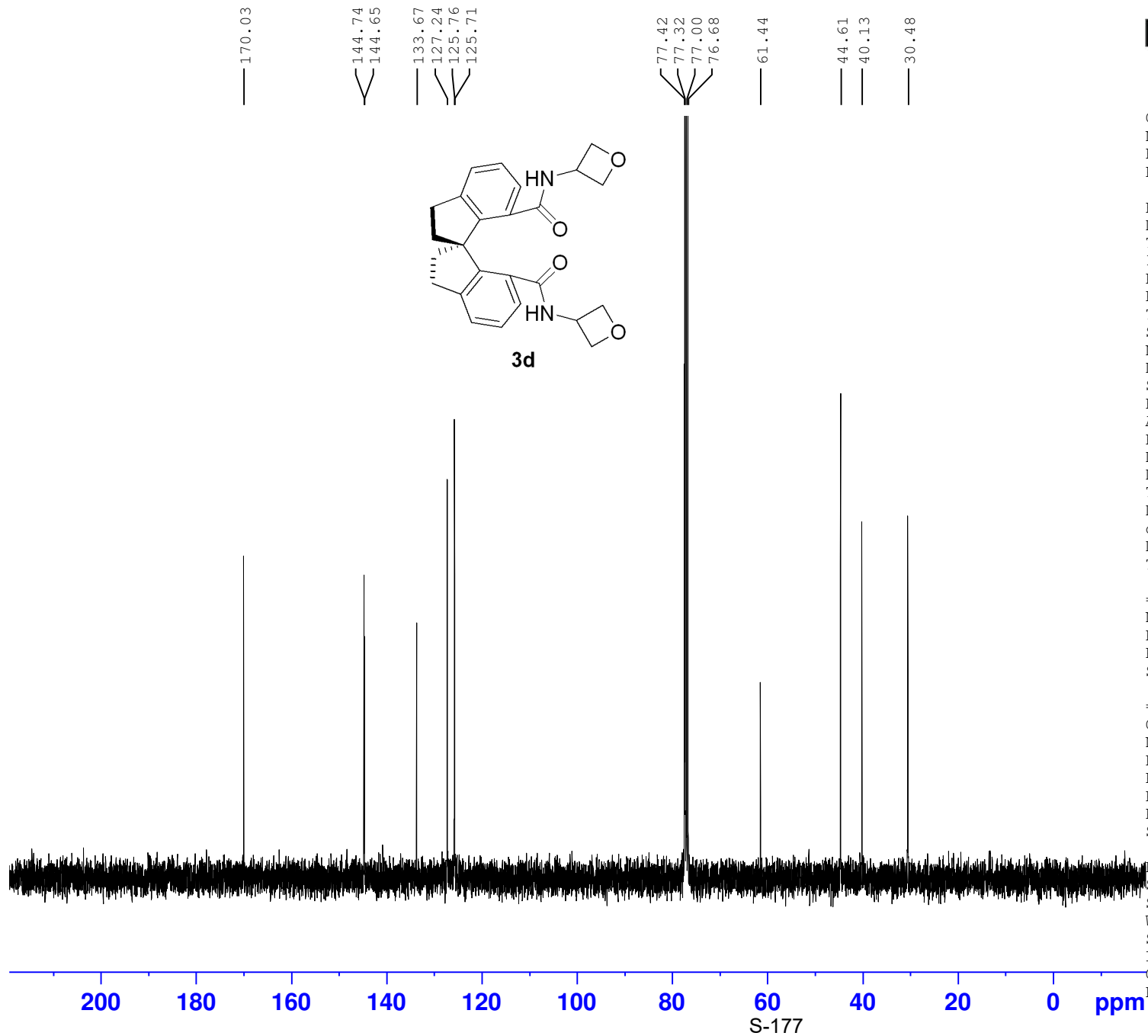
Current Data Parameters
NAME 20181025-WJL-1-35
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20181025
Time 22.13
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 112
DS 2
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 90.5
DW 20.800 usec
DE 6.00 usec
TE 295.5 K
D1 2.0000000 sec
d11 0.0300000 sec
DELTA 1.89999998 sec
TD0 1

==== CHANNEL f1 =====
NUC1 13C
P1 8.60 usec
PL1 -3.00 dB
SFO1 100.6228298 MHz

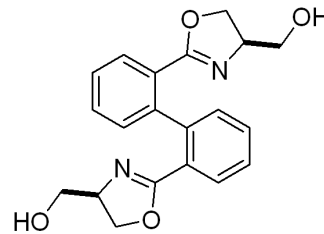
==== CHANNEL f2 =====
CPDPRG[2] waltz16
NUC2 1H
PCPD2 80.00 usec
PL12 14.39 dB
PL13 18.00 dB
PL2 -1.00 dB
SFO2 400.1316005 MHz

F2 - Processing parameters
SI 32768
SF 100.6127792 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40





7.561
7.545
7.529
7.527
7.511
7.508
7.439
7.436
7.417
7.407
7.398
7.388
7.260
4.207
4.203
4.181
4.160
4.157
4.140
4.122
4.114
4.096
4.072
4.070
4.041
4.038
3.917
3.897
3.878
3.384
3.377
3.352
3.345



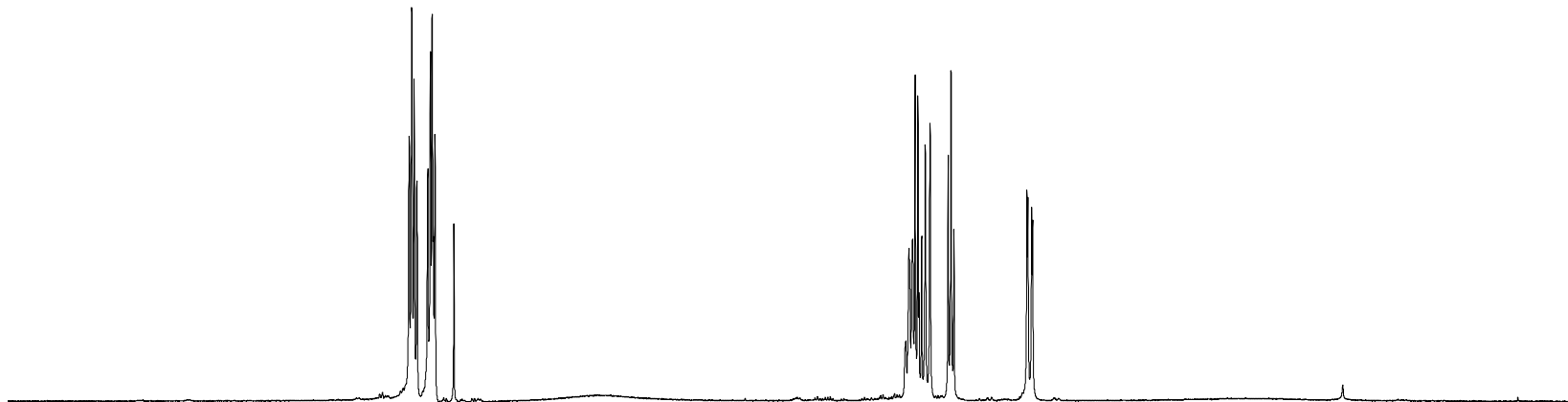
(±)-4a

Current Data Parameters
NAME czl-2-5
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20170826
Time 10.02
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT CDC13
NS 4
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 187.77
DW 62.400 usec
DE 6.50 usec
TE 297.5 K
D1 1.00000000 sec
TD0 1

==== CHANNEL f1 =====
SFO1 400.1324710 MHz
NUC1 1H
P1 14.50 usec
PLW1 11.99499989 W

F2 - Processing parameters
SI 65536
SF 400.1300105 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

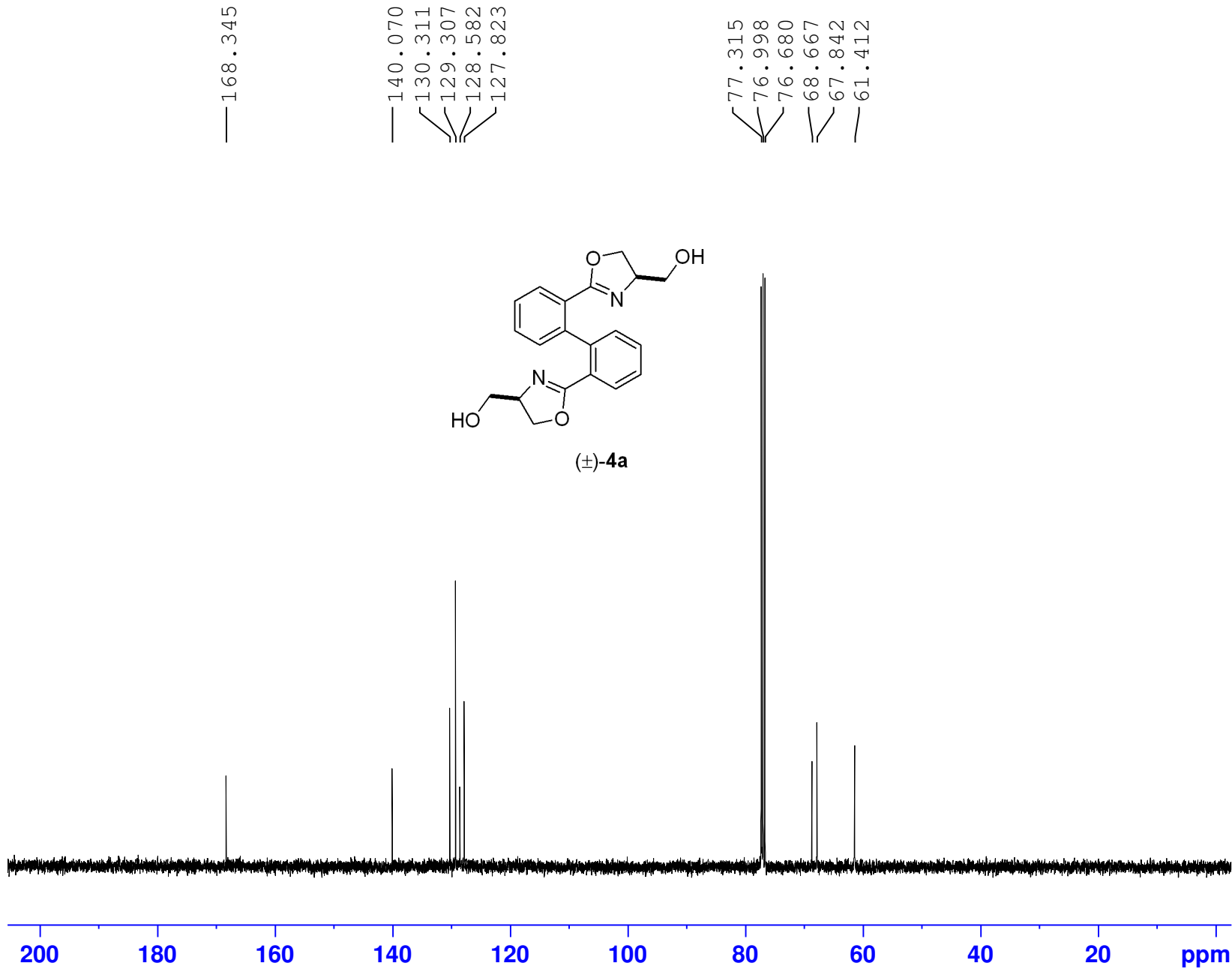
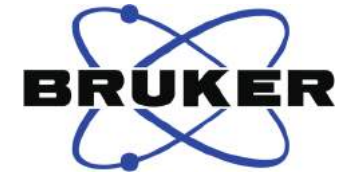


10 9 8 7 6 5 4 3 2 1 ppm

4.06
4.03

6.04
2.00
2.05

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Current Data Parameters
NAME czl-2-5
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20170826
Time 10.07
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 78
DS 2
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 196.92
DW 20.800 usec
DE 6.50 usec
TE 297.8 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

==== CHANNEL f1 =====
SFO1 100.6228298 MHz
NUC1 13C
P1 9.70 usec
PLW1 46.98899841 W

==== CHANNEL f2 =====
SFO2 400.1316005 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 90.00 usec
PLW2 11.99499989 W
PLW12 0.34213999 W
PLW13 0.27713001 W

F2 - Processing parameters
SI 32768
SF 100.6127736 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



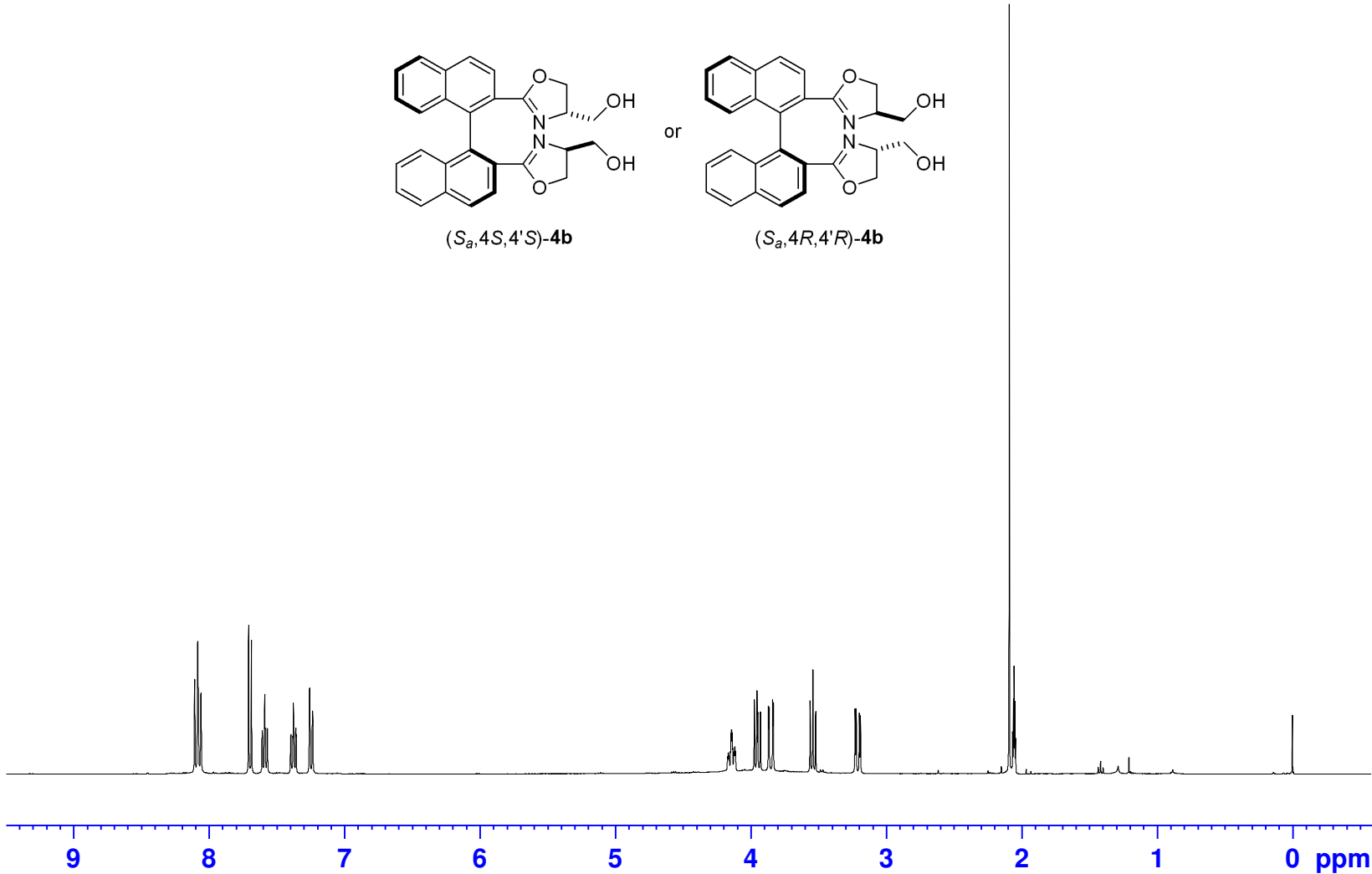
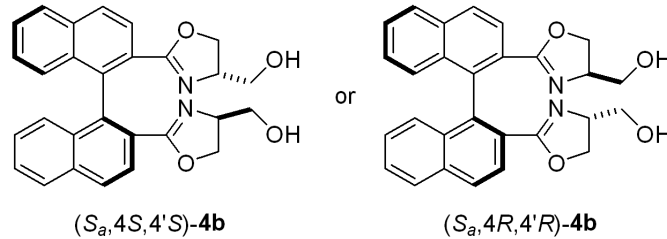
Current Data Parameters
NAME hh-2-97B-h-fr1
EXPNO 3
PROCNO 1

F2 - Acquisition Parameters
Date_ 20181201
Time 10.06
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT Acetone
NS 6
DS 0
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 88.84
DW 62.400 usec
DE 6.50 usec
TE 298.0 K
D1 1.00000000 sec
TD0 1

==== CHANNEL f1 =====
SFO1 400.1324710 MHz
NUC1 1H
P1 14.50 usec
PLW1 11.99499989 W

F2 - Processing parameters
SI 65536
SF 400.1300056 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

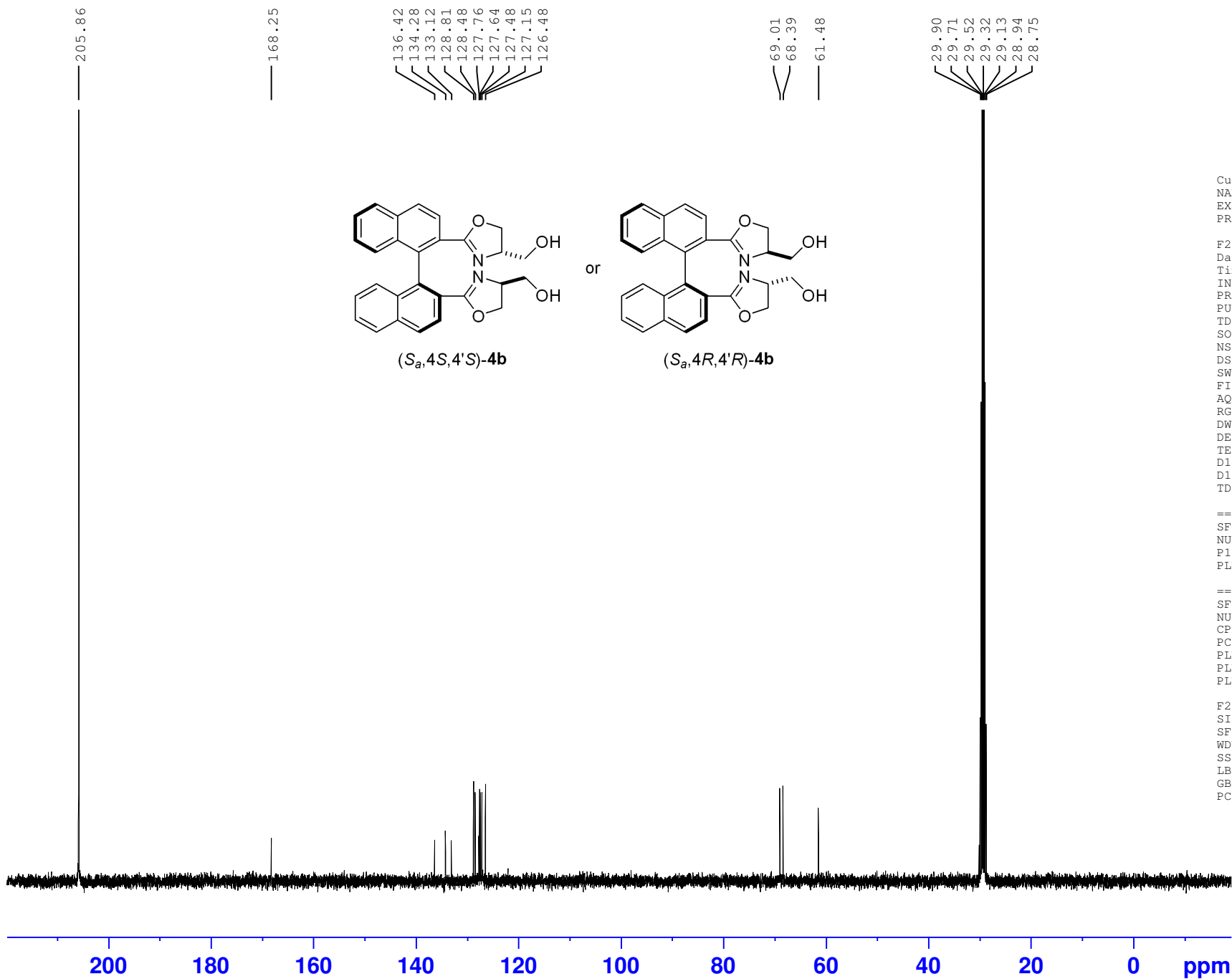
7.686
7.608
7.605
7.591
7.588
7.585
7.570
7.567
7.397
7.394
7.380
7.376
7.373
7.359
7.356
7.255
7.234
4.145
4.141
4.137
4.133
4.119
4.116
3.972
3.952
3.947
3.927
3.868
3.863
3.837
3.832
3.560
3.540
3.519
3.228
3.220
3.197
3.189
2.090
2.059
2.054
2.048



2.03
0.98
1.03
1.00
0.98

1.11
1.11
1.08
1.04
1.00

0.86



Current Data Parameters
NAME hh-2-97B-c-fr1
EXPNO 4
PROCNO 1

F2 - Acquisition Parameters
Date_ 20181201
Time 10.29
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT Acetone
NS 38
DS 0
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 196.92
DW 20.800 usec
DE 6.50 usec
TE 298.4 K
D1 2.0000000 sec
D11 0.0300000 sec
TD0 1

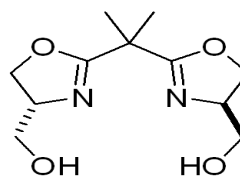
==== CHANNEL f1 =====
SFO1 100.6228298 MHz
NUC1 13C
P1 9.70 usec
PLW1 46.98899841 W

==== CHANNEL f2 =====
SFO2 400.1316005 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 90.00 usec
PLW2 11.99499989 W
PLW12 0.34213999 W
PLW13 0.27713001 W

F2 - Processing parameters
SI 32768
SF 100.6127344 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



4.328
4.313
4.302
4.293
4.211
4.200
4.184
3.659
3.628
3.557
3.546
3.530
3.518
2.090
2.065
2.059
2.054
2.048
2.043
1.461

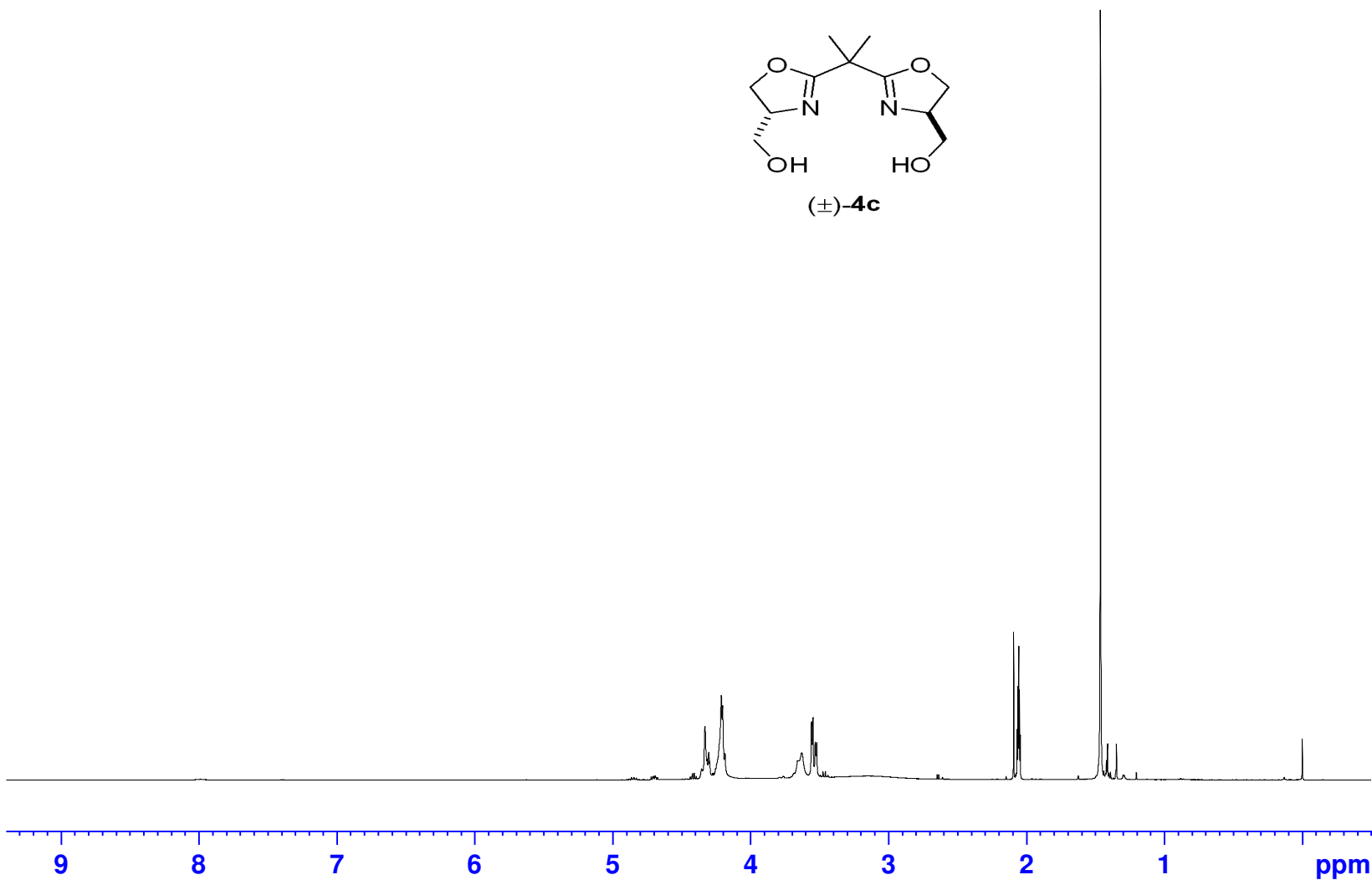


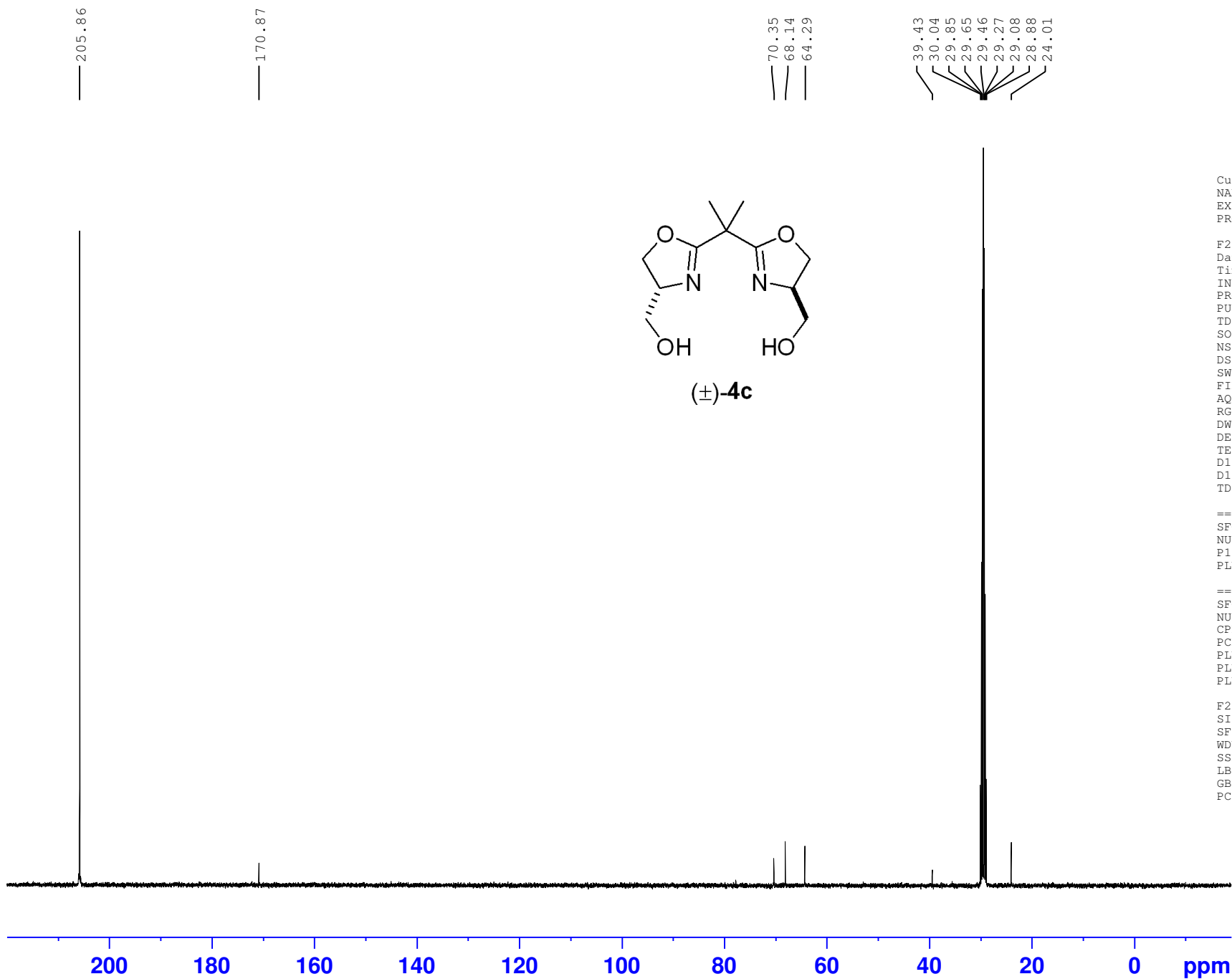
Current Data Parameters
NAME hh-2-97-h-fr1
EXPNO 4
PROCNO 1

F2 - Acquisition Parameters
Date_ 20181201
Time 19.57
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT Acetone
NS 6
DS 0
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 103.52
DW 62.400 usec
DE 6.50 usec
TE 297.3 K
D1 1.00000000 sec
TD0 1

==== CHANNEL f1 =====
SFO1 400.1324710 MHz
NUC1 1H
P1 14.50 usec
PLW1 11.99499989 W

F2 - Processing parameters
SI 65536
SF 400.1300056 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00





Current Data Parameters
NAME hh-2-97-c-fr1
EXPNO 4
PROCNO 1

F2 - Acquisition Parameters
Date_ 20181201
Time 20.14
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT Acetone
NS 244
DS 0
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 196.92
DW 20.800 usec
DE 6.50 usec
TE 298.5 K
D1 2.0000000 sec
D11 0.0300000 sec
TDO 1

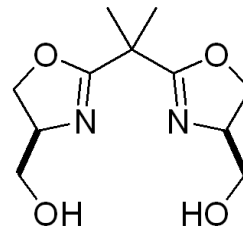
==== CHANNEL f1 =====
SFO1 100.6228298 MHz
NUC1 13C
P1 9.70 usec
PLW1 46.98899841 W

==== CHANNEL f2 =====
SFO2 400.1316005 MHz
NUC2 1H
PCPD2 waltz16
PLW2 90.00 usec
PLW12 11.99499989 W
PLW13 0.34213999 W
PLW13 0.27713001 W

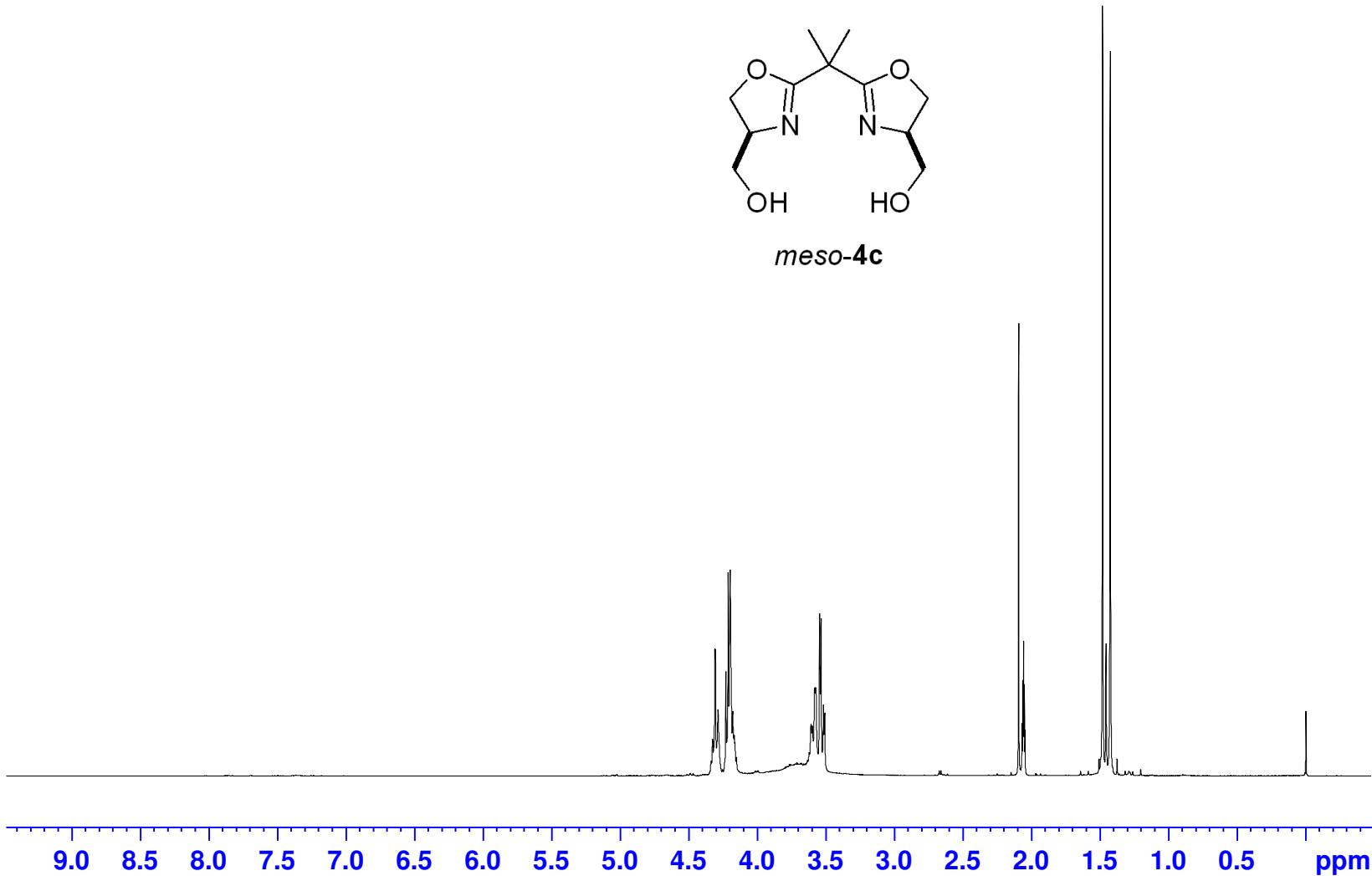
F2 - Processing parameters
SI 32768
SF 100.6127172 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



4.323
4.306
4.303
4.284
4.226
4.209
4.194
4.176
4.165
4.160
3.605
3.595
3.578
3.571
3.542
3.532
3.514
3.509
3.504
2.090
2.059
2.054
2.048
1.478
1.452
1.422



meso-4c

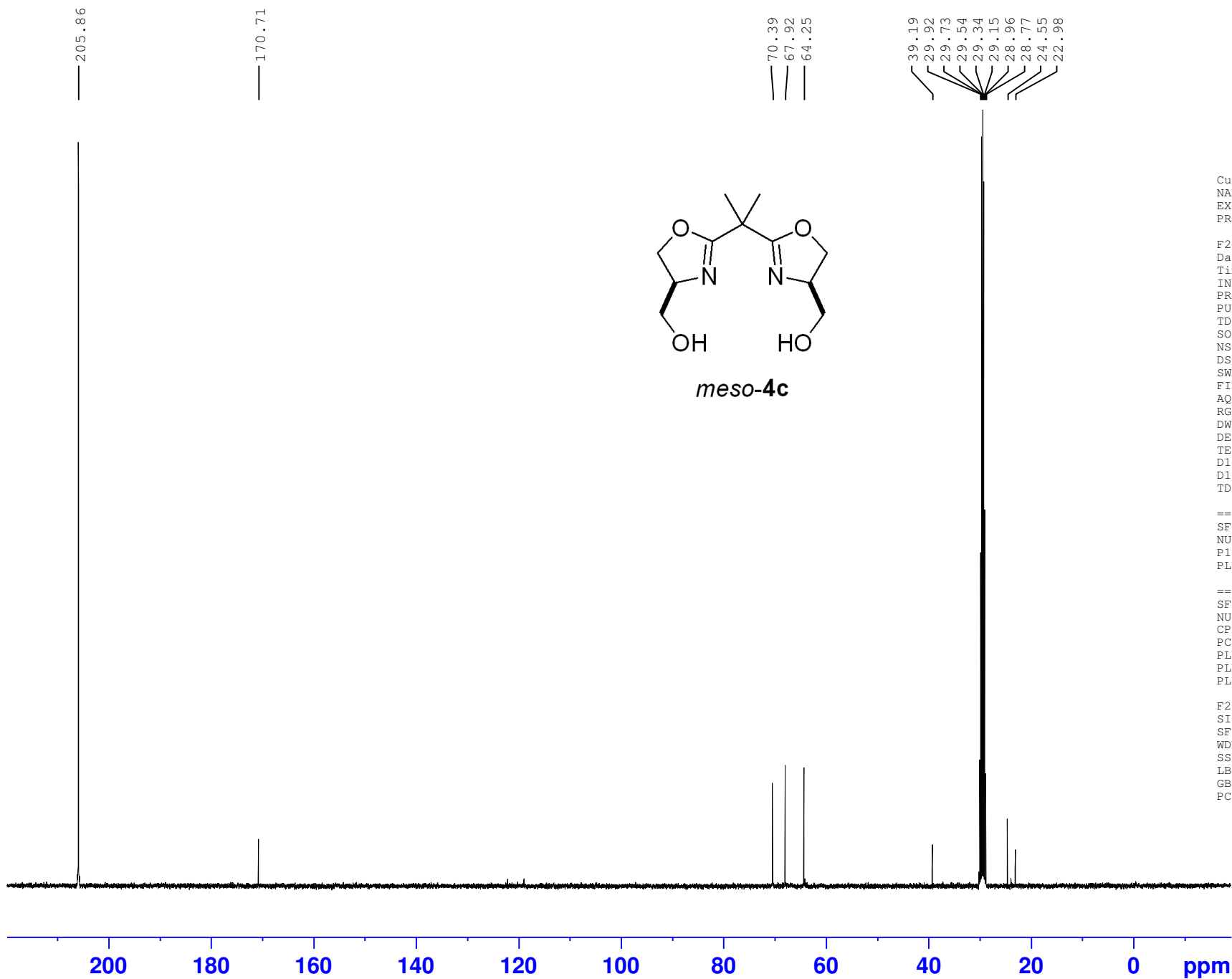


Current Data Parameters
NAME hh-2-97-h-fr2
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20181201
Time 14.14
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT Acetone
NS 5
DS 0
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 82.92
DW 62.400 usec
DE 6.50 usec
TE 295.9 K
D1 1.00000000 sec
TD0 1

==== CHANNEL f1 =====
SFO1 400.1324710 MHz
NUC1 1H
P1 14.50 usec
PLW1 11.99499989 W

F2 - Processing parameters
SI 65536
SF 400.1300056 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



Current Data Parameters
NAME hh-2-97-c-fr2
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20181201
Time 14.26
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT Acetone
NS 200
DS 0
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 196.92
DW 20.800 usec
DE 6.50 usec
TE 296.9 K
D1 2.0000000 sec
D11 0.03000000 sec
TDO 1

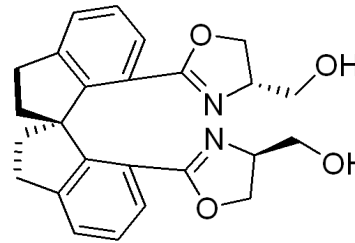
==== CHANNEL f1 =====
SFO1 100.6228298 MHz
NUC1 13C
P1 9.70 usec
PLW1 46.98899841 W

==== CHANNEL f2 =====
SFO2 400.1316005 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 90.00 usec
PLW2 11.99499989 W
PLW12 0.34213999 W
PLW13 0.27713001 W

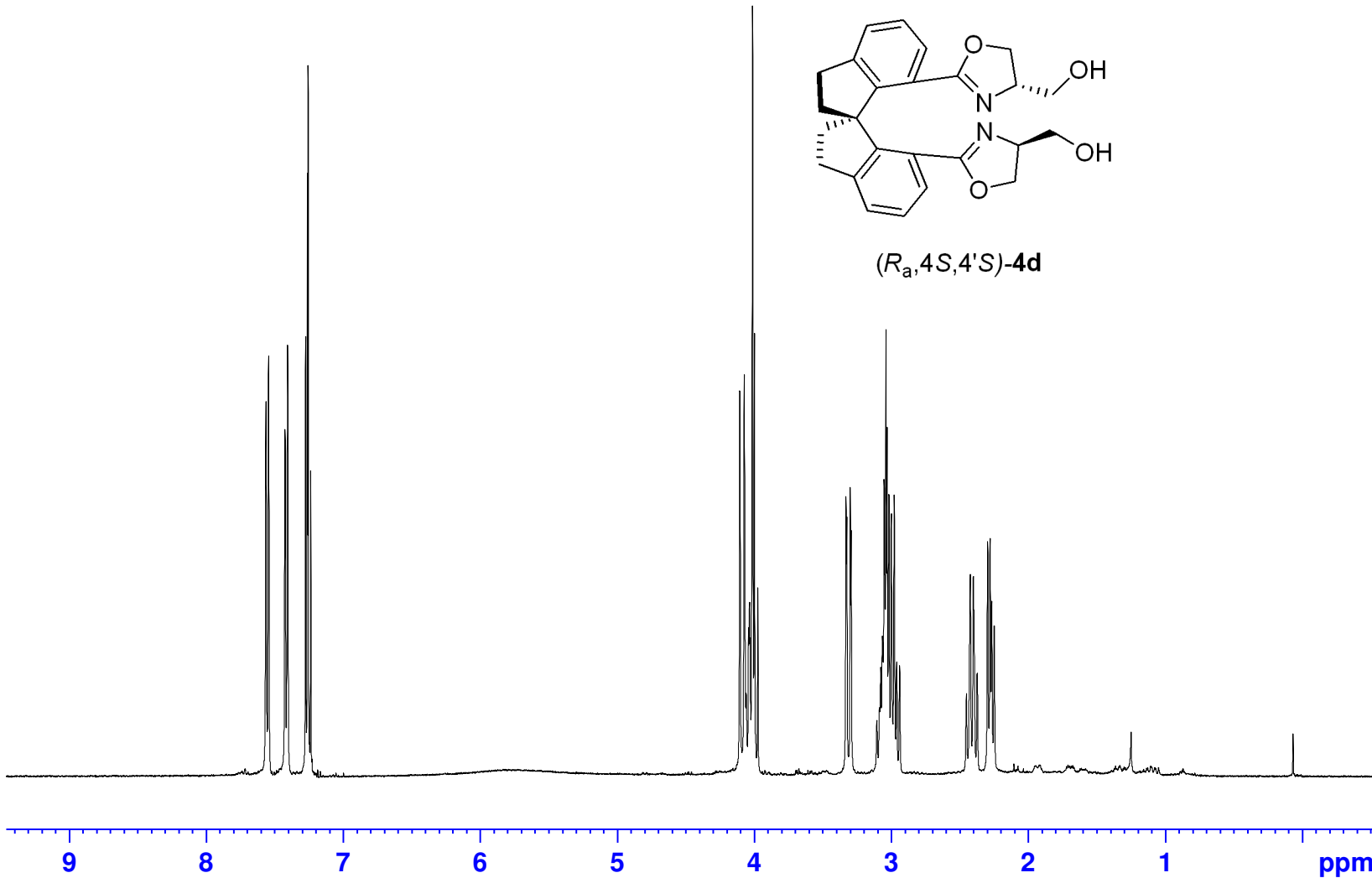
F2 - Processing parameters
SI 32768
SF 100.6127317 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



7.562
7.543
7.424
7.405
7.273
7.260
7.254
7.236
5.825
4.104
4.073
4.070
4.057
4.040
4.035
4.033
4.028
4.011
3.997
3.972
3.329
3.322
3.298
3.291
3.075
3.063
3.050
3.036
3.028
3.015
2.998
2.977
2.958
2.937
2.449
2.421
2.399
2.372
2.294
2.277
2.265
2.247



(*R_a*,4*S*,4'*S*)-4d

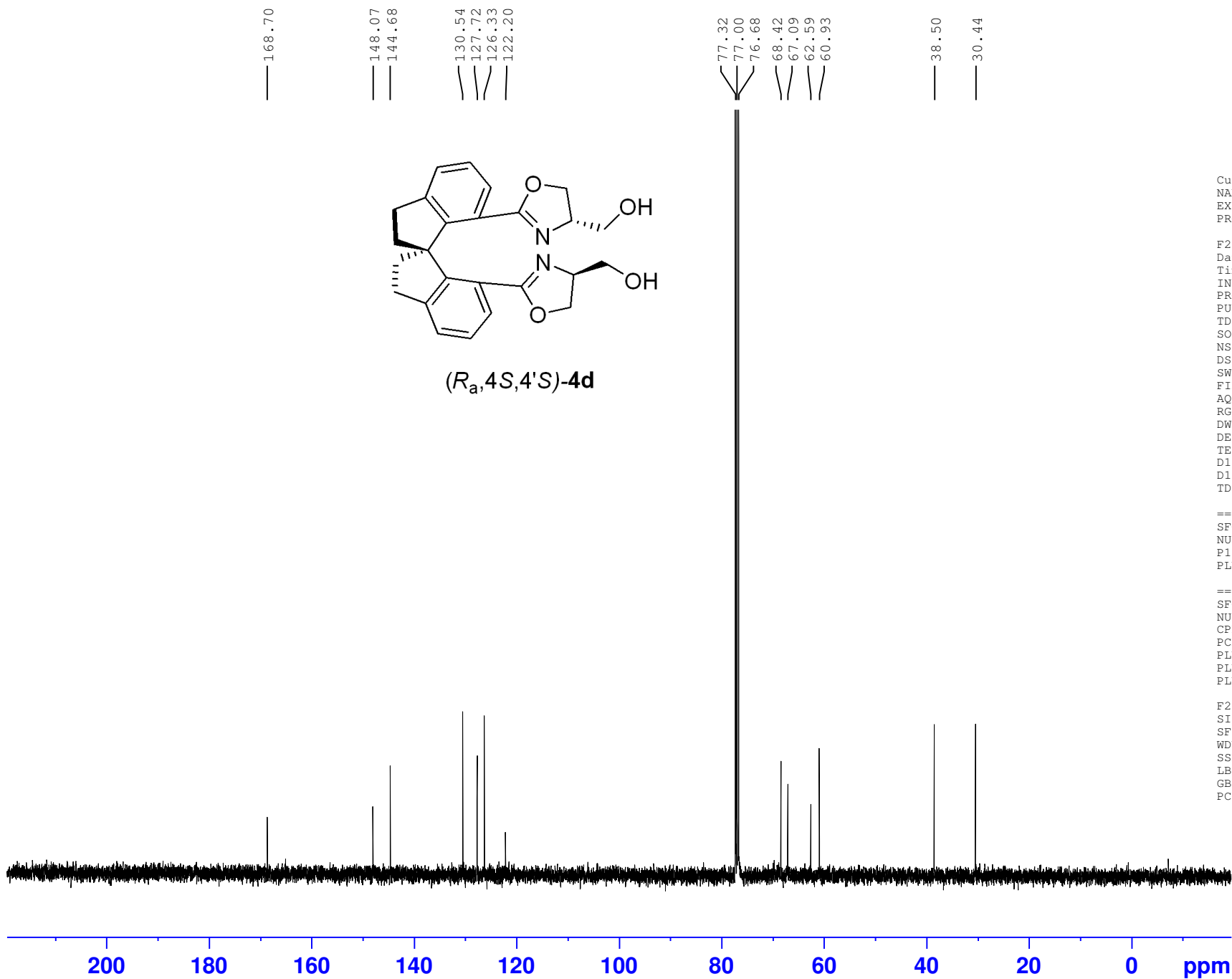
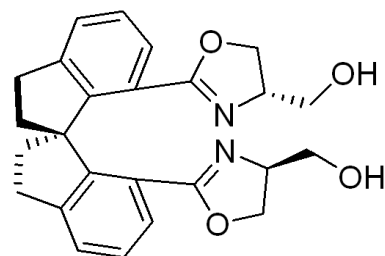


Current Data Parameters
NAME hh-2-106A-h-fr1
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20181203
Time 19.16
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT CDC13
NS 4
DS 0
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 142.88
DW 62.400 usec
DE 6.50 usec
TE 295.5 K
D1 1.00000000 sec
TD0 1

==== CHANNEL f1 =====
SFO1 400.1324710 MHz
NUC1 1H
P1 14.50 usec
PLW1 11.99499989 W

F2 - Processing parameters
SI 65536
SF 400.1300102 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



Current Data Parameters
NAME hh-2-106A-c-fr1
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20181203
Time 19.23
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 110
DS 0
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 196.92
DW 20.800 usec
DE 6.50 usec
TE 296.6 K
D1 2.0000000 sec
D11 0.0300000 sec
TD0 1

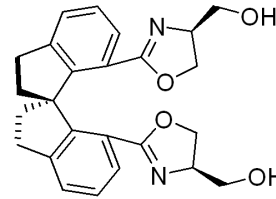
==== CHANNEL f1 =====
SFO1 100.6228298 MHz
NUC1 13C
P1 9.70 usec
PLW1 46.98899841 W

==== CHANNEL f2 =====
SFO2 400.1316005 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 90.00 usec
PLW2 11.99499989 W
PLW12 0.34213999 W
PLW13 0.27713001 W

F2 - Processing parameters
SI 32768
SF 100.6127722 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

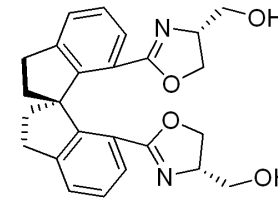


7.652
7.633
7.525
7.506
7.397
7.380
7.366
7.260
7.227
7.222
7.208
7.203
7.189
7.184
3.958
3.940
3.934
3.922
3.916
3.910
3.885
3.880
3.368
3.358
3.354
3.343
3.299
3.289
3.269
3.259
3.145
3.126
3.122
3.103
3.048
3.041
3.021
2.997
2.988
2.975
2.966
2.938
2.919
2.913
2.894
2.477
2.260
2.242

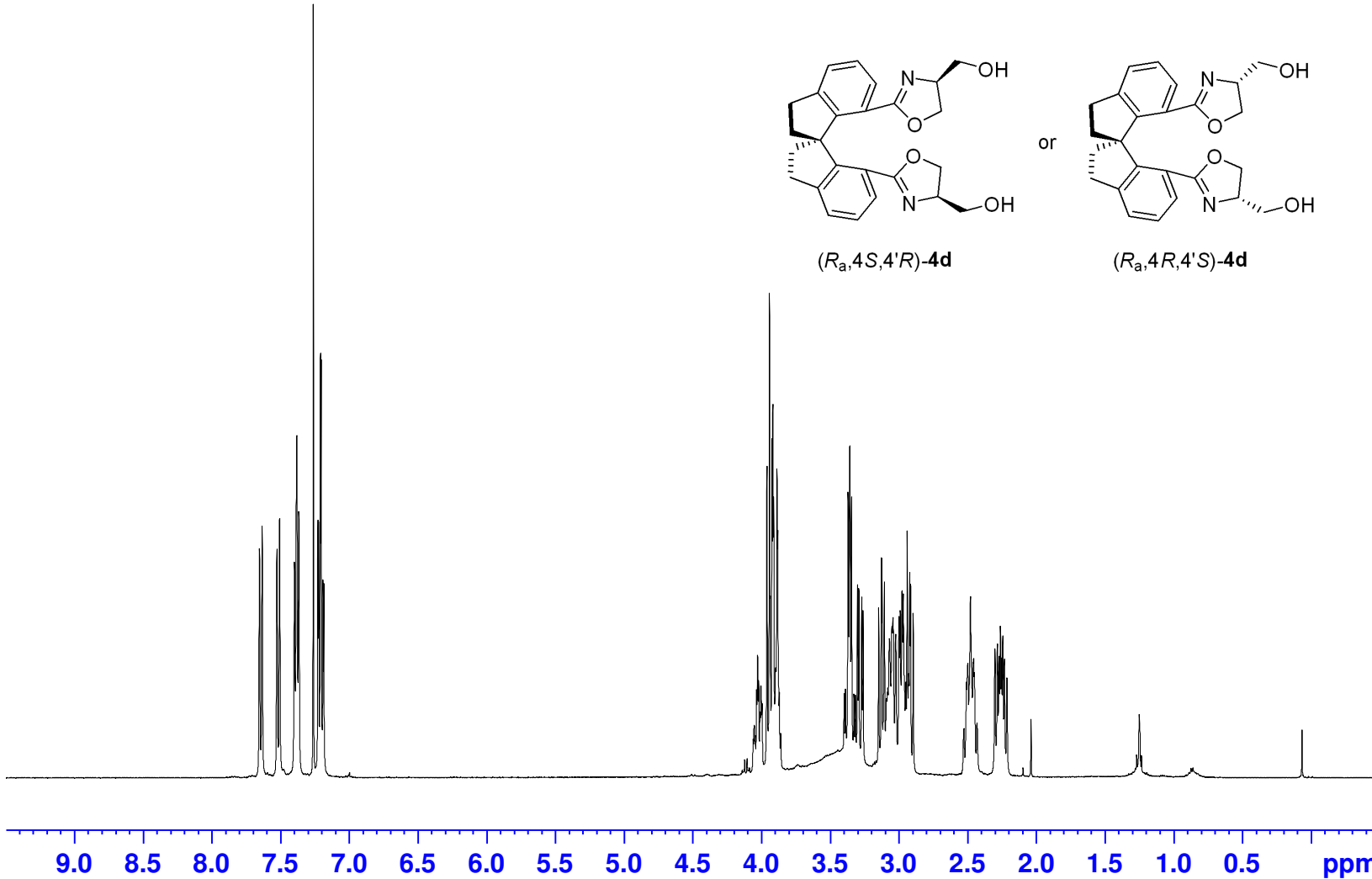


(R_a,4S,4'R)-4d

or



(R_a,4R,4'S)-4d

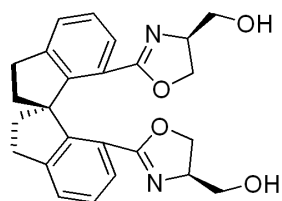


Current Data Parameters
NAME hh-2-106A-h-fr2
EXPNO 5
PROCNO 1

F2 - Acquisition Parameters
Date_ 20181208
Time 12.59
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT CDC13
NS 5
DS 0
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 82.92
DW 62.400 usec
DE 6.50 usec
TE 295.6 K
D1 1.00000000 sec
TD0 1

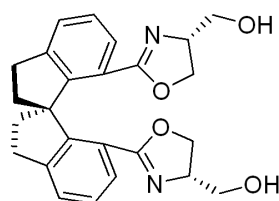
==== CHANNEL f1 =====
SFO1 400.1324710 MHz
NUC1 1H
P1 14.50 usec
PLW1 11.99499989 W

F2 - Processing parameters
SI 65536
SF 400.1300101 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

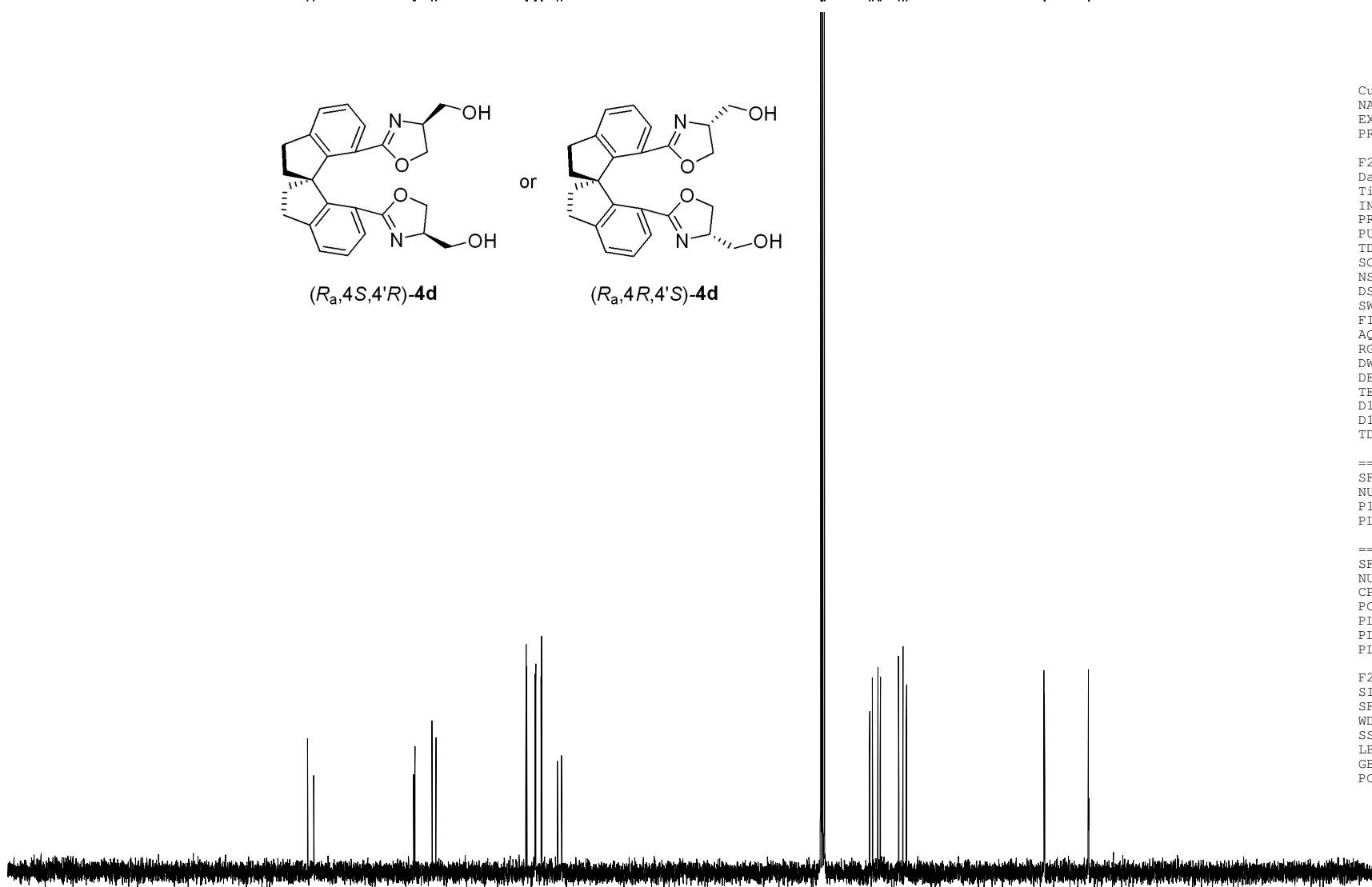


(*R_a*,4*S*,4'*R*)-4d

or



(*R_a*,4*R*,4'*S*)-4d



200 180 160 140 120 100 80 60 40 20 0 ppm

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Current Data Parameters
NAME hh-2-106A-c-fr2
EXPNO 5
PROCNO 1

F2 - Acquisition Parameters
Date_ 20181208
Time 13.09
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 159
DS 0
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 196.92
DW 20.800 usec
DE 6.50 usec
TE 296.6 K
D1 2.0000000 sec
D11 0.0300000 sec
TD0 1

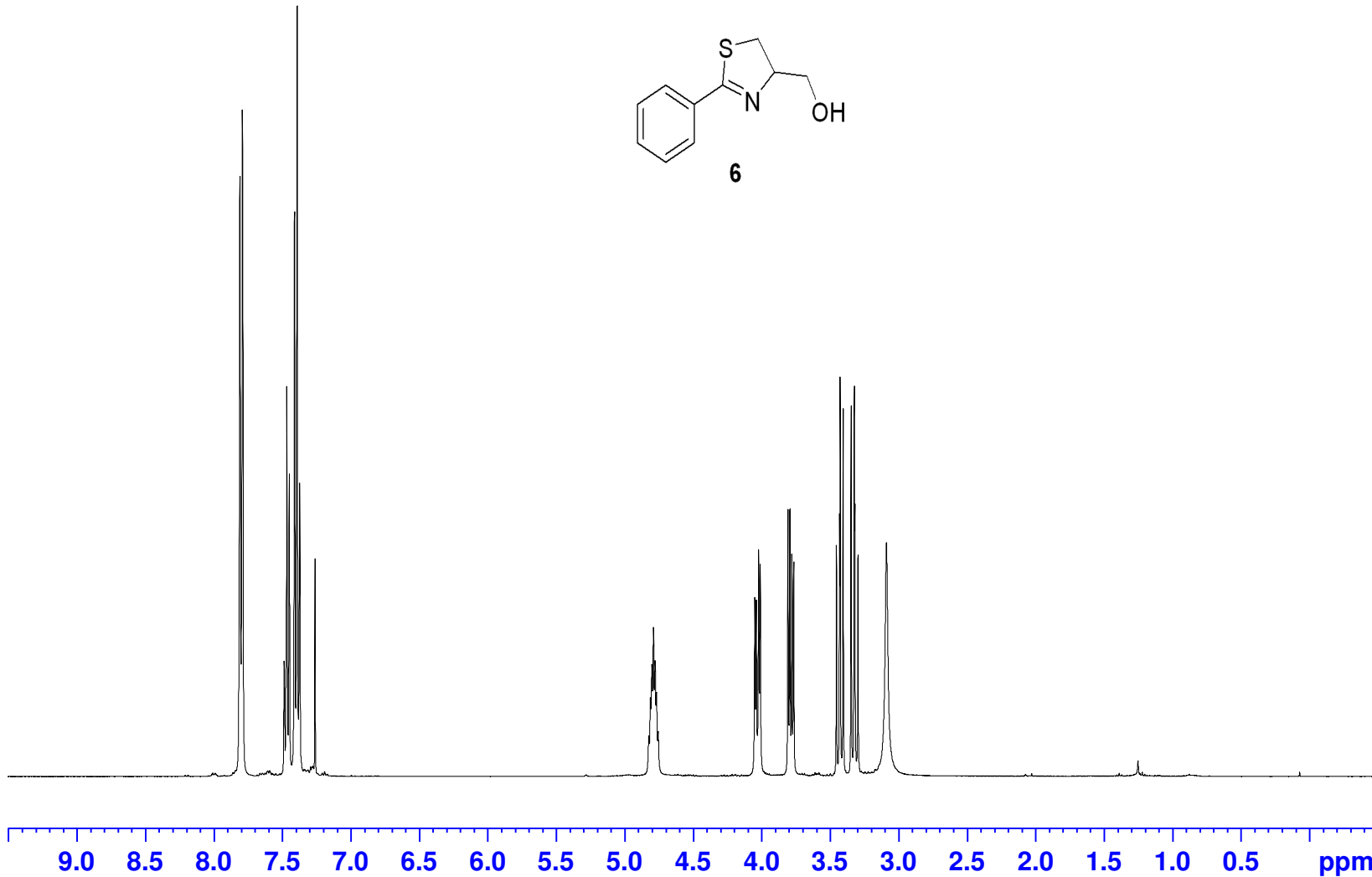
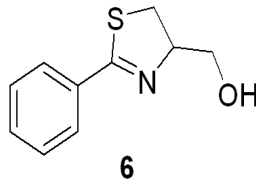
==== CHANNEL f1 =====
SFO1 100.6228298 MHz
NUC1 13C
P1 9.70 usec
PLW1 46.98899841 W

==== CHANNEL f2 =====
SFO2 400.1316005 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 90.00 usec
PLW2 11.99499989 W
PLW12 0.34213999 W
PLW13 0.27713001 W

F2 - Processing parameters
SI 32768
SF 100.6127743 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



7.809
7.791
7.788
7.485
7.472
7.467
7.462
7.448
7.410
7.391
7.373
7.260
4.823
4.811
4.800
4.789
4.777
4.767
4.754
4.049
4.037
4.021
4.009
3.806
3.792
3.778
3.764
3.452
3.430
3.425
3.403
3.345
3.322
3.318
3.295
3.087

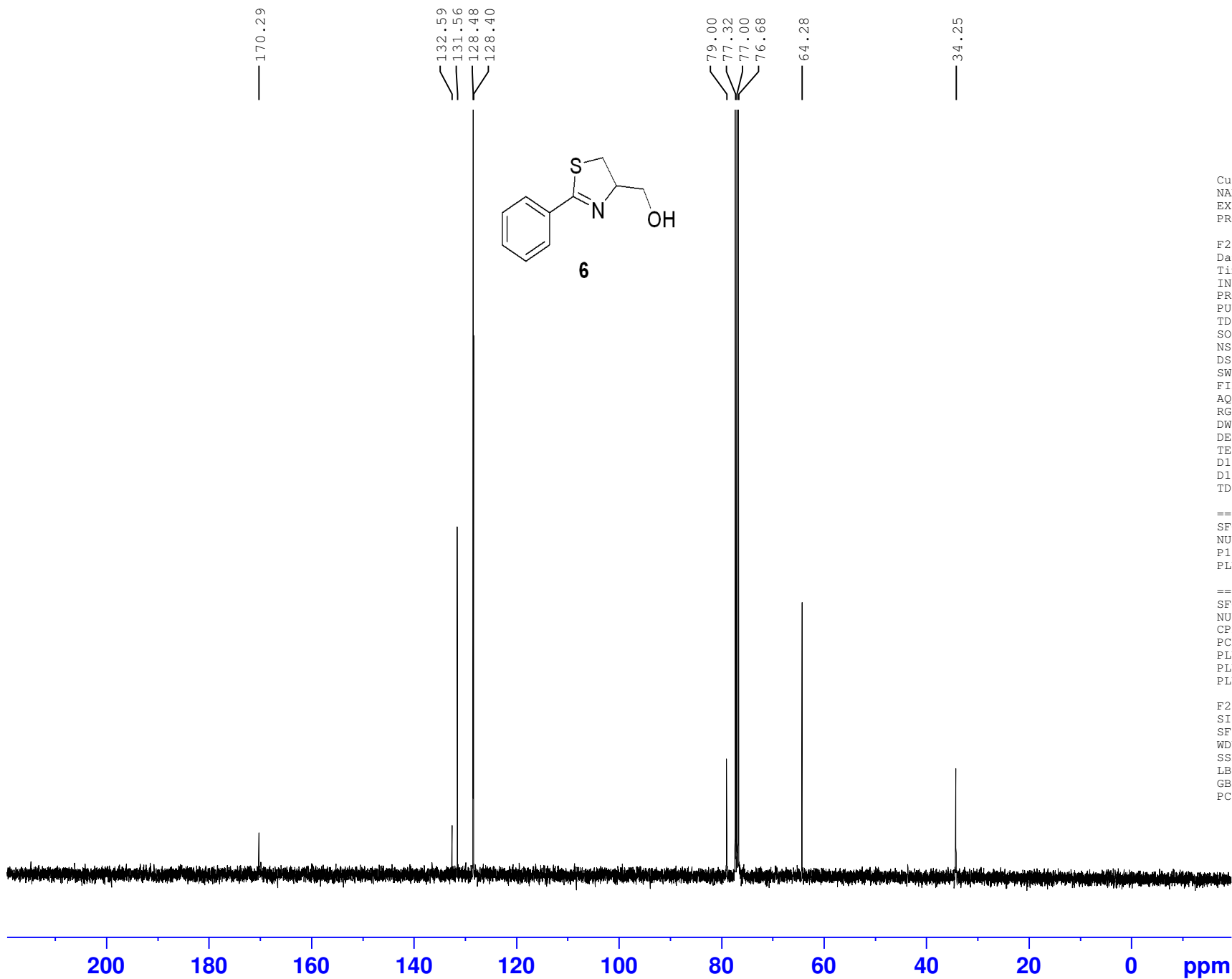


Current Data Parameters
NAME hh-3-149-h-fr1
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20190704
Time 15.43
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT CDC13
NS 10
DS 0
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 103.52
DW 62.400 usec
DE 6.50 usec
TE 295.4 K
D1 1.00000000 sec
TD0 1

==== CHANNEL f1 =====
SFO1 400.1324710 MHz
NUC1 1H
P1 14.50 usec
PLW1 11.99499989 W

F2 - Processing parameters
SI 65536
SF 400.1300101 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



Current Data Parameters
NAME hh-3-149-c-fr1
EXPNO 4
PROCNO 1

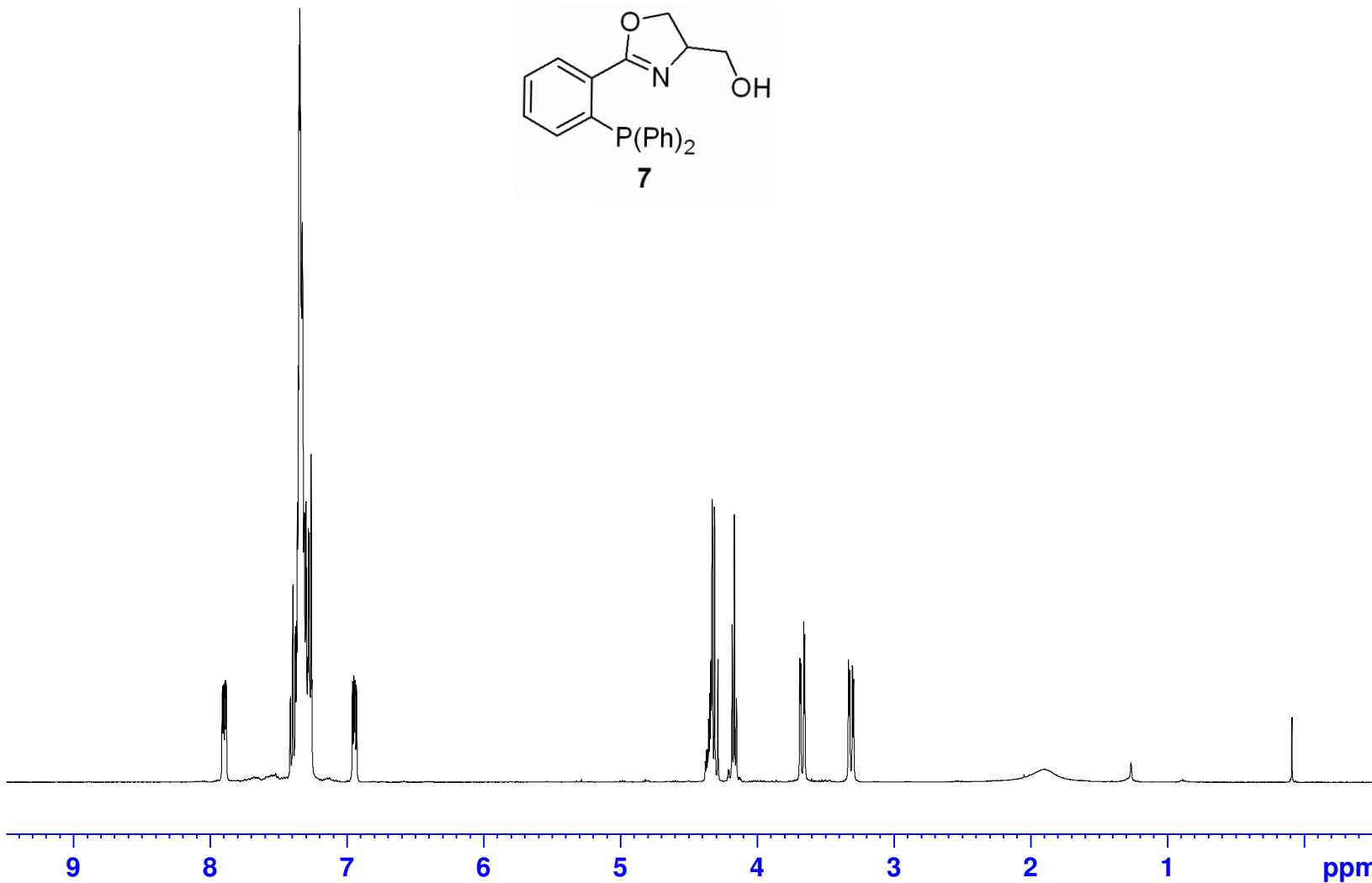
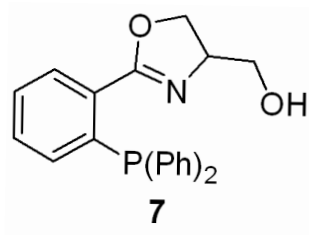
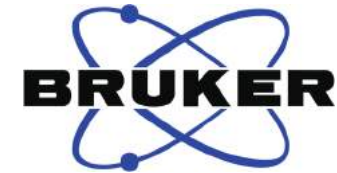
F2 - Acquisition Parameters
Date_ 20190704
Time 15.56
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 119
DS 0
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 196.92
DW 20.800 usec
DE 6.50 usec
TE 296.4 K
D1 2.0000000 sec
D11 0.03000000 sec
TDO 1

==== CHANNEL f1 =====
SFO1 100.6228298 MHz
NUC1 13C
P1 9.70 usec
PLW1 46.98899841 W

==== CHANNEL f2 =====
SFO2 400.1316005 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 90.00 usec
PLW2 11.99499989 W
PLW12 0.34213999 W
PLW13 0.27713001 W

F2 - Processing parameters
SI 32768
SF 100.6127751 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

7.899
7.892
7.889
7.883
7.396
7.393
7.377
7.374
7.366
7.361
7.355
7.347
7.343
7.339
7.331
7.326
7.323
7.313
7.309
7.302
7.298
7.294
7.286
7.279
7.275
7.269
7.260
7.255
6.959
6.956
6.949
6.946
6.940
6.930
4.336
4.326
4.309
4.285
4.181
4.165
3.686
3.679
3.657
3.650
3.330
3.321
3.301
3.292



Current Data Parameters
 NAME hh-2-160-h-fr1
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20181229
 Time 13.25
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zg30
 TD 65536
 SOLVENT CDC13
 NS 4
 DS 0
 SWH 8012.820 Hz
 FIDRES 0.122266 Hz
 AQ 4.0894465 sec
 RG 39.46
 DW 62.400 usec
 DE 6.50 usec
 TE 295.4 K
 D1 1.00000000 sec
 TD0 1

===== CHANNEL f1 =====
 SFO1 400.1324710 MHz
 NUC1 1H
 P1 14.50 usec
 PLW1 11.99499989 W

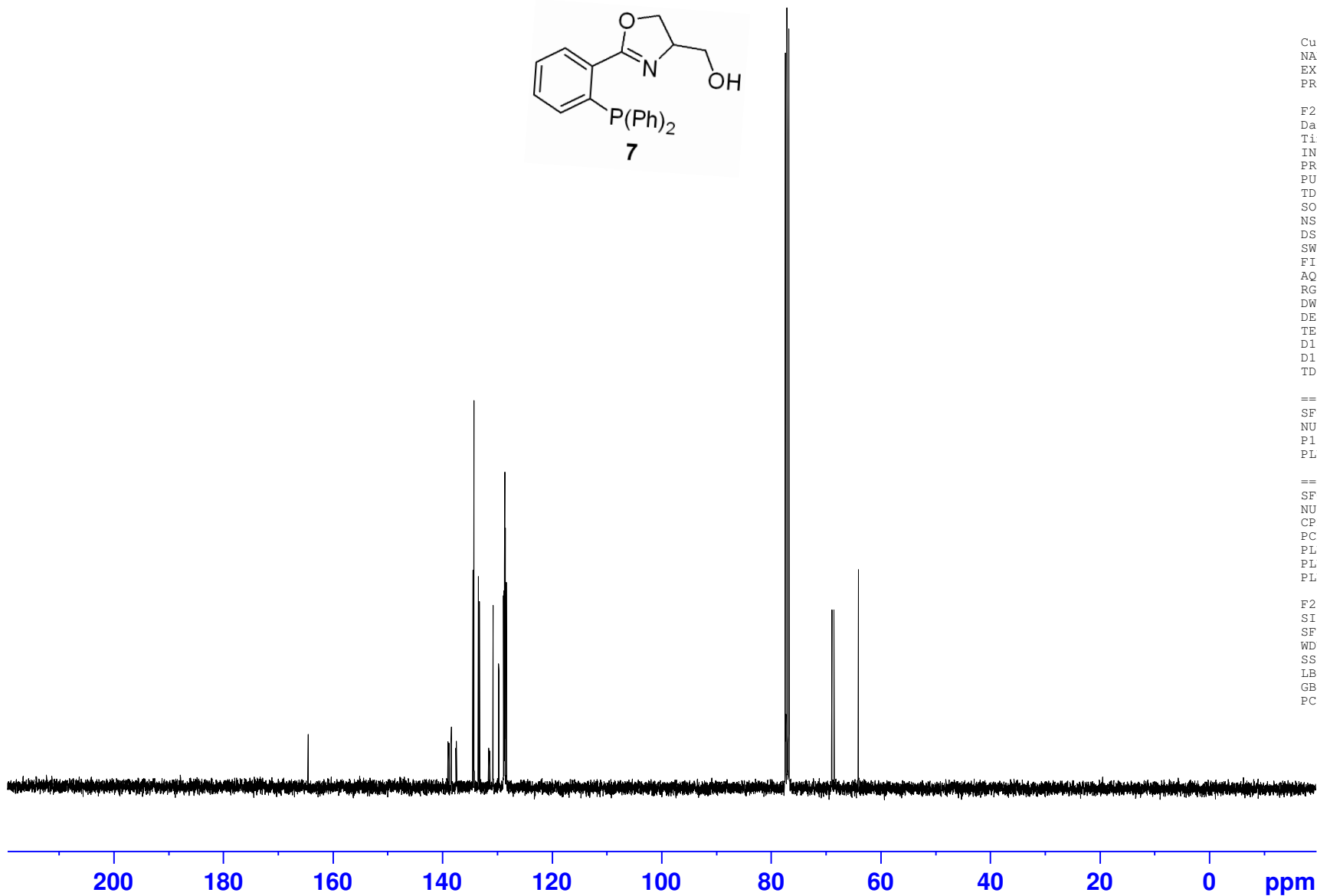
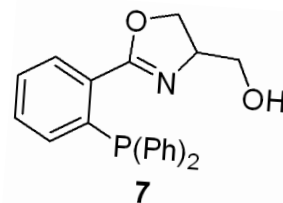
F2 - Processing parameters
 SI 65536
 SF 400.1300103 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

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164.45
164.43
138.92
138.70
138.35
138.28
137.46
137.37
134.39
134.18
133.39
133.19
131.51
131.31
130.70
129.67
129.64
128.79
128.66
128.57
128.50
128.26

77.32
77.20
77.00
76.68
68.83
68.43
63.98



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Current Data Parameters
NAME hh-2-160-c-fr1
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20181228
Time 21.23
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 100
DS 0
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 196.92
DW 20.800 usec
DE 6.50 usec
TE 296.5 K
D1 2.0000000 sec
D11 0.0300000 sec
TDO 1

==== CHANNEL f1 =====
SFO1 100.6228298 MHz
NUC1 13C
P1 9.70 usec
PLW1 46.98899841 W

==== CHANNEL f2 =====
SFO2 400.1316005 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 90.00 usec
PLW2 11.99499989 W
PLW12 0.34213999 W
PLW13 0.27713001 W

F2 - Processing parameters
SI 32768
SF 100.6127766 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



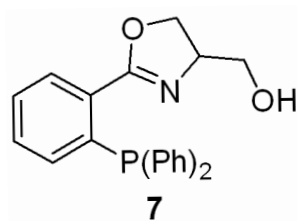
Current Data Parameters
NAME hh-2-160-p-frl
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20181229
Time 13.28
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 1
DS 0
SWH 64102.563 Hz
FIDRES 0.978127 Hz
AQ 0.5111808 sec
RG 196.92
DW 7.800 usec
DE 6.50 usec
TE 295.4 K
D1 2.0000000 sec
D11 0.0300000 sec
TD0 1

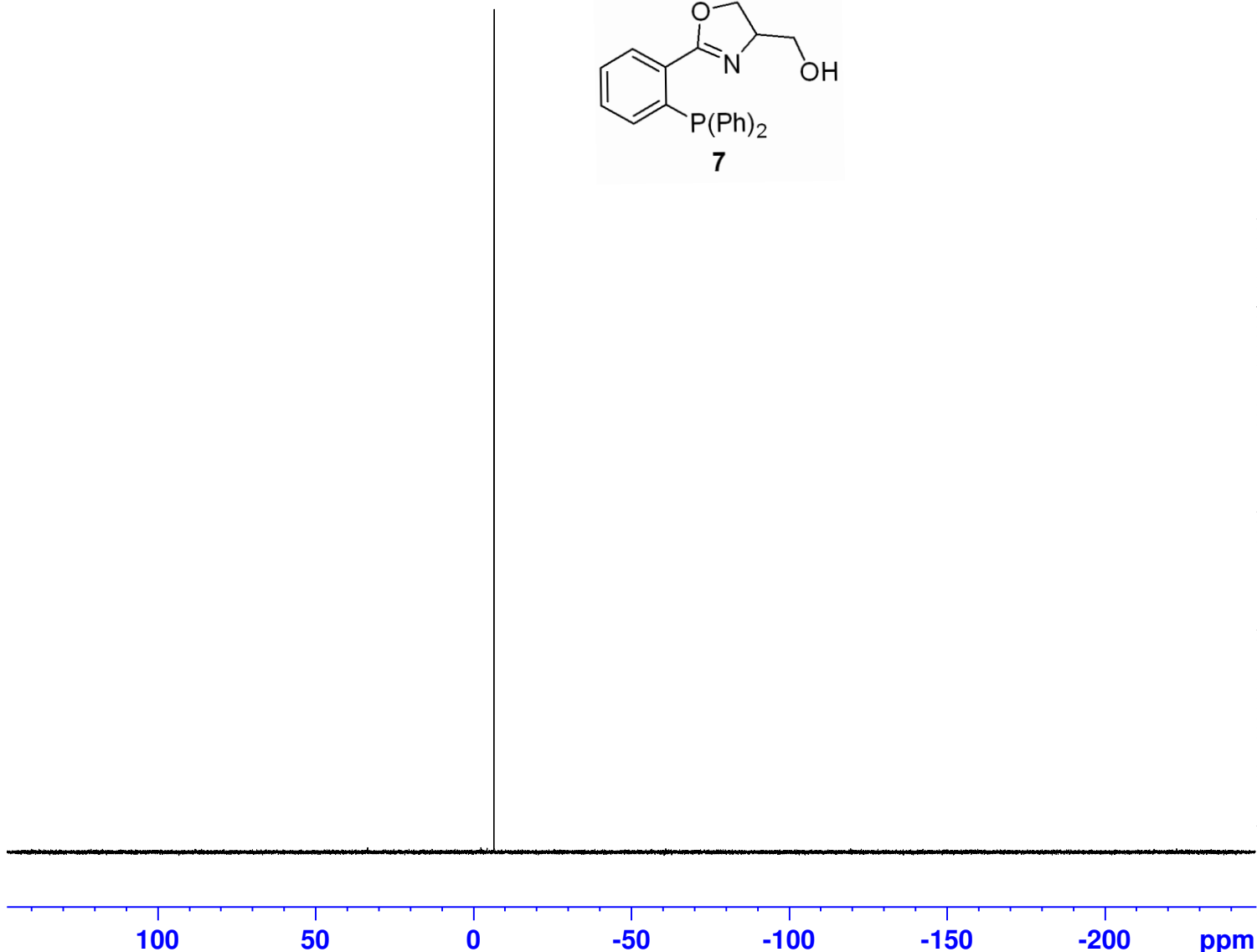
=====
CHANNEL f1
SFO1 161.9674942 MHz
NUC1 31P
P1 14.70 usec
PLW1 11.99499989 W

=====
CHANNEL f2
SFO2 400.1316005 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 90.00 usec
PLW2 11.99499989 W
PLW12 0.34213999 W
PLW13 0.27713001 W

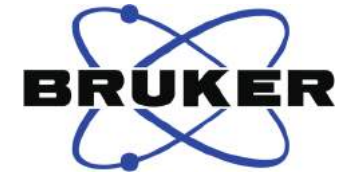
F2 - Processing parameters
SI 32768
SF 161.9755930 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



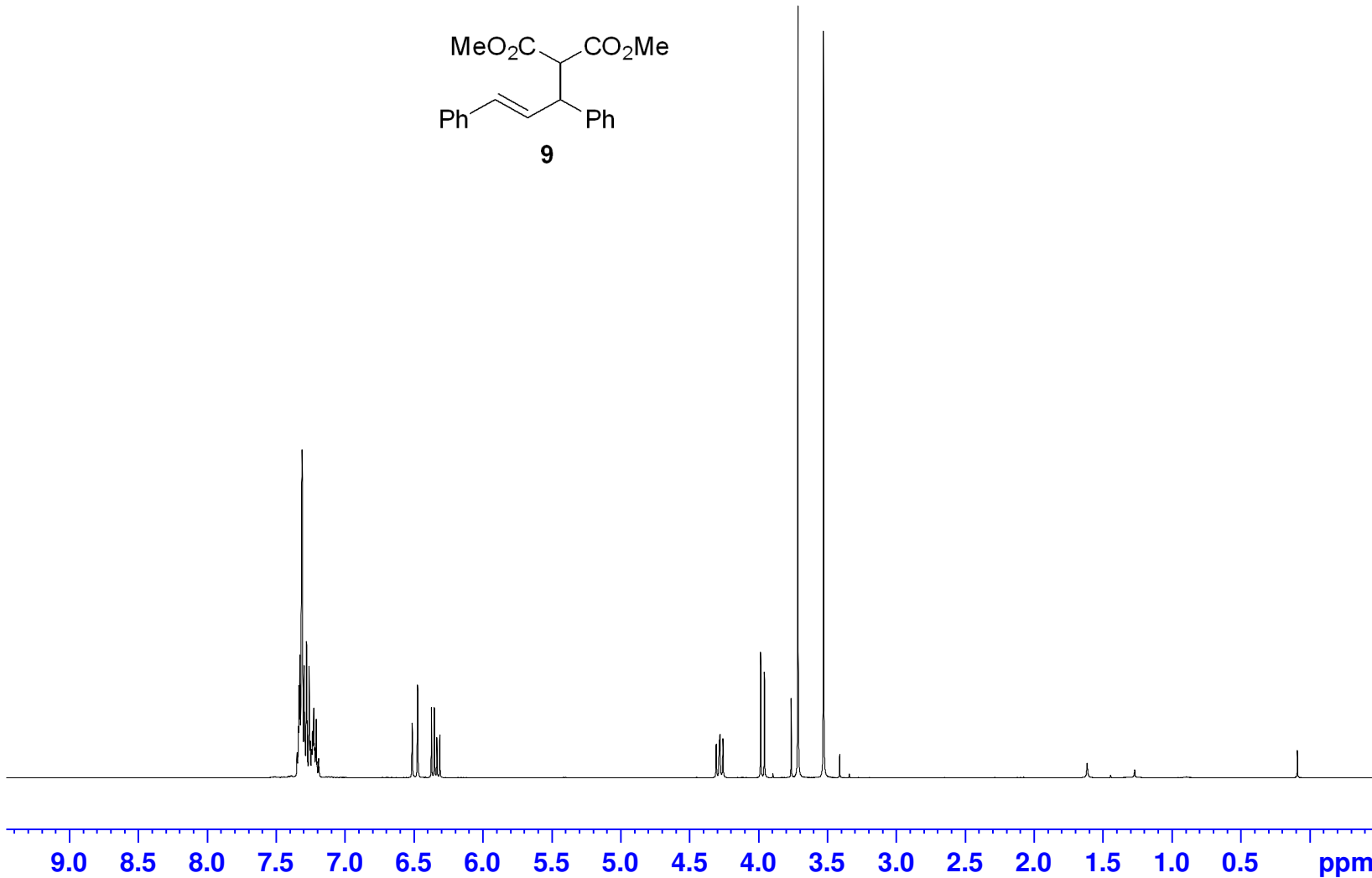
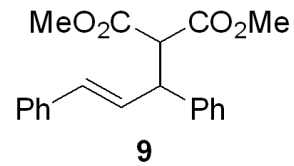
-6.59



S-194



7.310
7.308
7.295
7.286
7.278
7.274
7.260
7.251
7.241
7.239
7.234
7.229
7.225
7.221
7.218
7.213
7.207
7.190
6.511
6.472
6.372
6.350
6.332
6.311
4.283
4.277
4.256
3.982
3.955
3.761
3.712
3.526



Current Data Parameters
NAME hh-2-185-h-fr1
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20190109
Time 16.08
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT CDC13
NS 6
DS 0
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 70.97
DW 62.400 usec
DE 6.50 usec
TE 295.4 K
D1 1.00000000 sec
TD0 1

==== CHANNEL f1 =====
SFO1 400.1324710 MHz
NUC1 1H
P1 14.50 usec
PLW1 11.99499989 W

F2 - Processing parameters
SI 65536
SF 400.1300102 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

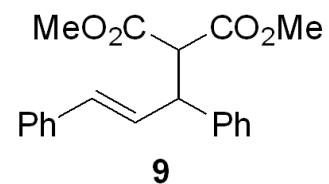


168.16
167.74

140.12
136.77
131.79
129.06
128.69
128.44
127.83
127.54
127.13
126.35

77.31
77.00
76.68

57.60
52.60
52.42
49.16



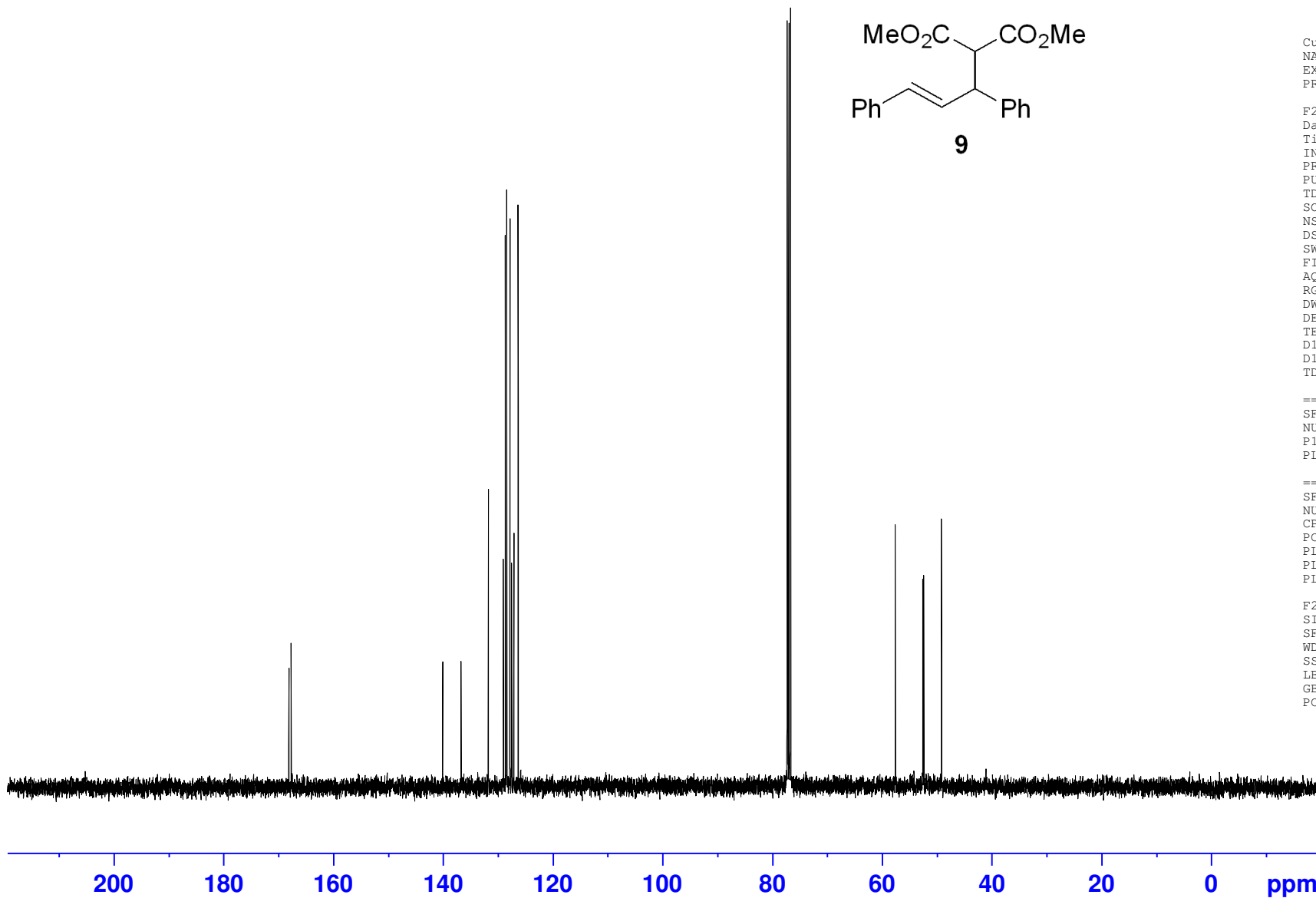
Current Data Parameters
NAME hh-2-185-c-fr1
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20190109
Time 20.11
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 66
DS 0
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 196.92
DW 20.800 usec
DE 6.50 usec
TE 296.1 K
D1 2.0000000 sec
D11 0.0300000 sec
TDO 1

==== CHANNEL f1 =====
SFO1 100.6228298 MHz
NUC1 13C
P1 9.70 usec
PLW1 46.98899841 W

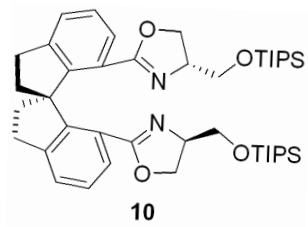
==== CHANNEL f2 =====
SFO2 400.1316005 MHz
NUC2 1H
PCPD2 waltz16
PCPD2 90.00 usec
PLW2 11.99499989 W
PLW12 0.34213999 W
PLW13 0.27713001 W

F2 - Processing parameters
SI 32768
SF 100.6127758 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40





7.520
7.503
7.333
7.314
7.260
7.144
7.126
7.107
3.960
3.834
3.824
3.810
3.800
3.753
3.731
3.720
3.709
3.698
3.687
3.331
3.308
3.285
3.263
3.244
3.081
3.069
3.049
3.042
3.022
2.992
2.970
2.953
2.931
2.695
2.668
2.644
2.617
2.260
2.242
2.231
2.212
1.027

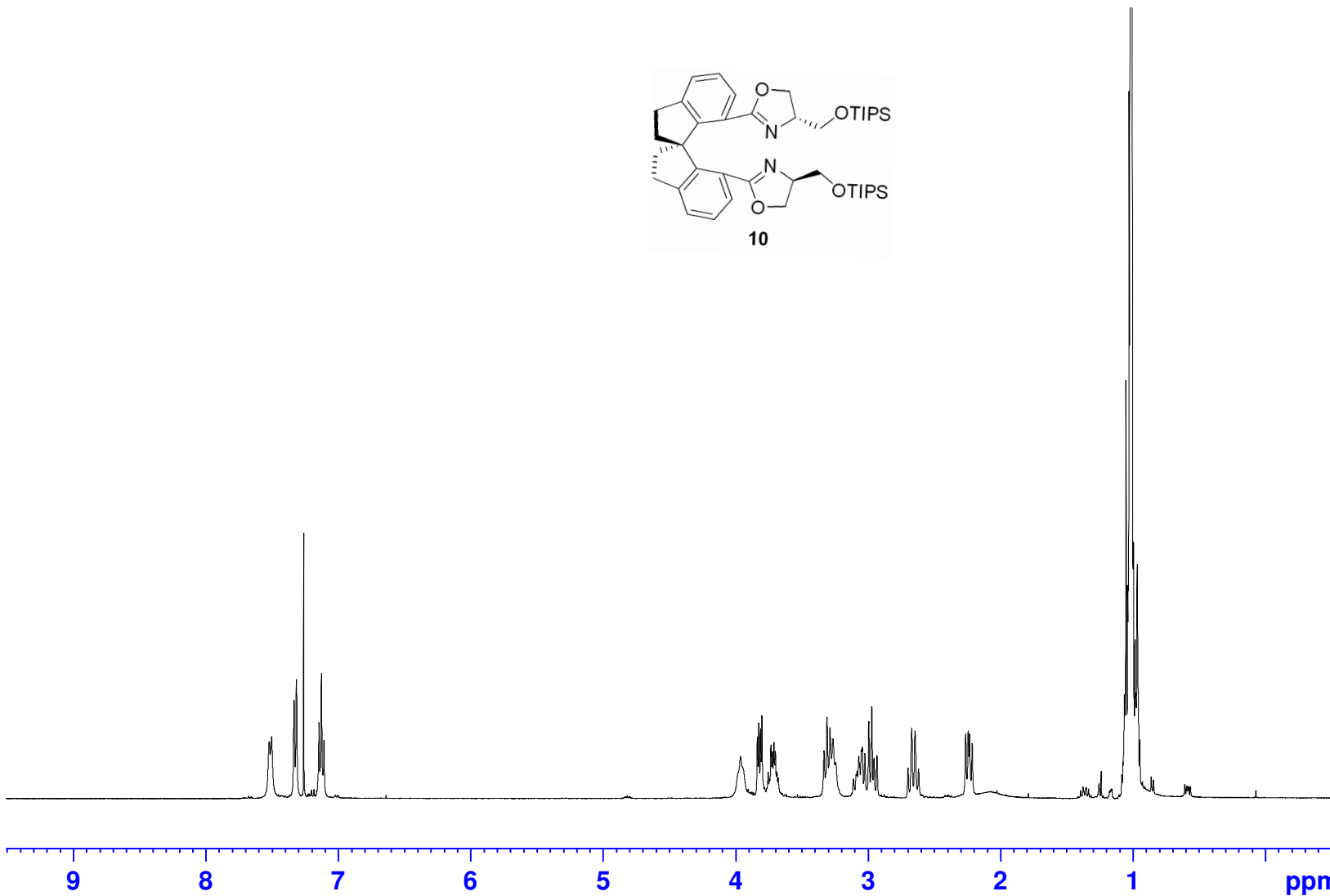


Current Data Parameters
NAME hh-3-38-h-fr1
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20190215
Time 19.59
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT CDC13
NS 6
DS 0
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 82.92
DW 62.400 usec
DE 6.50 usec
TE 296.2 K
D1 1.00000000 sec
TD0 1

==== CHANNEL f1 =====
SFO1 400.1324710 MHz
NUC1 1H
P1 14.50 usec
PLW1 11.99499989 W

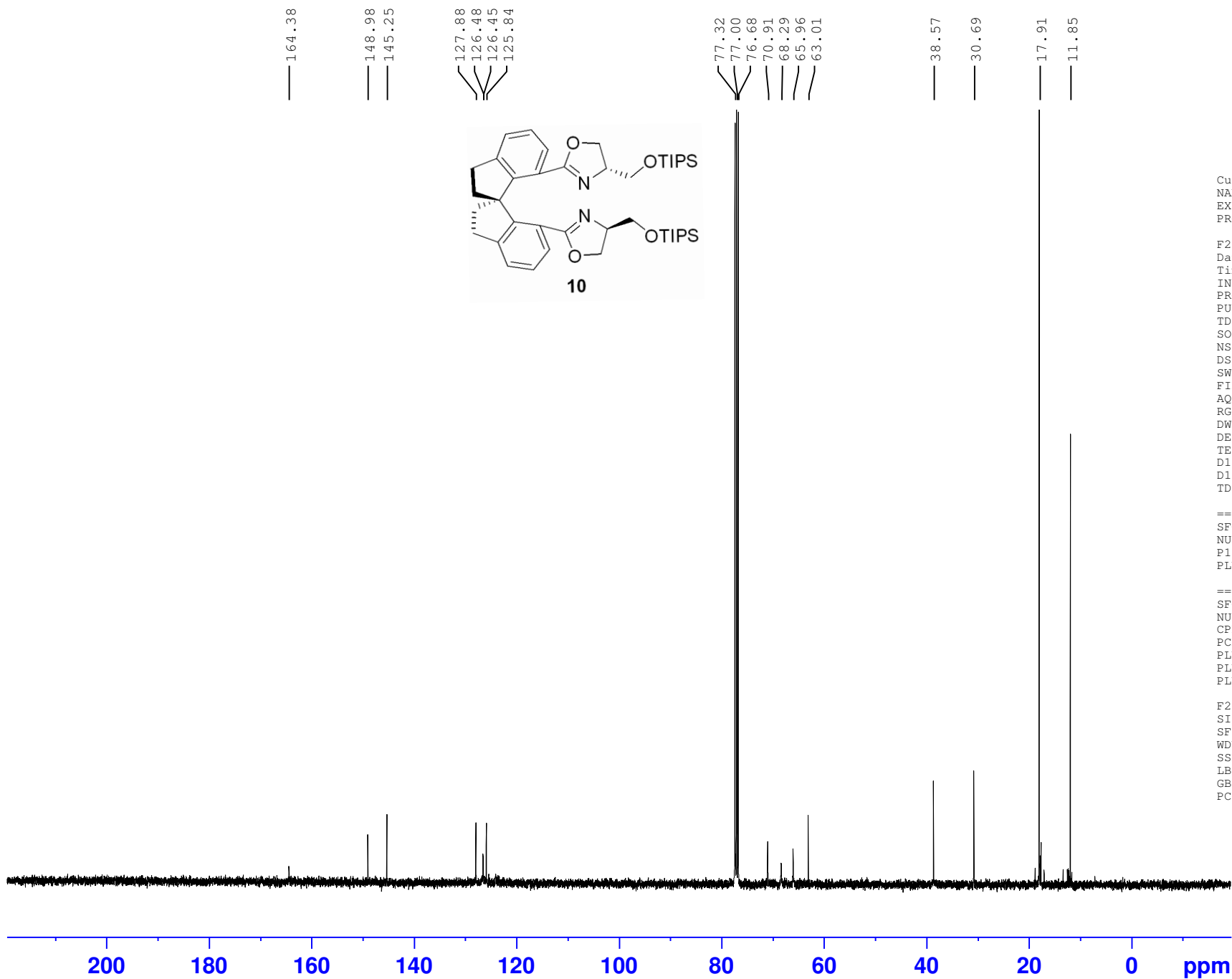
F2 - Processing parameters
SI 65536
SF 400.1300102 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



1.77
1.94
1.94

1.75
1.89
2.09
3.68
4.14
2.00
2.04

42.87



Current Data Parameters
NAME hh-3-38-c-fr1
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20190216
Time 12.50
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 426
DS 0
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 196.92
DW 20.800 usec
DE 6.50 usec
TE 297.5 K
D1 2.0000000 sec
D11 0.0300000 sec
TDO 1

=====
CHANNEL f1
SFO1 100.6228298 MHz
NUC1 13C
P1 9.70 usec
PLW1 46.98899841 W

=====
CHANNEL f2
SFO2 400.1316005 MHz
NUC2 1H
PCPD2 waltz16
PLW2 90.00 usec
PLW12 11.99499989 W
PLW13 0.34213999 W
PLW13 0.27713001 W

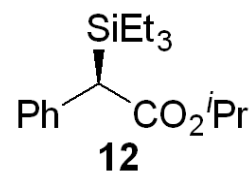
F2 - Processing parameters
SI 32768
SF 100.6127714 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

7.369
7.366
7.348
7.346
7.288
7.283
7.269
7.258
7.249
7.176
7.158
7.140

5.044
5.028
5.013
4.997
4.981

— 3.478

1.282
1.267
1.240
1.224
0.931
0.911
0.892
0.626
0.622
0.608
0.602
0.588
0.582

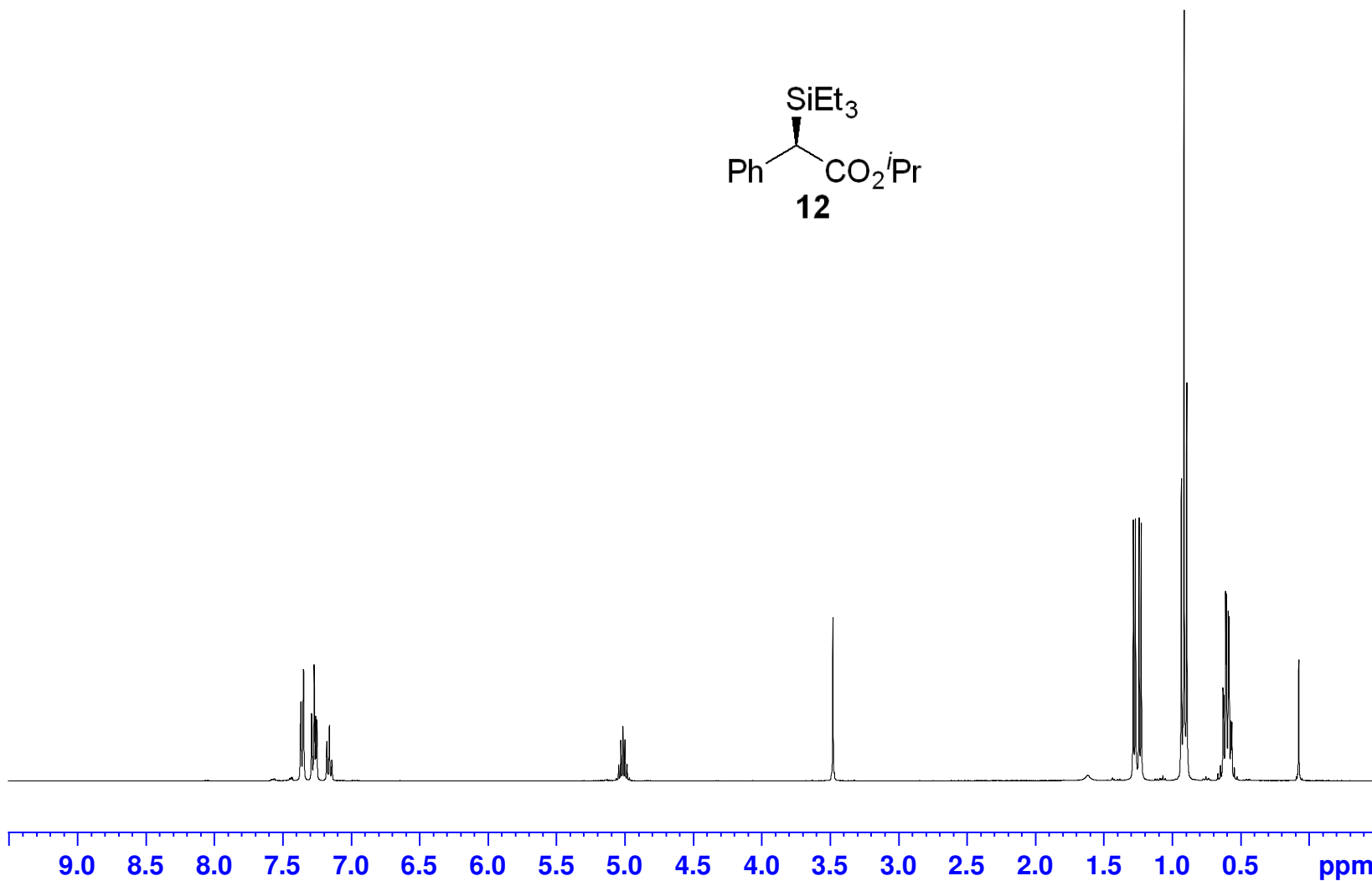


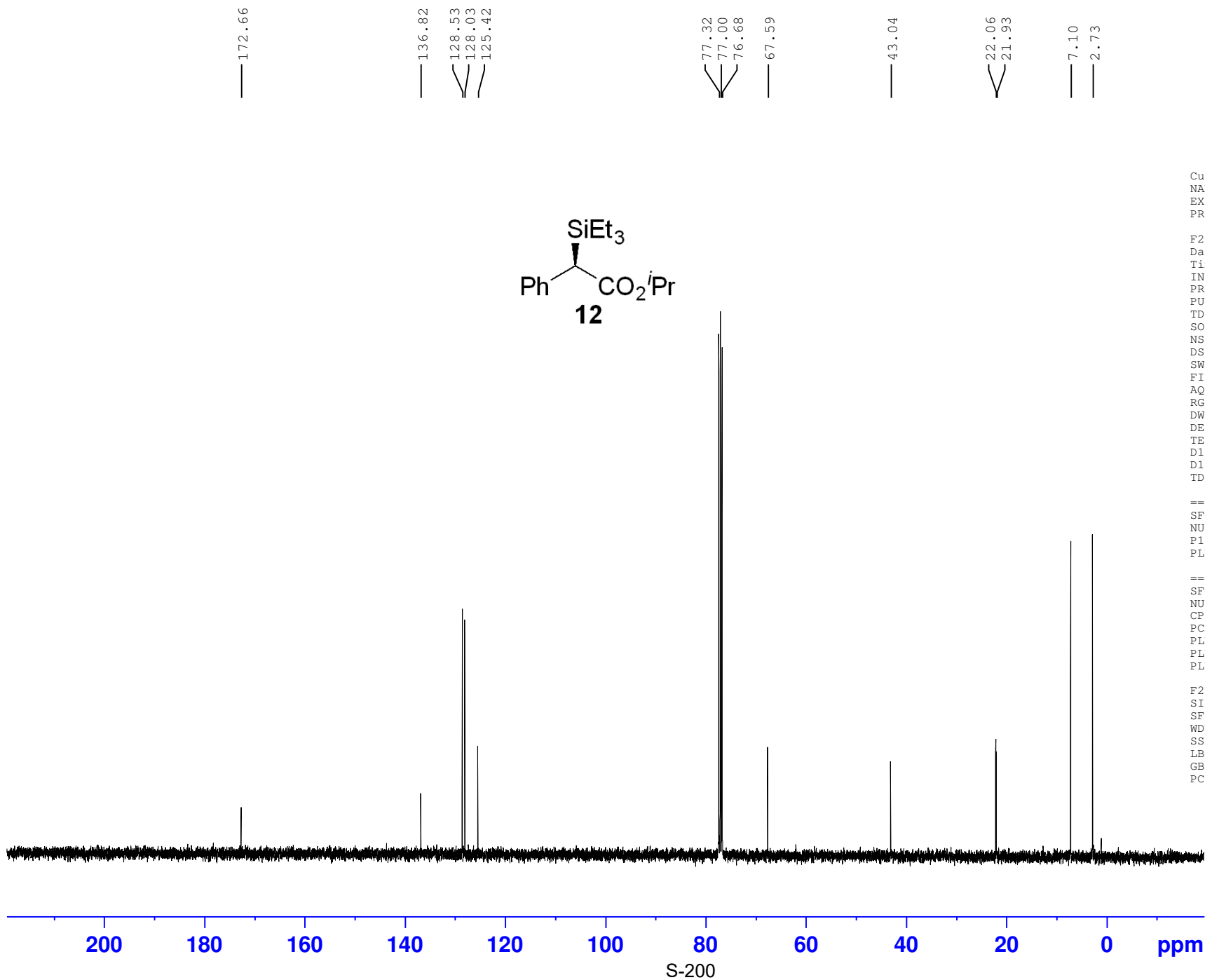
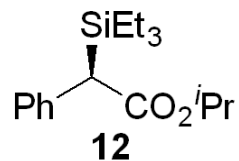
Current Data Parameters
NAME hh-3-97B-h-fr1
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20190413
Time 19.11
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 4
DS 0
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 70.97
DW 62.400 usec
DE 6.50 usec
TE 297.8 K
D1 1.00000000 sec
TD0 1

==== CHANNEL f1 =====
SFO1 400.1324710 MHz
NUC1 1H
P1 14.50 usec
PLW1 11.99499989 W

F2 - Processing parameters
SI 65536
SF 400.1300109 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00





Current Data Parameters
NAME hh-3-97B-c-fr1
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20190413
Time 19.15
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 63
DS 0
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 196.92
DW 20.800 usec
DE 6.50 usec
TE 298.7 K
D1 2.0000000 sec
D11 0.0300000 sec
TD0 1

==== CHANNEL f1 =====
SFO1 100.6228298 MHz
NUC1 13C
P1 9.70 usec
PLW1 46.98899841 W

==== CHANNEL f2 =====
SFO2 400.1316005 MHz
NUC2 1H
PCPDG[2] waltz16
PCPD2 90.00 usec
PLW2 11.99499989 W
PLW12 0.34213999 W
PLW13 0.27713001 W

F2 - Processing parameters
SI 32768
SF 100.6127715 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



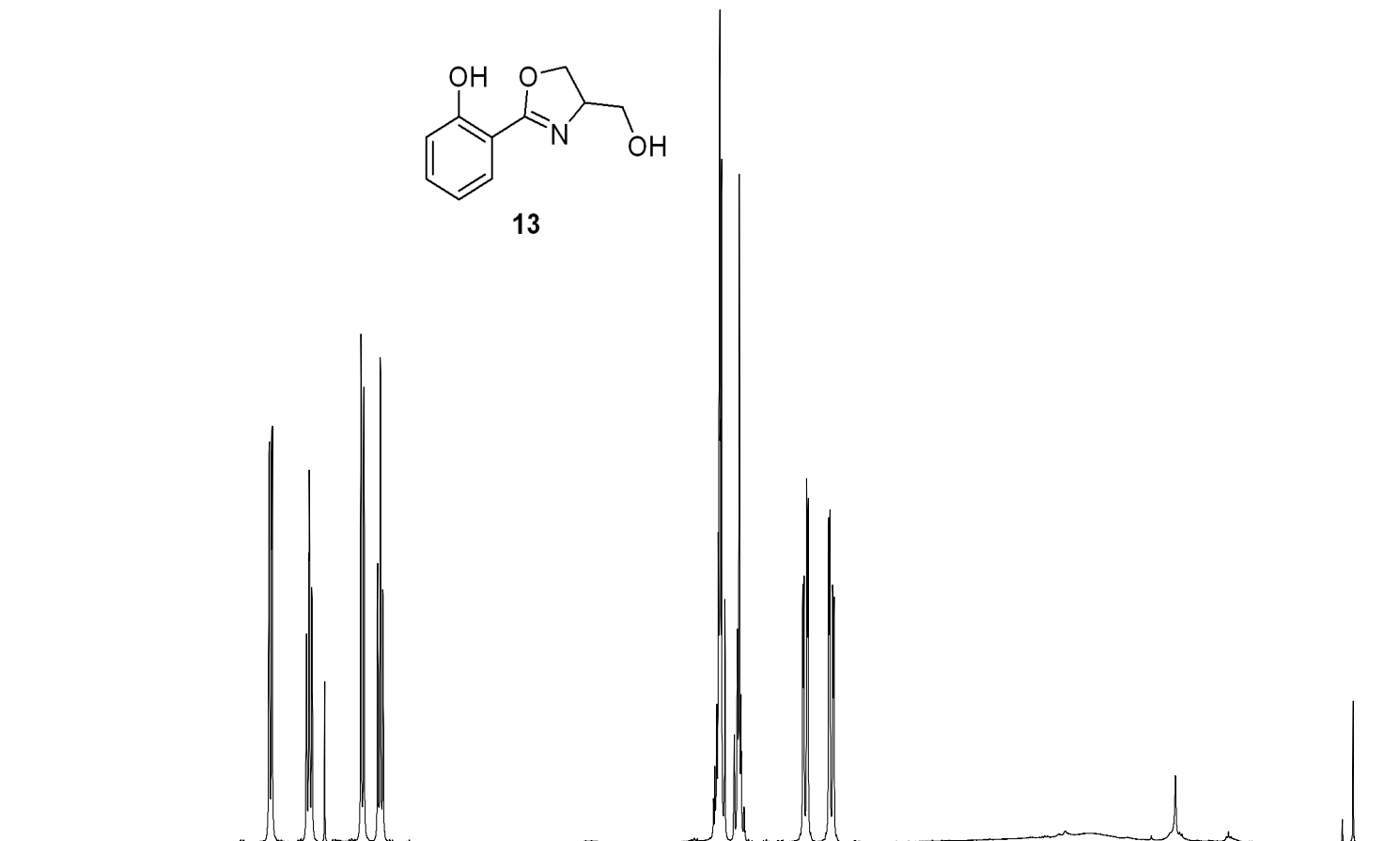
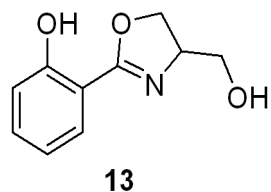
Current Data Parameters
NAME hh-1-6-h-frl
EXPNO 7
PROCNO 1

F2 - Acquisition Parameters
Date_ 20190624
Time 8.49
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 8
DS 2
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 2.0447233 sec
RG 100.49
DW 62.400 usec
DE 6.50 usec
TE 295.4 K
D1 1.00000000 sec
TD0 1

==== CHANNEL f1 =====
NUC1 1H
P1 9.90 usec
PLW1 23.00000000 W
SFO1 400.1932015 MHz

F2 - Processing parameters
SI 65536
SF 400.1900151 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 0.50

7.66
7.65
7.64
7.63
7.39
7.39
7.37
7.37
7.37
7.35
7.26
7.01
7.00
6.98
6.89
6.89
6.87
6.85
6.85
4.49
4.48
4.48
4.47
4.46
4.44
4.44
4.37
4.35
4.34
4.33
4.32
4.32
3.89
3.88
3.86
3.85
3.85
3.70
3.70
3.69
3.67
3.66



9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 ppm

1.00
1.02
1.01
1.03

2.14
1.07
1.08
1.07



Current Data Parameters
NAME hh-1-6-c-frl
EXPNO 8
PROCNO 1

F2 - Acquisition Parameters
Date_ 20190624
Time 8.54
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 31
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 193.13
DW 20.800 usec
DE 6.50 usec
TE 295.8 K
D1 2.0000000 sec
D11 0.0300000 sec
TD0 1

=====
CHANNEL f1
NUC1 13C
P1 9.90 usec
PLW1 53.0000000 W
SFO1 100.6379178 MHz

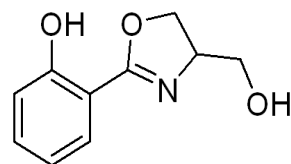
=====
CHANNEL f2
CPDPRG[2] waltz16
NUC2 1H
PCPD2 90.00 usec
PLW2 14.0000000 W
PLW12 0.35839999 W
PLW13 0.29030001 W
SFO2 400.1916008 MHz

F2 - Processing parameters
SI 32768
SF 100.6278646 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

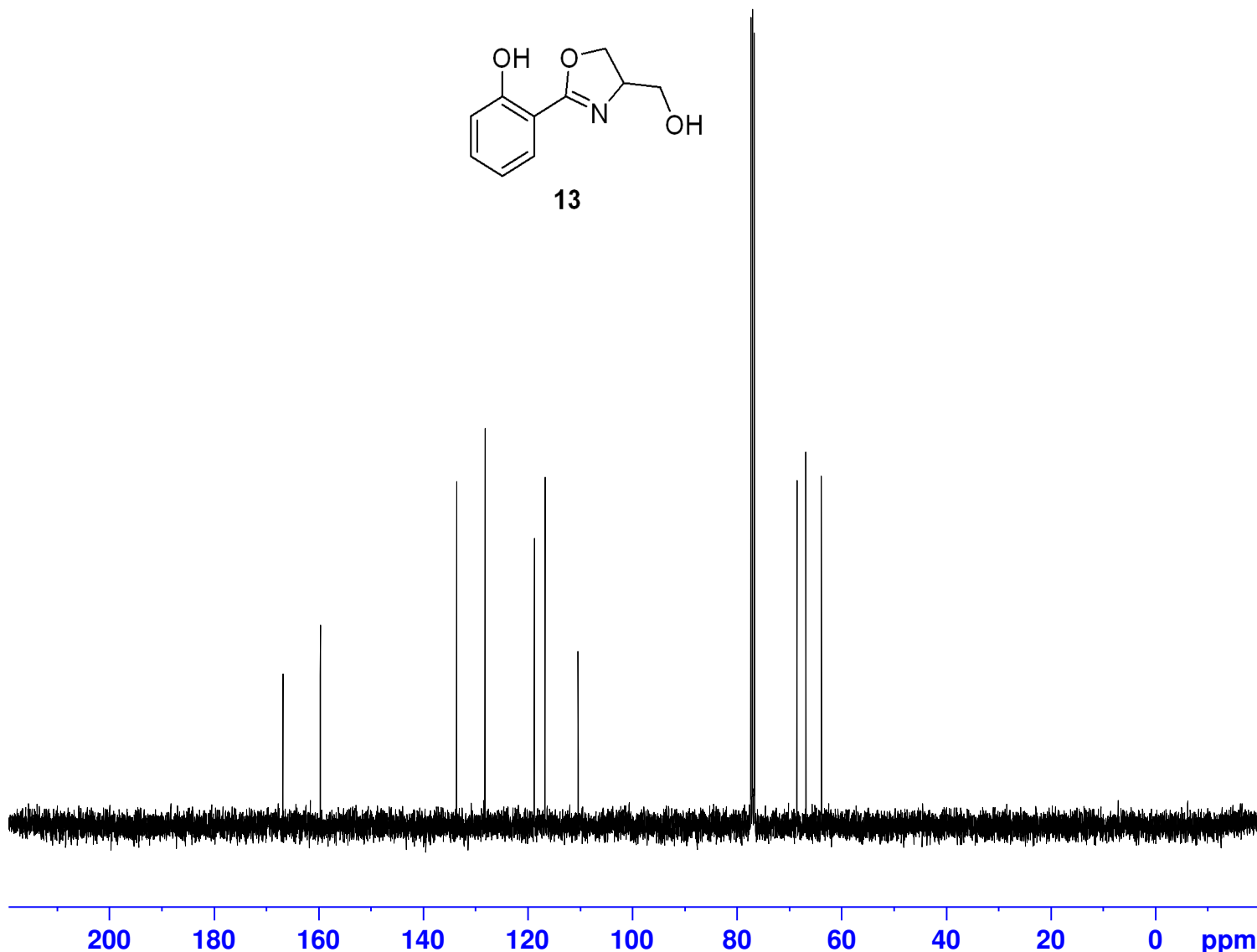
166.81
159.68

133.59
128.15
118.76
116.66
110.36

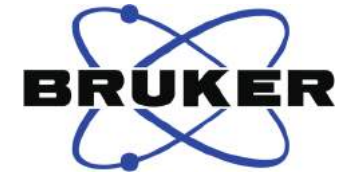
77.32
77.00
76.68
68.52
66.83
63.88



13



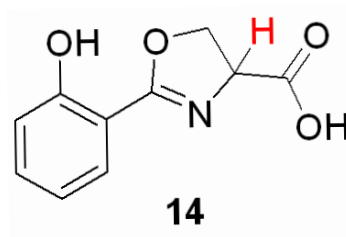
S-202



7.893
7.682
7.663
7.414
7.395
7.377
6.963
6.943
6.903
6.884
6.866

4.980
4.650
4.639

3.310



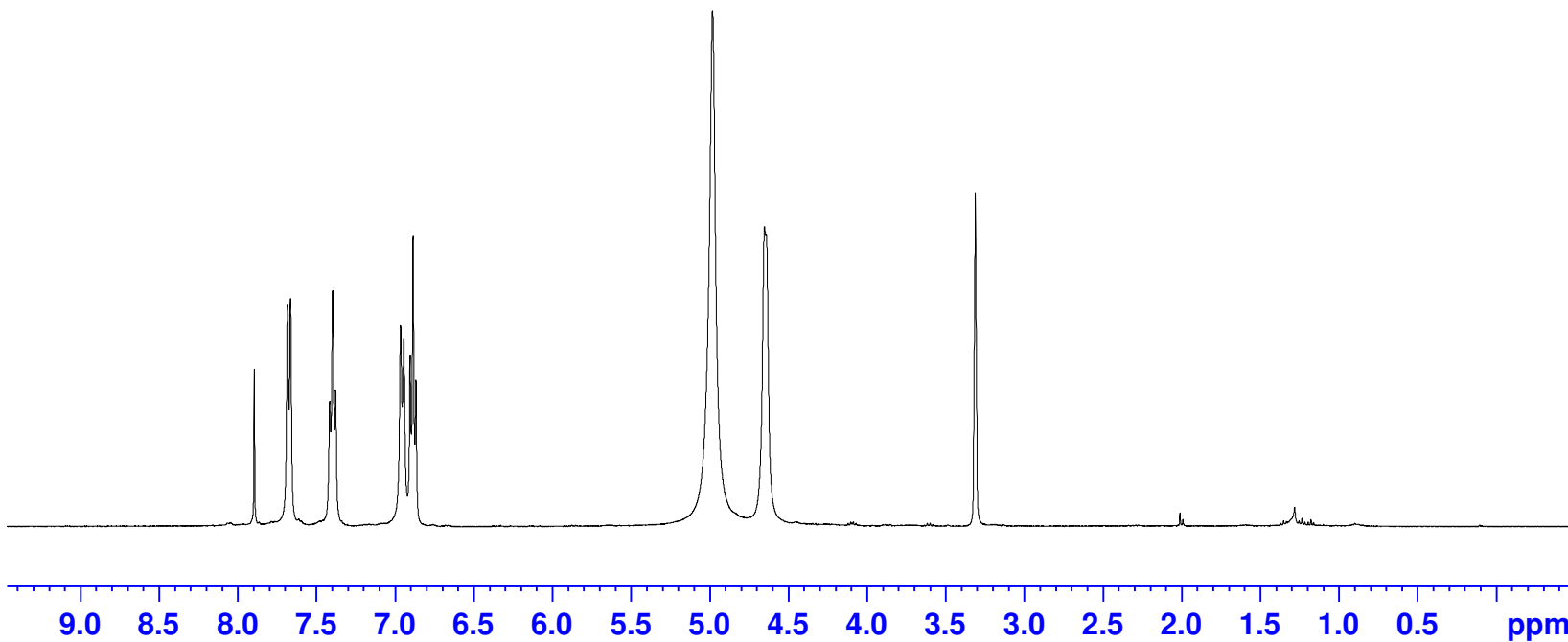
Current Data Parameters
NAME hh-3-151-h-fr1
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20190705
Time 14.45
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT MeOD
NS 6
DS 0
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 112.31
DW 62.400 usec
DE 6.50 usec
TE 295.0 K
D1 1.00000000 sec
TD0 1

==== CHANNEL f1 =====
SFO1 400.1324710 MHz
NUC1 1H
P1 14.50 usec
PLW1 11.99499989 W

F2 - Processing parameters
SI 65536
SF 400.1300082 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

H₂O & H





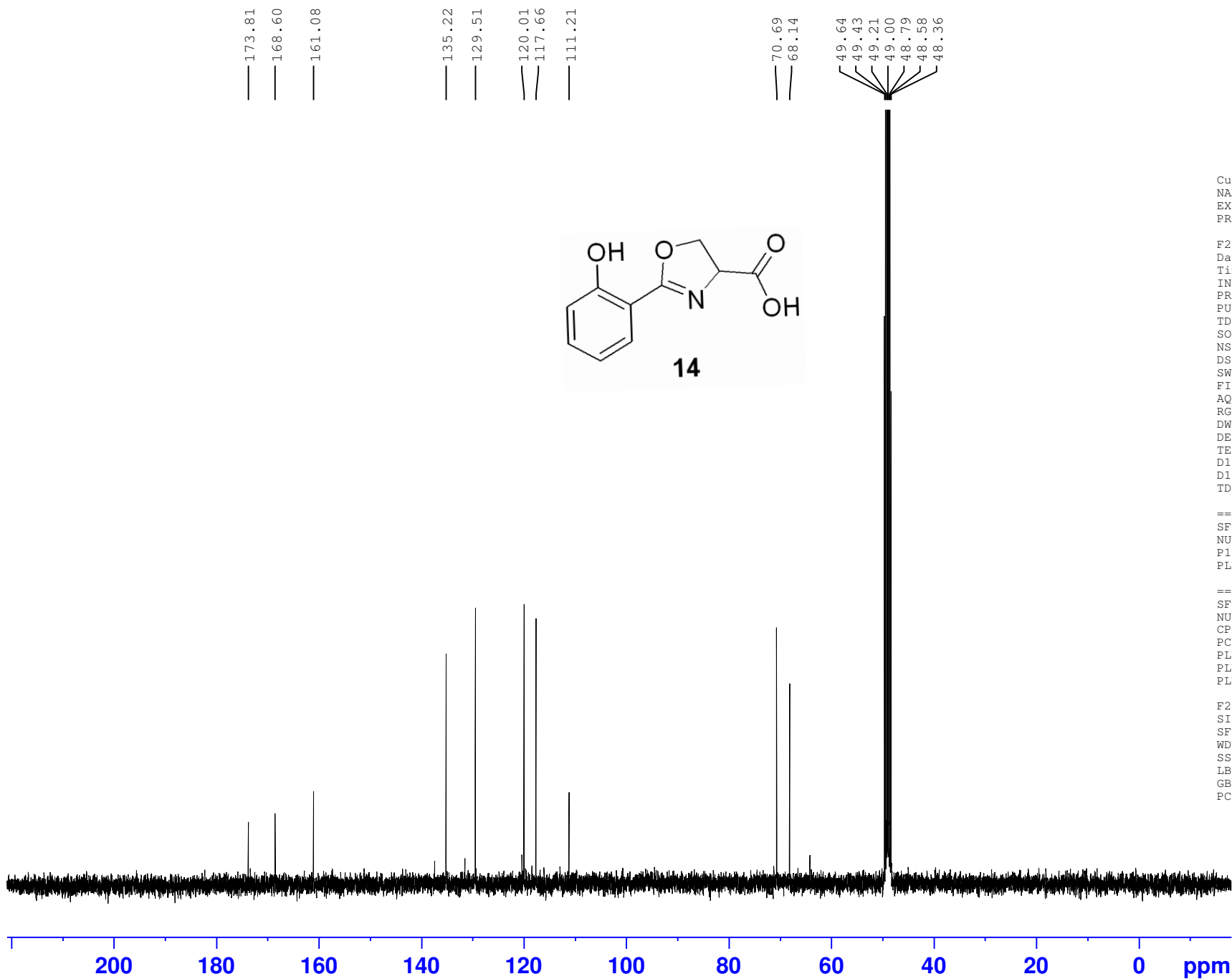
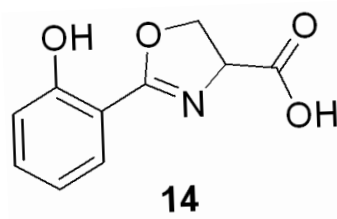
Current Data Parameters
NAME hh-3-151-c-crude
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20190708
Time 20.29
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT MeOD
NS 231
DS 0
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 196.92
DW 20.800 usec
DE 6.50 usec
TE 296.3 K
D1 2.0000000 sec
D11 0.03000000 sec
TD0 1

=====
CHANNEL f1
SFO1 100.6228298 MHz
NUC1 13C
P1 9.70 usec
PLW1 46.98899841 W

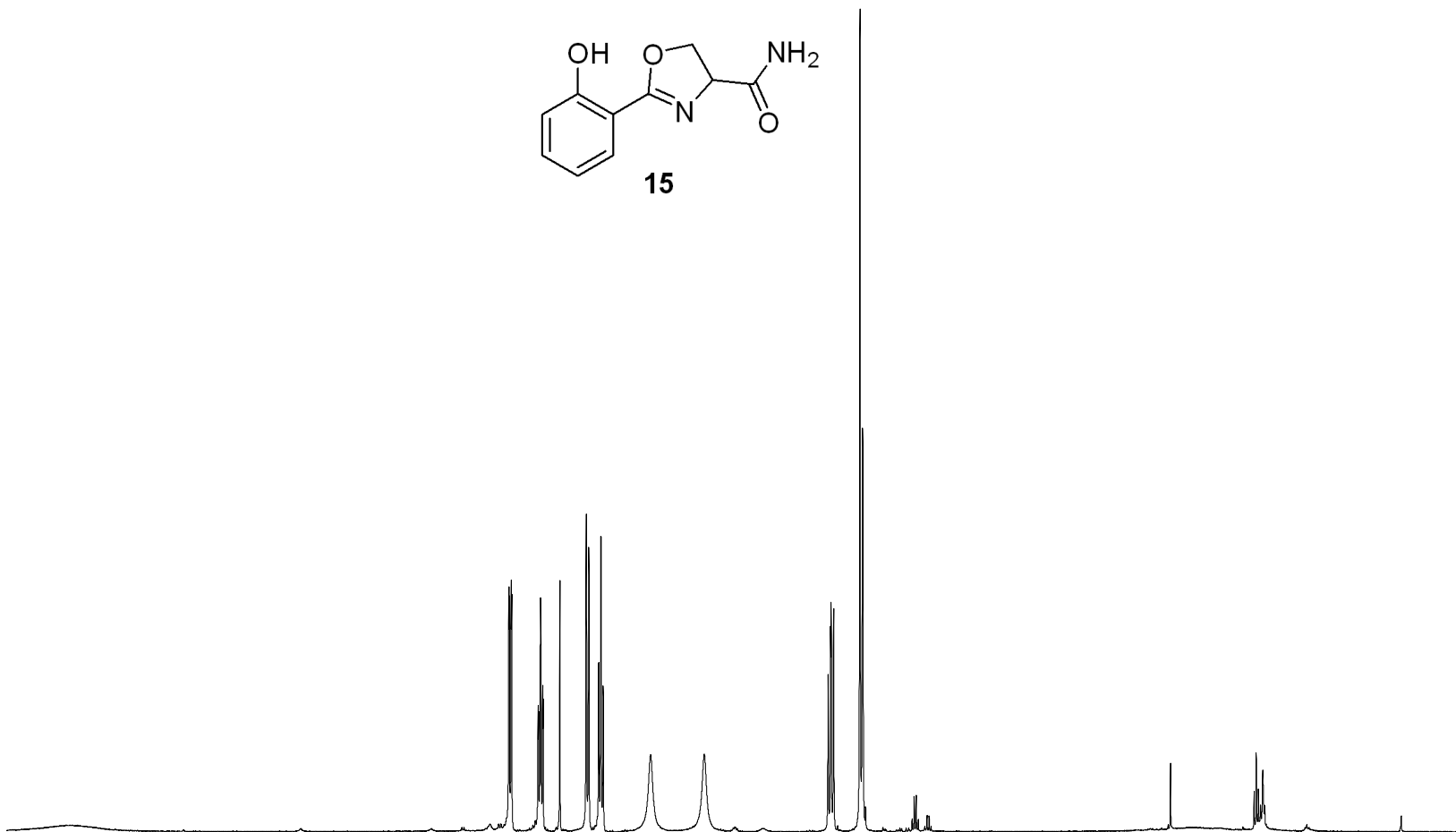
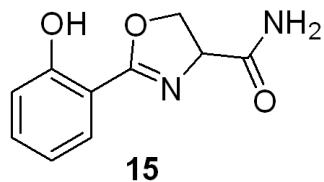
=====
CHANNEL f2
SFO2 400.1316005 MHz
NUC2 1H
PCPD2 waltz16
PLW2 90.00 usec
PLW12 11.99499989 W
PLW13 0.34213999 W
PLW13 0.27713001 W

F2 - Processing parameters
SI 32768
SF 100.6126285 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



— 11.457

7.696
7.692
7.676
7.672
7.446
7.442
7.425
7.407
7.403
7.260
7.034
7.013
6.928
6.926
6.908
6.890
6.483
6.025
4.966
4.945
4.940
4.919
4.694
4.672
4.669



11 10 9 8 7 6 5 4 3 2 1 ppm

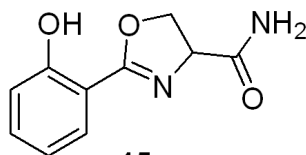
0.84
1.06
1.04
1.03
1.03
0.91
0.90
1.00
2.00

Current Data Parameters
NAME hh-3-161-h-fr1
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20190711
Time 19.09
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT CDC13
NS 4
DS 0
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 142.88
DW 62.400 usec
DE 6.50 usec
TE 295.2 K
D1 1.00000000 sec
TD0 1

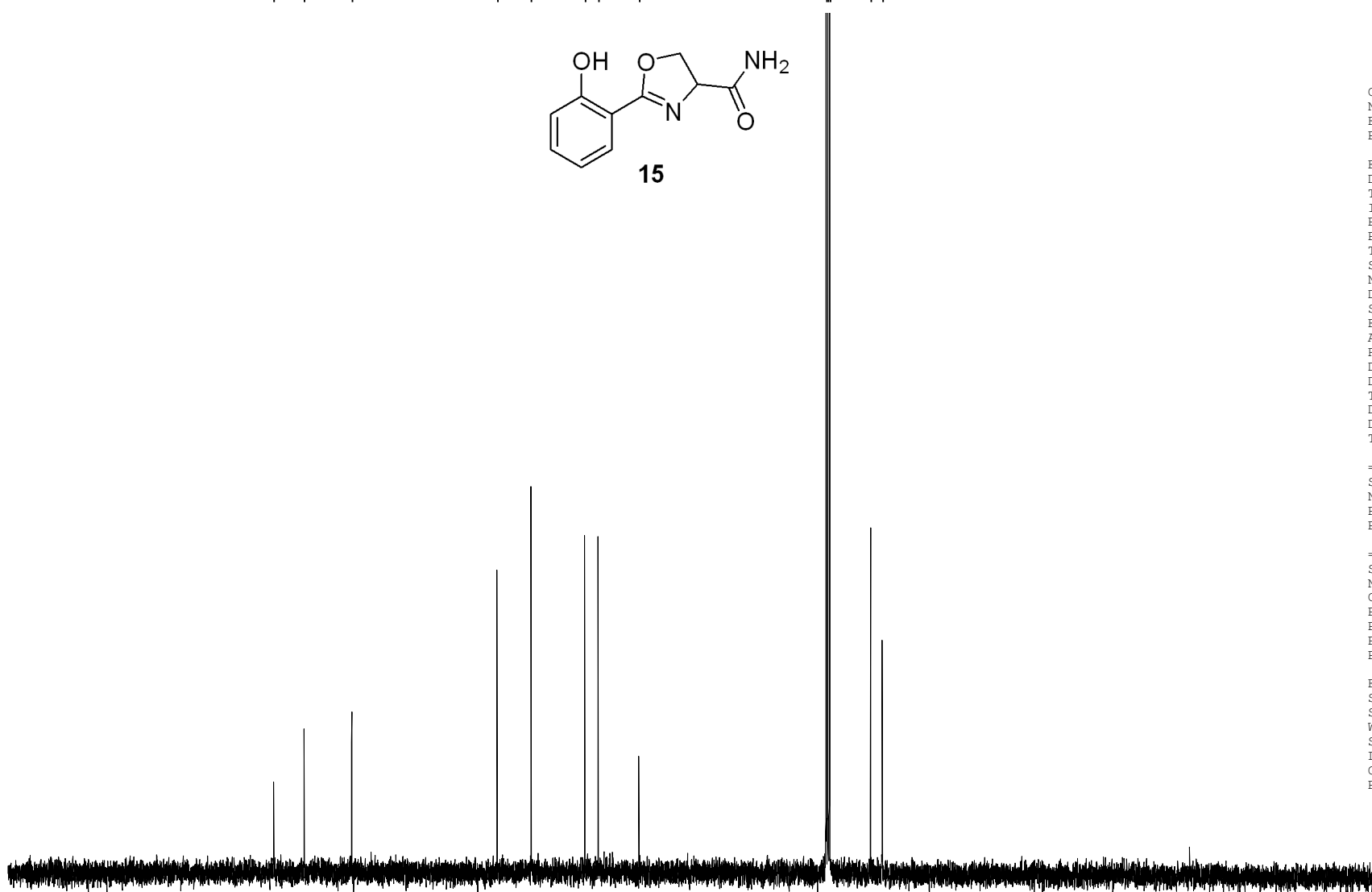
==== CHANNEL f1 =====
SFO1 400.1324710 MHz
NUC1 1H
P1 14.50 usec
PLW1 11.99499989 W

F2 - Processing parameters
SI 65536
SF 400.1300102 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



15

173.23
167.96
159.68
134.44
128.56
119.22
116.90
109.81
77.32
77.00
76.68
69.58
67.56



Current Data Parameters
NAME hh-3-161-c-fr1
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20190711
Time 19.19
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 150
DS 0
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 196.92
DW 20.800 usec
DE 6.50 usec
TE 296.3 K
D1 2.0000000 sec
D11 0.0300000 sec
TD0 1

==== CHANNEL f1 =====
SFO1 100.6228298 MHz
NUC1 13C
P1 9.70 usec
PLW1 46.98899841 W

==== CHANNEL f2 =====
SFO2 400.1316005 MHz
NUC2 1H
PCPDG[2] waltz16
PCPD2 90.00 usec
PLW2 11.99499989 W
PLW12 0.34213999 W
PLW13 0.27713001 W

F2 - Processing parameters
SI 32768
SF 100.6127736 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

200 180 160 140 120 100 80 60 40 20 0 ppm

S-206