Supporting Information

Ruthenium-Catalyzed Cycloisomerization of 2-Alkynylanilides: Synthesis of 3-Substituted Indoles by 1,2-Carbon Migration

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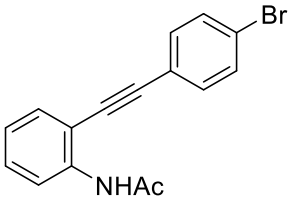
Contents

1. General Information

Reagents were commercially available and used without further purification unless otherwise noted. Chemical shifts were reported in delta units (δ) relative to residual $CHCl_3$ (7.24 ppm) for ^1H NMR, $CDCl_3$ (77.23 ppm) for ^{13}C NMR, and external H_3PO_4 (0.0 ppm) for $^{31}P\{^1H\}$ NMR. All reactions were carried out under an argon atmosphere. All solvents were anhydrous. Chlorobenzene was degassed by three freeze-pump-thaw cycles and stored under an argon atmosphere. [CpRuCl(dppe)],[1] [CpRuCl(dppbz)],[2] [IndRuCl(dppe)],[3] [CpRuCl(PPh_3)$_2$],[4] $NaBAr^F{}_4 \cdot 3H_2O$,[5] and **1o**[6] were prepared as described in the literature.

2.1 Synthesis of Substrates 1



***N*-(2-((4-Bromophenyl)ethynyl)phenyl)acetamide (1e)**

N-(2-Ethynylphenyl)acetamide[7] (0.478 g, 3.00 mmol), 1-bromo-4-iodobenzene (1.02 g, 3.60 mmol), [$PdCl_2(PPh_3)_2$] (0.0421 g, 0.06 mmol), and CuI (0.0230 g, 0.12 mmol) were dissolved in THF (12 mL). After addition of NEt_3 (0.50 mL, 3.6 mmol), the reaction mixture was allowed to stir at room temperature for 3.5 h. The resulting mixture was filtered through Celite and evaporated *in vacuo*. The crude product was purified by flash column chromatography over silica gel (hexane / methylene chloride 1:3) to give **1e** as a colorless solid. Yield: 0.271 g (0.862 mmol, 29%).

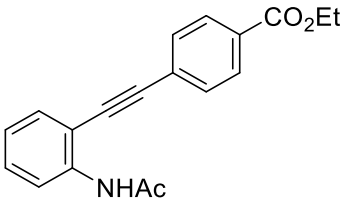
mp 201.0–202.0 °C.

IR (ATR): 3106, 3049, 1706, 1605, 1582, 1567, 1558, 1488, 1450, 1384, 1350, 1331, 1300, 1273, 1226, 1186, 1156, 1141, 1069 cm^{-1}.

^1H NMR (300 MHz, $CDCl_3$): δ 8.38 (d, *J* = 7.9 Hz, 1H), 7.87 (s, 1H), 7.51 (d, *J* = 8.7 Hz, 2H), 7.47 (dd, *J* = 7.7, 1.3 Hz, 1H), 7.41–7.30 (m, 3H), 7.06 (t, *J* = 7.7 Hz, 1H), 2.22 (s, 3H).

^{13}C NMR (76 MHz, $CDCl_3$): δ 168.3, 139.1, 133.1, 132.1, 132.0, 130.3, 123.7, 123.5, 121.5, 119.7, 111.7, 95.5, 85.7, 25.2.

HR-MS (ESI-FT-ICR) calcd for $C_{16}H_{13}NOBr$ ($[M + H]^+$): 314.01750, found 314.01742.



Ethyl 4-((2-acetamidophenyl)ethynyl)benzoate (1f)

N-(2-Ethynylphenyl)acetamide[7] (0.537 g, 3.37 mmol), ethyl 4-iodobenzoate (0.67 mL, 4.0 mmol), $[PdCl_2(PPh_3)_2]$ (0.0473 g, 0.067 mmol), and CuI (0.0257 g, 0.135 mmol) were dissolved in THF (30 mL). After addition of NEt_3 (0.56 mL, 4.0 mmol), the reaction mixture was allowed to stir at room temperature for 2 h. The resulting mixture was filtered through Celite and evaporated *in vacuo*. The crude product was purified by flash column chromatography over silica gel (hexane / methylene chloride 1:5) to give **1f** as a colorless solid. Yield: 1.00 g (3.26 mmol, 97%).

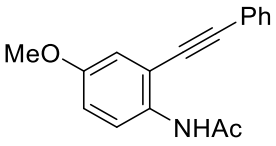
mp 157.6–158.6 °C.

IR (ATR): 3293, 2359, 1718, 1661, 1575, 1527, 1446, 1365, 1303, 1270, 1103 cm^{-1}.

^1H NMR (300 MHz, $CDCl_3$): δ 8.39 (d, *J* = 8.3 Hz, 1H), 8.05 (d, *J* = 8.5 Hz, 2H), 7.89 (s, 1H), 7.57 (d, *J* = 8.5 Hz, 2H), 7.49 (dd, *J* = 7.7, 1.5 Hz, 1H), 7.36 (td, *J* = 7.9, 1.3 Hz, 1H), 7.07 (t, *J* = 7.6 Hz, 1H), 4.38 (q, *J* = 7.2 Hz, 2H), 2.24 (s, 3H), 1.40 (t, *J* = 7.1 Hz, 3H).

^{13}C NMR (76 MHz, $CDCl_3$): δ 168.3, 166.0, 139.2, 132.1, 131.5, 130.6, 130.4, 129.9, 127.0, 123.7, 119.8, 111.5, 95.7, 87.3, 61.5, 25.2, 14.5.

HR-MS (ESI-FT-ICR) calcd for $C_{19}H_{18}NO_3$ ($[M + H]^+$): 308.12812, found 308.12785.



***N*-(4-Methoxy-2-(phenylethynyl)phenyl)acetamide (1g)**

4-Methoxy-2-(phenylethynyl)aniline[8] (0.893 g, 4.00 mmol) was dissolved in methylene chloride (30 mL). To the solution was added dry pyridine (0.34 mL, 4.8 mmol) and acetyl chloride (0.64 mL, 8.0 mmol) at 0 °C. The solution was warmed to room temperature and allowed to stir for 3.5 h. The reaction mixture was quenched by water and extracted with methylene chloride. The combined organic layer was washed with brine, dried with anhydrous Na_2SO_4, filtered, and evaporated *in vacuo*. The crude product was purified by flash column chromatography over silica gel (hexane / ethyl acetate 2.5:1) to give **1g** as a colorless solid. Yield: 0.642 g (2.42 mmol, 60%).

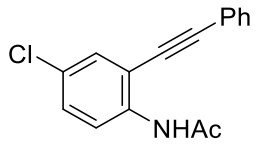
mp 150.6–151.3 °C.

IR (ATR): 3299, 3005, 2938, 2837, 1652, 1613, 1532, 1495, 1480, 1468, 1417, 1364, 1275, 1234, 1214, 1101, 1041 cm^{-1}.

^1H NMR (300 MHz, $CDCl_3$): δ 8.25 (d, *J* = 9.3 Hz, 1H), 7.77 (s, 1H), 7.56–7.48 (m, 2H), 7.41–7.34 (m, 3H), 7.00 (d, *J* = 3.1 Hz, 1H), 6.90 (dd, *J* = 9.1, 2.9 Hz, 1H), 3.79 (s, 3H), 2.20 (s, 3H).

^{13}C NMR (76 MHz, $CDCl_3$): δ 168.1, 155.5, 132.8, 131.8, 129.2, 128.8, 122.5, 121.4, 116.21, 116.16, 113.4, 96.3, 84.6, 55.8, 25.0.

HR-MS (ESI-FT-ICR) calcd for $C_{17}H_{16}NO_2$ ($[M + H]^+$): 266.11756, found 266.11741.



***N*-(4-Chloro-2-(phenylethynyl)phenyl)acetamide (1h)**

4-Chloro-2-(phenylethynyl)aniline[9] (1.14 g, 5.00 mmol) was dissolved in methylene chloride (40 mL). To the solution was added dry pyridine (0.42 mL, 6.0 mmol) and acetyl chloride (0.81 mL, 10 mmol) at 0 °C. The solution was allowed to warm to room temperature and stirred for 4.5 h. The reaction mixture was quenched by water and extracted with methylene chloride. The combined organic layer was washed with brine, dried with anhydrous Na_2SO_4, filtered, and evaporated *in vacuo*. The crude product was purified by recrystallization (hot methylene chloride / hexane) to give **1h** as a colorless solid. Yield: 0.673 g (2.49 mmol, 50%).

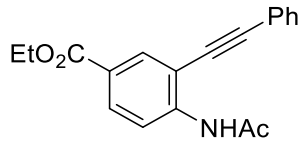
mp 180.4–181.1 °C.

IR (ATR): 3301, 3058, 2220, 1901, 1658, 1601, 1572, 1521, 1492, 1472, 1442, 1399, 1367, 1306, 1253, 1149, 1113, 1086, 1071, 1025 cm^{-1}.

^1H NMR (300 MHz, $CDCl_3$): δ 8.37 (d, *J* = 8.9 Hz, 1H), 7.89 (s, 1H), 7.52 (dd, *J* = 6.7, 3.1 Hz, 2H), 7.45 (d, *J* = 2.4 Hz, 1H), 7.42–7.36 (m, 3H), 7.29 (dd, *J* = 9.0, 2.4 Hz, 1H), 2.22 (s, 3H).

^{13}C NMR (76 MHz, $CDCl_3$): δ 168.3, 137.7, 131.8, 131.3, 129.9, 129.5, 128.9, 128.4, 122.0, 120.7, 113.6, 97.6, 83.2, 25.1.

HR-MS (ESI-FT-ICR) calcd for $C_{16}H_{13}NOCl$ ($[M + H]^+$): 270.06802, found 270.06801.



Ethyl 4-acetamido-3-(phenylethynyl)benzoate (1i)

Ethyl 4-amino-3-(phenylethynyl)benzoate[9] (0.929 g, 3.50 mmol) was dissolved in methylene chloride (28 mL). To the solution was added dry pyridine (0.30 mL, 4.2 mmol) and acetyl chloride (0.56 mL, 7.0 mmol) at 0 °C. The solution was allowed to warm to room temperature and stirred for 2 h. The reaction mixture was quenched by water and extracted with methylene chloride. The combined organic layer was washed with brine, dried with anhydrous Na_2SO_4, filtered, and evaporated *in vacuo*. The crude product was purified by flash column chromatography over silica gel (hexane / ethyl acetate 3:1) to give **1i** as a colorless solid. Yield: 0.912 g (2.97 mmol, 85%).

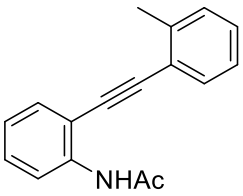
mp 119.9–120.3 °C.

IR (ATR): 3309, 2987, 1714, 1666, 1579, 1523, 1493, 1467, 1418, 1364, 1310, 1282, 1262, 1227, 1154, 1135, 1112, 1092, 1028 cm^{-1}.

^1H NMR (300 MHz, $CDCl_3$): δ 8.51 (d, J = 8.9 Hz, 1H), 8.17 (d, J = 2.1 Hz, 1H), 8.11 (s, 1H), 8.00 (dd, J = 8.7, 2.1 Hz, 1H), 7.56–7.50 (m, 2H), 7.43–7.36 (m, 3H), 4.35 (q, J = 7.2 Hz, 2H), 2.26 (s, 3H), 1.38 (t, J = 7.1 Hz, 3H).

^{13}C NMR (76 MHz, $CDCl_3$): δ 168.6, 165.7, 142.5, 133.4, 131.8, 131.4, 129.5, 128.9, 125.6, 122.1, 118.6, 111.8, 97.3, 83.5, 61.3, 25.3, 14.6.

HR-MS (ESI-FT-ICR) calcd for $C_{19}H_{18}NO_3$ ($[M + H]^+$): 308.12812, found 308.12804.



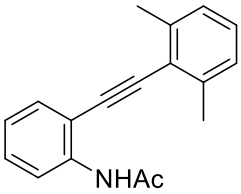
***N*-(2-(*o*-Tolylethynyl)phenyl)acetamide (1j)**

N-(2-Ethynylphenyl)acetamide[7] (0.637 g, 4.00 mmol), 2-iodotoluene (0.60 mL, 4.8 mmol), $[PdCl_2(PPh_3)_2]$ (0.0562 g, 0.0800 mmol), and CuI (0.0305 g, 0.160 mmol) were dissolved in THF (20 mL). After addition of NEt_3 (4 mL), the reaction mixture was allowed to stir at room temperature for 14 h. The resulting mixture was filtered through Celite and evaporated *in vacuo*. The crude product was purified by flash column chromatography over silica gel (hexane / methylene chloride 1:4) to give **1j** as a pale yellow solid. Yield: 0.877 g (3.52 mmol, 88%).

mp 133.5–134.0 °C.

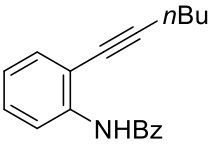
IR (ATR): 3293, 3057, 1684, 1661, 1577, 1530, 1491, 1449, 1369, 1305, 1257, 1042 cm^{-1}.

^{1}H NMR (300 MHz, $CDCl_3$): δ 8.39 (d, J = 8.3 Hz, 1H), 7.97 (s, 1H), 7.48–7.45 (m, 2H), 7.34–7.18 (m, 4H), 7.04 (t, J = 7.2 Hz, 1H), 2.51 (s, 3H), 2.19 (s, 3H).
^{13}C NMR (76 MHz, $CDCl_3$): δ 168.3, 139.8, 138.9, 132.1, 131.8, 129.9, 129.8, 129.2, 126.1, 123.6, 122.4, 119.5, 112.3, 95.5, 88.5, 25.1, 21.2.
HR-MS (ESI-FT-ICR) calcd for $C_{17}H_{16}NO$ ($[M + H]^+$): 250.12264, found 250.12223.



_N_-(2-((2,6-Dimethylphenyl)ethynyl)phenyl)acetamide (1k)

_N_-(2-Ethynylphenyl)acetamide[7] (0.716 g, 4.50 mmol), 2-iodo-1,3-dimethylbenzene (0.78 mL, 5.4 mmol), $[PdCl_2(PPh_3)_2]$ (0.0632 g, 0.09 mmol), CuI (0.0345 g, 0.18 mmol), and PPh_3 (0.0472 g, 0.18 mmol) were dissolved in NEt_3 (25 mL). The resulting mixture was refluxed for 16 h. The reaction mixture was filtered through Celite and evaporated *in vacuo*. The crude product was purified by flash column chromatography over silica gel (hexane / ethyl acetate 5:1) to give **1k** as a colorless solid. Yield: 0.836 g (3.17 mmol, 71%).
mp 129.4–129.7 °C.
IR (ATR): 3295, 2963, 2914, 1660, 1577, 1538, 1480, 1464, 1448, 1367, 1308, 1281, 1260, 1038 cm^{-1}.
^{1}H NMR (300 MHz, $CDCl_3$): δ 8.42 (d, J = 8.3 Hz, 1H), 8.01 (s, 1H), 7.50 (dd, J = 7.6, 1.4 Hz, 1H), 7.34 (t, J = 7.9 Hz, 1H), 7.21–7.03 (m, 4H), 2.53 (s, 6H), 2.21 (s, 3H).
^{13}C NMR (76 MHz, $CDCl_3$): δ 168.3, 140.0, 138.7, 131.8, 129.8, 128.6, 127.2, 123.6, 122.5, 119.5, 112.6, 94.3, 93.0, 25.1, 21.6.
HR-MS (ESI-FT-ICR) calcd for $C_{18}H_{18}NO$ ($[M + H]^+$): 264.13829, found 264.13872.



_N_-(2-(Hex-1-yn-1-yl)phenyl)benzamide (1m)

2-(Hex-1-yn-1-yl)aniline[10] (0.480 g, 2.77 mmol) was dissolved in THF (9 mL). To the solution was added NEt_3 (0.77 mL, 5.5 mmol) and benzoyl chloride (0.39 mL, 3.3 mmol) at 0 °C. The solution was allowed to warm to room temperature and stirred for

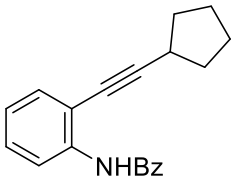
16 h. The reaction mixture was quenched by water and extracted with methylene chloride. The combined organic layer was washed with brine, dried with anhydrous Na_2SO_4, filtered, and evaporated *in vacuo*. The crude product was purified by flash column chromatography over silica gel (hexane / methylene chloride 1:2) to give **1m** as a pale yellow oil. Yield: 0.726 g (2.62 mmol, 94%).

IR (ATR): 3394, 2958, 2931, 1683, 1579, 1523, 1495, 1450, 1310, 1251 cm^{-1}.

^1H NMR (300 MHz, $CDCl_3$): δ 8.83 (s, 1H), 8.58 (d, J = 8.3 Hz, 1H), 7.91 (d, J = 6.5 Hz, 2H), 7.57–7.41 (m, 3H), 7.38 (d, J = 7.9 Hz, 1H), 7.31 (t, J = 7.9 Hz, 1H), 7.02 (t, J = 7.6 Hz, 1H), 2.49 (td, J = 7.1, 2.3 Hz, 2H), 1.67–1.53 (m, 2H), 1.53–1.35 (m, 2H), 0.90 (t, J = 7.2 Hz, 3H).

^{13}C NMR (76 MHz, $CDCl_3$): δ 165.2, 139.1, 135.1, 132.0, 131.6, 129.0, 128.9, 127.1, 123.4, 119.0, 113.1, 98.4, 76.1, 31.0, 22.2, 19.4, 13.7.

HR-MS (ESI-FT-ICR) calcd for $C_{19}H_{20}NO$ ($[M + H]^+$): 278.15394, found 278.15386.



***N*-(2-(Cyclopentylethynyl)phenyl)benzamide (1n)**

N-(2-Iodophenyl)benzamide[11] (1.13 g, 3.50 mmol), cyclopentylacetylene (0.53 mL, 4.6 mmol), $[PdCl_2(PPh_3)_2]$ (0.197 g, 0.28 mmol), and CuI (0.107 g, 0.56 mmol) were dissolved in THF (20 mL). After addition of NEt_3 (2.9 mL, 21 mmol), the reaction mixture was allowed to stir at room temperature for 2 h. The resulting mixture was filtered through Celite and evaporated in *vacuo*. The crude product was purified by flash column chromatography over silica gel (hexane / ethyl acetate 15:1) to give **1n** as a pale brown solid. Yield: 0.935 g (3.23 mmol, 92%).

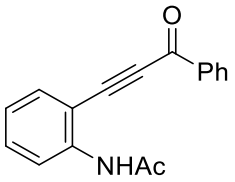
mp 89.6–90.6 °C.

IR (ATR): 3303, 2959, 2868, 1655, 1576, 1531, 1493, 1447, 1309 cm^{-1}.

^1H NMR (400 MHz, $CDCl_3$): δ 8.85 (1H, s), 8.57 (1H, d, J = 8.2 Hz), 7.92 (2H, d, J = 7.3 Hz), 7.56 (1H, t, J = 6.6 Hz), 7.49 (2H, t, J = 7.3 Hz), 7.39 (1H, d, J = 7.8 Hz), 7.33 (1H, t, J = 8.0 Hz), 7.03 (1H, t, J = 7.5 Hz), 2.96–2.89 (1H, m), 2.10–1.99 (2H, m), 1.83–1.58 (6H, m).

^{13}C NMR (100 MHz, $CDCl_3$): δ 165.3, 139.2, 135.3, 132.1, 131.6, 129.2, 129.0, 127.2, 123.5, 119.0, 113.2, 102.8, 75.7, 34.3, 31.1, 25.3.

HR-MS (ESI-FT-ICR) calcd for $C_{20}H_{20}NO$ ($[M + H]^+$): 290.15394, found 290.15383.



_N_-(2-(3-Oxo-3-phenylprop-1-yn-1-yl)phenyl)acetamide (1p)

_N_-(2-(3-Hydroxy-3-phenylprop-1-yn-1-yl)phenyl)acetamide[12] (0.795 g, 3.00 mmol) were dissolved in methylene chloride (50 mL). After the addition of activated MnO_2 (2.09 g, 24.0 mmol), the reaction mixture was stirred at room temperature for 3 h. The mixture was filtered through Celite and evaporated *in vacuo*. The crude product was purified by flash column chromatography over silica gel (hexane / methylene chloride 1:6) and recrystallization (methylene chloride / hexane) to give **1p** as a colorless solid. Yield: 0.230 g (0.872 mmol, 29%).

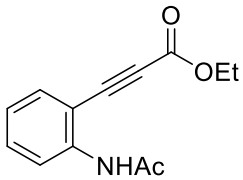
mp 134.0–135.0 °C.

IR (ATR): 3271, 2194, 1661, 1634, 1577, 1525, 1447, 1315, 1297 cm^{-1}.

^1H NMR (300 MHz, $CDCl_3$): δ 8.43 (d, J = 8.3 Hz, 1H), 8.21–8.16 (m , 2H), 7.97 (s, 1H), 7.68–7.60 (m, 2H), 7.57–7.43 (m, 3H), 7.12 (td, J = 7.7, 0.8 Hz, 1H), 2.26 (s, 3H).

^{13}C NMR (76 MHz, $CDCl_3$): δ 177.7, 168.7, 141.4, 136.8, 134.7, 133.4, 132.8, 129.7, 129.1, 123.9, 120.3, 108.9, 94.2, 88.5, 25.2.

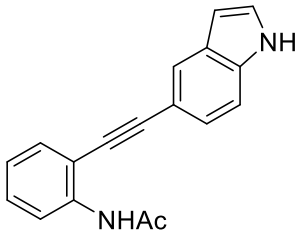
HR-MS (ESI-FT-ICR) calcd for $C_{17}H_{14}NO_2$ ($[M + H]^+$): 264.10191, found 264.10190.



Ethyl 3-(2-acetamidophenyl)propiolate (1q)

_N_-(2-Iodophenyl)acetamide[13] (0.131 g, 0.500 mmol), 3,3,3-triethoxyprop-1-yne[14] (0.129 g, 0.750 mmol), $[PdCl_2(PPh_3)_2]$ (0.0175 g, 0.0250 mmol), and CuI (0.0095 g, 0.050 mmol) were dissolved in THF (5 mL). After addition of NEt_3 (0.21 mL, 1.5 mmol), the reaction mixture was allowed to stir at room temperature for 2 h. The resulting mixture was filtered through Celite and evaporated in *vacuo*. The residue was passed through a pad of silica gel (hexane / ethyl acetate / NEt_3 70:30:1). The crude product was dissolved in THF (6 mL), and cooled at 0 °C. After the addition of 1 drop of water and $TsOH \cdot H_2O$ (0.0037 g, 0.020 mmol), the reaction mixture was stirred at 0 °C for 5 min. The reaction mixture was quenched by K_2CO_3 aq. and extracted with ethyl acetate. The organic layer was washed with brine, dried with anhydrous $MgSO_4$, filtered, and evaporated *in vacuo*. The crude product was purified by flash column chromatography

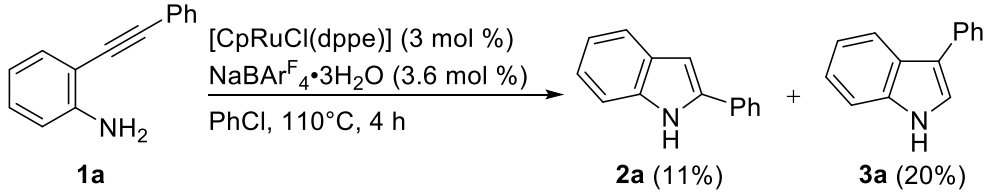
over silica gel (hexane / ethyl acetate / NEt_3 75:25:3) and recrystallization (methylene chloride / hexane) to give **1q** as a colorless solid. Yield: 0.0219 g (0.0195 mmol, 19%).
mp 120.7–122.2 °C.
IR (ATR): 3276, 2979, 2217, 1707, 1666, 1579, 1538, 1531, 1447, 1299, 1217, 1193 cm^{-1}.
^1H NMR (400 MHz, $CDCl_3$): δ 8.39 (1H, d, *J* = 8.7 Hz), 7.83 (1H, s), 7.51 (1H, d, *J* = 7.8 Hz), 7.44 (1H, t, *J* = 8.0 Hz), 7.06 (1H, t, *J* = 7.3 Hz), 4.30 (2H, q, *J* = 7.1 Hz), 2.24 (3H, s), 1.35 (3H, t, *J* = 7.1 Hz).
^{13}C NMR (MHz, $CDCl_3$): δ 168.6, 153.8, 141.1, 133.4, 132.5, 123.8, 120.1, 108.3, 87.9, 81.6, 62.6, 25.1, 14.3.
HR-MS (ESI-FT-ICR) calcd for $C_{13}H_{14}NO_3$ ($[M + H]^+$): 232.09682, found 232.09674.



***N*-(2-((1*H*-Indol-5-yl)ethynyl)phenyl)acetamide (1r)**
N-(2-Ethynylphenyl)acetamide[7] (0.159 g, 1.00 mmol), 5-iodoindole (0.267 g, 1.1 mmol) , $[PdCl_2(PPh_3)_2]$ (0.0351 g, 0.05 mmol), and CuI (0.0190 g, 0.10 mmol) were dissolved in THF (10 mL). After addition of NEt_3 (0.42 mL, 3.0 mmol), the reaction mixture was allowed to stir at room temperature for 18 h. The resulting mixture was filtered through Celite and evaporated in *vacuo*. The crude product was purified by flash column chromatography over silica gel (methylene chloride / ethyl acetate 40:1) to give **1r** as a pale yellow solid. Yield: 0.214 g (0.782 mmol, 78%).
mp 162.3–163.8 °C.
IR (ATR): 3296, 2202, 1637, 1618, 1575, 1531, 1479, 1450 cm^{-1}.
^1H NMR (400 MHz, $CDCl_3$): δ 8.40 (1H, d, *J* = 8.2 Hz), 8.31 (1H, s), 8.08 (1H, s), 7.85 (1H, s), 7.49 (1H, d, *J* = 6.8 Hz), 7.42–7.25 (4H, m), 7.05 (1H, t, *J* = 7.3 Hz), 6.59–6.56 (1H, m), 2.24 (3H, s).
^{13}C NMR (100 MHz, $CDCl_3$): δ 168.5, 130.0, 136.0, 131.7, 129.4, 128.1, 125.7, 125.6, 124.9, 123.6, 119.3, 113.6, 112.7, 111.6, 103.2, 98.5, 82.1, 25.3.
HR-MS (ESI-TOF) calcd for $C_{18}H_{14}N_2ONa$ ($[M + Na]^+$): 297.0998, found 297.1011.

2.2 Table 1. Ruthenium-Catalyzed Cycloisomerization 2-Aminodiphenylacetylene (1a) and Related Compounds

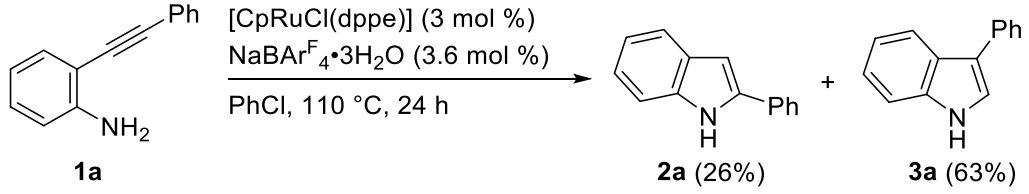
General procedure. A mixture of **1** (0.50 mmol), [CpRuCl(dppe)] (9.0 mg, 0.015 mmol), and $NaBAr^F_4 \cdot 3H_2O$ (16.8 mg, 0.018 mmol) in anhydrous PhCl (2.5 mL) was stirred at 110 °C under Ar. The reaction was monitored by TLC. The solvent was removed by evaporation, and the crude mixture was purified by flash column chromatography over silica gel.



1a **2a** (11%) **3a** (20%)

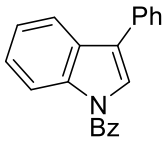
2-Phenyl-1*H*-indole[10] (2a) and 3-phenyl-1*H*-indole[15] (3a)

General procedure was followed using alkyne **1a**[7] (96.6 mg, 0.500 mmol), [CpRuCl(dppe)] (9.0 mg, 0.015 mmol), and $NaBAr^F_4 \cdot 3H_2O$ (16.8 mg, 0.018 mmol). The mixture was heated at 110 °C for 4 h. The crude product was purified by flash column chromatography over silica gel (hexane / ethyl acetate 10:1, then 7:1) to give a mixture of **1a** and **2a** (70.6 mg, 0.365 mmol, 73%), and **3a** (19.2 mg, 0.0994 mmol, 20%) as a brown solid. Since **1a** and **2a** were inseparable, the recovery of **1a** and the yield of **2a** was determined by ^{1}H NMR analysis of the mixture.



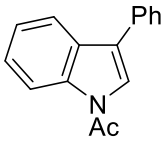
1a **2a** (26%) **3a** (63%)

General procedure was followed using alkyne **1a** (96.6 mg, 0.500 mmol), [CpRuCl(dppe)] (9.0 mg, 0.015 mmol), and $NaBAr^F_4 \cdot 3H_2O$ (16.8 mg, 0.018 mmol). The mixture was heated at 110 °C for 24 h. The crude product was purified by flash column chromatography over silica gel (hexane / ethyl acetate 10:1, then 7:1) to give **2a** (25.6 mg, 0.132 mmol, 26%) as a pale yellow solid and **3a** (60.4 mg, 0.313 mmol, 63%) as a brown solid.



Phenyl(3-phenyl-1*H*-indol-1-yl)methanone[16] (3b)

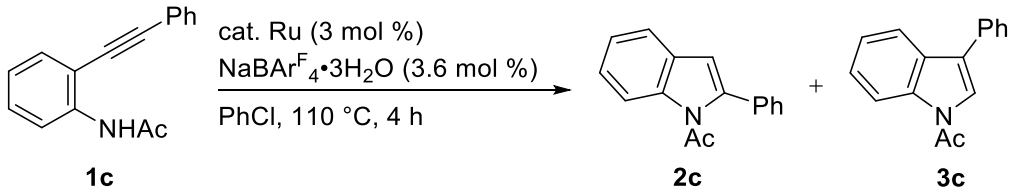
General procedure was followed using alkyne **1b**[17] (149 mg, 0.500 mmol), [CpRuCl(dppe)] (9.0 mg, 0.015 mmol), and $NaBAr^F_4 \cdot 3H_2O$ (16.8 mg, 0.018 mmol). The mixture was heated at 110 °C for 4 h. The crude product was purified by flash column chromatography over silica gel (hexane / methylene chloride 2.5:1, then 1.5:1) to give **3b** as a colorless solid. Yield: 55.2 mg (0.186 mmol, 34%). Starting material (**1b**) was also isolated (87.9 mg, 0.296 mmol, 59%).



1-(3-Phenyl-1*H*-indol-1-yl)ethan-1-one[18] (3c)

General procedure was followed using alkyne **1c**[17] (118 mg, 0.500 mmol), [CpRuCl(dppe)] (9.0 mg, 0.015 mmol), and $NaBAr^F_4 \cdot 3H_2O$ (16.8 mg, 0.018 mmol). The mixture was heated at 110 °C for 4 h. The crude product was purified by flash column chromatography over silica gel (hexane / ethyl acetate 8:1) to give **3c** as a colorless solid. Yield: 114 mg (0.483 mmol, 97%).

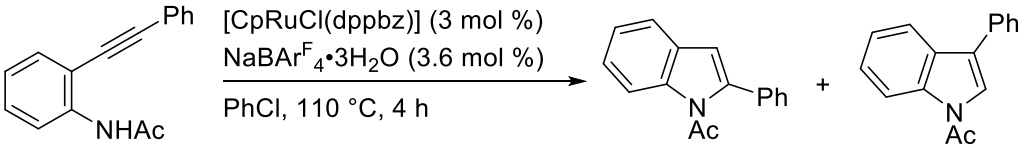
2.3 Table S1. Screening of the Catalyst



1c **2c** **3c**

entry	cat. Ru	product (yield, %)	recovery of **1c** (%)
1	[CpRuCl(dppe)]	**3c** (97)	–
2	[CpRuCl(dppbz)]	**2c** (6), **3c** (61)	29
3	[IndRuCl(dppe)]	**3c** (24)	67
4	[CpRuCl(PPh$_3$)$_2$]	no reaction	–

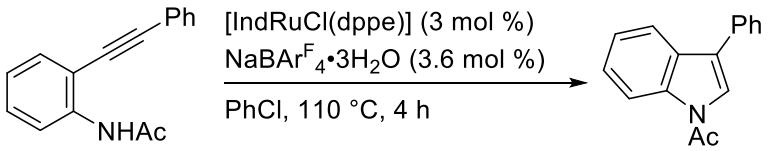
The catalysts were screened under similar reaction conditions described in Table 1. The dppbz complex was less reactive and gave **3c** in 61% yield, together with **1c** (29% recovery, entry 2). The 2-phenylindole (**2c**) was also isolated as a minor product (6% yield). [IndRuCl(dppe)] was a much less reactive catalyst, and **3c** was obtained in 24% yield, together with **1c** (67% recovery, entry 3). [CpRuCl(PPh$_3$)$_2$] gave neither **3c** nor **2c** (entry 4).



1c **2c** (6%) **3c** (61%)

1-(2-Phenyl-1*H*-indol-1-yl)ethan-1-one[19] (2c) and
1-(3-Phenyl-1*H*-indol-1-yl)ethan-1-one (3c)

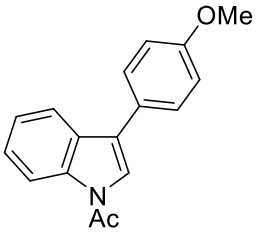
General procedure was followed using alkyne **1c** (118 mg, 0.500 mmol), [CpRuCl(dppbz)] (9.7 mg, 0.015 mmol), and NaBAr$^F_4$·3H$_2$O (16.8 mg, 0.018 mmol). The mixture was heated at 110 °C for 4 h. The crude product was purified by flash column chromatography over silica gel (hexane / ethyl acetate 8:1, then 3:1) to give **2c** (7.0 mg, 0.030 mmol, 6%) as a colorless oil and **3c** (72.0 mg, 0.306 mmol, 61%) as a colorless solid. Compound **1c** was recovered (33.9 mg, 0.144 mmol, 29%).



1c **3c** (24%)

General procedure was followed using alkyne **1c** (118 mg, 0.500 mmol), [IndRuCl(dppe)] (9.8 mg, 0.015 mmol), and NaBAr$^F_4$·3H$_2$O (16.8 mg, 0.018 mmol). The mixture was heated at 110 °C for 4 h. The crude product was purified by flash column chromatography over silica gel (hexane / ethyl acetate 8:1, then 3:1) to give **3c** (28.4 mg, 0.121 mmol, 24%) as a colorless solid. Compound **1c** was recovered (79.1 mg, 0.336 mmol, 67%).

2.4 Table 2. Synthesis of 3-Substituted Indoles by the Ruthenium-Catalyzed Cycloisomerization of 2-Alkynylanilides



1-(3-(4-Methoxyphenyl)-1*H*-indol-1-yl)ethan-1-one (3d)

General procedure was followed using alkyne **1d**[6] (133 mg, 0.500 mmol), [CpRuCl(dppe)] (9.0 mg, 0.015 mmol), and $NaBAr^F_4 \cdot 3H_2O$ (16.8 mg, 0.018 mmol). The mixture was heated at 110 °C for 2 h. The crude product was purified by flash column chromatography over silica gel (hexane / ethyl acetate 5:1) to give **3d** as a pale yellow solid. Yield: 128 mg (0.482 mmol, 96%).

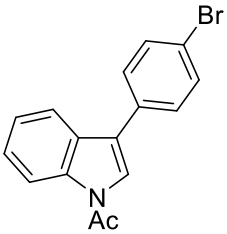
mp 115.2–116.1 °C.

IR (ATR): 1705, 1510, 1454, 1384, 1354, 1274, 1244, 1231, 1029 cm^{-1}.

^1H NMR (300 MHz , $CDCl_3$): δ 8.50 (d, *J* = 8.3 Hz, 1H), 7.76 (d, *J* = 7.6 Hz, 1H), 7.55 (d, *J* = 8.6 Hz, 2H), 7.43 (s, 1H), 7.39 (td, *J* = 7.6, 1.3 Hz, 1H), 7.31 (td, *J* = 7.5, 1.1 Hz, 1H), 7.01 (d, *J* = 8.6 Hz, 2H), 3.86 (s, 3H), 2.66 (s, 3H).

^{13}C NMR (76 MHz, $CDCl_3$): δ 168.8, 159.4, 136.5, 129.5, 129.3, 125.9, 125.7, 124.1, 123.9, 121.6, 120.1, 117.0, 114.6, 55.6, 24.3.

HR-MS (ESI-FT-ICR) calcd for $C_{17}H_{16}NO_2$ ($[M + H]^+$): 266.11756, found 266.11780.



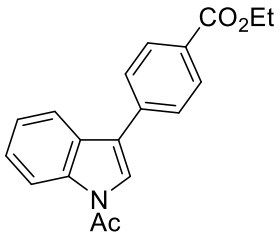
1-(3-(4-Bromophenyl)-1*H*-indol-1-yl)ethan-1-one (3e)

General procedure was followed using alkyne **1e** (157 mg, 0.500 mmol), [CpRuCl(dppe)] (9.0 mg, 0.015 mmol), and $NaBAr^F_4 \cdot 3H_2O$ (16.8 mg, 0.018 mmol). The mixture was heated at 110 °C for 6 h. The crude product was purified by flash column chromatography over silica gel (hexane / methylene chloride 1:5) to give **3e** as a colorless solid. Yield: 130 mg (0.414 mmol, 83%).

mp 152.6–153.3 °C.

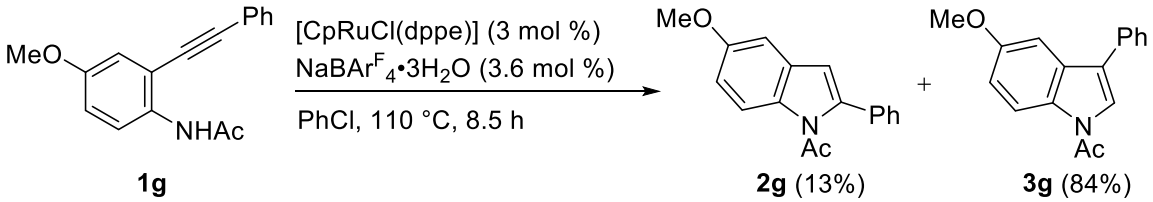
IR (ATR): 1706, 1450, 1384, 1351, 1331, 1274, 1226 cm^{-1}.

^{1}H NMR (300 MHz, $CDCl_3$): δ 8.49 (d, *J* = 8.3 Hz, 1H), 7.73 (d, *J* = 7.7 Hz, 1H), 7.59 (d, *J* = 8.7 Hz, 2H), 7.53–7.46 (m, 3H), 7.41 (td, *J* = 7.7, 1.1 Hz, 1H), 7.33 (td, *J* = 7.5, 1.1 Hz, 1H), 2.68 (s, 3H).
^{13}C NMR (76 MHz, $CDCl_3$): δ 168.7, 136.5, 132.5, 132.3, 129.7, 128.9, 125.9, 124.3, 123.1, 122.4, 121.7, 119.8, 117.1, 24.3.
HR-MS (ESI-FT-ICR) calcd for $C_{16}H_{13}NOBr$ ($[M + H]^+$): 314.01750, found 314.01774.



Ethyl 4-(1-acetyl-1*H*-indol-3-yl)benzoate (3f)

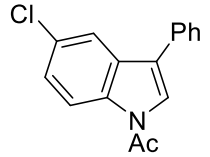
General procedure was followed using alkyne **1f** (154 mg, 0.500 mmol), [CpRuCl(dppe)] (9.0 mg, 0.015 mmol), and $NaBAr^F_4 \cdot 3H_2O$ (16.8 mg, 0.018 mmol). The mixture was heated at 110 °C for 12 h. The crude product was purified by flash column chromatography over silica gel (hexane / ethyl acetate 7:1, then 4:1) to give **3f** as a colorless solid. Yield: 139 mg (0.453 mmol, 91%).
mp 147.5–147.8 °C.
IR (ATR): 1705, 1609, 1448, 1385, 1356, 1278, 1228 cm^{-1}.
^{1}H NMR (300 MHz, $CDCl_3$): δ 8.50 (d, *J* = 8.3 Hz, 1H), 8.13 (d, *J* = 8.6 Hz, 2H), 7.79 (d, *J* = 7.6 Hz, 1H), 7.69 (d, *J* = 8.3 Hz, 2H), 7.58 (s, 1H), 7.41 (t, *J* = 7.1 Hz, 1H), 7.34 (t, *J* = 7.1 Hz, 1H), 4.40 (q, *J* = 7.1 Hz, 2H), 2.69 (s, 3H), 1.41 (t, *J* = 7.2 Hz, 3H).
^{13}C NMR (76 MHz, $CDCl_3$): δ 168.8, 166.6, 138.2, 136.6, 130.4, 129.6, 128.8, 127.9, 126.0, 124.4, 123.2, 123.0, 120.0, 117.1, 61.3, 24.3, 14.6.
HR-MS (ESI-FT-ICR) calcd for $C_{19}H_{18}NO_3$ ($[M + H]^+$): 308.12812, found 308.12828.



1g **2g** (13%) **3g** (84%)

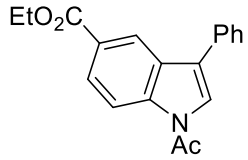
1-(5-Methoxy-2-phenyl-1*H*-indol-1-yl)ethan-1-one[19] (2g) and
1-(5-methoxy-3-phenyl-1*H*-indol-1-yl)ethan-1-one[20] (3g)

General procedure was followed using alkyne **1g** (133 mg, 0.500 mmol), [CpRuCl(dppe)] (9.0 mg, 0.015 mmol), and $NaBAr^F_4 \cdot 3H_2O$ (16.8 mg, 0.018 mmol). The mixture was heated at 110 °C for 8.5 h. The crude product was purified by flash column chromatography over silica gel (hexane / ethyl acetate 10:1, then 5:1) to give **2g** (17.5 mg, 0.066 mmol, 13%) as a pale brown oil and **3g** (111 mg, 0.418 mmol, 84%) as a colorless solid.



1-(5-Chloro-3-phenyl-1*H*-indol-1-yl)ethan-1-one[20] (3h)

General procedure was followed using alkyne **1h** (135 mg, 0.500 mmol), [CpRuCl(dppe)] (9.0 mg, 0.015 mmol), and $NaBAr^F_4 \cdot 3H_2O$ (16.8 mg, 0.018 mmol). The mixture was heated at 110 °C for 8.5 h. The crude product was purified by flash column chromatography over silica gel (hexane / ethyl acetate 6.5:1) to give **3h** as a colorless solid. Yield: 118 mg (0.438 mmol, 88%).



Ethyl 1-acetyl-3-phenyl-1*H*-indole-5-carboxylate (3i)

General procedure was followed using alkyne **1i** (154 mg, 0.500 mmol), [CpRuCl(dppe)] (9.0 mg, 0.015 mmol), and $NaBAr^F_4 \cdot 3H_2O$ (16.8 mg, 0.018 mmol). The mixture was heated at 145 °C for 9.5 h. The crude product was purified by flash column chromatography over silica gel (hexane / ethyl acetate 6:1) to give **3i** as a colorless solid. Yield: 138 mg (0.450 mmol, 90%).

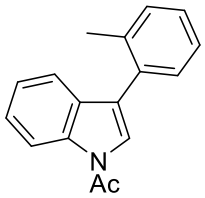
mp 146.2–147.2 °C.

IR (ATR): 2361, 1705, 1449, 1383, 1350, 1330, 1273, 1225 cm^{-1}.

^1H NMR (300 MHz, $CDCl_3$): δ 8.53 (d, *J* = 8.9 Hz, 1H), 8.49 (d, *J* = 1.1 Hz, 1H), 8.09 (dd, *J* = 8.8, 1.6 Hz, 1H), 7.63 (d, *J* = 7.0 Hz, 2H), 7.55 (s, 1H), 7.49 (t, *J* = 7.4 Hz, 2H), 7.42–7.38 (m, 1H), 4.39 (q, *J* = 7.1 Hz, 2H), 2.69 (s, 3H), 1.39 (t, *J* = 7.2 Hz, 3H).

^{13}C NMR (76 MHz, $CDCl_3$): δ 168.8, 167.0, 139.0, 132.9, 129.3, 129.1, 128.3, 128.1, 127.0, 126.5, 124.7, 123.3, 122.3, 116.7, 61.2, 24.3, 14.6.

HR-MS (ESI-FT-ICR) calcd for $C_{19}H_{18}NO_3$ ($[M + H]^+$): 308.12812, found 308.12843.



1-(3-(*o*-tolyl)-1*H*-indol-1-yl)ethan-1-one (3j)

General procedure was followed using alkyne **1j** (125 mg, 0.500 mmol), [CpRuCl(dppe)] (30.0 mg, 0.050 mmol), and $NaBAr^F_4 \cdot 3H_2O$ (56.1 mg, 0.060 mmol). The mixture was heated at 145 °C for 2.5 h. The crude product was purified by flash column chromatography over silica gel (hexane / ethyl acetate 9:1) to give **3j** as a colorless solid. Yield: 116 mg (0.466 mmol, 93%).

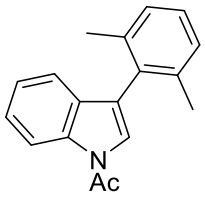
mp 84.5–85.2 °C.

IR (ATR): 1697, 1449, 1383, 1354, 1340, 1265, 1227 cm^{-1}.

^1H NMR (300 MHz, $CDCl_3$): δ 8.49 (d, J = 8.3 Hz, 1H), 7.42–7.25 (m, 8H), 2.66 (s, 3H), 2.28 (s, 3H).

^{13}C NMR (76 MHz, $CDCl_3$): δ 168.8, 137.2, 135.8, 132.6, 130.74, 130.66, 130.58, 128.2, 126.0, 125.6, 124.0, 123.8, 123.2, 120.5, 116.9, 24.3, 20.7.

HR-MS (ESI-FT-ICR) calcd for $C_{17}H_{16}NO$ ($[M + H]^+$): 250.12264, found 250.12275.



1-(3-(2,6-Dimethylphenyl)-1*H*-indol-1-yl)ethan-1-one (3k)

General procedure was followed using alkyne **1k** (132 mg, 0.500 mmol), [CpRuCl(dppe)] (30.0 mg, 0.050 mmol), and $NaBAr^F_4 \cdot 3H_2O$ (56.1 mg, 0.060 mmol). The mixture was heated at 145 °C for 24 h. The crude product was purified by flash column chromatography over silica gel (hexane / ethyl acetate 9:1, then 3:1) to give the **3k** (71.3 mg, 0.271 mmol, 54%) as a pale brown solid. Compound **1k** was recovered (46.3 mg, 0.176 mmol, 35%).

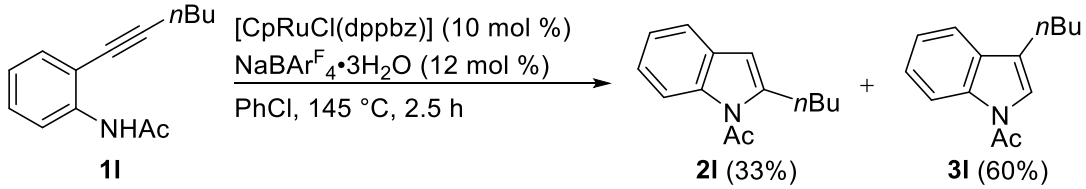
mp 120.3–121.1 °C.

IR (ATR): 3001, 2921, 1706, 1449, 1378, 1352, 1334, 1256, 1222, 1183, 1143, 1035 cm^{-1}.

^1H NMR (300 MHz, $CDCl_3$): δ 8.48 (d, J = 7.9 Hz, 1H), 7.37 (t, J = 7.7 Hz, 1H), 7.27 (s, 1H), 7.23–7.18 (m, 2H), 7.14 (d, J = 8.1 Hz, 3H), 2.65 (s, 3H), 2.09 (s, 6H).^{13}C NMR

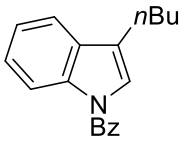
(76 MHz, $CDCl_3$): δ 168.7, 138.2, 135.9, 132.0, 130.5, 128.0, 127.5, 125.5, 123.9, 122.9, 122.4, 120.1, 116.8, 24.2, 20.9.

HR-MS (ESI-FT-ICR) calcd for $C_{18}H_{17}NNaO$ ($[M + Na]^+$): 286.12024, found 286.11923.



1-(2-Butyl-1*H*-indol-1-yl)ethan-1-one[21] (2l) and
1-(3-Butyl-1*H*-indol-1-yl)ethan-1-one[18] (3l)

General procedure was followed using alkyne **1l**[22] (108 mg, 0.500 mmol), [CpRuCl(dppbz)] (32.4 mg, 0.050 mmol), and NaBAr$^F_4$·3H$_2$O (56.1 mg, 0.060 mmol). The mixture was heated at 145 °C for 2.5 h. The crude product was purified by flash column chromatography over silica gel (hexane / ethyl acetate 20:1) to give **2l** (35.8 mg, 0.166 mmol, 33%) as a colorless solid and **3l** (64.8 mg, 0.301 mmol, 60%) as a pale yellow solid.



(3-Butyl-1*H*-indol-1-yl)(phenyl)methanone (3m)

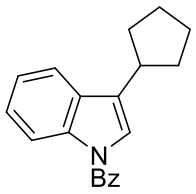
General procedure was followed using alkyne **1m** (137 mg, 0.492 mmol), [CpRuCl(dppbz)] (31.9 mg, 0.049 mmol), and NaBAr$^F_4$·3H$_2$O (55.2 mg, 0.059 mmol). The mixture was heated at 145 °C for 2 h. The crude product was purified by flash column chromatography over silica gel (hexane / methylene chloride 7:1, then 3:1) to give **3m** as a pale yellow oil. Yield: 119 mg (0.428 mmol, 87%).

IR (ATR): 2955, 2928, 1683, 1453, 1374, 1333, 1261 cm^{-1}.

^1H NMR (300 MHz, $CDCl_3$): δ 8.36 (d, J = 7.3 Hz, 1H), 7.71 (t, J = 4.1 Hz, 2H), 7.59–7.49 (m, 4H), 7.40–7.27 (m, 2H), 7.04 (s, 1H), 2.65 (t, J = 7.7 Hz, 2H), 1.70–1.58 (m, 2H), 1.46–1.32 (m, 2H), 0.92 (t, J = 7.3 Hz, 3H).

^{13}C NMR (76 MHz, $CDCl_3$): δ 168.6, 136.7, 135.2, 131.8, 131.5, 129.3, 128.8, 125.1, 124.0, 123.8, 123.2, 119.3, 116.8, 31.5, 24.8, 22.8, 14.1.

HR-MS (ESI-FT-ICR) calcd for $C_{19}H_{20}NO$ ($[M + H]^+$): 278.15394, found 278.15390.



(3-Cyclopentyl-1*H*-indol-1-yl)(phenyl)methanone (3n)

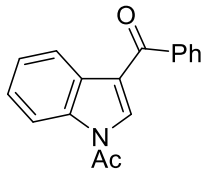
General procedure was followed at using alkyne **1n** (145 mg, 0.500 mmol), [CpRuCl(dppbz)] (32.4 mg, 0.050 mmol), and $NaBAr^F_4 \cdot 3H_2O$ (56.1 mg, 0.060 mmol). The mixture was heated at 145 °C for 2.5 h. The crude product was purified by flash column chromatography over silica gel (hexane / ethyl acetate 30:1) to give **3n** as a pale yellow oil. Yield: 134 mg (0.462 mmol, 92%).

IR (ATR): 2952, 2867, 1682, 1451, 1370, 1332, 1260 cm^{-1}.

^1H NMR (400 MHz, $CDCl_3$): δ 8.34 (1H, d, *J* = 7.8 Hz), 7.71 (2H, d, *J* = 7.3 Hz), 7.59 (2H, t, *J* = 8.2 Hz), 7.51 (2H, t, *J* = 7.5 Hz), 7.38–7.26 (2H, m), 7.03 (1H, s), 3.21–3.13 (1H, m), 2.17–2.05 (2H, m), 1.81–1.56 (7H, m).

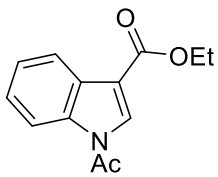
^{13}C NMR (100 MHz, $CDCl_3$): δ 168.7, 137.0, 135.2, 131.9, 131.3, 129.3, 128.8, 127.3, 125.1, 123.8, 122.6, 119.9, 116.8, 36.8, 32.7, 25.4.

HR-MS (ESI-FT-ICR) calcd for $C_{20}H_{20}NO$ ($[M + H]^+$): 290.15394, found 290.15373.



1-(3-Benzoyl-1*H*-indol-1-yl)ethan-1-one[23] (3p)

General procedure was followed using alkyne **1p** (132 mg, 0.500 mmol), [CpRuCl(dppe)] (9.0 mg, 0.015 mmol), and $NaBAr^F_4 \cdot 3H_2O$ (16.8 mg, 0.018 mmol). The mixture was heated at 110 °C for 1.5 h. The crude product was purified by flash column chromatography over silica gel (hexane / ethyl acetate 4:1) to give **3p** as a colorless solid. Yield: 122 mg (0.464 mmol, 93%).



Ethyl 1-acetyl-1*H*-indole-3-carboxylate (3q)

The glasswares for this reaction were flame dried. Before starting the reaction, $NaBAr^F_4 \cdot 3H_2O$ was treated with anhydrous toluene (2.5 mL) and the mixture was evaporated (three times). General procedure was followed using alkyne **1q** (117 mg, 0.500 mmol), [CpRuCl(dppe)] (15.0 mg, 0.025 mmol), and $NaBAr^F_4 \cdot 3H_2O$ (28.0 mg, 0.030 mmol). The mixture was heated at 145 °C for 1 h. The crude product was purified by flash column chromatography over silica gel (hexane / ethyl acetate 5:1) to give **3q** as a colorless solid. Yield: 91.5 mg (0.396 mmol, 79%).

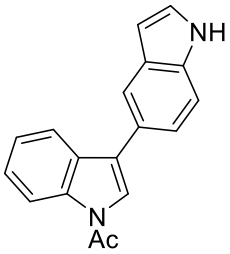
mp 94.7–95.3 °C.

IR (ATR): 2979, 1709, 1557, 1444, 1380, 1194 cm^{-1}.

^1H NMR (400 MHz, $CDCl_3$): δ 8.40 (1H, d, J = 8.7 Hz), 8.12 (1H, dd, J = 6.2, 2.1 Hz), 8.07 (1H, s), 7.41–7.32 (2H, m), 4.40 (2H, q, J = 7.1 Hz), 2.66 (3H, s), 1.42 (3H, t, J = 7.1 Hz).

^{13}C NMR (100 MHz, $CDCl_3$): δ 168.9, 164.2, 136.1, 131.3, 127.5, 126.1, 125.0, 121.8, 116.7, 114.3, 60.8, 24.1, 14.6.

HR-MS (ESI-FT-ICR) calcd for $C_{13}H_{14}NO_3$ ($[M + H]^+$): 232.09682, found 232.09704.



1-(1*H*,1'*H*-[3,5'-Biindol]-1-yl)ethan-1-one (3r)

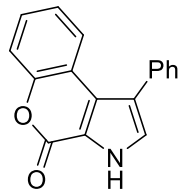
General procedure was followed using alkyne **1r** (137 mg, 0.500 mmol), [CpRuCl(dppe)] (9.0 mg, 0.015 mmol), and $NaBAr^F_4 \cdot 3H_2O$ (16.8 mg, 0.018 mmol). The mixture in PhCl (4 mL) was heated at 90 °C for 1.5 h. The crude product was purified by flash column chromatography over silica gel (methylene chloride / hexane 3:1) to give **3r** as a brown amorphous solid. Yield: 126 mg (0.460 mmol, 92%).

IR (ATR): 3419, 2359, 1698, 1684, 1449, 1381, 1349 cm^{-1}.

^1H NMR (400 MHz, $CDCl_3$): δ 8.54 (1H, d, J = 6.8 Hz), 8.29 (1H, s), 7.91 (1H, s), 7.87 (1H, d, J = 7.8 Hz), 7.51–7.45 (3H, m), 7.45–7.38 (1H, m), 7.34 (1H, t, J = 7.5 Hz), 7.27–7.25 (1H, m), 6.64–6.60 (1H, m), 2.67 (3H, s).

^{13}C NMR (100 MHz, $CDCl_3$): δ 168.9, 136.5, 135.6, 129.9, 128.6, 125.6, 125.5, 125.2, 125.1, 124.0, 122.7, 121.7, 120.4, 120.3, 117.0, 111.7, 103.0, 24.3.

HR-MS (APCI-FT-ICR) calcd for $C_{18}H_{15}N_2O$ ($[M + H]^+$): 275.11789, found 275.11790.



1-Phenylchromeno[3,4-*b*]pyrrol-4(3*H*)-one (3s)

General procedure was followed using alkyne **1s**[24] (131 mg, 0.500 mmol), [CpRuCl(dppe)] (15.0 mg, 0.025 mmol), and $NaBAr^F_4 \cdot 3H_2O$ (28.0 mg, 0.030 mmol). The mixture was heated at 145 °C for 2.5 h. The crude product was purified by flash column chromatography over silica gel (methylene chloride / ethyl acetate 30:1) to give **3s** as a colorless solid. Yield: 125 mg (0.477 mmol, 95%).

mp 244.8–245.4 °C.

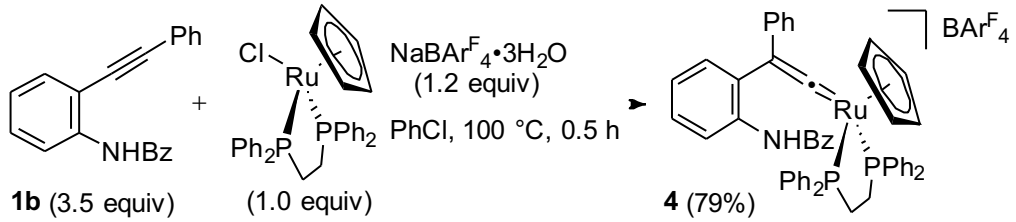
IR (ATR): 3236, 1704, 1396, 1105 cm^{-1}.

^1H NMR (300 MHz, $CDCl_3$): δ 10.54 (1H, s), 7.69 (1H, dd, J = 7.9, 1.4 Hz), 7.55-7.38 (6H, m), 7.38-7.30 (2H, m), 7.12-7.06 (1H, m).

^{13}C NMR (75 MHz, $CDCl_3$): δ156.4, 151.4, 134.4, 130.0, 128.9, 128.1, 127.93, 126.2, 124.3, 123.8, 122.9, 118.6, 117.7 (two signals are missing).

HR-MS (ESI-TOF) calcd for $C_{17}H_{12}NO_2$ ($[M + H]^+$): 262.08626, found 262.08629.

2.5 Scheme 2. Synthesis and Reaction of Vinylidene Complex 4



A solution of [CpRuCl(dppe)] (240 mg, 0.400 mmol), $NaBAr^F_4 \cdot 3H_2O$ (449 mg, 0.480 mmol), and **1b** (416 mg, 1.4 mmol) in chlorobenzene (7 mL) was heated at 100 °C for 30 min. The reaction mixture was evaporated *in vacuo*. The crude product was purified by flash column chromatography over silica gel (hexane / methylene chloride 1:1, then 1:1.3) to give **4** as a pink amorphous solid. Yield: 547 mg (0.317 mmol, 79%).

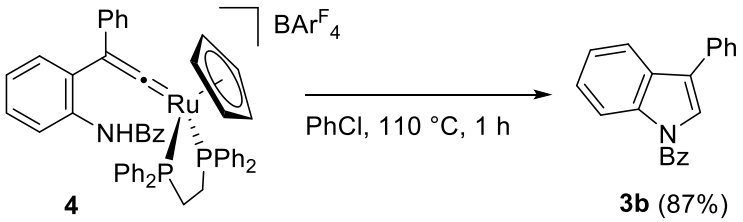
IR (ATR): 1682, 1625, 1521, 1438, 1355, 1279, 1126 cm^{-1}.

^1H NMR (300 MHz, $CDCl_3$): δ 7.91 (d, J = 7.9 Hz, 1H), 7.70 (br s, 8H), 7.49 (br s, 4H), 7.46–7.27 (m, 12H), 7.21–7.09 (m, 7H), 7.03–6.87 (m, 11H), 6.61–6.53 (m, 2H), 6.34 (d, J = 7.2 Hz, 2H), 5.35 (s, 5H), 3.19–2.86 (m, 4H).

^{13}C NMR (76 MHz, $CDCl_3$): δ 346.2 (t, J_{PC} = 15.6 Hz), 165.5 (s), 161.9 (q, J = 50.3 Hz, Ar^F), 135.8 (s), 135.5 (s), 135.0 (s), 134.8 (s), 134.2 (s), 133.2 (s), 132.6 (s), 132.4 (s), 132.2–131.8 (m), 131.4 (t, J_{PC} = 5.2 Hz), 130.2 (s), 129.7 (s), 129.6 (s), 129.5–129.00 (m), 128.95–128.8 (m), 128.5–128.4 (m), 127.8 (s), 127.7 (s), 126.9 (s), 125.53 (s), 125.49 (s), 125.0 (s), 124.8 (q, J_{FC} = 273.1 Hz), 120.9 (s), 117.8–117.5 (m), 92.5 (s), 28.2–27.4 (m).

$^{31}P\{^1H\}$ (121 MHz, $CDCl_3$): δ 75.8.

HR-MS (ESI-FT-ICR) calcd for $C_{52}H_{44}NOP_2Ru$ ($[M - BAr^F_4]^+$): 862.19496, found 862.19477.



A solution of **4** (345 mg, 0.200 mmol) in chlorobenzene (2 mL) was heated at 110 °C for 1 h. The reaction mixture was evaporated *in vacuo*. The crude product was purified by flash column chromatography over silica gel (hexane / methylene chloride 2.5:1) to give **3b** as a colorless solid. Yield: 51.9 mg (0.175 mmol, 87%).

3. References

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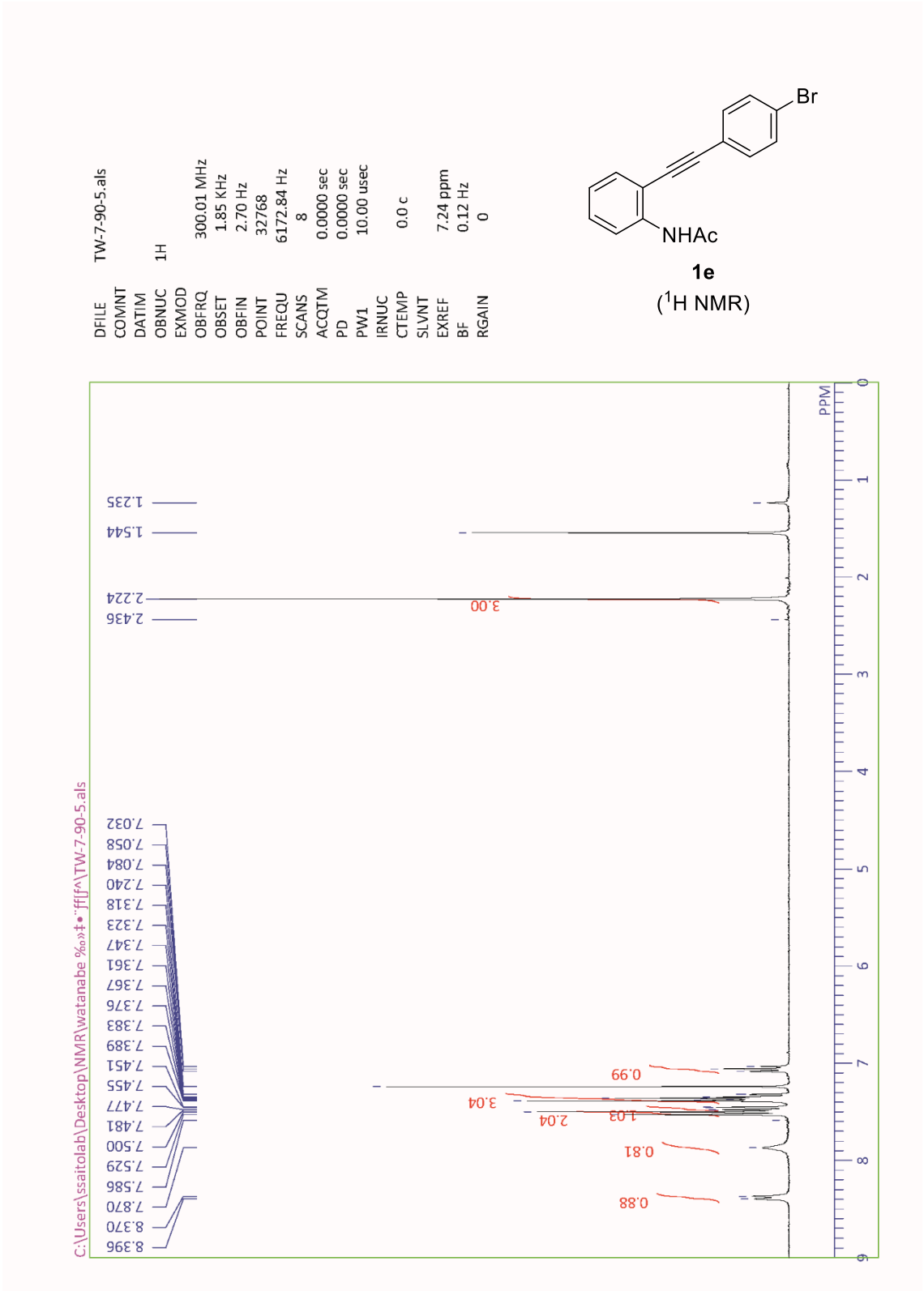
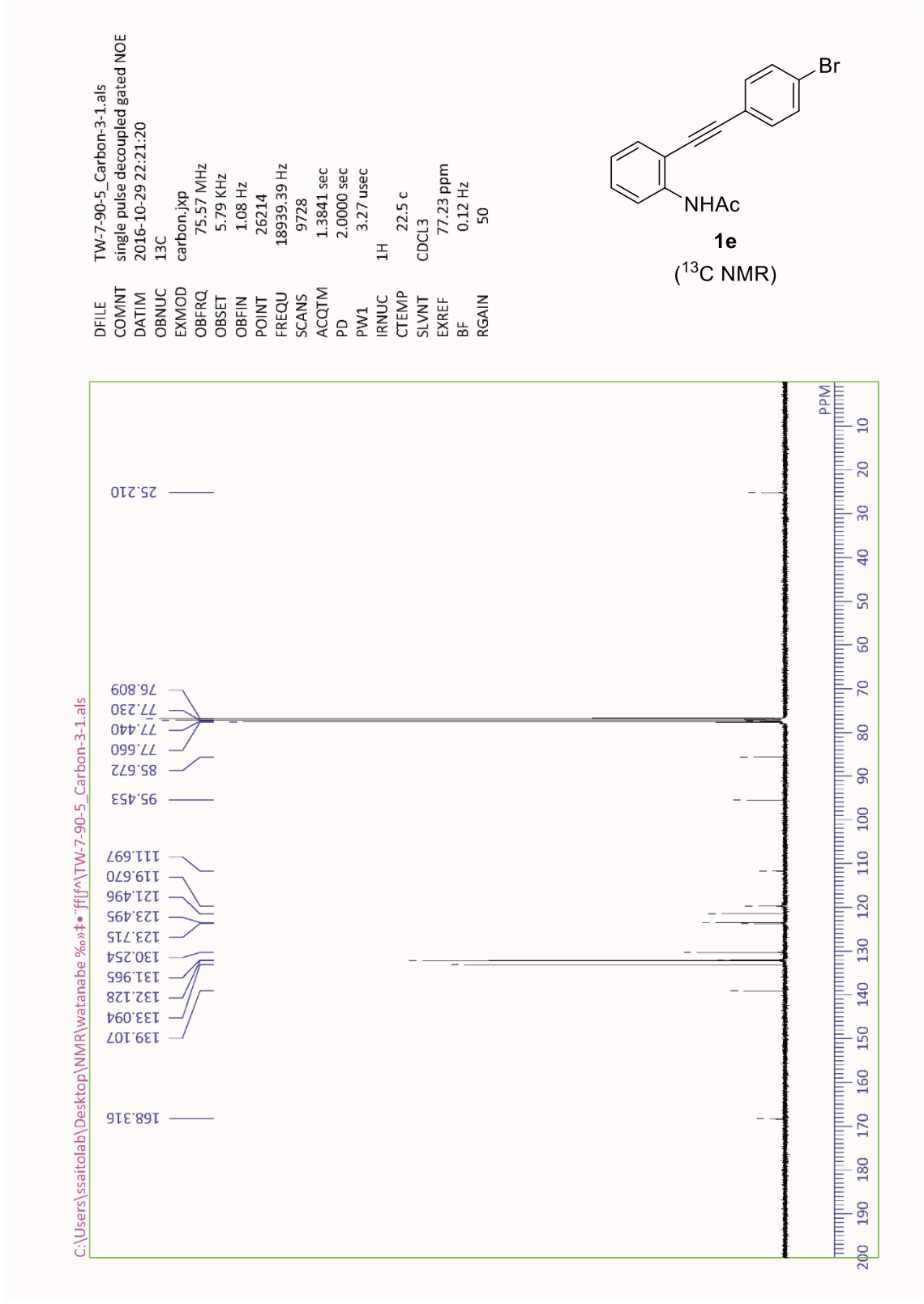
4. Copies of NMR Spectra

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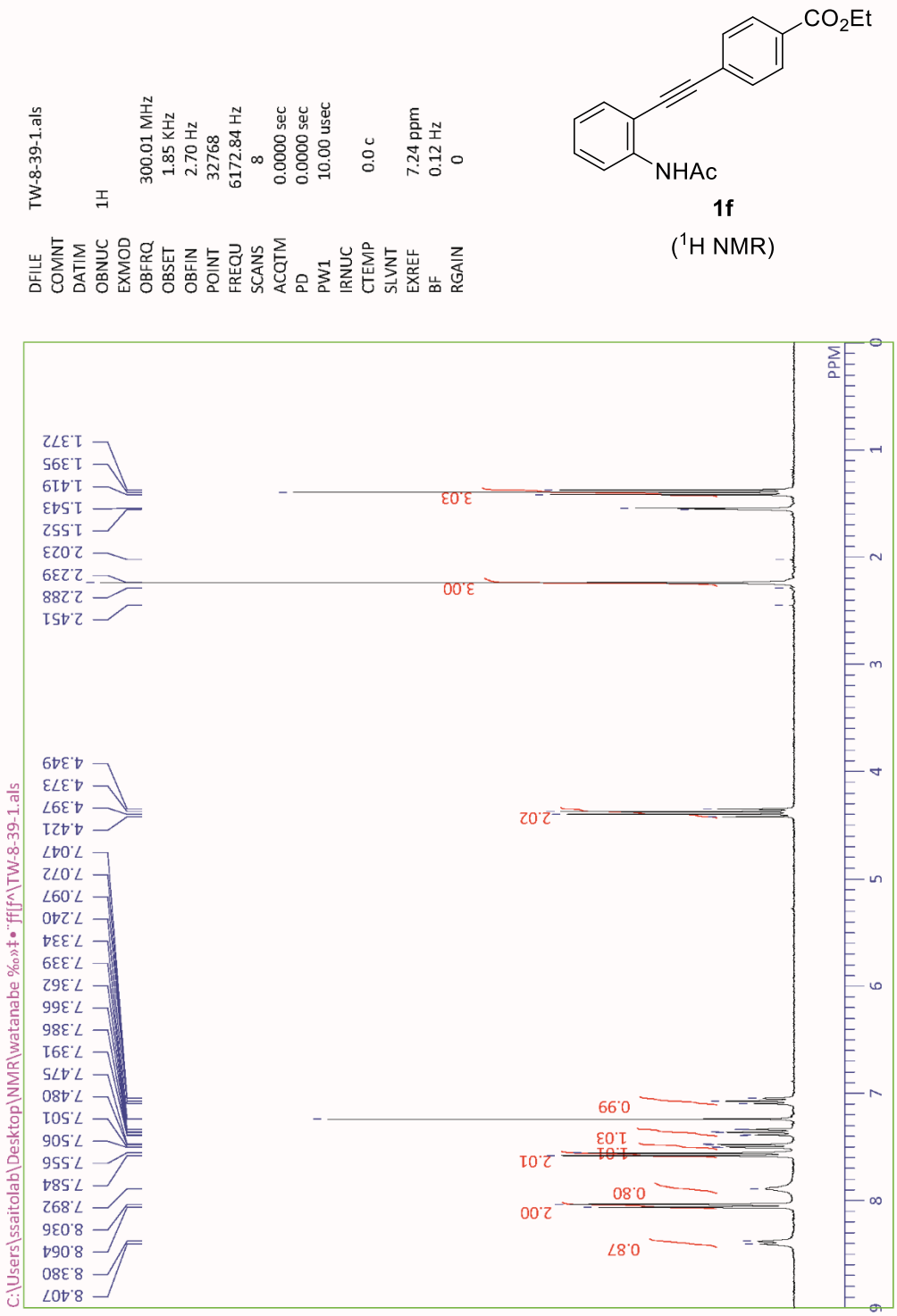
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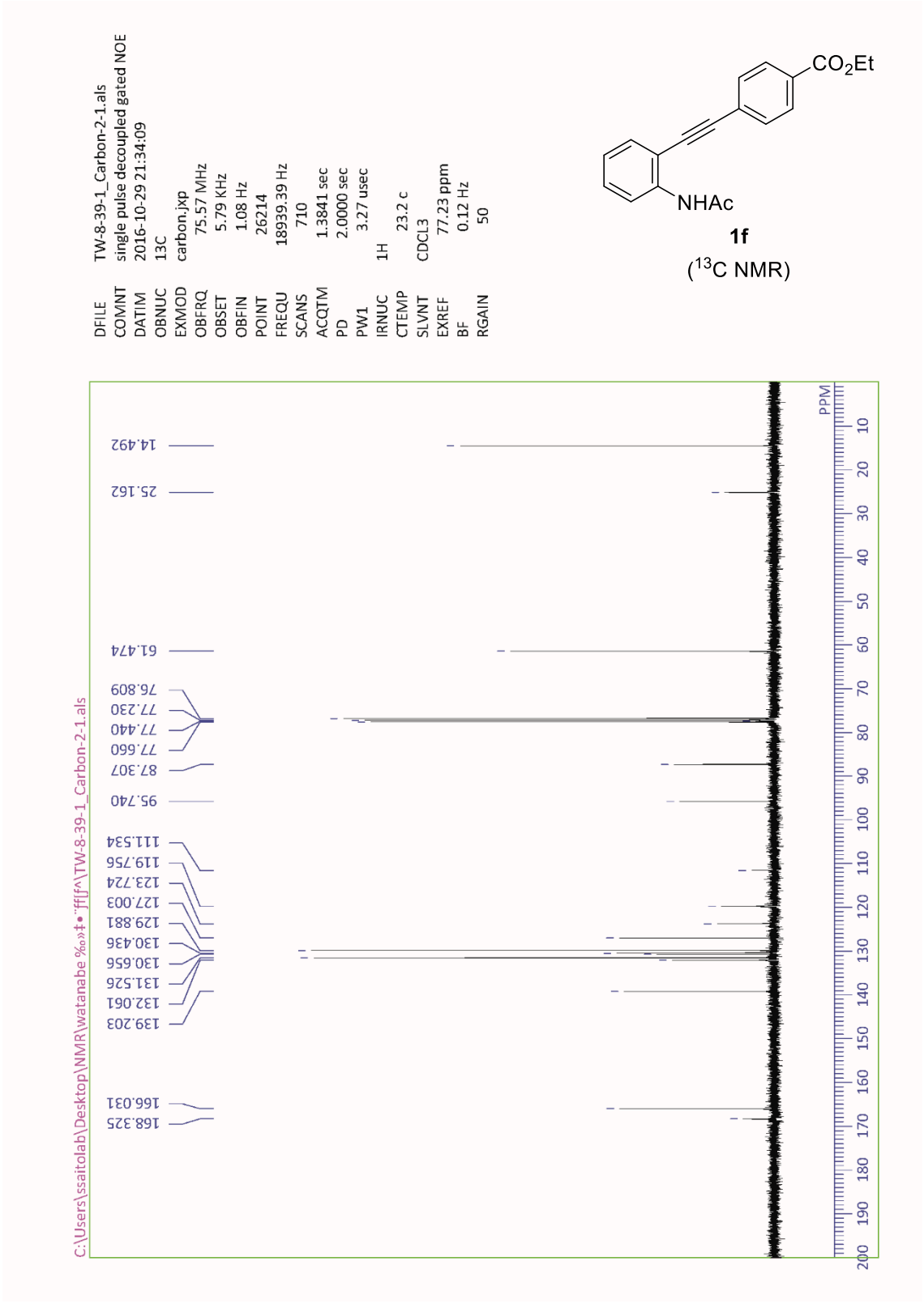
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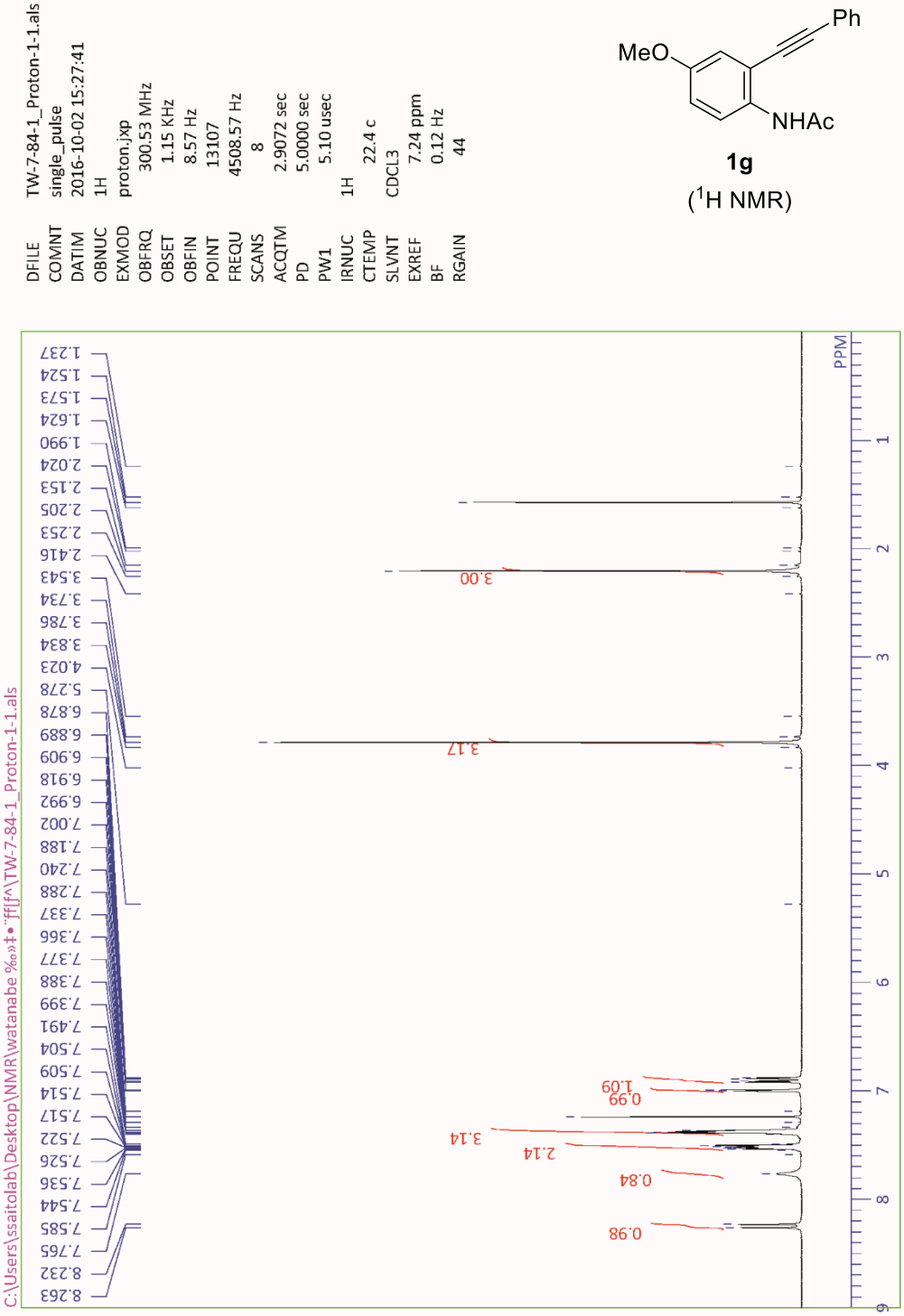
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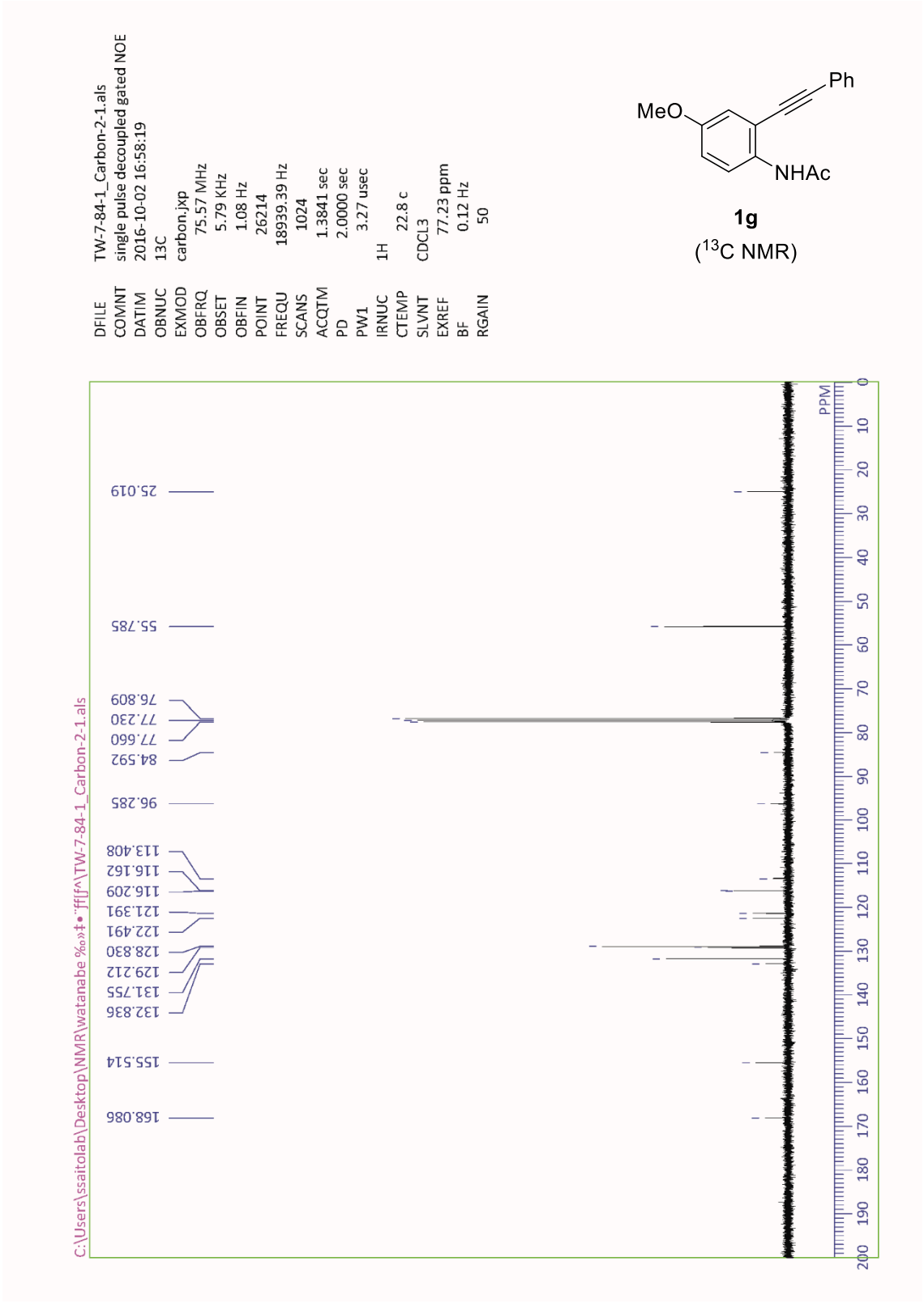
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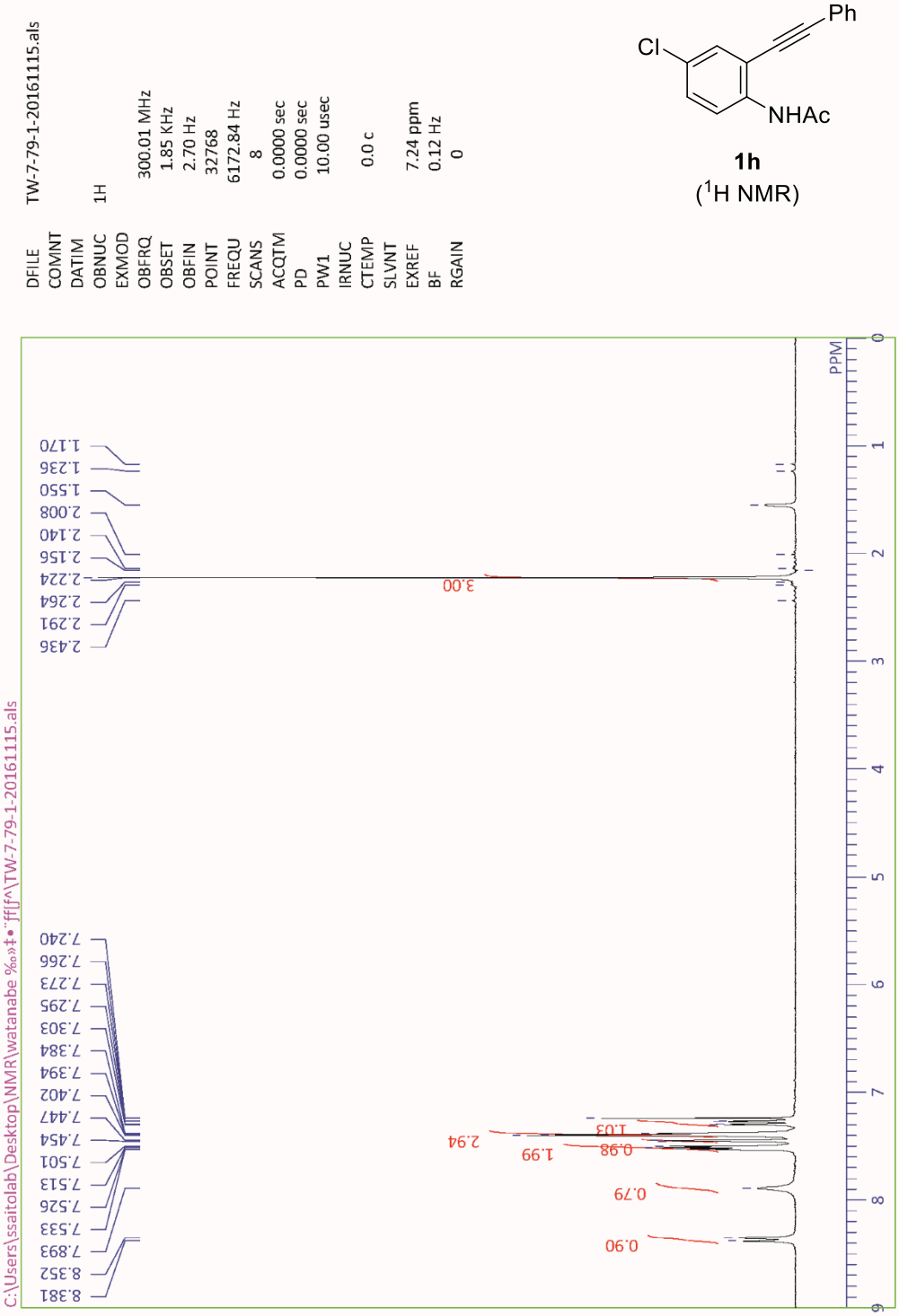
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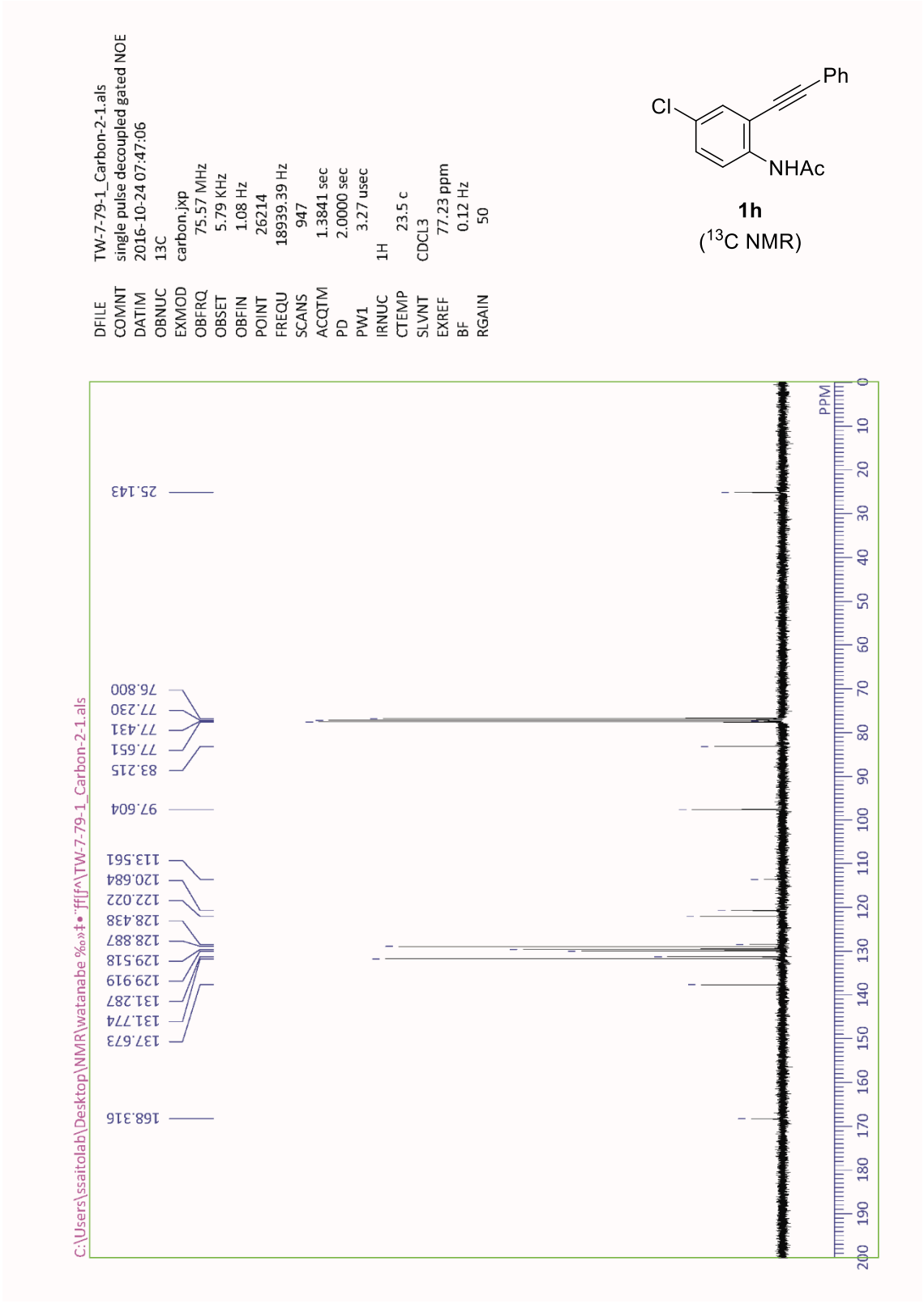
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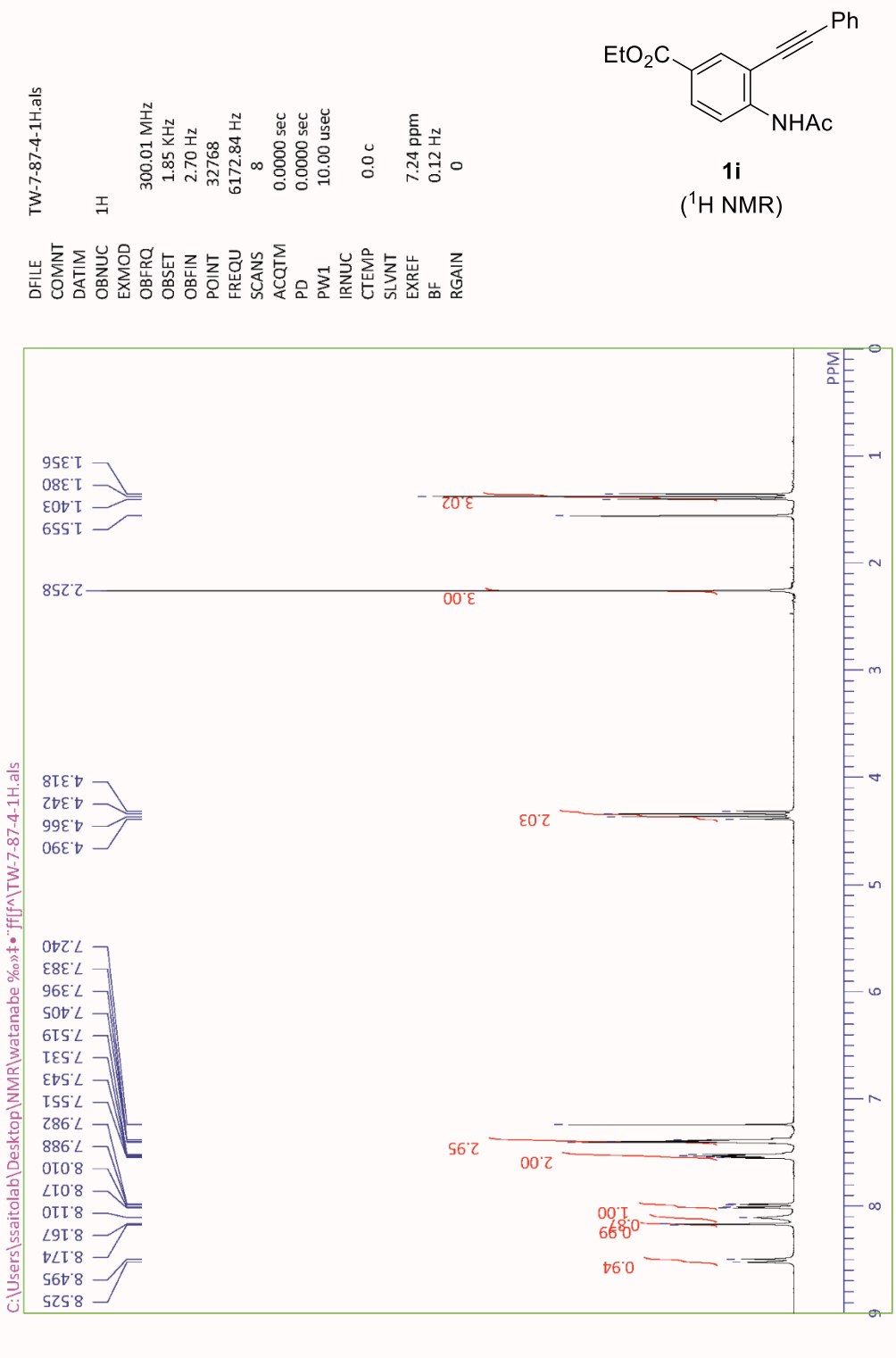
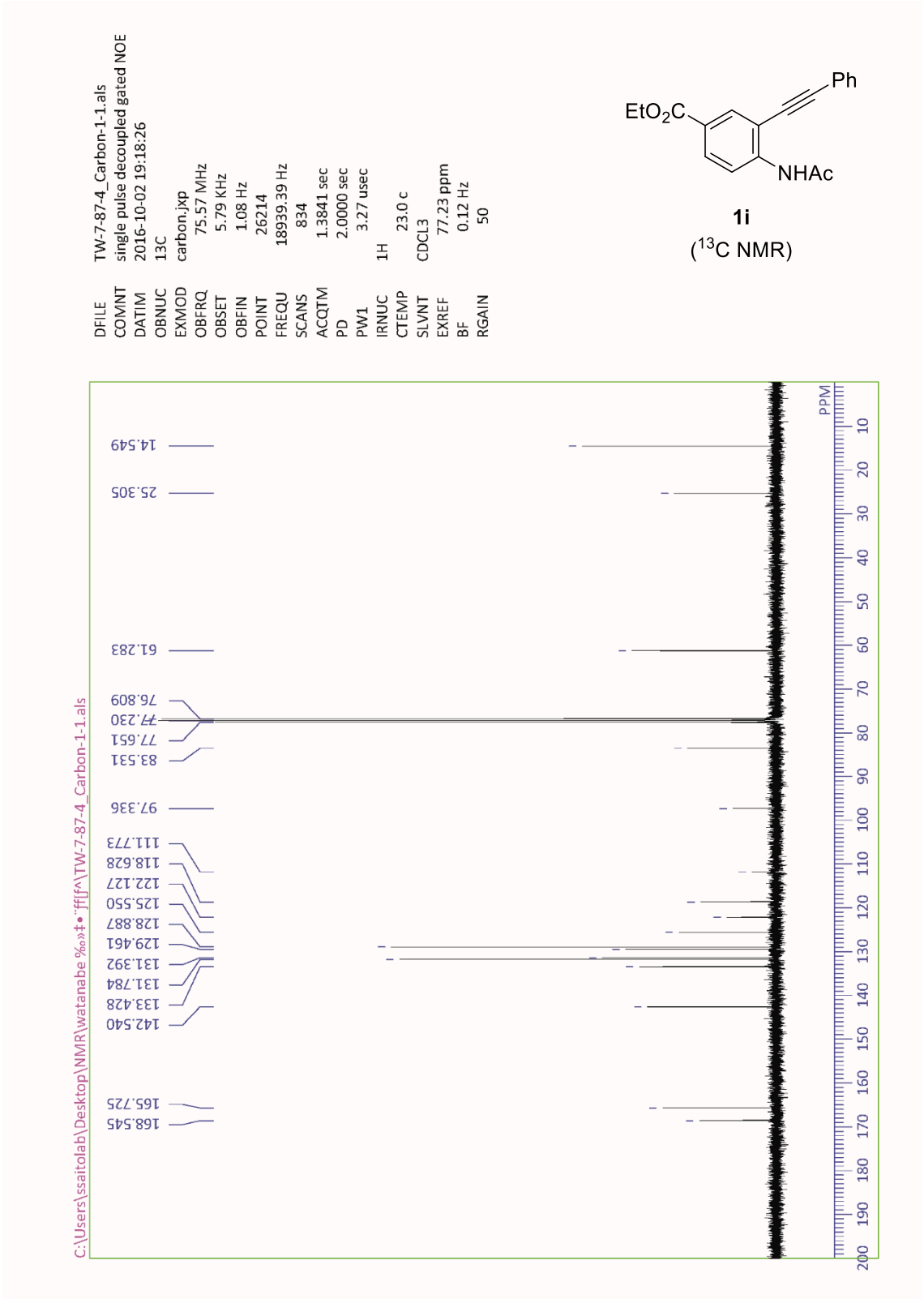
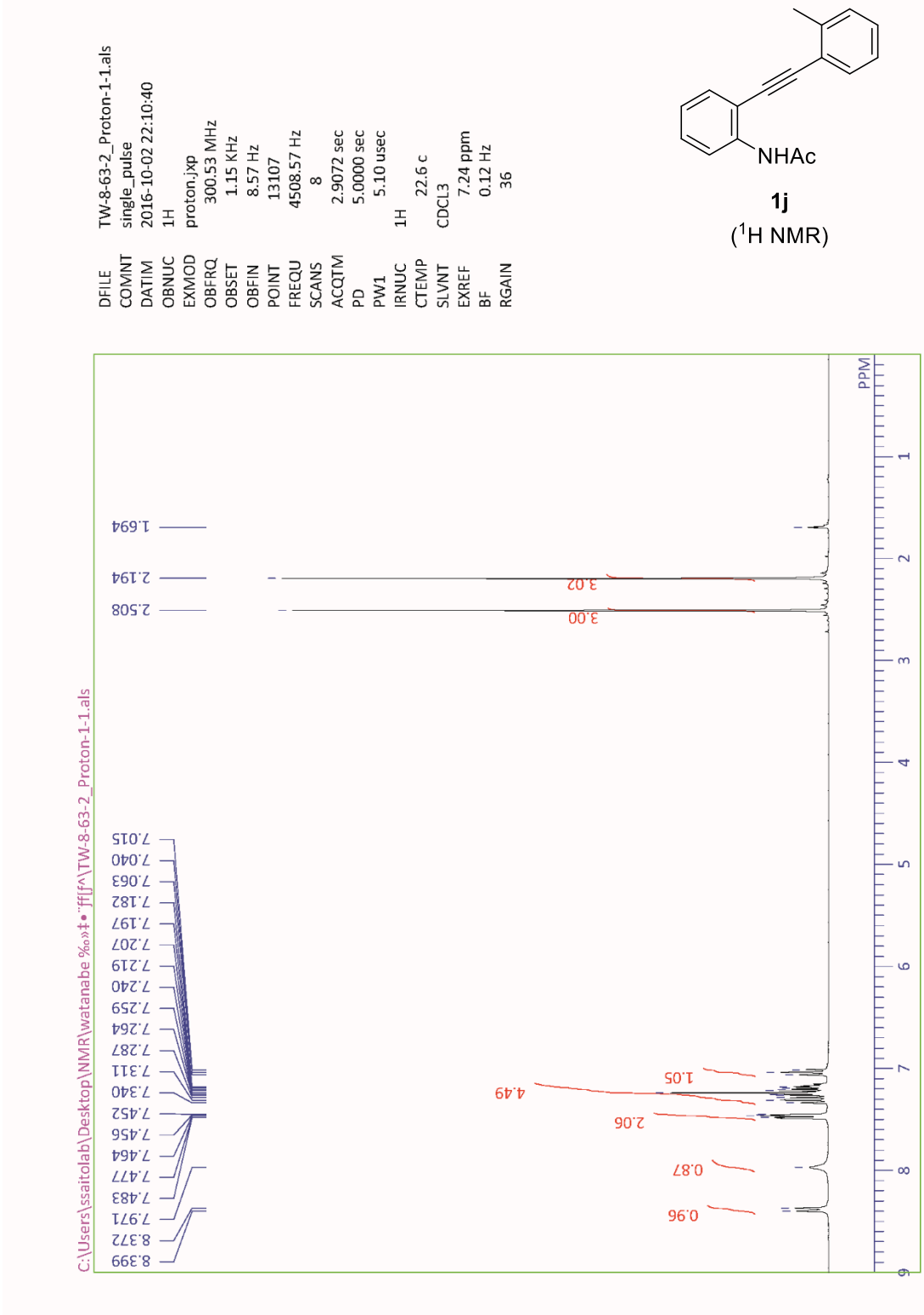
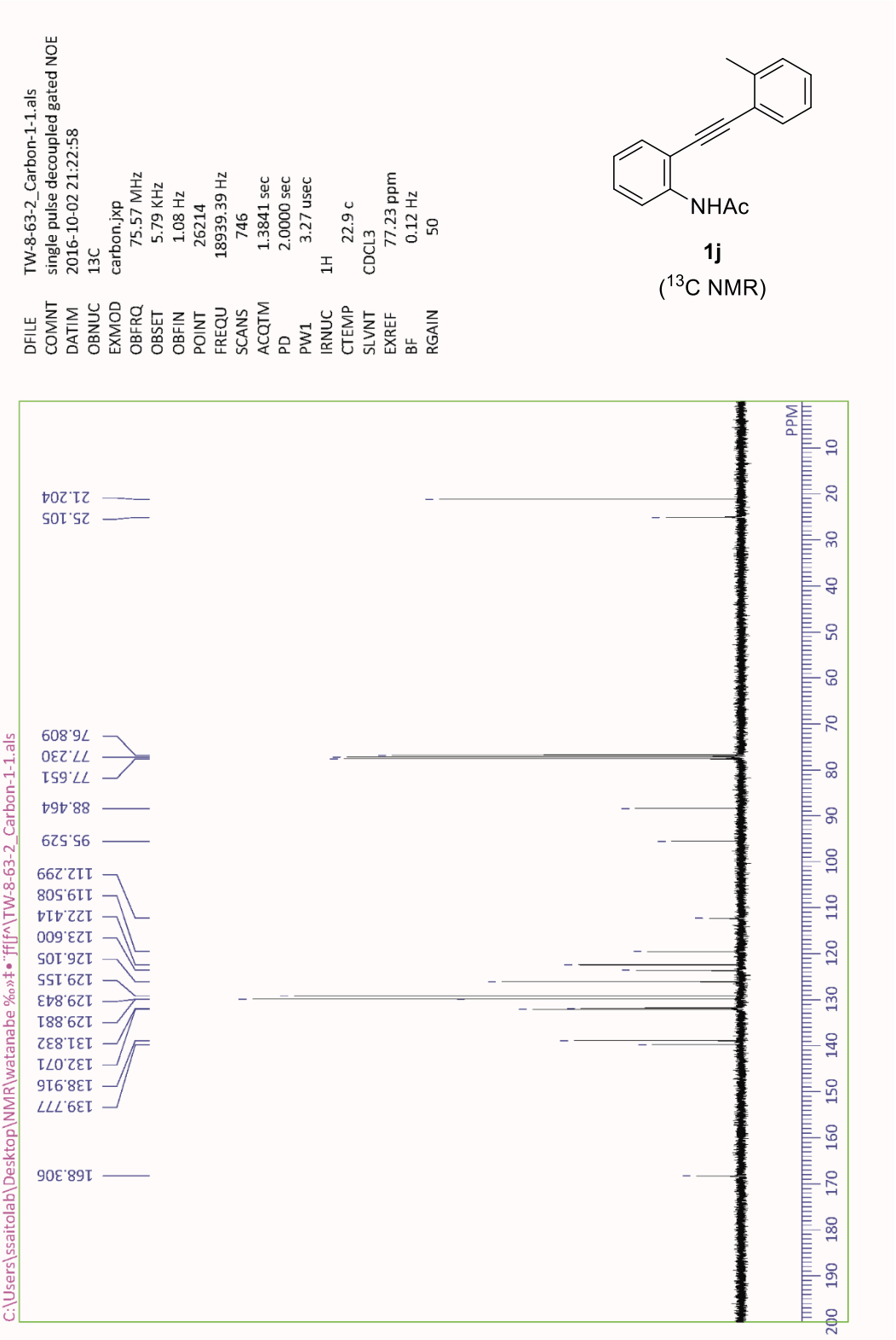
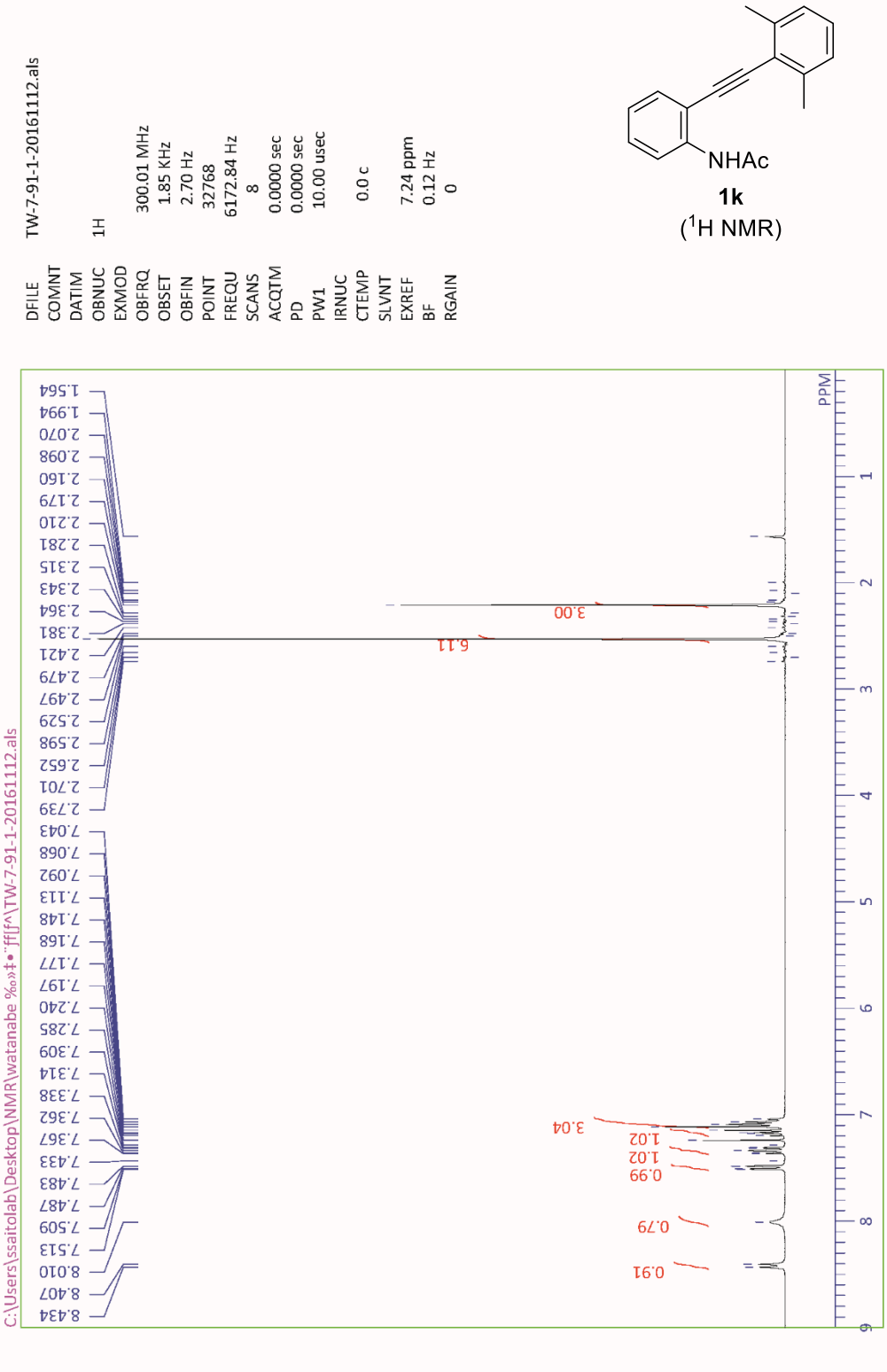
COMNT single pulse decoupled gated NOE
DATIM 2016-10-24 07:47:06
OBNUC 13C
EXMOD carbon.jxp
OBFRQ 75.57 MHz
OBSET 5.79 KHz
OBFIN 1.08 Hz
POINT 26214
FREQU 18939.39 Hz
SCANS 947
ACQTM 1.3841 sec
PD 2.0000 sec
PW1 3.27 usec
IRNUC 1H
CTEMP 23.5 c
SLVNT CDCl3
EXREF 77.23 ppm
BF 0.12 Hz
RGAIN 50
Cl
Ph
NHAc
1h
(13C NMR)
C:\Users\ssaitolab\Desktop\NMR\watanabe %‰»‡•"ff[f^\TW-7-79-1_Carbon-2-1.als
25.143
76.800
77.230
77.431
77.651
83.215
97.604
113.561
120.684
122.022
128.438
128.887
129.518
129.919
131.287
131.774
137.673
168.316
PPM

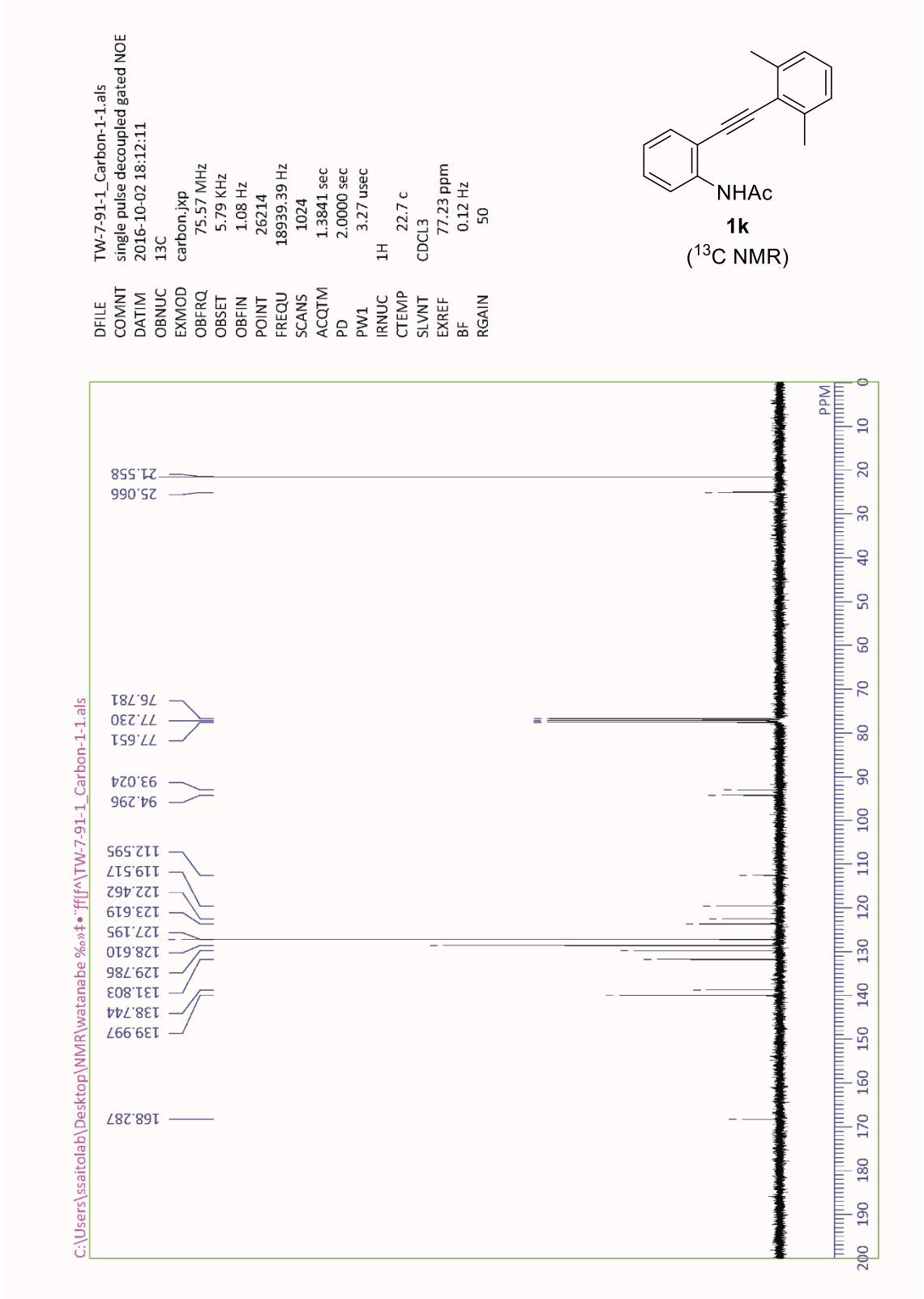

Ph
EtO2C
NHAc
1i
(1H NMR)
DFILE TW-7-87-4-1H.als
COMNT
DATIM
OBNUC 1H
EXMOD
OBFRQ 300.01 MHz
OBSET 1.85 KHz
OBFIN 2.70 Hz
POINT 32768
FREQU 6172.84 Hz
SCANS 8
ACQTM 0.0000 sec
PD 0.0000 sec
PW1 10.00 usec
IRNUC
CTEMP 0.0 c
SLVNT
EXREF 7.24 ppm
BF 0.12 Hz
RGAIN 0
C:\Users\ssaitolab\Desktop\NMR\watanabe ‰»‡•"ff[f^\TW-7-87-4-1H.als
PPM

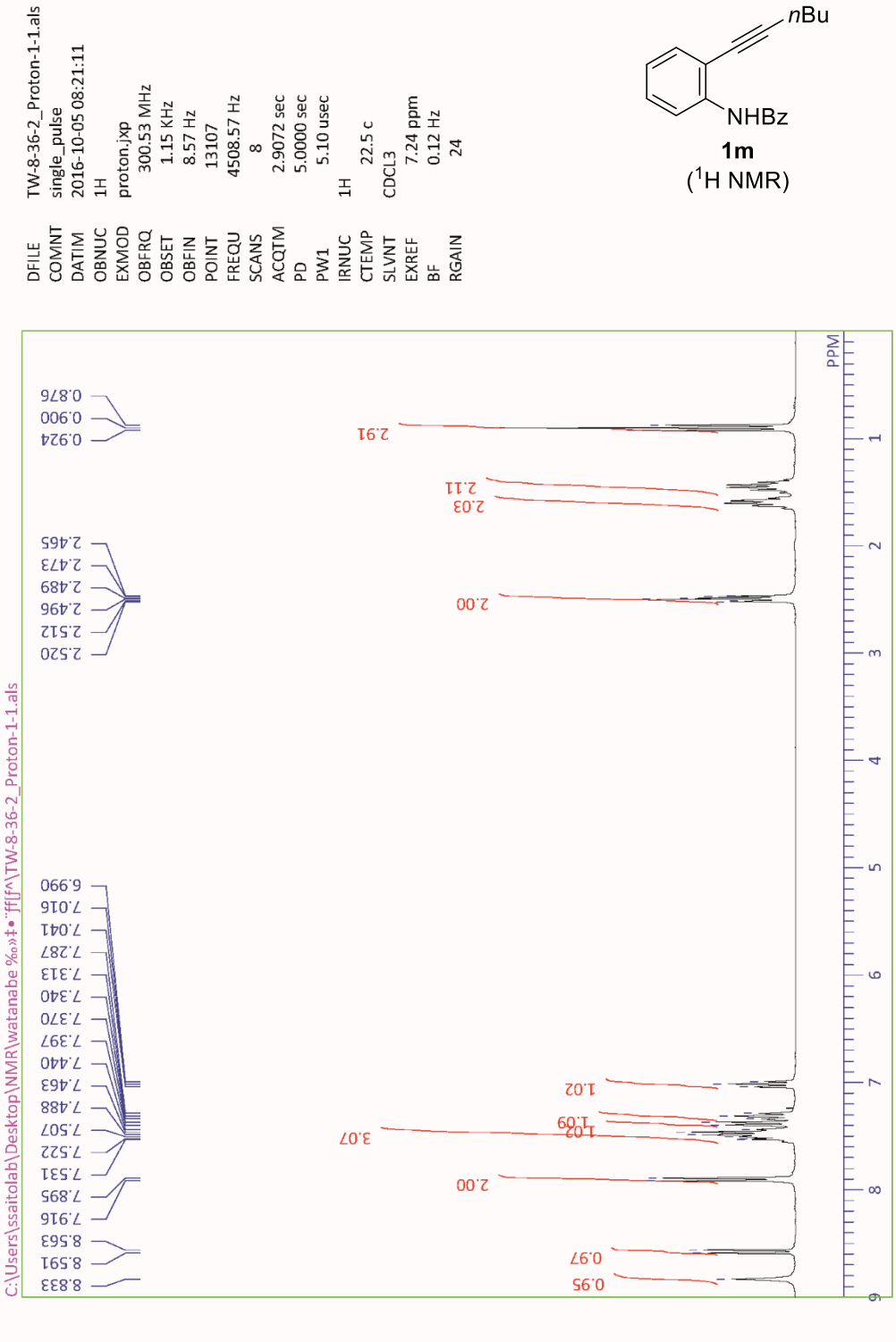

DFILE TW-7-87-4_Carbon-1-1.als
COMNT single pulse decoupled gated NOE
DATIM 2016-10-02 19:18:26
OBNUC 13C
EXMOD carbon.jxp
OBFRQ 75.57 MHz
OBSET 5.79 KHz
OBFIN 1.08 Hz
POINT 26214
FREQU 18939.39 Hz
SCANS 834
ACQTM 1.3841 sec
PD 2.0000 sec
PW1 3.27 usec
IRNUC 1H
CTEMP 23.0 c
SLVNT CDCl3
EXREF 77.23 ppm
BF 0.12 Hz
RGAIN 50
EtO2C
Ph
NHAc
1i
(13C NMR)
C:\Users\ssaitolab\Desktop\NMR\watanabe %»‡•"ff[^\TW-7-87-4_Carbon-1-1.als
14.549
25.305
61.283
76.809
77.230
77.651
83.531
97.336
111.773
118.628
122.127
125.550
128.887
129.461
131.392
131.784
133.428
142.540
165.725
168.545
PPM


DFILE TW-8-63-2_Proton-1-1.als
COMNT single_pulse
DATIM 2016-10-02 22:10:40
OBNUC 1H
EXMOD proton.jxp
OBFRQ 300.53 MHz
OBSET 1.15 KHz
OBFIN 8.57 Hz
POINT 13107
FREQU 4508.57 Hz
SCANS 8
ACQTM 2.9072 sec
PD 5.0000 sec
PW1 5.10 usec
IRNUC 1H
CTEMP 22.6 c
SLVNT CDCl3
EXREF 7.24 ppm
BF 0.12 Hz
RGAIN 36
NHAc
1j
(1H NMR)
C:\Users\ssaitolab\Desktop\NMR\watanabe %‰»‡•¨ff[f^\TW-8-63-2_Proton-1-1.als
PPM


DFILE TW-8-63-2_Carbon-1-1.als
COMNT single pulse decoupled gated NOE
DATIM 2016-10-02 21:22:58
OBNUC 13C
EXMOD carbon.jxp
OBFRQ 75.57 MHz
OBSET 5.79 KHz
OBFIN 1.08 Hz
POINT 26214
FREQU 18939.39 Hz
SCANS 746
ACQTM 1.3841 sec
PD 2.0000 sec
PW1 3.27 usec
IRNUC 1H
CTEMP 22.9 c
SLVNT CDCl3
EXREF 77.23 ppm
BF 0.12 Hz
RGAIN 50
NHAc
1j
(^{13}C NMR)
C:\Users\ssaitolab\Desktop\NMR\watanabe %»‡•"ff[f^\TW-8-63-2_Carbon-1-1.als
21.204
25.105
76.809
77.230
77.651
88.464
95.529
112.299
119.508
122.414
123.600
126.105
129.155
129.843
129.881
131.832
132.071
138.916
139.777
168.306
PPM
10
20
30
40
50
60
70
80
90
100
110
120
130
140
150
160
170
180
190
200


NHAc
1k
(1H NMR)
DFILE TW-7-91-1-20161112.als
COMNT
DATIM
OBNUC 1H
EXMOD
OBFRQ 300.01 MHz
OBSET 1.85 KHz
OBFIN 2.70 Hz
POINT 32768
FREQU 6172.84 Hz
SCANS 8
ACQTM 0.0000 sec
PD 0.0000 sec
PW1 10.00 usec
IRNUC
CTEMP 0.0 c
SLVNT
EXREF 7.24 ppm
BF 0.12 Hz
RGAIN 0
C:\Users\ssaitolab\Desktop\NMR\watanabe ‰»‡•"ff[f^\TW-7-91-1-20161112.als
PPM
3.00
6.11
3.04
1.02
1.02
0.99
0.79
0.91


DFILE TW-7-91-1_Carbon-1-1.als
COMNT single pulse decoupled gated NOE
DATIM 2016-10-02 18:12:11
OBNUC 13C
EXMOD carbon.jxp
OBFRQ 75.57 MHz
OBSET 5.79 KHz
OBFIN 1.08 Hz
POINT 26214
FREQU 18939.39 Hz
SCANS 1024
ACQTM 1.3841 sec
PD 2.0000 sec
PW1 3.27 usec
IRNUC 1H
CTEMP 22.7 c
SLVNT CDCl3
EXREF 77.23 ppm
BF 0.12 Hz
RGAIN 50
NHAc
1k
(13C NMR)
C:\Users\ssaitolab\Desktop\NMR\watanabe %»‡•"ff[f^\TW-7-91-1_Carbon-1-1.als
21.558
25.066
76.781
77.230
77.651
93.024
94.296
112.595
119.517
122.462
123.619
127.195
128.610
129.786
131.803
138.744
139.997
168.287
PPM


nBu
NHBz
1m
(1H NMR)
DFILE TW-8-36-2_Proton-1-1.als
COMNT single_pulse
DATIM 2016-10-05 08:21:11
OBNUC 1H
EXMOD proton.jxp
OBFRQ 300.53 MHz
OBSET 1.15 KHz
OBFIN 8.57 Hz
POINT 13107
FREQU 4508.57 Hz
SCANS 8
ACQTM 2.9072 sec
PD 5.0000 sec
PW1 5.10 usec
IRNUC 1H
CTEMP 22.5 c
SLVNT CDCl3
EXREF 7.24 ppm
BF 0.12 Hz
RGAIN 24
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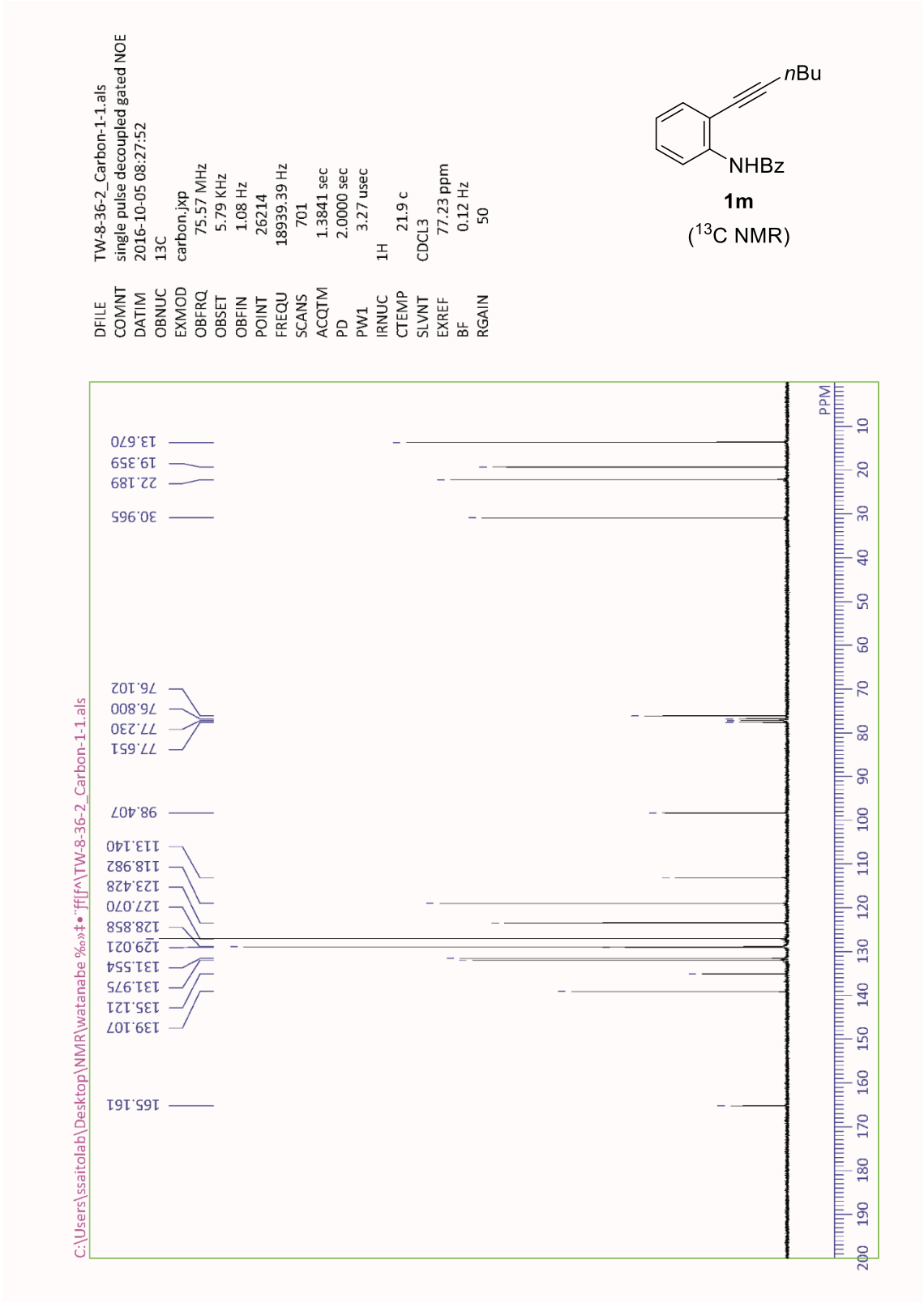
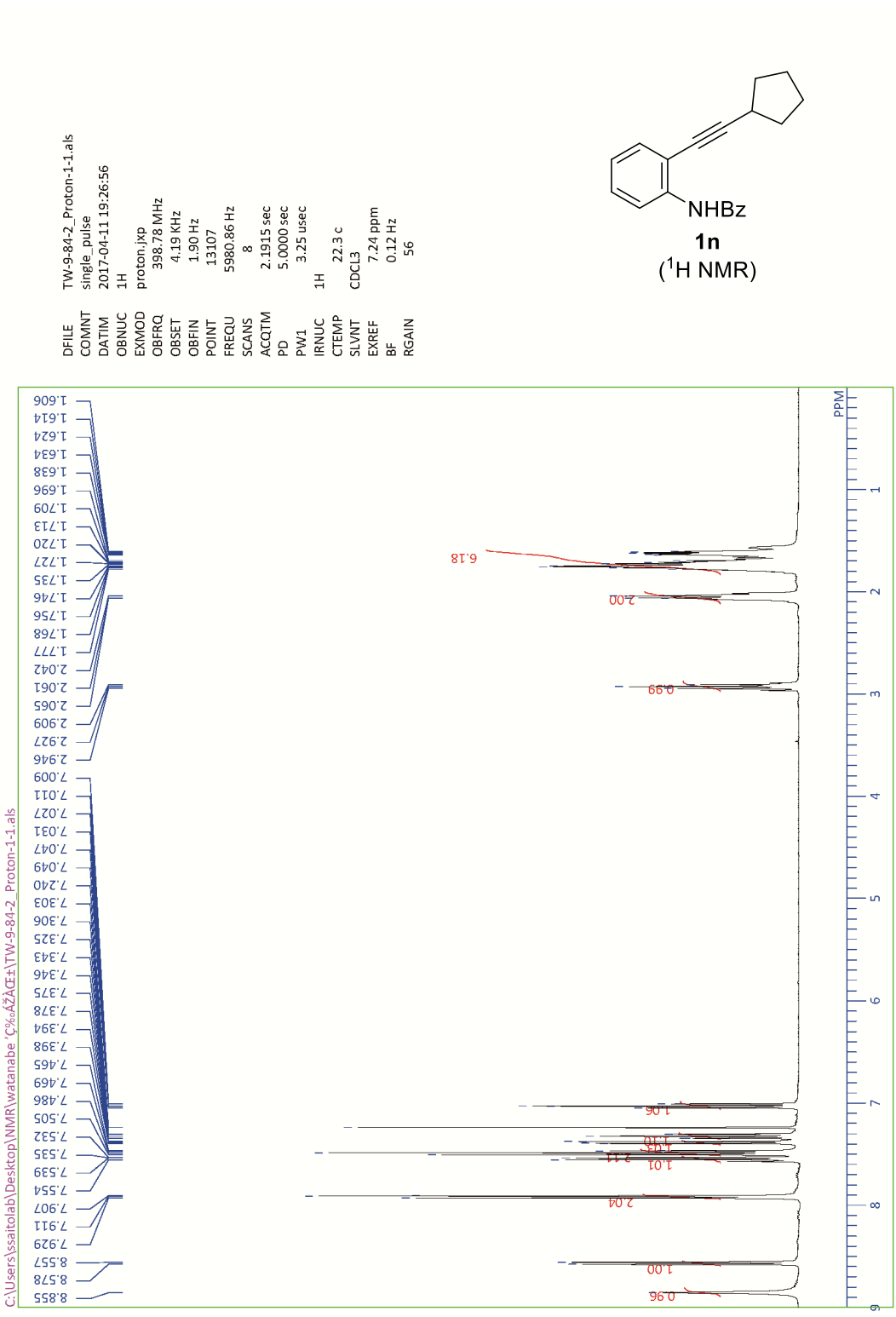
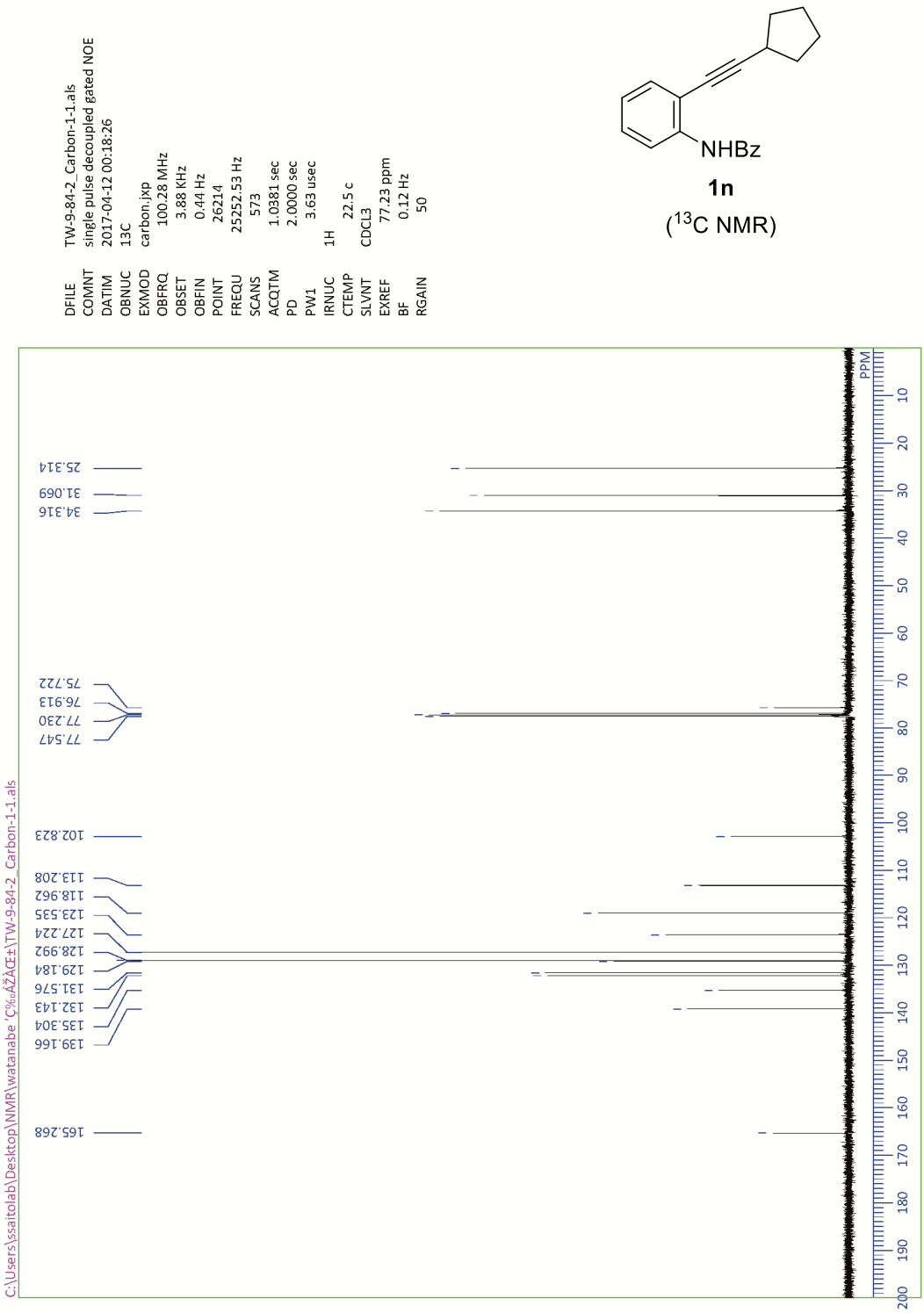
PPM


DFILE TW-8-36-2_Carbon-1-1.als
COMNT single pulse decoupled gated NOE
DATIM 2016-10-05 08:27:52
OBNUC 13C
EXMOD carbon.jxp
OBFRQ 75.57 MHz
OBSET 5.79 KHz
OBFIN 1.08 Hz
POINT 26214
FREQU 18939.39 Hz
SCANS 701
ACQTM 1.3841 sec
PD 2.0000 sec
PW1 3.27 usec
IRNUC 1H
CTEMP 21.9 c
SLVNT CDCl3
EXREF 77.23 ppm
BF 0.12 Hz
RGAIN 50
nBu
NHBz
1m
(13C NMR)
C:\Users\ssaitolab\Desktop\NMR\watanabe %»‡•ff[f^\TW-8-36-2_Carbon-1-1.als
13.670
19.359
22.189
30.965
76.102
76.800
77.230
77.651
98.407
113.140
118.982
123.428
127.070
128.858
129.021
131.554
131.975
135.121
139.107
165.161
PPM


DFILE TW-9-84-2_Proton-1-1.als
COMNT single_pulse
DATIM 2017-04-11 19:26:56
OBNUC 1H
EXMOD proton.jxp
OBFRQ 398.78 MHz
OBSET 4.19 KHz
OBFIN 1.90 Hz
POINT 13107
FREQU 5980.86 Hz
SCANS 8
ACQTM 2.1915 sec
PD 5.0000 sec
PW1 3.25 usec
IRNUC 1H
CTEMP 22.3 c
SLVNT CDCL3
EXREF 7.24 ppm
BF 0.12 Hz
RGAIN 56
NHBz
1n
(1H NMR)
C:\Users\ssaitolab\Desktop\NMR\watanabe 'Ç‰ÁŽÄŒ±\TW-9-84-2_Proton-1-1.als
PPM


NHBz
1n
(13C NMR)
DFILE TW-9-84-2_Carbon-1-1.als
COMNT single pulse decoupled gated NOE
DATIM 2017-04-12 00:18:26
OBNUC 13C
EXMOD carbon.jxp
OBFRQ 100.28 MHz
OBSET 3.88 KHz
OBFIN 0.44 Hz
POINT 26214
FREQU 25252.53 Hz
SCANS 573
ACQTM 1.0381 sec
PD 2.0000 sec
PW1 3.63 usec
IRNUC 1H
CTEMP 22.5 c
SLVNT CDCL3
EXREF 77.23 ppm
BF 0.12 Hz
RGAIN 50
25.314
31.069
34.316
75.722
76.913
77.230
77.547
102.823
113.208
118.962
123.535
127.224
128.992
129.184
131.576
132.143
135.304
139.166
165.268
PPM
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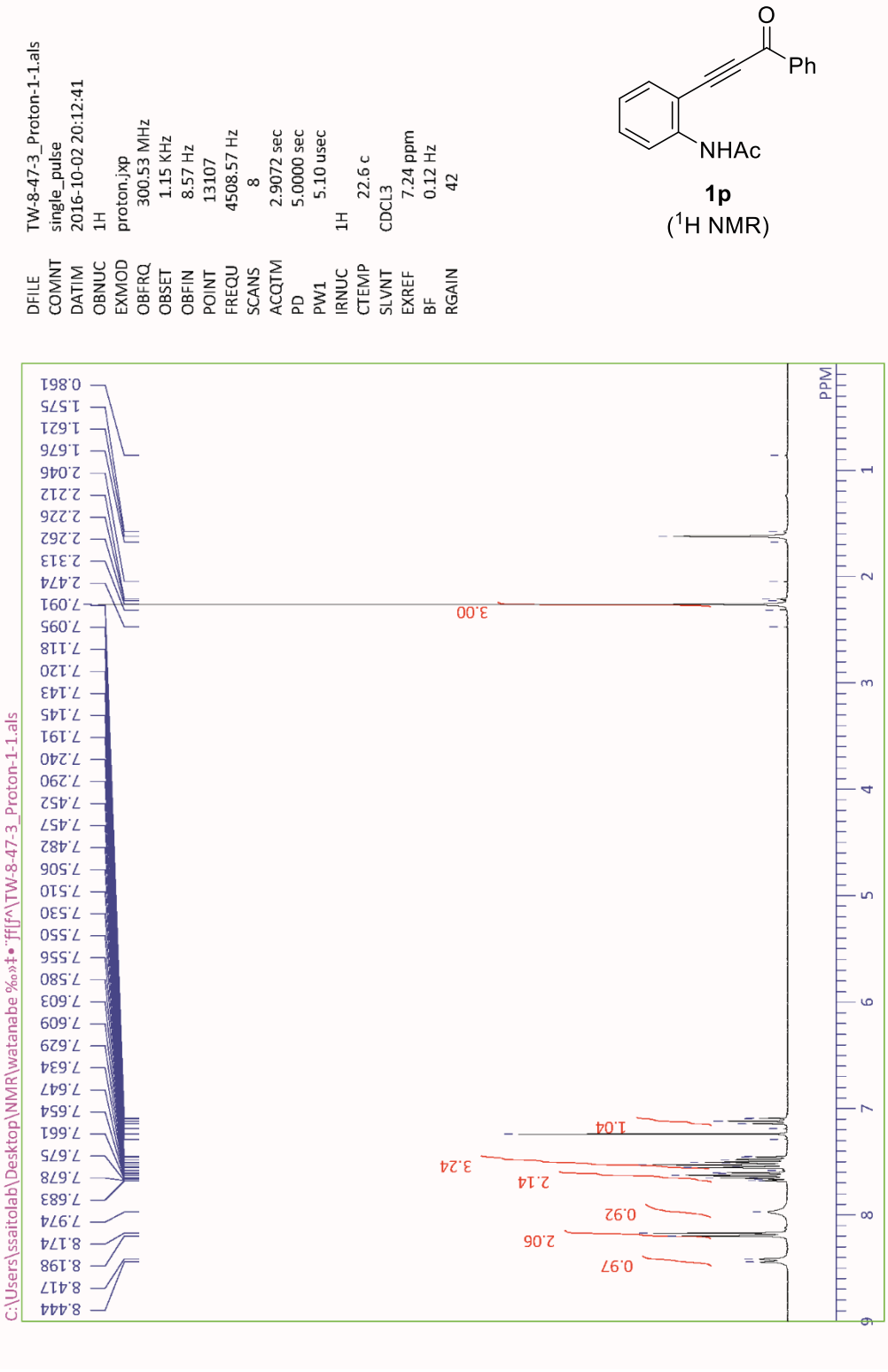
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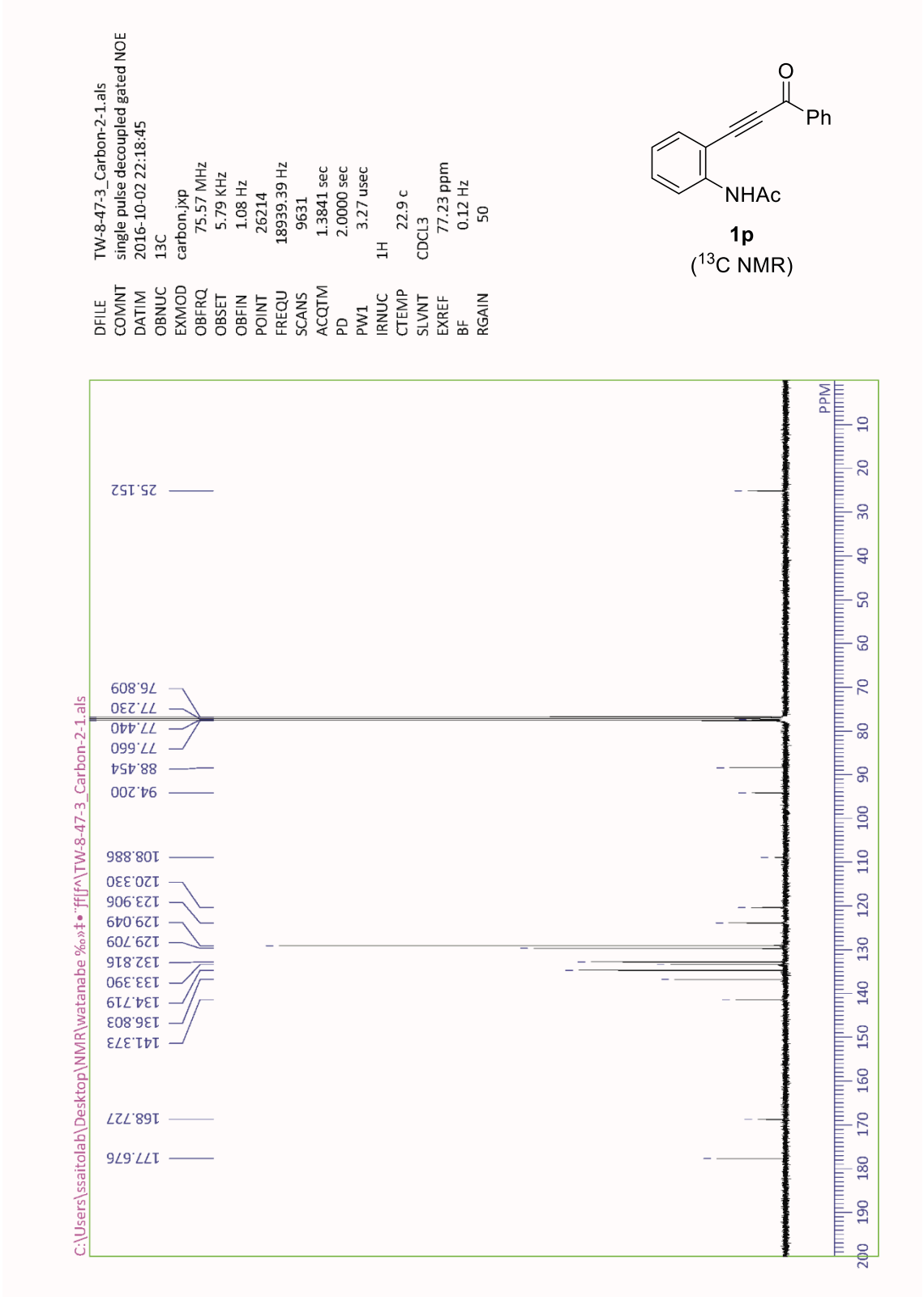
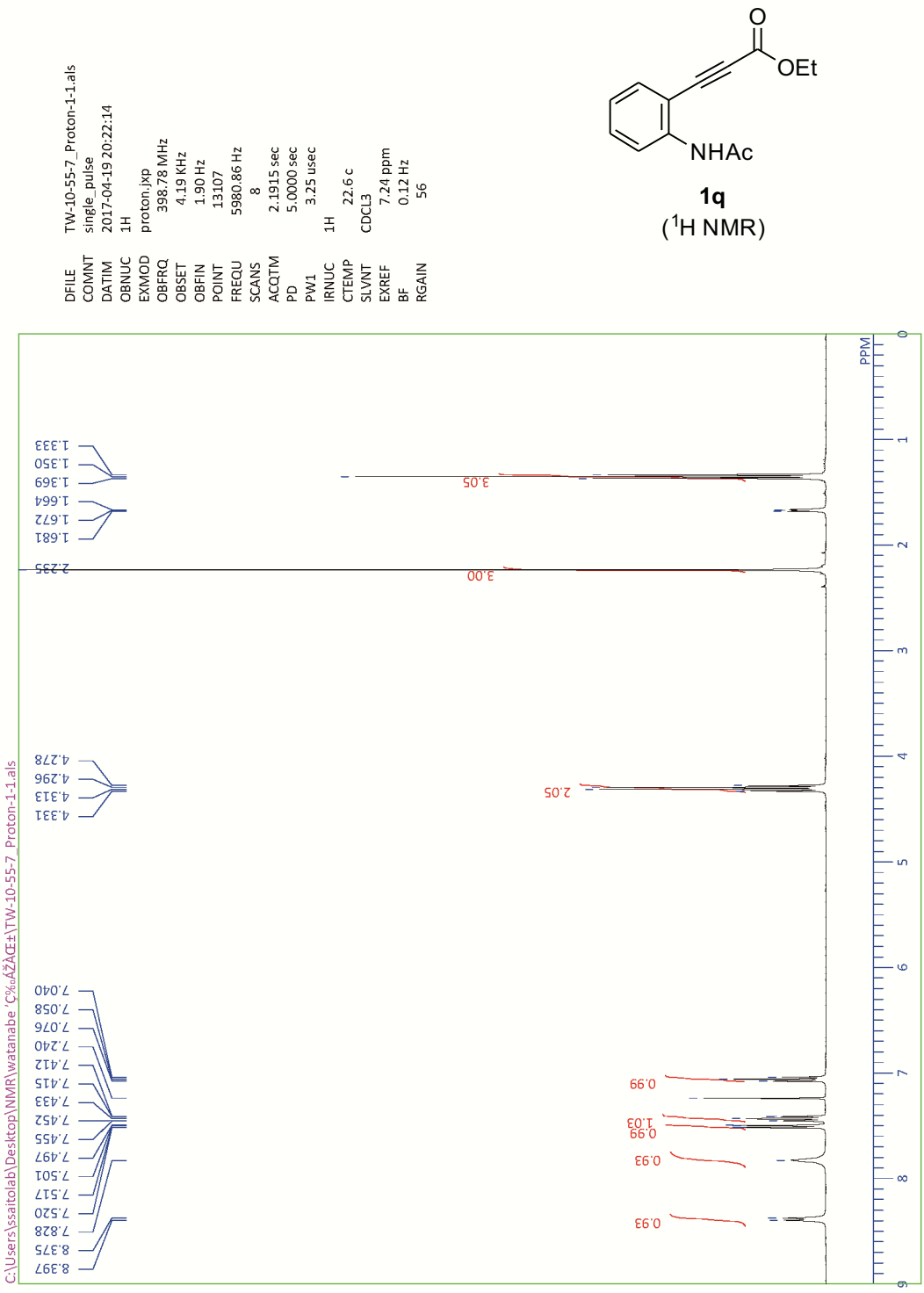
COMNT single_pulse
DATIM 2016-10-02 20:12:41
OBNUC 1H
EXMOD proton.jxp
OBFRQ 300.53 MHz
OBSET 1.15 KHz
OBFIN 8.57 Hz
POINT 13107
FREQU 4508.57 Hz
SCANS 8
ACQTM 2.9072 sec
PD 5.0000 sec
PW1 5.10 usec
IRNUC 1H
CTEMP 22.6 c
SLVNT CDCl3
EXREF 7.24 ppm
BF 0.12 Hz
RGAIN 42
O
Ph
NHAc
1p
(1H NMR)
C:\Users\ssaitolab\Desktop\NMR\watanabe %‰»‡•"ff[f^\TW-8-47-3_Proton-1-1.als
PPM
3.00
1.04
3.24
2.14
0.92
2.06
0.97


DFILE TW-8-47-3_Carbon-2-1.als
COMNT single pulse decoupled gated NOE
DATIM 2016-10-02 22:18:45
OBNUC 13C
EXMOD carbon.jxp
OBFRQ 75.57 MHz
OBSET 5.79 KHz
OBFIN 1.08 Hz
POINT 26214
FREQU 18939.39 Hz
SCANS 9631
ACQTM 1.3841 sec
PD 2.0000 sec
PW1 3.27 usec
IRNUC 1H
CTEMP 22.9 c
SLVNT CDCl3
EXREF 77.23 ppm
BF 0.12 Hz
RGAIN 50
O
Ph
NHAc
1p
(13C NMR)
C:\Users\ssaitolab\Desktop\NMR\watanabe %»‡•"ff[^\TW-8-47-3_Carbon-2-1.als
PPM


O
OEt
NHAc
1q
(1H NMR)
DFILE TW-10-55-7_Proton-1-1.als
COMNT single_pulse
DATIM 2017-04-19 20:22:14
OBNUC 1H
EXMOD proton.jxp
OBFRQ 398.78 MHz
OBSET 4.19 KHz
OBFIN 1.90 Hz
POINT 13107
FREQU 5980.86 Hz
SCANS 8
ACQTM 2.1915 sec
PD 5.0000 sec
PW1 3.25 usec
IRNUC 1H
CTEMP 22.6 c
SLVNT CDCL3
EXREF 7.24 ppm
BF 0.12 Hz
RGAIN 56
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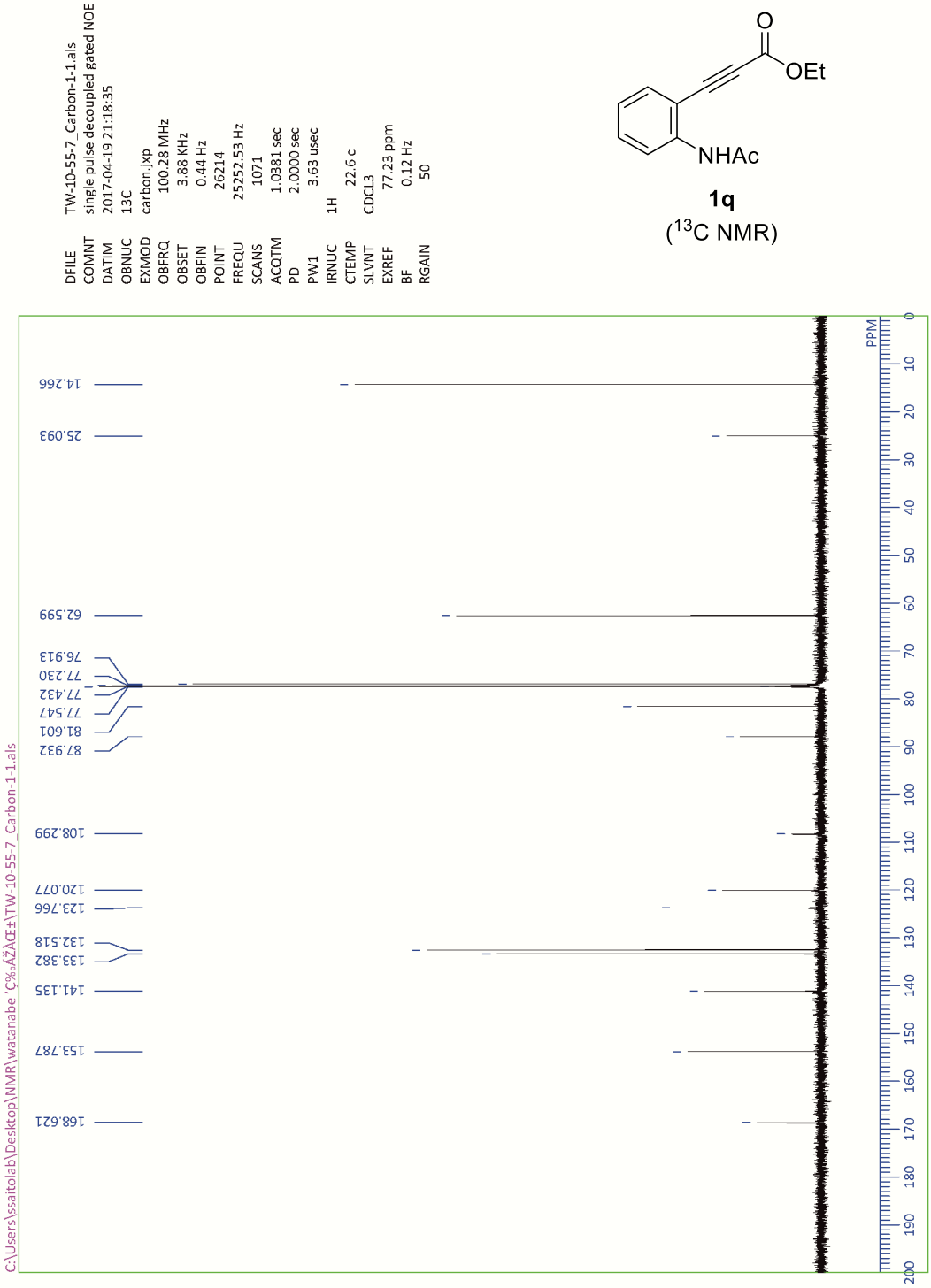
PPM


DFILE TW-10-55-7_Carbon-1-1.als
COMNT single pulse decoupled gated NOE
DATIM 2017-04-19 21:18:35
OBNUC 13C
EXMOD carbon.jxp
OBFRQ 100.28 MHz
OBSET 3.88 KHz
OBFIN 0.44 Hz
POINT 26214
FREQU 25252.53 Hz
SCANS 1071
ACQTM 1.0381 sec
PD 2.0000 sec
PW1 3.63 usec
IRNUC 1H
CTEMP 22.6 c
SLVNT CDCl3
EXREF 77.23 ppm
BF 0.12 Hz
RGAIN 50
O
OEt
NHAc
1q
(13C NMR)
14.266
25.093
62.599
76.913
77.230
77.432
77.547
81.601
87.932
108.299
120.077
123.766
132.518
133.382
141.135
153.787
168.621
PPM
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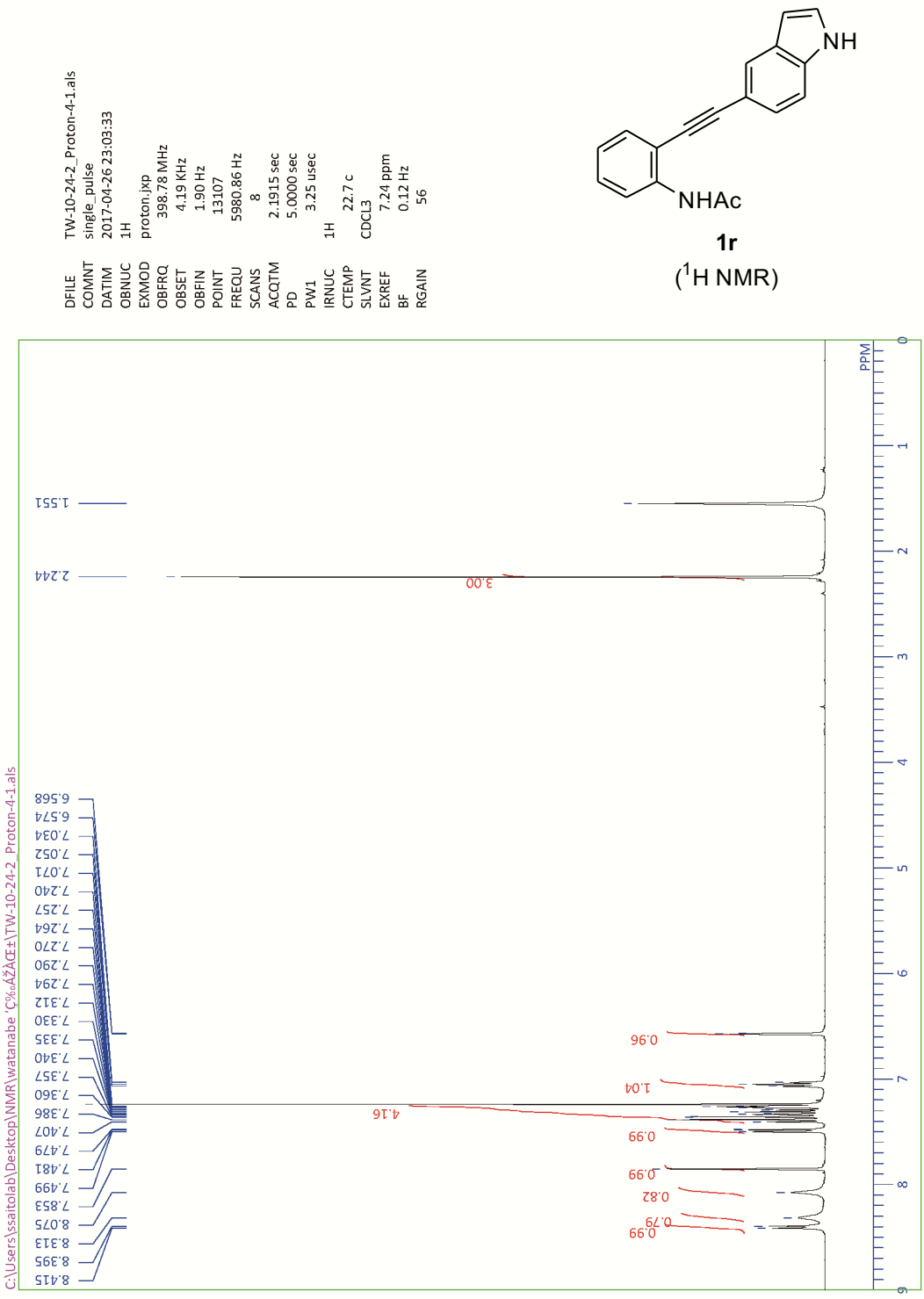
NH
NHAc
1r
(1H NMR)
DFILE TW-10-24-2_Proton-4-1.als
COMNT single_pulse
DATIM 2017-04-26 23:03:33
OBNUC 1H
EXMOD proton.jxp
OBFRQ 398.78 MHz
OBSET 4.19 KHz
OBFIN 1.90 Hz
POINT 13107
FREQU 5980.86 Hz
SCANS 8
ACQTM 2.1915 sec
PD 5.0000 sec
PW1 3.25 usec
IRNUC 1H
CTEMP 22.7 c
SLVNT CDCL3
EXREF 7.24 ppm
BF 0.12 Hz
RGAIN 56
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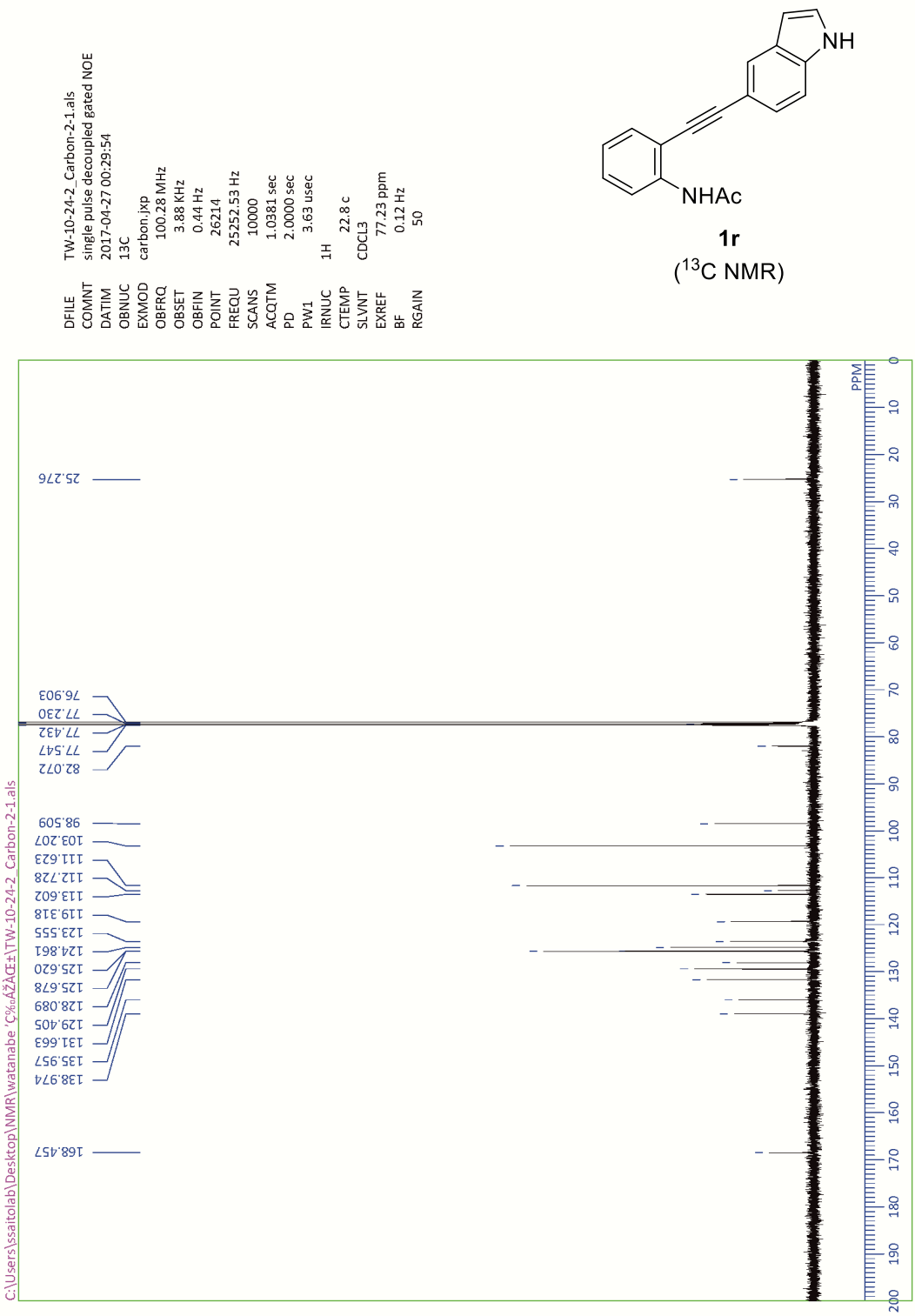
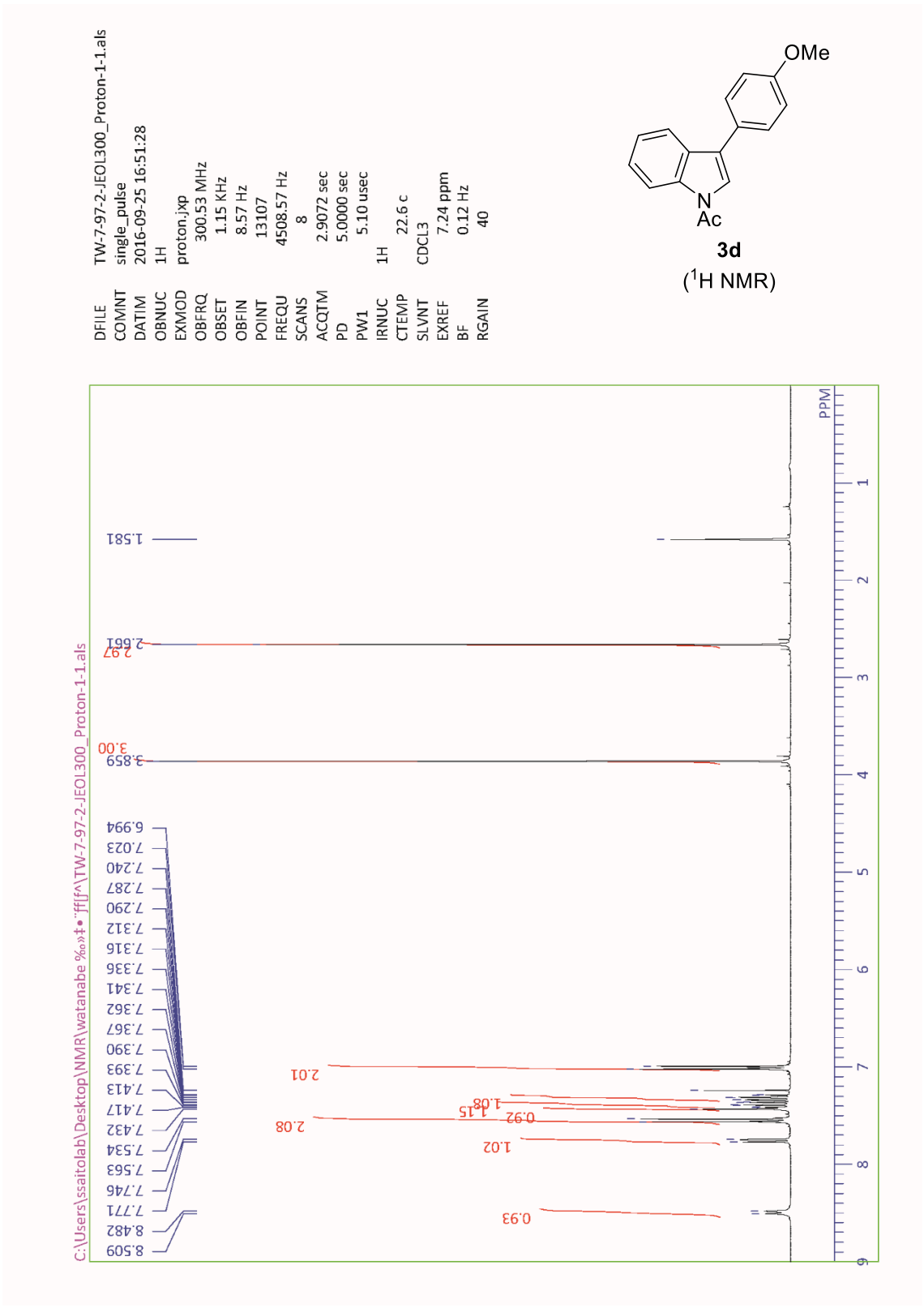
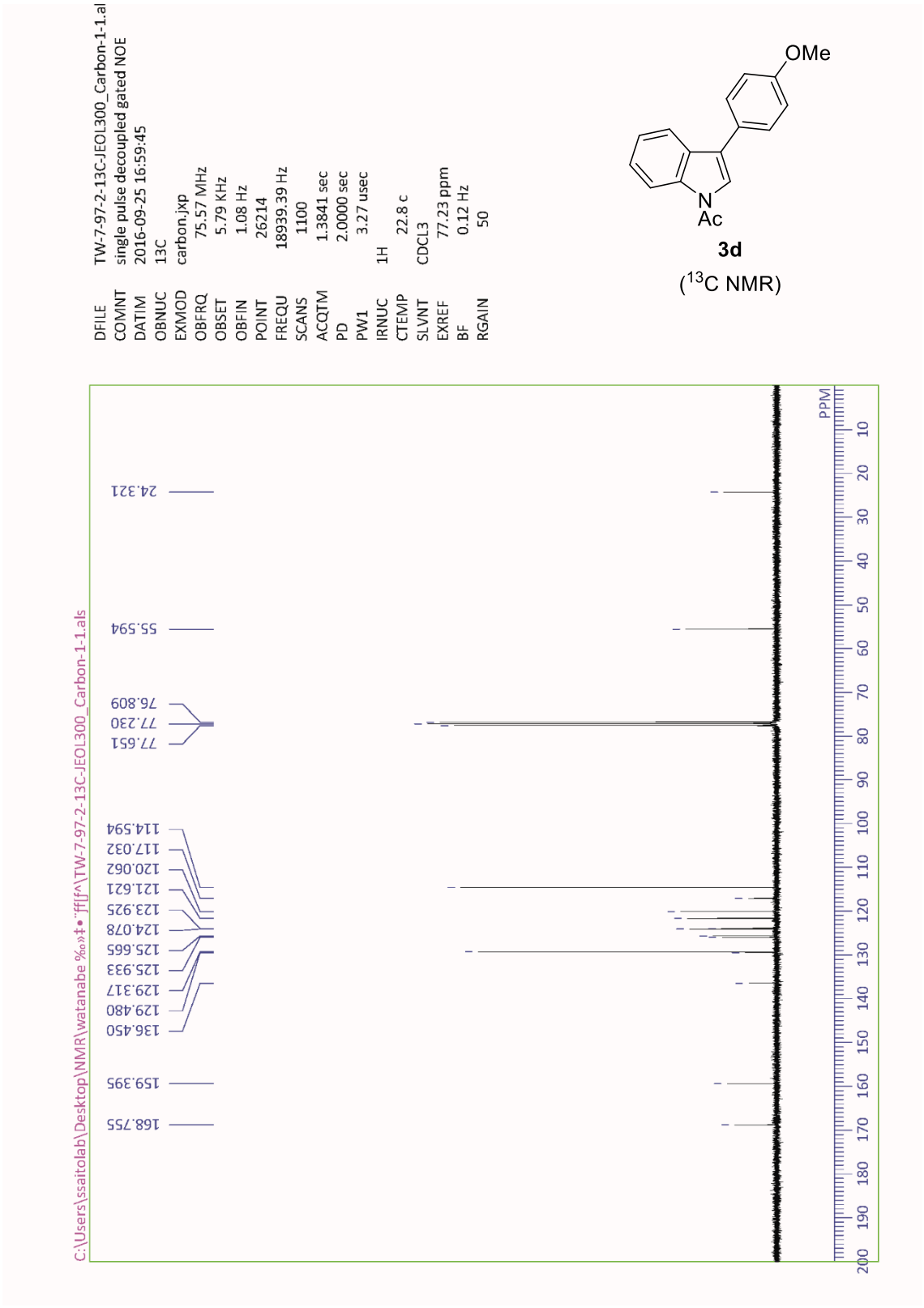
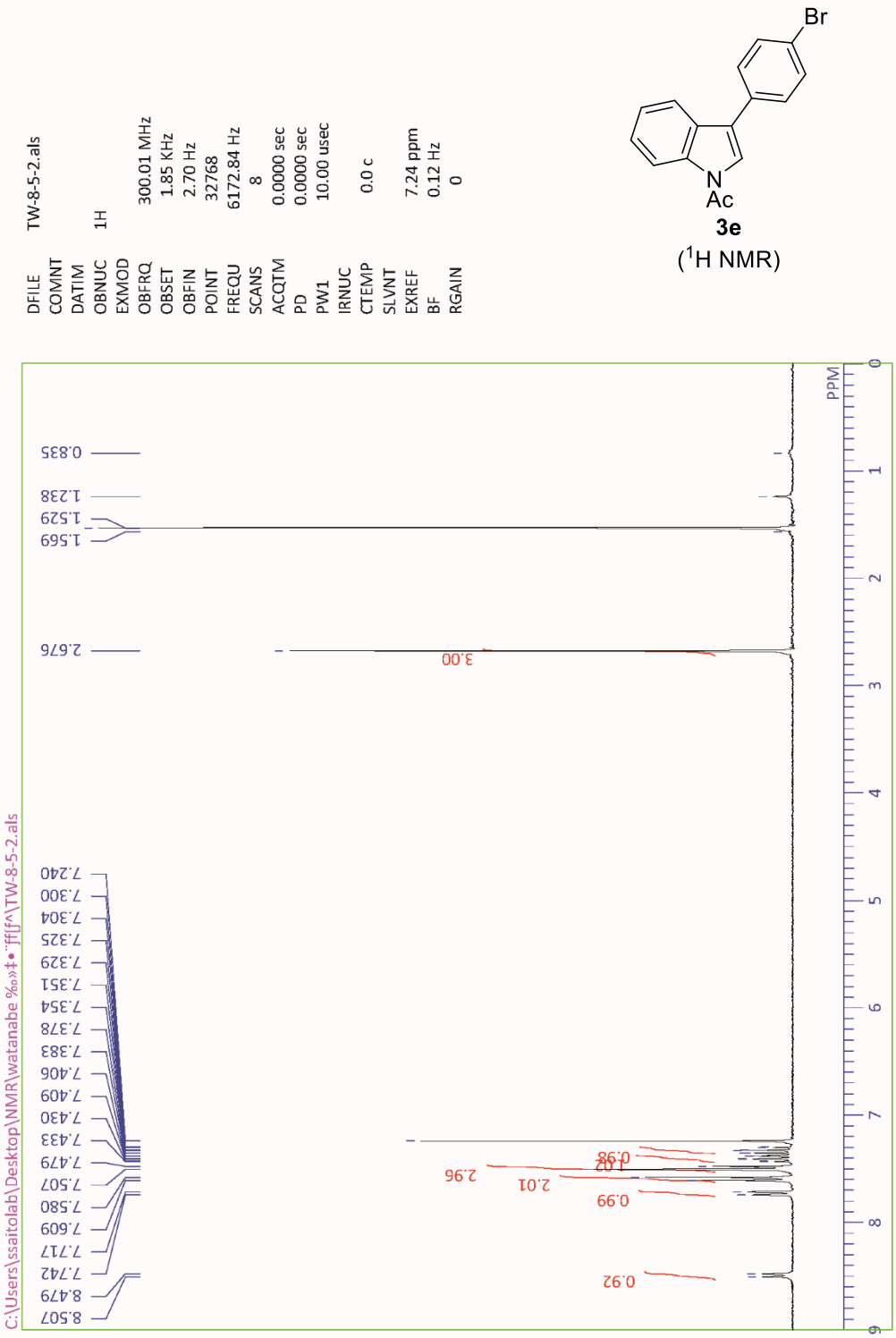
PPM


NH
NHAc
1r
(13C NMR)
DFILE TW-10-24-2_Carbon-2-1.als
COMNT single pulse decoupled gated NOE
DATIM 2017-04-27 00:29:54
OBNUC 13C
EXMOD carbon.jxp
OBFRQ 100.28 MHz
OBSET 3.88 KHz
OBFIN 0.44 Hz
POINT 26214
FREQU 25252.53 Hz
SCANS 10000
ACQTM 1.0381 sec
PD 2.0000 sec
PW1 3.63 usec
IRNUC 1H
CTEMP 22.8 c
SLVNT CDCL3
EXREF 77.23 ppm
BF 0.12 Hz
RGAIN 50
25.276
76.903
77.230
77.432
77.547
82.072
98.509
103.207
111.623
112.728
113.602
119.318
123.555
124.861
125.620
125.678
128.089
129.405
131.663
135.957
138.974
168.457
PPM
C:\Users\ssaitolab\Desktop\NMR\watanabe 'Ç‰ÁŽÀCŒ±\TW-10-24-2_Carbon-2-1.als


DFILE TW-7-97-2-JEOL300_Proton-1-1.als
COMNT single_pulse
DATIM 2016-09-25 16:51:28
OBNUC 1H
EXMOD proton.jxp
OBFRQ 300.53 MHz
OBSET 1.15 KHz
OBFIN 8.57 Hz
POINT 13107
FREQU 4508.57 Hz
SCANS 8
ACQTM 2.9072 sec
PD 5.0000 sec
PW1 5.10 usec
IRNUC 1H
CTEMP 22.6 c
SLVNT CDCl3
EXREF 7.24 ppm
BF 0.12 Hz
RGAIN 40
OMe
N
Ac
3d
(1H NMR)
C:\Users\ssaitolab\Desktop\NMR\watanabe %‰»‡•"ff[f^\TW-7-97-2-JEOL300_Proton-1-1.als
PPM


TW-7-97-2-13C-JEOL300_Carbon-1-1.al
single pulse decoupled gated NOE
2016-09-25 16:59:45
13C
carbon.jxp
75.57 MHz
5.79 KHz
1.08 Hz
26214
18939.39 Hz
1100
1.3841 sec
2.0000 sec
3.27 usec
1H
22.8 c
CDCl3
77.23 ppm
0.12 Hz
50
DFILE
COMNT
DATIM
OBNUC
EXMOD
OBFRQ
OBSET
OBFIN
POINT
FREQU
SCANS
ACQTM
PD
PW1
IRNUC
CTEMP
SLVNT
EXREF
BF
RGAIN
OMe
N
Ac
3d
(13C NMR)
C:\Users\ssaitolab\Desktop\NMR\watanabe %»‡•ff[f^\TW-7-97-2-13C-JEOL300_Carbon-1-1.als
24.321
55.594
76.809
77.230
77.651
114.594
117.032
120.062
121.621
123.925
124.078
125.665
125.933
129.317
129.480
136.450
159.395
168.755
PPM


Br
N
Ac
3e
(1H NMR)
DFILE TW-8-5-2.als
COMNT
DATIM
OBNUC 1H
EXMOD
OBFRQ 300.01 MHz
OBSET 1.85 KHz
OBFIN 2.70 Hz
POINT 32768
FREQU 6172.84 Hz
SCANS 8
ACQTM 0.0000 sec
PD 0.0000 sec
PW1 10.00 usec
IRNUC
CTEMP 0.0 c
SLVNT
EXREF 7.24 ppm
BF 0.12 Hz
RGAIN 0
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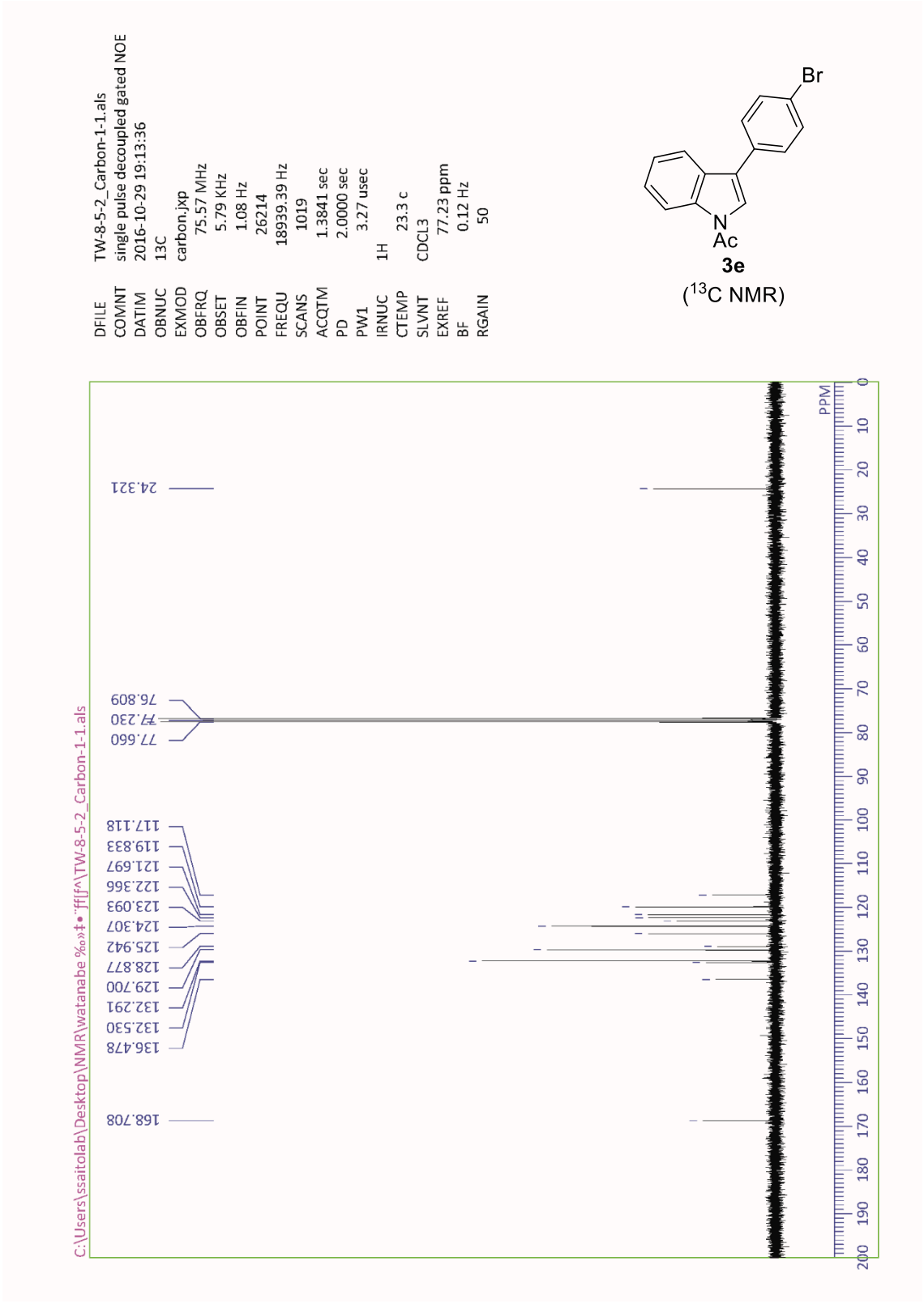
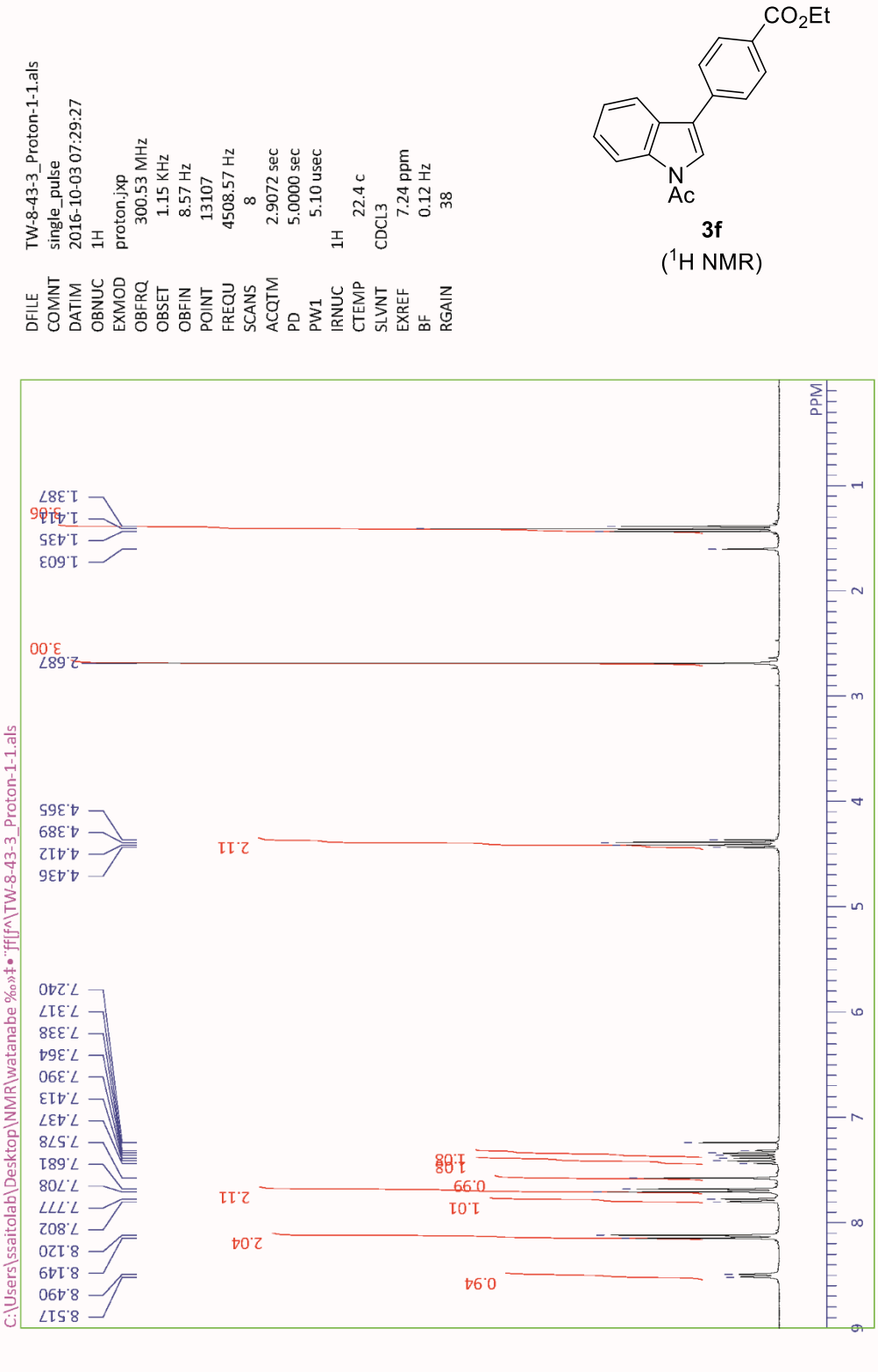
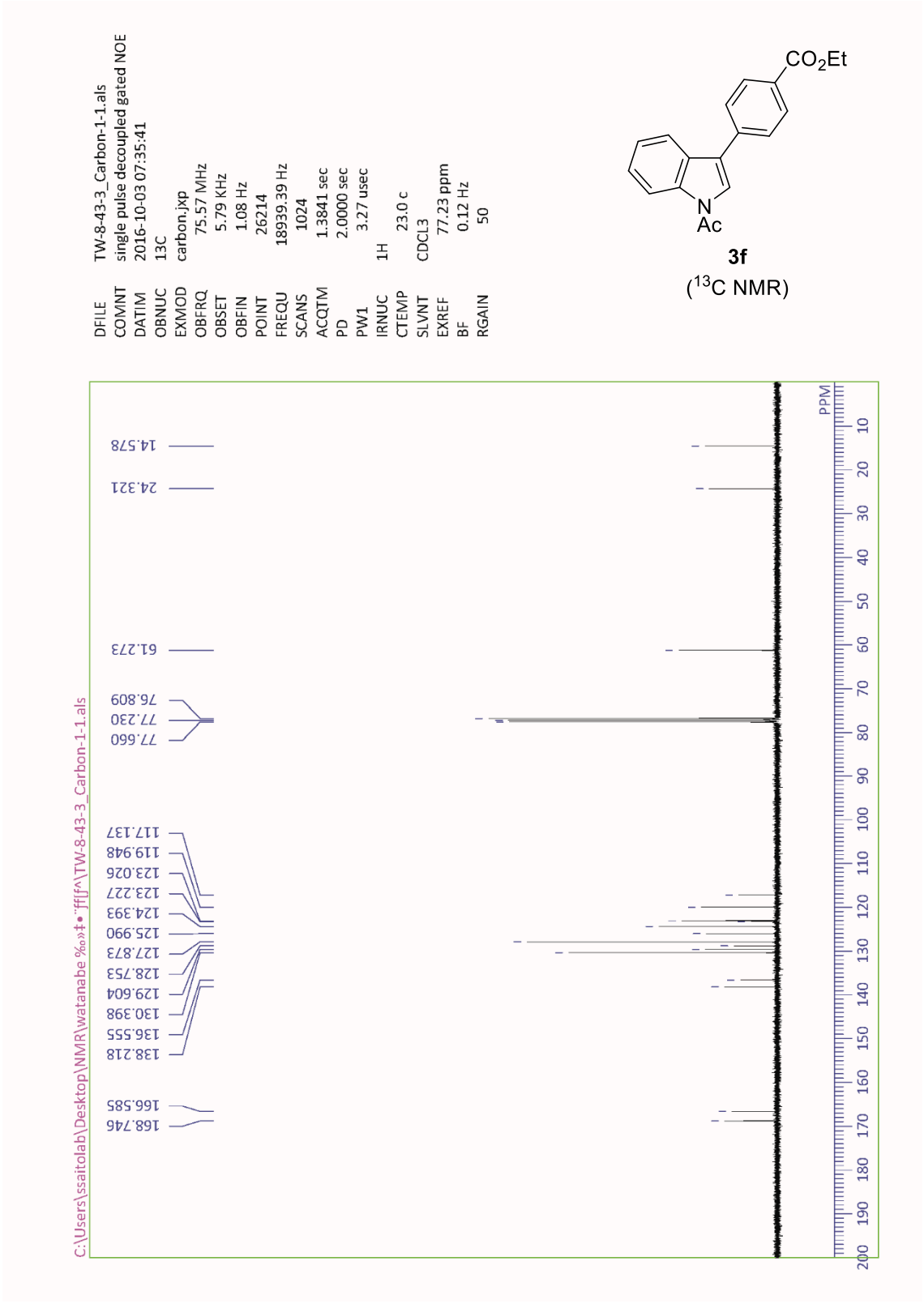
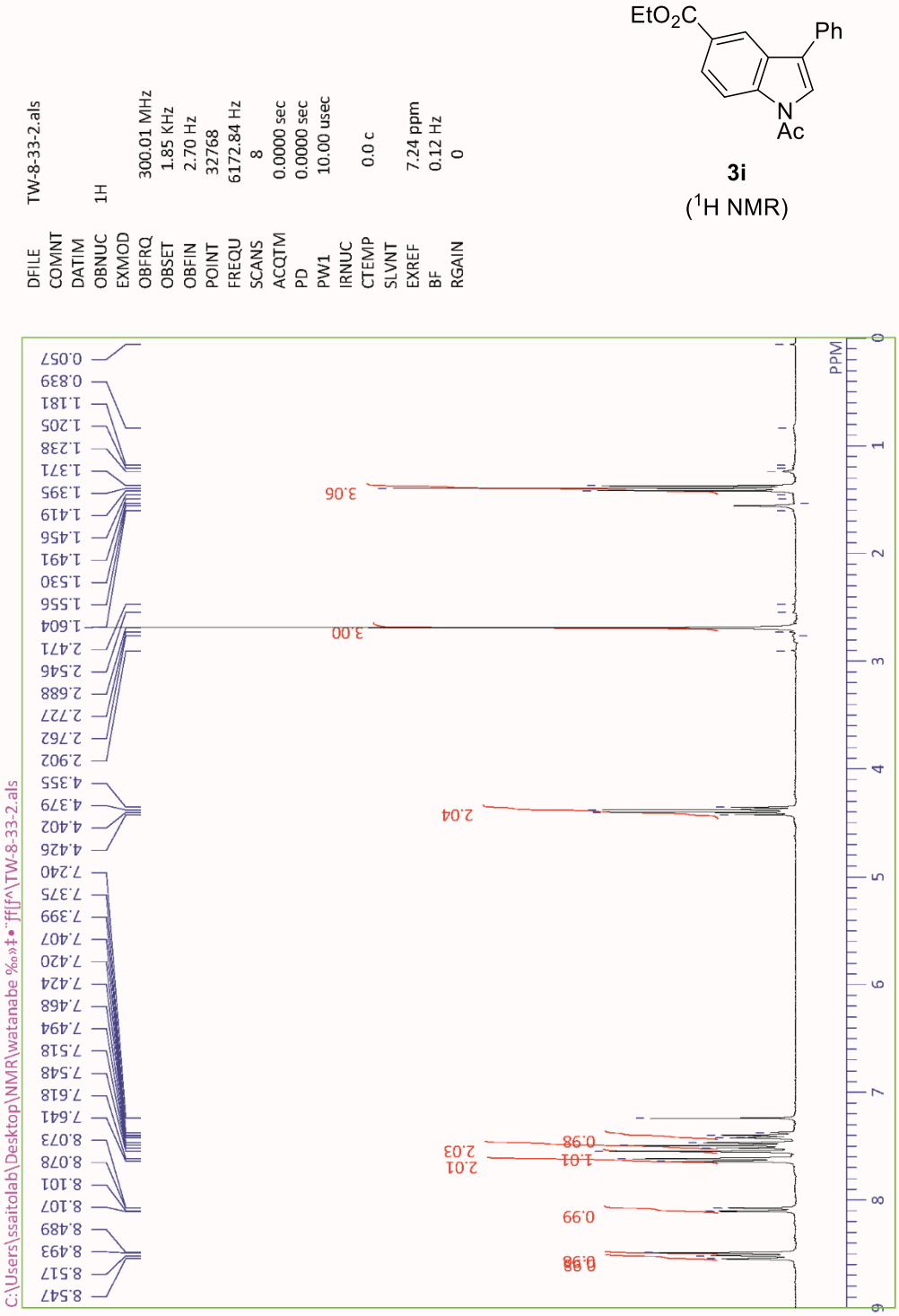
PPM


DFILE TW-8-5-2_Carbon-1-1.als
COMNT single pulse decoupled gated NOE
DATIM 2016-10-29 19:13:36
OBNUC 13C
EXMOD carbon.jxp
OBFRQ 75.57 MHz
OBSET 5.79 KHz
OBFIN 1.08 Hz
POINT 26214
FREQU 18939.39 Hz
SCANS 1019
ACQTM 1.3841 sec
PD 2.0000 sec
PW1 3.27 usec
IRNUC 1H
CTEMP 23.3 c
SLVNT CDCl3
EXREF 77.23 ppm
BF 0.12 Hz
RGAIN 50
Br
N
Ac
3e
(13C NMR)
C:\Users\ssaitolab\Desktop\NMR\watanabe %»‡•"ff[f^\TW-8-5-2_Carbon-1-1.als
24.321
76.809
77.230
77.660
117.118
119.833
121.697
122.366
123.093
124.307
125.942
128.877
129.700
132.291
132.530
136.478
168.708
PPM


DFILE TW-8-43-3_Proton-1-1.als
COMNT single_pulse
DATIM 2016-10-03 07:29:27
OBNUC 1H
EXMOD proton.jxp
OBFRQ 300.53 MHz
OBSET 1.15 KHz
OBFIN 8.57 Hz
POINT 13107
FREQU 4508.57 Hz
SCANS 8
ACQTM 2.9072 sec
PD 5.0000 sec
PW1 5.10 usec
IRNUC 1H
CTEMP 22.4 c
SLVNT CDCl3
EXREF 7.24 ppm
BF 0.12 Hz
RGAIN 38
CO2Et
N
Ac
3f
(1H NMR)
C:\Users\ssaitolab\Desktop\NMR\watanabe %‰»‡•"ff[f^\TW-8-43-3_Proton-1-1.als
PPM


DFILE TW-8-43-3_Carbon-1-1.als
COMNT single pulse decoupled gated NOE
DATIM 2016-10-03 07:35:41
OBNUC 13C
EXMOD carbon.jxp
OBFRQ 75.57 MHz
OBSET 5.79 KHz
OBFIN 1.08 Hz
POINT 26214
FREQU 18939.39 Hz
SCANS 1024
ACQTM 1.3841 sec
PD 2.0000 sec
PW1 3.27 usec
IRNUC 1H
CTEMP 23.0 c
SLVNT CDCl3
EXREF 77.23 ppm
BF 0.12 Hz
RGAIN 50
CO2Et
N
Ac
3f
(13C NMR)
C:\Users\ssaitolab\Desktop\NMR\watanabe %»‡•¨ff[f^\TW-8-43-3_Carbon-1-1.als
14.578
24.321
61.273
76.809
77.230
77.660
117.137
119.948
123.026
123.227
124.393
125.990
127.873
128.753
129.604
130.398
136.555
138.218
166.585
168.746
PPM


EtO2C
Ph
N
Ac
3i
(1H NMR)
DFILE TW-8-33-2.als
COMNT
DATIM
OBNUC 1H
EXMOD
OBFRQ 300.01 MHz
OBSET 1.85 KHz
OBFIN 2.70 Hz
POINT 32768
FREQU 6172.84 Hz
SCANS 8
ACQTM 0.0000 sec
PD 0.0000 sec
PW1 10.00 usec
IRNUC
CTEMP 0.0 c
SLVNT
EXREF 7.24 ppm
BF 0.12 Hz
RGAIN 0
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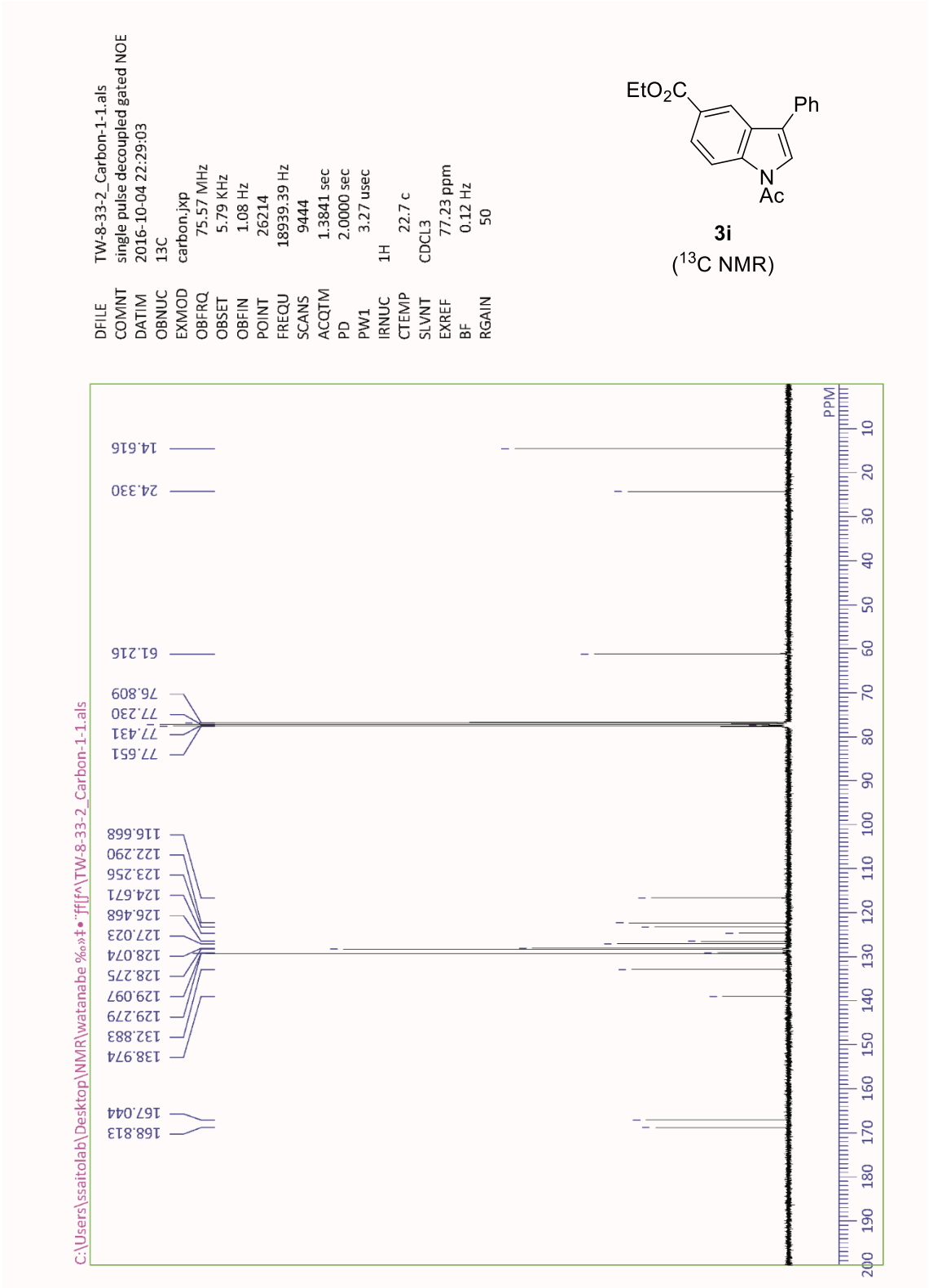
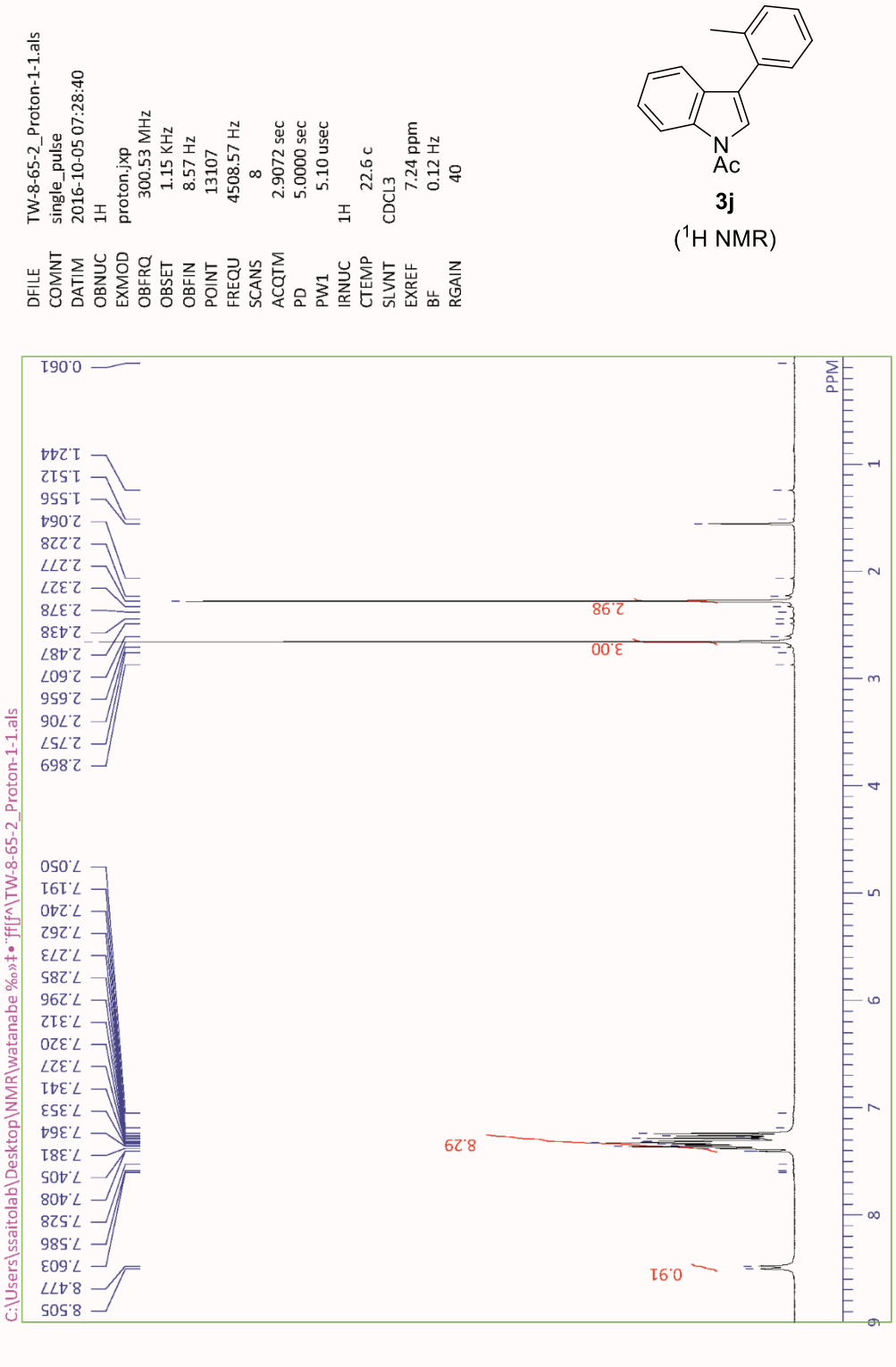
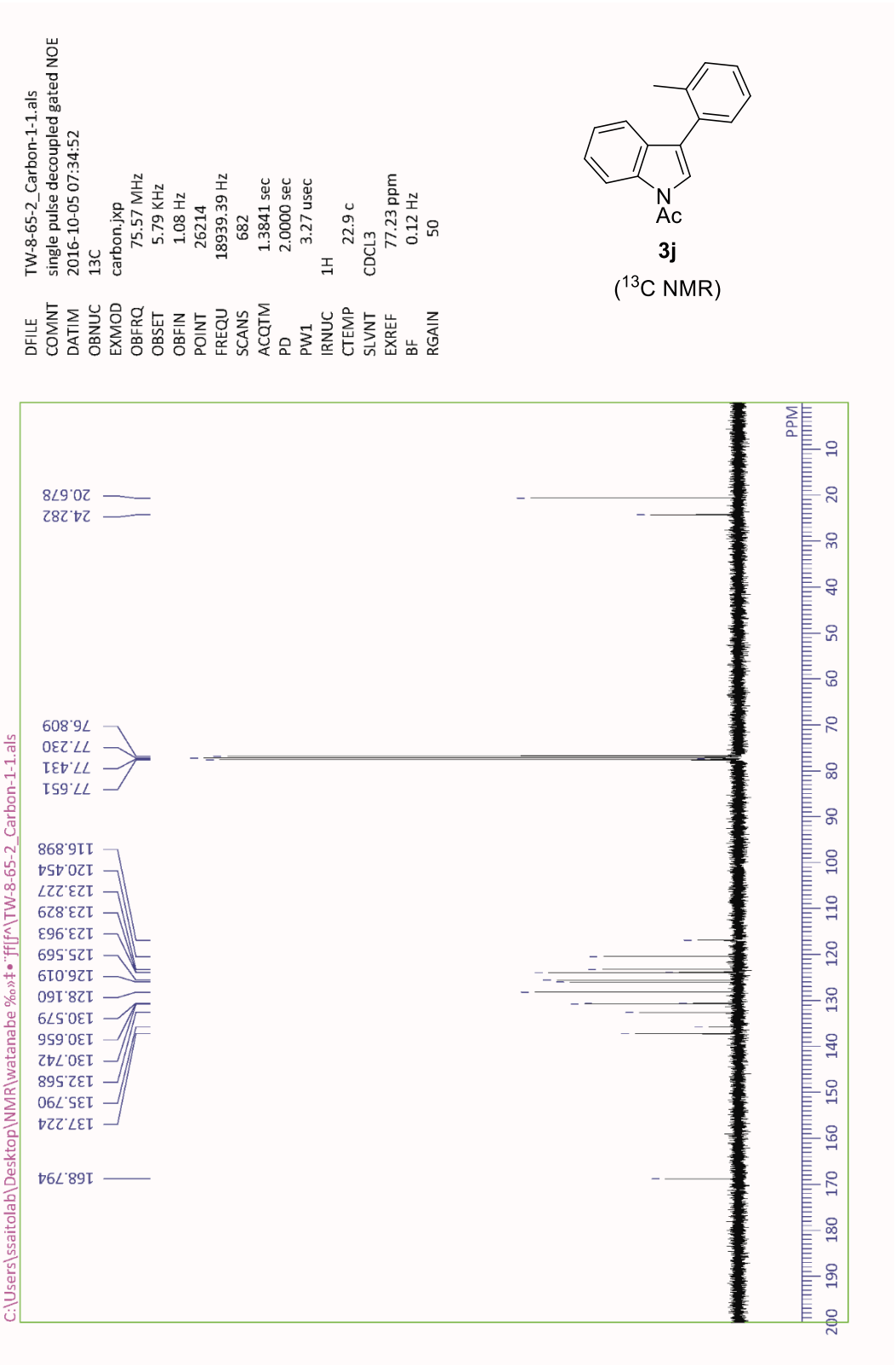
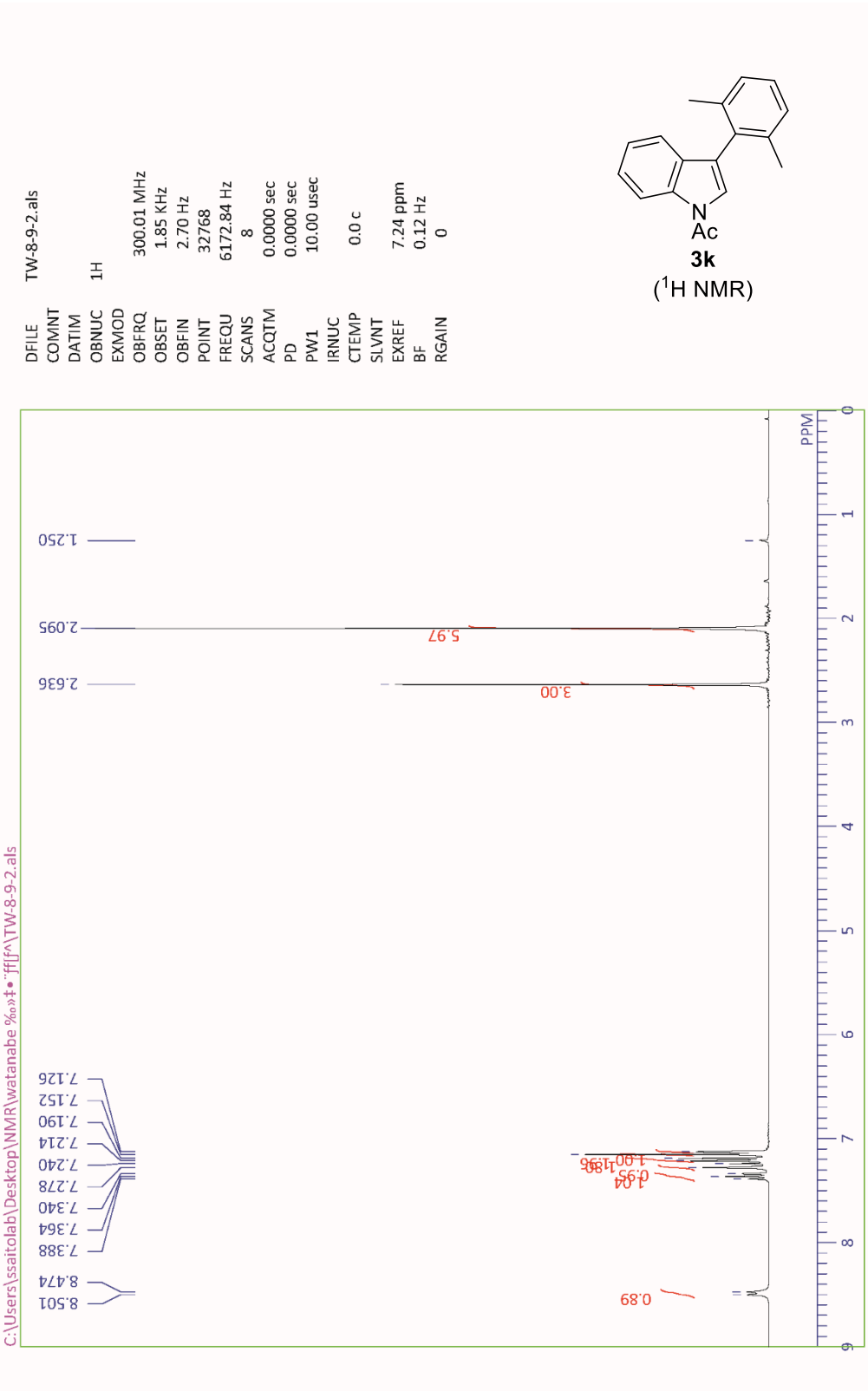
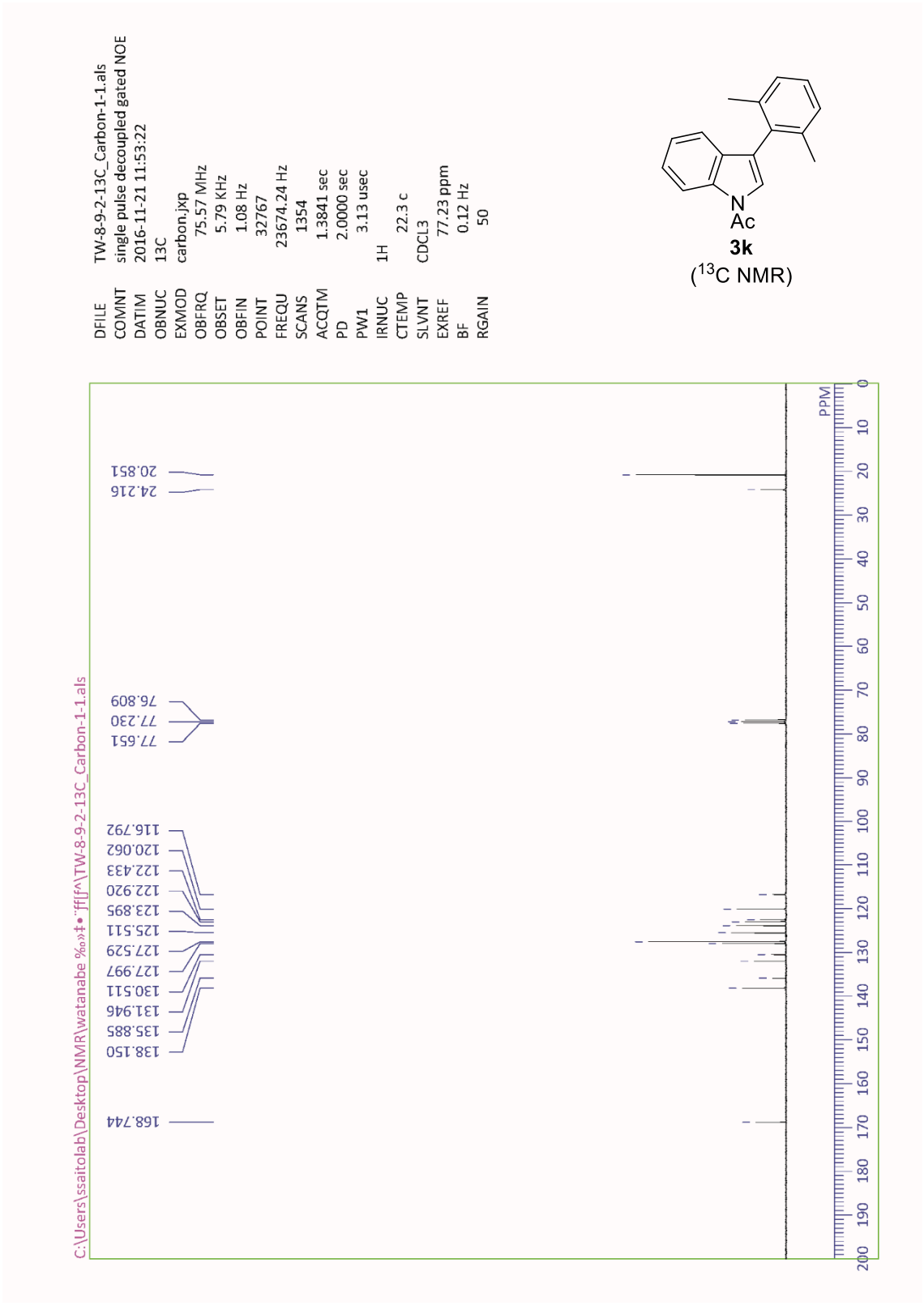
PPM

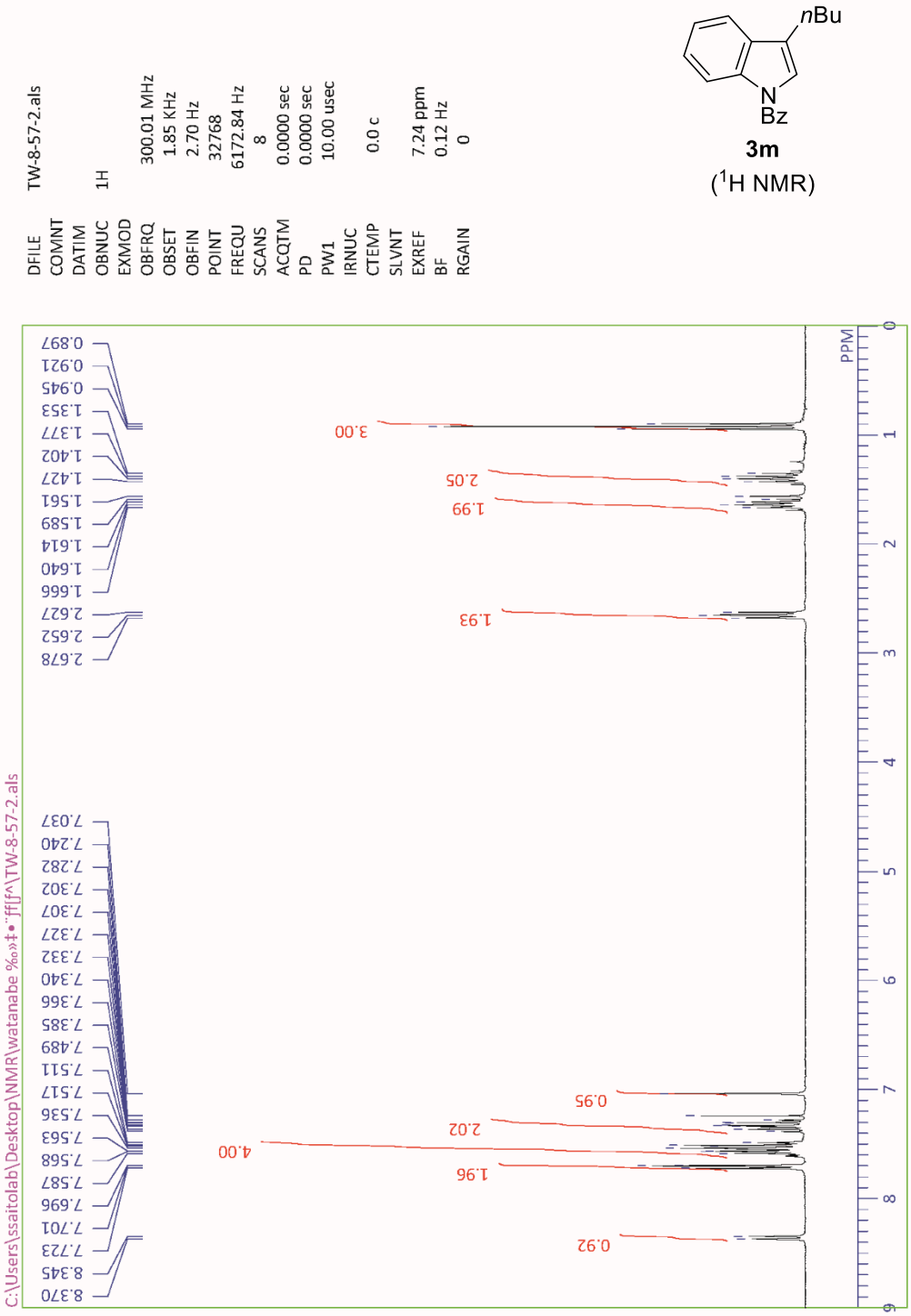

DFILE TW-8-33-2_Carbon-1-1.als
COMNT single pulse decoupled gated NOE
DATIM 2016-10-04 22:29:03
OBNUC 13C
EXMOD carbon.jxp
OBFRQ 75.57 MHz
OBSET 5.79 KHz
OBFIN 1.08 Hz
POINT 26214
FREQU 18939.39 Hz
SCANS 9444
ACQTM 1.3841 sec
PD 2.0000 sec
PW1 3.27 usec
IRNUC 1H
CTEMP 22.7 c
SLVNT CDCl3
EXREF 77.23 ppm
BF 0.12 Hz
RGAIN 50
EtO2C
Ph
N
Ac
3i
(13C NMR)
C:\Users\ssaitolab\Desktop\NMR\watanabe %»‡•¨ff[f^\TW-8-33-2_Carbon-1-1.als
14.616
24.330
61.216
76.809
77.230
77.431
77.651
116.668
122.290
123.256
124.671
126.468
127.023
128.074
128.275
129.097
129.279
132.883
138.974
167.044
168.813
PPM

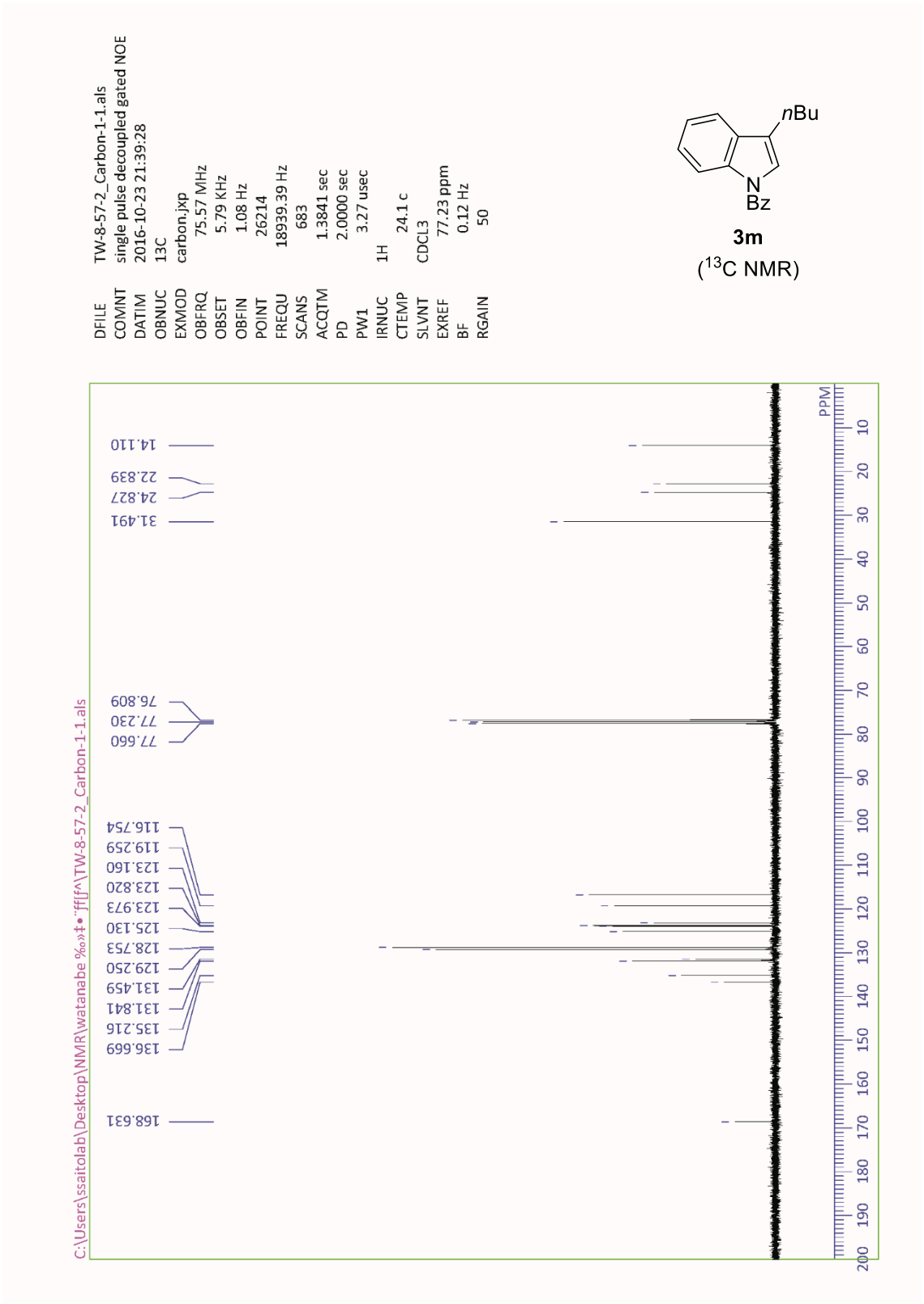

DFILE TW-8-65-2_Proton-1-1.als
COMNT single_pulse
DATIM 2016-10-05 07:28:40
OBNUC 1H
EXMOD proton.jxp
OBFRQ 300.53 MHz
OBSET 1.15 KHz
OBFIN 8.57 Hz
POINT 13107
FREQU 4508.57 Hz
SCANS 8
ACQTM 2.9072 sec
PD 5.0000 sec
PW1 5.10 usec
IRNUC 1H
CTEMP 22.6 c
SLVNT CDCl3
EXREF 7.24 ppm
BF 0.12 Hz
RGAIN 40
N
Ac
3j
(1H NMR)
C:\Users\ssaitolab\Desktop\NMR\watanabe %‰»‡•¨ff[f^\TW-8-65-2_Proton-1-1.als
PPM

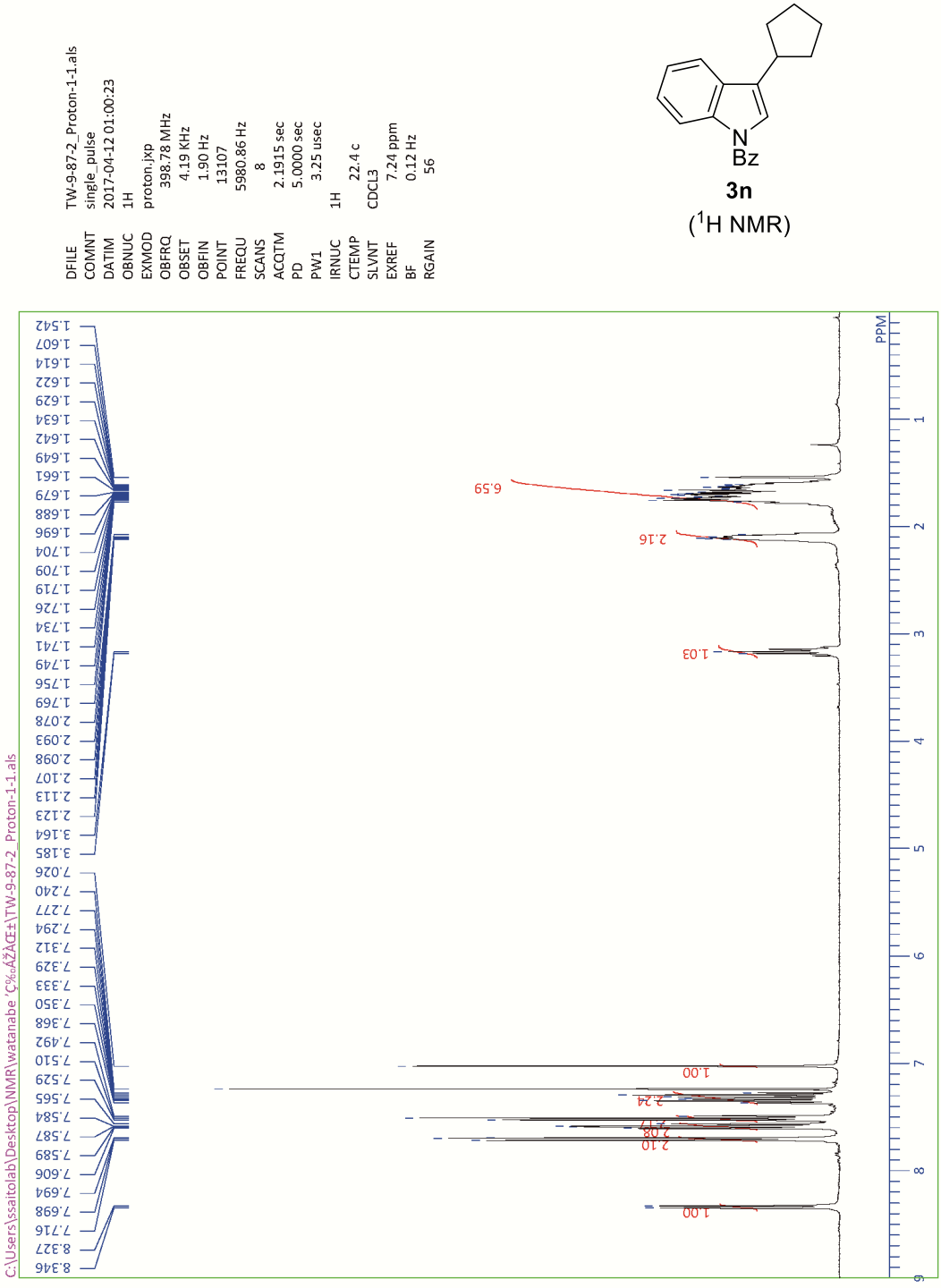

DFILE TW-8-65-2_Carbon-1-1.als
COMNT single pulse decoupled gated NOE
DATIM 2016-10-05 07:34:52
OBNUC 13C
EXMOD carbon.jxp
OBFRQ 75.57 MHz
OBSET 5.79 KHz
OBFIN 1.08 Hz
POINT 26214
FREQU 18939.39 Hz
SCANS 682
ACQTM 1.3841 sec
PD 2.0000 sec
PW1 3.27 usec
IRNUC 1H
CTEMP 22.9 c
SLVNT CDCl3
EXREF 77.23 ppm
BF 0.12 Hz
RGAIN 50
N
Ac
3j
(^{13}C NMR)
C:\Users\ssaitolab\Desktop\NMR\watanabe %‰»‡•¨ff[f^\TW-8-65-2_Carbon-1-1.als
20.678
24.282
76.809
77.230
77.431
77.651
116.898
120.454
123.227
123.829
123.963
125.569
126.019
128.160
130.579
130.656
130.742
132.568
135.790
137.224
168.794
PPM

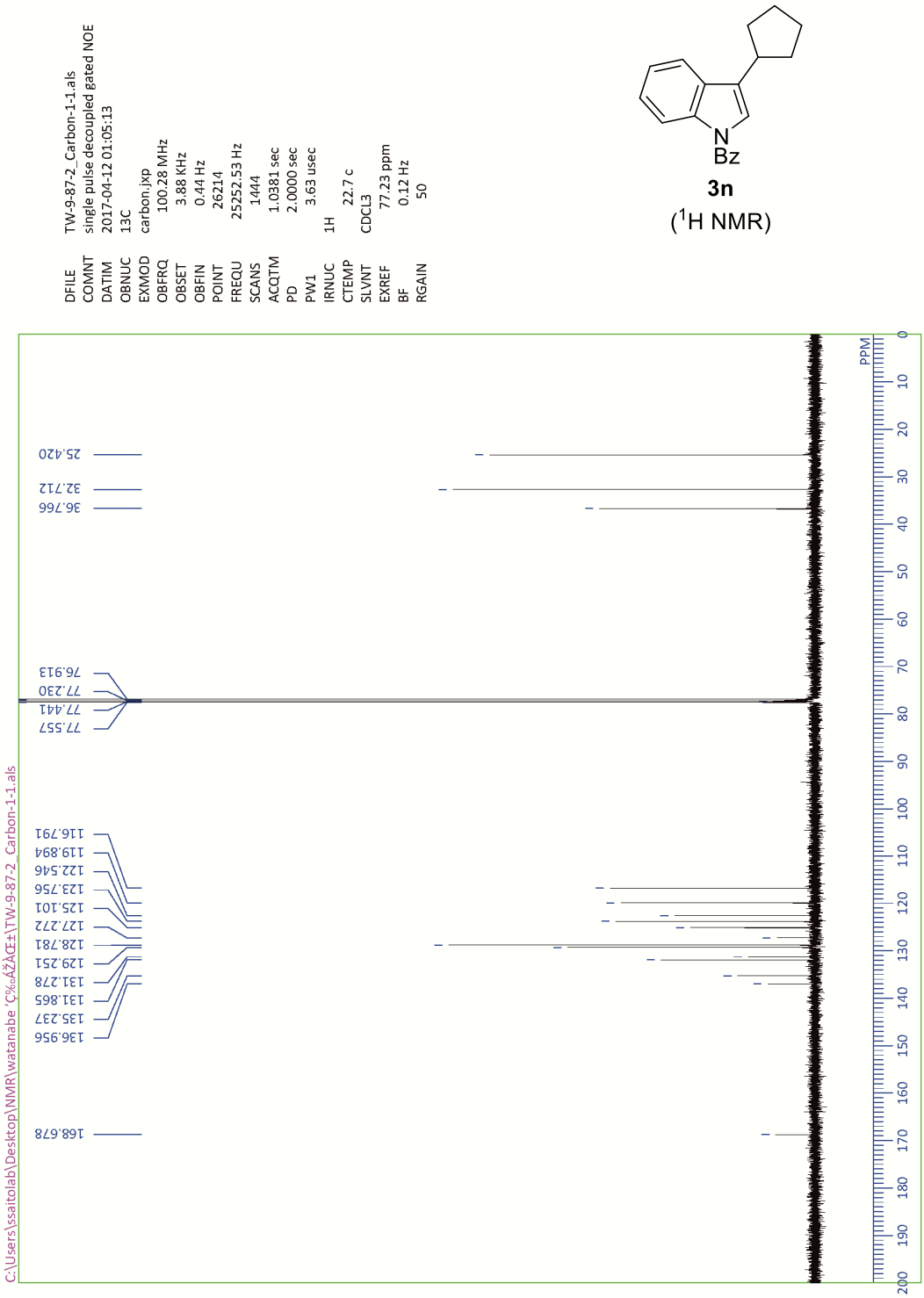

N
Ac
3k
(1H NMR)
DFILE TW-8-9-2.als
COMNT
DATIM
OBNUC 1H
EXMOD
OBFRQ 300.01 MHz
OBSET 1.85 KHz
OBFIN 2.70 Hz
POINT 32768
FREQU 6172.84 Hz
SCANS 8
ACQTM 0.0000 sec
PD 0.0000 sec
PW1 10.00 usec
IRNUC
CTEMP 0.0 c
SLVNT
EXREF 7.24 ppm
BF 0.12 Hz
RGAIN 0
C:\Users\ssaitolab\Desktop\NMR\watanabe ‰»‡•"ff[^\TW-8-9-2.als
PPM


DFILE TW-8-9-2-13C_Carbon-1-1.als
COMNT single pulse decoupled gated NOE
DATIM 2016-11-21 11:53:22
OBNUC 13C
EXMOD carbon.jxp
OBFRQ 75.57 MHz
OBSET 5.79 KHz
OBFIN 1.08 Hz
POINT 32767
FREQU 23674.24 Hz
SCANS 1354
ACQTM 1.3841 sec
PD 2.0000 sec
PW1 3.13 usec
IRNUC 1H
CTEMP 22.3 c
SLVNT CDCl3
EXREF 77.23 ppm
BF 0.12 Hz
RGAIN 50
N
Ac
3k
(13C NMR)
C:\Users\ssaitolab\Desktop\NMR\watanabe %»‡•"ff[f^\TW-8-9-2-13C_Carbon-1-1.als
20.851
24.216
76.809
77.230
77.651
116.792
120.062
122.433
122.920
123.895
125.511
127.529
127.997
130.511
131.946
135.885
138.150
168.744
PPM


nBu
N
Bz
3m
(1H NMR)
DFILE TW-8-57-2.als
COMNT
DATIM
OBNUC 1H
EXMOD
OBFRQ 300.01 MHz
OBSET 1.85 KHz
OBFIN 2.70 Hz
POINT 32768
FREQU 6172.84 Hz
SCANS 8
ACQTM 0.0000 sec
PD 0.0000 sec
PW1 10.00 usec
IRNUC
CTEMP 0.0 c
SLVNT
EXREF 7.24 ppm
BF 0.12 Hz
RGAIN 0
C:\Users\ssaitolab\Desktop\NMR\watanabe %‰»‡•"ff[f^\TW-8-57-2.als
PPM


DFILE TW-8-57-2_Carbon-1-1.als
COMNT single pulse decoupled gated NOE
DATIM 2016-10-23 21:39:28
OBNUC 13C
EXMOD carbon.jxp
OBFRQ 75.57 MHz
OBSET 5.79 KHz
OBFIN 1.08 Hz
POINT 26214
FREQU 18939.39 Hz
SCANS 683
ACQTM 1.3841 sec
PD 2.0000 sec
PW1 3.27 usec
IRNUC 1H
CTEMP 24.1 c
SLVNT CDCl3
EXREF 77.23 ppm
BF 0.12 Hz
RGAIN 50
nBu
N
Bz
3m
(13C NMR)
C:\Users\ssaitolab\Desktop\NMR\watanabe %»‡•"ff[^\TW-8-57-2_Carbon-1-1.als
14.110
22.839
24.827
31.491
76.809
77.230
77.660
116.754
119.259
123.160
123.820
123.973
125.130
128.753
129.250
131.459
131.841
135.216
136.669
168.631
PPM


DFILE TW-9-87-2_Proton-1-1.als
COMNT single_pulse
DATIM 2017-04-12 01:00:23
OBNUC 1H
EXMOD proton.jxp
OBFRQ 398.78 MHz
OBSET 4.19 KHz
OBFIN 1.90 Hz
POINT 13107
FREQU 5980.86 Hz
SCANS 8
ACQTM 2.1915 sec
PD 5.0000 sec
PW1 3.25 usec
IRNUC 1H
CTEMP 22.4 c
SLVNT CDCL3
EXREF 7.24 ppm
BF 0.12 Hz
RGAIN 56
N
Bz
3n
(1H NMR)
C:\Users\ssaitolab\Desktop\NMR\watanabe 'Ç‰ÁŽÆ±\TW-9-87-2_Proton-1-1.als
PPM


DFILE TW-9-87-2_Carbon-1-1.als
COMNT single pulse decoupled gated NOE
DATIM 2017-04-12 01:05:13
OBNUC 13C
EXMOD carbon.jxp
OBFRQ 100.28 MHz
OBSET 3.88 KHz
OBFIN 0.44 Hz
POINT 26214
FREQU 25252.53 Hz
SCANS 1444
ACQTM 1.0381 sec
PD 2.0000 sec
PW1 3.63 usec
IRNUC 1H
CTEMP 22.7 c
SLVNT CDCL3
EXREF 77.23 ppm
BF 0.12 Hz
RGAIN 50
N
Bz
3n
(1H NMR)
C:\Users\ssaitolab\Desktop\NMR\watanabe 'Ç‰ÁŽÆ±\TW-9-87-2_Carbon-1-1.als
PPM
25.420
32.712
36.766
76.913
77.230
77.441
77.557
116.791
119.894
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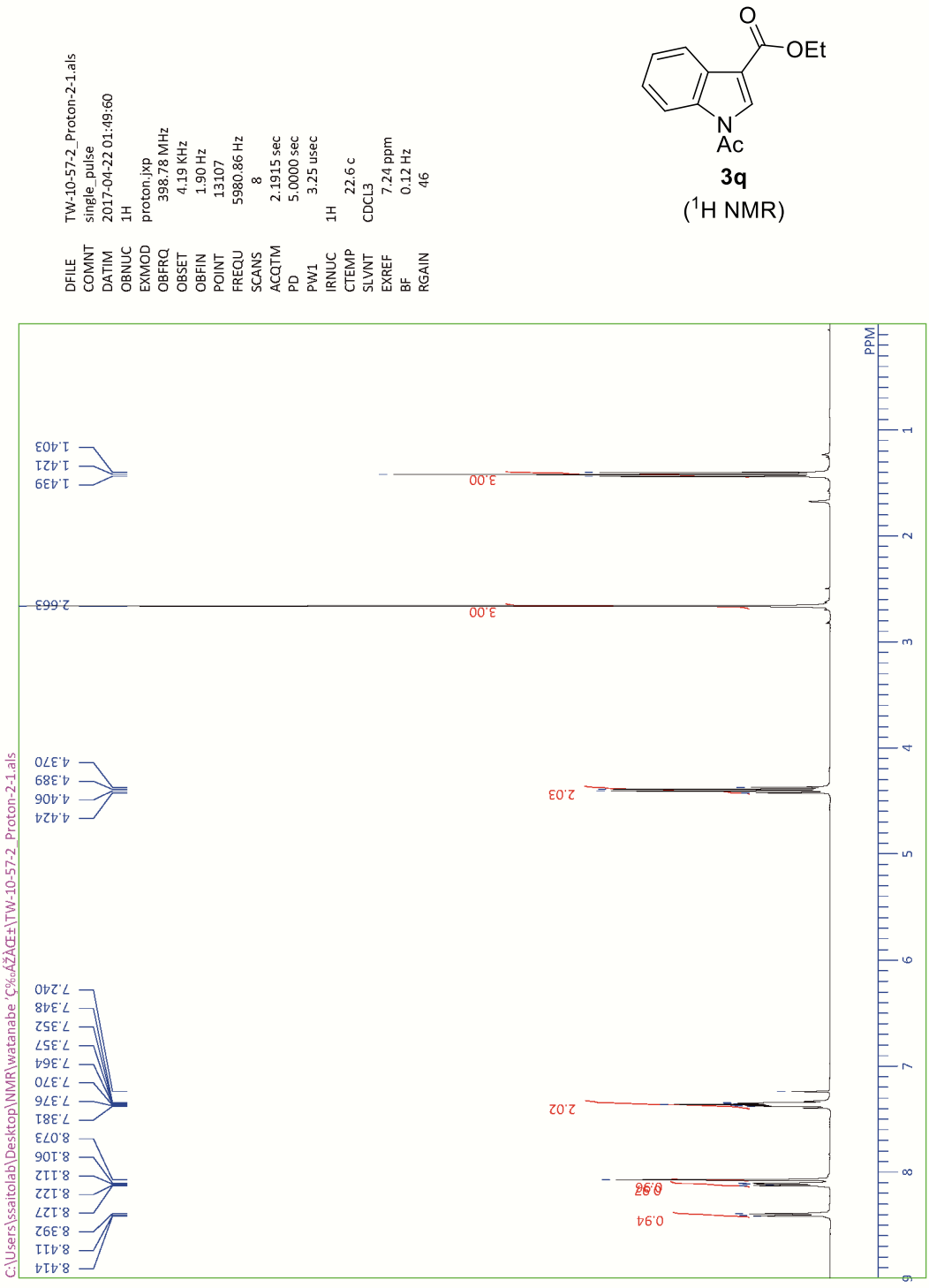
131.278
131.865
135.237
136.956
168.678


O
OEt
N
Ac
3q
(1H NMR)
DFILE TW-10-57-2_Proton-2-1.als
COMNT single_pulse
DATIM 2017-04-22 01:49:60
OBNUC 1H
EXMOD proton.jxp
OBFRQ 398.78 MHz
OBSET 4.19 KHz
OBFIN 1.90 Hz
POINT 13107
FREQU 5980.86 Hz
SCANS 8
ACQTM 2.1915 sec
PD 5.0000 sec
PW1 3.25 usec
IRNUC 1H
CTEMP 22.6 c
SLVNT CDCL3
EXREF 7.24 ppm
BF 0.12 Hz
RGAIN 46
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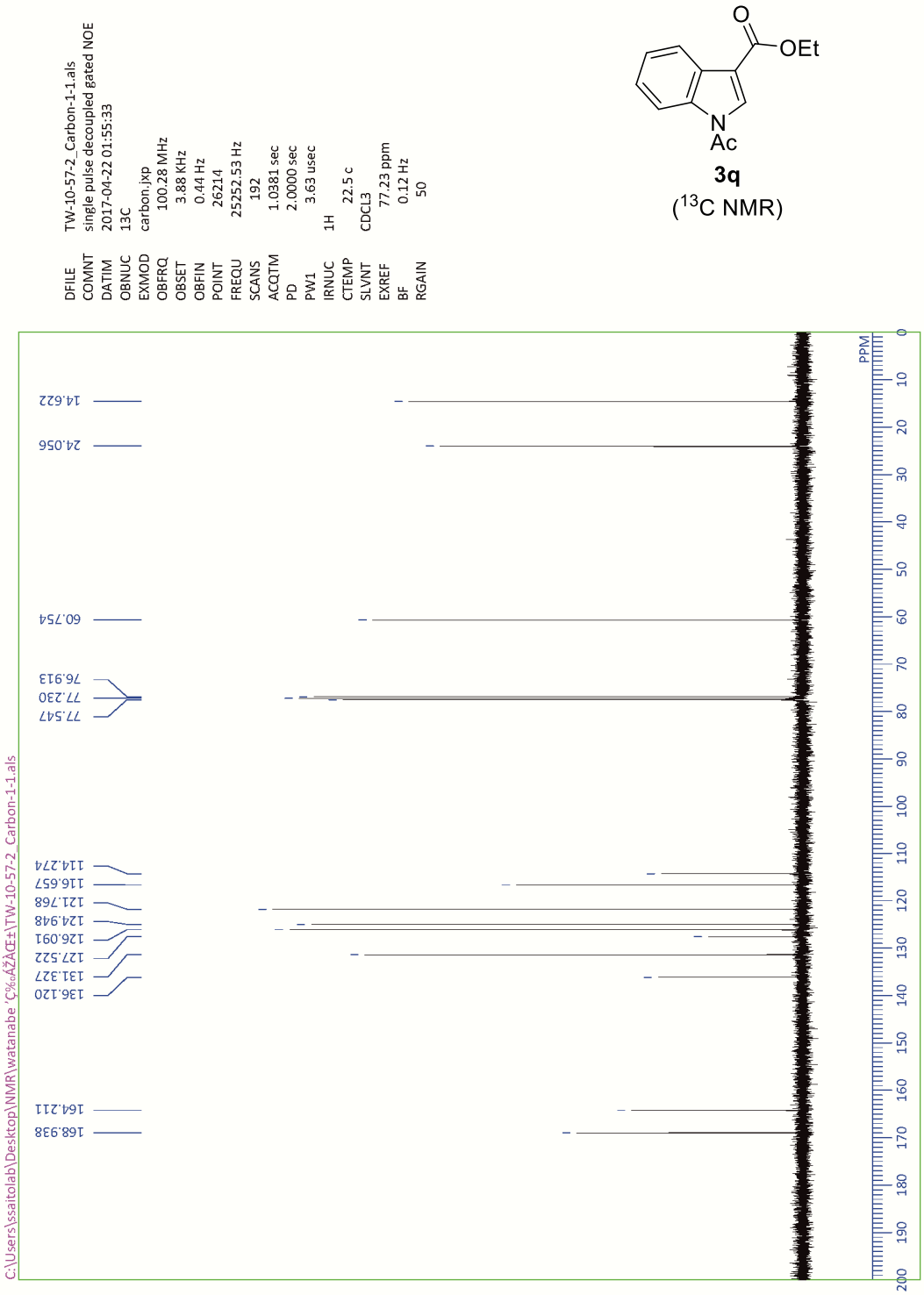
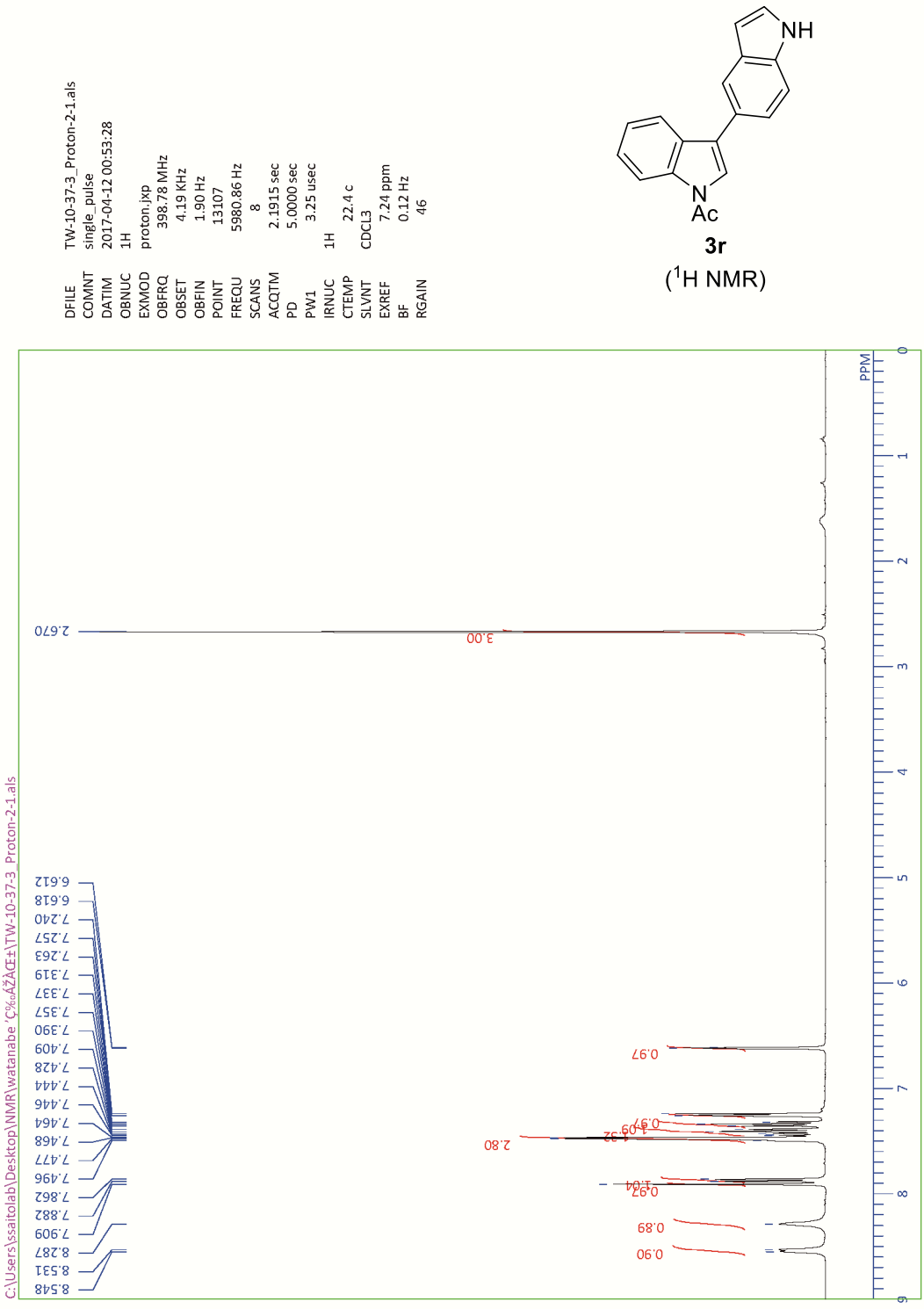
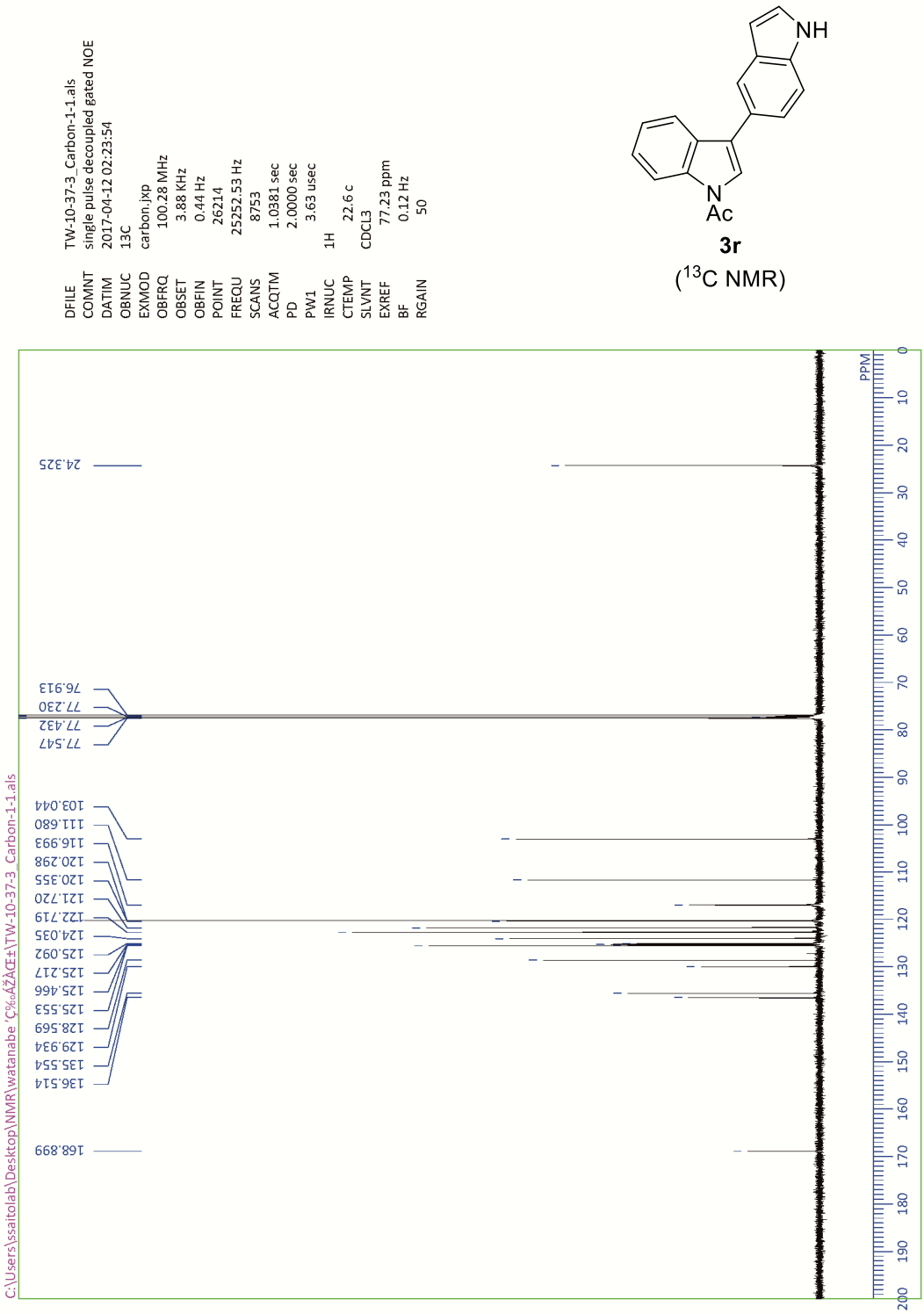
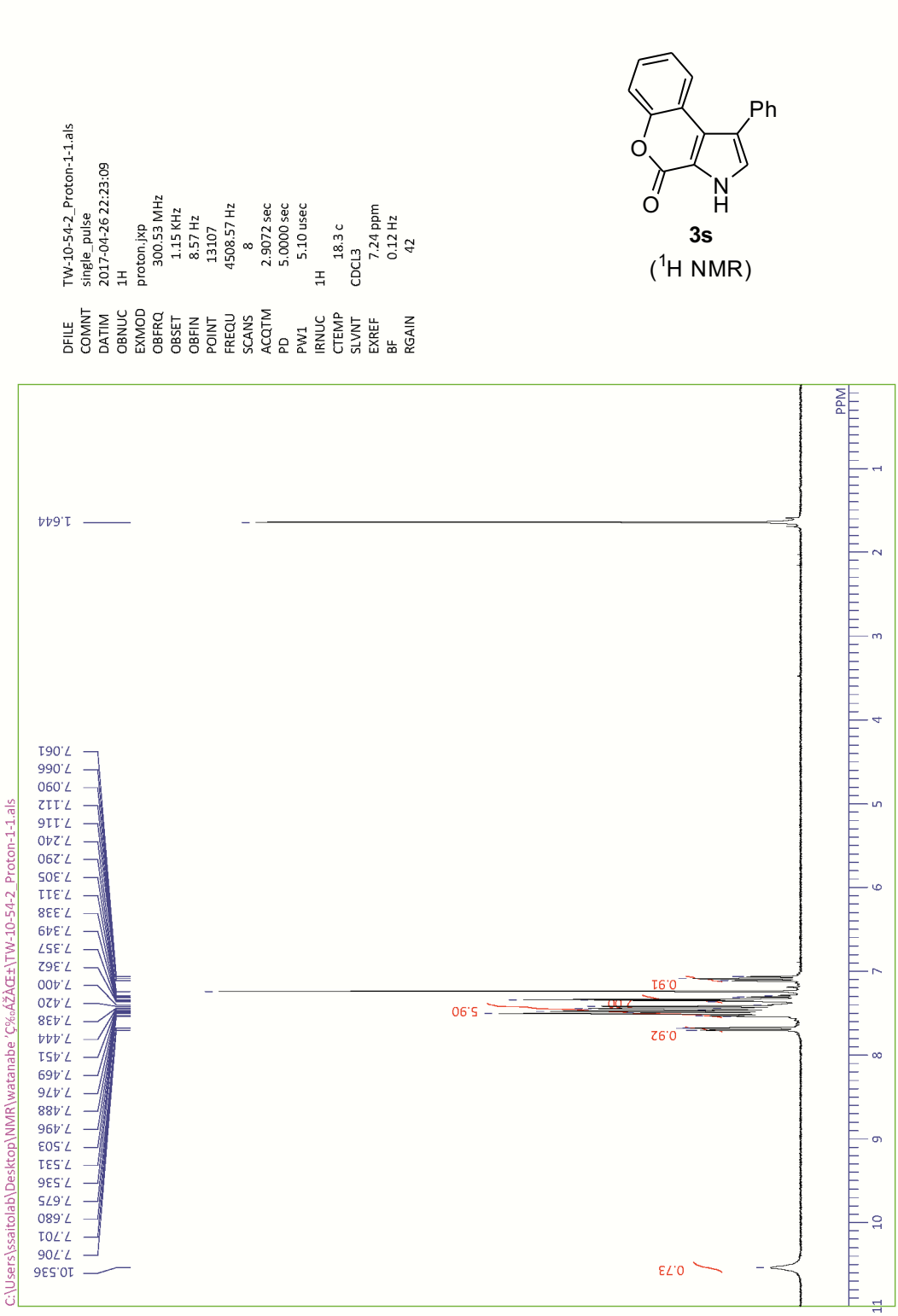
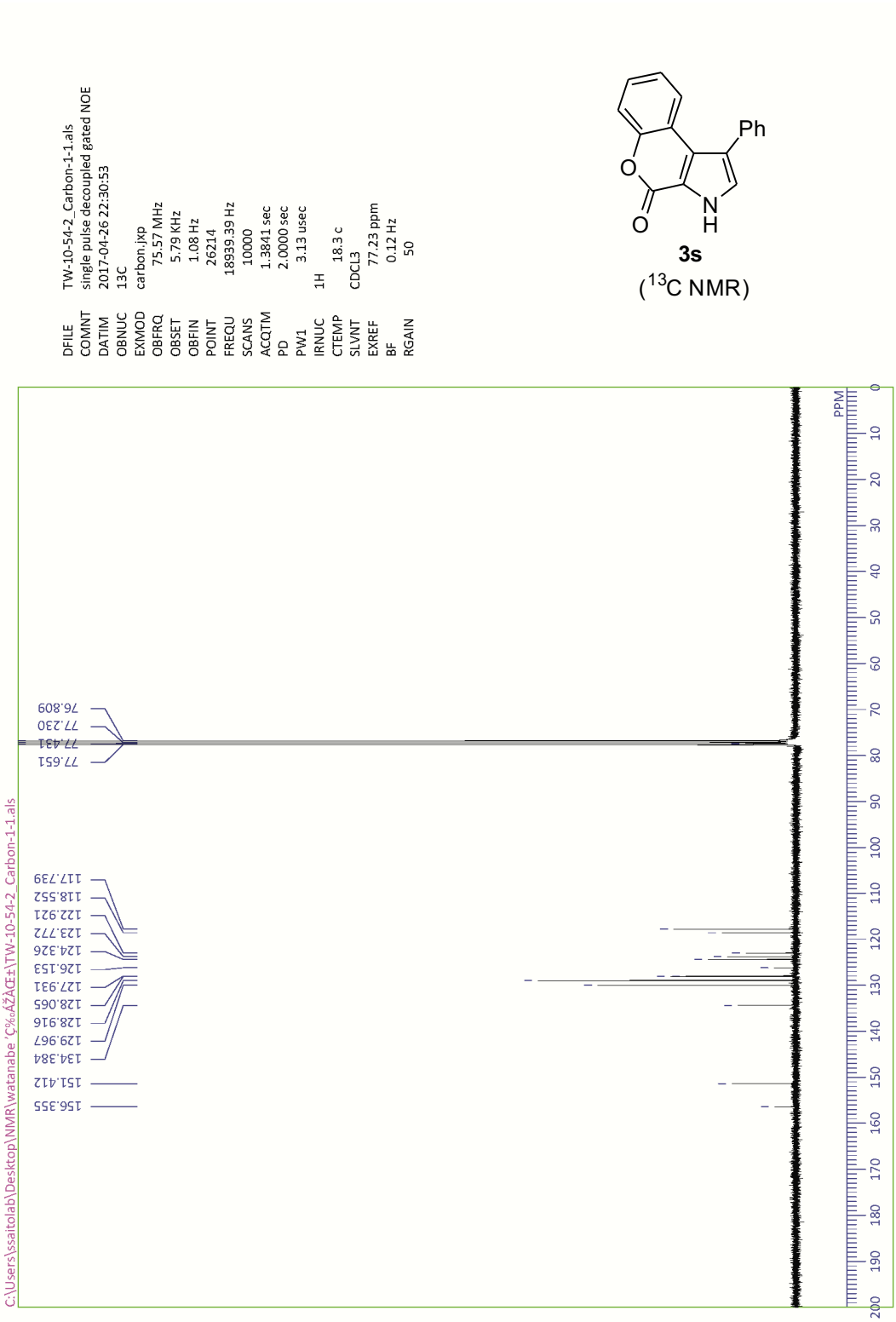
PPM

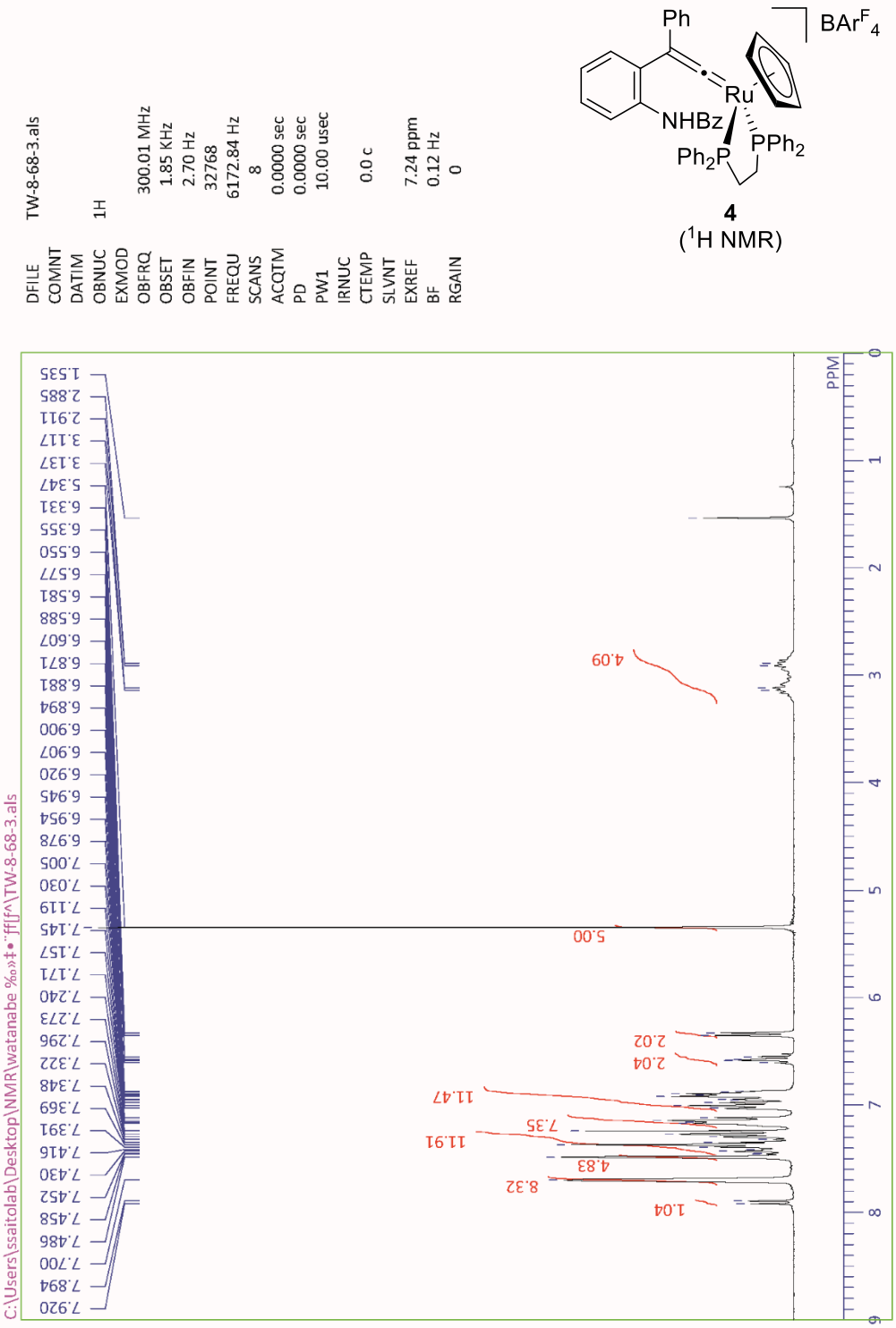

O
OEt
N
Ac
3q
(13C NMR)
DFILE TW-10-57-2_Carbon-1-1.als
COMNT single pulse decoupled gated NOE
DATIM 2017-04-22 01:55:33
OBNUC 13C
EXMOD carbon.jxp
OBFRQ 100.28 MHz
OBSET 3.88 KHz
OBFIN 0.44 Hz
POINT 26214
FREQU 25252.53 Hz
SCANS 192
ACQTM 1.0381 sec
PD 2.0000 sec
PW1 3.63 usec
IRNUC 1H
CTEMP 22.5 c
SLVNT CDCL3
EXREF 77.23 ppm
BF 0.12 Hz
RGAIN 50
14.622
24.056
60.754
76.913
77.230
77.547
114.274
116.657
121.768
124.948
126.091
127.522
131.327
136.120
164.211
168.938
PPM
C:\Users\ssaitolab\Desktop\NMR\watanabe 'Ç‰ÁŽÄŒ±\TW-10-57-2_Carbon-1-1.als

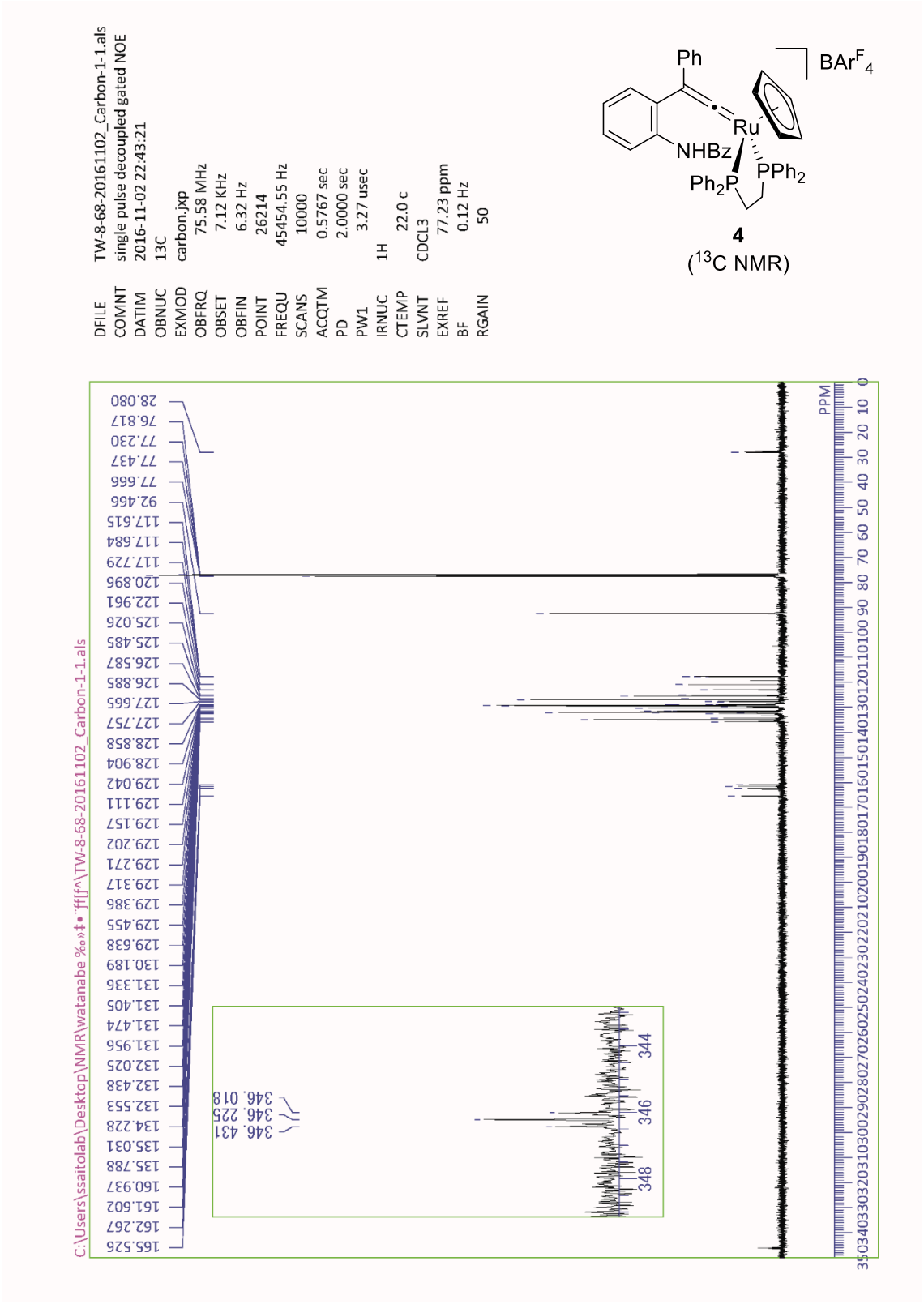

DFILE TW-10-37-3_Proton-2-1.als
COMNT single_pulse
DATIM 2017-04-12 00:53:28
OBNUC 1H
EXMOD proton.jxp
OBFRQ 398.78 MHz
OBSET 4.19 KHz
OBFIN 1.90 Hz
POINT 13107
FREQU 5980.86 Hz
SCANS 8
ACQTM 2.1915 sec
PD 5.0000 sec
PW1 3.25 usec
IRNUC 1H
CTEMP 22.4 c
SLVNT CDCL3
EXREF 7.24 ppm
BF 0.12 Hz
RGAIN 46
NH
N
Ac
3r
(1H NMR)
C:\Users\ssaitolab\Desktop\NMR\watanabe 'Ç‰ÁŽÆ±\TW-10-37-3_Proton-2-1.als
PPM

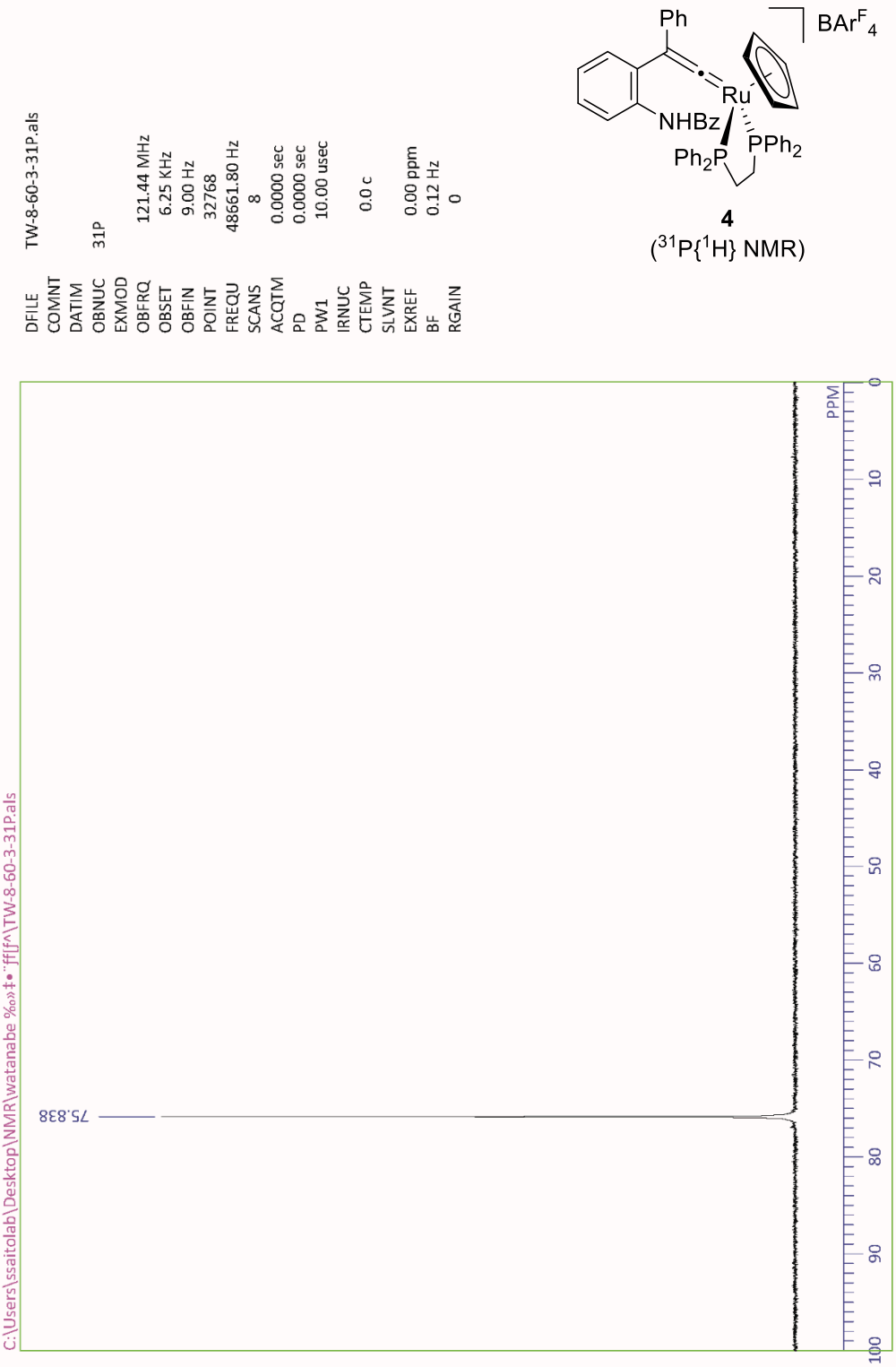

DFILE TW-10-37-3_Carbon-1-1.als
COMNT single pulse decoupled gated NOE
DATIM 2017-04-12 02:23:54
OBNUC 13C
EXMOD carbon.jxp
OBFRQ 100.28 MHz
OBSET 3.88 KHz
OBFIN 0.44 Hz
POINT 26214
FREQU 25252.53 Hz
SCANS 8753
ACQTM 1.0381 sec
PD 2.0000 sec
PW1 3.63 usec
IRNUC 1H
CTEMP 22.6 c
SLVNT CDCL3
EXREF 77.23 ppm
BF 0.12 Hz
RGAIN 50
NH
N
Ac
3r
(13C NMR)
C:\Users\ssaitolab\Desktop\NMR\watanabe 'Ç‰ÁŽÄŒ±\TW-10-37-3_Carbon-1-1.als
PPM


Ph
O
N
H
O
3s
(1H NMR)
DFILE TW-10-54-2_Proton-1-1.als
COMNT single_pulse
DATIM 2017-04-26 22:23:09
OBNUC 1H
EXMOD proton.jxp
OBFRQ 300.53 MHz
OBSET 1.15 KHz
OBFIN 8.57 Hz
POINT 13107
FREQU 4508.57 Hz
SCANS 8
ACQTM 2.9072 sec
PD 5.0000 sec
PW1 5.10 usec
IRNUC 1H
CTEMP 18.3 c
SLVNT CDCL3
EXREF 7.24 ppm
BF 0.12 Hz
RGAIN 42
C:\Users\ssaitolab\Desktop\NMR\watanabe 'Ç‰ÁŽÀCE±\TW-10-54-2_Proton-1-1.als
PPM
1.644
7.061
7.066
7.090
7.112
7.116
7.240
7.290
7.305
7.311
7.338
7.349
7.357
7.362
7.400
7.420
7.438
7.444
7.451
7.469
7.476
7.488
7.496
7.503
7.531
7.536
7.675
7.680
7.701
7.706
10.536
0.91
5.90
7.00
0.92
0.73


DFILE TW-10-54-2_Carbon-1-1.als
COMNT single pulse decoupled gated NOE
DATIM 2017-04-26 22:30:53
OBNUC 13C
EXMOD carbon.jxp
OBFRQ 75.57 MHz
OBSET 5.79 KHz
OBFIN 1.08 Hz
POINT 26214
FREQU 18939.39 Hz
SCANS 10000
ACQTM 1.3841 sec
PD 2.0000 sec
PW1 3.13 usec
IRNUC 1H
CTEMP 18.3 c
SLVNT CDCL3
EXREF 77.23 ppm
BF 0.12 Hz
RGAIN 50
Ph
O
N
H
O
3s
(^{13}C NMR)
C:\Users\ssaitolab\Desktop\NMR\watanabe 'Ç‰ÁŽÀCE±\TW-10-54-2_Carbon-1-1.als
PPM


Ph
BAr$^F_4$
Ru
NHBz
Ph$_2$P
PPh$_2$
4
(^{1}H NMR)
DFILE TW-8-68-3.als
COMNT
DATIM
OBNUC 1H
EXMOD
OBFRQ 300.01 MHz
OBSET 1.85 KHz
OBFIN 2.70 Hz
POINT 32768
FREQU 6172.84 Hz
SCANS 8
ACQTM 0.0000 sec
PD 0.0000 sec
PW1 10.00 usec
IRNUC
CTEMP 0.0 c
SLVNT
EXREF 7.24 ppm
BF 0.12 Hz
RGAIN 0
C:\Users\ssaitolab\Desktop\NMR\watanabe %»‡•"ff[^\TW-8-68-3.als
PPM
4.09
5.00
2.02
2.04
11.47
7.35
11.91
4.83
8.32
1.04


TW-8-68-20161102_Carbon-1-1.als
single pulse decoupled gated NOE
2016-11-02 22:43:21
13C
carbon.jxp
75.58 MHz
7.12 KHz
6.32 Hz
26214
45454.55 Hz
10000
0.5767 sec
2.0000 sec
3.27 usec
1H
22.0 c
CDCl3
77.23 ppm
0.12 Hz
50
DFILE
COMNT
DATIM
OBNUC
EXMOD
OBFRQ
OBSET
OBFIN
POINT
FREQU
SCANS
ACQTM
PD
PW1
IRNUC
CTEMP
SLVNT
EXREF
BF
RGAIN
Ph
BAr$^F_4$
Ru
NHBz
Ph$_2$P
PPh$_2$
4
(^{13}C NMR)
C:\Users\ssaitolab\Desktop\NMR\watanabe %‰»‡•"ff[f^\TW-8-68-20161102_Carbon-1-1.als
PPM


Ph
BAr$^F_4$
Ru
NHBz
Ph$_2$P
PPh$_2$
4
(^{31}P{^{1}H} NMR)
DFILE TW-8-60-3-31P.als
COMNT
DATIM
OBNUC 31P
EXMOD
OBFRQ 121.44 MHz
OBSET 6.25 KHz
OBFIN 9.00 Hz
POINT 32768
FREQU 48661.80 Hz
SCANS 8
ACQTM 0.0000 sec
PD 0.0000 sec
PW1 10.00 usec
IRNUC
CTEMP 0.0 c
SLVNT
EXREF 0.00 ppm
BF 0.12 Hz
RGAIN 0
75.838
PPM
0
10
20
30
40
50
60
70
80
90
100
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