

## Supporting Information

for

# Brønsted acid-mediated cyclization–dehydrosulfonylation/ reduction sequences: An easy access to pyrazinoisoquinolines and pyridopyrazines

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**<sup>1</sup>H and <sup>13</sup>C NMR spectra of synthesized compounds**

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## 1. General information

Melting points reported in this paper are uncorrected and were determined using BUCHI M-560, Buchi Labortechnik AG, Switzerland. Infrared spectra were recorded on Thermo Nicolet 6700 FT-IR Spectrophotometer and are reported in frequency of absorption ( $\text{cm}^{-1}$ ). Mass spectra were measured with Agilent-6530 B Q-TOF (ESI-HRMS),  $^1\text{H}$  and  $^{13}\text{C}$  NMR were recorded on Bruker AVANCE 400 spectrometer. NMR spectra for all the samples were measured in  $\text{CDCl}_3$  using TMS as an internal standard. The chemical shifts are expressed in  $\delta$  ppm down field from the signal of internal TMS.

Trifluoromethanesulfonic acid and iminodiacetic acid were purchased from Sigma-Aldrich and used without further purification. Aromatic/hetero aldehydes were also purchased from Sigma-Aldrich and purified (liquid sample) by distillation under reduced pressure.  $\beta$ -Arylethylamines were prepared from corresponding aromatic/hetero aldehydes using reported procedures.<sup>1-5</sup> Solvents used for the reactions were dried using standard procedures. Analytical thin layer chromatographic tests were carried out using pre-coated aluminum TLC plates. The spots were visualized by short exposure to iodine vapour or UV light. Column chromatography was carried out using Merck silica gel (100–200 mesh). All the glassware were pre-dried at 120 °C for 6 h and assembled while hot and cooled under stream of dry nitrogen gas. In all experiments, round bottom flasks of appropriate size were used.

## 2. Analytical data for compounds 7b–h

### 1-(3,5-Dimethoxyphenethyl)-4-(phenylsulfonyl)piperazine-2,6-dione (7b)

310 mg, (74% yield) white solid; m.p. 135-136 °C; IR (KBr,  $\text{cm}^{-1}$ ): 3003, 2937, 2835, 1740, 1687, 1590, 1515, 1447, 1354, 1268, 1171, 1114, 1026, 960, 851;  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  7.94 (dd,  $J = 8.0, 1.2$  Hz, 2H), 7.65 (s, 1H), 7.89-7.57 (m, 2H), 6.33-6.31 (m, 1H), 6.30-6.28 (m, 2H), 4.13 (s, 4H), 3.76 (s, 6H), 3.65-3.60 (m, 2H), 2.44-2.40 (m, 2H);  $^{13}\text{C}$  (100 MHz,  $\text{CDCl}_3$ ): 166.3, 160.9, 140.8, 135.6, 134.1, 129.9, 127.6, 107.0, 104.6, 98.8, 55.4, 48.9, 40.5, 34.0; HRMS-ESI ( $m/z$ ): Calculated for  $\text{C}_{20}\text{H}_{22}\text{N}_2\text{O}_6\text{S}$  (M+H): 419.1277, Found (M+H): 419.1271.

### 1-(3-Methoxyphenethyl)-4-(phenylsulfonyl)piperazine-2,6-dione (7c)

272 mg, (70% yield) colorless solid; m.p. 131-132 °C; IR (KBr,  $\text{cm}^{-1}$ ): 3005, 2936, 2832, 1741, 1687, 1608, 1444, 1354, 1172, 1112, 9666, 755, 575;  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  7.78-7.79 (m, 2H), 7.66-7.62 (m, 1H), 7.59-7.55 (m, 2H), 7.17 (d,  $J = 8.0$  Hz, 2H), 6.97-6.66 (m, 2H), 4.11 (s, 4H), 3.77 (s, 3H), 3.64-3.60 (m, 2H), 2.52–2.41 (m, 2H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ ):  $\delta$  166.3, 159.8, 139.3, 135.6, 134.1, 130.0, 129.6, 127.6, 121.1, 114.5, 112.2, 55.2, 48.8, 40.5, 33.7; HRMS-ESI ( $m/z$ ): Calculated for  $\text{C}_{19}\text{H}_{20}\text{N}_2\text{O}_5\text{S}$  (M+H): 389.1171, Found (M+H): 389.1140.

### 1-Phenethyl-4-(phenylsulfonyl)piperazine-2,6-dione (7h)

243 mg, (68% yield) colorless solid; m.p. 127-128 °C; IR (KBr,  $\text{cm}^{-1}$ ): 2937, 2835, 1741, 1687, 1608, 1443, 1354, 964, 752, 573;  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  7.80-7.78 (m,

2H), 7.66-7.62 (m, 1H), 7.58-7.55 (m, 2H), 7.29- 7.25 (m, 2H), 7.20-7.18 (m, 1H), 7.15-7.13 (m, 2H), 4.12 (s, 4H), 3.66-3.62 (m, 2H), 2.52–2.48 (m, 2H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ ):  $\delta$  166.3, 137.8, 135.6, 134.1, 130.0, 129.8, 128.6, 127.6, 126.8, 48.8, 40.7, 33.7; HRMS-ESI ( $m/z$ ): Calculated for  $\text{C}_{18}\text{H}_{18}\text{N}_2\text{O}_4\text{S}$  (M+H): 359.1066, Found (M+H): 359.1072.

**1-(2-(1*H*-Indol-3-yl)ethyl)-4-(phenylsulfonyl)piperazine-2,6-dione (7g)**

309 mg, (78% yield) yellow solid; m.p. 117-118 °C; IR (KBr,  $\text{cm}^{-1}$ ): 3403, 3121, 1742, 1687, 1541, 1486, 1447, 1398, 1325, 1171, 1060, 933, 835, 741, 660, 574;  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  7.97 (s, 1H), 7.81-7.78 (m, 2H), 7.64-7.60 (m, 2H), 7.57-7.53 (m, 2H), 7.33 (d,  $J = 8.0$  Hz, 1H), 7.17 (td,  $J = 7.6, 1.2$  Hz, 1H), 7.1 (td,  $J = 8.0, 7.6$  Hz, 1H), 6.99 (d,  $J = 2.4$  Hz, 1H), 4.11 (s, 4H), 3.73-3.69 (m, 2H), 2.69-2.65 (m, 2H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ ):  $\delta$  166.5, 134.1, 130.0, 127.7, 122.3, 119.7, 118.9, 111.3, 49.0, 40.2, 23.5; HRMS-ESI ( $m/z$ ): Calculated for  $\text{C}_{20}\text{H}_{19}\text{N}_3\text{O}_4\text{S}$  (M+H): 398.1175, Found (M+H): 398.1167.

**1-(2-(Benzo[*b*]thiophen-2-yl)ethyl)-4-(phenylsulfonyl)piperazine-2,6-dione (7f)**

298 mg, (72% yield) yellow liquid; IR (KBr,  $\text{cm}^{-1}$ ): 2920, 1680, 1335, 1154, 960, 738, 623, 578;  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  7.3 (d,  $J = 7.2$  Hz, 2H), 7.7 (d,  $J = 7.6$  Hz, 1H), 7.59 (dd,  $J = 6.8, 4.4$  Hz, 2H), 7.53-7.49 (m, 2H), 7.26-7.18 (m, 2H), 6.94 (s, 1H), 4.08 (s, 4H), 3.72-3.68 (m, 2H), 2.76–2.72 (m, 2H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ ):  $\delta$  166.4, 140.7, 140.0, 139.6, 139.4, 135.6, 134.0, 129.8, 127.7, 124.4, 124.0, 123.2, 122.3, 49.0,

40.0, 31.1, 28.6; HRMS-ESI ( $m/z$ ): Calculated for  $C_{20}H_{18}N_2O_4S_2$  (M+H): 415.0786, Found (M+H): 415.0760.

**4-(Phenylsulfonyl)-1-(3,4,5-trimethoxyphenethyl)piperazine-2,6-dione (7d)**

304 mg, (68% yield) yellow solid; m.p. 125-126 °C; IR (KBr,  $cm^{-1}$ ): 1739, 1687, 1647, 1588, 1507, 1446, 1335, 1240, 1170, 1125, 1004, 954,763, 737, 627, 523;  $^1H$  NMR (400 MHz,  $CDCl_3$ ):  $\delta$  7.80 (d,  $J = 7.6$  Hz, 2H), 7.66-7.67 (m, 1H), 7.60-7.56 (m, 2H), 6.36 (s, 2H), 4.12 (s, 4H), 3.84 (s, 6H), 3.80 (s, 3H), 3.67-3.63 (m, 2H), 2.56-2.39 (m, 2H);  $^{13}C$  NMR (100 MHz,  $CDCl_3$ ):  $\delta$  166.5, 153.4, 136.9, 135.5, 134.2, 133.5, 130.0, 127.7, 105.8, 60.9, 56.2, 48.9, 40.8, 34.2; HRMS-ESI ( $m/z$ ): Calculated for  $C_{21}H_{24}N_2O_7S$  (M+H): 449.1382, Found (M+H): 449.1372.

**4-(Phenylsulfonyl)-1-(2-(thiophen-2-yl)ethyl)piperazine-2,6-dione (7e)**

273 mg, (75% yield) yellow liquid ; IR (KBr,  $cm^{-1}$ ): 3007, 1743, 1688, 1616, 1345, 1283, 1170, 970, 854, 757, 627, 574;  $^1H$  NMR (400 MHz,  $CDCl_3$ ):  $\delta$  7.81-7.78 (m, 2H), 7.68-7.64 (m, 1H), 7.61-7.55 (m, 2H), 7.12 (dd,  $J = 5.2, 1.2$  Hz, 1H), 6.90 (dd,  $J = 5.2, 3.6$  Hz, 1H), 6.78-6.77 (m, 1H), 4.13 (s, 4H), 3.71-3.67 (m, 2H), 2.74 (m, 2H);  $^{13}C$  NMR (100 MHz,  $CDCl_3$ ):  $\delta$  166.4, 139.7, 135.7, 134.2, 130.0, 127.7, 127.1, 125.7, 124.2, 49.0, 40.6, 27.7; HRMS-ESI ( $m/z$ ): Calculated for  $C_{16}H_{16}N_2O_4S_2$  (M+H): 365.0630, Found (M+H): 365.0627.

### 3. Analytical data for compounds **8b–c**, **8h** and **8i**

#### **4-Benzyl-1-(3,5-dimethoxyphenethyl)piperazine-2,6-dione (8b)**

258 mg, (70% yield) yellow liquid; IR (KBr,  $\text{cm}^{-1}$ ): 2942, 2833, 1736, 1683, 1589, 1470, 1442, 1351, 1267, 1168, 1083, 1007, 748, 632;  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  7.33-7.30 (m, 1H), 7.29-7.26 (m, 2H), 7.26-7.22 (m, 2H), 6.94 (t,  $J = 8.0$  Hz, 1H), 6.78-6.74 (m, 2H), 3.97-3.93 (m, 2H), 3.82 (s, 3H), 3.80 (s, 3H), 3.56 (s, 2H), 3.38 (s, 4H), 2.86-2.82 (m, 2H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ ):  $\delta$  169.9, 152.9, 147.7, 135.7, 132.4, 129.2, 128.8, 128.0, 123.8, 122.6, 111.0, 60.9, 60.8, 56.5, 55.8, 39.7, 28.2; HRMS-ESI ( $m/z$ ): Calculated for  $\text{C}_{21}\text{H}_{24}\text{N}_2\text{O}_4$  (M+H): 369.1814, Found (M+H): 369.1806.

#### **4-Benzyl-1-(3-methoxyphenethyl)piperazine-2,6-dione (8c)**

230 mg, (68% yield) yellow liquid; IR (KBr,  $\text{cm}^{-1}$ ): 2955, 2834, 1734, 1682, 1596, 1350, 1261, 1162, 1043, 699;  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  7.27-7.21 (m, 3H), 7.18-7.16 (m, 2H), 7.14-7.10 (m, 1H), 6.75 (d,  $J = 7.6$  Hz, 1H), 6.70-6.66 (m, 2H), 3.91-3.87 (m, 2H), 3.70 (s, 3H), 3.48 (s, 2H), 3.28 (s, 4H), 2.75-2.71 (m, 2H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ ):  $\delta$  169.8, 159.7, 139.9, 135.5, 129.5, 129.0, 128.7, 128.0, 121.4, 114.5, 112.1, 60.6, 56.2, 55.1, 40.1, 33.9; HRMS-ESI ( $m/z$ ): Calculated for  $\text{C}_{20}\text{H}_{22}\text{N}_2\text{O}_3$  (M+H): 339.1709, Found (M+H): 339.1683.

#### **4-Benzyl-1-phenethylpiperazine-2,6-dione (8h)**

216 mg, (70% yield) yellow liquid; IR (KBr,  $\text{cm}^{-1}$ ): 2926, 1692, 1449, 1369, 1031, 747, 698;  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  7.31-7.27 (m, 1H), 7.27-7.22 (m, 2H), 7.22-7.17 (m, 1H), 7.17-7.12 (m, 2H), 4.02-3.83 (m, 2H), 3.51 (s, 2H), 3.30 (s, 4H), 2.88-2.68 (m, 2H);

$^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ ):  $\delta$  169.9, 138.4, 135.5, 129.2, 129.0, 128.8, 128.6, 128.0, 126.7, 60.6, 56.4, 40.4, 34.0; HRMS-ESI ( $m/z$ ): Calculated for  $\text{C}_{19}\text{H}_{20}\text{N}_2\text{O}_2$  (M+H): 309.1603, Found (M+H): 309.1590.

#### **4-Benzyl-1-(2-(1-ethyl-1*H*-pyrrol-2-yl)ethyl)piperazine-2,6-dione (8i)**

254 mg, (78% yield) yellow liquid; IR (KBr,  $\text{cm}^{-1}$ ): 3098, 2973, 2780, 2247, 1743, 1684, 1439, 1351, 1148, 1068, 965, 922, 709, 629;  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  7.38-7.35 (m, 1H), 7.34-7.31 (m, 2H), 7.30-7.28 (m, 3H), 6.63 (dd,  $J = 2.8, 2.0$  Hz, 1H), 6.09-6.07 (m, 1H), 5.86 (dd,  $J = 3.6, 1.6$  Hz, 1H), 3.96-3.92 (m, 4H), 3.61 (s, 2H), 3.40 (s, 4H), 2.82-2.79 (m, 2H), 1.31 (t,  $J = 7.3$  Hz, 3H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ ):  $\delta$  169.9, 135.4, 129.1, 128.7, 128.1, 128.0, 119.6, 107.1, 107.0, 60.8, 56.4, 41.0, 38.8, 24.5, 16.8; HRMS-ESI ( $m/z$ ): Calculated for  $\text{C}_{19}\text{H}_{23}\text{N}_3\text{O}_2$  (M+H): 326.1869, Found (M+H): 326.1863.

## **4. Analytical data for compounds 9b–g**

### **9,11-Dimethoxy-2-(phenylsulfonyl)-2,3,6,7-tetrahydro-4*H*-pyrazino[2,1-*a*]isoquinolin-4-one (9b)**

348 mg, (87% yield) colorless liquid; IR (KBr,  $\text{cm}^{-1}$ ): 2926, 2845, 1680, 1514, 1356, 1162, 1032, 825, 733;  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  7.83 (dd,  $J = 7.2, 1.6$  Hz, 2H), 7.61-7.57 (m, 1H), 7.53-7.49 (m, 1H), 7.16 (s, 1H), 6.42 (d,  $J = 2.0$  Hz, 1H), 6.27 (d,  $J = 2.4$  Hz, 1H), 4.18 (s, 2H), 3.89 (s, 3H), 3.81 (s, 3H), 3.47-3.44 (m, 2H), 2.57-2.54 (m, 2H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ ):  $\delta$  162.3, 138.0, 133.4, 129.1, 127.4, 104.6, 97.8, 55.8, 55.5, 48.3, 38.1, 29.9; HRMS-ESI ( $m/z$ ): Calculated for  $\text{C}_{20}\text{H}_{20}\text{N}_2\text{O}_5\text{S}$  (M+H): 401.1171, Found (M+H): 401.1156.



**9-Methoxy-2-(phenylsulfonyl)-2,3,6,7-tetrahydro-4H-pyrazino[2,1-a]isoquinolin-4-one (9c)**

337 mg, (91% yield) colorless liquid; IR (KBr,  $\text{cm}^{-1}$ ): 2933, 1682, 1494, 1456, 1361, 1280, 1172, 1024, 725;  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  7.81 (dd,  $J = 8.0, 0.8$  Hz, 2H), 7.60-7.56 (m, 1H), 7.49 (td,  $J = 6.8, 1.6$  Hz, 2H), 7.426 (d,  $J = 8.8$  Hz, 1H), 6.85-6.79 (m, 1H), 6.63 (d,  $J = 2.78$  Hz, 1H), 6.6 (d,  $J = 4.4$  Hz, 1H), 4.18 (s, 2H), 3.89 (s, 3H), 3.80 (s, 4H), 3.53-3.45 (m, 2H), 2.58-2.55 (m, 2H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ ):  $\delta$  161.9, 152.9, 145.7, 136.9, 133.6, 129.3, 128.4, 127.3, 126.5, 121.4, 119.6, 111.4, 104.4, 60.8, 56.0, 48.3, 37.9, 21.9; HRMS-ESI ( $m/z$ ): Calculated for  $\text{C}_{19}\text{H}_{18}\text{N}_2\text{O}_4\text{S}$  (M+H): 371.1066, Found (M+H): 371.1035.

**9,10,11-Trimethoxy-2-(phenylsulfonyl)-2,3,6,7-tetrahydro-4H-pyrazino[2,1-a]isoquinolin-4-one (9d)**

365 mg, (85% yield) colorless liquid; IR (KBr,  $\text{cm}^{-1}$ ): 2936, 2842, 1677, 1592, 1461, 1354, 1162, 1100, 1032, 726, 573;  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  7.81-7.79 (m, 2H), 7.59-7.55 (m, 1H), 7.52-7.47 (m, 2H), 7.23 (s, 1H), 6.40 (s, 1H), 4.11 (s, 2H), 3.83 (s, 3H), 3.81 (s, 6H), 3.53-3.46 (m, 2H), 2.56-2.53 (m, 2H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ ):  $\delta$  162.0, 153.1, 151.3, 141.7, 136.8, 133.5, 131.1, 129.2, 127.3, 121.0, 114.4, 109.6, 107.1, 61.1, 60.4, 56.0, 48.1, 38.3, 29.4; HRMS-ESI ( $m/z$ ): Calculated for  $\text{C}_{21}\text{H}_{22}\text{N}_2\text{O}_6\text{S}$  (M+H): 431.1277, Found (M+H): 431.1269.

**2-(Phenylsulfonyl)-2,3,6,7-tetrahydro-4*H*-thieno[3',2':3,4]pyrido[1,2-*a*]pyrazin-4-one (9e)**

294 mg, (85% yield) yellow liquid; IR (KBr,  $\text{cm}^{-1}$ ): 2925, 2857, 1689, 1456, 1359, 1168, 960, 726, 684;  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  7.83-7.80 (m, 2H), 7.6-7.56 (m, 1H), 7.53-7.49 (m, 2H), 7.16 (d,  $J = 5.2$  Hz, 1H), 7.10 (d,  $J = 5.2$  Hz, 1H), 6.60 (s, 1H), 4.15 (s, 2H), 3.63 (t,  $J = 6.0$  Hz, 2H), 2.83 (t,  $J = 6.0$  Hz, 2H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ ):  $\delta$  161.9, 136.8, 134.7, 133.6, 129.3, 127.7, 127.2, 125, 124.9, 122.1, 104.9, 48.6, 38.9, 24.0; HRMS-ESI ( $m/z$ ): Calculated for  $\text{C}_{16}\text{H}_{14}\text{N}_2\text{O}_3\text{S}_2$  (M+H): 347.0524, Found (M+H): 347.0526.

**2-(Phenylsulfonyl)-2,3,6,7-tetrahydro-4*H*-benzo[4',5']thieno[3',2':3,4]pyrido[1,2-*a*]pyrazin-4-one (9f)**

285 mg, (72% yield) yellow solid; m.p. 105-106  $^\circ\text{C}$ ; IR (KBr,  $\text{cm}^{-1}$ ): 2923, 2855, 1657, 1576, 1479, 1268, 1023, 803;  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  7.89 (d,  $J = 8.0$  Hz, 1H), 7.8-7.43 (m, 3H), 7.51 (d,  $J = 7.2$  Hz, 1H), 7.46-7.43 (m, 3H), 7.34-7.31 (m, 1H), 6.95 (s, 1H), 4.17 (s, 2H), 3.64-3.61 (m, 2H), 2.84-2.81 (m, 2H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ ):  $\delta$  162.5, 139.1, 138.4, 136.8, 135.1, 133.7, 129.4, 127.3, 125.6, 124.8, 124.0, 123.1, 122.3, 122.2, 105.9, 48.3, 38.4, 29.8; HRMS-ESI ( $m/z$ ): Calculated for  $\text{C}_{20}\text{H}_{16}\text{N}_2\text{O}_3\text{S}_2$  (M+H): 397.0681, Found (M+H): 397.0678.

**2-(Phenylsulfonyl)-2,6,7,12-tetrahydropyrazino[1',2':1,2]pyrido[3,4-*b*]indol-4(3H)-one (9g)**

326 mg, (86% yield) yellow oily liquid; IR (KBr,  $\text{cm}^{-1}$ ): 3319, 2924, 1679, 1358, 1169, 989, 737, 687, 639;  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  8.46 (s, 1H), 7.89-7.87 (m, 2H), 7.62-7.58 (m, 1H), 7.55-7.50 (m, 2H), 7.45 (d,  $J = 8.0$  Hz, 1H), 7.35 (dt,  $J = 8.4, 0.8$  Hz, 1H), 7.24-7.22 (m, 1H), 7.26-7.21 (m, 1H), 7.12 (td,  $J = 7.2, 1.2$  Hz, 1H), 4.23 (s, 2H), 3.68 (t,  $J = 6.0$  Hz, 2H), 2.84 (t,  $J = 6.0$  Hz, 2H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ ):  $\delta$  161.7, 137.6, 133.9, 129.5, 127.3, 126.4, 125.4, 124.3, 122.6, 120.5, 118.9, 112.6, 111.4, 102.6, 49.0, 39.6, 20.3; HRMS-ESI ( $m/z$ ): Calculated for  $\text{C}_{20}\text{H}_{17}\text{N}_3\text{O}_3\text{S}$  (M+H): 380.1069, Found (M+H): 380.1045.

## **5. Analytical data for compounds 10b–f**

**9,11-Dimethoxy-6,7-dihydro-4*H*-pyrazino[2,1-*a*]isoquinolin-4-one (10b)**

211 mg, (82% yield) yellow solid; m.p. 137-138 °C; IR (KBr,  $\text{cm}^{-1}$ ): 2926, 2850, 1680, 1514, 1354, 1162, 1030, 993, 732;  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  8.06 (s, 1H), 7.75 (s, 1H), 7.17 (s, 1H), 6.75 (s, 1H), 4.22-4.17 (m, 2H), 3.94 (s, 6H), 2.96-2.93 (m, 2H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ ):  $\delta$  155.9, 151.8, 149.0, 145.3, 135.6, 129.0, 119.9, 118.8, 110.8, 107.7, 56.4, 56.2, 38.8, 27.0; HRMS-ESI ( $m/z$ ): Calculated for  $\text{C}_{14}\text{H}_{14}\text{N}_2\text{O}_3$  (M+H): 259.1083, Found (M+H): 259.1070.

**9-Methoxy-6,7-dihydro-4*H*-pyrazino[2,1-*a*]isoquinolin-4-one (10c)**

194 mg, (85% yield) yellow solid; m.p. 120-138 °C; IR (KBr,  $\text{cm}^{-1}$ ): 2965, 2923, 2853, 1737, 1651, 1584, 1562, 1464, 1421, 1334, 1190, 825, 799, 734, 738, 552;  $^1\text{H}$  NMR

(400 MHz, CDCl<sub>3</sub>): δ 8.03 (s, 1H), 7.76 (s, 1H), 7.68 (d, *J* = 8.7 Hz, 1H), 6.88 (dd, *J* = 8.7, 2.6 Hz, 1H), 6.77 (d, *J* = 2.6 Hz, 1H), 4.21-4.18 (m, 2H), 3.84 (s, 3H), 3.00-2.96 (m, 2H); <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>): δ 161.8, 159.9, 155.8, 145.1, 137.2, 135.7, 129.7, 129.4, 127.4, 127.0, 119.8, 119.3, 114.5, 114.1, 113.4, 55.6, 38.7, 27.7; HRMS-ESI (*m/z*): Calculated for C<sub>13</sub>H<sub>12</sub>N<sub>2</sub>O<sub>2</sub> (M+H): 229.0977, Found (M+H): 229.0969.

**9,10,11-Trimethoxy-6,7-dihydro-4*H*-pyrazino[2,1-*a*]isoquinolin-4-one (10d)**

229 mg, (80% yield) yellow solid; m.p. 127-128 °C; IR (KBr, cm<sup>-1</sup>): 2926, 2853, 1661, 1596, 1338, 1190, 1116, 838, 810; <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>): δ 8.37 (s, 1H), 8.08 (s, 1H), 6.58 (s, 1H), 4.18 (m, 2H), 3.95-3.84 (m, 9H), 2.94-2.83 (m, 2H); <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>): δ 156.0, 155.5, 153.0, 145.2, 142.1, 133.1, 133.0, 124.6, 113.3, 107.1, 61.2, 56.2, 38.8, 29.8, 28.7; HRMS-ESI (*m/z*): Calculated for C<sub>15</sub>H<sub>16</sub>N<sub>2</sub>O<sub>4</sub> (M+H): 289.1188, Found (M+H): 289.1171.

**6,7-Dihydro-4*H*-thieno[3',2':3,4]pyrido[1,2-*a*]pyrazin-4-one (10e)**

184 mg, (90% yield) yellow solid; m.p. 132-133 °C; IR (KBr, cm<sup>-1</sup>): 2923, 2855, 1656, 1580, 1457, 1269, 1097; <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>): δ 8.02 (s, 1H), 7.58 (s, 1H), 7.26 (s, 2H), 4.27 (t, *J* = 6.8 Hz, 2H), 3.09 (t, *J* = 6.8 Hz, 2H); <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>): δ 155.8, 146.1, 139.1, 132.5, 128.0, 125.6, 123.0, 119.5, 39.3, 29.7, 22.7; HRMS-ESI (*m/z*): Calculated for C<sub>10</sub>H<sub>8</sub>N<sub>2</sub>OS (M+H): 205.0436, Found (M+H): 205.0419.

**6,7-Dihydro-4*H*-benzo[4',5']thieno[3',2':3,4]pyrido[1,2-*a*]pyrazin-4-one (10f)**

193 mg, (76% yield) yellow solid; m.p. 156-157 °C; IR (KBr,  $\text{cm}^{-1}$ ): 2925, 2855, 1657, 1576, 1479, 1268, 1023, 803, 734;  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  8.14 (s, 1H), 8.13-8.06 (m, 1H), 7.88 (s, 1H), 7.54-7.50 (m, 1H), 7.45-7.43 (m, 1H), 7.43-7.41 (m, 1H), 4.39-4.36 (m, 2H), 3.24-3.21 (m, 2H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ ):  $\delta$  156.0, 146.6, 143.3, 139.3, 134.9, 132.5, 126.0, 125.3, 123.3, 122.7, 122.5, 120.5, 38.8, 24.2; HRMS-ESI ( $m/z$ ): Calculated for  $\text{C}_{14}\text{H}_{10}\text{N}_2\text{OS}$  (M+H): 255.0592, Found (M+H): 255.0583.

**6. Analytical data for compounds 11a–c and 11i**

**2-Benzyl-9,10-dimethoxy-1,2,3,6,7,11*b*-hexahydro-4*H*-pyrazino[2,1-*a*]isoquinolin-4-one (11a)**

300 mg, (85% yield) colorless liquid; IR (KBr,  $\text{cm}^{-1}$ ): 2931, 2841, 1648, 1484, 1454, 1329, 1279, 1089, 744, 697;  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  7.35-7.26 (m, 4H), 7.32-7.26 (m, 1H), 6.62 (s, 1H), 6.50 (s, 1H), 4.85-4.79 (m, 2H), 3.86 (s, 3H), 3.80 (s, 3H), 3.72 (d,  $J = 12.8$  Hz, 1H), 3.56-3.52 (m, 1H), 3.48-3.43 (m, 2H), 2.95-2.78 (m, 3H), 2.63 (dd,  $J = 15.2, 2.8$  Hz, 1H), 2.38 (dd,  $J = 11.6, 10.0$  Hz, 1H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ ):  $\delta$  165.5, 148.2, 147.9, 136.8, 129.2, 128.6, 127.7, 127.5, 126.2, 111.9, 108.0, 61.9, 57.1, 56.5, 56.3, 56.0, 55.5, 39.0, 28.5; HRMS-ESI ( $m/z$ ): Calculated for  $\text{C}_{21}\text{H}_{24}\text{N}_2\text{O}_3$  (M+H): 353.1865, Found (M+H): 353.1861.

**2-Benzyl-9,11-dimethoxy-1,2,3,6,7,11b-hexahydro-4H-pyrazino[2,1-a]isoquinolin-4-one (11b)**

290 mg, (82% yield) colorless. liquid ; IR (KBr,  $\text{cm}^{-1}$ ): 2923, 2841, 1650, 1458, 1279, 1088, 744, 697;  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  7.28-7.26 (m, 4H), 7.25-7.19 (m, 1H), 6.69 (dd,  $J = 16.8, 8.8$  Hz, 2H), 4.72 (dd,  $J = 11.2, 4.4$  Hz, 2H), 3.8 (s, 3H), 3.73 (s, 3H), 3.59-3.51 (m, 2H), 3.47-3.43 (m, 1H), 3.41-3.37 (m, 1H), 2.88 (d,  $J = 4.4$  Hz, 1H), 2.84 (d,  $J = 6.0$  Hz, 1H), 2.74-2.68 (m, 2H), 2.26 (dd,  $J = 11.2, 10.0$  Hz, 1H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ ):  $\delta$  166.5, 151.4, 146.6, 136.9, 129.7, 129.2, 128.6, 127.8, 127.7, 120.3, 110.8, 61.9, 60.4, 57.3, 56.3, 55.9, 55.1, 38.6, 23.1; HRMS-ESI ( $m/z$ ): Calculated for  $\text{C}_{21}\text{H}_{24}\text{N}_2\text{O}_3$  (M+H): 353.1865, Found (M+H): 353.1861.

**2-Benzyl-9-methoxy-1,2,3,6,7,11b-hexahydro-4H-pyrazino[2,1-a]isoquinolin-4-one (11c)**

273 mg, (85% yield) colorless liquid; IR (KBr,  $\text{cm}^{-1}$ ): 2928, 2840, 1648, 1501, 1457, 1294, 1246, 1157, 1034, 744, 710, 600;  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  7.35 (d,  $J = 4.4$  Hz, 4H), 7.32-7.29 (m, 1H), 6.94 (d,  $J = 8.8$  Hz, 1H), 6.74 (dd,  $J = 8.8, 2.4$  Hz, 1H), 6.67 (d,  $J = 2.4$  Hz, 1H), 4.83-4.74 (m, 2H), 3.78 (s, 3H), 3.62 (d,  $J = 4.0$  Hz, 2H), 3.51-3.45 (m, 2H), 2.96-2.85 (m, 3H), 2.73-2.69 (m, 1H), 2.34-2.29 (m, 1H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ ):  $\delta$  166.6, 158.5, 136.9, 136.5, 129.2, 128.7, 127.7, 126.7, 126.0, 113.8, 113.0, 61.9, 57.3, 56.2, 55.4, 55.3, 38.9, 29.2; HRMS-ESI ( $m/z$ ): Calculated for  $\text{C}_{20}\text{H}_{22}\text{N}_2\text{O}_2$  (M+H): 323.1760, Found (M+H): 323.1775.

**2-Benzyl-8-ethyl-2,3,6,7,8,10b-hexahydropyrrolo[3',2':3,4]pyrido[1,2-a]pyrazin-4(1H)-one (11i)**

259 mg, (84% yield) green liquid; IR (KBr,  $\text{cm}^{-1}$ ): 2923, 2853, 1647, 1455, 1351, 1284, 1092 (br) 705, 477;  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  7.27-7.26 (m, 5H), 7.19 (s, 1H), 6.50 (d,  $J = 2.8$  Hz, 1H), 5.77 (d,  $J = 2.8$  Hz, 1H), 4.98-4.93 (m, 1H), 4.64 (dd,  $J = 10.4, 4.8$  Hz, 1H), 3.75-3.69 (m, 2H), 3.57-3.41 (m, 3H), 3.31-3.26 (m, 1H), 2.85-2.75 (m, 2H), 2.67-2.65 (m, 1H), 2.17 (d,  $J = 10.4$  Hz, 1H), 1.29-1.25 (m, 3H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ ):  $\delta$  166.8, 129.2, 128.6, 127.6, 125.7, 119.5, 116.4, 61.9, 57.6, 56.4, 53.7, 41.1, 38.6, 29.8, 21.9, 16.5; HRMS-ESI ( $m/z$ ): Calculated for  $\text{C}_{19}\text{H}_{23}\text{N}_3\text{O}$  (M+H): 310.1919, Found (M+H): 310.1913.

## 7. X-ray crystal structure of compound 9b and 10a

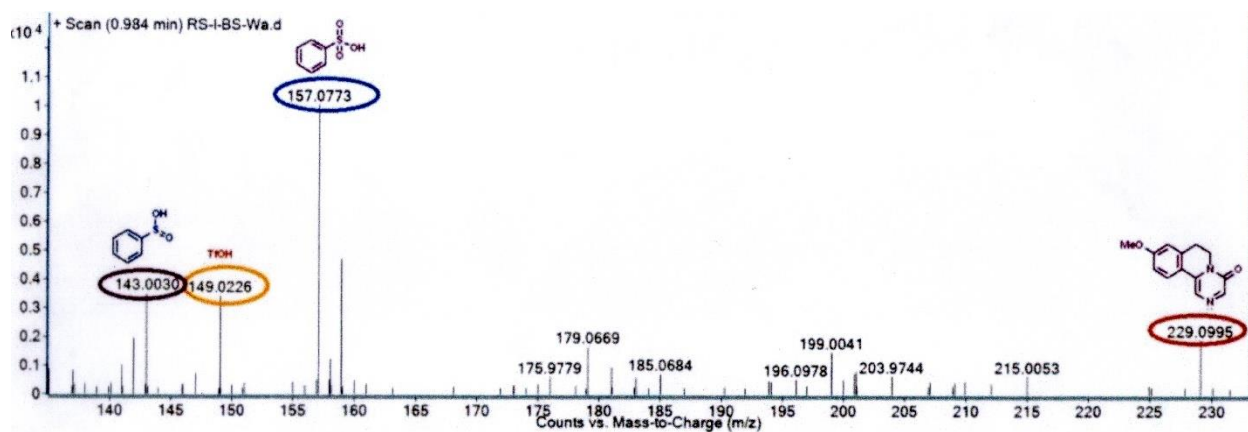
<b>Crystal data:</b>	<b>9b</b>	<b>10a</b>
Empirical formula	C <sub>41</sub> H <sub>42</sub> N <sub>4</sub> O <sub>10</sub> S <sub>2</sub> Cl <sub>2</sub>	C <sub>14</sub> H <sub>14</sub> N <sub>2</sub> O <sub>3</sub>
Formula weight	885.80	258.27
Temperature/K	298	298(2)
Crystal system	monoclinic	orthorhombic
Space group	<i>P</i> 2 <sub>1</sub>	<i>P</i> bca
<i>a</i> /Å	8.0605(10)	9.3599(7)
<i>b</i> /Å	26.933(3)	9.3599(7)
<i>c</i> /Å	9.4487(11)	17.9438(15)
$\alpha$ /°	90.00	90
$\beta$ /°	92.587(12)	90
$\gamma$ /°	90.00	90
Volume/Å <sup>3</sup>	2049.2(4)	2453.1(3)
<i>Z</i>	2	8
$\rho_{\text{calc}}$ /mg/mm <sup>3</sup>	1.436	1.399
<i>m</i> /mm <sup>-1</sup>	0.324	0.100
<i>F</i> (000)	924.0	1088.0
Crystal size/mm <sup>3</sup>	0.5 × 0.25 × 0.2	0.3 × 0.2 × 0.03
2 $\theta$ range for data collection	7.172 to 58.332°	7.194 to 58.37°
Index ranges	-10 ≤ <i>h</i> ≤ 8, -28 ≤ <i>k</i> ≤ 36, -12 ≤ <i>l</i> ≤ 12	-18 ≤ <i>h</i> ≤ 19, -12 ≤ <i>k</i> ≤ 10, -21 ≤ <i>l</i> ≤ 24
Reflections collected	11174	10303
Independent reflections	7170 [ <i>R</i> <sub>int</sub> = 0.0766, <i>R</i> <sub>sigma</sub> = 0.1184]	2961 [ <i>R</i> <sub>int</sub> = 0.0359, <i>R</i> <sub>sigma</sub> = 0.0429]
Data/restraints/parameters	7170/1/547	2961/0/174
Goodness-of-fit on <i>F</i> <sup>2</sup>	1.097	1.021
Final <i>R</i> indexes [ <i>I</i> ≥ 2σ( <i>I</i> )]	<i>R</i> <sub>1</sub> = 0.0861, <i>wR</i> <sub>2</sub> = 0.2042	<i>R</i> <sub>1</sub> = 0.0503, <i>wR</i> <sub>2</sub> = 0.1099
Final <i>R</i> indexes [all data]	<i>R</i> <sub>1</sub> = 0.1508, <i>wR</i> <sub>2</sub> = 0.2538	<i>R</i> <sub>1</sub> = 0.1020, <i>wR</i> <sub>2</sub> = 0.1352
Largest diff. peak/hole / e Å <sup>-3</sup>	0.40/-0.37	0.17/-0.22



## 8. References

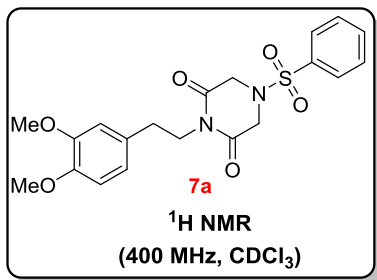
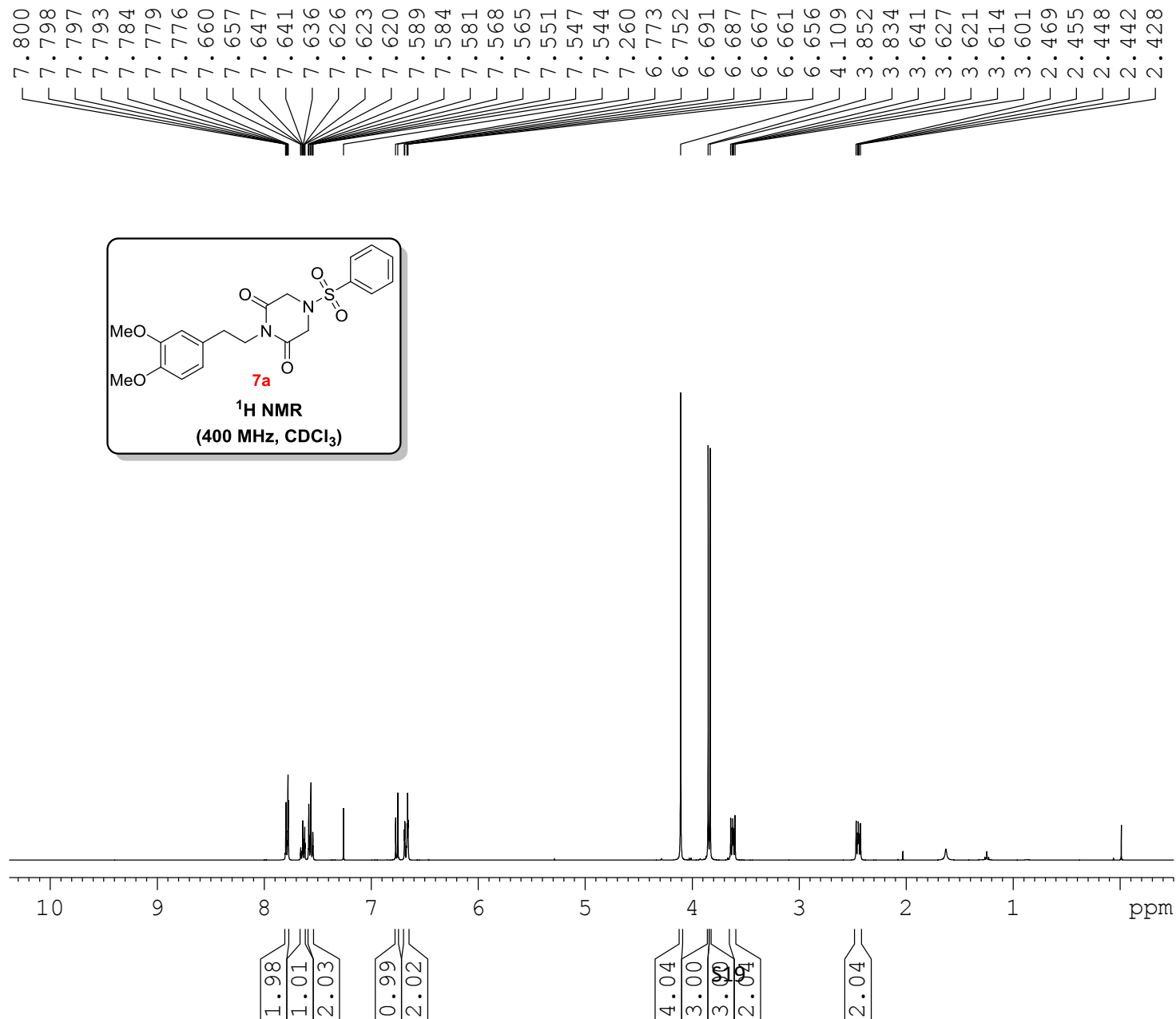
1. Merchant, J. R.; Mountwala, A. J. *J. Org. Chem.* **1958**, *23*, 1774
2. Sinhababu, A. K.; Borchardt, R. T. *Tetrahedron Lett.* **1983**, *24*, 227
3. Trost, B. M. ; Yeh, V. S. C. ; Ito, H. ; Bremeyer, N. *Org. Lett.* **2002**, *4*, 2621
4. Pei, Z. ; Li, L.; Geldern, T.W. ; Longenecker, K. ; Pireh, D.; Stewart, K. D. ; Backes, B. J. ; Lai, C.; Lubben, T. H. ; Ballaron, S. J ; Beno, D. W. A.; Grote, A. J. ; Sham, H. L. ; Trevillyan, J. M. *J. Med. Chem.* **2007**, *50*, 1983.
5. Gigant, N.; Claveau, E.; Bouyssou, P.; Gillaizeau, I. *Org. Lett.* **2012**, *7*, 3679.

## 9. HRMS spectra of an aliquot generated from cyclization reaction of 7c

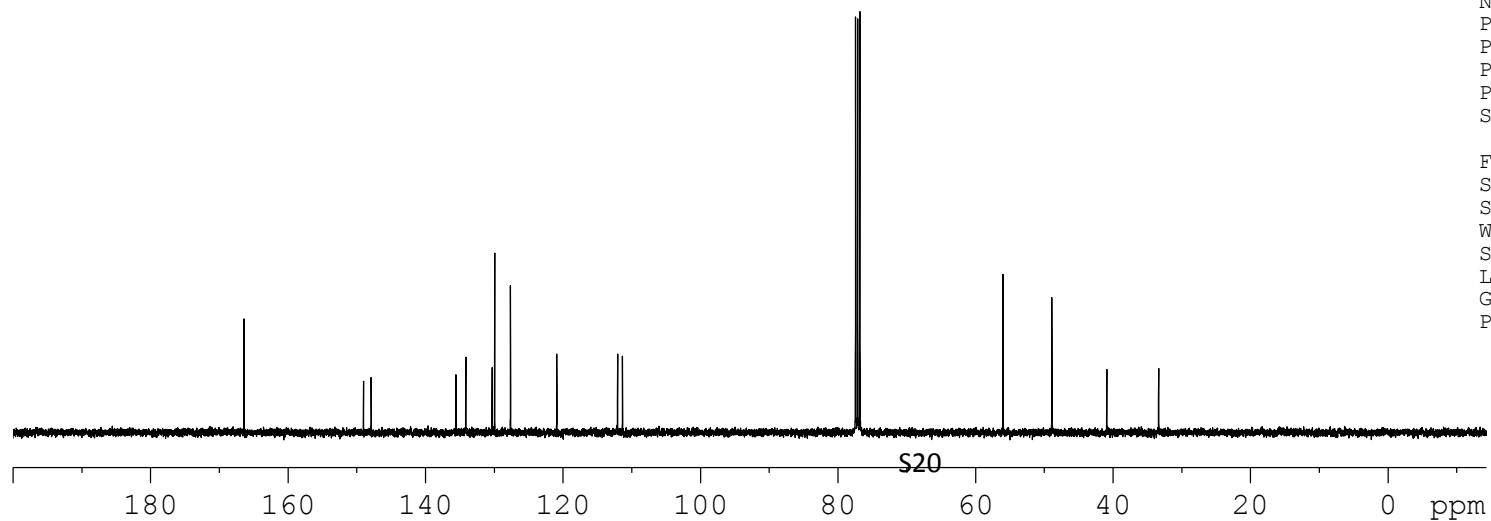
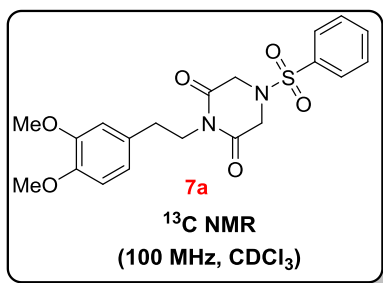
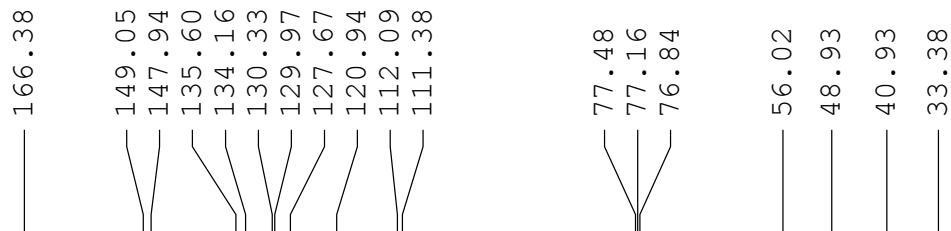


## 10. Copies of $^1\text{H}$ and $^{13}\text{C}$ NMR spectra

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C13CPD CDC13 {D:\CRR} KOPAL 1



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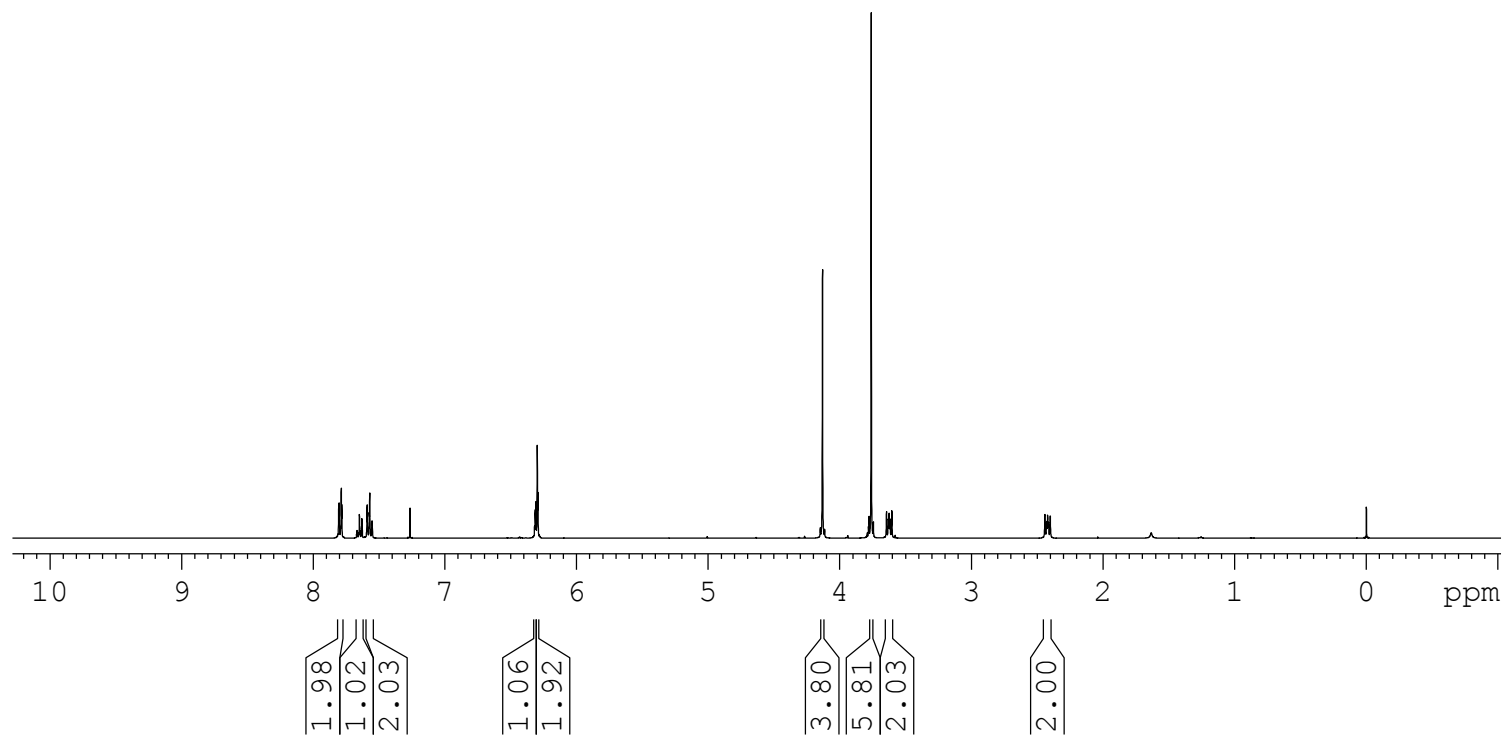
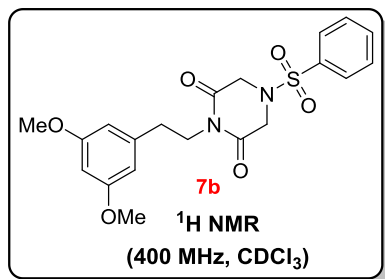
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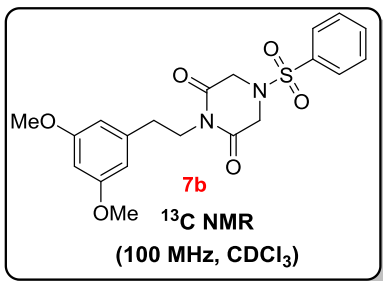
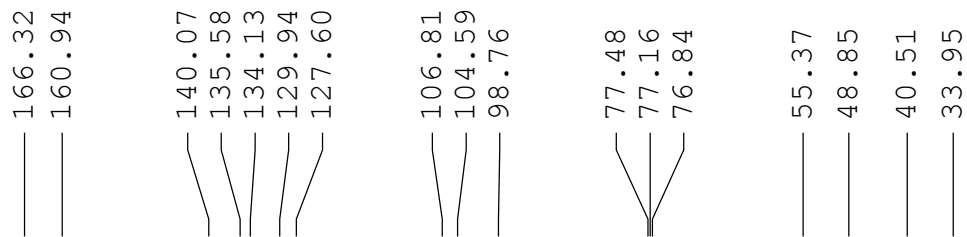
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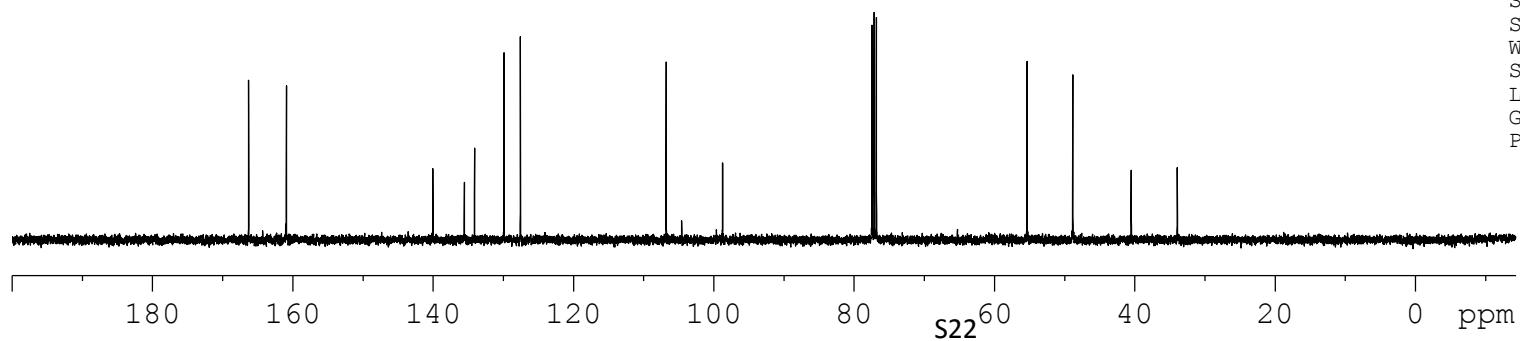
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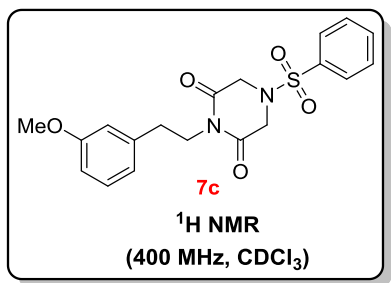


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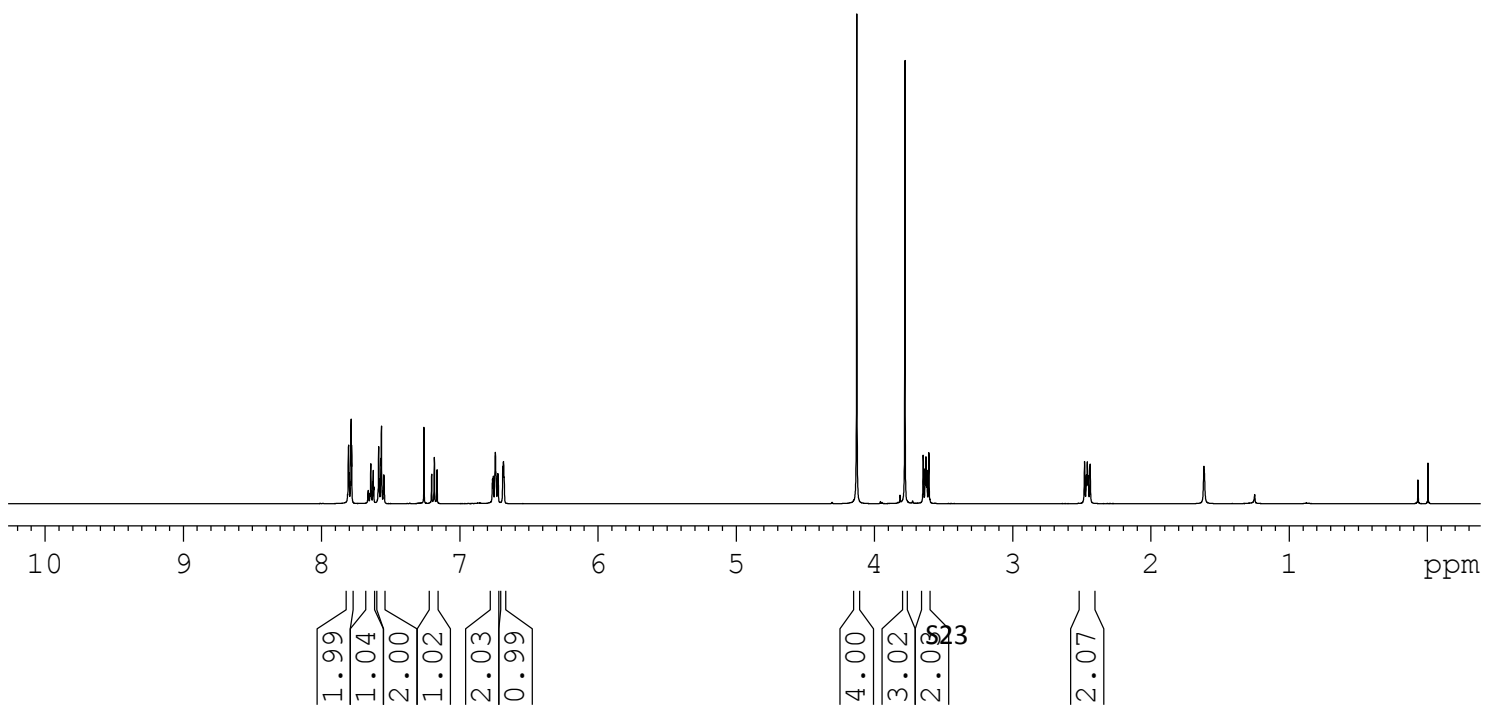
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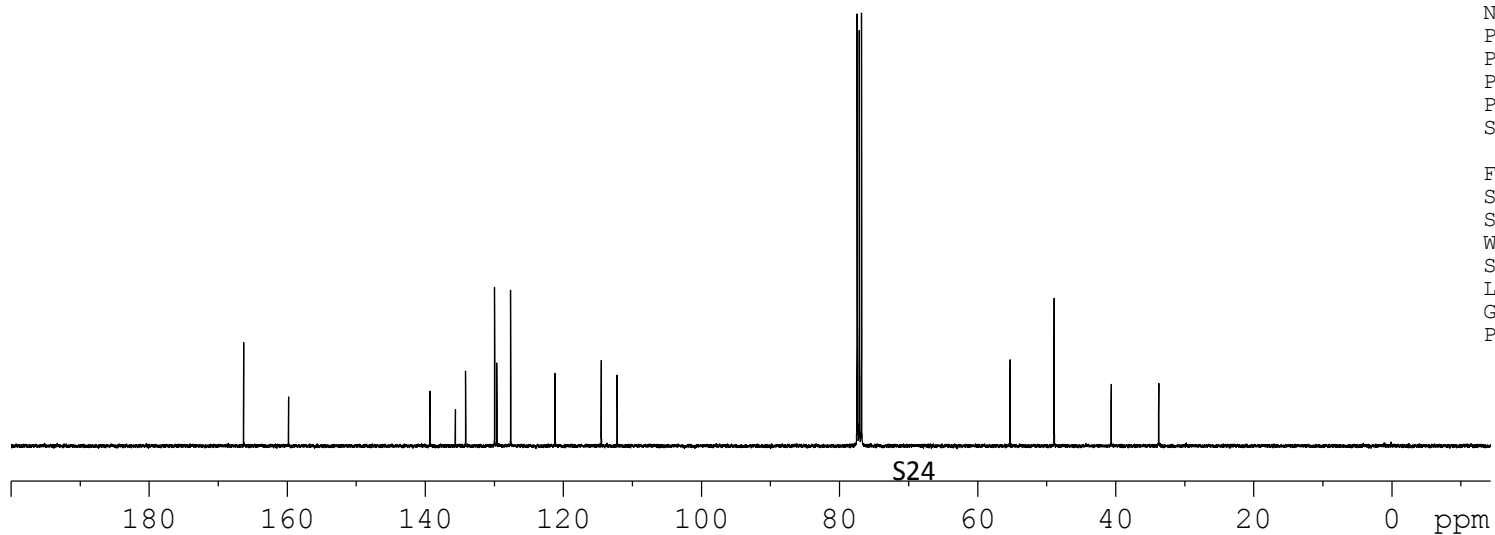
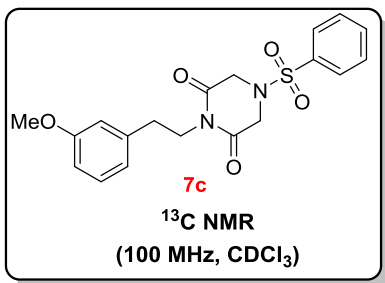
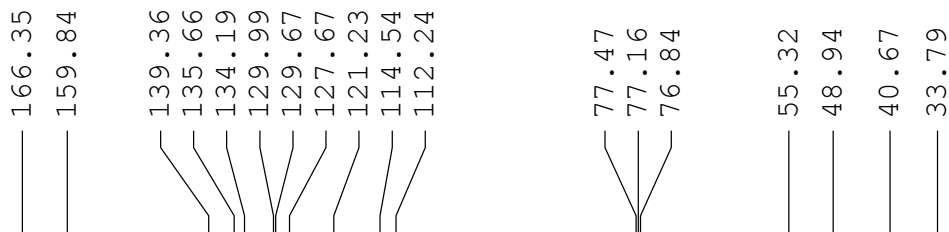
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INSTRUM spect  
PROBHD 5 mm DUL 13C-1  
PULPROG zg30  
TD 65536  
SOLVENT CDC13  
NS 12  
DS 2  
SWH 8223.685 Hz  
FIDRES 0.125483 Hz  
AQ 3.9846387 sec  
RG 161  
DW 60.800 usec  
DE 6.00 usec  
TE 293.0 K  
D1 1.0000000 sec  
TDO 1



==== CHANNEL f1 =====  
NUC1 1H  
P1 11.42 usec  
PL1 -3.00 dB  
SFO1 400.1324710 MHz  
  
F2 - Processing parameters  
SI 32768  
SF 400.1300051 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00



C13CPD CDC13 {D:\CRR} guest 1



Current Data Parameters  
NAME RS-I-3-OME-PZQ-IN  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20150215  
Time\_ 11.50  
INSTRUM spect  
PROBHD 5 mm DUL 13C-1  
PULPROG zgpg30  
TD 65536  
SOLVENT CDC13  
NS 1024  
DS 4  
SWH 24038.461 Hz  
FIDRES 0.366798 Hz  
AQ 1.3631988 sec  
RG 32  
DW 20.800 usec  
DE 6.00 usec  
TE 294.4 K  
D1 2.0000000 sec  
d11 0.0300000 sec  
DELTA 1.89999998 sec  
TD0 1

==== CHANNEL f1 =====  
NUC1 13C  
P1 9.15 usec  
PL1 0.00 dB  
SFO1 100.6228298 MHz

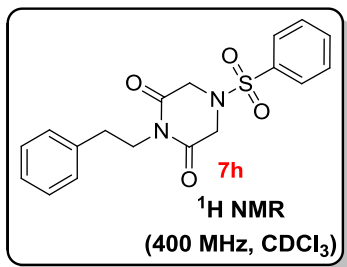
==== CHANNEL f2 =====  
CPDPRG2 waltz16  
NUC2 1H  
PCPD2 90.00 usec  
PL12 14.90 dB  
PL13 14.90 dB  
PL2 -3.00 dB  
SFO2 400.1316005 MHz

F2 - Processing parameters  
SI 32768  
SF 100.6127567 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40



PROTON CDCl3 {D:\CRR} KOPAL 1

7.646  
7.640  
7.634  
7.624  
7.621  
7.618  
7.583  
7.567  
7.564  
7.550  
7.546  
7.290  
7.287  
7.284  
7.270  
7.267  
7.260  
7.252  
7.222  
7.219  
7.209  
7.204  
7.197  
7.185  
7.156  
7.152  
7.135  
4.119  
3.659  
3.645  
3.639  
3.632  
3.619  
2.518  
2.504  
2.497  
2.491  
2.477

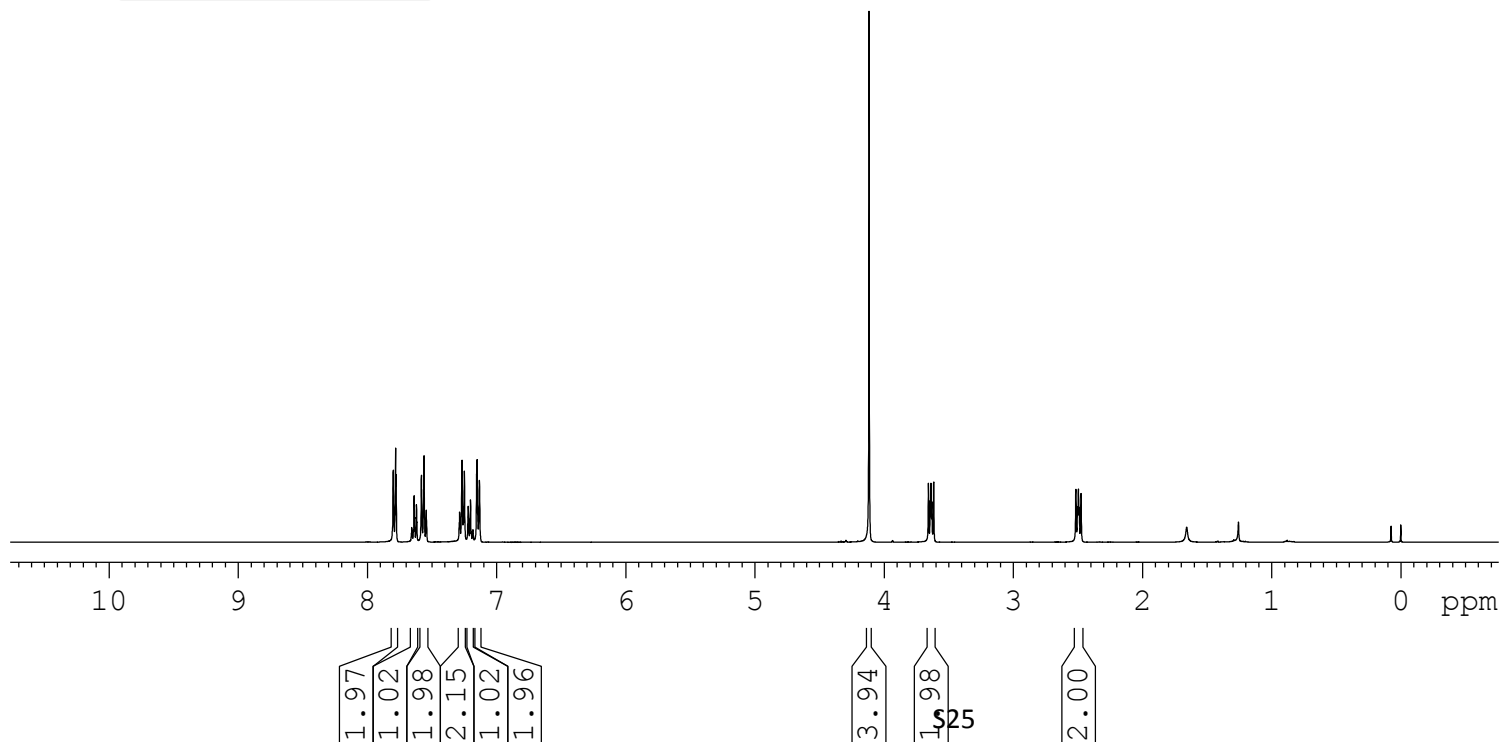


Current Data Parameters  
NAME RS-I-UN-PZQ-IMIDE  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20130821  
Time 14.55  
INSTRUM spect  
PROBHD 5 mm BBO BB-1H  
PULPROG zg30  
TD 65536  
SOLVENT CDCl3  
NS 16  
DS 2  
SWH 8223.685 Hz  
FIDRES 0.125483 Hz  
AQ 3.9846387 sec  
RG 128  
DW 60.800 usec  
DE 6.00 usec  
TE 297.6 K  
D1 1.00000000 sec  
TD0 1

==== CHANNEL f1 =====  
NUC1 1H  
P1 14.50 usec  
PL1 -0.90 dB  
SFO1 400.1324710 MHz

F2 - Processing parameters  
SI 32768  
SF 400.1300056 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00



C13CPD CDCl3 {D:\CRR} KOPAL 1

Current Data Parameters  
NAME RS-I-UN-PZQ-IMIDE  
EXPNO 2  
PROCNO 1

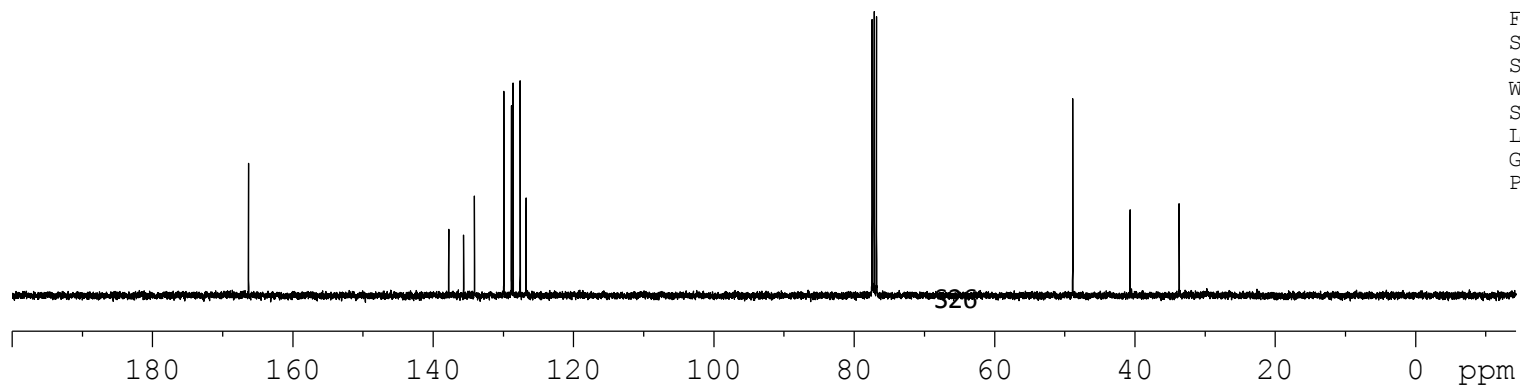
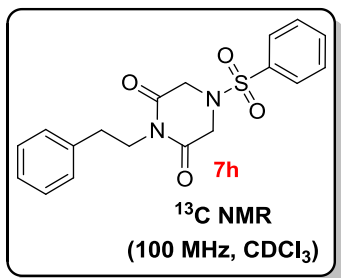
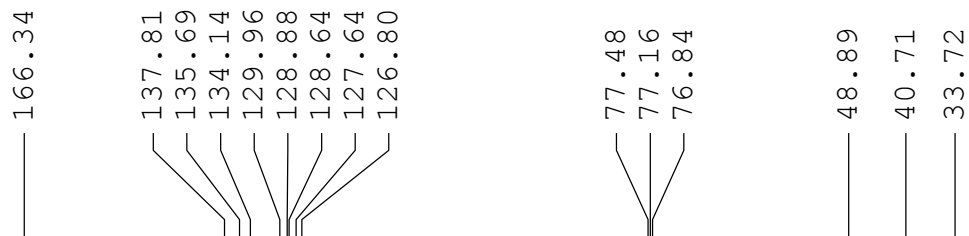
F2 - Acquisition Parameters

Date\_ 20130821  
Time\_ 15.01  
INSTRUM spect  
PROBHD 5 mm BBO BB-1H  
PULPROG zgpg30  
TD 65536  
SOLVENT CDCl3  
NS 120  
DS 4  
SWH 24038.461 Hz  
FIDRES 0.366798 Hz  
AQ 1.3631988 sec  
RG 57  
DW 20.800 usec  
DE 6.00 usec  
TE 298.0 K  
D1 2.00000000 sec  
d11 0.03000000 sec  
DELTA 1.89999998 sec  
TD0 1

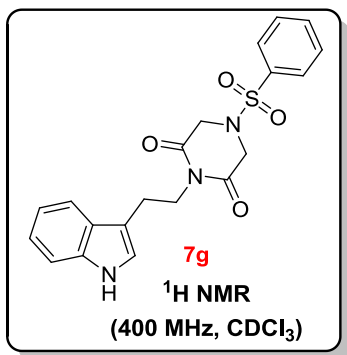
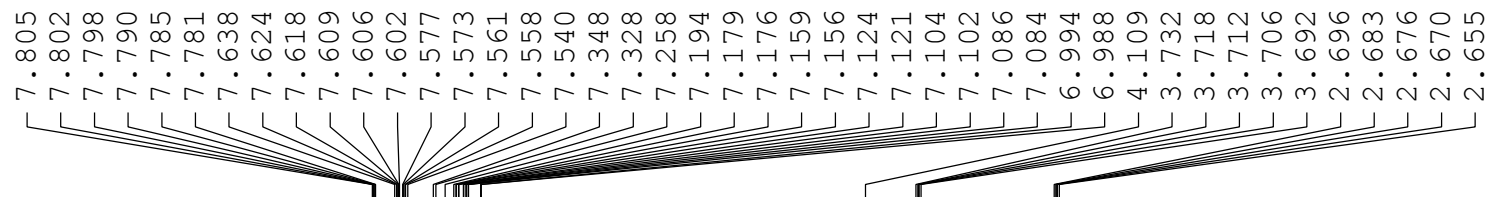
=====  
CHANNEL f1  
NUC1 13C  
P1 9.50 usec  
PL1 -0.60 dB  
SFO1 100.6228298 MHz

=====  
CHANNEL f2  
CPDPRG2 waltz16  
NUC2 1H  
PCPD2 90.00 usec  
PL12 14.96 dB  
PL13 15.60 dB  
PL2 -0.90 dB  
SFO2 400.1316005 MHz

F2 - Processing parameters  
SI 32768  
SF 100.6127596 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40



PROTON CDC13 {D:\CRR} KOPAL 1



Current Data Parameters  
NAME RS-I-TRY-PZQ  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters  
Date 20130802  
Time 11.10  
INSTRUM spect  
PROBHD 5 mm BBO BB-1H  
PULPROG zg30  
TD 65536  
SOLVENT CDCl3  
NS 16  
DS 2  
SWH 8223.685 Hz  
FIDRES 0.125483 Hz  
AQ 3.9846387 sec  
RG 1150  
DW 60.800 usec  
DE 6.00 usec  
TE 297.8 K  
D1 1.00000000 sec  
TD0 1

==== CHANNEL f1 =====  
NUC1 1H  
P1 14.50 usec  
PL1 -0.90 dB  
SF01 400.1324710 MHz

F2 - Processing parameters  
SI 32768  
SF 400.1300063 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00



C13CPD CDC13 {D:\CRR} KOPAL 1

Current Data Parameters  
NAME RS-I-TRY-PZQ  
EXPNO 2  
PROCNO 1

F2 - Acquisition Parameters

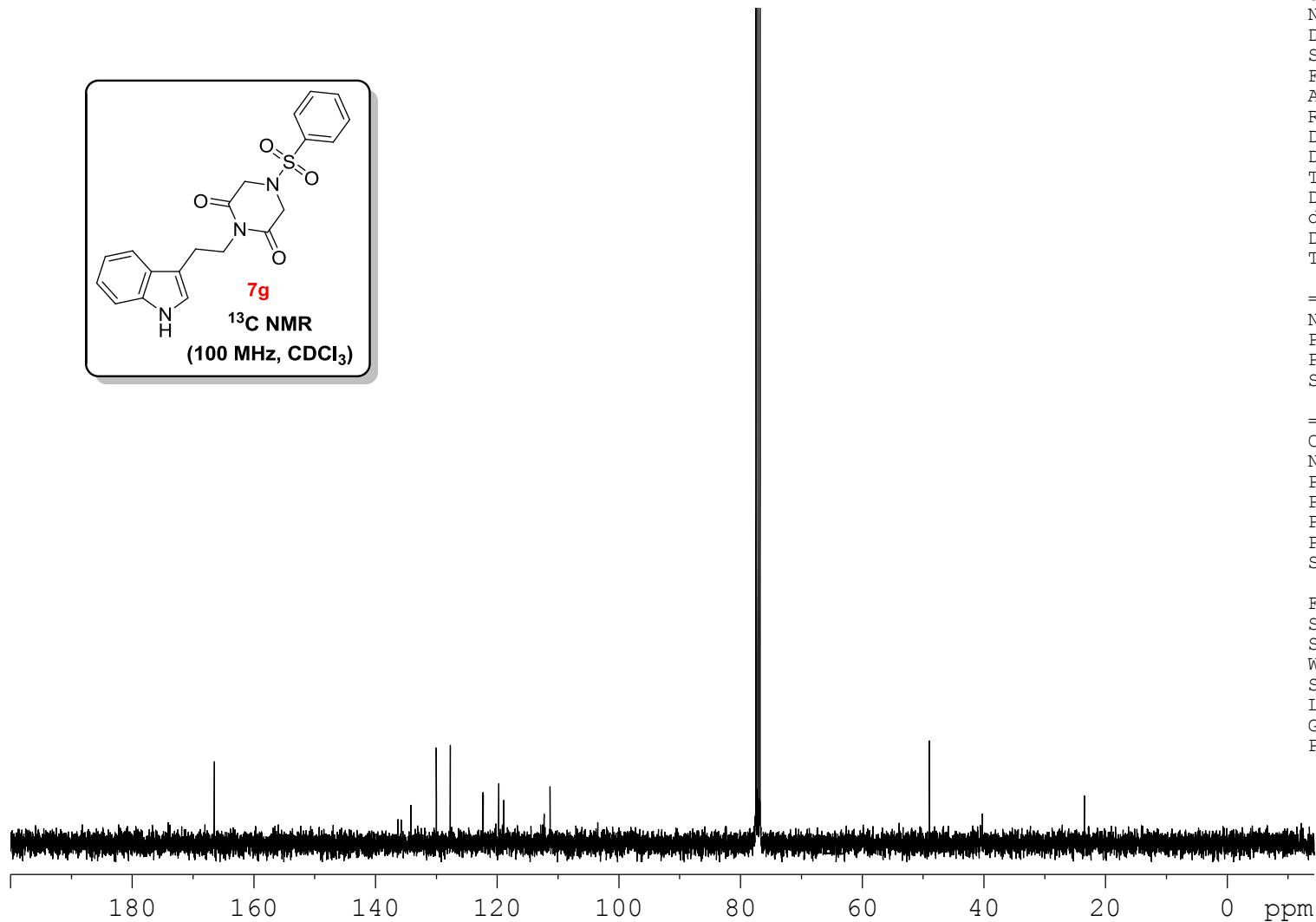
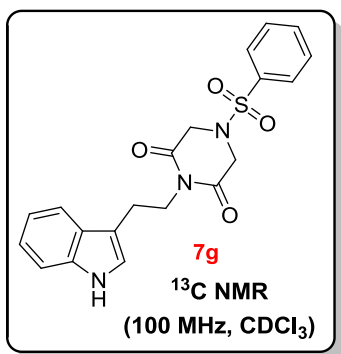
Date\_ 20130802  
Time\_ 11.25  
INSTRUM spect  
PROBHD 5 mm BBO BB-1H  
PULPROG zgpg30  
TD 65536  
SOLVENT CDC13  
NS 256  
DS 4  
SWH 24038.461 Hz  
FIDRES 0.366798 Hz  
AQ 1.3631988 sec  
RG 575  
DW 20.800 usec  
DE 6.00 usec  
TE 298.2 K  
D1 2.0000000 sec  
d11 0.03000000 sec  
DELTA 1.89999998 sec  
TD0 1

=====  
CHANNEL f1  
NUC1 13C  
P1 9.50 usec  
PL1 -0.60 dB  
SFO1 100.6228298 MHz

=====  
CHANNEL f2  
CPDPRG2 waltz16  
NUC2 1H  
PCPD2 90.00 usec  
PL12 14.96 dB  
PL13 15.60 dB  
PL2 -0.90 dB  
SFO2 400.1316005 MHz

F2 - Processing parameters  
SI 32768  
SF 100.6127531 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40

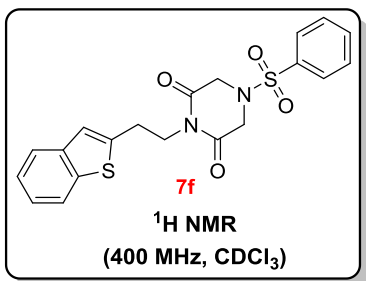
166.48  
134.18  
129.99  
127.70  
122.34  
122.27  
119.73  
118.93  
111.30  
77.48  
77.16  
76.84  
48.97  
40.27  
23.50



PROTON CDC13 {D:\CRR} KOPAL 1

7.742  
7.724  
7.687  
7.668  
7.604  
7.593  
7.587  
7.575  
7.529  
7.509  
7.491  
7.259  
7.243  
7.224  
7.221  
7.218  
7.214  
7.195  
7.180  
6.940

4.082  
3.725  
3.705  
3.686  
2.760  
2.740  
2.721

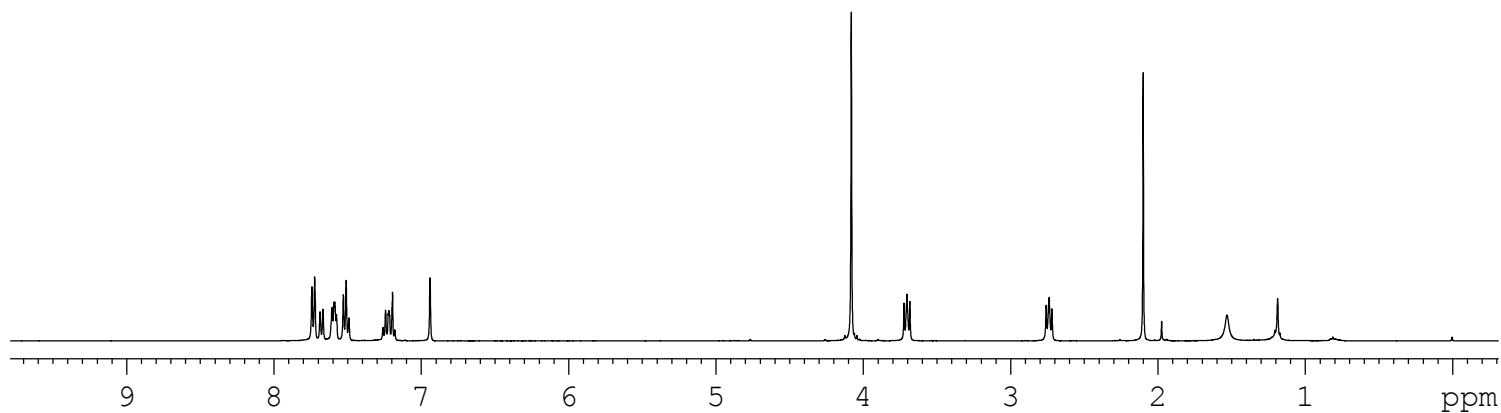


Current Data Parameters  
NAME RS-I-BT-PZQ-IM  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20150724  
Time\_ 11.32  
INSTRUM spect  
PROBHD 5 mm DUL 13C-1  
PULPROG zg30  
TD 65536  
SOLVENT CDC13  
NS 16  
DS 2  
SWH 8223.685 Hz  
FIDRES 0.125483 Hz  
AQ 3.9846387 sec  
RG 228  
DW 60.800 usec  
DE 6.00 usec  
TE 296.2 K  
D1 1.00000000 sec  
TD0 1

==== CHANNEL f1 =====  
NUC1 1H  
P1 11.42 usec  
PL1 -3.00 dB  
SFO1 400.1324710 MHz

F2 - Processing parameters  
SI 32768  
SF 400.1300314 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00



2.06  
1.07  
2.12  
2.06  
2.37  
1.00

4.02  
2.00  
2.10

S29

C13CPD CDC13 {D:\CRR} KOPAL 1

Current Data Parameters  
NAME RS-I-BT-PZQ-IM  
EXPNO 2  
PROCNO 1

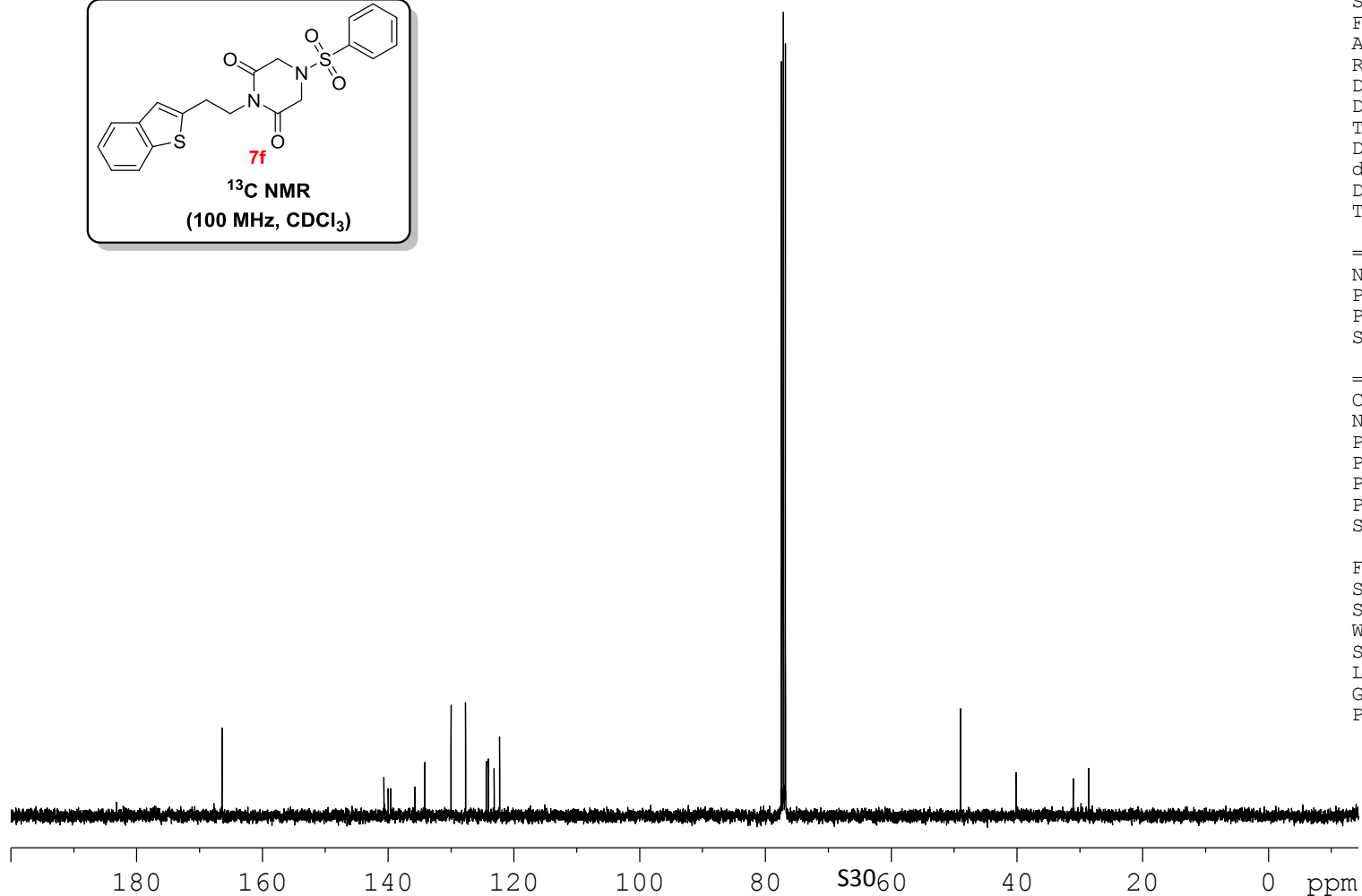
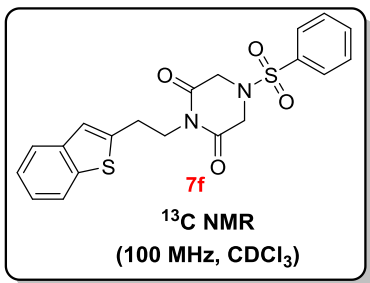
F2 - Acquisition Parameters  
Date\_ 20150724  
Time\_ 11.37  
INSTRUM spect  
PROBHD 5 mm DUL 13C-1  
PULPROG zgpg30  
TD 65536  
SOLVENT CDC13  
NS 223  
DS 4  
SWH 24038.461 Hz  
FIDRES 0.366798 Hz  
AQ 1.3631988 sec  
RG 40.3  
DW 20.800 usec  
DE 6.00 usec  
TE 296.9 K  
D1 2.00000000 sec  
d11 0.03000000 sec  
DELTA 1.89999998 sec  
TD0 1

==== CHANNEL f1 =====  
NUC1 13C  
P1 9.15 usec  
PL1 0.00 dB  
SFO1 100.6228298 MHz

==== CHANNEL f2 =====  
CPDPRG2 waltz16  
NUC2 1H  
PCPD2 90.00 usec  
PL12 14.90 dB  
PL13 14.90 dB  
PL2 -3.00 dB  
SFO2 400.1316005 MHz

F2 - Processing parameters  
SI 32768  
SF 100.6127543 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40

166.39  
140.70  
140.02  
139.61  
135.77  
134.21  
130.03  
127.71  
124.43  
124.07  
123.17  
122.30  
77.48  
77.16  
76.84  
48.98  
40.13  
31.06  
28.60



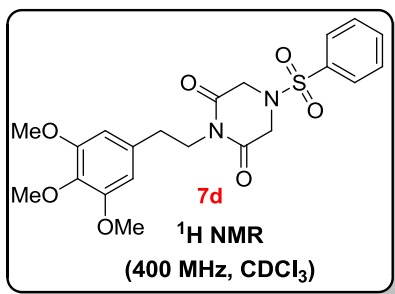
PROTON CDC13 {D:\CRR} KOPAL 1

7.811  
7.792  
7.676  
7.657  
7.639  
7.598  
7.579  
7.561  
7.260  
6.362

4.126  
3.837  
3.804  
3.671  
3.651  
3.630  
2.470  
2.450  
2.430

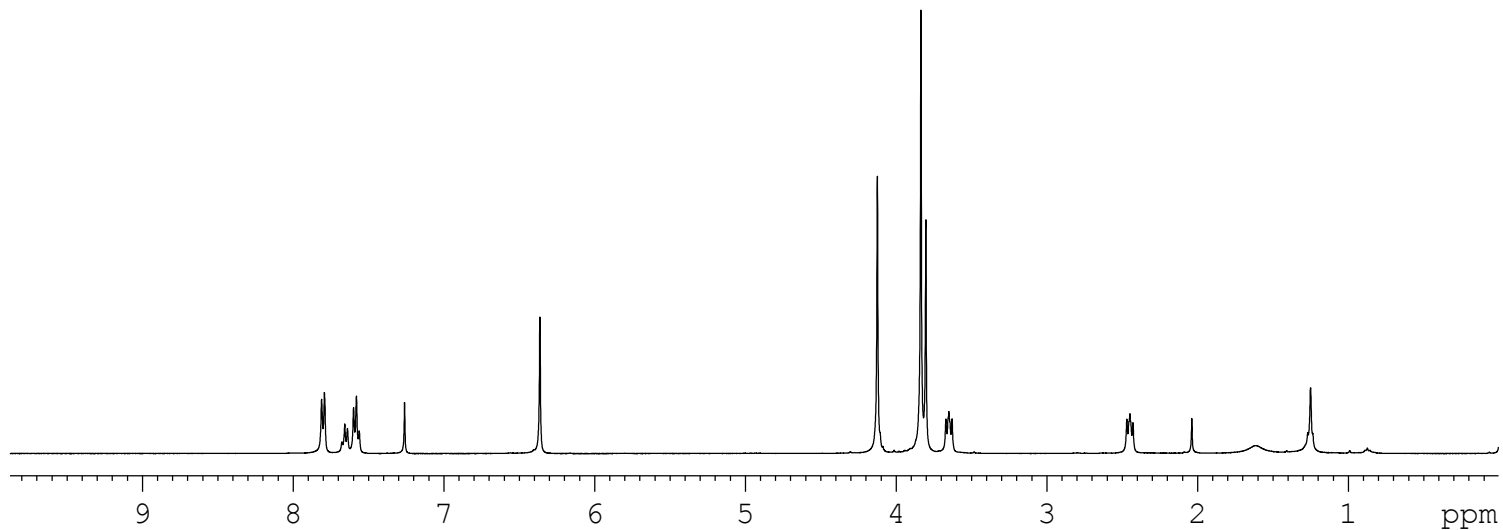
Current Data Parameters  
NAME RS-I-3,4,5-PZQ-Im  
EXPNO 2  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20150203  
Time\_ 10.37  
INSTRUM spect  
PROBHD 5 mm DUL 13C-1  
PULPROG zg30  
TD 65536  
SOLVENT CDC13  
NS 16  
DS 2  
SWH 8223.685 Hz  
FIDRES 0.125483 Hz  
AQ 3.9846387 sec  
RG 203  
DW 60.800 usec  
DE 6.00 usec  
TE 295.9 K  
D1 1.00000000 sec  
TD0 1



==== CHANNEL f1 =====  
NUC1 1H  
P1 11.42 usec  
PL1 -3.00 dB  
SFO1 400.1324710 MHz

F2 - Processing parameters  
SI 32768  
SF 400.1300050 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00



1.91  
1.00  
1.89

1.96

4.00  
5.83  
2.82  
1.91

1.90

C13CPD CDC13 {D:\CRR} KOPAL 1

Current Data Parameters  
NAME RS-I-3,4,5-PZQ-Im  
EXPNO 3  
PROCNO 1

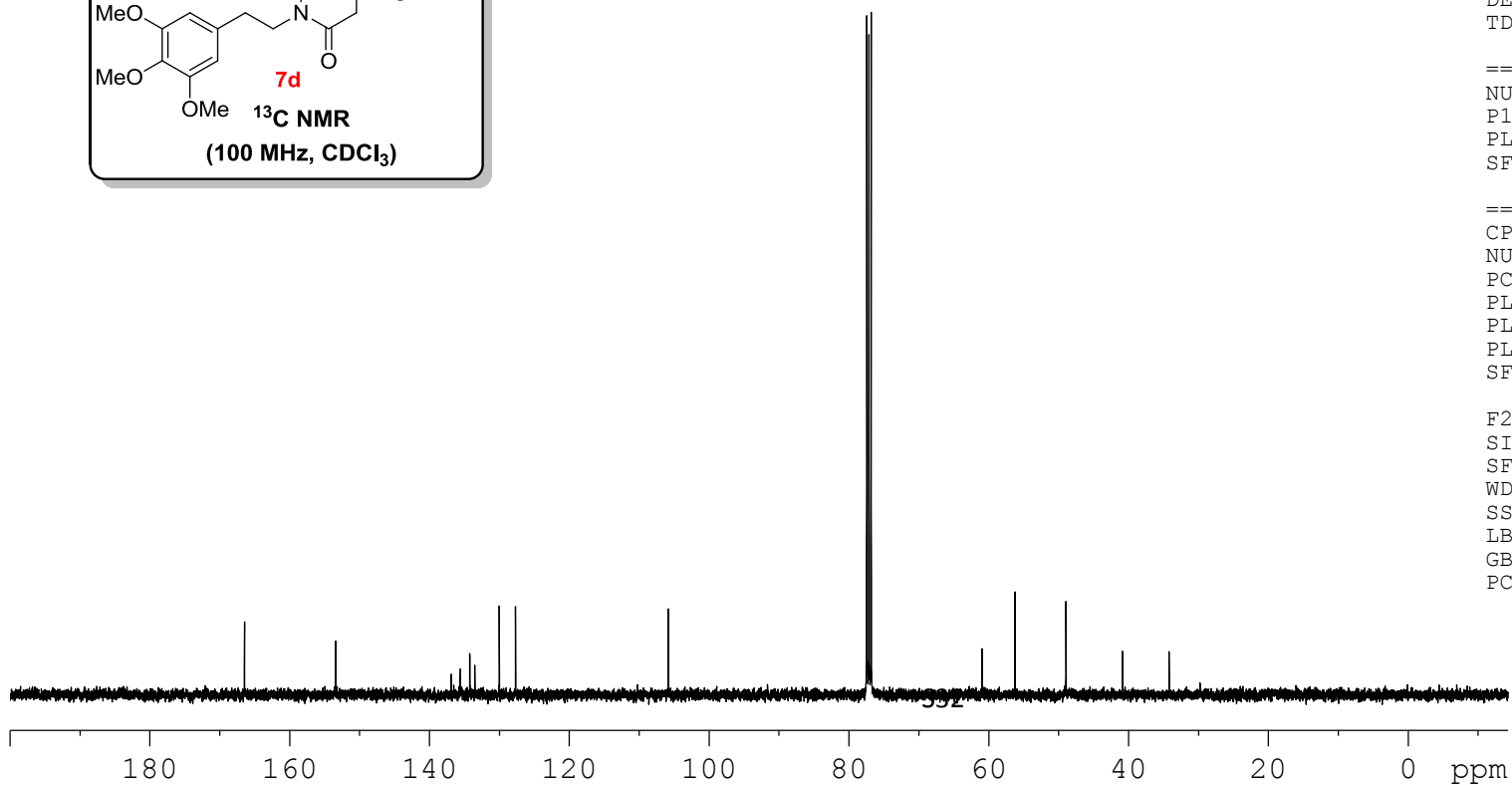
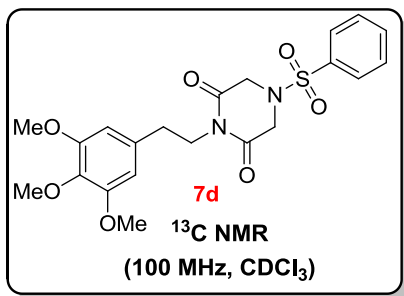
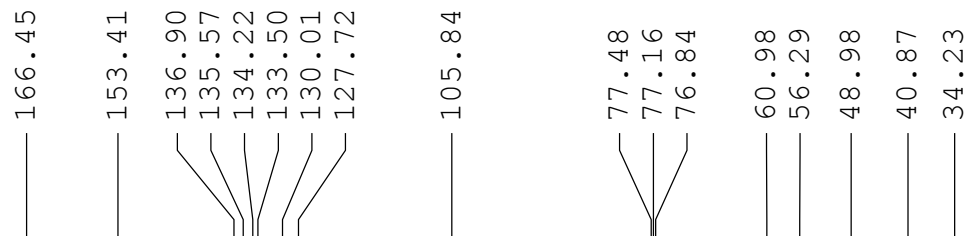
F2 - Acquisition Parameters

Date\_ 20150203  
Time\_ 10.44  
INSTRUM spect  
PROBHD 5 mm DUL 13C-1  
PULPROG zgpg30  
TD 65536  
SOLVENT CDC13  
NS 229  
DS 4  
SWH 24038.461 Hz  
FIDRES 0.366798 Hz  
AQ 1.3631988 sec  
RG 32  
DW 20.800 usec  
DE 6.00 usec  
TE 296.7 K  
D1 2.00000000 sec  
d11 0.03000000 sec  
DELTA 1.89999998 sec  
TD0 1

=====  
CHANNEL f1  
NUC1 13C  
P1 9.15 usec  
PL1 0.00 dB  
SFO1 100.6228298 MHz

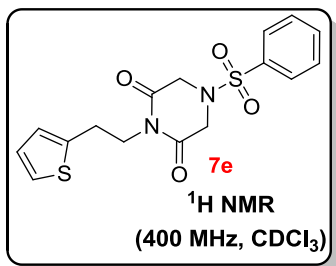
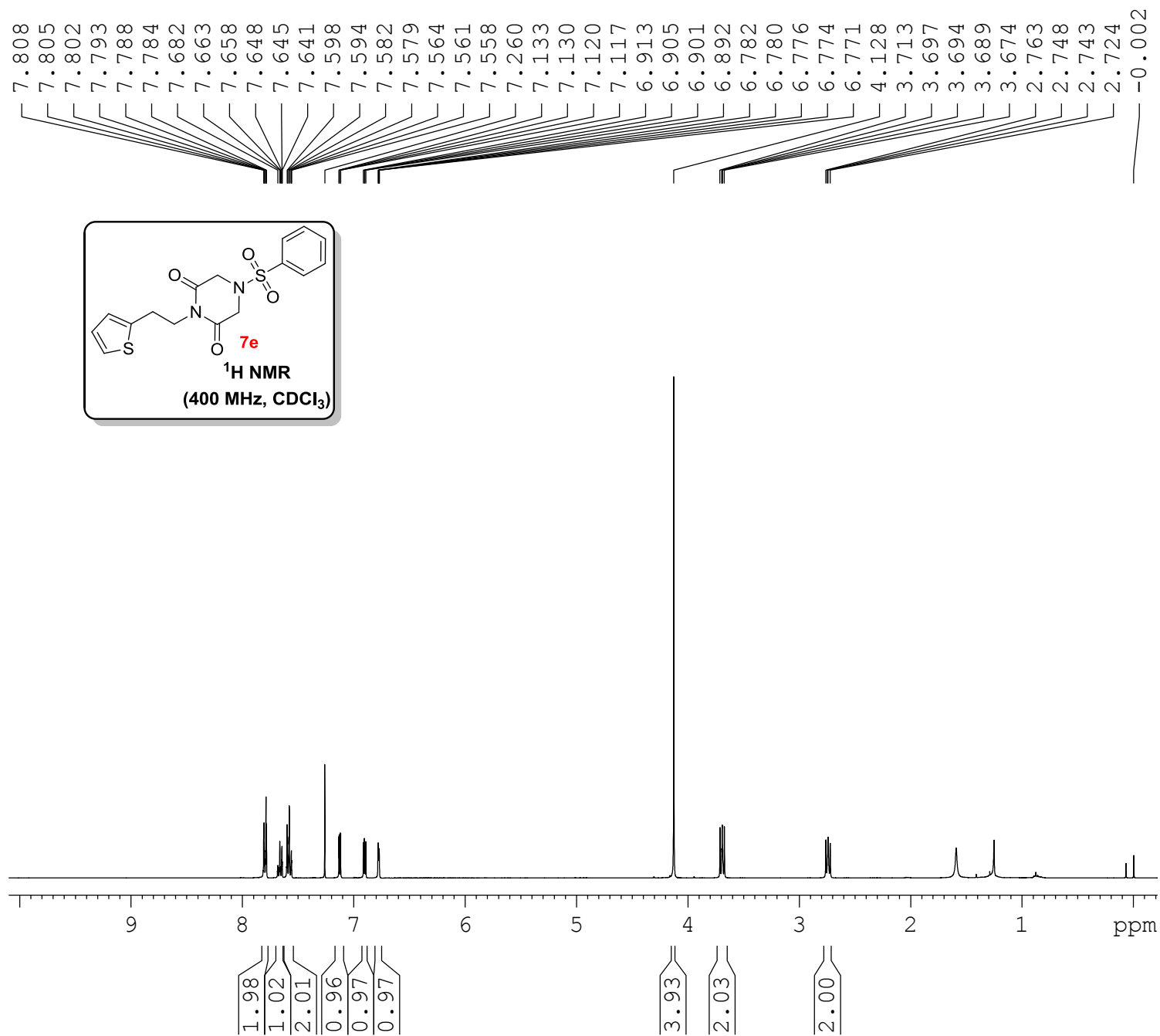
=====  
CHANNEL f2  
CPDPRG2 waltz16  
NUC2 1H  
PCPD2 90.00 usec  
PL12 14.90 dB  
PL13 14.90 dB  
PL2 -3.00 dB  
SFO2 400.1316005 MHz

F2 - Processing parameters  
SI 32768  
SF 100.6127543 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40





PROTON CDC13 {D:\CRR} KOPAL 1



Current Data Parameters  
NAME RS-I-THIO-PZQ-IM  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20150225  
Time 16.05  
INSTRUM spect  
PROBHD 5 mm DUL 13C-1  
PULPROG zg30  
TD 65536  
SOLVENT CDCl3  
NS 16  
DS 2  
SWH 8223.685 Hz  
FIDRES 0.125483 Hz  
AQ 3.9846387 sec  
RG 203  
DW 60.800 usec  
DE 6.00 usec  
TE 295.7 K  
D1 1.00000000 sec  
TDO 1

==== CHANNEL f1 =====  
NUC1 1H  
P1 11.42 usec  
PL1 -3.00 dB  
SF01 400.1324710 MHz

F2 - Processing parameters  
SI 32768  
SF 400.1300051 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00

Current Data Parameters  
 NAME RS-I-THIO-PZQ-IM  
 EXPNO 2  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20150226  
 Time\_ 12.22  
 INSTRUM spect  
 PROBHD 5 mm DUL 13C-1  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT CDC13  
 NS 162  
 DS 4  
 SWH 24038.461 Hz  
 FIDRES 0.366798 Hz  
 AQ 1.3631988 sec  
 RG 28.5  
 DW 20.800 usec  
 DE 6.00 usec  
 TE 295.1 K  
 D1 2.00000000 sec  
 d11 0.03000000 sec  
 DELTA 1.89999998 sec  
 TD0 1

==== CHANNEL f1 =====  
 NUC1 13C  
 P1 9.15 usec  
 PL1 0.00 dB  
 SFO1 100.6228298 MHz

==== CHANNEL f2 =====  
 CPDPRG2 waltz16  
 NUC2 1H  
 PCPD2 90.00 usec  
 PL12 14.90 dB  
 PL13 14.90 dB  
 PL2 -3.00 dB  
 SFO2 400.1316005 MHz

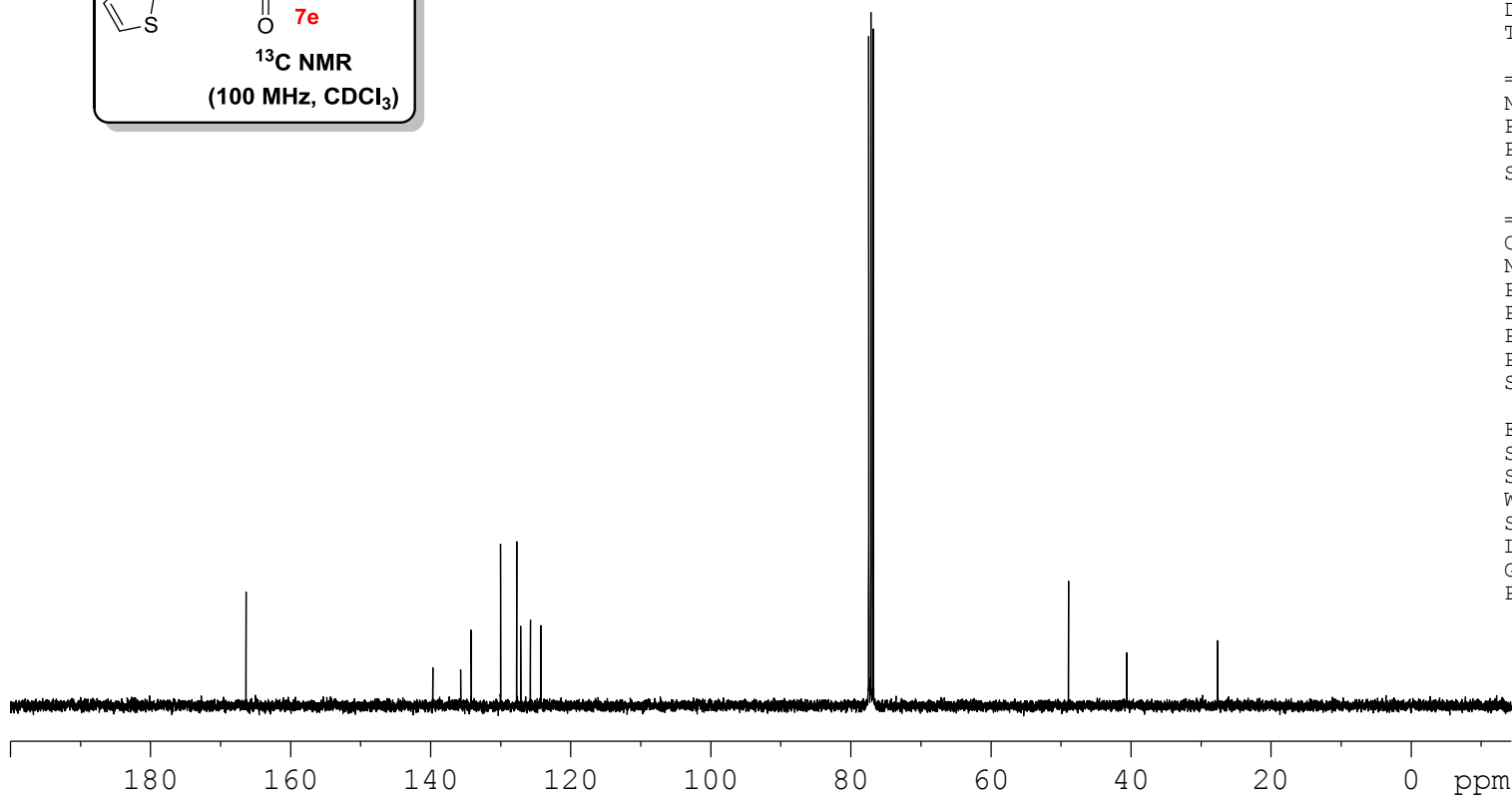
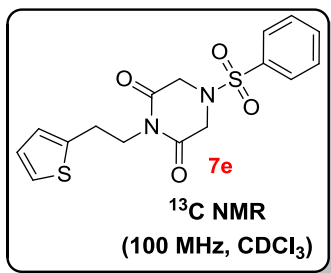
F2 - Processing parameters  
 SI 32768  
 SF 100.6127553 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40

166.35  
 139.67  
 135.70  
 134.20  
 130.01  
 127.70  
 127.14  
 125.75  
 124.25

77.48  
 77.16  
 76.84

48.95  
 40.61

27.67

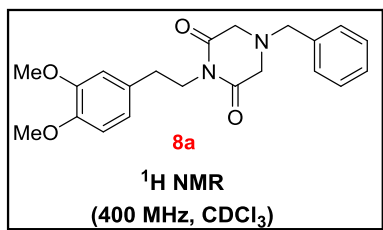


PROTON CDCl3 {D:\CRR} KOPAL 1

7.278  
7.261  
7.258  
7.247  
7.244  
7.237  
7.232  
7.228  
7.215  
7.187  
7.177  
7.173  
7.157  
6.703  
6.682

3.897  
3.882  
3.878  
3.872  
3.858  
3.789  
3.762  
3.488  
3.287  
2.724  
2.710  
2.705  
2.700  
2.685

0.000

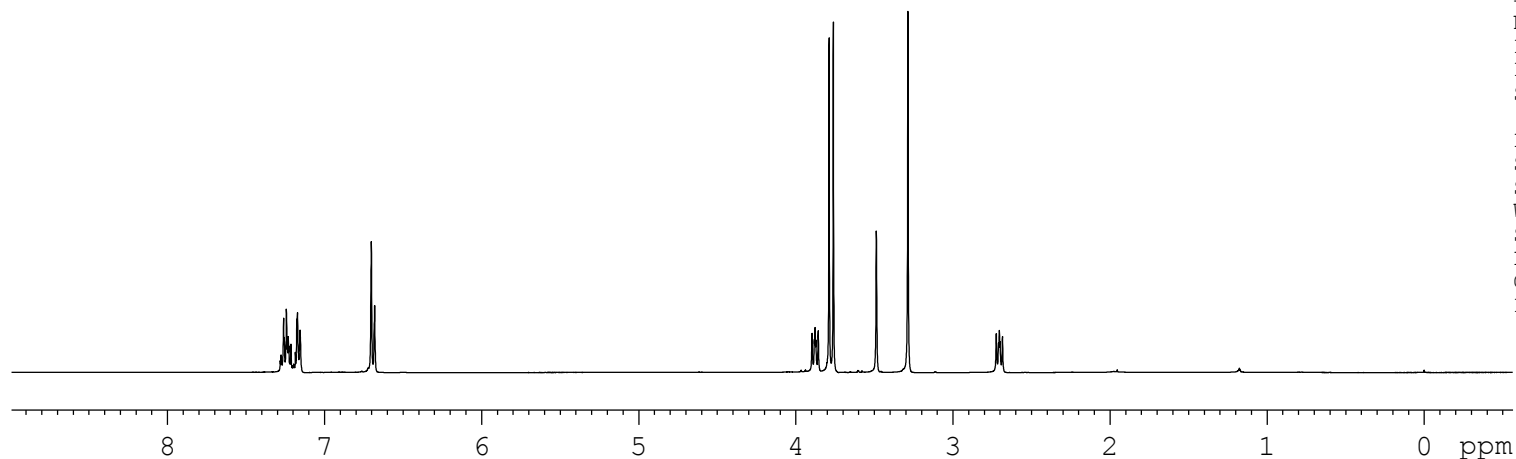


Current Data Parameters  
NAME RS-I-Bn-3,4-PZQ-Im  
EXPNO 3  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20150831  
Time\_ 11.39  
INSTRUM spect  
PROBHD 5 mm DUL 13C-1  
PULPROG zg30  
TD 65536  
SOLVENT CDCl3  
NS 16  
DS 2  
SWH 8223.685 Hz  
FIDRES 0.125483 Hz  
AQ 3.9846387 sec  
RG 71.8  
DW 60.800 usec  
DE 6.00 usec  
TE 295.7 K  
D1 1.00000000 sec  
TD0 1

==== CHANNEL f1 =====  
NUC1 1H  
P1 11.42 usec  
PL1 -3.00 dB  
SFO1 400.1324710 MHz

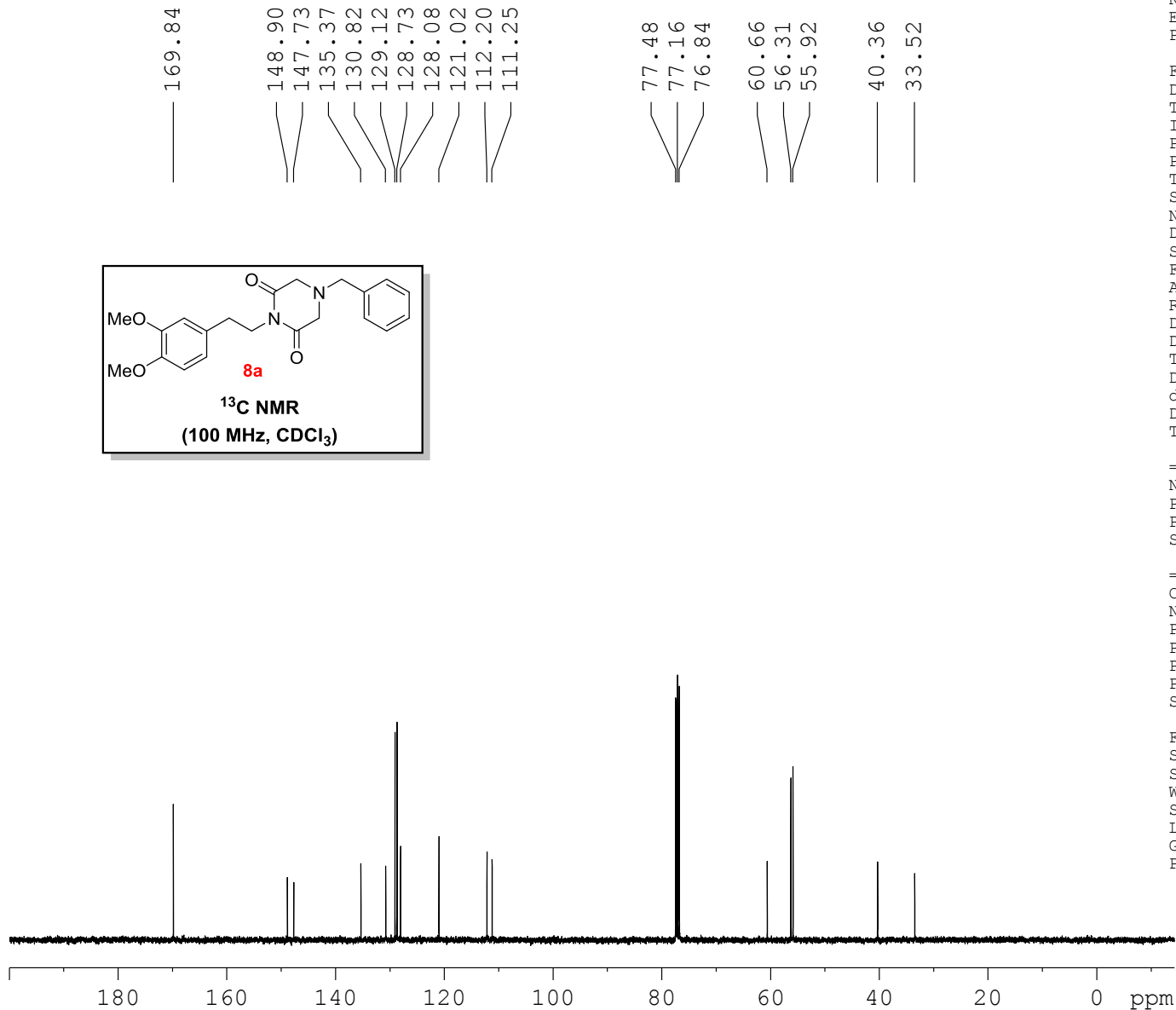
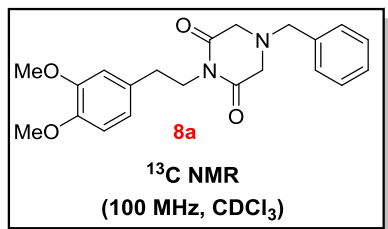
F2 - Processing parameters  
SI 32768  
SF 400.1300342 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00



0.98  
1.90  
2.04  
1.75  
0.89

2.01  
2.94  
2.94  
1.91  
3.87  
2.00

S35



Current Data Parameters  
 NAME RS-I-Bn-3,4-PZQ-Im  
 EXPNO 2  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20150831  
 Time\_ 11.34  
 INSTRUM spect  
 PROBHD 5 mm DUL 13C-1  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 70  
 DS 4  
 SWH 24038.461 Hz  
 FIDRES 0.366798 Hz  
 AQ 1.3631988 sec  
 RG 45.2  
 DW 20.800 usec  
 DE 6.00 usec  
 TE 296.2 K  
 D1 2.00000000 sec  
 d11 0.03000000 sec  
 DELTA 1.89999998 sec  
 TD0 1

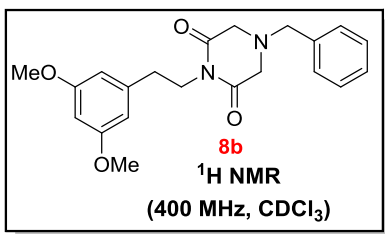
===== CHANNEL f1 =====  
 NUC1 13C  
 P1 9.15 usec  
 PL1 0.00 dB  
 SFO1 100.6228298 MHz

===== CHANNEL f2 =====  
 CPDPRG2 waltz16  
 NUC2 1H  
 PCPD2 90.00 usec  
 PL12 14.90 dB  
 PL13 14.90 dB  
 PL2 -3.00 dB  
 SFO2 400.1316005 MHz

F2 - Processing parameters  
 SI 32768  
 SF 100.6122859 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40

PROTON CDC13 {D:\CRR} KOPAL 1

7.328  
7.323  
7.319  
7.307  
7.302  
7.292  
7.289  
7.276  
7.272  
7.259  
7.246  
7.241  
7.223  
6.962  
6.942  
6.922  
6.777  
6.774  
6.768  
6.765  
6.758  
6.754  
6.748  
6.745  
3.971  
3.955  
3.952  
3.949  
3.933  
3.822  
3.807  
3.558  
3.329  
2.856  
2.841  
2.837  
2.819

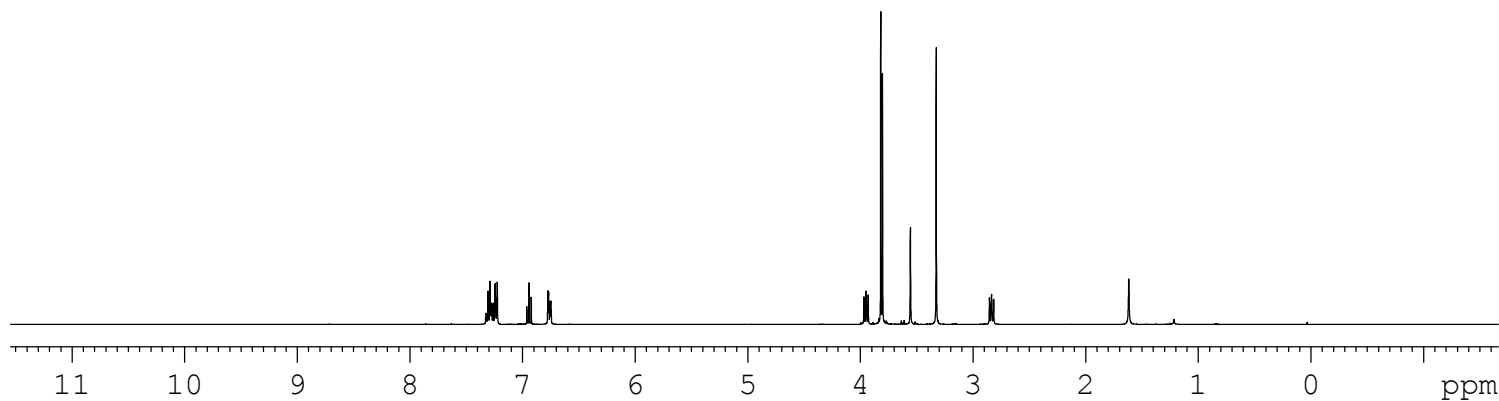


Current Data Parameters  
NAME RS-I-3,5-BN-PZQ-IM  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20151004  
Time\_ 17.08  
INSTRUM spect  
PROBHD 5 mm DUL 13C-1  
PULPROG zg30  
TD 65536  
SOLVENT CDCl3  
NS 16  
DS 2  
SWH 8223.685 Hz  
FIDRES 0.125483 Hz  
AQ 3.9846387 sec  
RG 161  
DW 60.800 usec  
DE 6.00 usec  
TE 294.1 K  
D1 1.00000000 sec  
TD0 1

==== CHANNEL f1 =====  
NUC1 1H  
P1 11.42 usec  
PL1 -3.00 dB  
SFO1 400.1324710 MHz

F2 - Processing parameters  
SI 32768  
SF 400.1300198 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00



1.09  
1.51  
2.23  
0.20  
0.46  
0.29  
2.00  
1.93  
2.96  
3.02  
1.87  
1.62  
2.00

C13CPD CDC13 {D:\CRR} KOPAL 1

Current Data Parameters  
NAME RS-I-3,5-BN-PZQ-IM  
EXPNO 2  
PROCNO 1

F2 - Acquisition Parameters

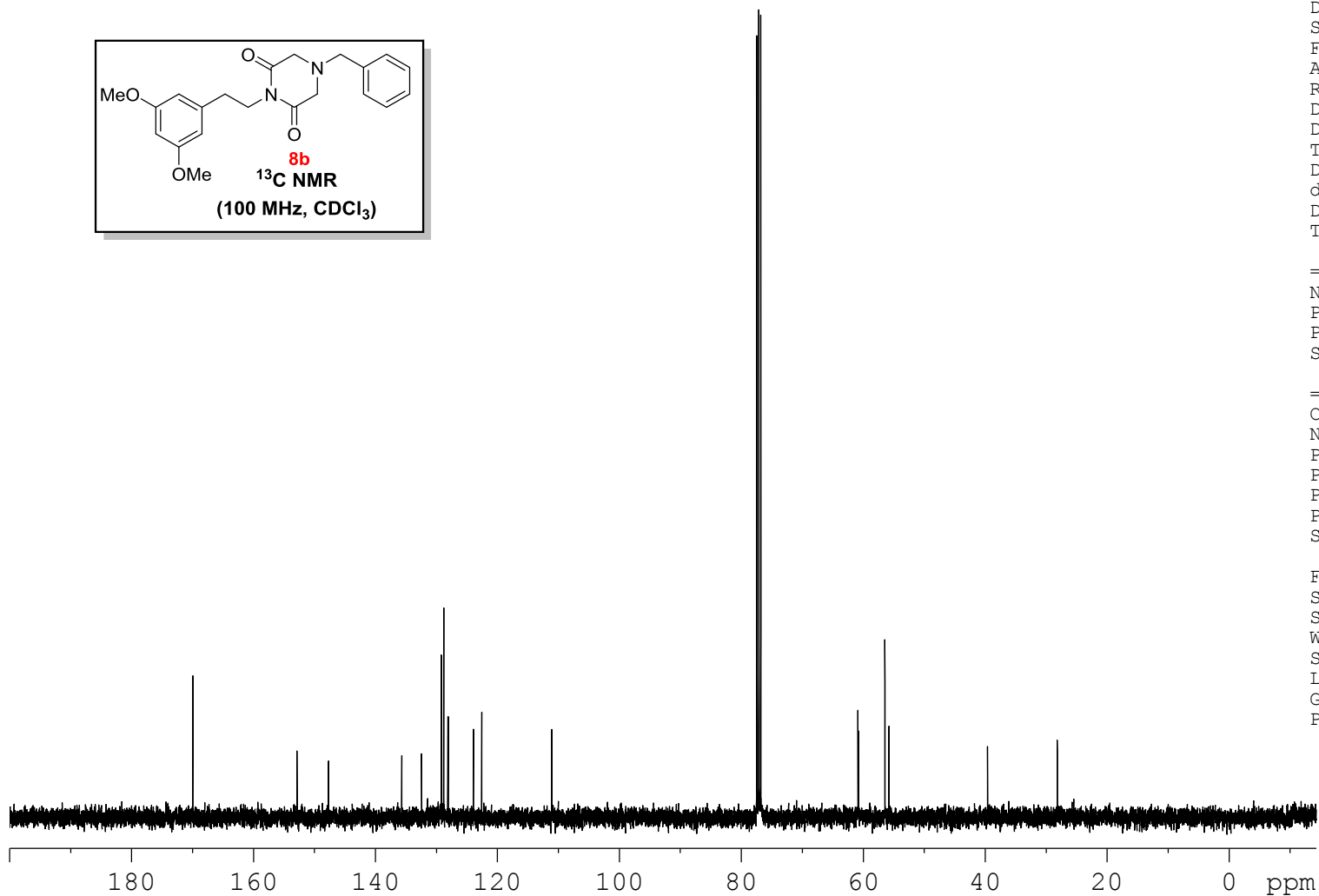
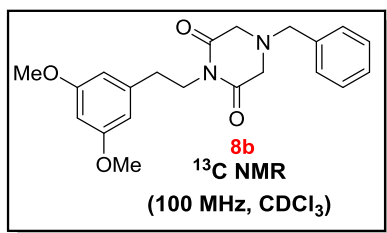
Date\_ 20151004  
Time 17.28  
INSTRUM spect  
PROBHD 5 mm DUL 13C-1  
PULPROG zgpg30  
TD 65536  
SOLVENT CDC13  
NS 83  
DS 4  
SWH 24038.461 Hz  
FIDRES 0.366798 Hz  
AQ 1.3631988 sec  
RG 32  
DW 20.800 usec  
DE 6.00 usec  
TE 294.4 K  
D1 2.00000000 sec  
d11 0.03000000 sec  
DELTA 1.89999998 sec  
TDO 1

==== CHANNEL f1 =====  
NUC1 13C  
P1 9.15 usec  
PL1 0.00 dB  
SFO1 100.6228298 MHz

==== CHANNEL f2 =====  
CPDPRG2 waltz16  
NUC2 1H  
PCPD2 90.00 usec  
PL12 14.90 dB  
PL13 14.90 dB  
PL2 -3.00 dB  
SFO2 400.1316005 MHz

F2 - Processing parameters  
SI 32768  
SF 100.6127562 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40

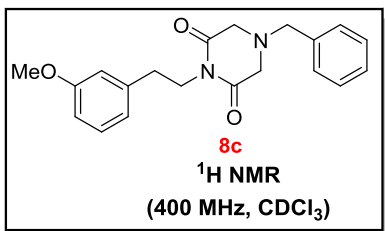
169.93  
152.86  
147.68  
135.66  
132.41  
129.19  
128.78  
128.10  
123.96  
122.60  
111.10  
77.47  
77.16  
76.84  
60.89  
60.82  
56.47  
55.81  
39.65  
28.20



S38

PROTON CDCl3 {D:\CRR} KOPAL 1

7.273  
7.257  
7.253  
7.239  
7.232  
7.228  
7.223  
7.210  
7.180  
7.176  
7.161  
7.139  
7.120  
7.100  
6.764  
6.745  
6.705  
6.691  
6.690  
6.686  
6.670  
6.665  
3.911  
3.896  
3.892  
3.886  
3.872  
3.699  
3.481  
3.281  
2.751  
2.736  
2.731  
2.711

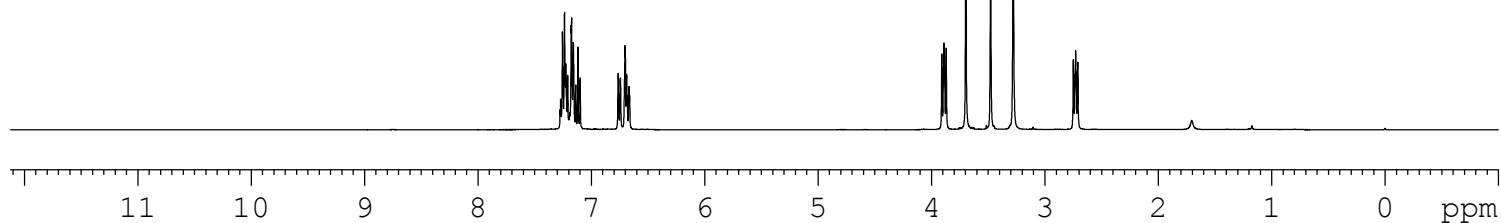


Current Data Parameters  
NAME RS-I-3-BN-PZQ-IM  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20150924  
Time\_ 14.09  
INSTRUM spect  
PROBHD 5 mm DUL 13C-1  
PULPROG zg30  
TD 65536  
SOLVENT CDCl3  
NS 16  
DS 2  
SWH 8223.685 Hz  
FIDRES 0.125483 Hz  
AQ 3.9846387 sec  
RG 64  
DW 60.800 usec  
DE 6.00 usec  
TE 294.5 K  
D1 1.00000000 sec  
TD0 1

==== CHANNEL f1 =====  
NUC1 1H  
P1 11.42 usec  
PL1 -3.00 dB  
SFO1 400.1324710 MHz

F2 - Processing parameters  
SI 32768  
SF 400.1300441 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00



2.90  
2.15  
1.06  
1.01  
2.01

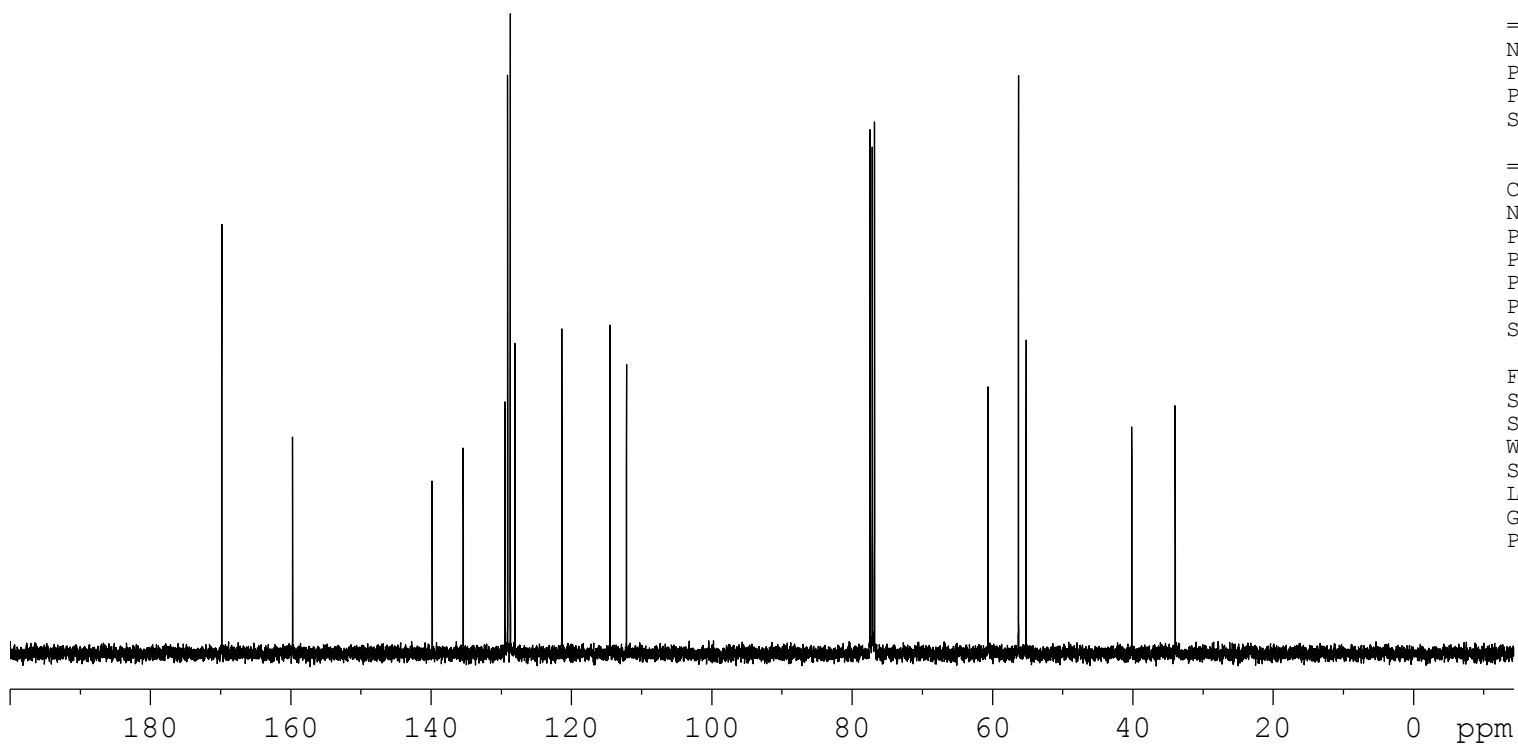
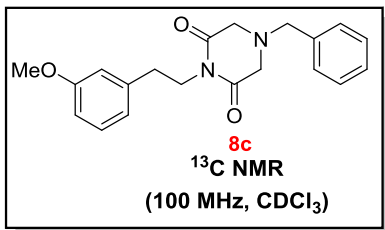
2.00  
3.00  
1.96  
3.96  
2.00

S39

Current Data Parameters  
 NAME RS-I-3-BN-PZQ-IM  
 EXPNO 2  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20150924  
 Time\_ 14.12  
 INSTRUM spect  
 PROBHD 5 mm DUL 13C-1  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT CDC13  
 NS 46  
 DS 4  
 SWH 24038.461 Hz  
 FIDRES 0.366798 Hz  
 AQ 1.3631988 sec  
 RG 64  
 DW 20.800 usec  
 DE 6.00 usec  
 TE 295.0 K  
 D1 2.00000000 sec  
 d11 0.03000000 sec  
 DELTA 1.89999998 sec  
 TD0 1

169.82  
 159.74  
 139.88  
 135.46  
 129.51  
 129.13  
 128.74  
 128.08  
 121.40  
 114.54  
 112.18  
 77.48  
 77.16  
 76.84  
 60.66  
 56.33  
 55.24  
 40.17  
 33.99



==== CHANNEL f1 =====  
 NUC1 13C  
 P1 9.15 usec  
 PL1 0.00 dB  
 SFO1 100.6228298 MHz

==== CHANNEL f2 =====  
 CPDPRG2 waltz16  
 NUC2 1H  
 PCPD2 90.00 usec  
 PL12 14.90 dB  
 PL13 14.90 dB  
 PL2 -3.00 dB  
 SFO2 400.1316005 MHz

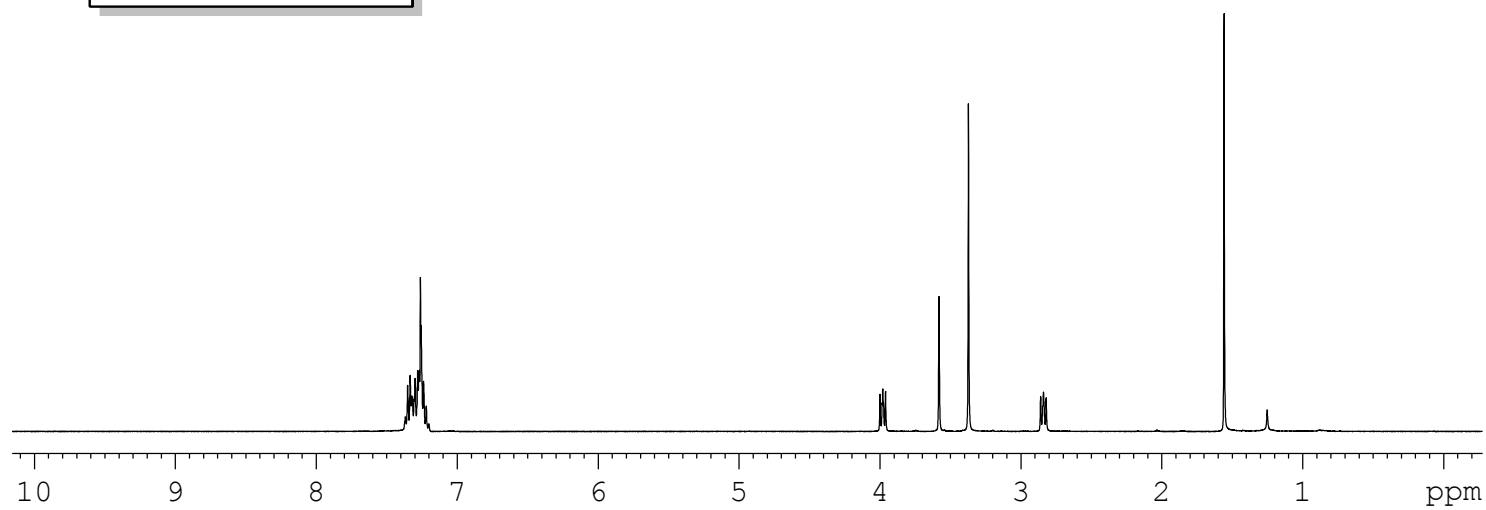
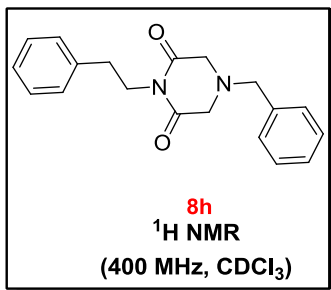
F2 - Processing parameters  
 SI 32768  
 SF 100.6127646 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40



PROTON CDC13 {D:\CRR} KOPAL 1

7.351  
7.333  
7.322  
7.319  
7.305  
7.298  
7.280  
7.272  
7.268  
7.260  
7.255  
7.238  
7.218

4.001  
3.986  
3.982  
3.976  
3.962  
3.583  
3.374  
2.861  
2.841  
2.822



1.18  
1.82  
1.25  
2.11  
3.30

1.98  
5.44  
1.94  
3.91  
2.00

Current Data Parameters  
NAME RS-I-Bn-UN-SUB -PZQ-IM  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20150825  
Time\_ 11.19  
INSTRUM spect  
PROBHD 5 mm DUL 13C-1  
PULPROG zg30  
TD 65536  
SOLVENT CDCl3  
NS 16  
DS 2  
SWH 8223.685 Hz  
FIDRES 0.125483 Hz  
AQ 3.9846387 sec  
RG 256  
DW 60.800 usec  
DE 6.00 usec  
TE 295.4 K  
D1 1.00000000 sec  
TD0 1

==== CHANNEL f1 =====  
NUC1 1H  
P1 11.42 usec  
PL1 -3.00 dB  
SFO1 400.1324710 MHz

F2 - Processing parameters  
SI 32768  
SF 400.1300048 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00

C13CPD CDC13 {D:\CRR} KOPAL 1

Current Data Parameters  
NAME RS-I-Bn-PZQ-Im  
EXPNO 1  
PROCNO 1

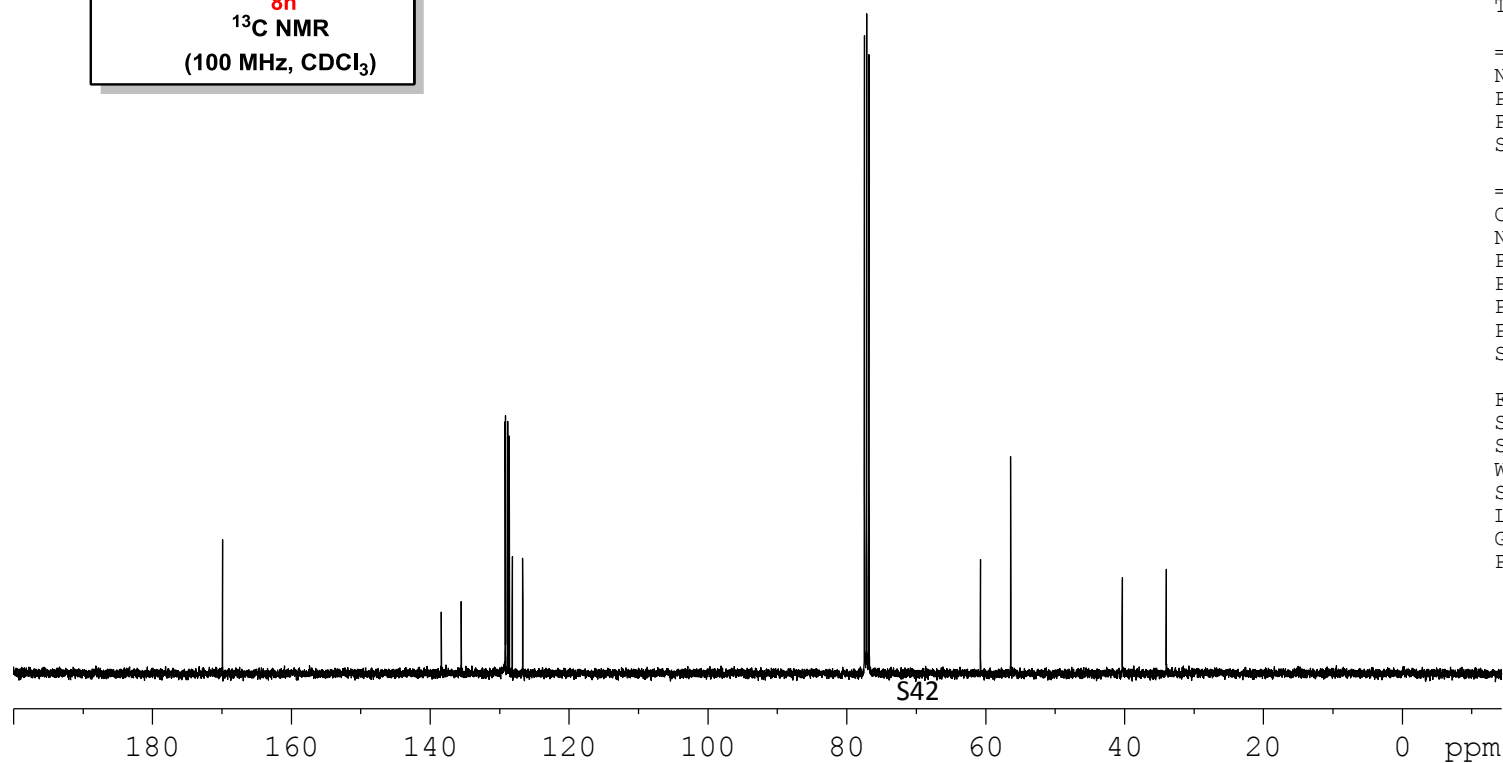
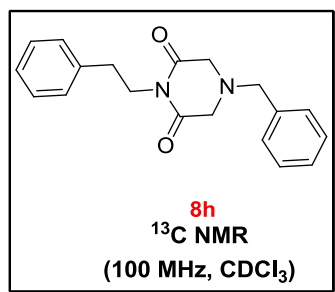
F2 - Acquisition Parameters  
Date\_ 20150825  
Time\_ 12.09  
INSTRUM spect  
PROBHD 5 mm DUL 13C-1  
PULPROG zgpg30  
TD 65536  
SOLVENT CDC13  
NS 256  
DS 4  
SWH 24038.461 Hz  
FIDRES 0.366798 Hz  
AQ 1.3631988 sec  
RG 40.3  
DW 20.800 usec  
DE 6.00 usec  
TE 295.8 K  
D1 2.00000000 sec  
d11 0.03000000 sec  
DELTA 1.89999998 sec  
TD0 1

==== CHANNEL f1 =====  
NUC1 13C  
P1 9.15 usec  
PL1 0.00 dB  
SFO1 100.6228298 MHz

==== CHANNEL f2 =====  
CPDPRG2 waltz16  
NUC2 1H  
PCPD2 90.00 usec  
PL12 14.90 dB  
PL13 14.90 dB  
PL2 -3.00 dB  
SFO2 400.1316005 MHz

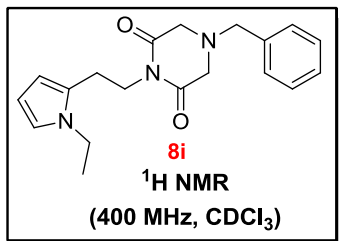
F2 - Processing parameters  
SI 32768  
SF 100.6127561 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40

169.90  
138.38  
135.52  
129.19  
129.13  
128.82  
128.59  
128.17  
126.67  
77.48  
77.16  
76.84  
60.78  
56.44  
40.35  
34.02



PROTON CDCl3 {D:\CRR} KOPAL 1

7.380  
7.377  
7.364  
7.360  
7.349  
7.346  
7.344  
7.334  
7.330  
7.317  
7.302  
7.298  
7.282  
7.260  
6.644  
6.639  
6.637  
6.632  
6.091  
6.082  
6.075  
5.958  
5.954  
5.949  
5.945  
3.962  
3.959  
3.941  
3.923  
3.618  
3.411  
3.398  
3.390  
2.829  
2.809  
2.790  
1.424  
1.406  
1.388

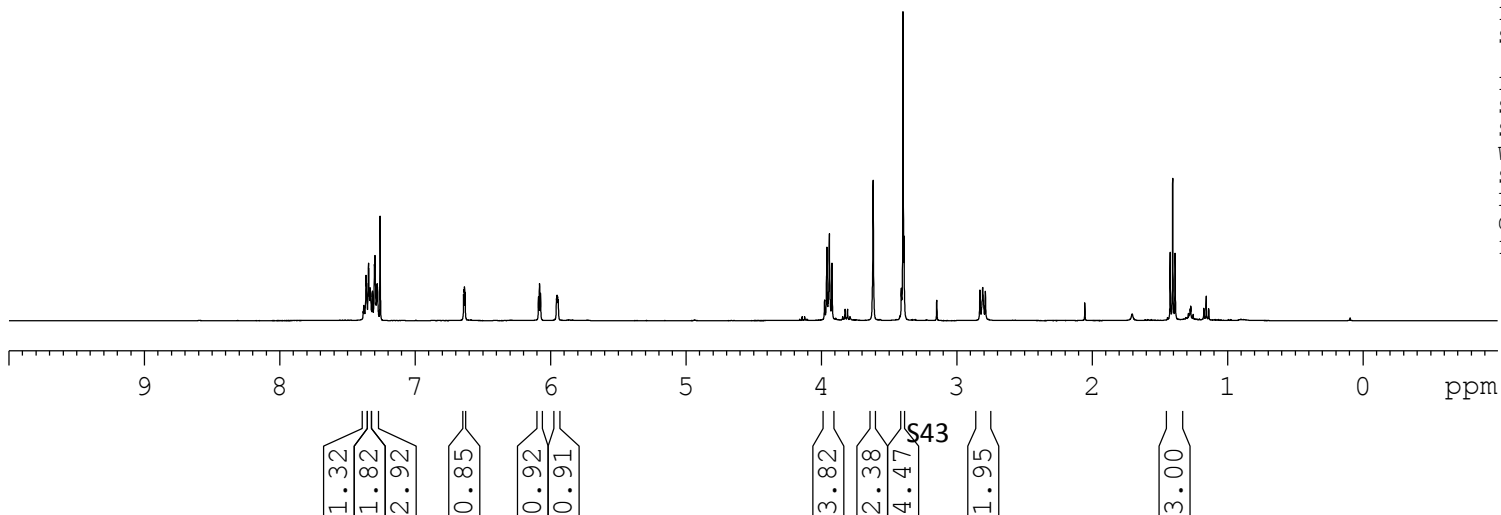


Current Data Parameters  
NAME RS-I-BN-NET-PY-PZQ  
EXPNO 1  
PROCNO 1

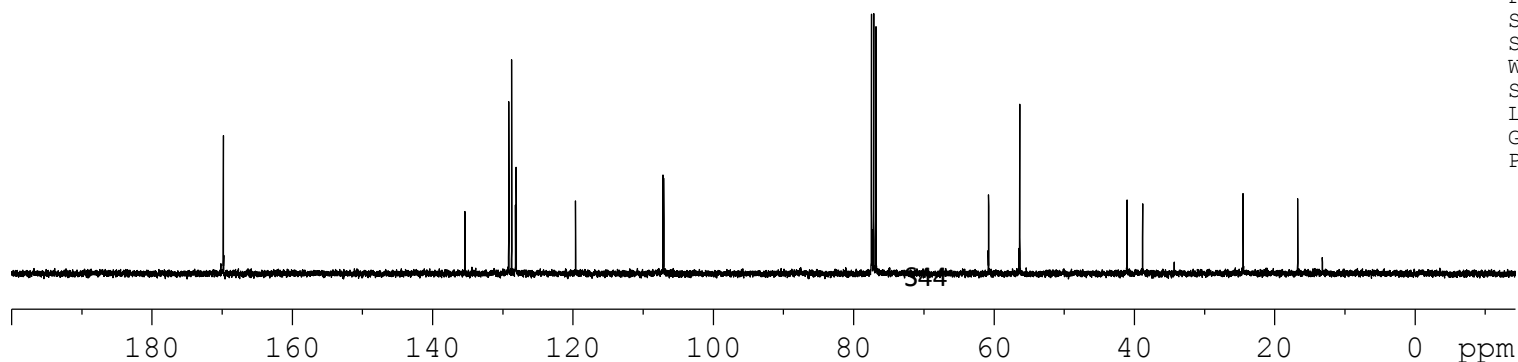
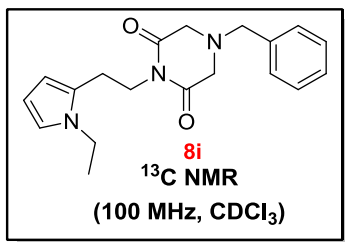
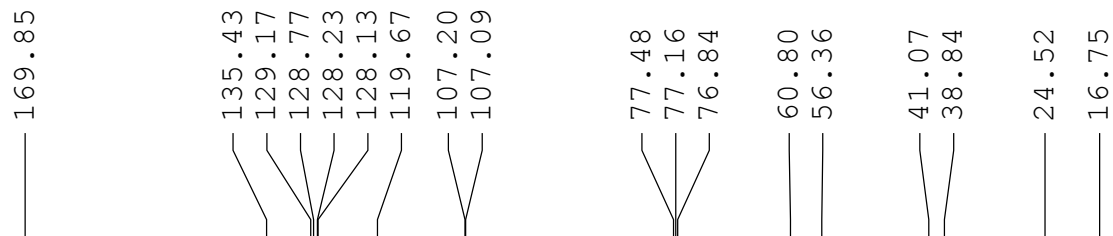
F2 - Acquisition Parameters  
Date\_ 20150831  
Time\_ 10.27  
INSTRUM spect  
PROBHD 5 mm DUL 13C-1  
PULPROG zg30  
TD 65536  
SOLVENT CDCl3  
NS 16  
DS 2  
SWH 8223.685 Hz  
FIDRES 0.125483 Hz  
AQ 3.9846387 sec  
RG 71.8  
DW 60.800 usec  
DE 6.00 usec  
TE 295.1 K  
D1 1.0000000 sec  
TD0 1

==== CHANNEL f1 =====  
NUC1 1H  
P1 11.42 usec  
PL1 -3.00 dB  
SFO1 400.1324710 MHz

F2 - Processing parameters  
SI 32768  
SF 400.1300050 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00



C13CPD CDC13 {D:\CRR} KOPAL 1



Current Data Parameters  
 NAME RS-I-BN-NET-PY-PZQ  
 EXPNO 2  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20150831  
 Time\_ 10.32  
 INSTRUM spect  
 PROBHD 5 mm DUL 13C-1  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT CDC13  
 NS 80  
 DS 4  
 SWH 24038.461 Hz  
 FIDRES 0.366798 Hz  
 AQ 1.3631988 sec  
 RG 36  
 DW 20.800 usec  
 DE 6.00 usec  
 TE 295.8 K  
 D1 2.00000000 sec  
 d11 0.03000000 sec  
 DELTA 1.89999998 sec  
 TD0 1

==== CHANNEL f1 =====  
 NUC1 13C  
 P1 9.15 usec  
 PL1 0.00 dB  
 SFO1 100.6228298 MHz

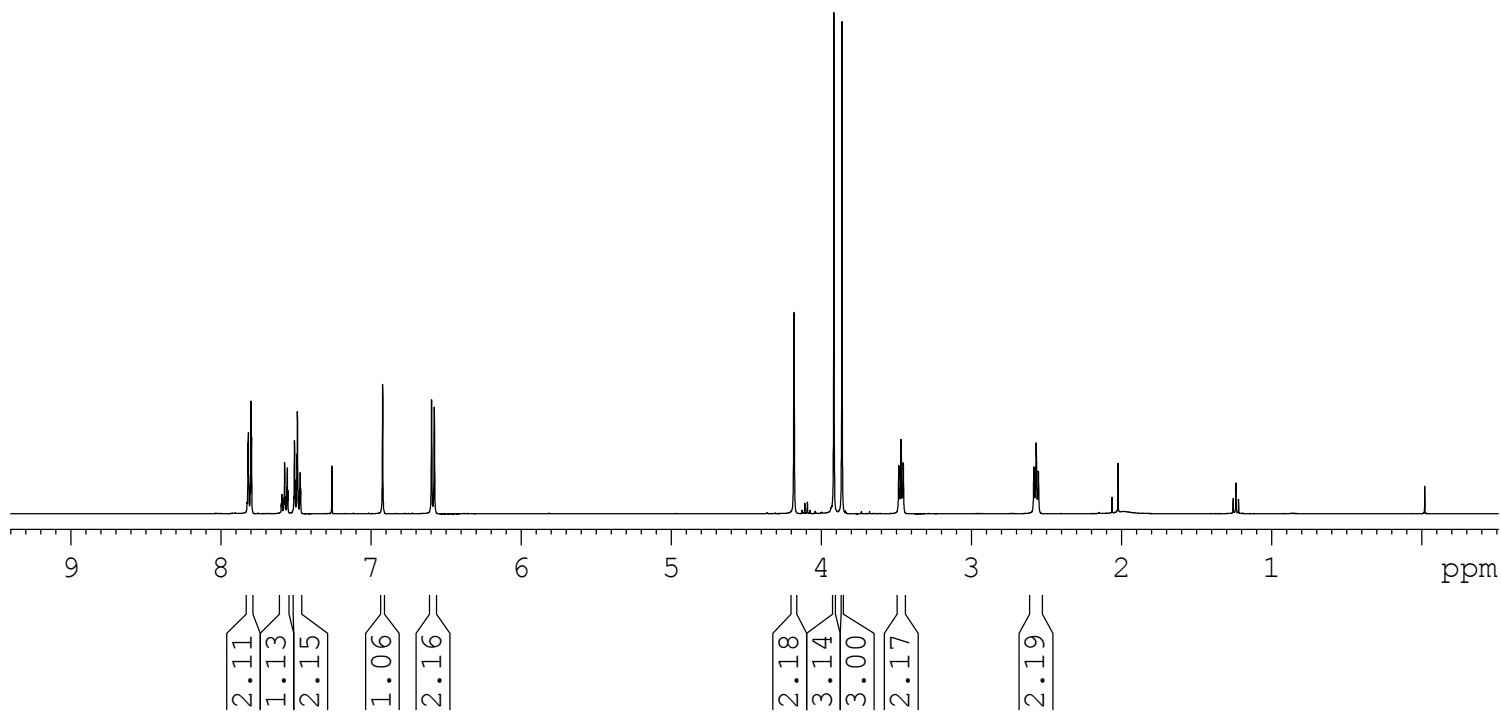
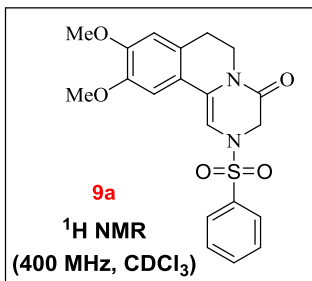
==== CHANNEL f2 =====  
 CPDPRG2 waltz16  
 NUC2 1H  
 PCPD2 90.00 usec  
 PL12 14.90 dB  
 PL13 14.90 dB  
 PL2 -3.00 dB  
 SFO2 400.1316005 MHz

F2 - Processing parameters  
 SI 32768  
 SF 100.6127626 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40

7.796  
7.594  
7.581  
7.576  
7.570  
7.560  
7.557  
7.554  
7.514  
7.509  
7.505  
7.493  
7.489  
7.486  
7.475  
7.471  
7.469  
7.260  
6.922  
6.596  
6.577

4.181  
3.915  
3.861  
3.483  
3.468  
3.453

2.584  
2.569  
2.555



Current Data Parameters  
NAME RS-I-PZQ-IM-CY-A  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20130711  
Time\_ 14.48  
INSTRUM spect  
PROBHD 5 mm BBO BB-1H  
PULPROG zg30  
TD 65536  
SOLVENT CDCl3  
NS 16  
DS 2  
SWH 8223.685 Hz  
FIDRES 0.125483 Hz  
AQ 3.9846387 sec  
RG 181  
DW 60.800 usec  
DE 6.00 usec  
TE 296.8 K  
D1 1.00000000 sec  
TDO 1

==== CHANNEL f1 =====  
NUC1 1H  
P1 14.50 usec  
PL1 -0.90 dB  
SFO1 400.1324710 MHz

F2 - Processing parameters  
SI 32768  
SF 400.1300056 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00

Current Data Parameters  
 NAME RS-I-3,4-BS-PZQ-XY  
 EXPNO 2  
 PROCNO 1

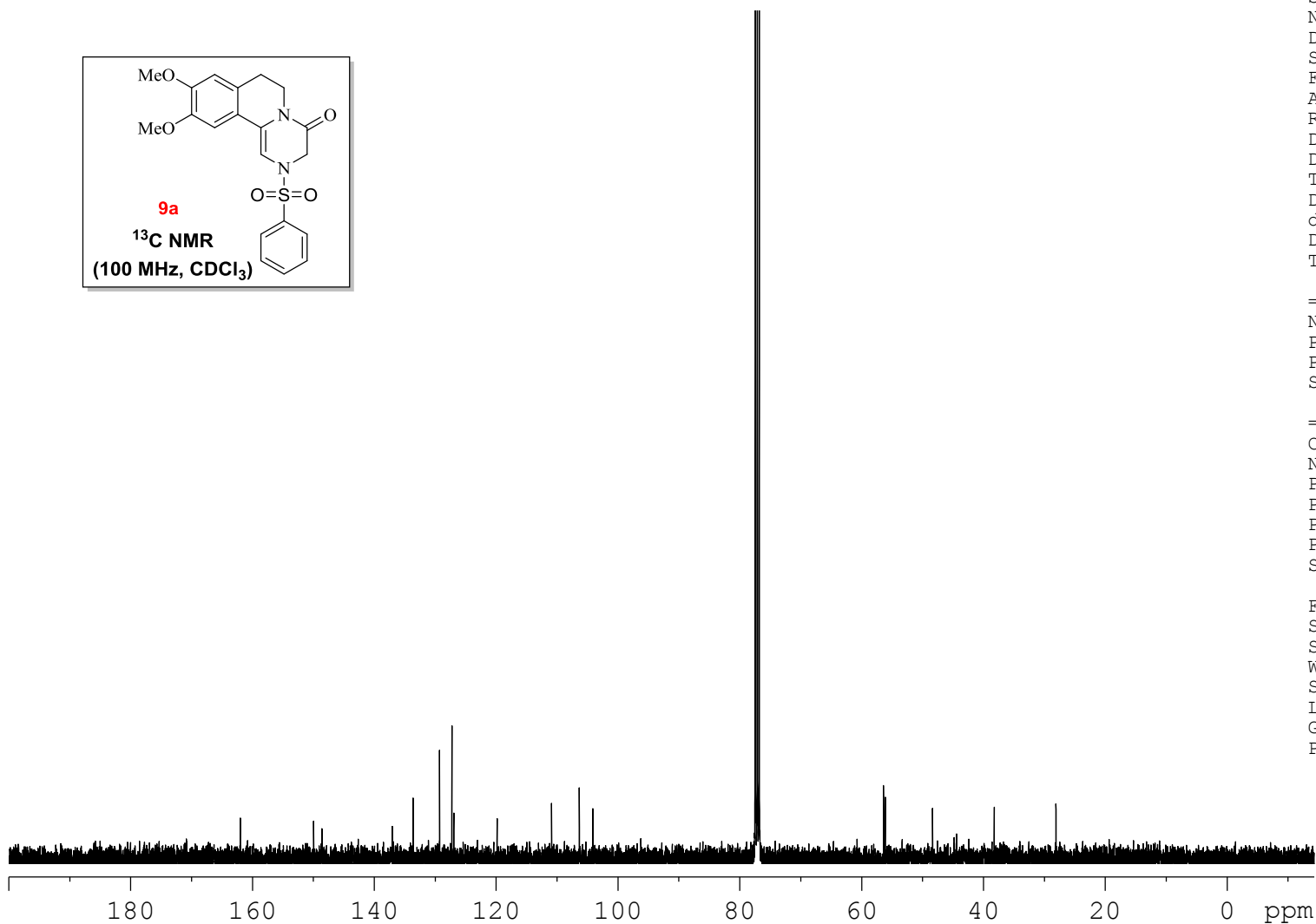
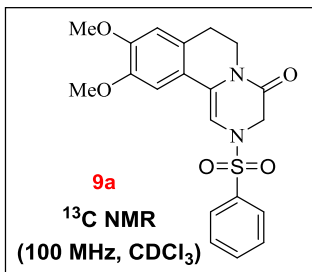
F2 - Acquisition Parameters  
 Date 20151008  
 Time 13.13  
 INSTRUM spect  
 PROBHD 5 mm DUL 13C-1  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT CDC13  
 NS 256  
 DS 4  
 SWH 24038.461 Hz  
 FIDRES 0.366798 Hz  
 AQ 1.3631988 sec  
 RG 57  
 DW 20.800 usec  
 DE 6.00 usec  
 TE 296.5 K  
 D1 2.0000000 sec  
 d11 0.0300000 sec  
 DELTA 1.8999999 sec  
 TDO 1

==== CHANNEL f1 =====  
 NUC1 13C  
 P1 9.15 usec  
 PL1 0.00 dB  
 SFO1 100.6228298 MHz

==== CHANNEL f2 =====  
 CPDPRG2 waltz16  
 NUC2 1H  
 PCPD2 90.00 usec  
 PL12 14.90 dB  
 PL13 14.90 dB  
 PL2 -3.00 dB  
 SFO2 400.1316005 MHz

F2 - Processing parameters  
 SI 32768  
 SF 100.6127535 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40

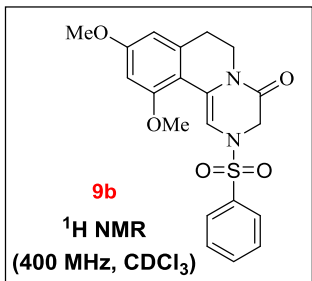
161.98  
 149.94  
 148.57  
 137.02  
 133.60  
 129.27  
 127.29  
 126.97  
 119.88  
 110.93  
 106.37  
 104.14  
 77.48  
 77.16  
 76.84  
 56.43  
 56.14  
 48.38  
 38.25  
 28.11



7.837  
7.823  
7.819  
7.611  
7.608  
7.605  
7.596  
7.590  
7.584  
7.574  
7.571  
7.568  
7.530  
7.527  
7.514  
7.510  
7.492  
7.490  
7.260  
7.164  
6.415  
6.410  
6.272  
6.266  
4.180  
3.890  
3.810  
3.476  
3.461  
3.446  
2.575  
2.559  
2.545

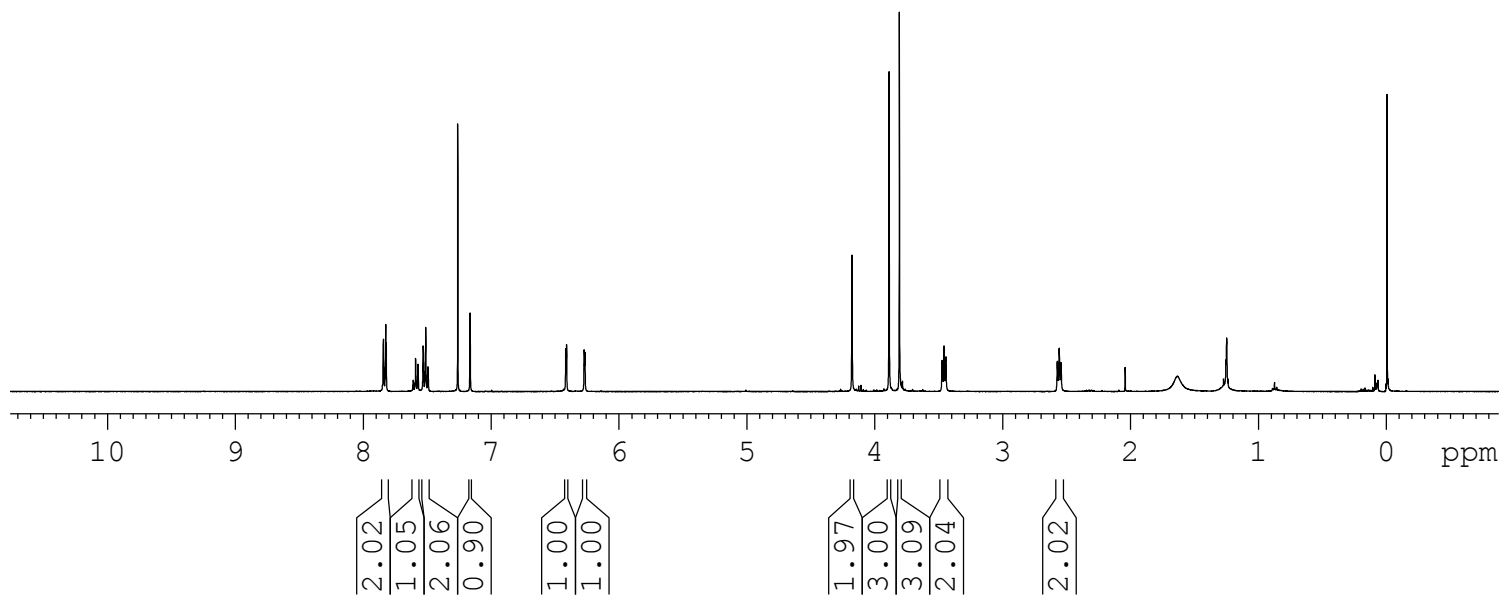
Current Data Parameters  
NAME RS-I-3,5-PZQ-CY  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20130913  
Time\_ 15.42  
INSTRUM spect  
PROBHD 5 mm BBO BB-1H  
PULPROG zg30  
TD 65536  
SOLVENT CDCl3  
NS 16  
DS 2  
SWH 8223.685 Hz  
FIDRES 0.125483 Hz  
AQ 3.9846387 sec  
RG 912  
DW 60.800 usec  
DE 6.00 usec  
TE 293.5 K  
D1 1.0000000 sec  
TD0 1



==== CHANNEL f1 =====  
NUC1 1H  
P1 14.50 usec  
PL1 -0.90 dB  
SFO1 400.1324710 MHz

F2 - Processing parameters  
SI 32768  
SF 400.1300058 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00



Current Data Parameters  
 NAME RS-I-3,5-PZQ-CY  
 EXPNO 2  
 PROCNO 1

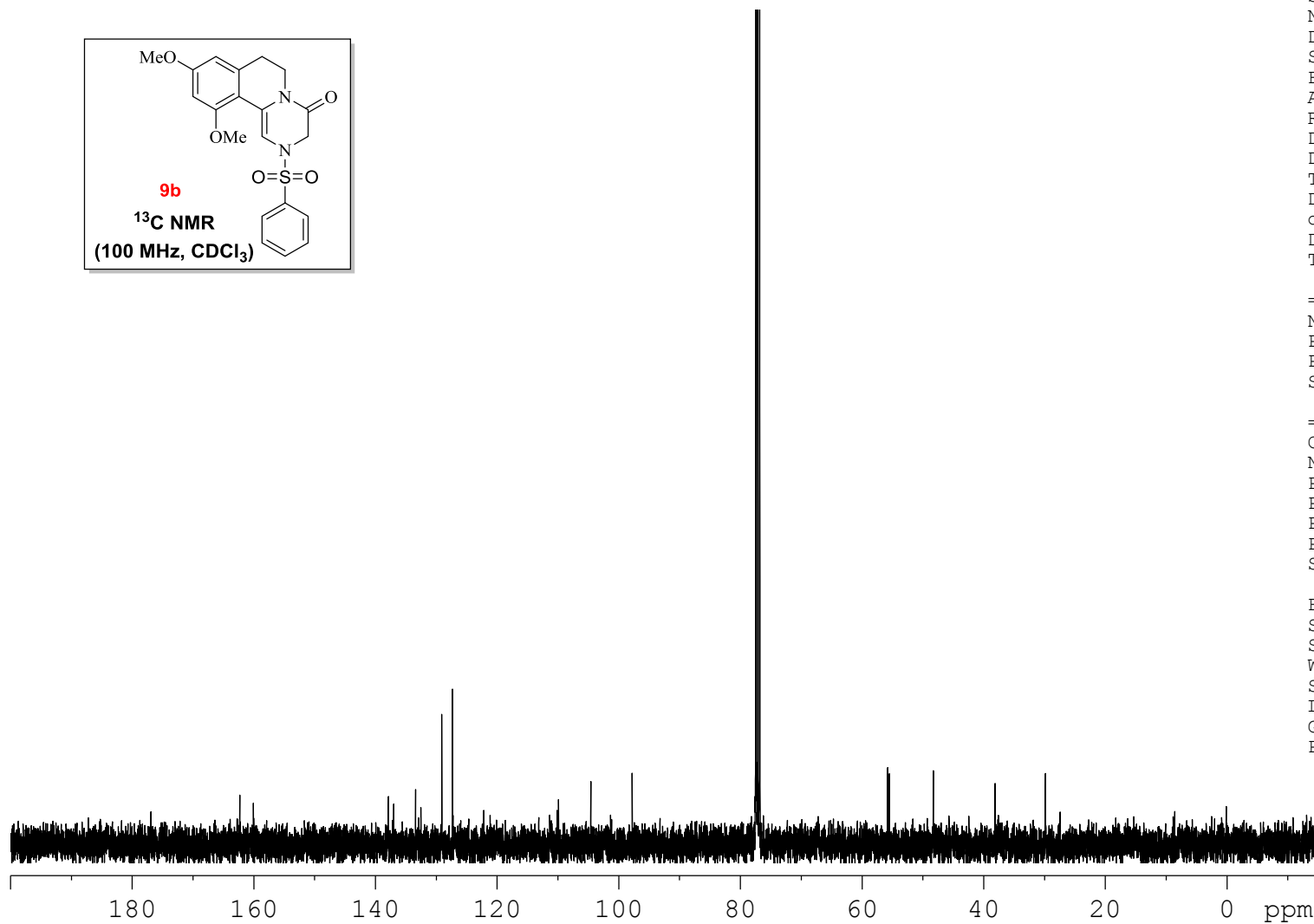
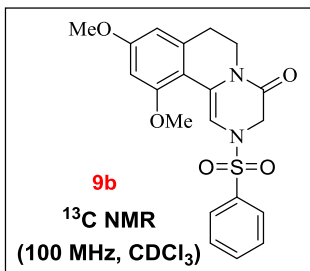
F2 - Acquisition Parameters  
 Date 20130913  
 Time 15.47  
 INSTRUM spect  
 PROBHD 5 mm BBO BB-1H  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT CDC13  
 NS 256  
 DS 4  
 SWH 24038.461 Hz  
 FIDRES 0.366798 Hz  
 AQ 1.3631988 sec  
 RG 645  
 DW 20.800 usec  
 DE 6.00 usec  
 TE 294.1 K  
 D1 2.00000000 sec  
 d11 0.03000000 sec  
 DELTA 1.89999998 sec  
 TD0 1

==== CHANNEL f1 =====  
 NUC1 13C  
 P1 9.50 usec  
 PL1 -0.60 dB  
 SFO1 100.6228298 MHz

==== CHANNEL f2 =====  
 CPDPRG2 waltz16  
 NUC2 1H  
 PCPD2 90.00 usec  
 PL12 14.96 dB  
 PL13 15.60 dB  
 PL2 -0.90 dB  
 SFO2 400.1316005 MHz

F2 - Processing parameters  
 SI 32768  
 SF 100.6127544 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40

162.29  
 137.91  
 133.42  
 129.15  
 127.36  
 104.62  
 97.82  
 77.48  
 77.16  
 76.84  
 55.83  
 55.55  
 48.31  
 38.16  
 29.88





PROTON CDCl3 {D:\CRR} guest 1

7.849  
7.832  
7.828  
7.617  
7.548  
7.531  
7.528  
7.287  
7.282  
7.260  
6.878  
6.856  
6.640

4.210  
3.915  
3.810  
3.507  
3.492  
3.477  
2.728  
2.713  
2.698

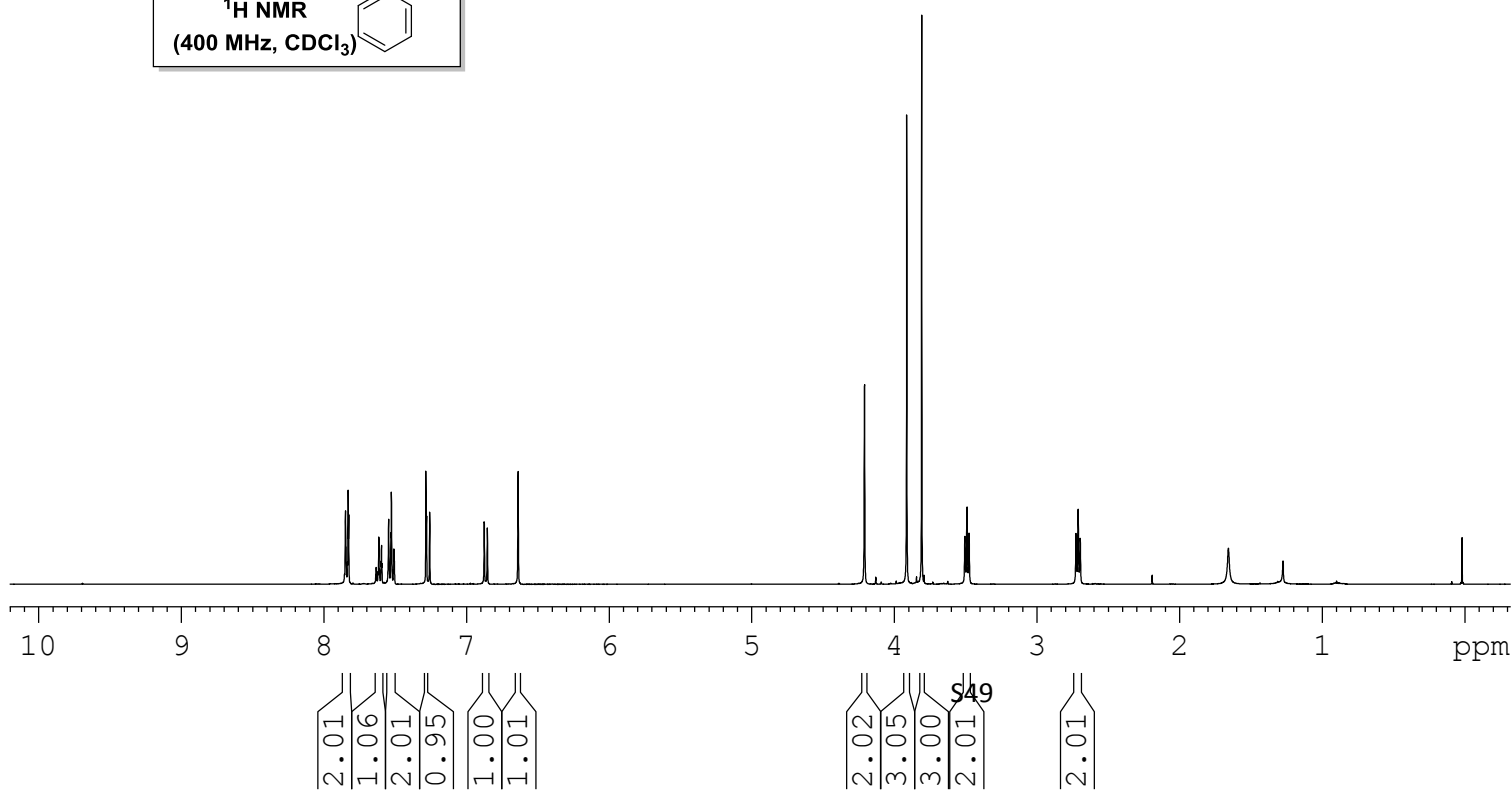
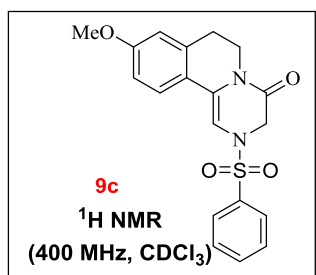
0.021

Current Data Parameters  
NAME RS-I-3-OMe-PzZQ-CY1  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20150222  
Time\_ 22.55  
INSTRUM spect  
PROBHD 5 mm DUL 13C-1  
PULPROG zg30  
TD 65536  
SOLVENT CDCl3  
NS 16  
DS 2  
SWH 8223.685 Hz  
FIDRES 0.125483 Hz  
AQ 3.9846387 sec  
RG 181  
DW 60.800 usec  
DE 6.00 usec  
TE 295.1 K  
D1 1.00000000 sec  
TD0 1

==== CHANNEL f1 =====  
NUC1 1H  
P1 11.42 usec  
PL1 -3.00 dB  
SFO1 400.1324710 MHz

F2 - Processing parameters  
SI 32768  
SF 400.1299944 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00



C13CPD CDC13 {D:\CRR} guest 1

Current Data Parameters  
NAME RS-I-3-OMe-PzZQ-CY1  
EXPNO 2  
PROCNO 1

F2 - Acquisition Parameters

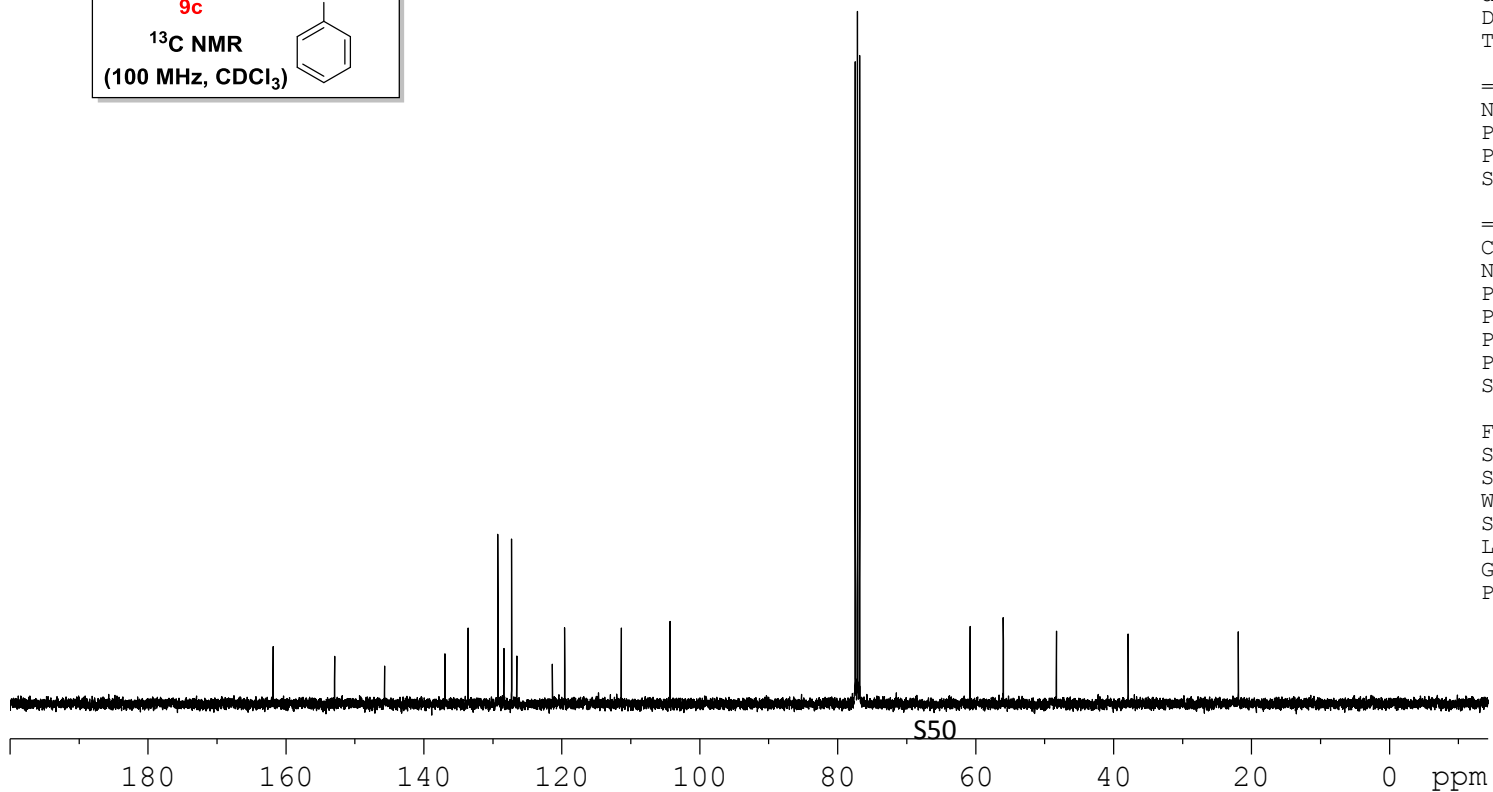
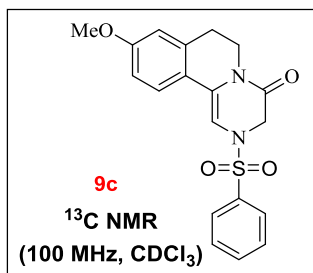
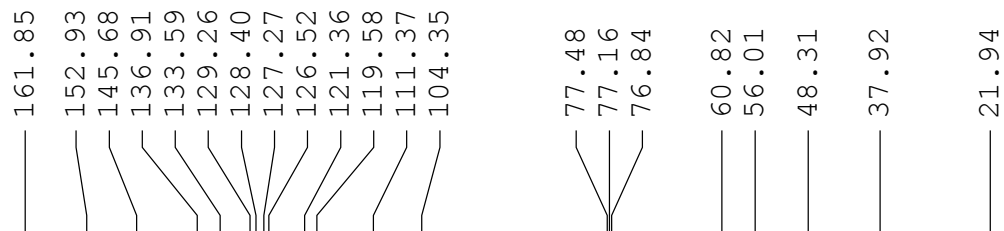
Date\_ 20150222  
Time\_ 23.06  
INSTRUM spect  
PROBHD 5 mm DUL 13C-1  
PULPROG zgpg30  
TD 65536  
SOLVENT CDC13  
NS 178  
DS 4  
SWH 24038.461 Hz  
FIDRES 0.366798 Hz  
AQ 1.3631988 sec  
RG 45.2  
DW 20.800 usec  
DE 6.00 usec  
TE 295.7 K  
D1 2.00000000 sec  
d11 0.03000000 sec  
DELTA 1.89999998 sec  
TD0 1

==== CHANNEL f1 =====  
NUC1 13C  
P1 9.15 usec  
PL1 0.00 dB  
SFO1 100.6228298 MHz

==== CHANNEL f2 =====  
CPDPRG2 waltz16  
NUC2 1H  
PCPD2 90.00 usec  
PL12 14.90 dB  
PL13 14.90 dB  
PL2 -3.00 dB  
SFO2 400.1316005 MHz

F2 - Processing parameters

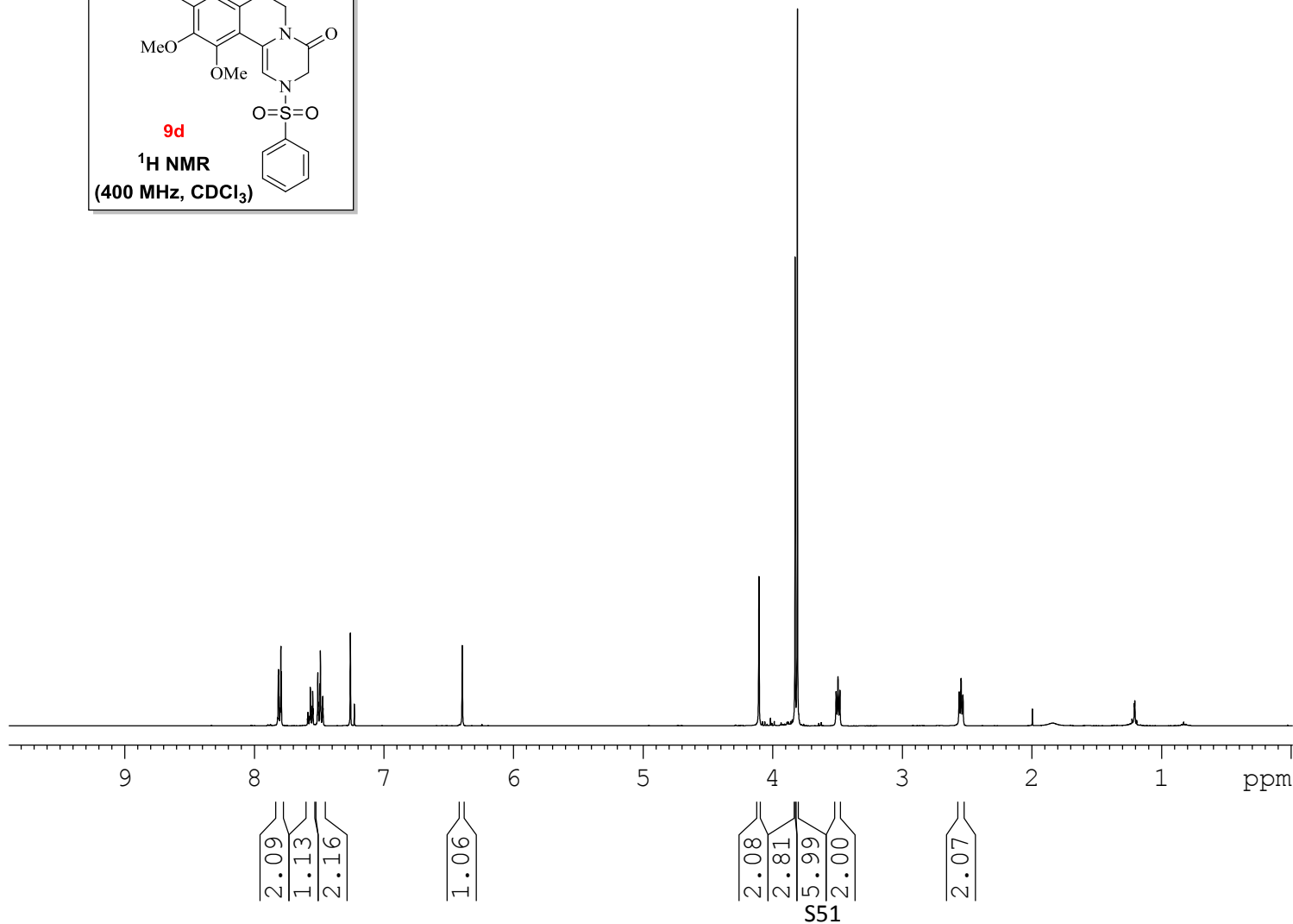
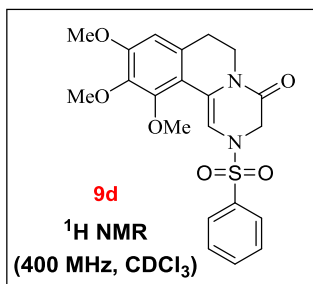
SI 32768  
SF 100.6127553 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40



PROTON CDCl3 {D:\CRR} KOPAL 1

7.797  
7.793  
7.591  
7.588  
7.585  
7.575  
7.570  
7.564  
7.554  
7.551  
7.548  
7.516  
7.511  
7.507  
7.495  
7.492  
7.478  
7.474  
7.471  
7.260  
7.230  
6.397

4.108  
3.829  
3.811  
3.512  
3.498  
3.483  
2.563  
2.547  
2.533



Current Data Parameters  
NAME RS-I-3,4,5-PZQ-CY-1  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20150128  
Time\_ 11.20  
INSTRUM spect  
PROBHD 5 mm DUL 13C-1  
PULPROG zg30  
TD 65536  
SOLVENT CDCl3  
NS 16  
DS 2  
SWH 8223.685 Hz  
FIDRES 0.125483 Hz  
AQ 3.9846387 sec  
RG 90.5  
DW 60.800 usec  
DE 6.00 usec  
TE 292.3 K  
D1 1.00000000 sec  
TD0 1

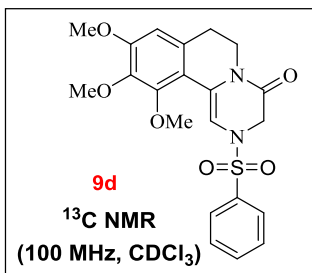
==== CHANNEL f1 =====  
NUC1 1H  
P1 11.42 usec  
PL1 -3.00 dB  
SFO1 400.1324710 MHz

F2 - Processing parameters  
SI 32768  
SF 400.1300169 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00

Current Data Parameters  
 NAME RS-I-3,4,5-PZQ-CY-1  
 EXPNO 2  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20150128  
 Time\_ 11.30  
 INSTRUM spect  
 PROBHD 5 mm DUL 13C-1  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT CDC13  
 NS 256  
 DS 4  
 SWH 24038.461 Hz  
 FIDRES 0.366798 Hz  
 AQ 1.3631988 sec  
 RG 64  
 DW 20.800 usec  
 DE 6.00 usec  
 TE 293.5 K  
 D1 2.00000000 sec  
 d11 0.03000000 sec  
 DELTA 1.89999999 sec  
 TDO 1

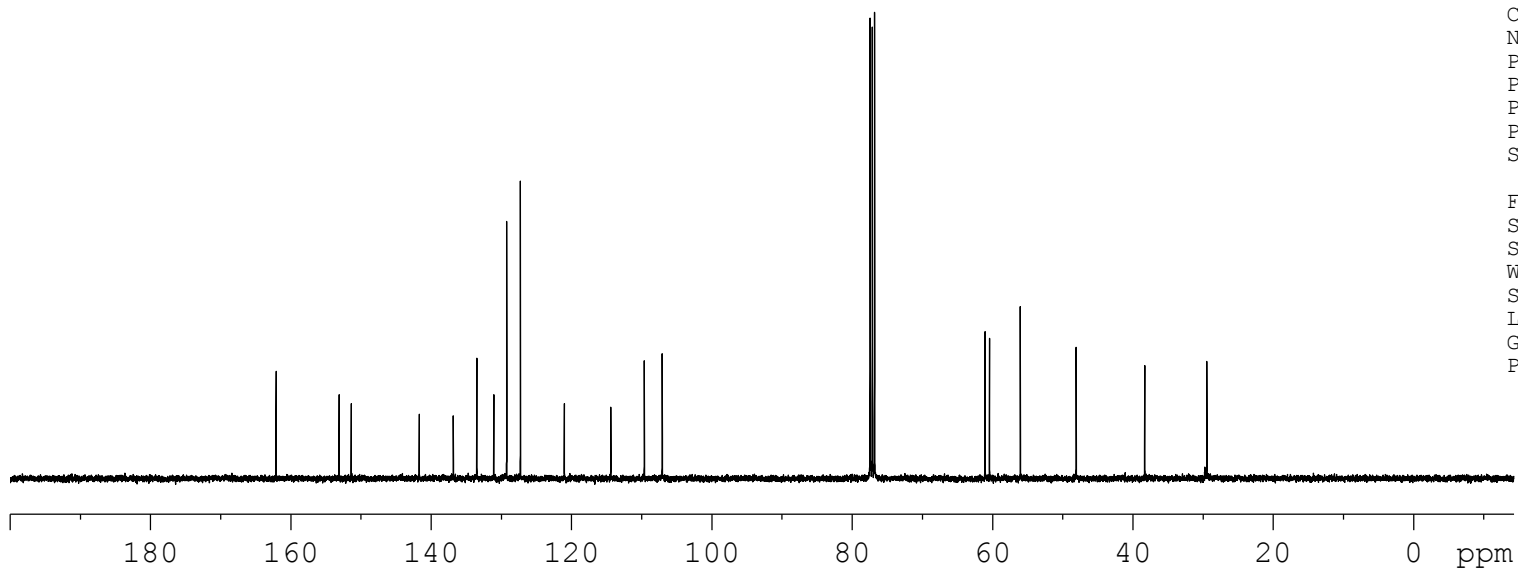
162.08  
 153.10  
 151.37  
 141.72  
 136.88  
 133.52  
 131.11  
 129.27  
 127.32  
 121.05  
 114.44  
 109.66  
 107.10  
 77.48  
 77.16  
 76.84  
 61.10  
 60.46  
 56.07  
 48.11  
 38.34  
 29.49



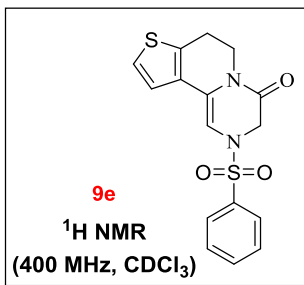
===== CHANNEL f1 =====  
 NUC1 13C  
 P1 9.15 usec  
 PL1 0.00 dB  
 SFO1 100.6228298 MHz

===== CHANNEL f2 =====  
 CPDPRG2 waltz16  
 NUC2 1H  
 PCPD2 90.00 usec  
 PL12 14.90 dB  
 PL13 14.90 dB  
 PL2 -3.00 dB  
 SFO2 400.1316005 MHz

F2 - Processing parameters  
 SI 32768  
 SF 100.6127595 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40



7.813  
7.808  
7.804  
7.604  
7.585  
7.580  
7.570  
7.567  
7.563  
7.533  
7.528  
7.524  
7.512  
7.508  
7.495  
7.490  
7.488  
7.260  
7.173  
7.160  
7.101  
7.088  
6.599  
4.750  
4.152  
3.643  
3.628  
3.613  
2.849  
2.834  
2.819  
1.248

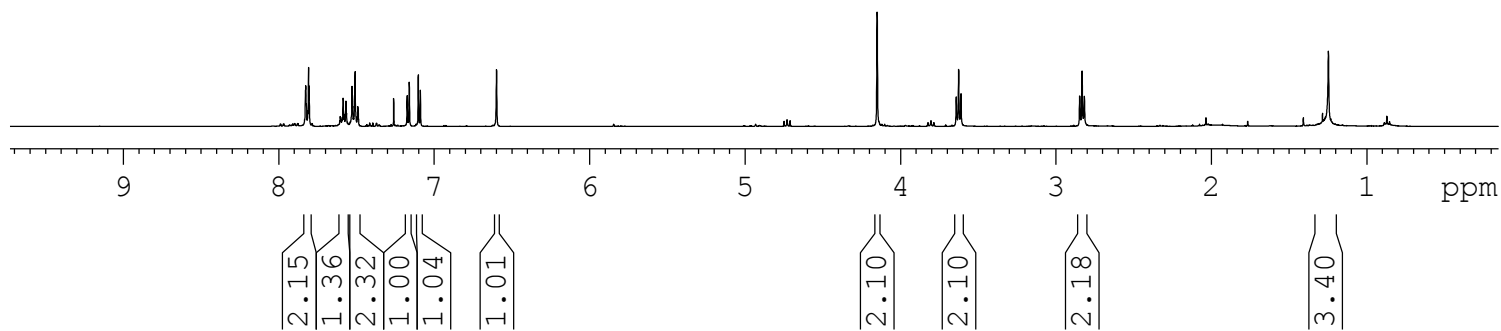


Current Data Parameters  
NAME RS-I-THIO-PZQ-CY-1  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20150226  
Time\_ 15.24  
INSTRUM spect  
PROBHD 5 mm DUL 13C-1  
PULPROG zg30  
TD 65536  
SOLVENT CDCl3  
NS 16  
DS 2  
SWH 8223.685 Hz  
FIDRES 0.125483 Hz  
AQ 3.9846387 sec  
RG 128  
DW 60.800 usec  
DE 6.00 usec  
TE 295.5 K  
D1 1.00000000 sec  
TD0 1

==== CHANNEL f1 =====  
NUC1 1H  
P1 11.42 usec  
PL1 -3.00 dB  
SFO1 400.1324710 MHz

F2 - Processing parameters  
SI 32768  
SF 400.1300051 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00



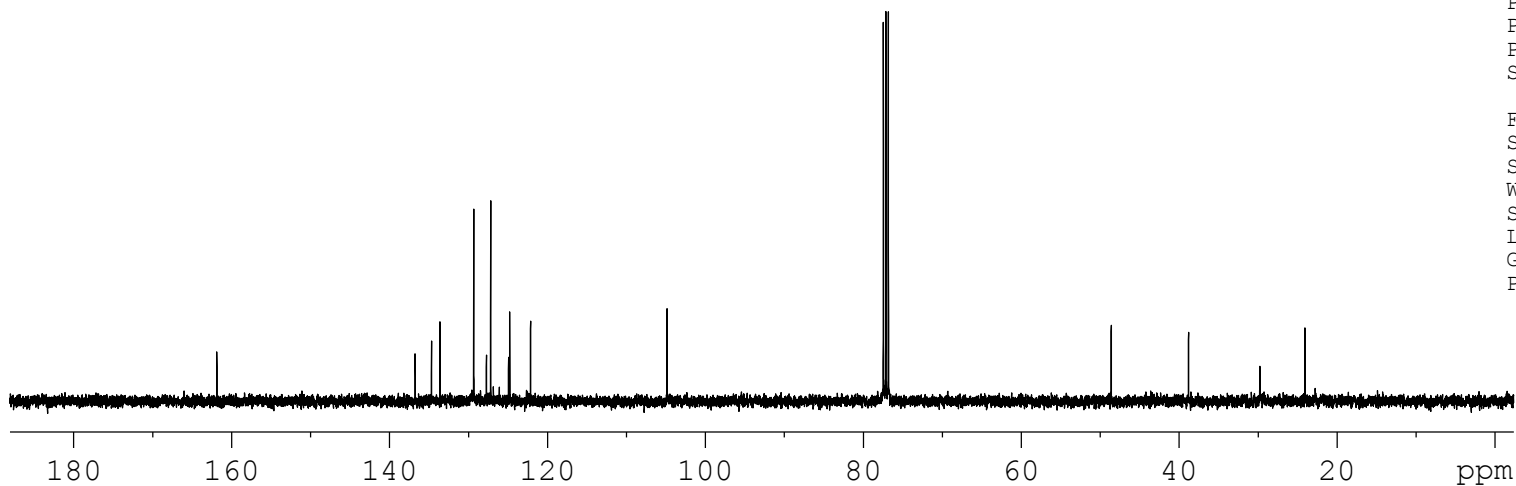
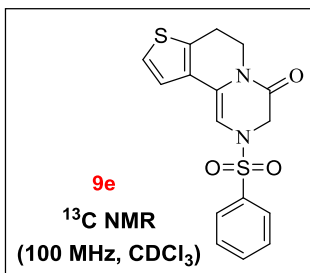
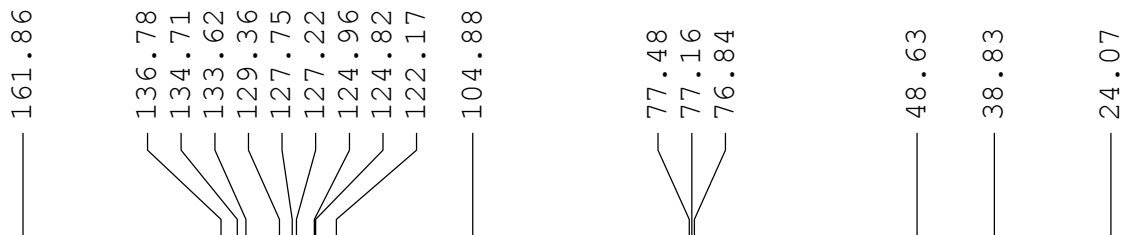
Current Data Parameters  
 NAME RS-I-THIO-PZQ-CY-1  
 EXPNO 2  
 PROCNO 1

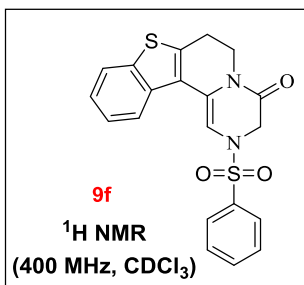
F2 - Acquisition Parameters  
 Date\_ 20150226  
 Time\_ 15.27  
 INSTRUM spect  
 PROBHD 5 mm DUL 13C-1  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT CDC13  
 NS 63  
 DS 4  
 SWH 24038.461 Hz  
 FIDRES 0.366798 Hz  
 AQ 1.3631988 sec  
 RG 32  
 DW 20.800 usec  
 DE 6.00 usec  
 TE 296.1 K  
 D1 2.00000000 sec  
 d11 0.03000000 sec  
 DELTA 1.89999998 sec  
 TD0 1

==== CHANNEL f1 =====  
 NUC1 13C  
 P1 9.15 usec  
 PL1 0.00 dB  
 SFO1 100.6228298 MHz

==== CHANNEL f2 =====  
 CPDPRG2 waltz16  
 NUC2 1H  
 PCPD2 90.00 usec  
 PL12 14.90 dB  
 PL13 14.90 dB  
 PL2 -3.00 dB  
 SFO2 400.1316005 MHz

F2 - Processing parameters  
 SI 32768  
 SF 100.6127574 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40





7.9019  
 7.8819  
 7.8004  
 7.7816  
 7.7636  
 7.7432  
 7.5282  
 7.5103  
 7.4642  
 7.4463  
 7.4343  
 7.3435  
 7.3248  
 7.3065  
 7.1879  
 6.9528

4.1723  
 3.6419  
 3.6284  
 3.6146  
 2.8402  
 2.8265  
 2.8128

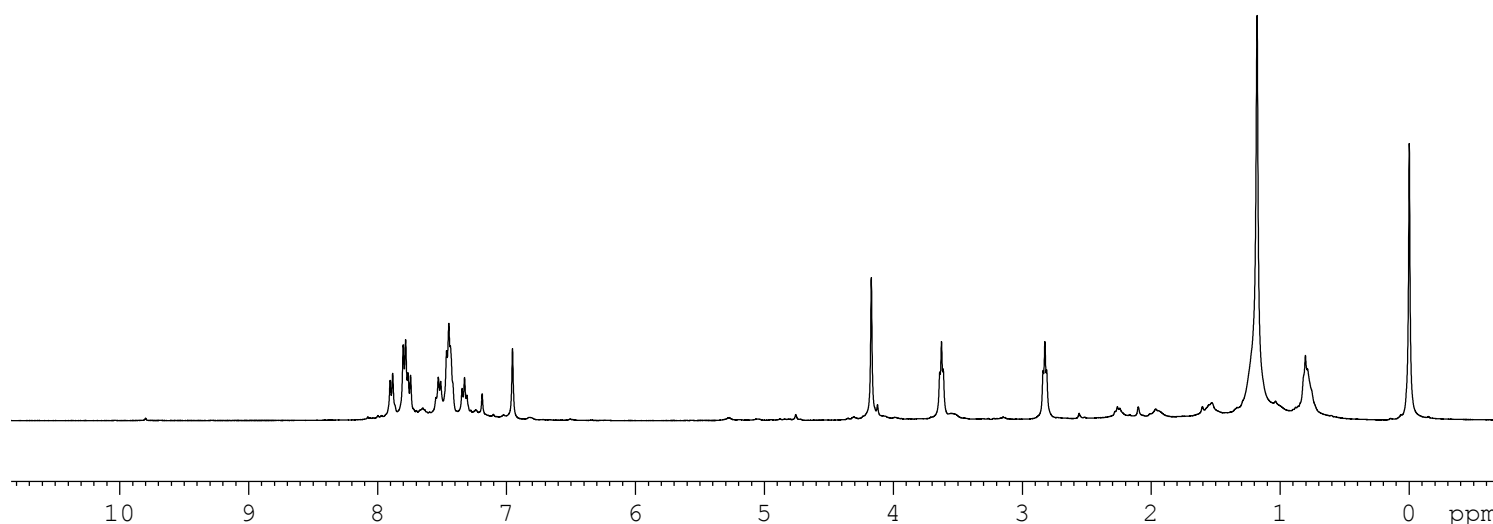
0.0003

Current Data Parameters  
 NAME RS-I-BT-PZQ-CY-1  
 EXPNO 1  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20150726  
 Time\_ 13.07  
 INSTRUM spect  
 PROBHD 5 mm DUL 13C-1  
 PULPROG zg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 16  
 DS 2  
 SWH 8223.685 Hz  
 FIDRES 0.125483 Hz  
 AQ 3.9846387 sec  
 RG 114  
 DW 60.800 usec  
 DE 6.00 usec  
 TE 294.0 K  
 D1 1.00000000 sec  
 TD0 1

===== CHANNEL f1 =====  
 NUC1 1H  
 P1 11.42 usec  
 PL1 -3.00 dB  
 SFO1 400.1324710 MHz

F2 - Processing parameters  
 SI 32768  
 SF 400.1300338 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00



1.20  
 3.33  
 1.79  
 3.62  
 1.44  
 1.03

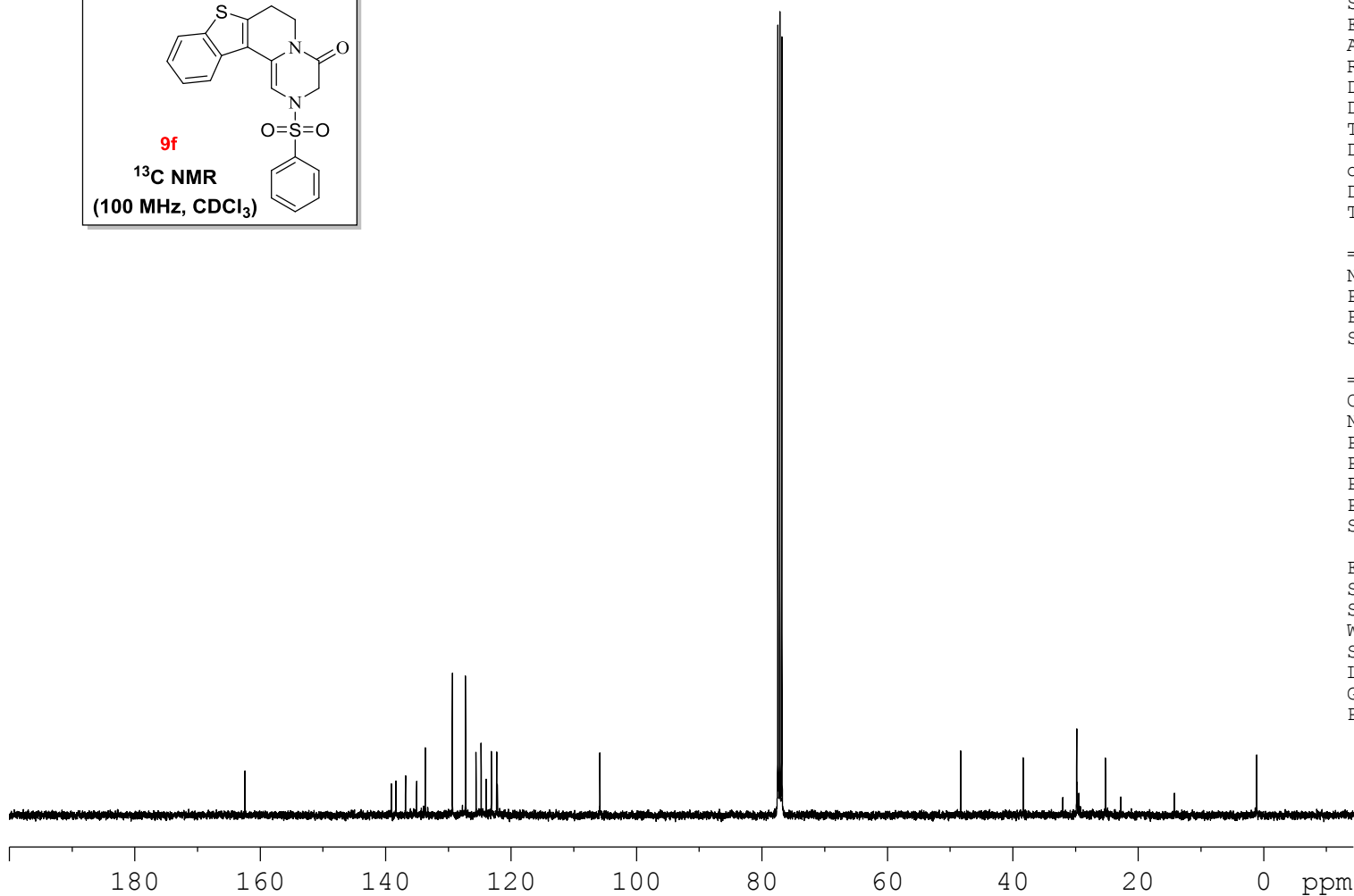
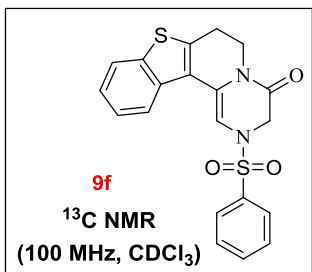
2.00  
 2.08  
 2.08

S55

Current Data Parameters  
 NAME RS-I-BT-PZQ-CY-1  
 EXPNO 2  
 PROCNO 1

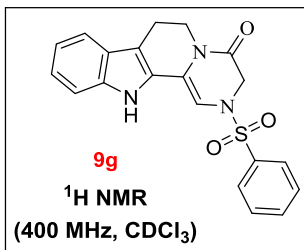
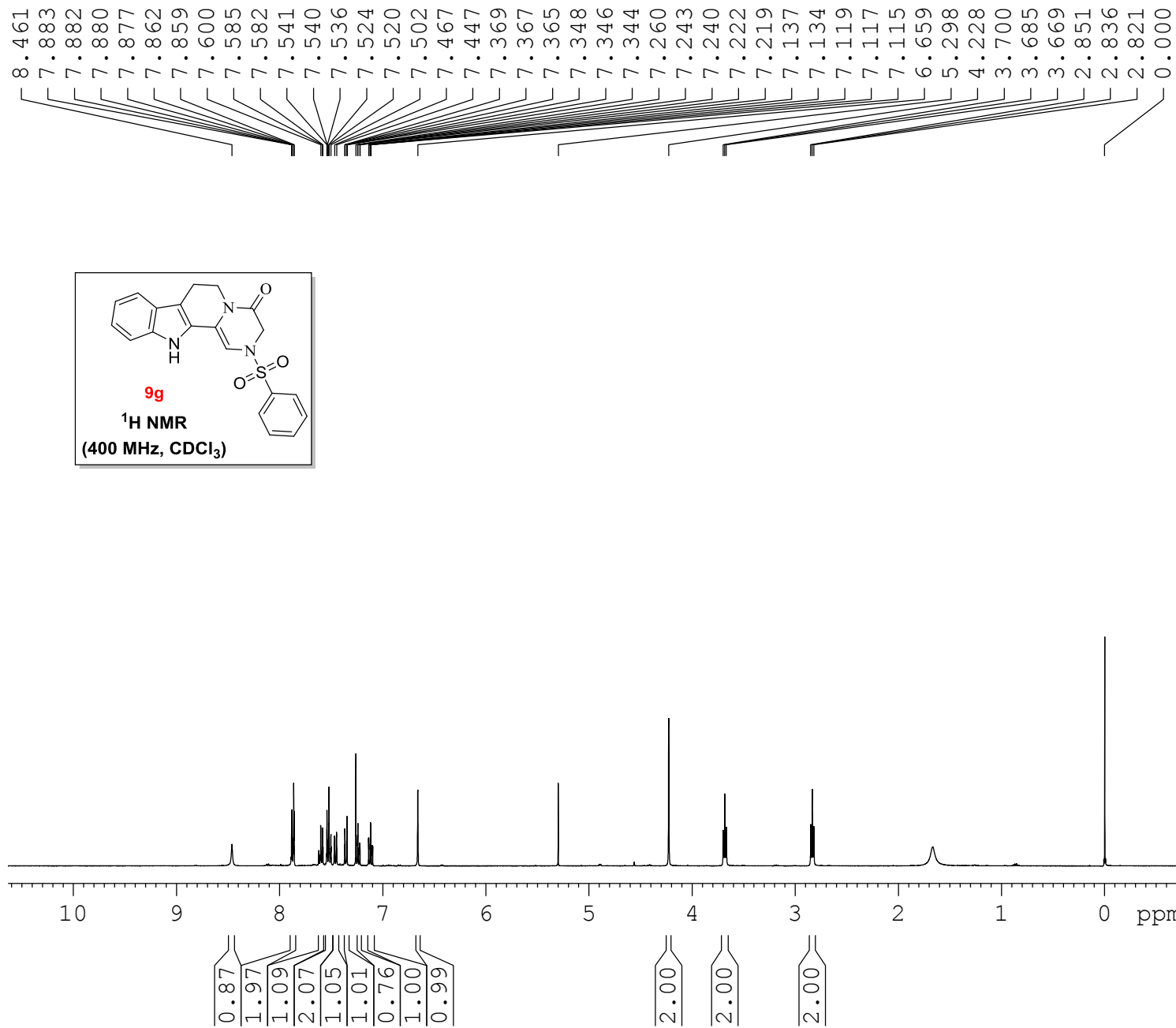
F2 - Acquisition Parameters  
 Date\_ 20150726  
 Time\_ 13.14  
 INSTRUM spect  
 PROBHD 5 mm DUL 13C-1  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT CDC13  
 NS 1024  
 DS 4  
 SWH 24038.461 Hz  
 FIDRES 0.366798 Hz  
 AQ 1.3631988 sec  
 RG 57  
 DW 20.800 usec  
 DE 6.00 usec  
 TE 294.7 K  
 D1 2.00000000 sec  
 d11 0.03000000 sec  
 DELTA 1.89999998 sec  
 TD0 1

162.47  
 139.09  
 138.38  
 136.85  
 135.08  
 133.70  
 129.39  
 127.30  
 125.62  
 124.80  
 123.98  
 123.18  
 122.32  
 122.21  
 105.87  
 77.48  
 77.16  
 76.84  
 48.33  
 38.37  
 29.83  
 25.26



==== CHANNEL f1 =====  
 NUC1 13C  
 P1 9.15 usec  
 PL1 0.00 dB  
 SFO1 100.6228298 MHz  
 ===== CHANNEL f2 =====  
 CPDPRG2 waltz16  
 NUC2 1H  
 PCPD2 90.00 usec  
 PL12 14.90 dB  
 PL13 14.90 dB  
 PL2 -3.00 dB  
 SFO2 400.1316005 MHz  
 F2 - Processing parameters  
 SI 32768  
 SF 100.6127560 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40





Current Data Parameters  
 NAME RS-I-IN-PZQ-CY  
 EXPNO 1  
 PROCNO 1

F2 - Acquisition Parameters  
 Date 20150106  
 Time 15.00  
 INSTRUM spect  
 PROBHD 5 mm DUL 13C-1  
 PULPROG zg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 16  
 DS 2  
 SWH 8223.685 Hz  
 FIDRES 0.125483 Hz  
 AQ 3.9846387 sec  
 RG 256  
 DW 60.800 usec  
 DE 6.00 usec  
 TE 296.8 K  
 D1 1.00000000 sec  
 TD0 1

==== CHANNEL f1 =====  
 NUC1 1H  
 P1 11.42 usec  
 PL1 -3.00 dB  
 SF01 400.1324710 MHz

F2 - Processing parameters  
 SI 32768  
 SF 400.1300051 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00

Current Data Parameters  
 NAME RS-I-IN-PZQ-CY  
 EXPNO 2  
 PROCNO 1

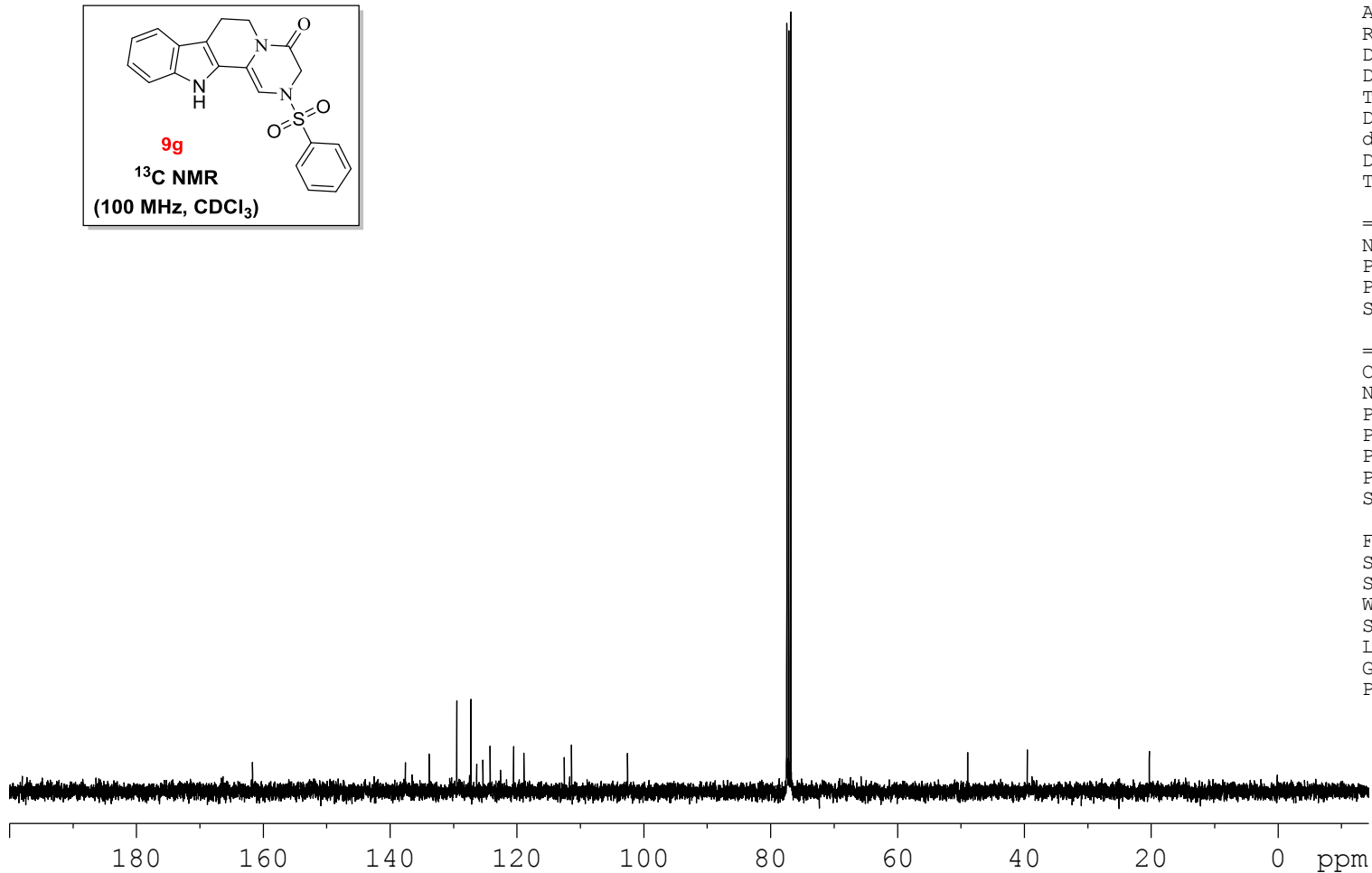
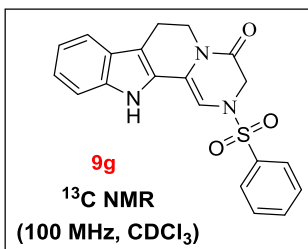
F2 - Acquisition Parameters  
 Date\_ 20150106  
 Time\_ 16.52  
 INSTRUM spect  
 PROBHD 5 mm DUL 13C-1  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT DMSO  
 NS 217  
 DS 4  
 SWH 24038.461 Hz  
 FIDRES 0.366798 Hz  
 AQ 1.3631988 sec  
 RG 50.8  
 DW 20.800 usec  
 DE 6.00 usec  
 TE 298.0 K  
 D1 2.00000000 sec  
 d11 0.03000000 sec  
 DELTA 1.89999998 sec  
 TD0 1

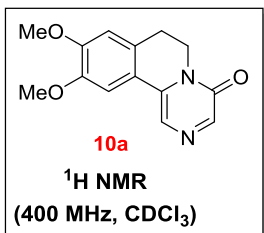
==== CHANNEL f1 =====  
 NUC1 13C  
 P1 9.15 usec  
 PL1 0.00 dB  
 SFO1 100.6228298 MHz

==== CHANNEL f2 =====  
 CPDPRG2 waltz16  
 NUC2 1H  
 PCPD2 90.00 usec  
 PL12 14.90 dB  
 PL13 14.90 dB  
 PL2 -3.00 dB  
 SFO2 400.1316005 MHz

F2 - Processing parameters  
 SI 32768  
 SF 100.6122739 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40

161.67  
 137.63  
 133.86  
 129.51  
 127.30  
 126.39  
 125.39  
 124.26  
 122.62  
 120.55  
 118.93  
 112.57  
 111.42  
 102.59  
 77.48  
 77.16  
 76.84  
 48.96  
 39.56  
 20.32





8.042  
 7.740  
 7.260  
 7.168  
 6.745

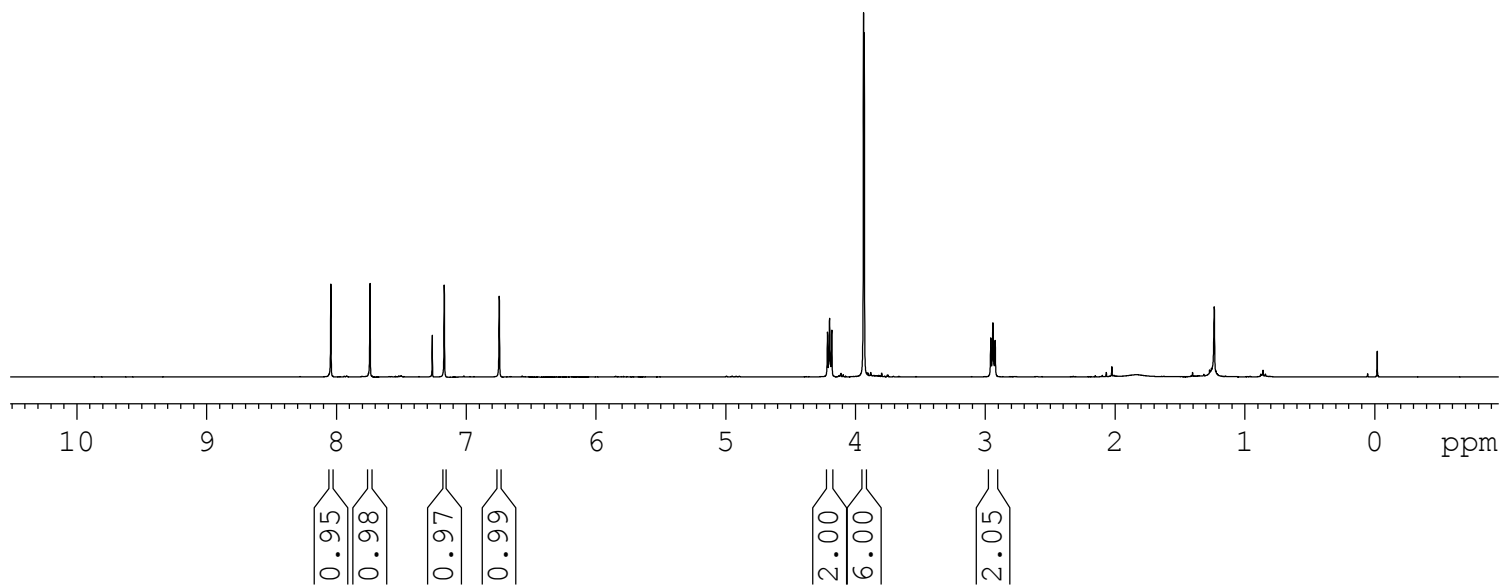
4.215  
 4.199  
 4.182  
 3.938  
 3.932  
 2.959  
 2.943  
 2.926

Current Data Parameters  
 NAME RS-I-PZQ-IM-CY-B  
 EXPNO 1  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20130711  
 Time\_ 12.51  
 INSTRUM spect  
 PROBHD 5 mm BBO BB-1H  
 PULPROG zg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 16  
 DS 2  
 SWH 8223.685 Hz  
 FIDRES 0.125483 Hz  
 AQ 3.9846387 sec  
 RG 256  
 DW 60.800 usec  
 DE 6.00 usec  
 TE 296.9 K  
 D1 1.00000000 sec  
 TD0 1

===== CHANNEL f1 =====  
 NUC1 1H  
 P1 14.50 usec  
 PL1 -0.90 dB  
 SF01 400.1324710 MHz

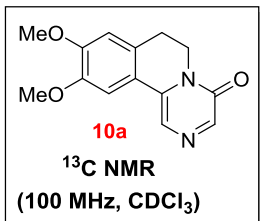
F2 - Processing parameters  
 SI 32768  
 SF 400.1300056 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00



Current Data Parameters  
 NAME RS-I-PZQ-IM-CY-B  
 EXPNO 2  
 PROCNO 1

F2 - Acquisition Parameters  
 Date 20130711  
 Time 13.04  
 INSTRUM spect  
 PROBHD 5 mm BBO BB-1H  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT CDC13  
 NS 211  
 DS 4  
 SWH 24038.461 Hz  
 FIDRES 0.366798 Hz  
 AQ 1.3631988 sec  
 RG 724  
 DW 20.800 usec  
 DE 6.00 usec  
 TE 297.3 K  
 D1 2.00000000 sec  
 d11 0.03000000 sec  
 DELTA 1.89999998 sec  
 TDO 1

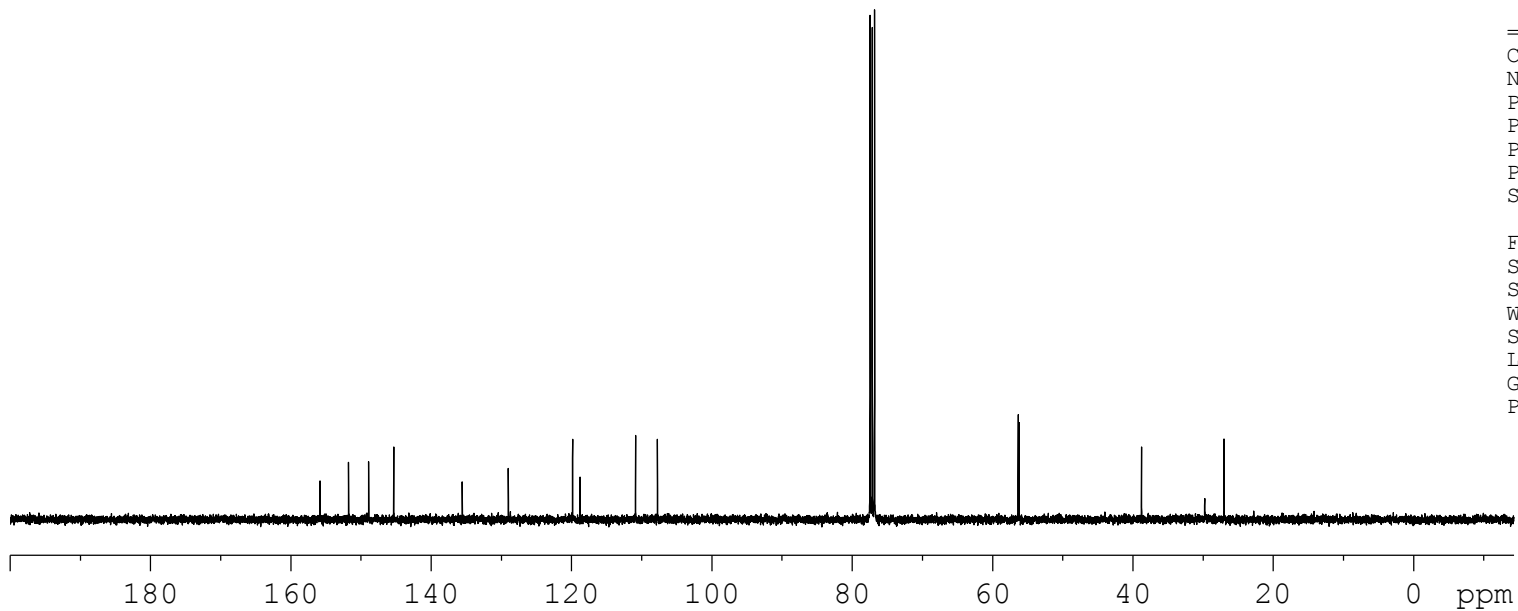
155.84  
 151.76  
 148.90  
 145.31  
 135.55  
 128.99  
 119.83  
 118.78  
 110.86  
 107.74  
 77.48  
 77.16  
 76.84  
 56.38  
 56.22  
 38.79  
 27.04

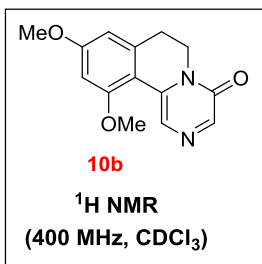


==== CHANNEL f1 =====  
 NUC1 13C  
 P1 9.50 usec  
 PL1 -0.60 dB  
 SFO1 100.6228298 MHz

==== CHANNEL f2 =====  
 CPDPRG2 waltz16  
 NUC2 1H  
 PCPD2 90.00 usec  
 PL12 14.96 dB  
 PL13 15.60 dB  
 PL2 -0.90 dB  
 SFO2 400.1316005 MHz

F2 - Processing parameters  
 SI 32768  
 SF 100.6127564 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40





8.061  
 7.754  
 7.260  
 7.173  
 6.750

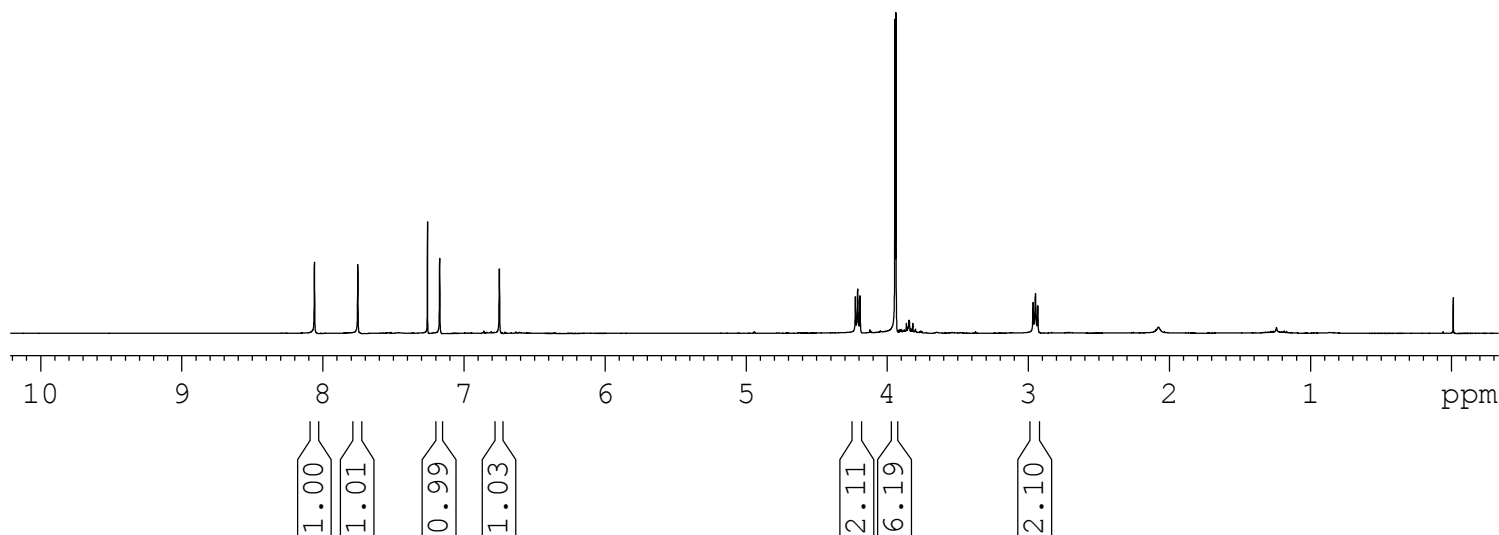
4.226  
 4.210  
 4.194  
 3.946  
 3.940  
 2.967  
 2.950  
 2.934

Current Data Parameters  
 NAME RS-I-3,5-PZQ-CY-2  
 EXPNO 2  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20150204  
 Time\_ 15.56  
 INSTRUM spect  
 PROBHD 5 mm DUL 13C-1  
 PULPROG zg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 16  
 DS 2  
 SWH 8223.685 Hz  
 FIDRES 0.125483 Hz  
 AQ 3.9846387 sec  
 RG 181  
 DW 60.800 usec  
 DE 6.00 usec  
 TE 294.7 K  
 D1 1.0000000 sec  
 TD0 1

==== CHANNEL f1 =====  
 NUC1 1H  
 P1 11.42 usec  
 PL1 -3.00 dB  
 SFO1 400.1324710 MHz

F2 - Processing parameters  
 SI 32768  
 SF 400.1300051 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00



Current Data Parameters  
 NAME RS-I-3,5-PZQ-CY-2  
 EXPNO 3  
 PROCNO 1

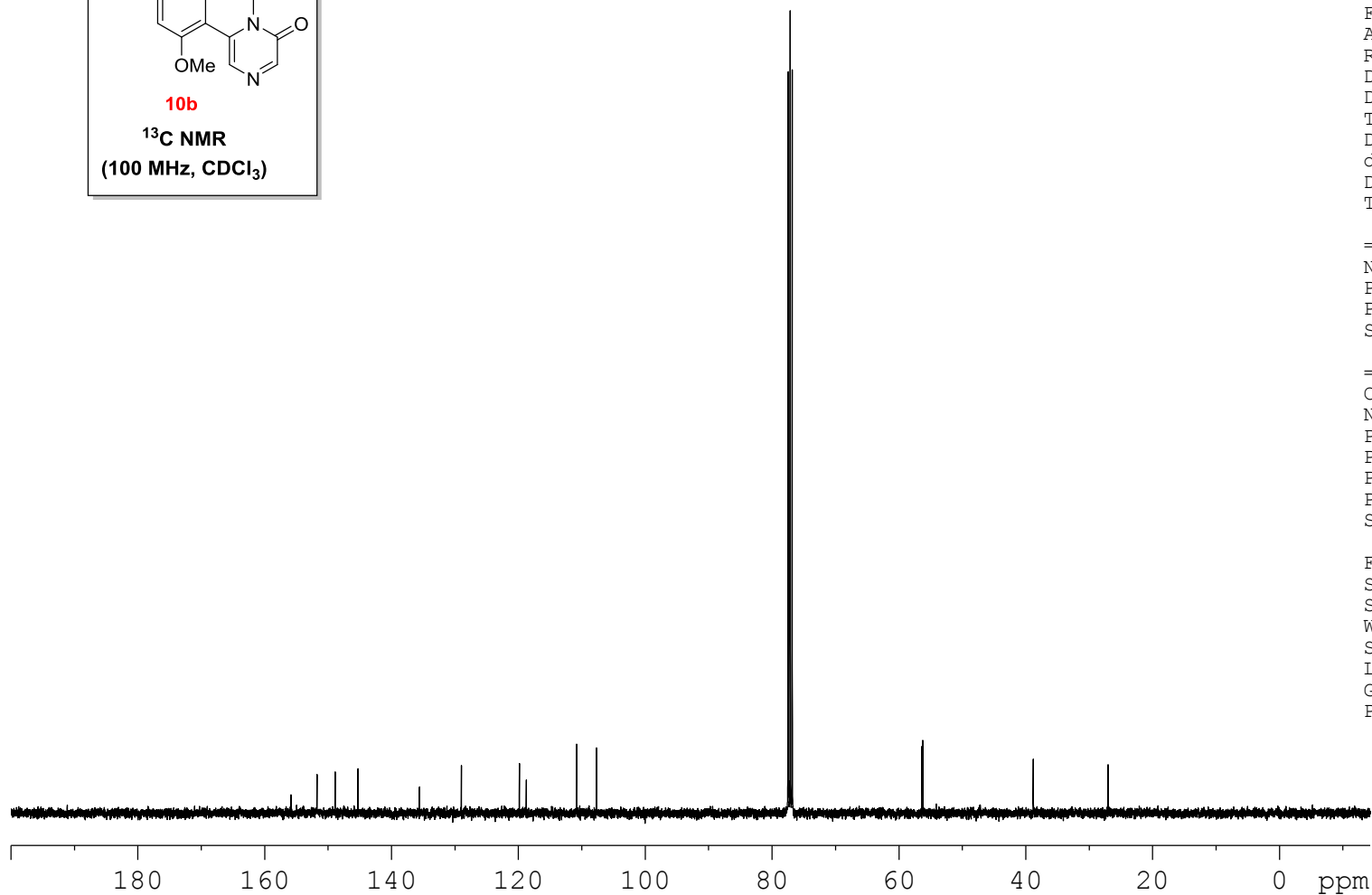
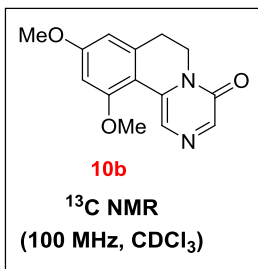
F2 - Acquisition Parameters  
 Date\_ 20150204  
 Time\_ 16.10  
 INSTRUM spect  
 PROBHD 5 mm DUL 13C-1  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT CDC13  
 NS 256  
 DS 4  
 SWH 24038.461 Hz  
 FIDRES 0.366798 Hz  
 AQ 1.3631988 sec  
 RG 32  
 DW 20.800 usec  
 DE 6.00 usec  
 TE 295.0 K  
 D1 2.00000000 sec  
 d11 0.03000000 sec  
 DELTA 1.89999998 sec  
 TDO 1

==== CHANNEL f1 =====  
 NUC1 13C  
 P1 9.15 usec  
 PL1 0.00 dB  
 SFO1 100.6228298 MHz

==== CHANNEL f2 =====  
 CPDPRG2 waltz16  
 NUC2 1H  
 PCPD2 90.00 usec  
 PL12 14.90 dB  
 PL13 14.90 dB  
 PL2 -3.00 dB  
 SFO2 400.1316005 MHz

F2 - Processing parameters  
 SI 32768  
 SF 100.6127553 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40

155.89  
 151.77  
 148.90  
 145.30  
 135.61  
 129.01  
 119.87  
 118.77  
 110.85  
 107.72  
 77.48  
 77.16  
 76.84  
 56.39  
 56.24  
 38.83  
 27.04



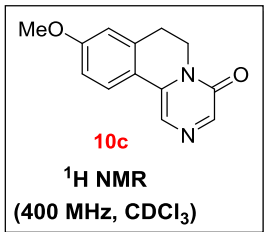
8.035  
7.762  
7.691  
7.669  
7.260  
6.909  
6.902  
6.887  
6.881  
6.788  
6.782

4.219  
4.203  
4.201  
4.186  
3.856  
2.992  
2.976  
2.960

0.058

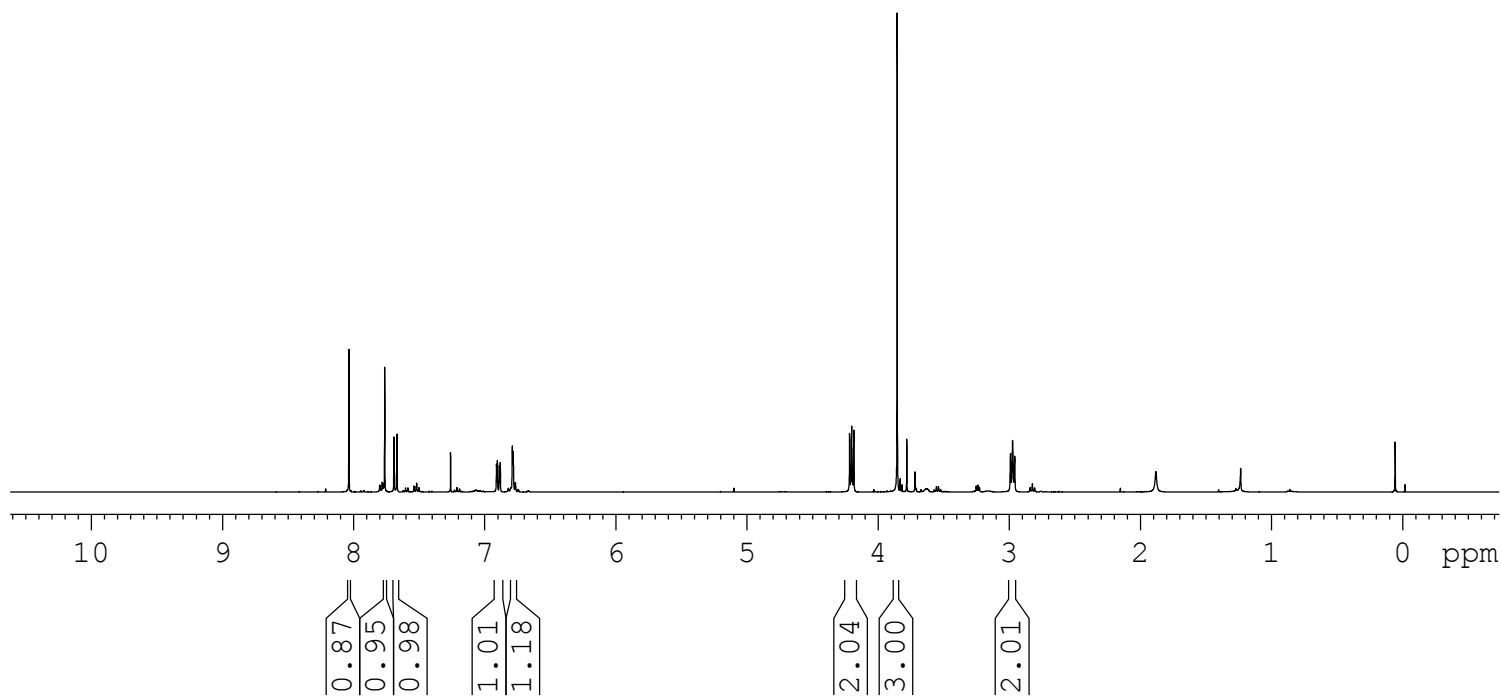
Current Data Parameters  
NAME RS-I-2,3-ome-PZ-QCY-2  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20150223  
Time 16.40  
INSTRUM spect  
PROBHD 5 mm DUL 13C-1  
PULPROG zg30  
TD 65536  
SOLVENT CDC13  
NS 16  
DS 2  
SWH 8223.685 Hz  
FIDRES 0.125483 Hz  
AQ 3.9846387 sec  
RG 144  
DW 60.800 usec  
DE 6.00 usec  
TE 296.0 K  
D1 1.00000000 sec  
TD0 1



==== CHANNEL f1 =====  
NUC1 1H  
P1 11.42 usec  
PL1 -3.00 dB  
SFO1 400.1324710 MHz

F2 - Processing parameters  
SI 32768  
SF 400.1300051 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00



Current Data Parameters  
 NAME RS-I-2,3-ome-PZ-QCY-2  
 EXPNO 2  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20150223  
 Time\_ 16.47  
 INSTRUM spect  
 PROBHD 5 mm DUL 13C-1  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT CDC13  
 NS 130  
 DS 4  
 SWH 24038.461 Hz  
 FIDRES 0.366798 Hz  
 AQ 1.3631988 sec  
 RG 57  
 DW 20.800 usec  
 DE 6.00 usec  
 TE 296.7 K  
 D1 2.00000000 sec  
 d11 0.03000000 sec  
 DELTA 1.89999998 sec  
 TD0 1

===== CHANNEL f1 =====  
 NUC1 13C  
 P1 9.15 usec  
 PL1 0.00 dB  
 SFO1 100.6228298 MHz

===== CHANNEL f2 =====  
 CPDPRG2 waltz16  
 NUC2 1H  
 PCPD2 90.00 usec  
 PL12 14.90 dB  
 PL13 14.90 dB  
 PL2 -3.00 dB  
 SFO2 400.1316005 MHz

F2 - Processing parameters  
 SI 32768  
 SF 100.6127575 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40

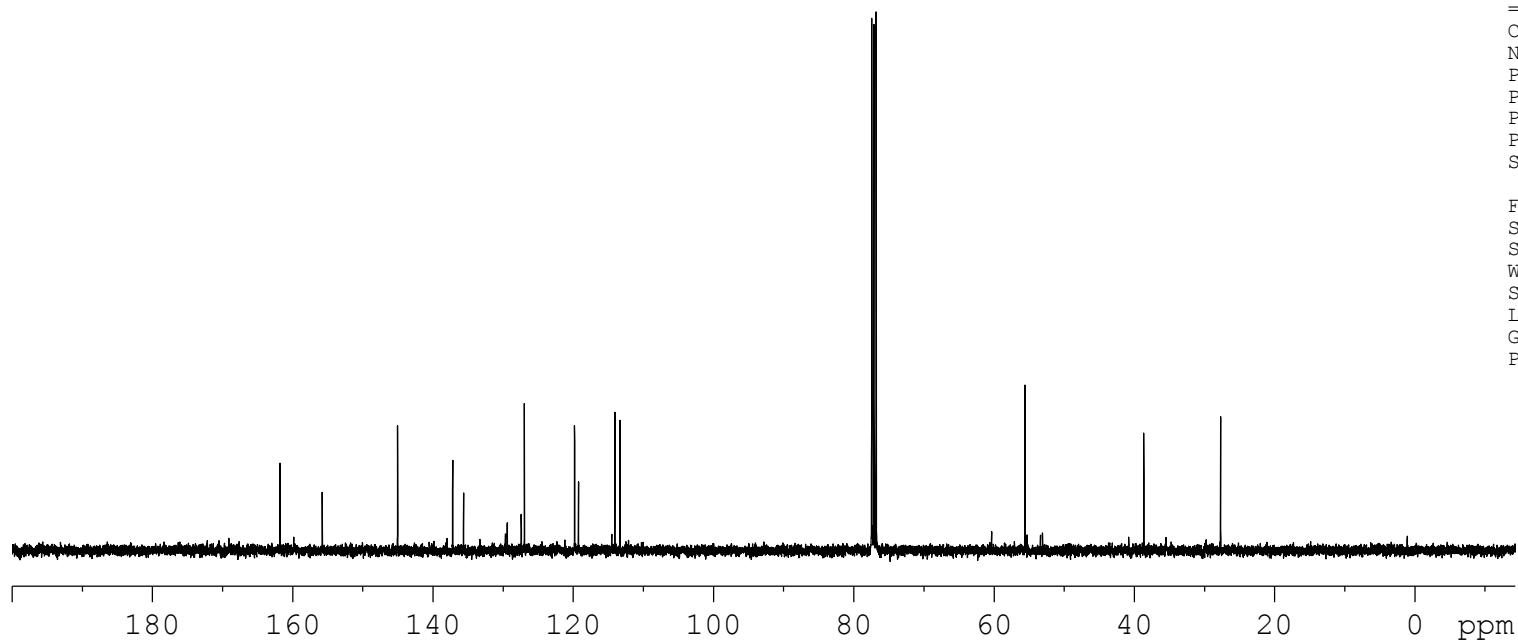
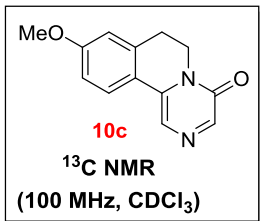
161.84  
 159.89  
 155.82  
 145.06  
 137.22  
 135.67  
 129.69  
 129.44  
 127.44  
 127.00  
 119.83  
 119.27  
 114.53  
 114.08  
 113.37

77.48  
 77.16  
 76.84

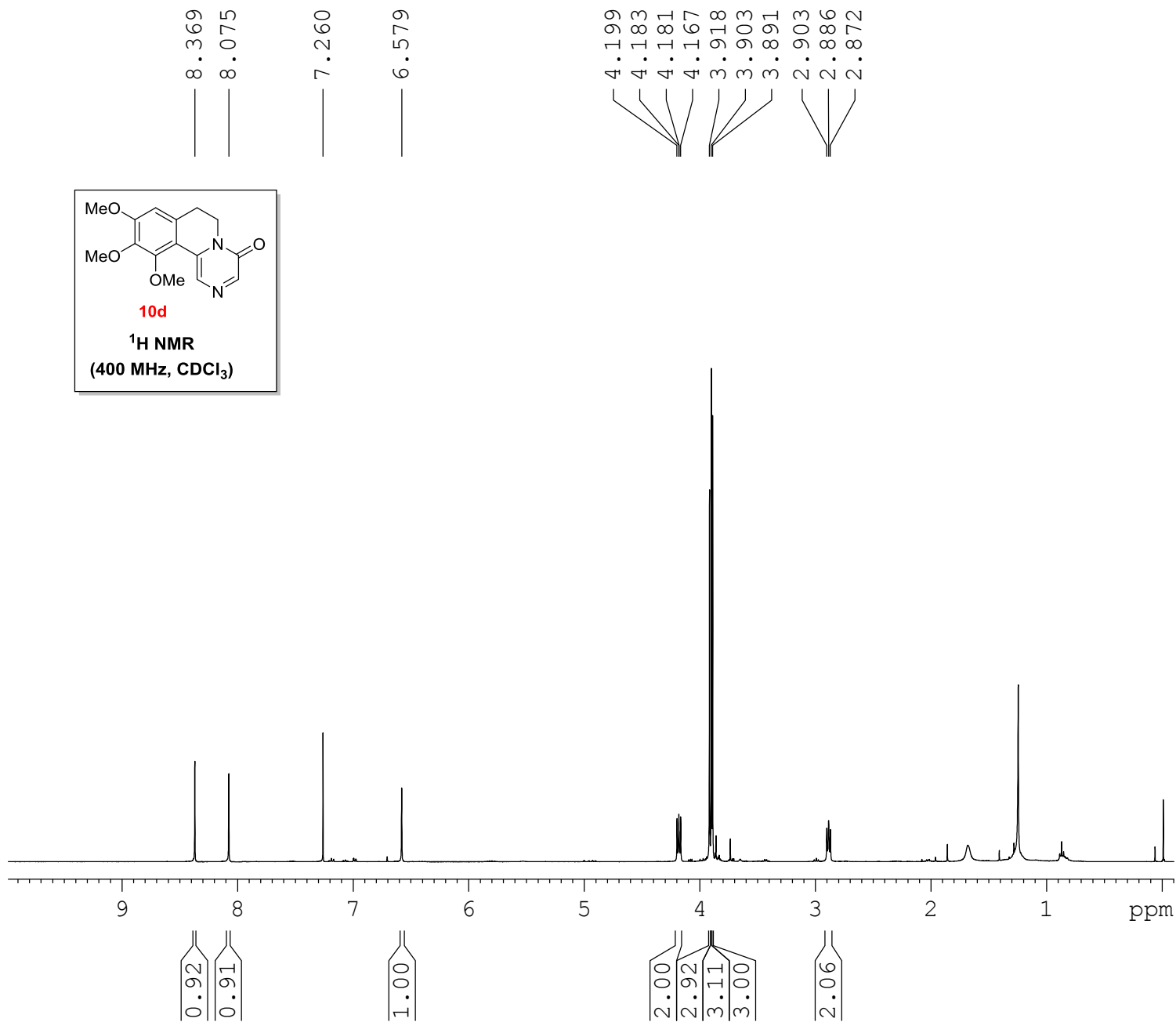
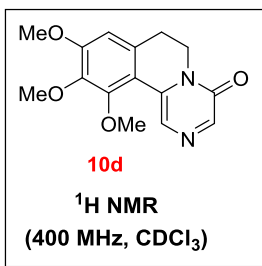
55.62

38.67

27.72







Current Data Parameters  
 NAME RS-I-3,4,5-PZQ-CY-2  
 EXPNO 3  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20150203  
 Time\_ 10.57  
 INSTRUM spect  
 PROBHD 5 mm DUL 13C-1  
 PULPROG zg30  
 TD 65536  
 SOLVENT CDC13  
 NS 16  
 DS 2  
 SWH 8223.685 Hz  
 FIDRES 0.125483 Hz  
 AQ 3.9846387 sec  
 RG 203  
 DW 60.800 usec  
 DE 6.00 usec  
 TE 296.1 K  
 D1 1.00000000 sec  
 TD0 1

==== CHANNEL f1 =====  
 NUC1 1H  
 P1 11.42 usec  
 PL1 -3.00 dB  
 SF01 400.1324710 MHz

F2 - Processing parameters  
 SI 32768  
 SF 400.1300051 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00

Current Data Parameters  
 NAME RS-I-3,4,5-PZQ-CY-2  
 EXPNO 4  
 PROCNO 1

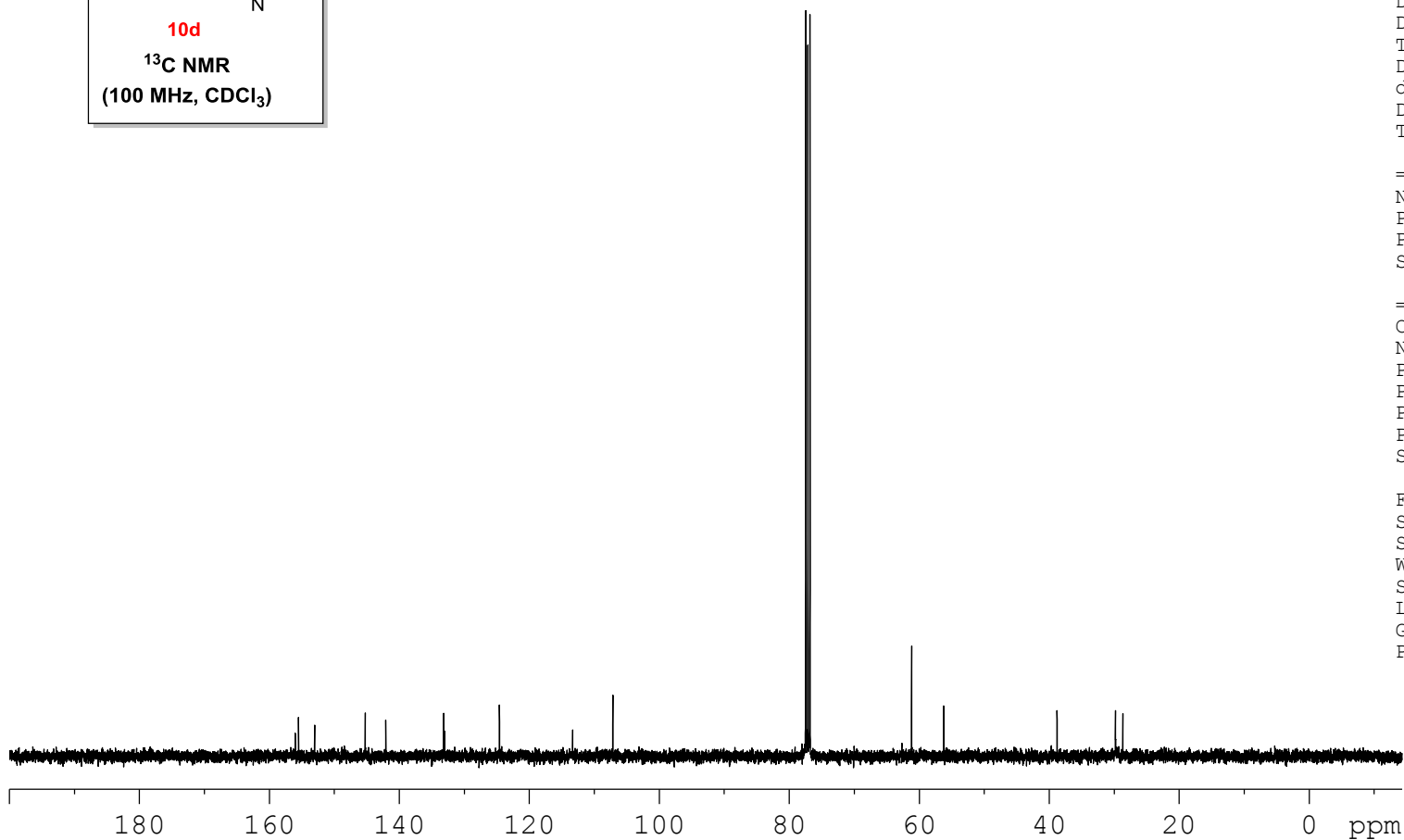
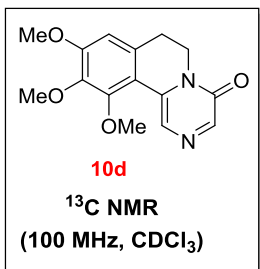
F2 - Acquisition Parameters  
 Date\_ 20150203  
 Time\_ 10.58  
 INSTRUM spect  
 PROBHD 5 mm DUL 13C-1  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT CDC13  
 NS 163  
 DS 4  
 SWH 24038.461 Hz  
 FIDRES 0.366798 Hz  
 AQ 1.3631988 sec  
 RG 45.2  
 DW 20.800 usec  
 DE 6.00 usec  
 TE 296.7 K  
 D1 2.00000000 sec  
 d11 0.03000000 sec  
 DELTA 1.89999999 sec  
 TDO 1

==== CHANNEL f1 =====  
 NUC1 13C  
 P1 9.15 usec  
 PL1 0.00 dB  
 SFO1 100.6228298 MHz

==== CHANNEL f2 =====  
 CPDPRG2 waltz16  
 NUC2 1H  
 PCPD2 90.00 usec  
 PL12 14.90 dB  
 PL13 14.90 dB  
 PL2 -3.00 dB  
 SFO2 400.1316005 MHz

F2 - Processing parameters  
 SI 32768  
 SF 100.6127542 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40

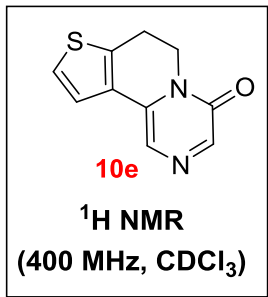
156.01  
 155.49  
 153.02  
 145.22  
 142.07  
 133.16  
 133.01  
 124.58  
 113.31  
 107.13  
 77.48  
 77.16  
 76.84  
 61.20  
 56.25  
 38.81  
 29.83  
 28.68



8.020  
7.587  
7.260

4.339  
4.322  
4.305

3.159  
3.142  
3.125

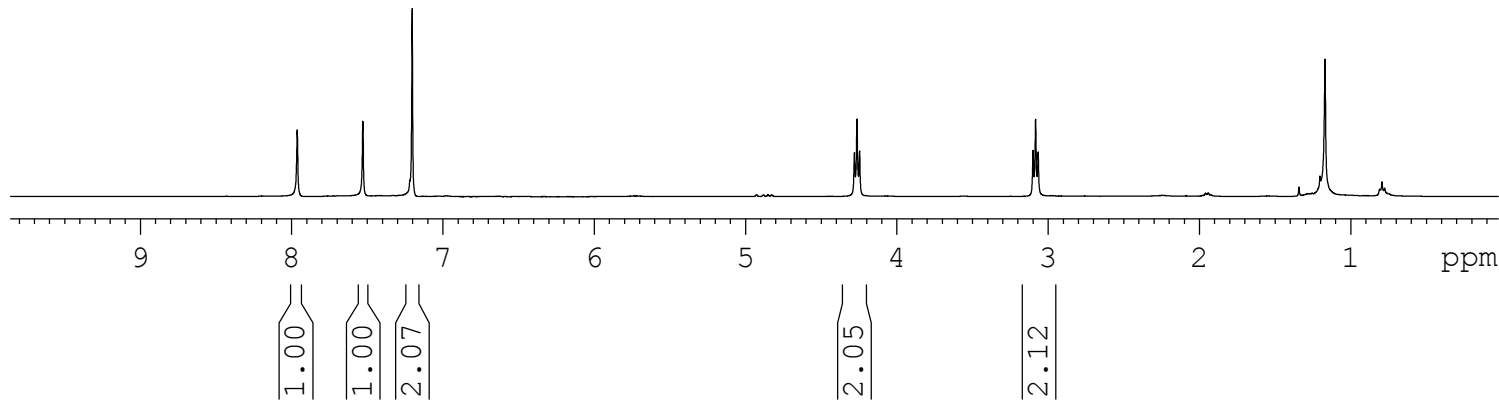


Current Data Parameters  
NAME RS-I-THIO-PZQ-CY-2  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20160227  
Time\_ 15.29  
INSTRUM spect  
PROBHD 5 mm DUL 13C-1  
PULPROG zg30  
TD 65536  
SOLVENT CDCl3  
NS 16  
DS 2  
SWH 8223.685 Hz  
FIDRES 0.125483 Hz  
AQ 3.9846387 sec  
RG 80.6  
DW 60.800 usec  
DE 6.00 usec  
TE 295.1 K  
D1 1.0000000 sec  
TD0 1

==== CHANNEL f1 =====  
NUC1 1H  
P1 11.42 usec  
PL1 -3.00 dB  
SFO1 400.1324710 MHz

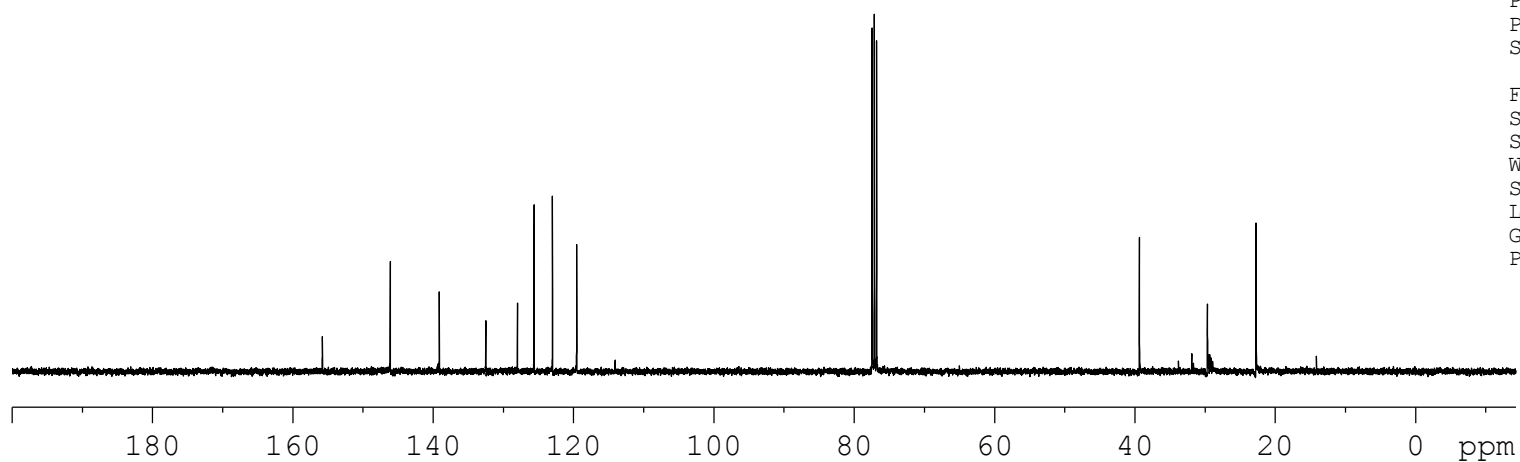
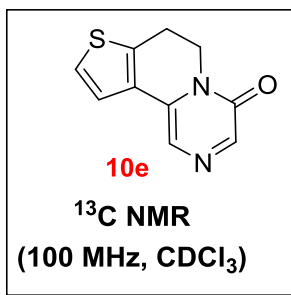
F2 - Processing parameters  
SI 32768  
SF 400.1300212 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00



155.77  
146.09  
139.11  
132.47  
127.98  
125.61  
122.99  
119.54

77.48  
77.16  
76.84

39.38  
29.69  
22.78



S68

Current Data Parameters  
NAME RS-I-THIO-PZQ-CY-2  
EXPNO 2  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20160227  
Time\_ 15.33  
INSTRUM spect  
PROBHD 5 mm DUL 13C-1  
PULPROG zgpg30  
TD 65536  
SOLVENT CDC13  
NS 73  
DS 4  
SWH 24038.461 Hz  
FIDRES 0.366798 Hz  
AQ 1.3631988 sec  
RG 64  
DW 20.800 usec  
DE 6.00 usec  
TE 295.6 K  
D1 2.00000000 sec  
d11 0.03000000 sec  
DELTA 1.89999998 sec  
TD0 1

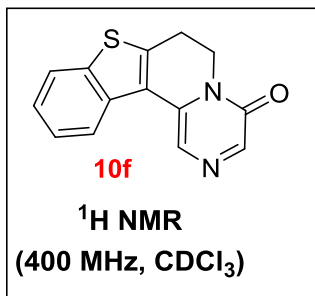
===== CHANNEL f1 =====  
NUC1 13C  
P1 9.15 usec  
PL1 0.00 dB  
SFO1 100.6228298 MHz

===== CHANNEL f2 =====  
CPDPRG2 waltz16  
NUC2 1H  
PCPD2 90.00 usec  
PL12 14.90 dB  
PL13 14.90 dB  
PL2 -3.00 dB  
SFO2 400.1316005 MHz

F2 - Processing parameters  
SI 32768  
SF 100.6127649 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40

8.147  
8.131  
8.110  
8.063  
7.894  
7.875  
7.547  
7.544  
7.528  
7.526  
7.523  
7.508  
7.505  
7.457  
7.454  
7.437  
7.435  
7.419  
7.416  
7.260

4.398  
4.382  
4.365  
  
3.244  
3.227  
3.211

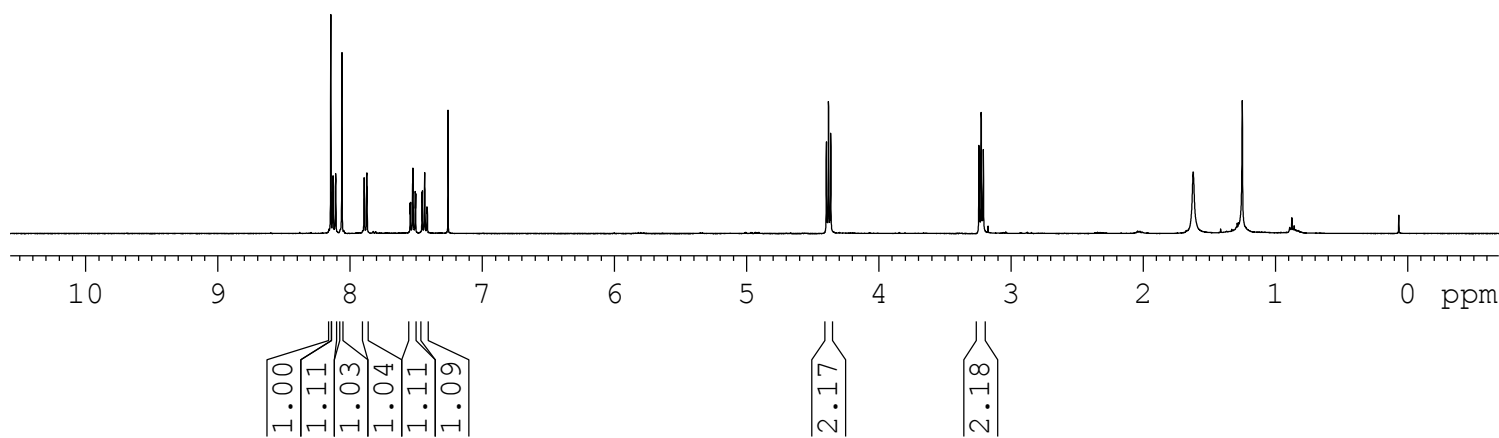


Current Data Parameters  
NAME RS-I-BT-PZQ-CY-2  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20150727  
Time\_ 15.36  
INSTRUM spect  
PROBHD 5 mm DUL 13C-1  
PULPROG zg30  
TD 65536  
SOLVENT CDC13  
NS 12  
DS 2  
SWH 8223.685 Hz  
FIDRES 0.125483 Hz  
AQ 3.9846387 sec  
RG 256  
DW 60.800 usec  
DE 6.00 usec  
TE 296.5 K  
D1 1.00000000 sec  
TD0 1

==== CHANNEL f1 =====  
NUC1 1H  
P1 11.42 usec  
PL1 -3.00 dB  
SF01 400.1324710 MHz

F2 - Processing parameters  
SI 32768  
SF 400.1300051 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00



Current Data Parameters  
 NAME RS-I-BT-PZQ-CY-2  
 EXPNO 2  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20150727  
 Time\_ 15.40  
 INSTRUM spect  
 PROBHD 5 mm DUL 13C-1  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT CDC13  
 NS 256  
 DS 4  
 SWH 24038.461 Hz  
 FIDRES 0.366798 Hz  
 AQ 1.3631988 sec  
 RG 50.8  
 DW 20.800 usec  
 DE 6.00 usec  
 TE 297.2 K  
 D1 2.00000000 sec  
 d11 0.03000000 sec  
 DELTA 1.89999998 sec  
 TD0 1

==== CHANNEL f1 =====  
 NUC1 13C  
 P1 9.15 usec  
 PL1 0.00 dB  
 SFO1 100.6228298 MHz

==== CHANNEL f2 =====  
 CPDPRG2 waltz16  
 NUC2 1H  
 PCPD2 90.00 usec  
 PL12 14.90 dB  
 PL13 14.90 dB  
 PL2 -3.00 dB  
 SFO2 400.1316005 MHz

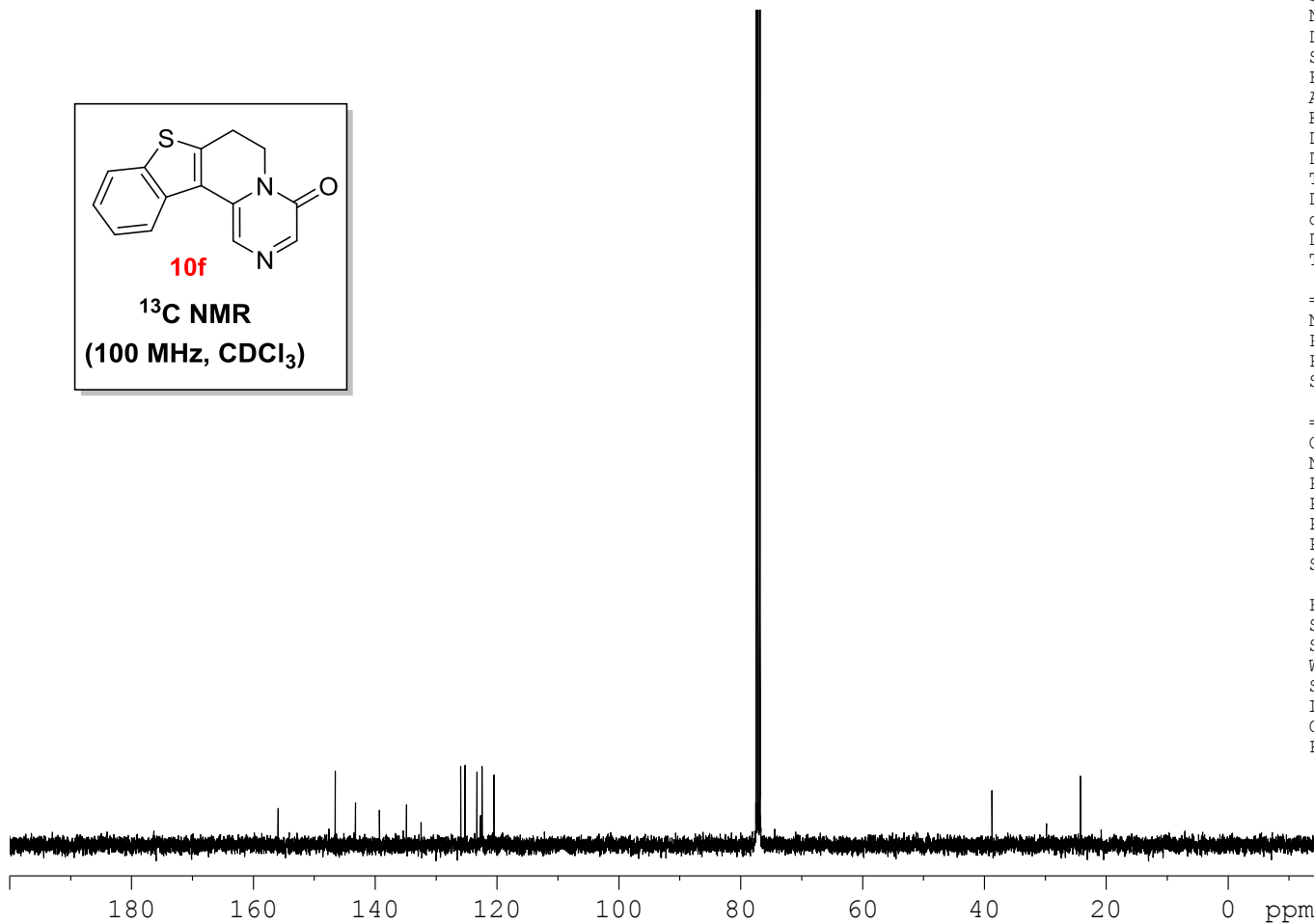
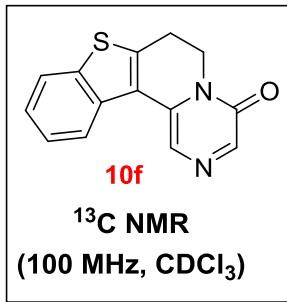
F2 - Processing parameters  
 SI 32768  
 SF 100.6127537 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40

155.92  
 146.58  
 143.28  
 139.33  
 134.88  
 132.49  
 126.00  
 125.28  
 123.33  
 122.75  
 122.49  
 120.53

77.48  
 77.16  
 76.84

38.78

24.25



PROTON CDC13 {D:\CRR} KOPAL 1

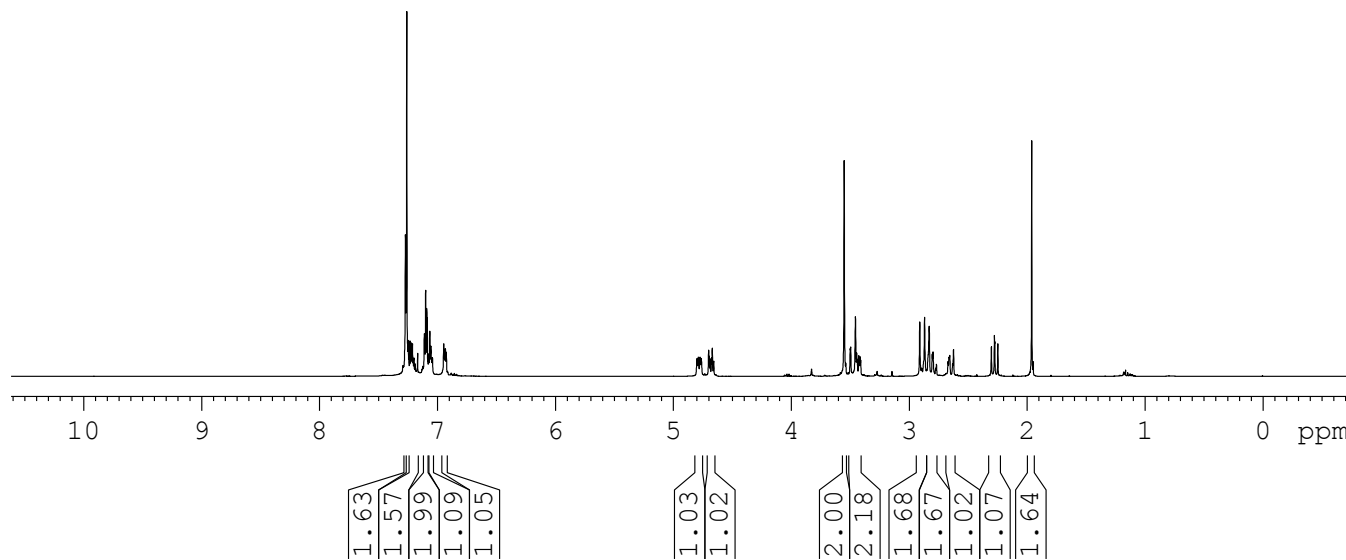
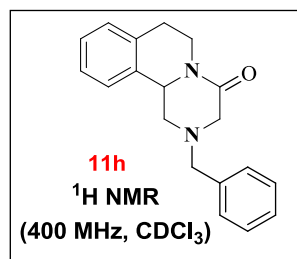
7.271  
7.260  
7.248  
7.243  
7.233  
7.225  
7.222  
7.211  
7.168  
7.111  
7.110  
7.100  
7.091  
7.086  
7.074  
7.065  
7.055  
6.947  
6.933  
6.924  
4.790  
4.776  
4.702  
4.697  
3.553  
3.502  
3.498  
3.457  
3.447  
3.429  
3.418  
2.912  
2.871  
2.832  
2.807  
2.800  
2.664  
2.658  
2.626  
2.305  
2.279  
2.276  
2.250  
1.963

Current Data Parameters  
NAME RS-I-Un-SUB-PZQ-CY-Bn  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20150901  
Time 15.32  
INSTRUM spect  
PROBHD 5 mm DUL 13C-1  
PULPROG zg30  
TD 65536  
SOLVENT CDCl3  
NS 16  
DS 2  
SWH 8223.685 Hz  
FIDRES 0.125483 Hz  
AQ 3.9846397 sec  
RG 57  
DW 60.800 usec  
DE 6.00 usec  
TE 296.5 K  
D1 1.00000000 sec  
TD0 1

==== CHANNEL f1 =====  
NUC1 1H  
P1 11.42 usec  
PL1 -3.00 dB  
SF01 400.1324710 MHz

F2 - Processing parameters  
SI 32768  
SF 400.1300417 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00



C13CPD CDC13 {D:\CRR} KOPAL 1

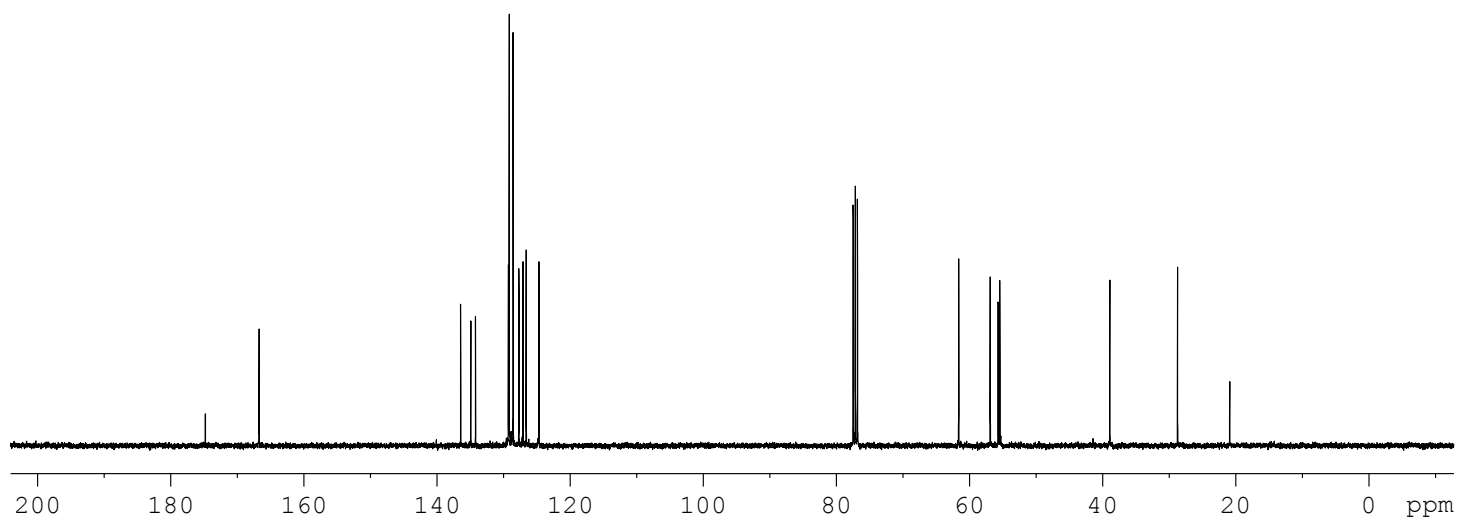
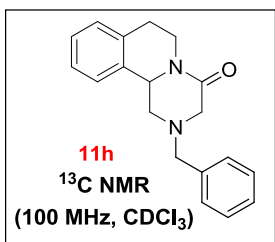
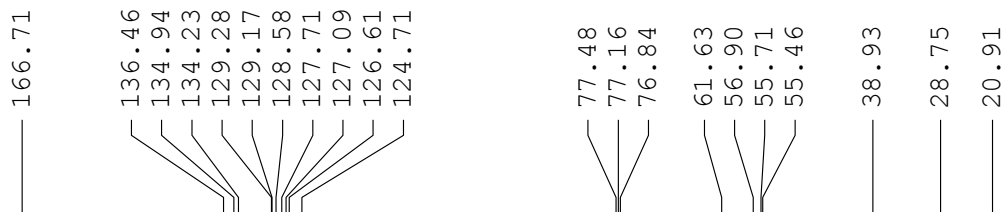
Current Data Parameters  
NAME RS-I-Un-SUB-PZQ-CY-Bn  
EXPNO 2  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20150901  
Time\_ 15.43  
INSTRUM spect  
PROBHD 5 mm DUL 13C-1  
PULPROG zgpg30  
TD 65536  
SOLVENT CDC13  
NS 168  
DS 4  
SWH 24038.461 Hz  
FIDRES 0.366798 Hz  
AQ 1.3631988 sec  
RG 64  
DW 20.800 usec  
DE 6.00 usec  
TE 297.3 K  
D1 2.00000000 sec  
d11 0.03000000 sec  
DELTA 1.89999998 sec  
TD0 1

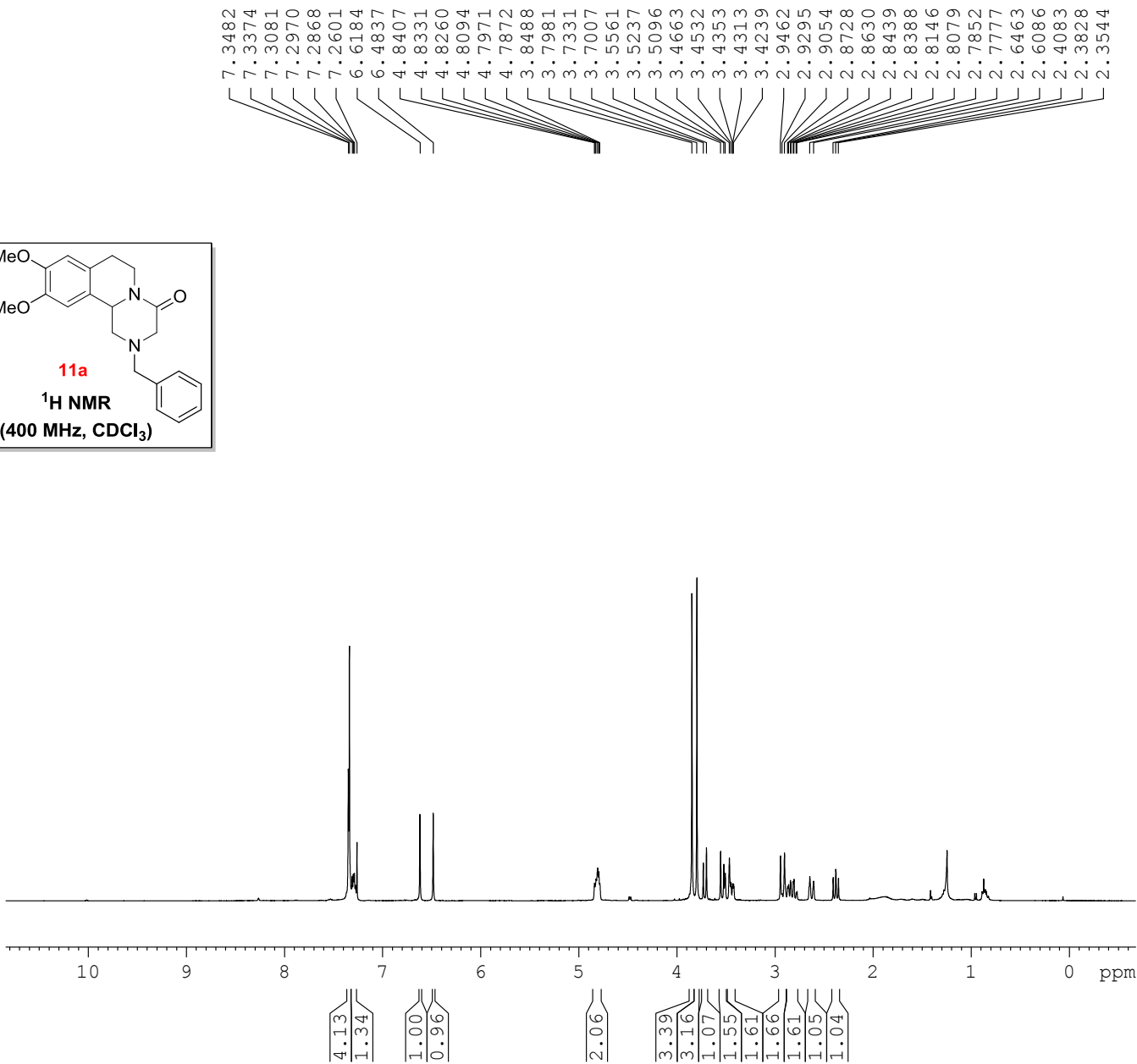
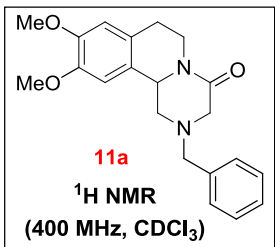
===== CHANNEL f1 =====  
NUC1 13C  
P1 9.15 usec  
PL1 0.00 dB  
SFO1 100.6228298 MHz

===== CHANNEL f2 =====  
CPDPRG2 waltz16  
NUC2 1H  
PCPD2 90.00 usec  
PL12 14.90 dB  
PL13 14.90 dB  
PL2 -3.00 dB  
SFO2 400.1316005 MHz

F2 - Processing parameters  
SI 32768  
SF 100.6127684 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40







Current Data Parameters  
 NAME RS-I-3,4-BN-PZQ-CY  
 EXPNO 1  
 PROCNO 1

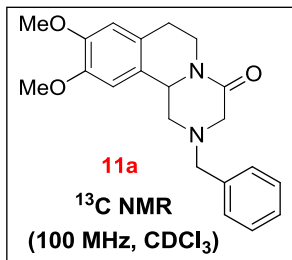
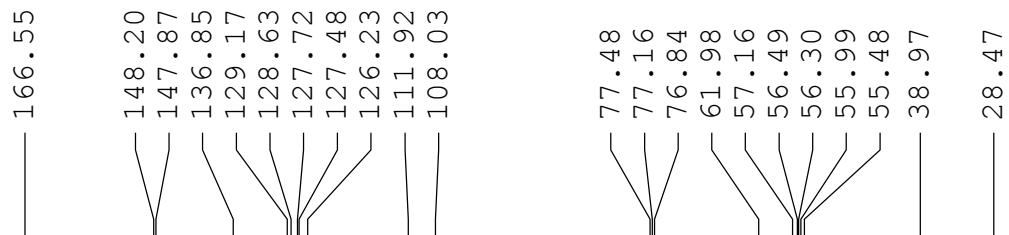
F2 - Acquisition Parameters  
 Date\_ 20150924  
 Time\_ 14.17  
 INSTRUM spect  
 PROBHD 5 mm DUL 13C-1  
 PULPROG zg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 16  
 DS 2  
 SWH 8223.685 Hz  
 FIDRES 0.125483 Hz  
 AQ 3.9846387 sec  
 RG 114  
 DW 60.800 usec  
 DE 6.00 usec  
 TE 294.7 K  
 D1 1.00000000 sec  
 TD0 1

===== CHANNEL f1 =====  
 NUC1 1H  
 P1 11.42 usec  
 PL1 -3.00 dB  
 SFO1 400.1324710 MHz

F2 - Processing parameters  
 SI 32768  
 SF 400.1300050 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00

Current Data Parameters  
 NAME RS-I-3,4-BN-PZQ-CY  
 EXPNO 2  
 PROCNO 1

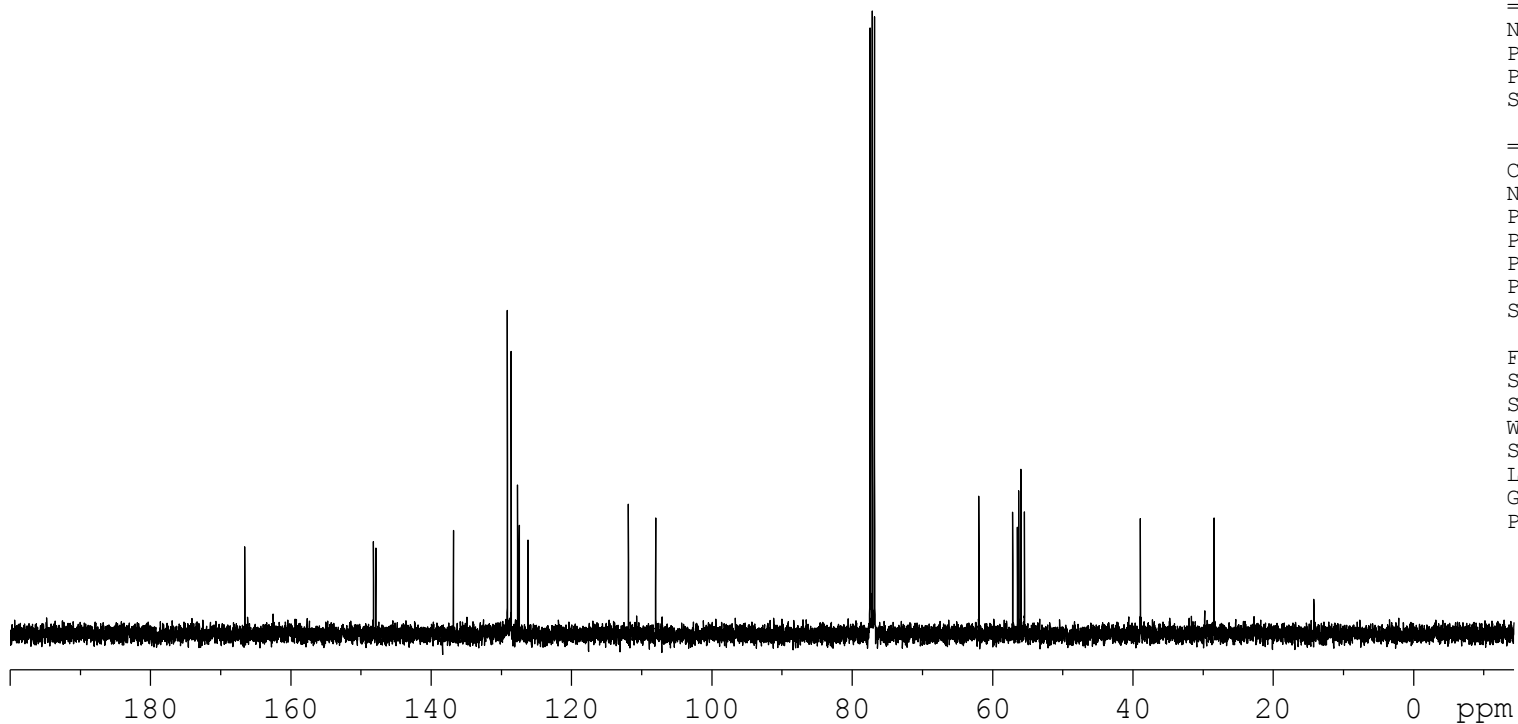
F2 - Acquisition Parameters  
 Date\_ 20150924  
 Time\_ 14.36  
 INSTRUM spect  
 PROBHD 5 mm DUL 13C-1  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT CDC13  
 NS 65  
 DS 4  
 SWH 24038.461 Hz  
 FIDRES 0.366798 Hz  
 AQ 1.3631988 sec  
 RG 57  
 DW 20.800 usec  
 DE 6.00 usec  
 TE 295.5 K  
 D1 2.00000000 sec  
 d11 0.03000000 sec  
 DELTA 1.89999998 sec  
 TD0 1



==== CHANNEL f1 =====  
 NUC1 13C  
 P1 9.15 usec  
 PL1 0.00 dB  
 SFO1 100.6228298 MHz

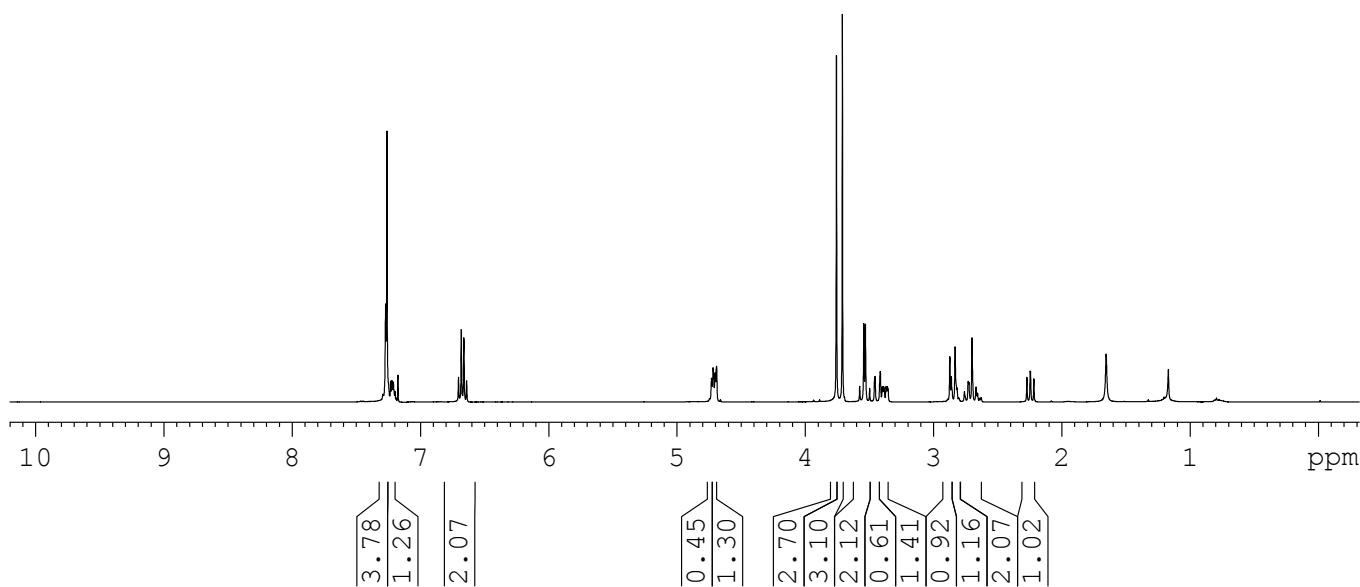
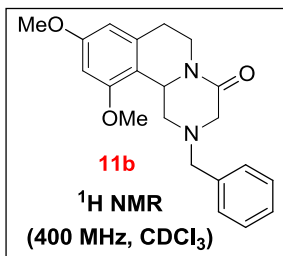
==== CHANNEL f2 =====  
 CPDPRG2 waltz16  
 NUC2 1H  
 PCPD2 90.00 usec  
 PL12 14.90 dB  
 PL13 14.90 dB  
 PL2 -3.00 dB  
 SFO2 400.1316005 MHz

F2 - Processing parameters  
 SI 32768  
 SF 100.6127580 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40



PROTON CDC13 {D:\CRR} KOPAL 1

7.283  
7.273  
7.260  
7.247  
7.236  
7.225  
7.190  
6.718  
6.696  
6.676  
6.654  
4.745  
4.733  
4.716  
4.705  
3.771  
3.725  
3.590  
3.558  
3.545  
3.513  
3.470  
3.429  
3.414  
3.410  
3.402  
3.398  
3.385  
3.380  
3.373  
3.369  
2.887  
2.876  
2.846  
2.831  
2.744  
2.738  
2.714  
2.683  
2.286



Current Data Parameters  
NAME RS-I-3,5-BN-PZQ-CY  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20151006  
Time 22.05  
INSTRUM spect  
PROBHD 5 mm DUL 13C-1  
PULPROG zg30  
TD 65536  
SOLVENT CDC13  
NS 16  
DS 2  
SWH 8223.685 Hz  
FIDRES 0.125483 Hz  
AQ 3.9846387 sec  
RG 161  
DW 60.800 usec  
DE 6.00 usec  
TE 296.4 K  
D1 1.0000000 sec  
TD0 1

==== CHANNEL f1 =====  
NUC1 1H  
P1 11.42 usec  
PL1 -3.00 dB  
SFO1 400.1324710 MHz

F2 - Processing parameters  
SI 32768  
SF 400.1300382 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00

Current Data Parameters  
 NAME RS-I-3,5-BN-PZQ-CY  
 EXPNO 2  
 PROCNO 1

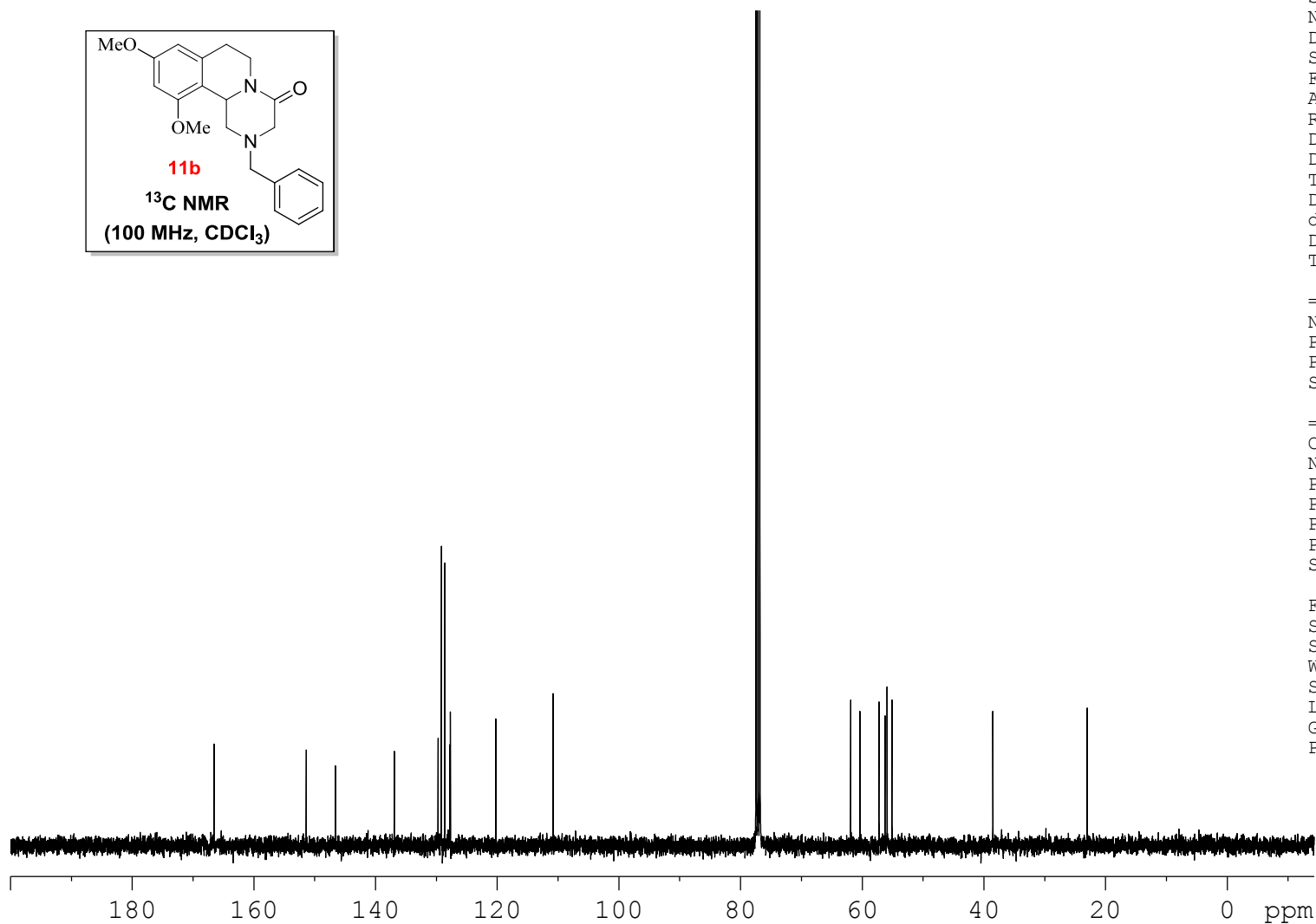
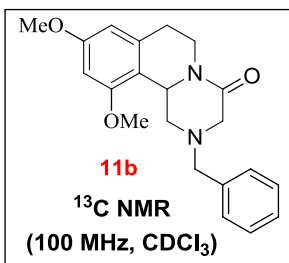
F2 - Acquisition Parameters  
 Date\_ 20151006  
 Time\_ 22.15  
 INSTRUM spect  
 PROBHD 5 mm DUL 13C-1  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT CDC13  
 NS 198  
 DS 4  
 SWH 24038.461 Hz  
 FIDRES 0.366798 Hz  
 AQ 1.3631988 sec  
 RG 71.8  
 DW 20.800 usec  
 DE 6.00 usec  
 TE 297.0 K  
 D1 2.00000000 sec  
 d11 0.03000000 sec  
 DELTA 1.89999998 sec  
 TDO 1

==== CHANNEL f1 =====  
 NUC1 13C  
 P1 9.15 usec  
 PL1 0.00 dB  
 SFO1 100.6228298 MHz

==== CHANNEL f2 =====  
 CPDPRG2 waltz16  
 NUC2 1H  
 PCPD2 90.00 usec  
 PL12 14.90 dB  
 PL13 14.90 dB  
 PL2 -3.00 dB  
 SFO2 400.1316005 MHz

F2 - Processing parameters  
 SI 32768  
 SF 100.6127558 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40

166.53  
 151.36  
 146.57  
 136.89  
 129.74  
 129.20  
 128.65  
 127.81  
 127.72  
 120.26  
 110.83  
 77.48  
 77.16  
 76.84  
 61.92  
 60.40  
 57.27  
 56.28  
 55.95  
 55.14  
 38.56  
 23.06



PROTON CDC13 {D:\CRR} KOPAL 1

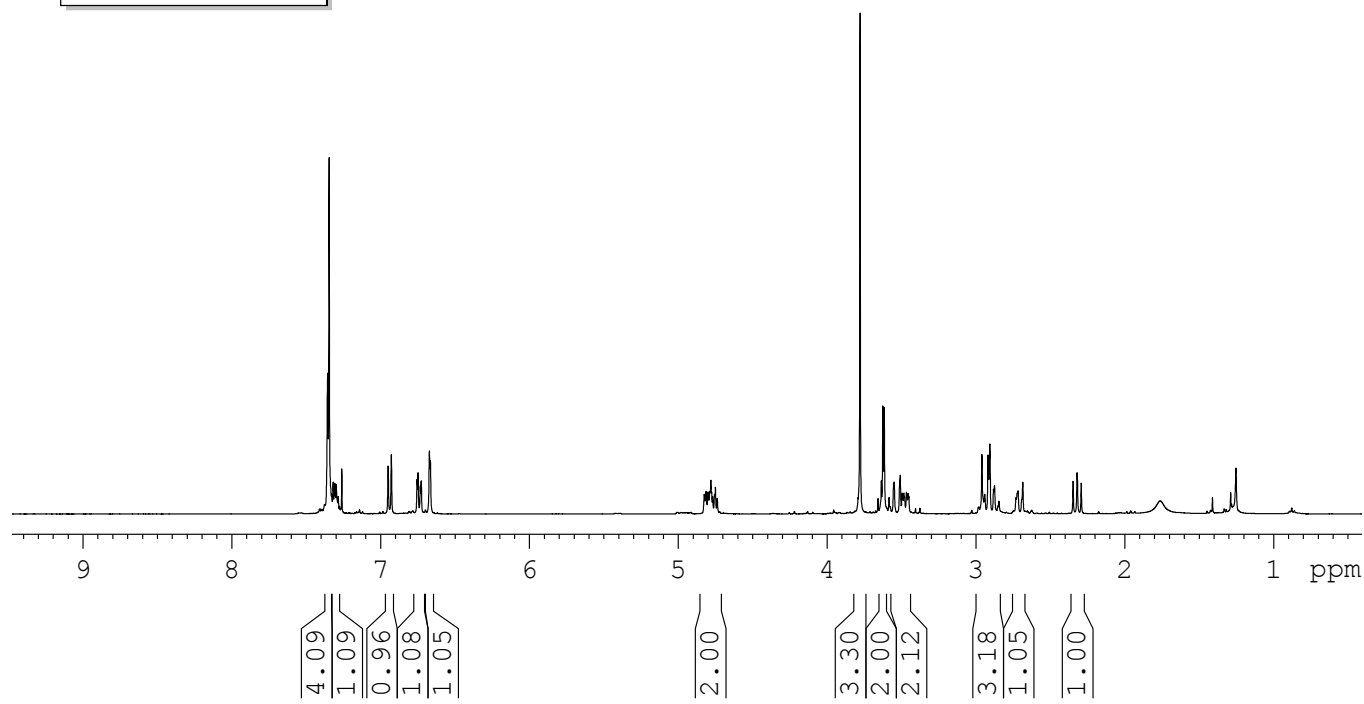
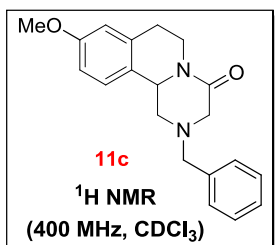
7.356  
7.345  
7.318  
7.311  
7.307  
7.297  
7.260  
6.951  
6.929  
6.756  
6.750  
6.734  
6.728  
6.673  
6.667  
4.815  
4.801  
4.789  
4.782  
4.777  
4.751  
3.780  
3.627  
3.617  
3.554  
3.551  
3.510  
3.497  
3.486  
3.468  
3.463  
3.456  
2.961  
2.920  
2.908  
2.882  
2.876  
2.724  
2.718  
2.686  
2.348  
2.322  
2.319  
2.293

Current Data Parameters  
NAME RS-I-3-BN-PZQ-CY  
EXPNO 3  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20150927  
Time\_ 15.18  
INSTRUM spect  
PROBHD 5 mm DUL 13C-1  
PULPROG zg30  
TD 65536  
SOLVENT CDC13  
NS 16  
DS 2  
SWH 8223.685 Hz  
FIDRES 0.125483 Hz  
AQ 3.9846387 sec  
RG 181  
DW 60.800 usec  
DE 6.00 usec  
TE 294.5 K  
D1 1.00000000 sec  
TD0 1

==== CHANNEL f1 =====  
NUC1 1H  
P1 11.42 usec  
PL1 -3.00 dB  
SFO1 400.1324710 MHz

F2 - Processing parameters  
SI 32768  
SF 400.1300050 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00



Current Data Parameters  
 NAME RS-I-3-BN-PZQ-CY  
 EXPNO 4  
 PROCNO 1

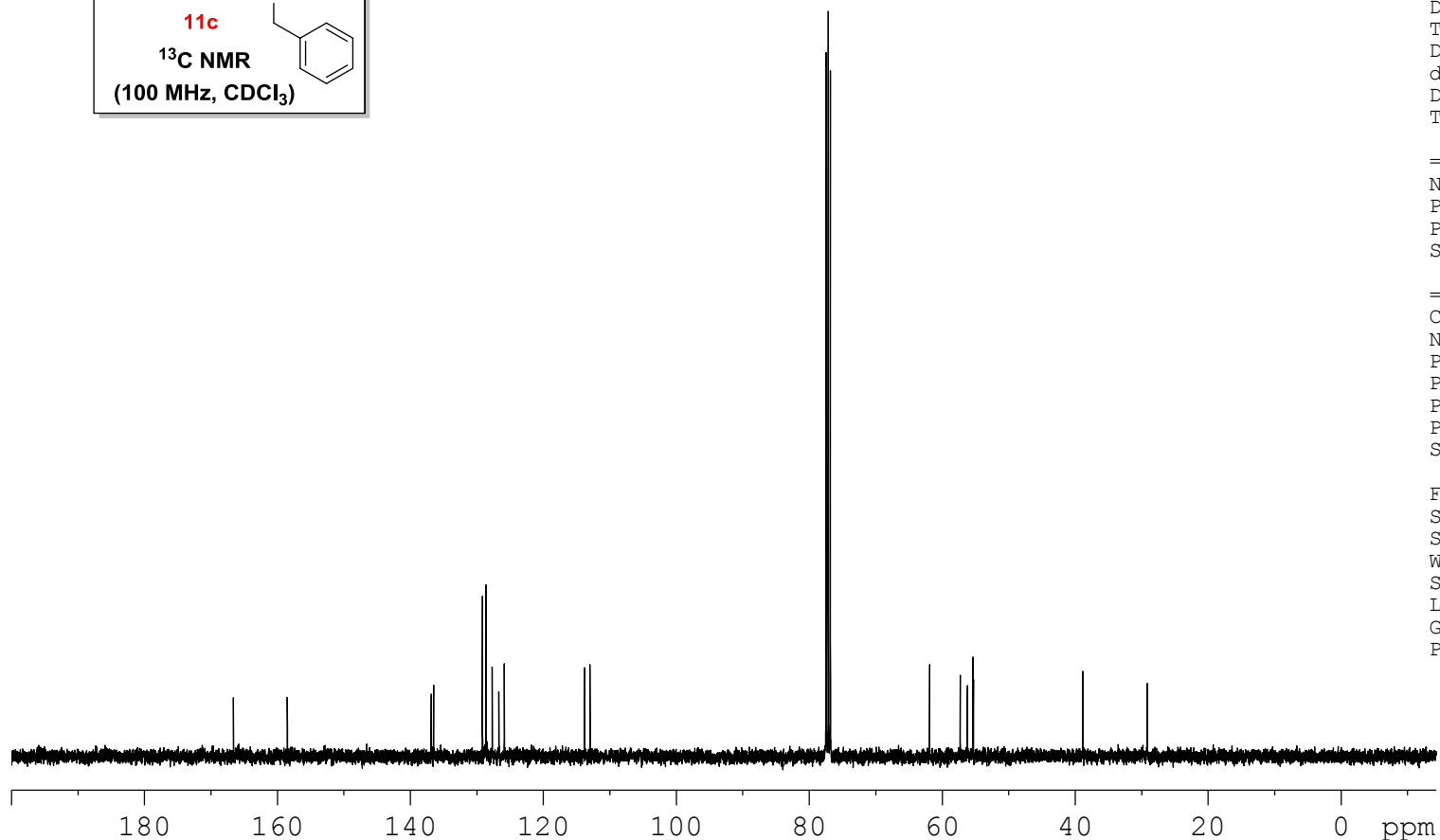
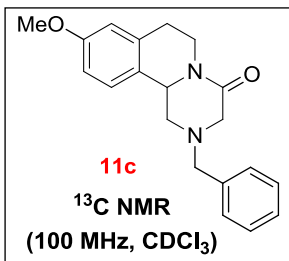
F2 - Acquisition Parameters  
 Date\_ 20150927  
 Time\_ 15.26  
 INSTRUM spect  
 PROBHD 5 mm DUL 13C-1  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 137  
 DS 4  
 SWH 24038.461 Hz  
 FIDRES 0.366798 Hz  
 AQ 1.3631988 sec  
 RG 64  
 DW 20.800 usec  
 DE 6.00 usec  
 TE 295.2 K  
 D1 2.00000000 sec  
 d11 0.03000000 sec  
 DELTA 1.89999998 sec  
 TDO 1

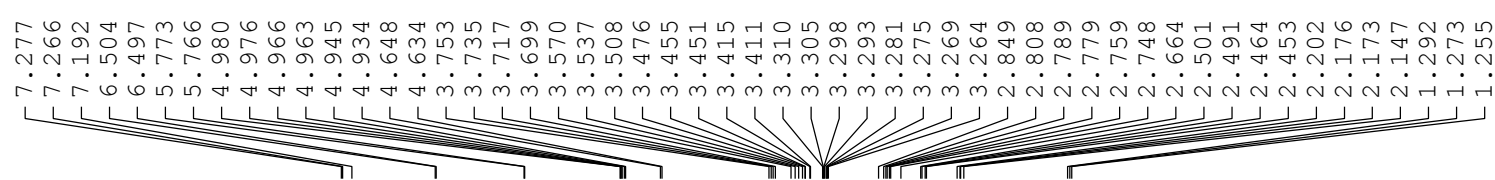
==== CHANNEL f1 =====  
 NUC1 13C  
 P1 9.15 usec  
 PL1 0.00 dB  
 SFO1 100.6228298 MHz

==== CHANNEL f2 =====  
 CPDPRG2 waltz16  
 NUC2 1H  
 PCPD2 90.00 usec  
 PL12 14.90 dB  
 PL13 14.90 dB  
 PL2 -3.00 dB  
 SFO2 400.1316005 MHz

F2 - Processing parameters  
 SI 32768  
 SF 100.6127551 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40

166.62  
 158.49  
 136.89  
 136.54  
 129.20  
 128.66  
 127.74  
 126.73  
 125.92  
 113.81  
 113.01  
 77.48  
 77.16  
 76.85  
 61.92  
 57.31  
 56.24  
 55.41  
 55.32  
 38.86  
 29.18



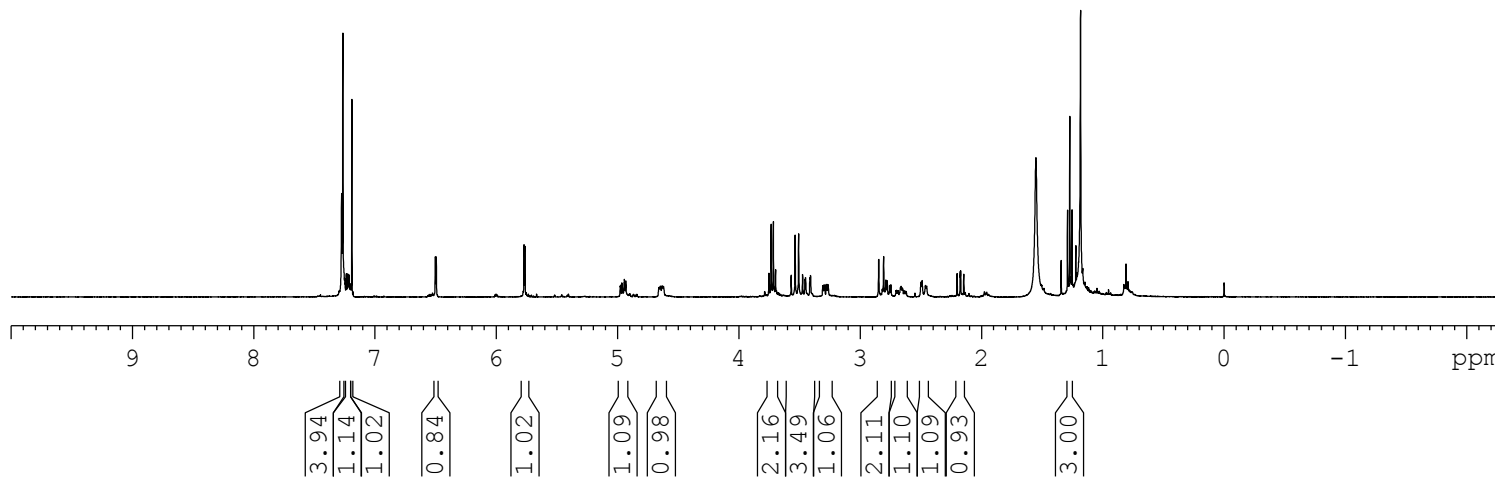
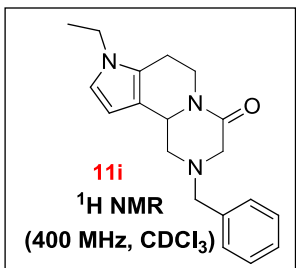


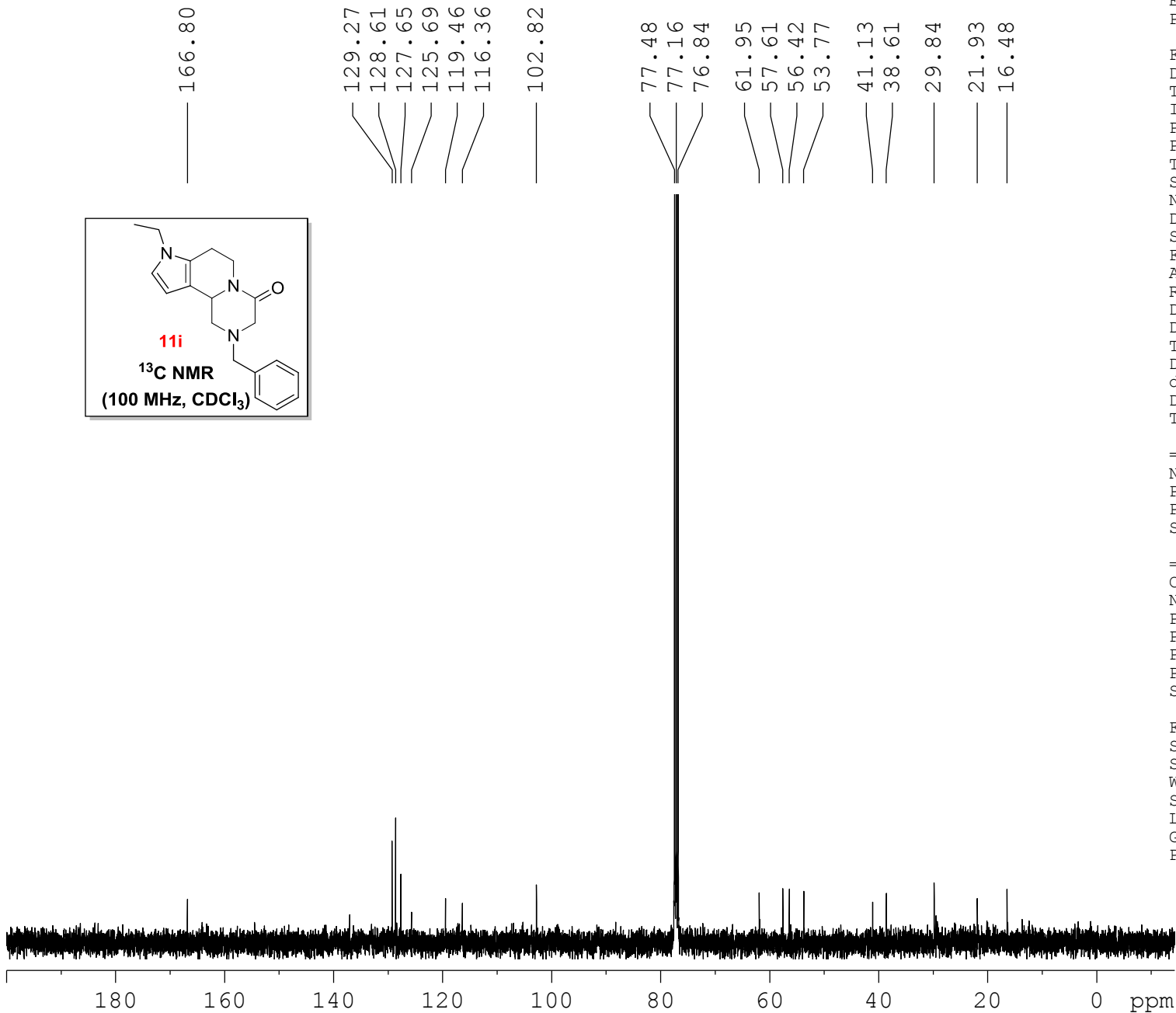
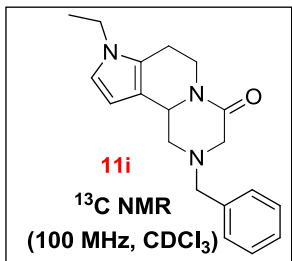
Current Data Parameters  
 NAME RS-I-PY-CY  
 EXPNO 2  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20151002  
 Time\_ 17.59  
 INSTRUM spect  
 PROBHD 5 mm DUL 13C-1  
 PULPROG zg30  
 TD 65536  
 SOLVENT CDC13  
 NS 16  
 DS 2  
 SWH 8223.685 Hz  
 FIDRES 0.125483 Hz  
 AQ 3.9846387 sec  
 RG 256  
 DW 60.800 usec  
 DE 6.00 usec  
 TE 294.6 K  
 D1 1.00000000 sec  
 TD0 1

==== CHANNEL f1 =====  
 NUC1 1H  
 P1 11.42 usec  
 PL1 -3.00 dB  
 SFO1 400.1324710 MHz

F2 - Processing parameters  
 SI 32768  
 SF 400.1300323 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00





Current Data Parameters  
 NAME RS-I-PY-CY  
 EXPNO 3  
 PROCNO 1

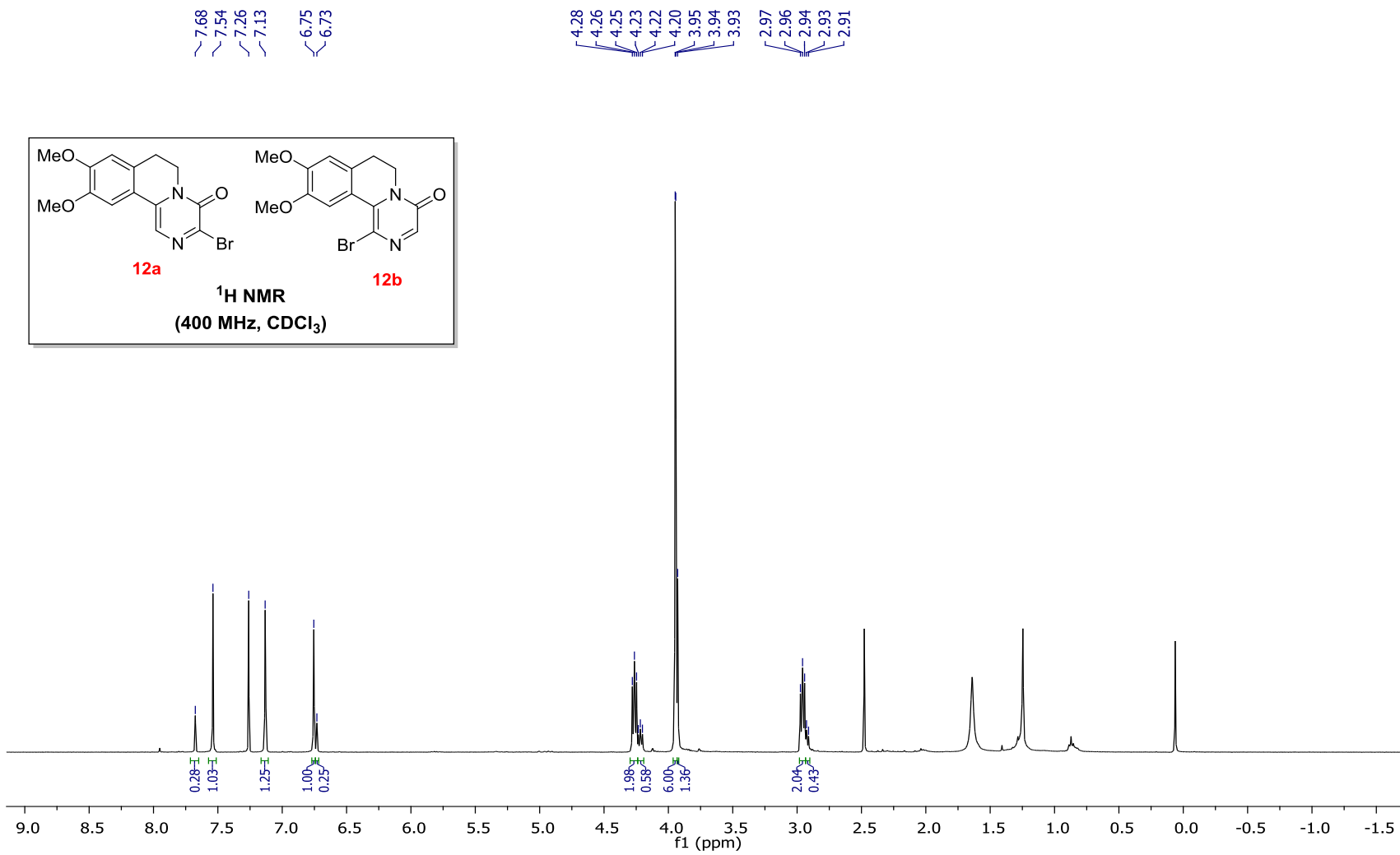
F2 - Acquisition Parameters  
 Date 20151002  
 Time 18.29  
 INSTRUM spect  
 PROBHD 5 mm DUL 13C-1  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT CDC13  
 NS 512  
 DS 4  
 SWH 24038.461 Hz  
 FIDRES 0.366798 Hz  
 AQ 1.3631988 sec  
 RG 57  
 DW 20.800 usec  
 DE 6.00 usec  
 TE 295.1 K  
 D1 2.00000000 sec  
 d11 0.03000000 sec  
 DELTA 1.89999998 sec  
 TD0 1

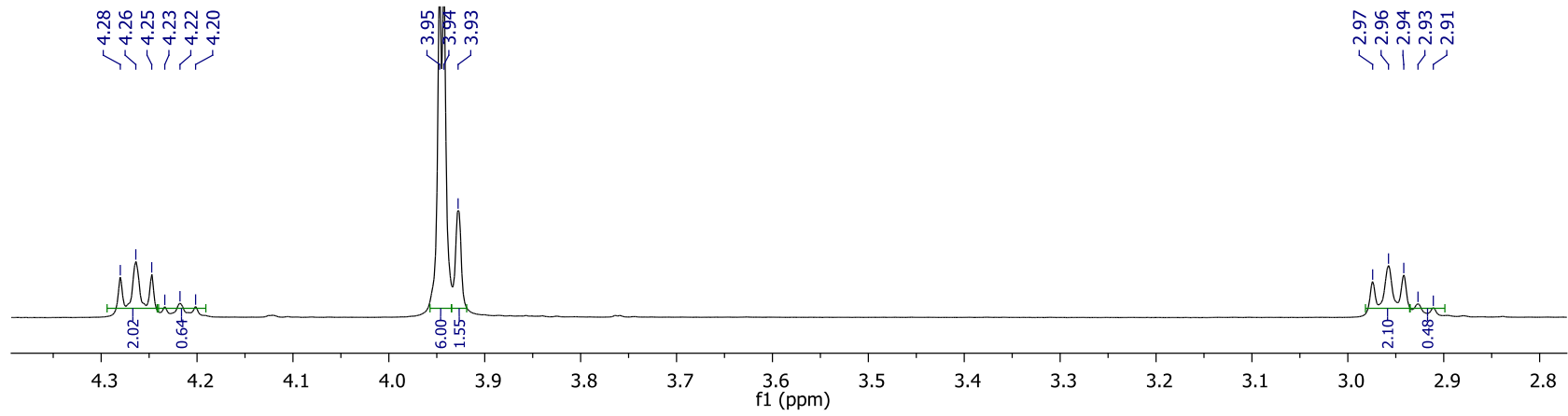
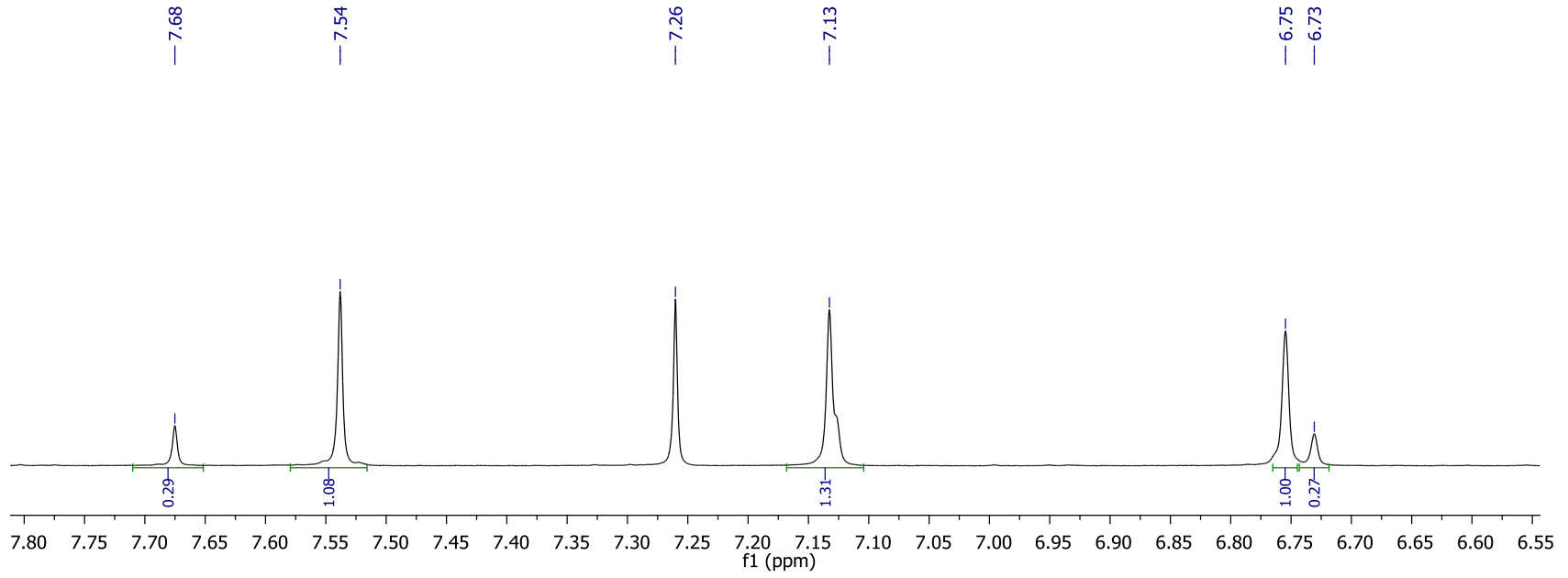
==== CHANNEL f1 =====  
 NUC1 13C  
 P1 9.15 usec  
 PL1 0.00 dB  
 SFO1 100.6228298 MHz

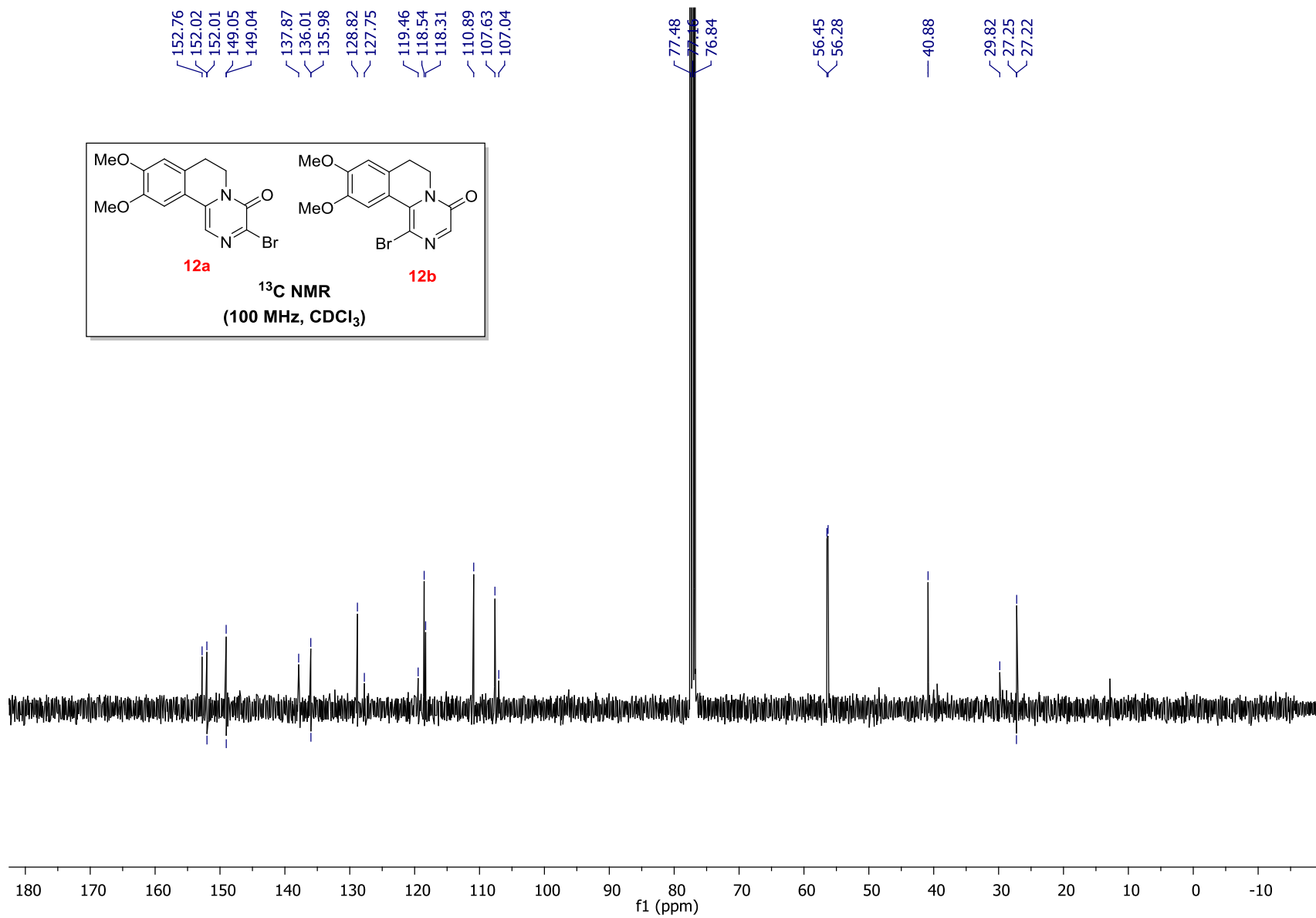
==== CHANNEL f2 =====  
 CPDPRG2 waltz16  
 NUC2 1H  
 PCPD2 90.00 usec  
 PL12 14.90 dB  
 PL13 14.90 dB  
 PL2 -3.00 dB  
 SFO2 400.1316005 MHz

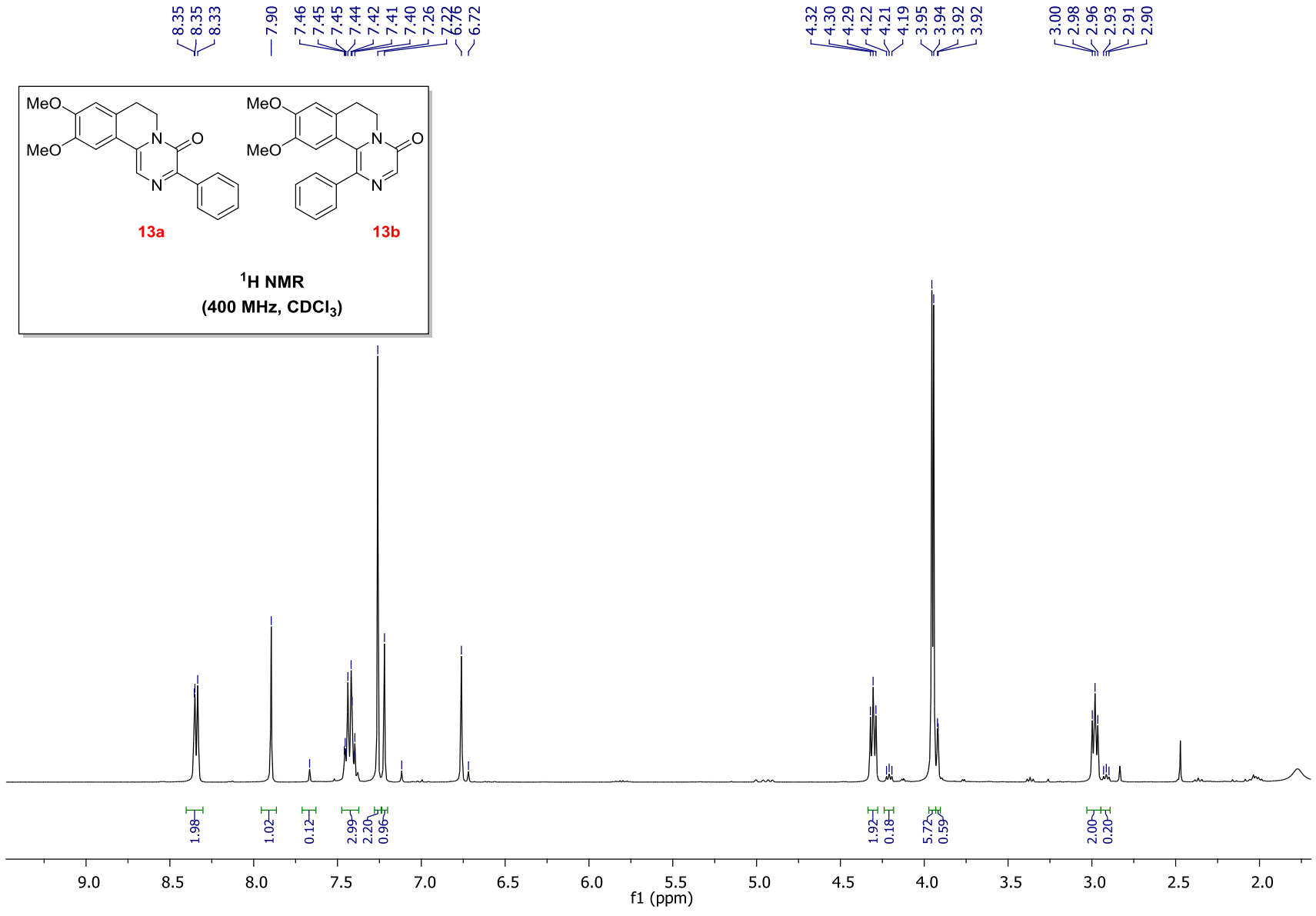
F2 - Processing parameters  
 SI 32768  
 SF 100.6127539 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40

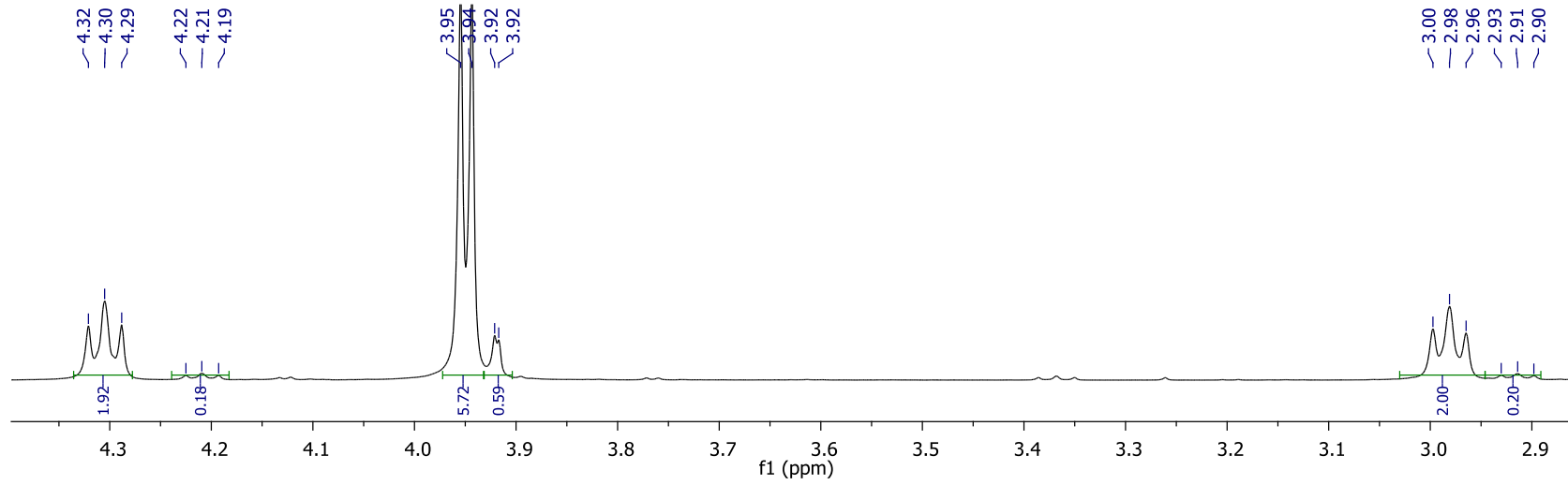
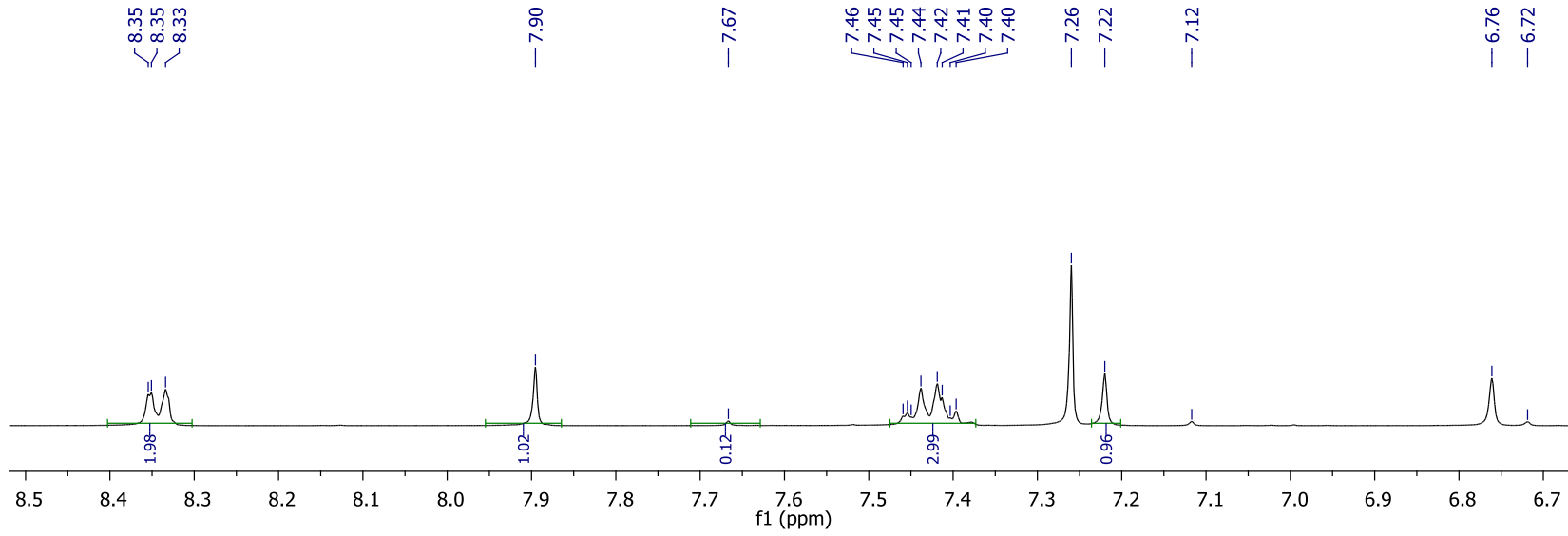




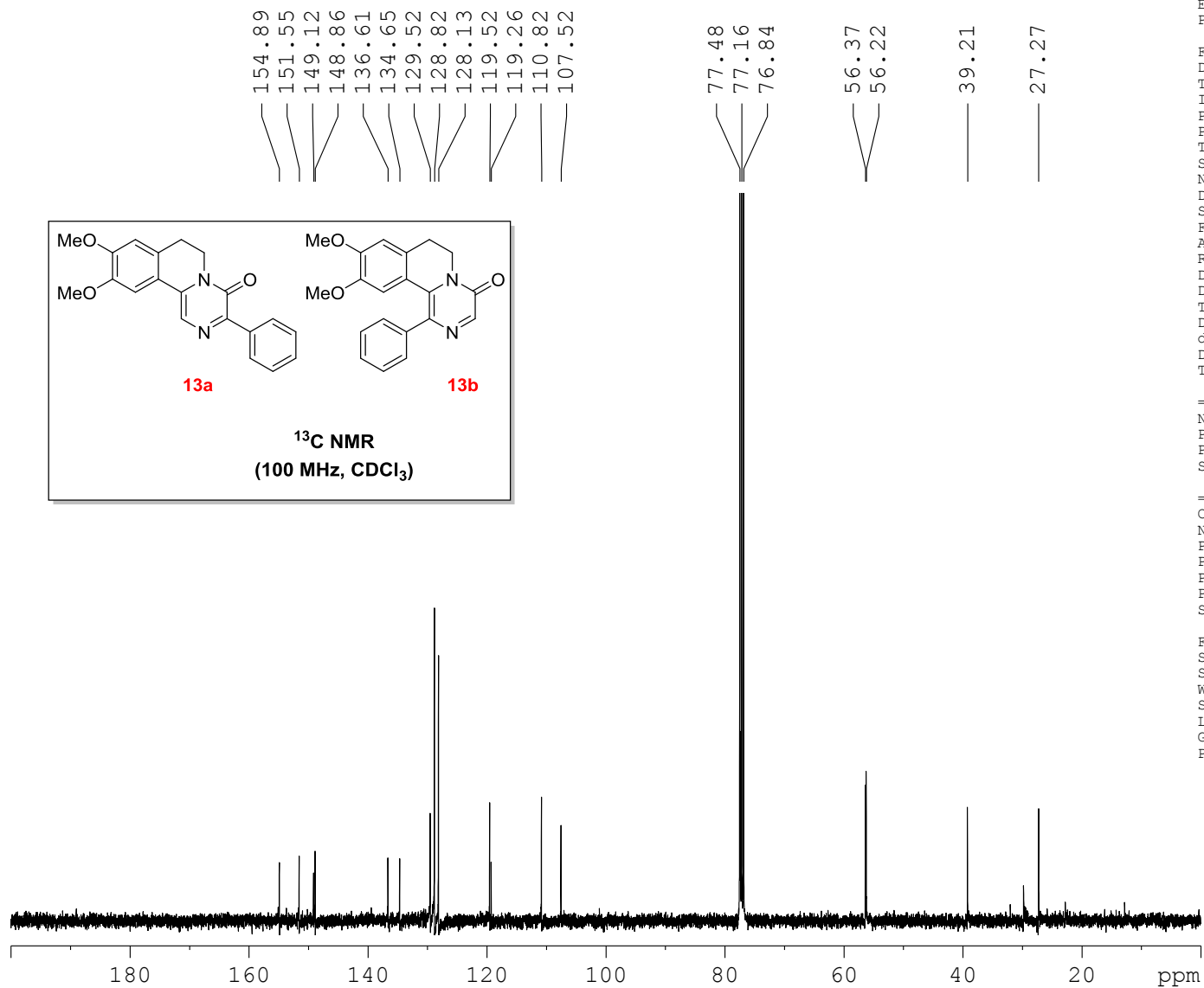








C13CPD CDCl3 {D:\CRR} KOPAL 1



Current Data Parameters  
NAME RS-I-3,4-PZQ-CY-2-COUP  
EXPNO 2  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20160227  
Time 20.08  
INSTRUM spect  
PROBHD 5 mm DUL 13C-1  
PULPROG zgpg30  
TD 65536  
SOLVENT CDCl3  
NS 264  
DS 4  
SWH 24038.461 Hz  
FIDRES 0.366798 Hz  
AQ 1.3631988 sec  
RG 28.5  
DW 20.800 usec  
DE 6.00 usec  
TE 295.5 K  
D1 2.0000000 sec  
d11 0.03000000 sec  
DELTA 1.89999998 sec  
TD0 1

=====  
CHANNEL f1  
NUC1 13C  
P1 9.15 usec  
PL1 0.00 dB  
SFO1 100.6228298 MHz

=====  
CHANNEL f2  
CPDPRG2 waltz16  
NUC2 1H  
PCPD2 90.00 usec  
PL12 14.90 dB  
PL13 14.90 dB  
PL2 -3.00 dB  
SFO2 400.1316005 MHz

F2 - Processing parameters  
SI 32768  
SF 100.6127569 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40

