Visible Light Mediated sp^3 C-H Bond Functionalization of N-Aryl-1,2,3,4-tetrahydroisoquinolines via Ugi-type Three Components Reaction

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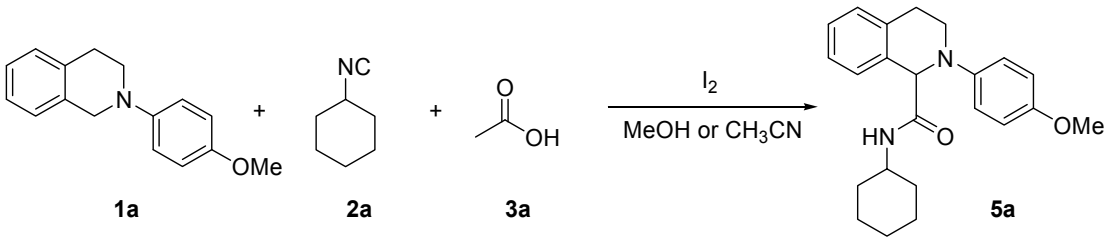
Supporting Information

1. General information
2. General procedure for iodine catalyzed Ugi-type reaction
3. Characterization data of compounds **4a-y**
4. Copies of ^{1}H-NMR and ^{13}C-NMR Spectra

1. General information

^{1}H and ^{13}C NMR spectra were recorded on Brucker AVANCE 400MHz spectrameter (400 MHz for ^{1}H or 100 MHz for ^{13}C, respectively). NMR chemical shifts are expressed in δ values with reference to the residual solvents or TMS as internal standard. IR spectra were taken on an FTIR spectrophotometer. Mass spectra (MS) were measured by the +ESI method. Melting points were determined in open capillary tubes and are uncorrected. The reaction mixture was checked by thin-layer chromatography on silica gel plates (60 F-254) using UV light, or 7% ethanolic phosphomolybdic acid and heating as the visualizing methods. Flash column chromatography over silica gel was used for purification. Yields refer to chromatographically and spectroscopically (^{1}H-NMR) homogeneous materials. Reagents were obtained commercially and used as received.

2. General procedure for iodine catalyzed Ugi-type reaction

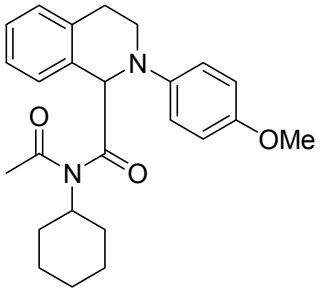


1a **2a** **3a** **5a**

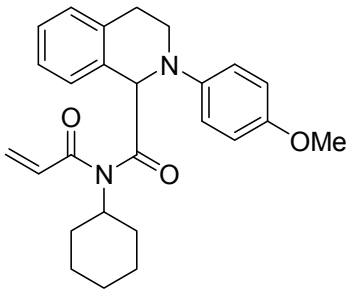
To a 10 mL reaction vial was charged with magnetic stir bar, acetonitrile (2 mL), N-aryl-1,2,3,4-tetrahydroisoquinoline (0.25 mmol), acids (0.3 mmol), isocyanide (0.3 mmol), and I_2 (0.025 mmol) sequentially. After stirring at room temperature for 3 days, the reaction mixture was directly purified by column chromatography on silica gel to provide **5a** as a pale yellowish solid.

1-cyclohexylaminocarbonyl-N-(4-methoxyphenyl)-1,2,3,4-tetrahydroisoquinoline (5a): A pale yellowish solid. R_f=0.55 (25% EtOAc–PE). IR (KBr) 3305, 2929, 1658, 1511, 1245, 1189, 1038, 816, 743 cm^{-1}. ^{1}H NMR (400MHz, $CDCl_3$) δ ppm 7.59 (dd, *J*=8.4, 1.6 Hz, 1H), 7.24–7.19 (m, 2H), 7.13 (dd, *J*=6.8, 2.4Hz, 1H), 6.91–6.85 (m, 1H), 6.90 (d, *J*=9.2 Hz, 2H), 6.86 (d, *J*=9.2 Hz, 2H), 3.77 (s, 3H), 3.75–3.65 (m, 2H), 3.27–3.21 (m, 1H), 3.05–2.98 (m, 1H), 2.94–2.89 (m, 1H), 1.80–1.69 (m, 2H), 1.61–1.51 (m, 3H), 1.32–1.23 (m, 2H), 1.12–0.97 (m, 3H). ^{13}C NMR (100MHz, $CDCl_3$) δ ppm 171.3, 153.7, 143.8, 134.3, 132.8, 128.7, 127.7, 127.2, 126.5, 117.2(×2), 114.6(×2), 66.1, 55.6, 48.0, 46.5, 32.9, 32.7, 28.9, 25.4, 24.7, 24.6. MS (+ESI): *m*/*z* (%) = 365 (100) $[M+H]^+$. HRMS (+CI) calcd for $C_{23}H_{29}N_2O_2$ 365.2229 $[M+H]^+$, found 365.2230.

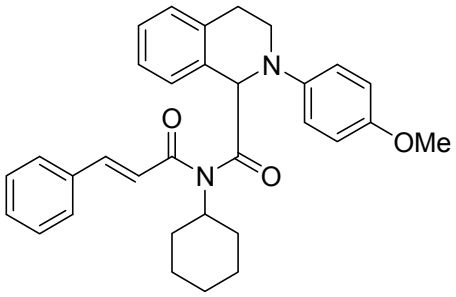
3. Characterization data of compounds 4a-y.



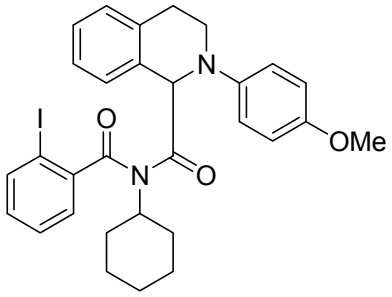
2-(4-methoxylphenyl)-N-acetyl-N-cyclohexyl-1,2,3,4-tetrahydroisoquinoline-1-carboxamide (4a): (96 mg, 95%). A pale brownish oil. R_f=0.49 (25% EtOAc–PE). IR (film) 2932, 1679, 1510, 1244, 1039, 754 cm^{-1}. ^1H NMR (400MHz, $CDCl_3$) δ ppm 7.39–7.36 (m, 1H), 7.28–7.23 (m, 2H), 7.18–7.15 (m, 1H), 6.98 (d, *J*=9.2 Hz, 2H), 6.85 (d, *J*=9.2 Hz, 2H), 5.76 (s, 1H), 3.80–3.72 (m, 1H), 3.78 (s, 3H), 3.59 –3.53 (m, 1H), 3.49–3.43 (m, 1H), 2.97–2.85 (m, 2H), 2.13 (s, 3H), 1.97–1.87 (m, 2H), 1.76–1.65 (m, 2H), 1.56–1.53 (m, 1H), 1.44–1.36 (m, 2H), 1.19–1.06 (m, 2H), 1.00–0.93 (m, 1H). ^{13}C NMR (100MHz, $CDCl_3$) δ ppm 176.1, 174.5, 154.2, 142.7, 134.8, 132.0, 128.9, 127.9 127.6, 126.2, 119.1(×2), 114.6(×2), 64.2, 58.5, 55.6, 46.7, 30.1, 30.0, 27.1, 26.6, 26.5, 26.4, 25.1. MS (+ESI): *m*/*z* (%) = 407 (100) $[M+H]^+$. HRMS (+EI) calcd for $C_{25}H_{28}N_2O_3$ 404.2100 $[M-H_2]^+$, found 404.2104.



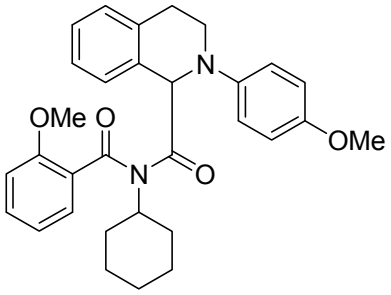
2-(4-methoxylphenyl)-N-acrylyl-N-cyclohexyl-1,2,3,4-tetrahydroisoquinoline-1-carboxamide (4b): (71 mg, 68%). 122-124 ^oC (from EtOAc-hexance). A pale yellow crystalline solid. R_f=0.76 (25% EtOAc–PE). IR (KBr) 2950, 1694, 1659, 1609, 1511, 1253, 1204, 1038, 766 cm^{-1}. ^1H NMR (400MHz, $CDCl_3$) δ ppm 7.38 (d, *J*=7.2 Hz, 1H), 7.26–7.22 (m, 2H), 7.06 (d, *J*=7.2 Hz, 1H), 6.81 (d, *J*=9.2 Hz, 2H), 6.75 (d, *J*=9.2 Hz, 2H), 6.02 (dd, *J*=17.2, 10.4 Hz, 1H), 5.86 (dd, *J*=17.2, 1.2 Hz, 1H), 5.52 (dd, *J*=10.4, 1.2 Hz, 1H), 5.11 (s, 1H), 4.12–4.06 (m, 1H), 3.73 (s, 3H), 3.48–3.43 (m, 1H), 3.29–3.22 (m, 1H), 2.75–2.68 (m, 1H), 2.65–2.59 (m, 1H), 2.05–1.95 (m, 1H), 1.80–1.73 (m, 4H), 1.59–1.52 (m, 2H), 1.27–1.08 (m, 3H). ^{13}C NMR (100MHz, $CDCl_3$) δ ppm 173.4, 168.9, 154.8, 141.0, 135.0, 134.3, 131.5, 129.7, 128.9, 127.5, 126.2, 126.0, 120.0 (×2), 114.4 (×2), 61.9, 57.4, 55.4, 46.0, 31.4, 29.2, 26.3, 26.3, 25.3, 25.2. MS (+ESI): *m*/*z* (%) = 419 (100) $[M+H]^+$. Found: C, 74.37; H, 7.30; N, 6.50. Calc. for $C_{26}H_{30}N_2O_3$: C, 74.61; H, 7.22; N, 6.69%.



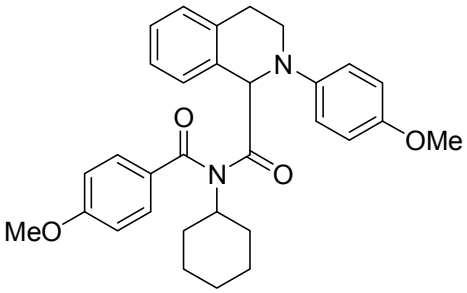
2-(4-methoxylphenyl)-N-*trans*-cinnamoyl-N-cyclohexyl-1,2,3,4-tetrahydroisoquinoline-1-carboxamide (**4c**)**:** (104 mg, 84%). A yellowish amorphous solid. R_f=0.44 (25% EtOAc–PE). IR (KBr) 2930, 1690, 1654, 1620, 1509, 1243, 1134, 1038, 760 cm^{-1}. ^1H NMR (400MHz, $CDCl_3$) δ ppm 7.39 (d, *J*=7.2 Hz, 1H), 7.34–7.28 (m, 3H), 7.23–7.17 (m, 4H), 7.05 (d, *J*=7.2 Hz, 1H), 6.78 (d, *J*=8.8 Hz, 2H), 6.70 (d, *J*=8.8 Hz, 2H), 6.32 (d, *J*=16.0 Hz, 1H), 4.18–4.11 (m, 1H), 3.68 (s, 3H), 3.52–3.47 (m, 1H), 3.37–3.30 (m, 1H), 2.75–2.71 (m, 1H), 2.68–2.63 (m, 1H), 2.01–1.95 (m, 1H), 1.84–1.73 (m, 4H), 1.60–1.59 (m, 2H), 1.27–1.09 (m, 3H). ^{13}C NMR (100MHz, $CDCl_3$) δ ppm 173.4, 169.3, 154.8, 141.8, 141.2, 134.4, 134.3, 131.6, 130.1, 129.4, 128.9, 128.8 (×2), 128.0 (×2), 127.4, 126.0, 125.0, 119.9 (×2), 114.4 (×2), 62.2, 57.4, 55.5, 46.2, 31.4, 29.6, 26.4, 26.3, 25.6, 25.3. MS (+ESI): *m*/*z* (%) = 495 (100) $[M+H]^+$. HRMS (+EI) calcd for $C_{32}H_{34}N_2O_3$ 494.2569 $[M^+]$, found 494.2584.



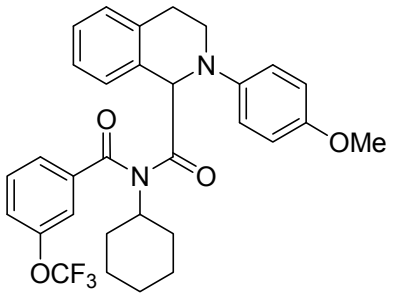
2-(4-methoxylphenyl)-N-(2-iodobenzoyl)-N-cyclohexyl-1,2,3,4-tetrahydroisoquinoline-1-carboxamide (**4d**): (113 mg, 76%). 108-110 ^oC (from EtOAc-hexance). A pale yellowish solid. R_f=0.77 (25% EtOAc–PE). IR (KBr) 2925, 1681, 1666, 1510, 1452, 1243, 1037, 743 cm^{-1}. ^1H NMR (400MHz, $CDCl_3$) δ ppm 7.85 (d, *J*=7.6 Hz, 1H), 7.45–7.43 (m, 1H), 7.23–7.20 (m, 3H), 7.13–7.11 (m, 1H), 7.05 (ddd, *J*=7.6, 7.6, 0.8 Hz, 1H), 6.86 (d, *J*=7.2 Hz, 1H), 6.82 (d, *J*=9.2 Hz, 2H), 6.75 (d, *J*=9.2 Hz, 2H), 5.95 (s, 1H), 3.74 (s, 3H), 3.68–3.60 (m, 1H), 3.57–3.50 (m, 2H), 2.86–2.78 (m, 2H), 2.06–1.97 (m, 2H), 1.68–1.60 (m, 4H), 1.48–1.46 (m, 1H), 1.05–1.01 (m, 2H), 0.96–0.86 (m, 1H). ^{13}C NMR (100MHz, $CDCl_3$) δ ppm 176.4, 173.6, 153.9, 143.0, 140.8, 140.5, 135.2, 132.3, 131.5, 128.8, 128.3, 127.9, 127.8, 127.5, 126.1, 119.2, 119.1, 114.6 (×2). 93.6, 63.4, 60.7, 55.6, 45.9, 30.5, 29.7, 26.4, 26.3, 26.3, 25.0. MS (+ESI): *m*/*z* (%) = 595 (100) $[M+H]^+$. Found: C, 60.34; H, 5.39; N, 4.64. Calc. for $C_{30}H_{31}IN_2O_3$: C, 60.61; H, 5.26; N, 4.71%.



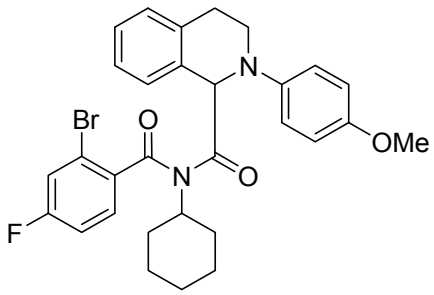
2-(4-methoxyphenyl)-N-(2-methoxybenzoyl)-N-cyclohexyl-1,2,3,4-tetrahydroisoquinoline-1-carboxamide (**4e**): (101 mg, 81%). A pale yellowish amorphous solid. R_f=0.30 (25% EtOAc–PE). IR (KBr) 2931, 1710, 1650, 1599, 1511, 1244, 1134, 1038, 753 cm^{-1}. ^1H NMR (400MHz, $CDCl_3$) δ ppm 7.36–7.32(m, 1H), 7.31–7.28 (m, 1H), 7.23 (dd, *J*=7.6, 1.6Hz, 1H), 7.21–7.18 (m, 2H), 7.07–7.05 (m, 1H), 6.81 (d, *J*=8.4 Hz, 1H), 6.80 (dd, *J*=7.6, 7.6 Hz, 1H), 6.67 (d, *J*=9.2 Hz, 2H), 6.62 (d, *J*=9.2 Hz, 2H), 5.53 (s, 1H), 3.92–3.86 (m, 1H), 3.71 (s, 3H), 3.61–3.53 (m, 2H), 2.79–2.69 (m, 2H), 1.99–1.93 (m, 2H), 1.68–1.60 (m, 3H), 1.53–1.50 (m, 2H), 1.07–1.05 (m, 3H). ^{13}C NMR (100MHz, $CDCl_3$) δ ppm 176.1, 171.7, 157.2, 153.2, 142.2, 135.1, 132.7, 132.5, 130.3, 129.1, 128.6, 127.4, 125.8, 124.8, 120.3, 117.7(×2), 114.3(×2), 111.2, 63.0, 59.7, 55.6, 55.4, 44.9, 30.7, 29.7, 26.44, 26.41, 25.7, 25.3. MS (+ESI): *m*/*z* (%) = 499 (100) $[M+H]^+$. HRMS (+EI) calcd for $C_{31}H_{32}N_2O_4$ 496.2362 $[M-H_2]^+$, found 496.2368.



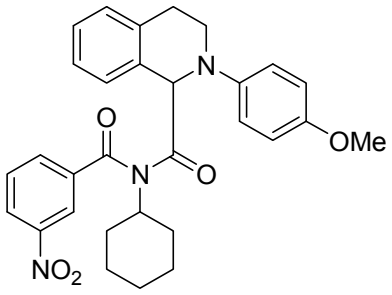
2-(4-methoxyphenyl)-N-(4-methoxybenzoyl)-N-cyclohexyl-1,2,3,4-tetrahydroisoquinoline-1-carboxamide (**4f**): (106 mg, 85%). A pale yellowish amorphous solid. R_f=0.57 (25% EtOAc–PE). IR (KBr) 2931, 1684, 1653, 1602, 1508, 1256, 1168, 1033 cm^{-1}. ^1H NMR (400MHz, $CDCl_3$) δ ppm 7.51 (d, *J*=9.2Hz, 2H), 7.33(d, *J*=7.2Hz,1H), 7.22 (ddd, *J*=7.6, 7.6, 1.6Hz, 1H), 7.17 (ddd, *J*=7.6, 7.6, 1.6Hz, 1H), 6.99 (d, *J*=7.2Hz, 1H), 6.69 (d, *J*=9.2Hz, 2H), 6.55 (d, *J*=9.2 Hz, 2H), 6.34 (d, *J*=9.2Hz, 2H), 4.86 (s, 1H), 4.17–4.10 (m, 1H), 3.80 (s, 3H), 3.68 (s, 3H), 3.50–3.45 (m, 1H), 3.30–3.23 (m, 1H), 2.69–2.60 (m, 1H), 2.50 (dd, *J*=16.8, 2.4Hz, 1H), 2.10–2.00 (m, 1H), 1.89–1.81 (m, 2H), 1.78–1.79 (m, 3H), 1.58 (d, *J*=12.4Hz, 1H), 1.28–1.18 (m, 2H), 1.16–1.08 (m, 1H). ^{13}C NMR (100MHz, $CDCl_3$) δ ppm 173.4, 170.7, 163.0, 154.3, 140.3, 134.3, 131.6(×2), 131.1, 130.1, 128.8, 127.8, 127.3, 125.7, 118.7(×2), 114.0(×2), 113.2(×2), 61.5, 58.2, 55.48, 55.46, 45.5, 31.5, 29.1, 26.32, 26.27, 25.4, 24.8. MS (+ESI): *m*/*z* (%) = 499 (100) $[M+H]^+$. HRMS (+EI) calcd for $C_{31}H_{32}N_2O_4$ 496.2362 $[M-H_2]^+$, found 496.2365.



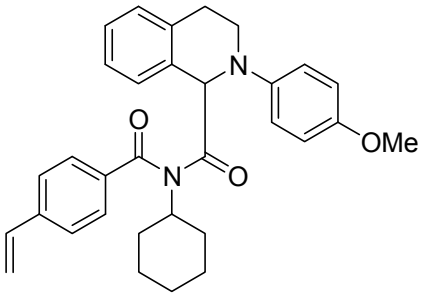
2-(4-methoxyphenyl)-N-(3-trifluoromethoxybenzoyl)-N-cyclohexyl-1,2,3,4-tetrahydroisoquinoline-1-carboxamide (**4g)**: (119 mg, 86%). 90-93 ^{o}C (from EtOAc-hexance). A yellowish crystalline solid. R_f=0.64 (14% EtOAc–PE). IR (KBr) 2932, 1699, 1660, 1510, 1256, 1215, 1041, 829, 751 cm^{-1}. ^{1}H NMR (400MHz, $CDCl_3$) δ ppm 7.49–7.46 (m, 1H), 7.41 (s, 1H), 7.34 (d, *J*=7.6Hz, 1H), 7.27–7.17 (m, 4H), 6.99 (d, *J*=7.2Hz, 1H), 6.55 (d, *J*=8.8 Hz, 2H), 6.32 (d, *J*=9.2 Hz, 2H), 4.79 (s, 1H), 4.26–4.19 (m, 1H), 3.67 (s, 3H), 3.51–3.46 (m, 1H), 3.22–3.14 (m, 1H), 2.64–2.59 (m, 1H), 2.54–2.49 (m, 1H), 2.13–2.03 (m, 1H), 1.90 (d, *J*=12.4Hz, 1H), 1.81–1.75 (m, 3H), 1.69 (d, *J*=9.2Hz, 1H), 1.60 (d, *J*=12.4Hz, 1H), 1.30–1.21 (m, 2H), 1.20–1.10(m,1H). ^{13}C NMR (100MHz, $CDCl_3$) δ ppm 172.9, 168.6, 154.7, 148.9(d, *J*=1.5Hz), 139.1, 137.1, 134.1, 130.9, 130.3, 129.4, 128.8, 127.5, 126.6, 125.9, 124.3, 121.0, 120.3 (*J*=256.4Hz), 118.3(×2), 114.1(×2), 61.1, 58.3, 55.4, 45.2, 31.7, 29.0, 26.2(×2), 25.3, 24.7. MS (+ESI): *m*/*z* (%) = 553 (87) $[M+H]^+$, 1127 (100) $[2M+Na]^+$. HRMS (+EI) calcd for $C_{31}H_{29}F_3N_2O_4$ 550.2079 $[M-H_2]^+$, found 550.2073.



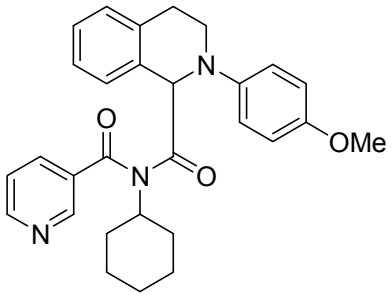
2-(4-methoxyphenyl)-N-(2-bromo-4-fluorobenzoyl)-N-cyclohexyl-1,2,3,4-tetrahydroisoquinoline-1-carboxamide (**4h)**: (100 mg, 71%). 151-153 ^{o}C (from EtOAc-hexance). A pale yellowish crystalline solid. R_f=0.75 (25% EtOAc–PE). IR (KBr) 3064, 2930, 1683, 1666, 1510, 1508, 1300, 1245, 1112, 1037, 830, 755 cm^{-1}. ^{1}H NMR (400MHz, $CDCl_3$) δ ppm 7.40–7.38 (m, 1H), 7.29 (dd, *J*=8.0, 2.4Hz, 1H), 7.25–7.21 (m, 2H), 7.12–7.10 (m, 1H), 6.92 (dd, *J*=8.4, 6.0Hz, 1H), 6.84–6.74 (m, 1H), 6.79 (d, *J*=9.2Hz, 2H), 6.75 (d, *J*=9.2Hz, 2H), 5.71 (s, 1H), 3.75 (s, 3H), 3.82–3.73 (m, 1H), 3.63 –3.57 (m, 1H), 3.53–3.48 (m, 1H), 2.84–2.79 (m, 1H), 2.03–1.94 (m, 2H), 1.71–1.67 (m, 2H), 1.60–1.50 (m, 3H), 1.10–1.01 (m, 2H), .0.99–0.94 (m, 1H). ^{13}C NMR (100MHz, $CDCl_3$) δ ppm 175.9, 171.3, 162.9 (*J*=254.4 Hz), 154.2, 142.7, 135.0, 133.5 (*J*=3.4 Hz), 131.9, 130.7 (*J*=9.7Hz), 128.9, 128.3, 127.6, 126.1, 121,5(*J*=9.6Hz), 121.1(*J*=24.5Hz), 119.4(×2), 114.5(×2), 114.4 (*J*=21.5Hz), 63.6, 60.3, 55.6, 46.3, 30.5, 29.7, 26.42, 26.37, 26.3, 25.1. MS (+ESI): *m*/*z* (%) =565 (100) $[M+H]^+$. HRMS (+CI) calcd for $C_{30}H_{31}FBrN_2O_3$ 565.1502 $[M+H]^+$, found 565.1511. Found: C, 63.55; H, 5.18; N, 4.67. Calc. for $C_{30}H_{30}FBrN_2O_3$: C, 63.72; H, 5.35; N, 4.95%.



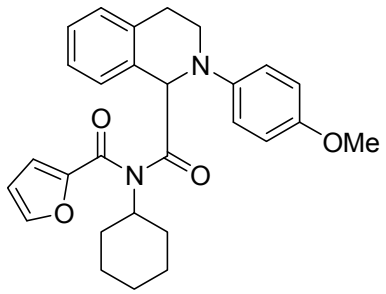
2-(4-methoxyphenyl)-N-(3-nitrobenzoyl)-N-cyclohexyl-1,2,3,4-tetrahydroisoquinoline-1-carb oxamide (**4i)**: (89 mg, 69 %). 174-176 ^{o}C (from EtOAc-hexance). A yellowish crystalline solid. R_f= 0.62 (17% EtOAc–PE). IR (KBr) 3113, 2933, 1869, 1654, 1526, 1512, 1345, 1216, 1036, 821, 713, cm^{-1}. ^{1}H NMR (400MHz, $CDCl_3$) δ ppm 8.29 (dd, *J*=2.0, 2.0Hz, 1H), 8.14–8.12 (m, 1H), 7.82–7.79 (m, 1H), 7.39 (dd, *J*=8.0, 8.0Hz, 1H), 7.34 (d, *J*=7.2Hz, 1H), 7.24 (ddd, *J*=7.6, 7.6, 1.2Hz, 1H), 7.19 (ddd, *J*=7.2, 7.2, 1.2Hz, 1H), 6.99 (d, *J*=7.2Hz, 1H), 6.52 (d, *J*=9.2Hz, 2H), 6.32 (d, *J*=9.2Hz, 2H), 4.63 (s, 1H), 4.38–4.31 (m, 1H), 3.65 (s, 3H), 3.56–3.51 (m, 1H), 3.20–3.12 (m, 1H), 2.68–2.59 (m, 1H), 2.56–2.51 (m, 1H), 2.13–2.04 (m, 1H), 1.93 (d, *J*=12.0Hz, 1H), 1.80–1.69 (m, 4H), 1.61 (d, *J*=12.8Hz, 1H), 1.34–1.25 (m, 2H), 1.23–1.11(m, 1H). ^{13}C NMR (100MHz, $CDCl_3$) δ ppm 172.4, 167.5, 154.8, 147.7, 138.6, 136.8, 133.9, 132.9, 130.5, 130.3, 128.9, 128.8, 127.7, 126.0, 125.9, 123.5, 118.0 (×2), 114.3 (×2), 60.9, 58.3, 55.4, 44.9, 32.0, 29.1, 26.22, 26.20, 25.3, 24.8. MS (+ESI): *m*/*z* (%) = 514 (100) $[M+H]^+$. Found: C, 70.50; H, 6.27; N, 8.49. Calc. for $C_{30}H_{31}N_3O_5$: C, 70.16; H, 6.08; N, 8.18%.



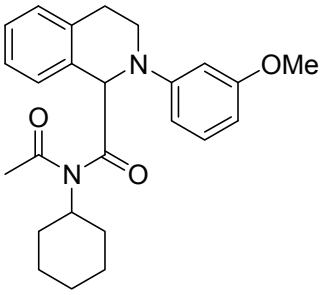
2-(4-methoxyphenyl)-N-(4-vinylbenzoyl)-N-cyclohexyl-1,2,3,4-tetrahydroisoquinoline-1-carb oxamide (**4j)**: (98 mg, 79%). 123-125 ^{o}C (from EtOAc-hexance).A yellowish crystalline solid. R_f=0.69 (14% EtOAc–PE). IR (KBr) 2929, 1684, 1653, 1509, 1243, 1036, 829, 751 cm^{-1}. ^{1}H NMR (400MHz, $CDCl_3$) δ ppm 7.50 (d, *J*=8.4Hz, 2H), 7.33 (d, *J*=7.2Hz, 1H), 7.24 (dd, *J*=6.8, 6.8Hz, 1H), 7.23 (d, *J*=8.0Hz, 2H), 7.18 (ddd, *J*=7.6, 7.6, 1.6Hz, 1H), 6.99 (d, *J*=7.2Hz, 1H), 6.67 (dd, *J*=17.6, 11.2 Hz, 1H), 6.53 (d, *J*=9.2 Hz, 2H), 6.33 (d, *J*=8.8Hz, 2H), 5.79 (d, *J*=17.6Hz, 1H), 5.35 (d, *J*=11.2Hz, 1H), 4.87 (s, 1H), 4.21–4.13 (m, 1H), 3.67 (s, 3H), 3.52–3.47 (m, 1H), 3.28–3.20 (m, 1H), 2.69–2.61 (m, 1H), 2.54–2.49 (m, 1H), 2.13–2.03 (m, 1H), 1.91–1.78 (m, 2H), 1.74–1.70 (m, 3H), 1.58 (d, *J*=12.8Hz, 1H), 1.29–1.21 (m, 2H), 1.18–1.09 (m, 1H). ^{13}C NMR (100MHz, $CDCl_3$) δ ppm 173.4, 170.6, 154.4, 141.4, 139.9, 135.9, 134.3, 134.2, 131.4, 130.2, 129.1(×2), 128.8, 127.4, 125.7, 125.66(×2), 118.5(×2), 116.5, 114.0 (×2), 61.4, 58.3, 55.5, 45.2, 31.6, 29.1, 26.31, 26.27, 25.3, 24.8. MS (+ESI): *m*/*z* (%) = 495 (100) $[M+H]^+$, 1011 (48) $[2M+Na]^+$. HRMS (+EI) calcd for $C_{32}H_{32}N_2O_3$ 492.2413 $[M-H_2]^+$, found 492.2425.



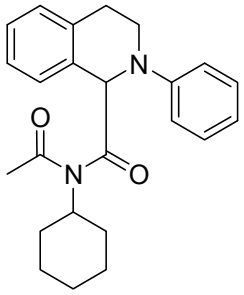
2-(4-methoxyphenyl)-N-(3-pyridyl)-N-cyclohexyl-1,2,3,4-tetrahydroisoquinoline-1-carboxamide (4k): (115 mg, 98%). 148-149 ^{o}C (from EtOAc-hexance). A pale yellowish solid. R_f=0.44 (25% EtOAc–PE). IR (KBr) 2925, 1693, 1658, 1511, 1245, 1035, 830 cm^{-1}. ^{1}H NMR (400MHz, $CDCl_3$) δ ppm 8.81 (d, *J*=2.0 Hz, 1H), 8.55 (dd, *J*=5.2, 2.0 Hz, 1H), 7.75 (ddd, *J*=8.0, 1.6, 1.6 Hz, 1H), 7.35 (d, *J*=7.6 Hz, 1H), 7.26 (dd, *J*=7.6, 7.6 Hz, 1H), 7.19 (ddd, *J*=8.4, 8.4, 1.2 Hz, 1H), 7.04 (dd, *J*=8.0, 4.8 Hz, 1H), 6.99 (d, *J*=8.0 Hz, 1H), 6.56 (d, *J*=8.8 Hz, 2H), 6.33 (d, *J*=9.2Hz, 2H), 4.77 (s, 1H), 4.29–4.21 (m, 1H), 3.67 (s, 3H), 3.52–3.47 (m, 1H), 3.22–3.15 (m, 1H), 2.67–2.59 (m, 1H), 2.52 (dd, J= 17.2, 2.8 Hz, 1H), 2.12–2.02 (m, 1H), 1.92–1.89 (m, 1H), 1.80–1.68 (m, 4H), 1.61–1.58 (m, 1H), 1.34–1.22 (m, 2H), 1.18–1.10 (m, 1H). ^{13}C NMR (100MHz, $CDCl_3$) δ ppm 172.7, 168.5, 154.7, 152.5, 149.1, 139.1, 135.9, 134.0, 131.0, 130.7, 130.3, 128.8, 127.6, 125.9, 122.8, 118.4(×2), 114.2(×2), 61.0, 58.3, 55.5, 45.2, 31.9, 29.1, 26.2, 25.3, 24.7. MS (+ESI): *m*/*z* (%) = 470 (100) $[M+H]^+$. Found: C, 73.97; H, 6.79; N, 9.06. Calc. for $C_{29}H_{31}N_3O_3$: C, 74.18; H, 6.65; N, 8.95%.



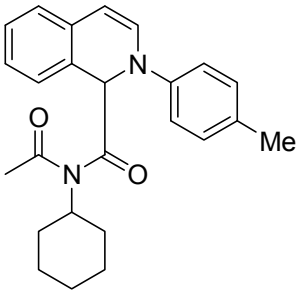
2-(4-methoxyphenyl)-N-(2-furyl)-N-cyclohexyl-1,2,3,4-tetrahydroisoquinoline-1-carboxamide (4l): (84 mg, 73%). 147-148 ^{o}C (from EtOAc-hexance).A pale yellowish crystalline solid. R_f=0.32 (17% EtOAc–PE). IR (KBr) 3059, 2930, 1686, 1649, 1509, 1467, 1274, 1039, 830, 757, 609 cm^{-1}. ^{1}H NMR (400MHz, $CDCl_3$) δ ppm 7.44 (d, *J*=7.6Hz, 1H), 7.29–7.25 (m, 2H), 7.19 (ddd, *J*=7.6, 7.6, 1.2Hz, 1H), 7.00 (d, *J*=7.6Hz, 1H), 6.78 (dd, *J*=3.6, 0.4Hz, 1H), 6.60 (d, *J*=8.8Hz, 2H), 6.51 (d, *J*=9.2Hz, 2H), 6.24 (dd, *J*=3.6, 2.0Hz, 1H), 4.93 (s, 1H), 4.24–4.17 (m,1H), 3.68 (s, 3H), 3.44–3.39 (m, 1H), 3.24–3.16 (m, 1H), 2.67–2.59 (m,1H), 2.48 (dd, *J*=16.8, 2.8Hz, 1H), 2.05–1.95 (m, 1H), 1.89 (d, *J*=9.6Hz, 1H), 1.77–1.67 (m, 4H), 1.58 (d, *J*=12.8Hz, 1H), 1.32–1.22 (m, 2H), 1.17–1.09 (m, 1H). ^{13}C NMR (100MHz, $CDCl_3$) δ ppm 172.2, 159.5, 154.8, 150.0, 145.4, 139.8, 134.3, 131.4, 130.4, 128.8, 127.4, 125.8, 119.4(×2), 116.7, 113.9(×2), 111.8, 61.1, 57.7, 55.4, 45.9, 32.0, 29.2, 26.24, 26.22, 25.3, 24.5. MS (+ESI): *m*/*z* (%) = 459 (100) $[M+H]^+$, 940 (50) $[2M+Na]^+$. Found: C, 73.10; H, 5.78; N, 6.51. Calc. for $C_{28}H_{30}N_2O_4$: C, 73.34; H, 6.59; N, 6.11%.



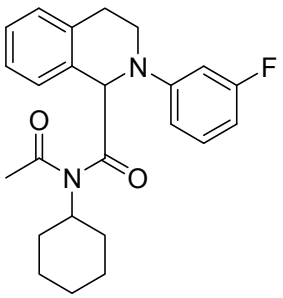
2-(3-methoxyphenyl)-N-acetyl-N-cyclohexyl-1,2,3,4-tetrahydroisoquinoline-1-carboxamide (4m): (72 mg, 71 %). A pale yellowish oil. R_f=30 (11% EtOAc–PE). IR (film) 1674, 1608, 735 cm^{-1}. ^1H NMR (400MHz, $CDCl_3$) δ ppm 7.34–7.32 (m, 1H), 7.24–7.21 (m, 2H), 7.17–7.14 (m, 2H), 6.58 (dd, *J*=9.6, 2.0Hz, 1H), 6.57 (s, 1H), 6.39 (dd, *J*=9.6, 2.4Hz, 1H), 6.22 (s, 1H), 3.80 (s, 3H), 3.72–3.67 (m, 1H), 3.56–3.48 (m, 2H), 3.05–2.98 (m,1H), 2.94–2.87 (m, 1H), 2.22 (s, 3H), 2.03–1.92 (m, 1H), 1.74–1.66 (m, 3H), 1.54–1.51 (m, 1H), 1.12–1.02 (m, 4H). ^{13}C NMR (100MHz, $CDCl_3$) δ ppm 177.6, 174.5, 160.7, 150.0, 135.7, 132.6, 129.9, 128.3, 127.8, 127.7, 126.5, 107.6, 103.8, 101.3, 63.5, 59.3, 55.2, 44.6, 31.0, 29.2, 27.5, 26.5, 26.4, 25.4, 25.1. MS (+ESI): *m*/*z* (%) = 407 (100) $[M+H]^+$. HRMS (+EI) calcd for $C_{25}H_{28}N_2O3$ 404.2100 $[M-H_2]^+$, found 404.2103.



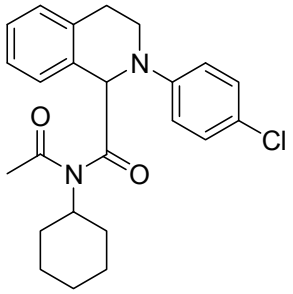
2-(phenyl)-N-acetyl-N-cyclohexyl-1,2,3,4-tetrahydroisoquinoline-1-carboxamide (4n): (81 mg, 86 %). A pale yellowish oil. R_f=55 (15% EtOAc–PE). IR (film) 1676, 1505, 1178, 749 cm^{-1}. ^1H NMR (400MHz, $CDCl_3$) δ ppm 7.38–7.36 (m, 1H), 7.30–7.23 (m, 4H), 7.18–7.15 (m, 1H), 6.99 (d, *J*=8.4Hz, 2H), 6.84 (dd, *J*=7.6, 7.6 Hz, 1H), 6.19 (s, 1H), 3.72–3.66 (m, 1H), 3.59–3.52 (m, 2H), 3.04–2.97 (m, 1H), 2.94–2.88 (m, 1H), 2.20 (s, 3H), 2.02–1.92 (m, 1H), 1.82–1.68 (m, 3H), 1.56–1.48 (m, 2H), 1.14–1.02 (m, 4H). ^{13}C NMR (100MHz, $CDCl_3$) δ ppm 177.3, 174.6, 148.6, 135.5, 132.5, 129.3(×2), 128.4, 127.8, 127.7, 126.4, 119.1, 115.3, 63.4, 59.2, 44.8, 30.8, 29.4, 27.5, 26.5(×2), 25.6, 25.1. MS (+ESI): *m*/*z* (%) = 377 (100) $[M+H]^+$. HRMS (+EI) calcd for $C_{24}H_{26}N_2O_2$ 374.1994 $[M-H_2]^+$, found 374.1999.



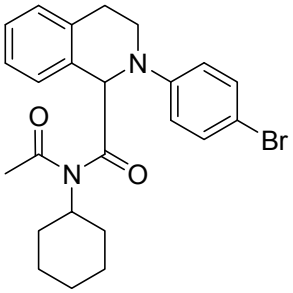
2-(4-methylphenyl)-N-acetyl-N-cyclohexyl-1,2,3,4-tetrahydroisoquinoline-1-carboxamide (4o) : (82 mg, 84%). A brownish oil. R_f=0.49 (15% EtOAc–PE). IR (film) 1678, 1515, 752 cm^{-1}. ^1H NMR (400MHz, $CDCl_3$) δ ppm 7.38–7.36 (m, 1H), 7.26–7.21 (m, 2H), 7.17–7.13 (m, 1H), 7.08 (d, *J*=8.8Hz, 2H), 6.90 (d, *J*=8.4 Hz, 2H), 5.95 (s, 1H), 3.71–3.64 (m, 1H), 3.62–3.58 (m, 1H), 3.56–3.50 (m, 1H), 2.98–2.85 (m, 2H), 2.27 (s, 3H), 2.16 (s, 3H), 1.98–1.82(m, 2H), 1.74–1.67 (m, 2H), 1.55 (d, *J*=10.8 Hz, 1H), 1.43 (d, *J*=11.6 Hz, 1H), 1.33–1.28 (m, 1H), 1.20–0.98 (m, 3H). ^{13}C NMR (100MHz, $CDCl_3$) δ ppm 176.6, 174.5, 146.4, 135.1, 132.3, 129.8(×2), 129.3, 128.7, 127.9, 127.6, 126.3, 116.5(×2), 63.5, 58.8, 45.5, 30.4, 29.9, 27.2, 26.5, 26.4, 26.1, 25.1, 20.5. MS (+ESI): *m*/*z* (%) =387 (100), 391(33) $[M+H]^+$. HRMS (+EI) calcd for $C_{25}H_{28}N_2O_2$ 388.2151 $[M-H_2]^+$, found 388.2143.



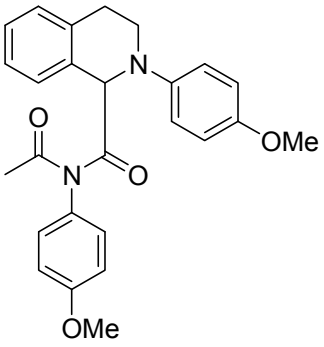
2-(3-fluorophenyl)-N-acetyl-N-cyclohexyl-1,2,3,4-tetrahydroisoquinoline-1-carboxamide (4p): (78 mg, 79%). A pale yellowish amorphous solid. R_f=0.50 (25% EtOAc–PE). IR (KBr) 2934, 1693, 1664, 1613 1500, 1395, 1177, 1044, 754 cm^{-1}. ^1H NMR (400MHz, $CDCl_3$) δ ppm 7.35–7.33 (m, 1H), 7.29–7.24 (m, 2H), 7.23–7.18 (m, 2H), 6.75 (dd, *J*=8.4, 2.8 Hz, 1H), 6.69 (ddd, *J*=12.8, 2.4, 2.4 Hz, 1H), 6.49 (ddd, *J*=8.4, 8.4, 2.4 Hz, 1H), 6.40 (s, 1H), 3.79–3.73 (m, 1H), 3.54–3.49 (m, 1H), 3.48–3.40 (m, 1H), 3.12–3.06 (m, 1H), 2.93 (ddd, *J*=15.6, 4.2, 4.2Hz, 1H), 2.28 (s, 3H), 2.07–1.99 (m, 1H), 1.77–1.74 (m, 1H), 1.68–1.56 (m, 4H), 1.13–1.07 (m, 2H), 0.93–0.84 (m, 2H). ^{13}C NMR (100MHz, $CDCl_3$) δ ppm 178.0, 174.6, 164.0 (d, *J*=241 Hz), 150.3 (d, *J*=11.2Hz), 135.9, 132.6, 130.3 (d, *J*=10.2), 128.1, 128.1, 127.5, 126.7, 109.3 (d, *J*=1.7Hz), 104.4 (d, *J*=20.8), 100.9 (d, *J*=26.0), 63.5, 59.8, 44.4, 31.4, 28.6, 27.6, 26.5, 26.3, 25.0, 24.9. MS (+ESI): *m*/z (%) = 395 (100) $[M+H]^+$. HRMS (+EI) calcd for $C_{24}H_{25}N_2O_2F$ 392.1900 $[M-H_2]^+$, found 392.1893.



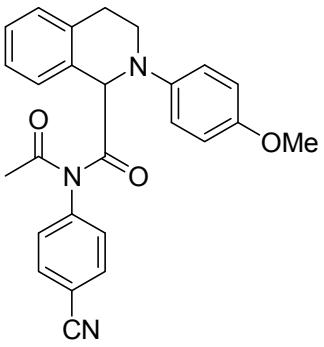
2-(4-chlorophenyl)-N-acetyl-N-cyclohexyl-1,2,3,4-tetrahydroisoquinoline-1-carboxamide (**4q**): (85 mg, 83%). A pale yellowish amorphous solid. R_f=0.50 (25% EtOAc–PE). IR (KBr) 2930, 1720, 1674, 1596 1499, 1333, 1177, 1044, 750 cm^{-1}. ^1H NMR (400MHz, $CDCl_3$) δ ppm 7.35–7.33 (m, 1H), 7.29–7.21 (m, 4H), 7.20–7.17 (m, 1H), 6.93–6.90 (m, 2H), 6.29 (s, 1H), 3.74–3.68 (m, 1H), 3.54–3.45 (m, 2H), 3.09–3.02 (m, 1H), 2.91 (ddd, J=16.0, 5.2, 5.2 Hz, 1H), 2.25 (s, 3H), 2.04–2.00 (m, 1H), 1.76–1.74 (m, 1H), 1.70–1.64 (m, 2H), 1.61–1.56 (m, 2H), 1.12–1.06 (m, 2H), 0.94–0.88 (m, 2H). ^{13}C NMR (100MHz, $CDCl_3$) δ ppm 177.7, 174.6, 147.2, 135.6, 132.5, 129.1 (×2), 128.2, 128.1, 127.6, 126.6, 123.2, 115.5 (×2), 63.5, 59.6, 44.7, 31.2, 28.8, 27.5, 26.4, 26.3, 25.2, 25.0. MS (+ESI): *m*/*z* (%) = 411 (100) $[M+H]^+$. HRMS (+EI) calcd for $C_{24}H_{25}N_2O_2Cl$ 408.1605 $[M-H_2]^+$, found 408.1602.



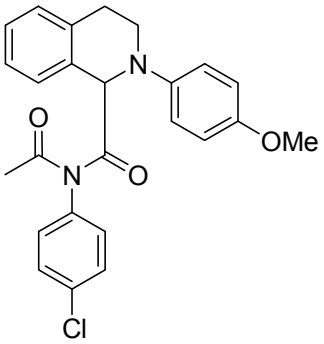
2-(4-bromophenyl)-N-acetyl-N-cyclohexyl-1,2,3,4-tetrahydroisoquinoline-1-carboxamide (4r): (103 mg, 91 %). A pale yellowish oil. R_f= 0.36(11% EtOAc–PE). IR (film) 1672, 1496, 907, 729 cm^{-1}. ^1H NMR (400MHz, $CDCl_3$) δ ppm 7.34(d, *J*=8.8Hz, 2H), 735–7.30(m, 1H), 7.25–7.22 (m, 2H), 7.16 (d, *J*=7.6 Hz, 1H), 6.84 (d, *J*=9.2 Hz, 2H), 6.29 (s, 1H), 3.70–3.66 (m, 1H), 3.51–3.41 (m, 2H), 3.04–3.00 (m, 1H), 2.92–2.87 (m, 1H), 2.24 (s, 3H), 2.02–1.98 (m, 1H), 1.74–1.55 (m, 5H), 1.10–1.04 (m, 3H), 0.90–0.87 (m, 1H). ^{13}C NMR (100MHz, $CDCl_3$) δ ppm 177.7, 174.6, 147.6, 135.7, 132.5, 131.9(×2), 128.2, 128.1, 127.6, 126.6, 115.8(×2), 110.3, 63.5, 59.6, 44.6, 31.3, 28.8, 27.5, 26.5, 26.3, 25.1, 25.0. MS (+ESI): *m*/*z* (%) = 455 (100) $[M+H]^+$, 457 (82) $[M+H+2]^+$. HRMS (+EI) calcd for $C_{24}H_{25}BrN_2O_2$ 452.1099 $[M-H_2]^+$, found 452.1099.



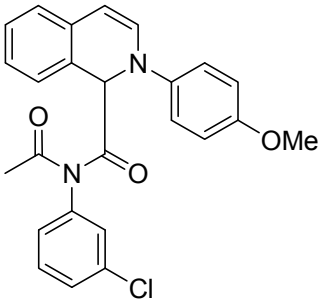
2-(4-methoxyphenyl)-N-acetyl-N-(4-methoxyphenyl)-1,2,3,4-tetrahydroisoquinoline-1-carboxamide (4s): (86 mg, 80%). A yellowish oil. R_f= 0.22(15% EtOAc–PE). IR (film) 1701, 1509, 1246, 731 cm^{-1}. ^1H NMR (400MHz, $CDCl_3$) δ ppm 7.41 (d, *J*=8.0Hz, 1H), 7.25–7.21 (m, 2H), 7.18 (d, *J*=7.6 Hz, 1H), 6.92 (d, *J*=9.2Hz, 2H), 6.86 (d, *J*=8.8 Hz, 2H), 6.79 (d, *J*=8.8Hz, 2H), 6.64 (d, *J*=8.4Hz, 2H), 6.39 (s, 1H), 3.79 (s, 3H), 3.77–3.74 (m, 1H), 3.76 (s, 3H), 3.50–3.45 (m, 1H), 2.98–2.87 (m, 2H), 2.08 (s, 3H). ^{13}C NMR (100MHz, $CDCl_3$) δ ppm 176.2, 174.0, 159.5, 153.8, 143.3, 135.6, 132.4, 131.1, 129.8(×2), 128.9, 127.6, 127.0, 126.1, 118.5(×2), 114.7(×2), 114.6(×2), 62.4, 55.7, 55.4, 44.1, 27.5, 26.1. MS (+ESI): *m*/*z* (%) = 427 (100), 431(33) $[M+H]^+$. HRMS (+CI) calcd for $C_{26}H_{27}N_2O_4$ 431.1971 $[M+H]^+$, found 431.1966.



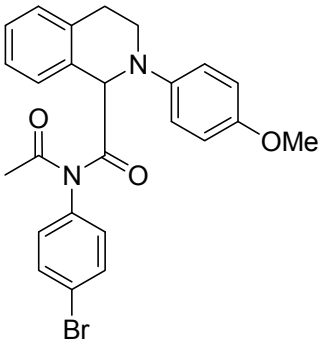
2-(4-methoxyphenyl)-N-acetyl-N-(4-cyanophenyl)-1,2,3,4-tetrahydroisoquinoline-1-carboxamide (4t): (93 mg, 88%). A yellowish amorphous solid. R_f=0.28 (20% EtOAc–PE). IR (film) 1710, 1510, 1244, 734 cm^{-1}. ^1H NMR (400MHz, acetone-d_6) δ ppm 7.72–7.69 (m, 2H), 7.48–7.46(m, 1H), 7.27–7.22 (m, 2H), 7.19–7.17 (m, 1H), 7.15–7.11 (m, 2H), 6.88–6.83 (m, 4H), 6.24 (s, 1H), 3.75 (s, 3H), 3.66–3.53 (m, 2H), 2.91–2.74 (m, 2H), 2.13 (s, 3H). ^{13}C NMR (100MHz, acetone-d_6) δ ppm 175.2, 172.7, 154.0, 143.0, 142.8, 135.7, 133.1(×2), 132.3, 130.3(×2), 128.8, 127.6, 127.4, 126.0, 118.2(×2), 117.8, 114.4(×2), 112.0, 62.0, 54.9, 44.0, 26.7, 25.5. MS (+ESI): *m*/*z* (%) = 426 (84) $[M+H]^+$, 448 (100) $[M+Na]^+$. HRMS (+EI) calcd for $C_{26}H_{21}N_3O_3$ 423.1583 $[M-H_2]^+$, found 423.1586.



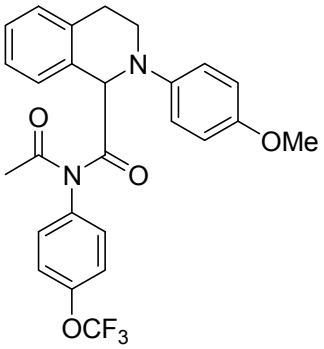
2-(4-methoxyphenyl)-N-acetyl-N-(4-chlorophenyl)-1,2,3,4-tetrahydroisoquinoline-1-carboxa mide (4u) : (85 mg, 78%). A brownish oil. R_f=0.33 (15% EtOAc–PE). IR (film) 1708, 1510, 1265, 736 cm^{-1}. ^1H NMR (400MHz, $CDCl_3$) δ ppm 7.40–7.38 (m, 1H), 7.24–7.20 (m, 2H), 7.22 (d, *J*=8.4Hz, 2H), 7.17–7.15 (m, 1H), 6.88 (d, *J*=9.6Hz, 2H), 6.84 (d, *J*=9.2Hz, 2H), 6.62 (d, *J*=8.8Hz, 2H), 6.28 (s, 1H), 3.78 (s, 3H), 3.71–3.65 (m, 1H), 3.46–3.41 (m, 1H), 2.95–2.87 (m, 1H), 2.84–2.78 (m, 1H), 2.07 (s, 3H). ^{13}C NMR (100MHz, $CDCl_3$) δ ppm 175.9, 173.4, 153.9, 143.3, 136.9, 135.6, 134.7, 132.1, 130.2(×2), 129.6(×2), 129.0, 127.7, 127.0, 126.2, 118.6(×2), 114.6(×2), 62.6, 55.7, 44.2, 27.5, 26.1. MS (+ESI): *m*/*z* (%) =391(100), 435 (95) $[M+H]^+$. HRMS (+CI) calcd for $C_{25}H_{24}ClN_2O_3$ 435.1475 $[M+H]^+$, found 435.1474.



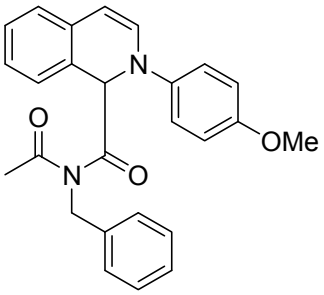
2-(4-methoxyphenyl)-N-acetyl-N-(3-chlorophenyl)-1,2,3,4-tetrahydroisoquinoline-1-carboxa mide (4v): (99 mg, 91%). A brownish oil. R_f=0.33 (15% EtOAc–PE). IR (film) 1705, 1510, 736 cm^{-1}. ^1H NMR (400MHz, $CDCl_3$) δ ppm 7.43–7.41 (m, 1H), 7.28–7.17 (m, 5H), 6.92–6.86 (m, 4H), 6.68 (d, *J*=7.6 Hz, 1H), 6.58 (dd, *J*=1.6, 2.0 Hz, 1H), 6.28 (s, 1H), 3.81 (s, 3H), 3.71–3.65 (m, 1H), 3,47–3.41 (m, 1H), 2.97–2.90 (m, 1H), 2.85–2.78 (m, 1H), 2.09 (s, 3H). ^{13}C NMR (100MHz, $CDCl_3$) δ ppm 175.7, 173.3, 154.1, 143.3, 139.4, 135.5, 134.9, 132.0, 130.2, 129.3, 129.1, 129.0, 127.6, 127.2, 127.0, 126.2, 119.0(×2), 114.6(×2), 62.7, 55.7, 44.2, 27.6, 26.1. MS (+ESI): *m*/*z* (%) =238(100), 435(45) $[M+H]^+$, 457(39) $[M+Na]^+$. HRMS (+CI) calcd for $C_{25}H_{24}ClN_2O_3$ 435.1475 $[M+H]^+$, found 435.1463.



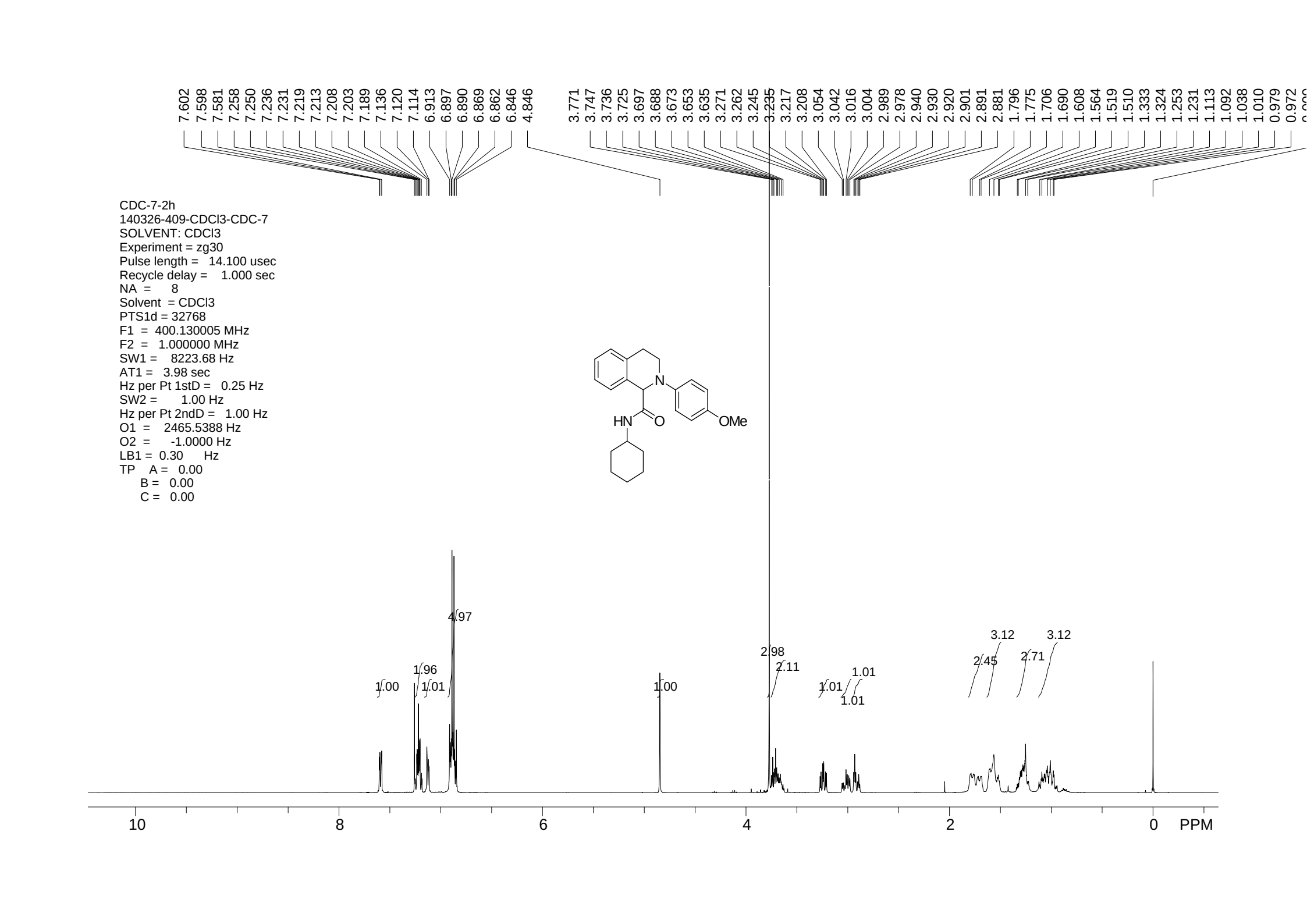
2-(4-methoxyphenyl)-N-acetyl-N-(4-bromophenyl)-1,2,3,4-tetrahydroisoquinoline-1-carboxamide (4w): (106 mg, 89%). A brownish amorphous solid. R_f=0.43 (25% EtOAc–PE). IR (film) 1705, 1510, 1243, 736 cm^{-1}. ^1H NMR (400MHz, $CDCl_3$) δ ppm 7.41–7.38 (m, 1H), 7.40 (d, *J*=8.8Hz, 2H), 7.28–7.23 (m, 2H), 7.19–7.17 (m, 1H), 6.89 (d, *J*=9.2Hz, 2H), 6.86 (d, *J*=9.2 Hz, 2H), 6.58 (d, *J*=8.4Hz, 2H), 6.29 (s, 1H), 3.80 (s, 3H), 3.73–3.67 (m, 1H), 3.48–3.43 (m, 1H), 2.97–2.89 (m, 1H), 2.86-2.79 (m, 1H), 2.09 (s, 3H). ^{13}C NMR (100MHz, $CDCl_3$) δ ppm 175.7, 173.3, 154.0, 143.2, 137.4, 135.5, 132.6(×2), 132.0, 130.5(×2), 129.0, 127.7, 127.0, 126.2, 122.8, 118.7(×2), 114.6(×2), 62.6, 55.7, 44.3, 27.5, 26.1. MS (+ESI): *m*/*z* (%) = 479(100) $[M+H]^+$. HRMS (+EI) calcd for $C_{25}H_{21}BrN_2O_3$ 476.0736 $[M-H_2]^+$, found 476.0742.



2-(4-methoxyphenyl)-N-acetyl-N-(4-trifluoromethoxyphenyl)-1,2,3,4-tetrahydroisoquinoline-1-carboxamide (4x): (111 mg, 92%). A brownish oil. R_f=0.26 (11% EtOAc–PE). IR (film) 1707, 1509, 1256, 736 cm^{-1}. ^1H NMR (400MHz, $CDCl_3$) δ ppm 7.41–7.39 (m, 1H), 7.28–7.22 (m, 2H), 7.18–7.16 (m, 1H), 7.10 (d, *J*=8.4Hz, 2H), 6.89 (d, *J*=9.2Hz, 2H), 6.85 (d, *J*=9.2 Hz, 2H), 6.76 (d, *J*=8.4Hz, 2H), 6.20 (s, 1H), 3.79 (s, 3H), 3.72–3.66 (m, 1H), 3.48–3.43 (m, 1H), 2.94–2.86 (m, 1H), 2.81–2.75 (m, 1H), 2.13 (s, 3H). ^{13}C NMR (100MHz, $CDCl_3$) δ ppm 175.8, 173.4, 154.0, 149.0, 143.2, 136.7, 135.6, 131.9, 130.5(×2), 129.1, 127.7, 127.0, 126.2, 121.6(×2), 120.3(q, *J*=250.6Hz), 118.8(×2), 114.6(×2), 62.7, 55.6, 44.6, 27.3, 26.2. MS (+ESI): *m*/*z* (%) =238 (100), 485 (85) $[M+H]^+$. HRMS (+CI) calcd for $C_{26}H_{24}F_3N_2O_4$ 485.1688 $[M+H]^+$, found 485.1681.



2-(4-methoxyphenyl)-N-acetyl-N-benzyl-1,2,3,4-tetrahydroisoquinoline-1-carboxamide (4y): (95 mg, 92%). A brownish oil. R_f=0.27 (15% EtOAc–PE). IR (film) 1697, 1510, 752 cm^{-1}. ^1H NMR (400MHz, $CDCl_3$) δ ppm 7.25–7.21 (m, 4H), 7.20–7.13 (m, 3H), 6.92–6.85 (m, 6H), 6.22 (s, 1H), 5.11 and 4.61 (ABq, *J*=16.4, 16.8Hz, 2H), 3.79 (s, 3H), 3.73–3.66 (m, 1H), 3.56–3.51 (m, 1H), 2.95–2.83 (m, 2H), 2.31 (s, 3H). ^{13}C NMR (100MHz, $CDCl_3$) δ ppm 176.1, 174.5, 154.0, 143.2, 137.1, 135.6, 132.2, 129.0, 128.7(×2), 127.6, 127.33, 127.28, 126.2(×3), 118.9(×2), 114.7(×2), 62.8, 55.6, 47.6, 45.3, 26.7, 26.1. MS (+ESI): *m*/*z* (%) =415 (100) $[M+H]^+$. HRMS (+CI) calcd for $C_{26}H_{27}N_2O_3$ 415.2022 $[M+H]^+$, found 415.2018.


7.602 7.598 7.581 7.258 7.250 7.236 7.231 7.219 7.213 7.208 7.203 7.189 7.136 7.120 7.114 6.913 6.897 6.890 6.869 6.862 6.846 4.846
3.771 3.747 3.736 3.725 3.697 3.688 3.673 3.653 3.635 3.271 3.262 3.245 3.235 3.217 3.208 3.054 3.042 3.016 3.004 2.989 2.978 2.940 2.930 2.920 2.901 2.891 2.881 1.796 1.775 1.706 1.690 1.608 1.564 1.519 1.510 1.333 1.324 1.253 1.231 1.113 1.092 1.038 1.010 0.979 0.972
CDC-7-2h
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SOLVENT: CDCl3
Experiment = zg30
Pulse length = 14.100 usec
Recycle delay = 1.000 sec
NA = 8
Solvent = CDCl3
PTS1d = 32768
F1 = 400.130005 MHz
F2 = 1.000000 MHz
SW1 = 8223.68 Hz
AT1 = 3.98 sec
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SW2 = 1.00 Hz
Hz per Pt 2ndD = 1.00 Hz
O1 = 2465.5388 Hz
O2 = -1.0000 Hz
LB1 = 0.30 Hz
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B = 0.00
C = 0.00
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OMe
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1.01
4.97
1.00
2.98
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1.01
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2.71
3.12
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2
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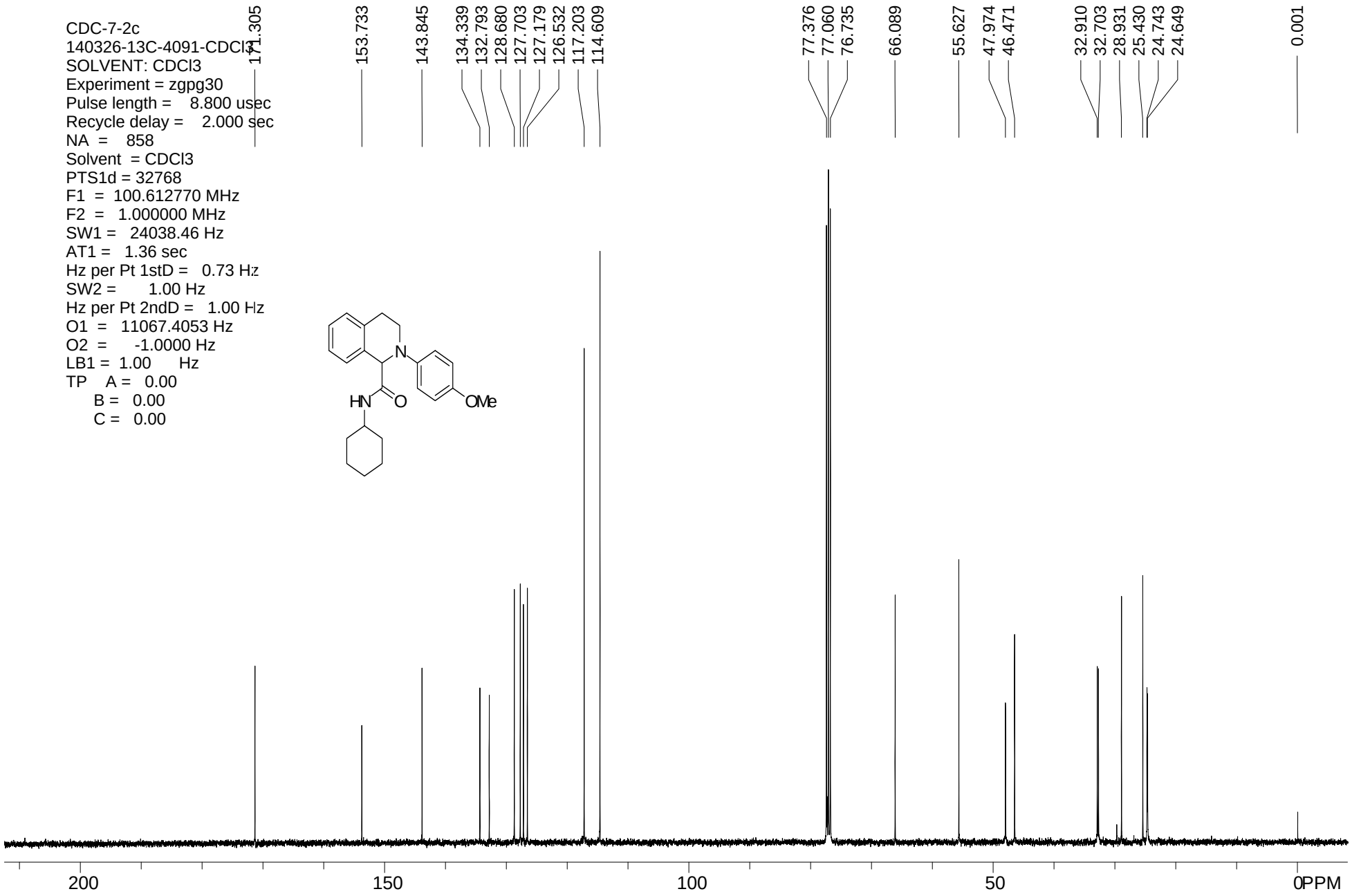
PPM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140326-13C-4091-CDCl3
SOLVENT: CDCl3
Experiment = zgpg30
Pulse length = 8.800 usec
Recycle delay = 2.000 sec
NA = 858
Solvent = CDCl3
PTS1d = 32768
F1 = 100.612770 MHz
F2 = 1.000000 MHz
SW1 = 24038.46 Hz
AT1 = 1.36 sec
Hz per Pt 1stD = 0.73 Hz
SW2 = 1.00 Hz
Hz per Pt 2ndD = 1.00 Hz
O1 = 11067.4053 Hz
O2 = -1.0000 Hz
LB1 = 1.00 Hz
TP A = 0.00
B = 0.00
C = 0.00
171.305
153.733
143.845
134.339
132.793
128.680
127.703
127.179
126.532
117.203
114.609
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76.735
66.089
55.627
47.974
46.471
32.910
32.703
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N
HN
O
OMe
200
150
100
50
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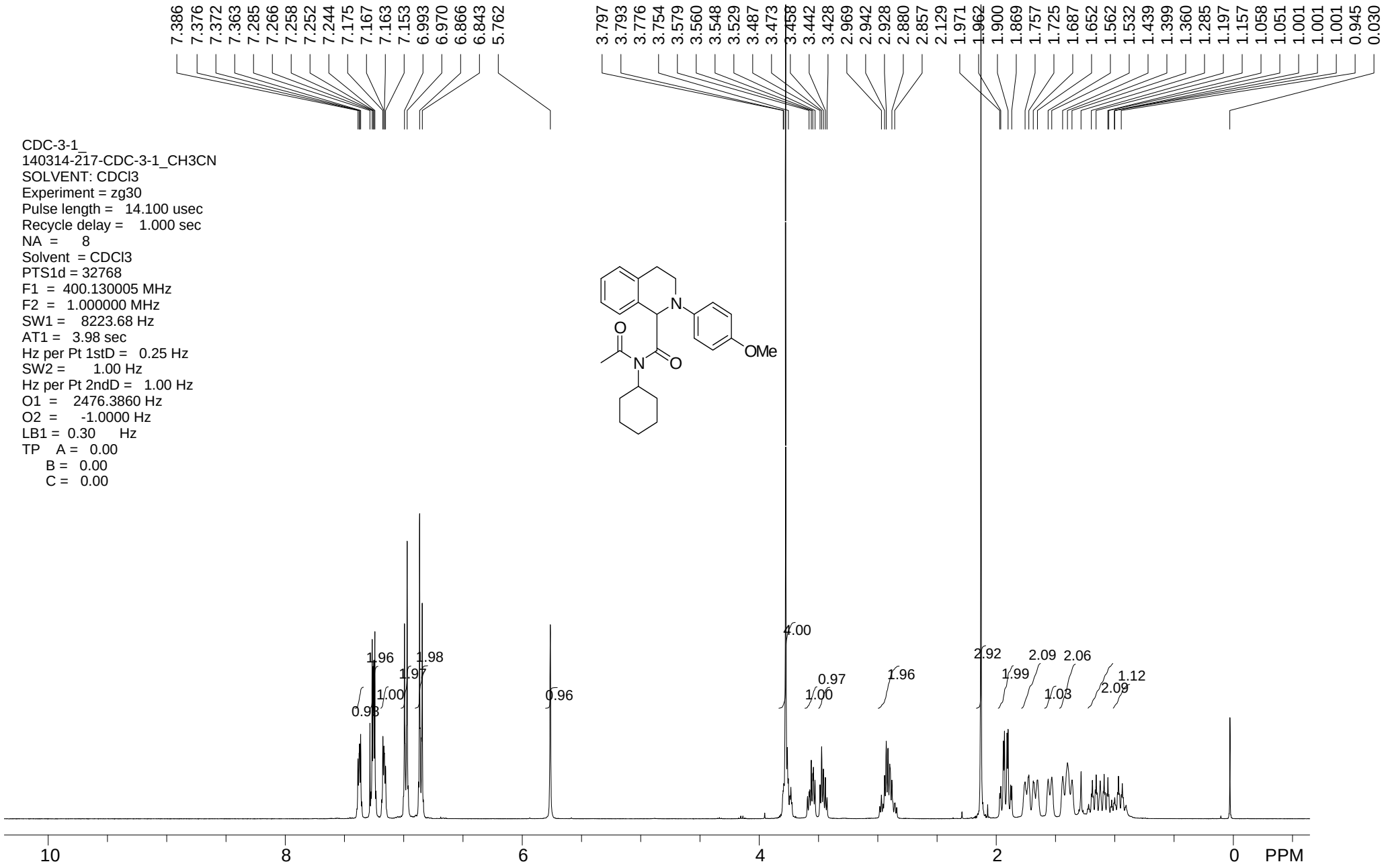
PPM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6.970
6.866
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5.762
3.797
3.793
3.776
3.754
3.579
3.560
3.548
3.529
3.487
3.473
3.458
3.442
3.428
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2.928
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2.857
2.129
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1.962
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1.439
1.399
1.360
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1.157
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1.051
1.001
1.001
1.001
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0.030
CDC-3-1_
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SOLVENT: CDCl3
Experiment = zg30
Pulse length = 14.100 usec
Recycle delay = 1.000 sec
NA = 8
Solvent = CDCl3
PTS1d = 32768
F1 = 400.130005 MHz
F2 = 1.000000 MHz
SW1 = 8223.68 Hz
AT1 = 3.98 sec
Hz per Pt 1stD = 0.25 Hz
SW2 = 1.00 Hz
Hz per Pt 2ndD = 1.00 Hz
O1 = 2476.3860 Hz
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LB1 = 0.30 Hz
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B = 0.00
C = 0.00
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O
N
O
OMe
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1.96
1.00
1.97
1.98
0.96
4.00
1.00
0.97
1.96
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2.09
1.03
2.06
2.09
1.12
10
8
6
4
2
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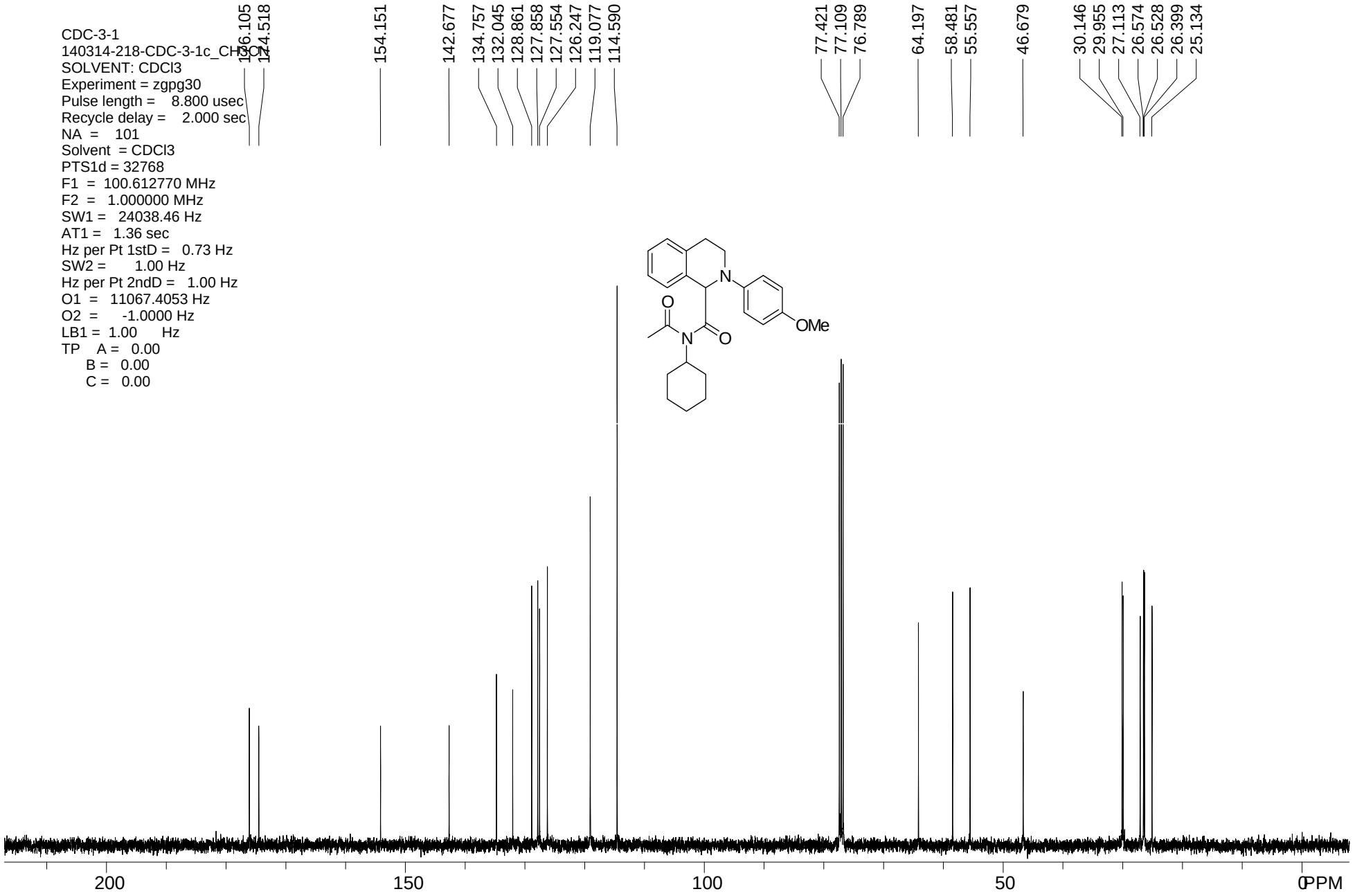
PPM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140314-218-CDC-3-1c_CH3Cl
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Experiment = zgpg30
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Recycle delay = 2.000 sec
NA = 101
Solvent = CDCl3
PTS1d = 32768
F1 = 100.612770 MHz
F2 = 1.000000 MHz
SW1 = 24038.46 Hz
AT1 = 1.36 sec
Hz per Pt 1stD = 0.73 Hz
SW2 = 1.00 Hz
Hz per Pt 2ndD = 1.00 Hz
O1 = 11067.4053 Hz
O2 = -1.0000 Hz
LB1 = 1.00 Hz
TP A = 0.00
B = 0.00
C = 0.00
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154.518
154.151
142.677
134.757
132.045
128.861
127.858
127.554
126.247
119.077
114.590
77.421
77.109
76.789
64.197
58.481
55.557
46.679
30.146
29.955
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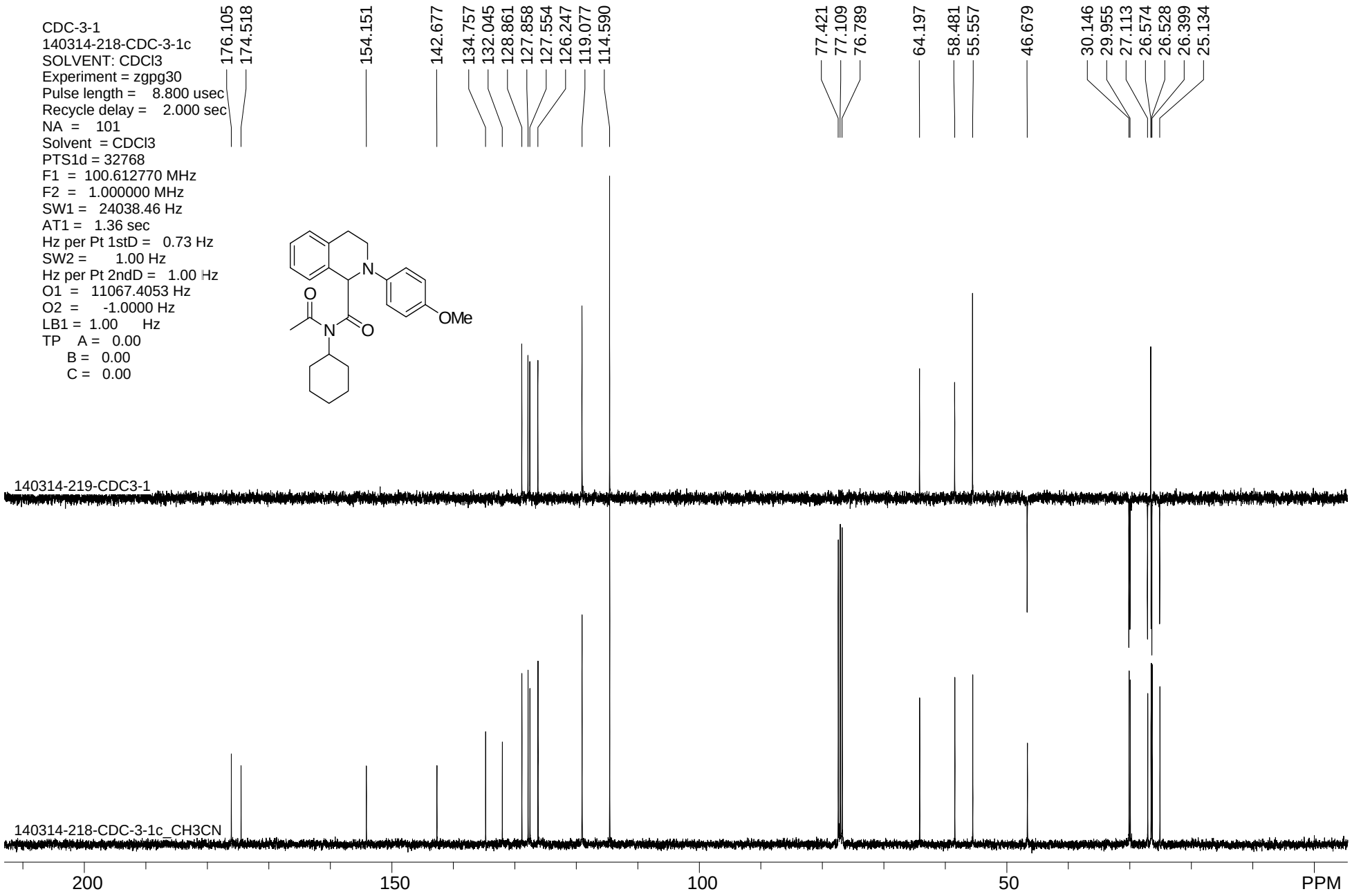
26.528
26.399
25.134
N
O
N
O
OMe
200
150
100
50
0
PPM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Experiment = zgpg30
Pulse length = 8.800 usec
Recycle delay = 2.000 sec
NA = 101
Solvent = CDCl3
PTS1d = 32768
F1 = 100.612770 MHz
F2 = 1.000000 MHz
SW1 = 24038.46 Hz
AT1 = 1.36 sec
Hz per Pt 1stD = 0.73 Hz
SW2 = 1.00 Hz
Hz per Pt 2ndD = 1.00 Hz
O1 = 11067.4053 Hz
O2 = -1.0000 Hz
LB1 = 1.00 Hz
TP A = 0.00
B = 0.00
C = 0.00
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174.518
154.151
142.677
134.757
132.045
128.861
127.858
127.554
126.247
119.077
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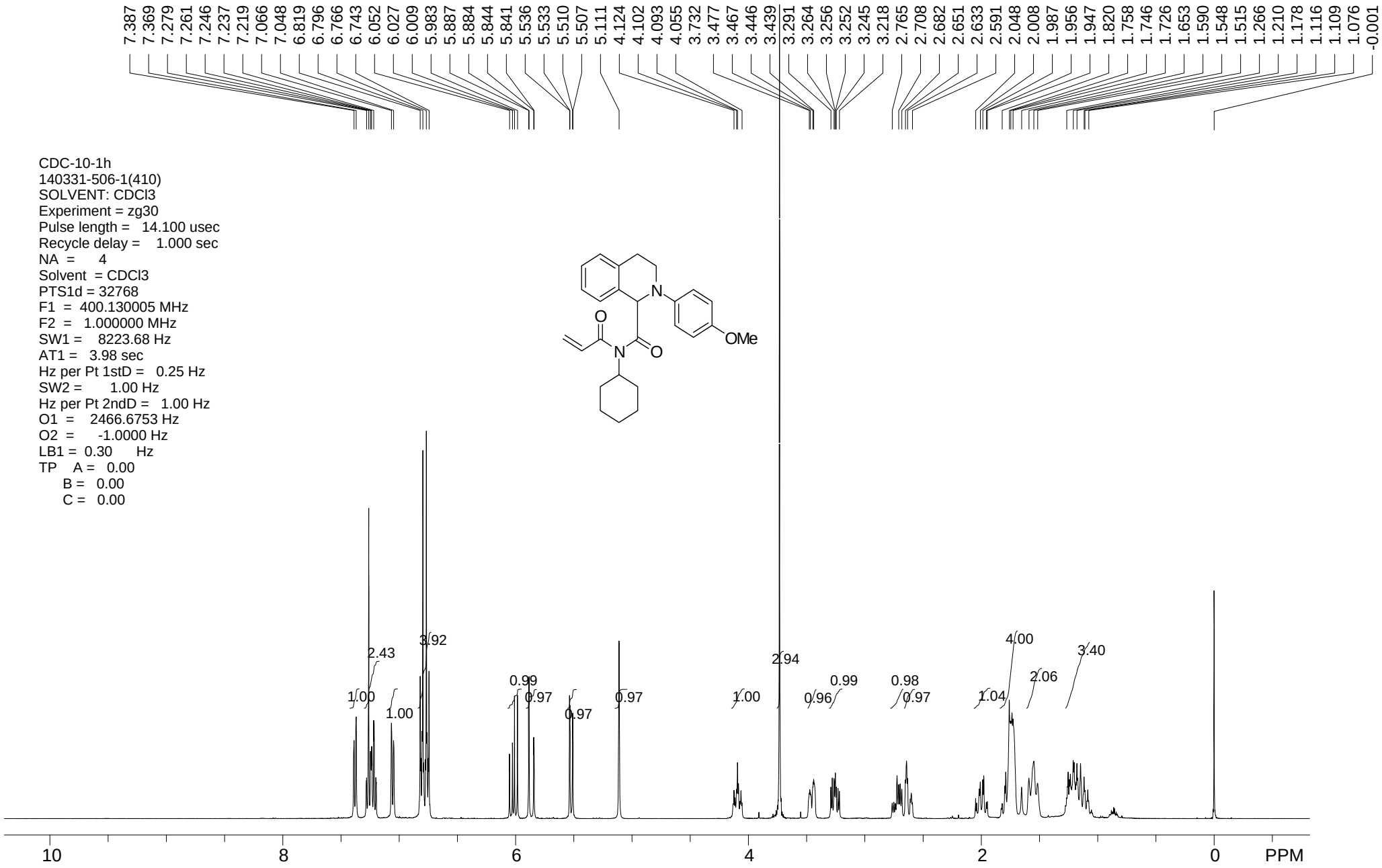
150
100
50
PPM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5.533
5.510
5.507
5.111
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4.093
4.055
3.732
3.477
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3.439
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1.746
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1.116
1.109
1.076
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CDC-10-1h
140331-506-1(410)
SOLVENT: CDCl3
Experiment = zg30
Pulse length = 14.100 usec
Recycle delay = 1.000 sec
NA = 4
Solvent = CDCl3
PTS1d = 32768
F1 = 400.130005 MHz
F2 = 1.000000 MHz
SW1 = 8223.68 Hz
AT1 = 3.98 sec
Hz per Pt 1stD = 0.25 Hz
SW2 = 1.00 Hz
Hz per Pt 2ndD = 1.00 Hz
O1 = 2466.6753 Hz
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LB1 = 0.30 Hz
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B = 0.00
C = 0.00
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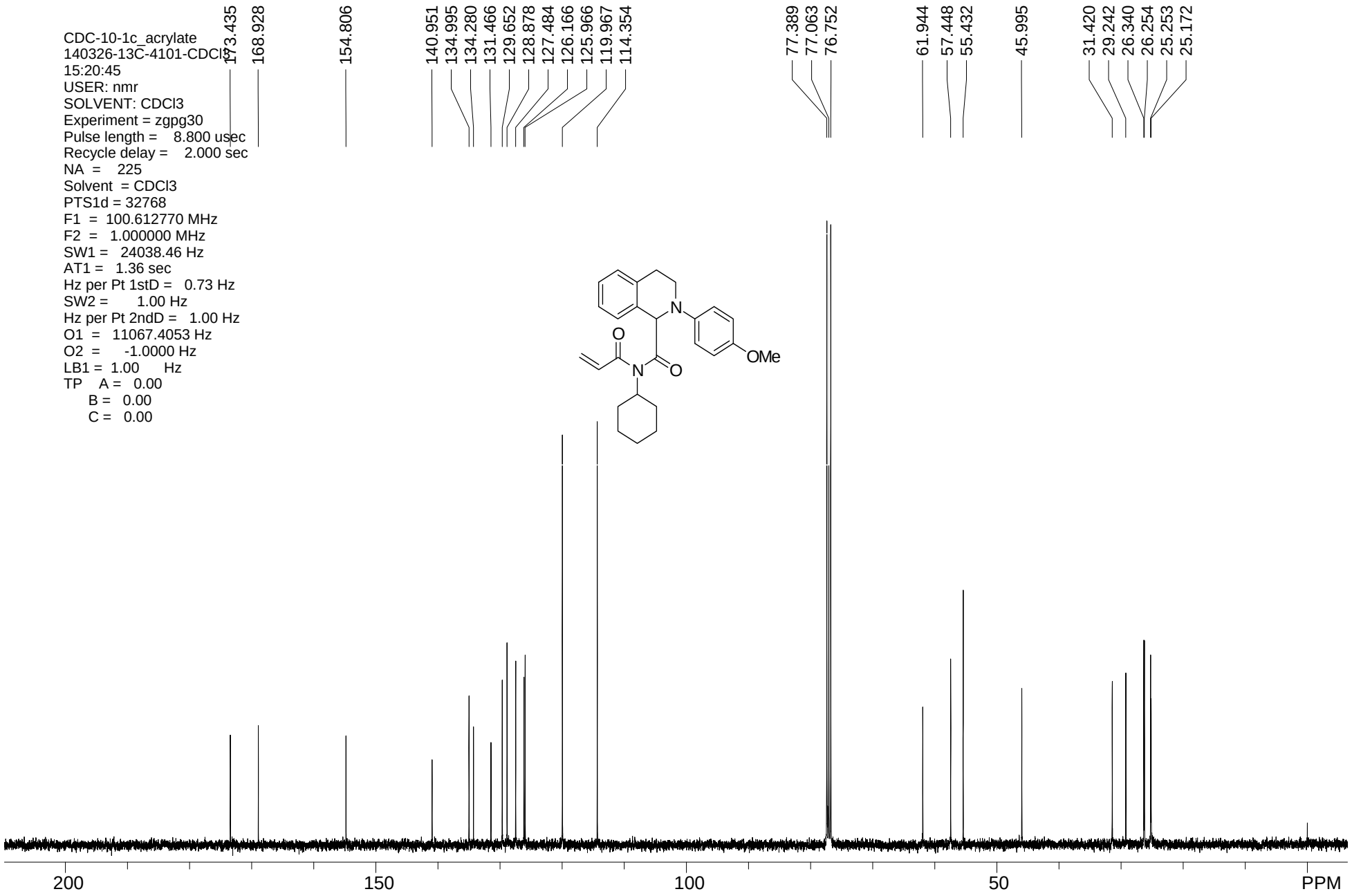
O
N
O
OMe
1.00
2.43
1.00
3.92
0.99
0.97
0.97
0.97
1.00
2.94
0.96
0.99
0.98
0.97
1.04
4.00
2.06
3.40
10
8
6
4
2
0
PPM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SOLVENT: CDCl3
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Recycle delay = 2.000 sec
NA = 225
Solvent = CDCl3
PTS1d = 32768
F1 = 100.612770 MHz
F2 = 1.000000 MHz
SW1 = 24038.46 Hz
AT1 = 1.36 sec
Hz per Pt 1stD = 0.73 Hz
SW2 = 1.00 Hz
Hz per Pt 2ndD = 1.00 Hz
O1 = 11067.4053 Hz
O2 = -1.0000 Hz
LB1 = 1.00 Hz
TP A = 0.00
B = 0.00
C = 0.00
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134.280
131.466
129.652
128.878
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126.166
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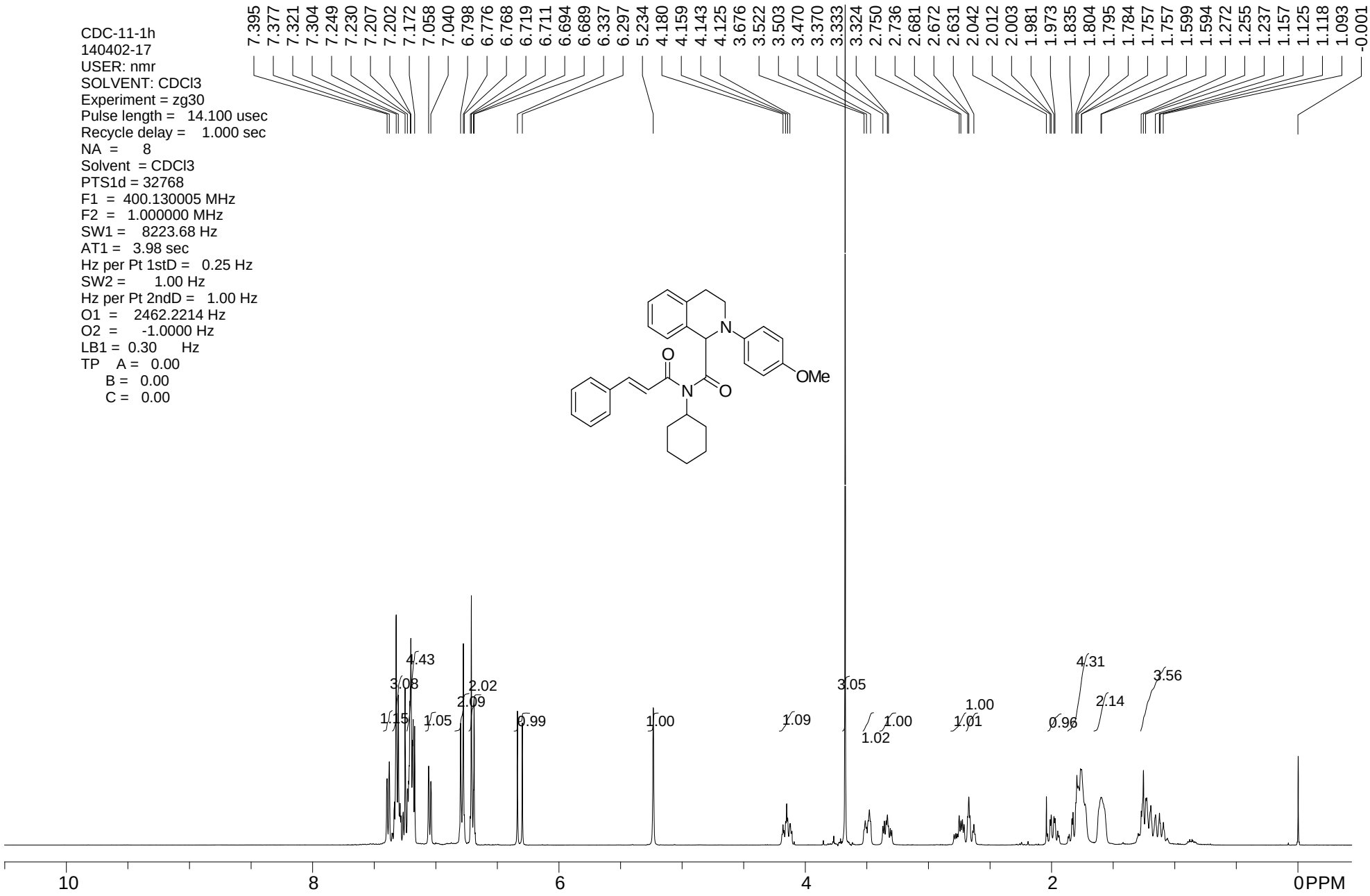
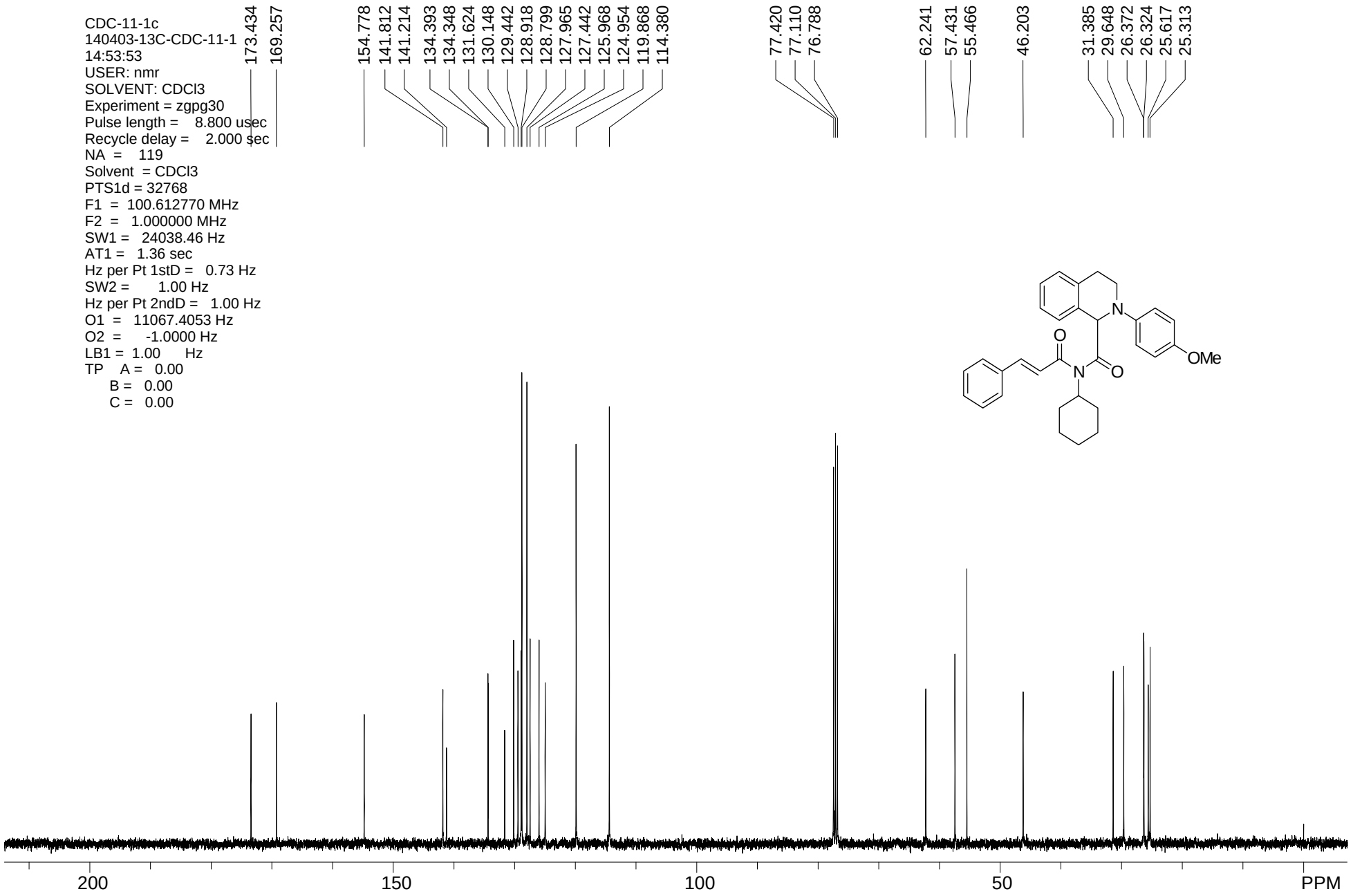
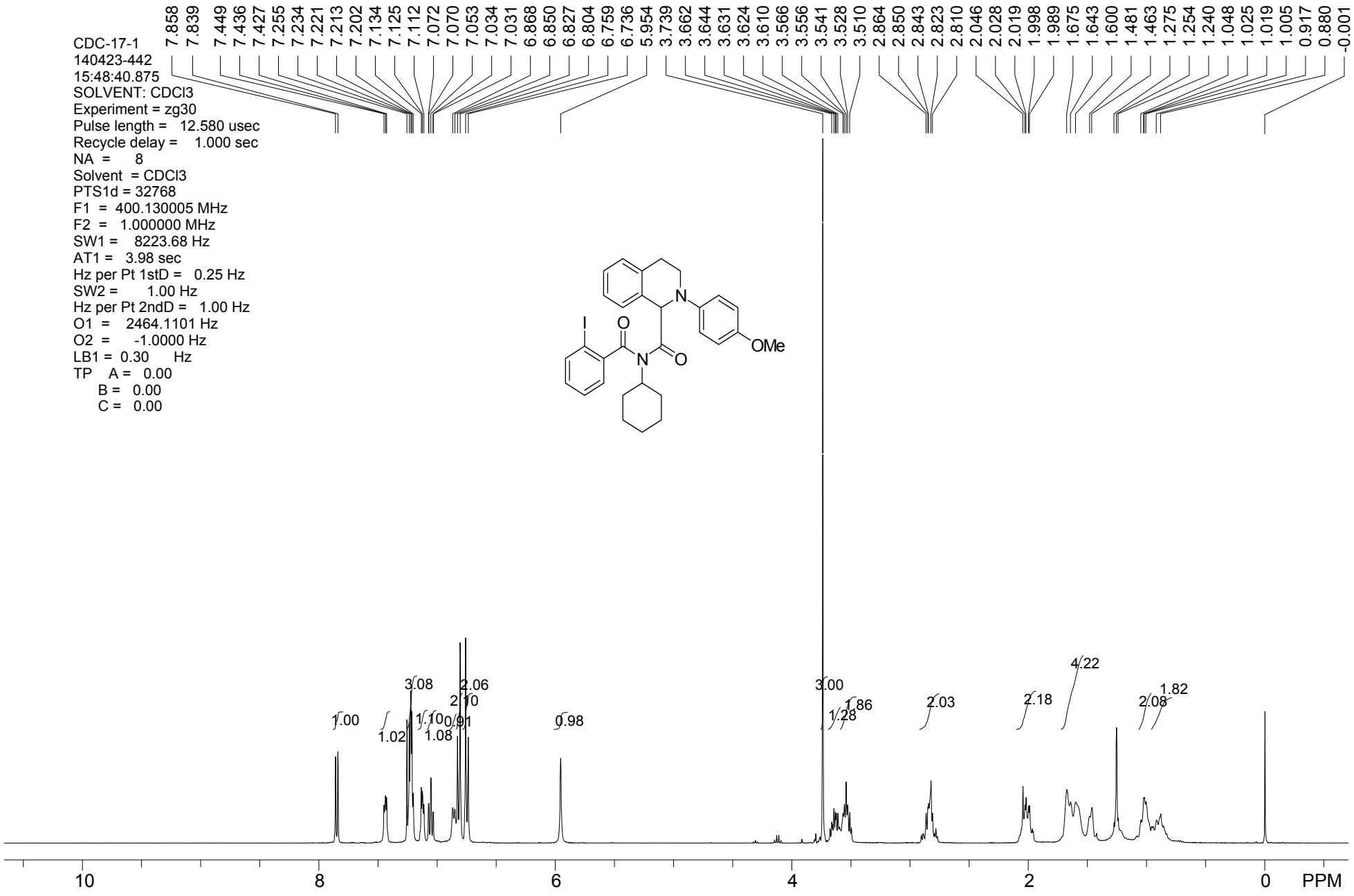
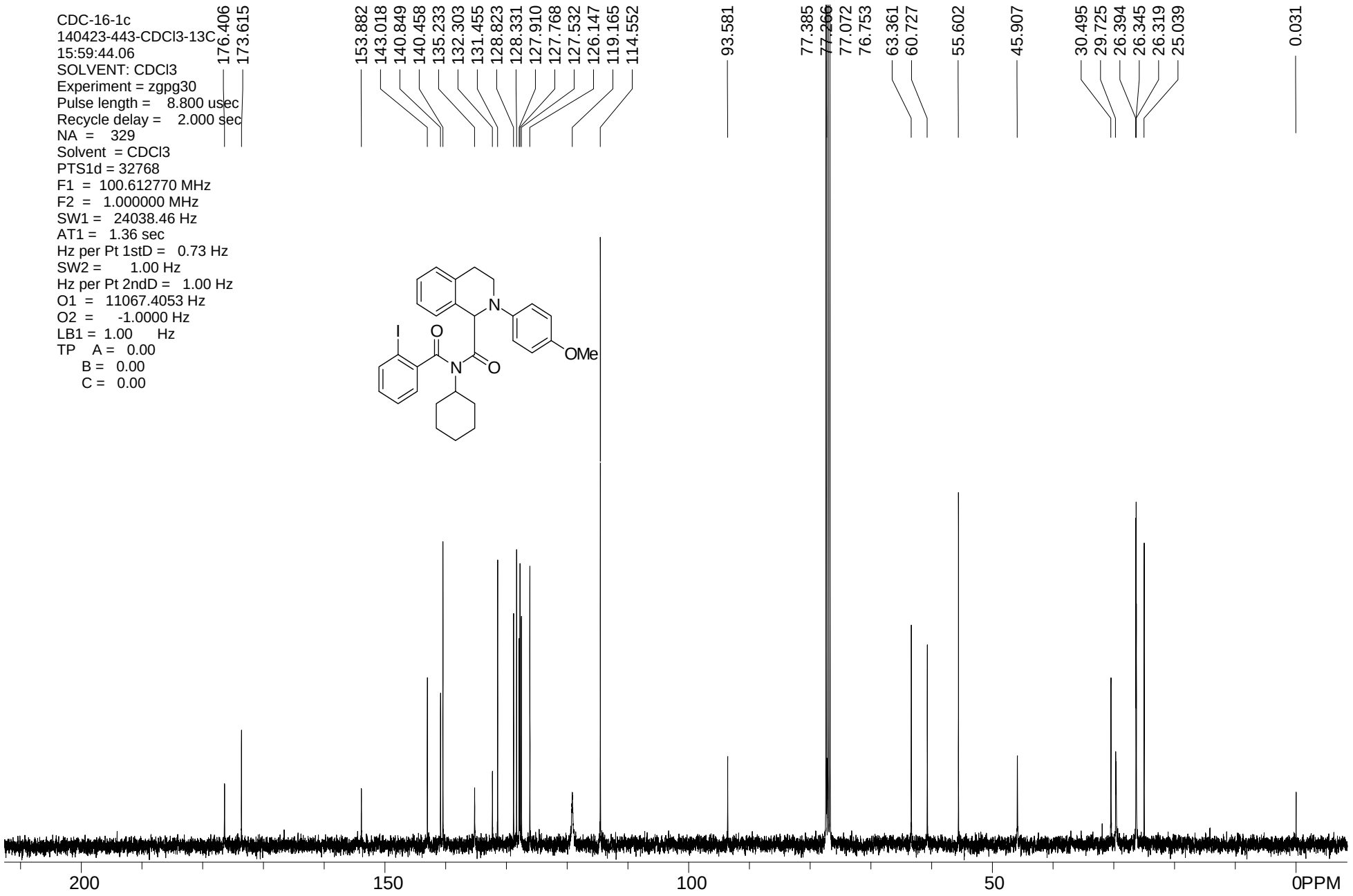
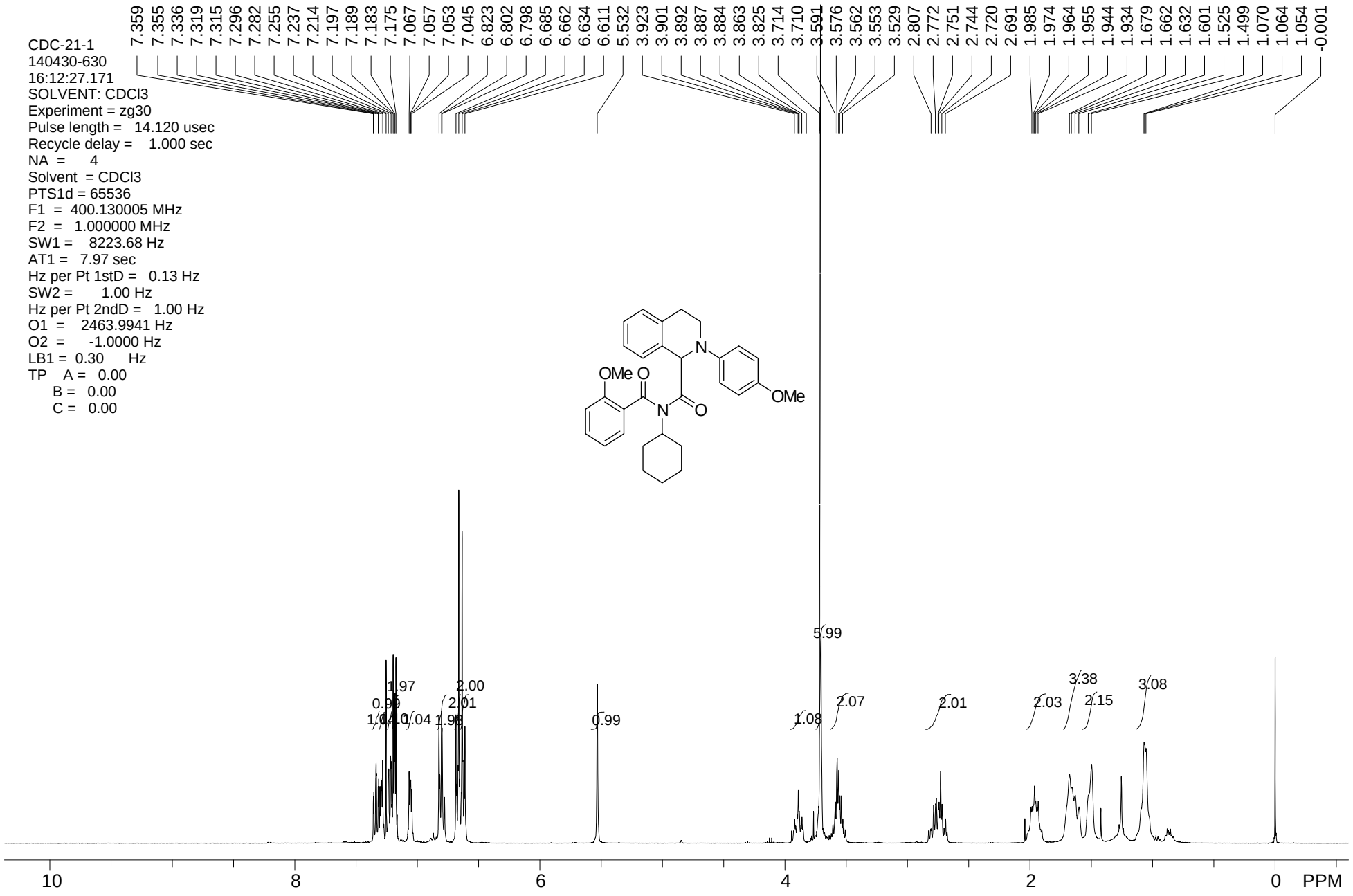
119.967
114.354
77.389
77.063
76.752
61.944
57.448
55.432
45.995
31.420
29.242
26.340
26.254
25.253
25.172
N
O
N
O
OMe
200
150
100
50
PPM

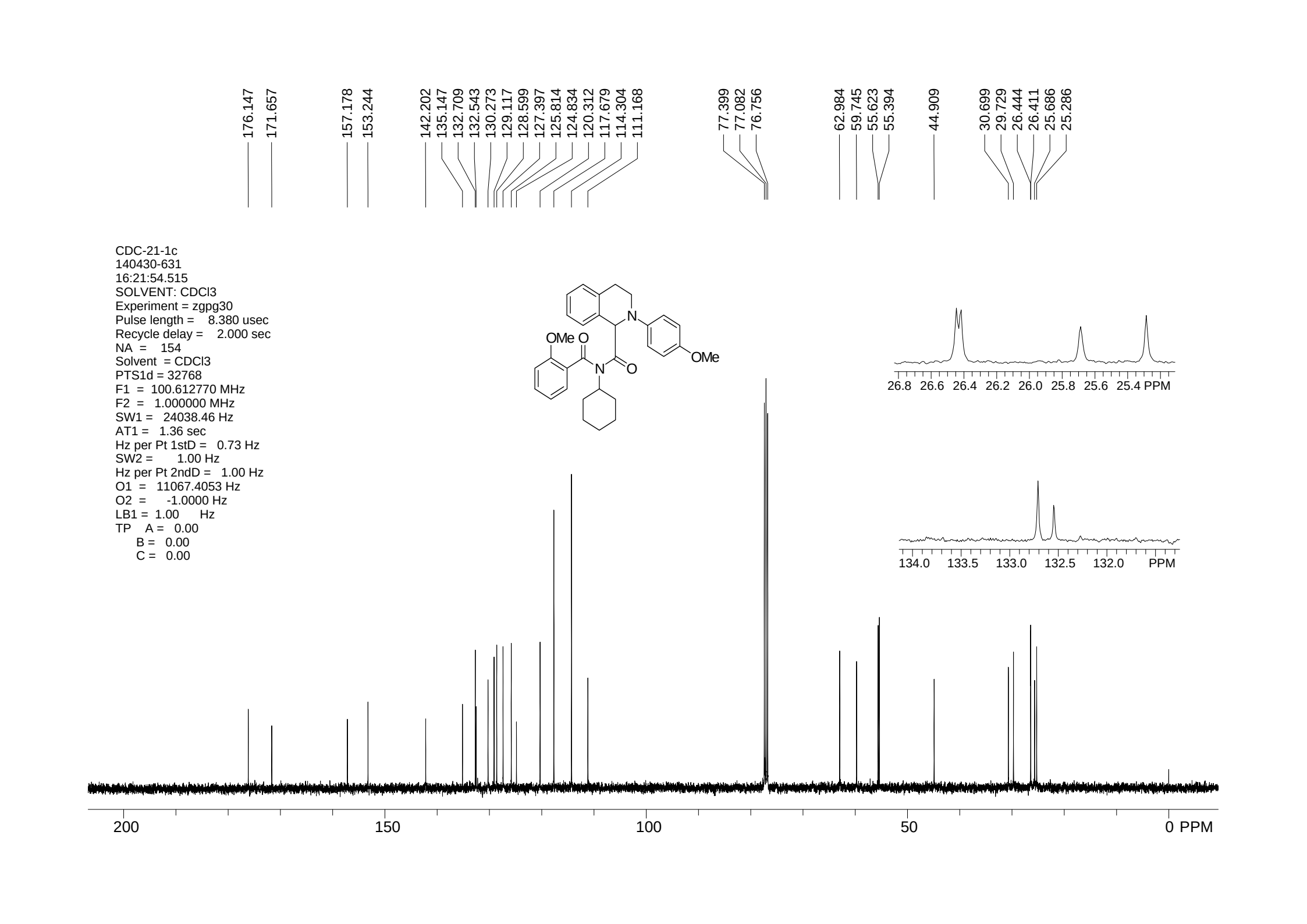

CDC-11-1h
140402-17
USER: nmr
SOLVENT: CDCl3
Experiment = zg30
Pulse length = 14.100 usec
Recycle delay = 1.000 sec
NA = 8
Solvent = CDCl3
PTS1d = 32768
F1 = 400.130005 MHz
F2 = 1.000000 MHz
SW1 = 8223.68 Hz
AT1 = 3.98 sec
Hz per Pt 1stD = 0.25 Hz
SW2 = 1.00 Hz
Hz per Pt 2ndD = 1.00 Hz
O1 = 2462.2214 Hz
O2 = -1.0000 Hz
LB1 = 0.30 Hz
TP A = 0.00
B = 0.00
C = 0.00
7.395 7.377 7.321 7.304 7.249 7.230 7.207 7.202 7.172 7.058 7.040 6.798 6.776 6.768 6.719 6.711 6.694 6.689 6.337 6.297 5.234 4.180 4.159 4.143 4.125 3.676 3.522 3.503 3.470 3.370 3.333 3.324 2.750 2.736 2.681 2.672 2.631 2.042 2.012 2.003 1.981 1.973 1.835 1.804 1.795 1.784 1.757 1.757 1.599 1.594 1.272 1.255 1.237 1.157 1.125 1.118 1.093 -0.001
N
O
N
O
OMe
4.43
3.08
1.15
1.05
2.02
2.09
0.99
1.00
1.09
3.05
1.02
1.00
1.00
1.01
0.96
4.31
2.14
3.56
10
8
6
4
2
0 PPM

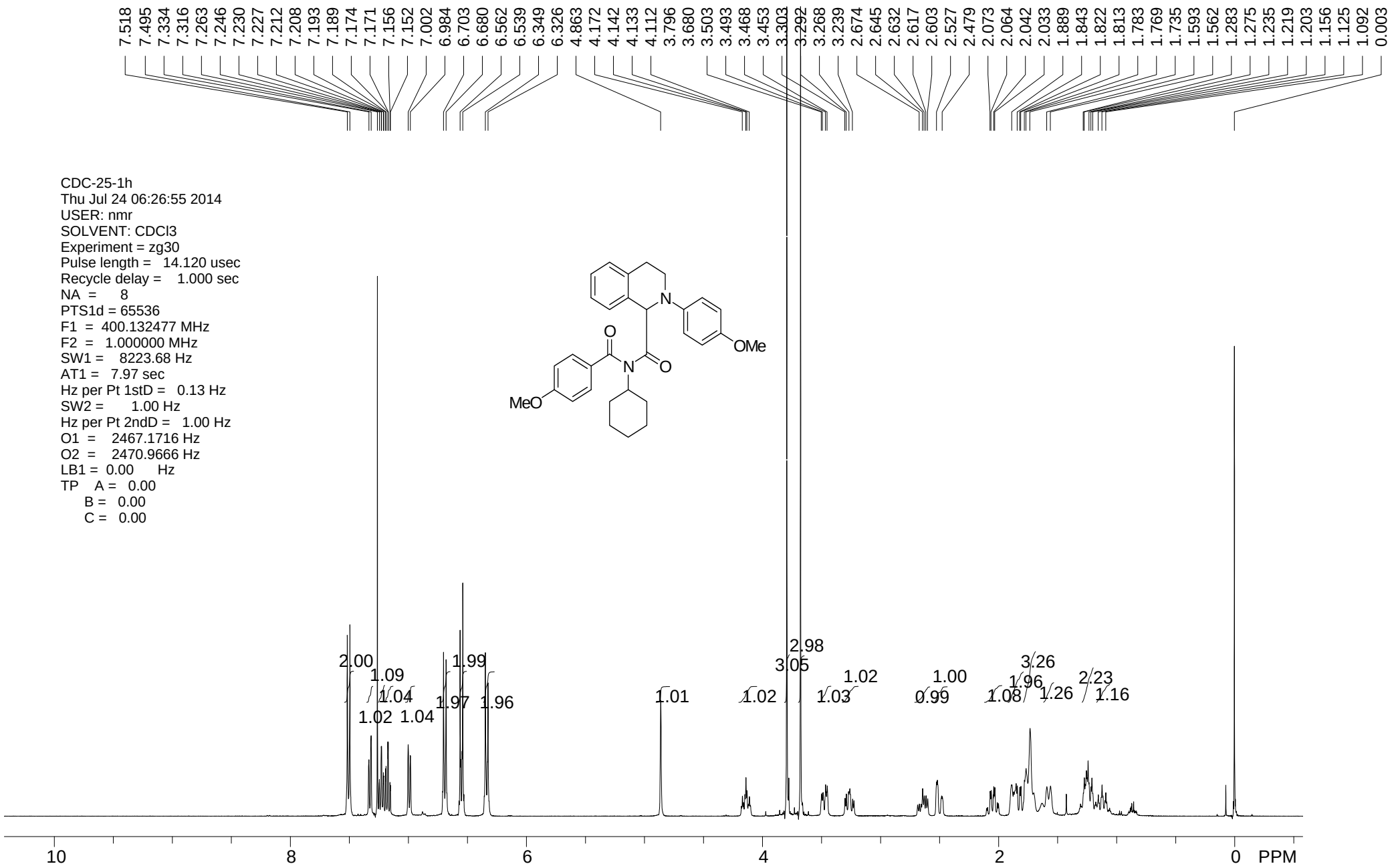

CDC-11-1c
140403-13C-CDC-11-1
14:53:53
USER: nmr
SOLVENT: CDCl3
Experiment = zgpg30
Pulse length = 8.800 usec
Recycle delay = 2.000 sec
NA = 119
Solvent = CDCl3
PTS1d = 32768
F1 = 100.612770 MHz
F2 = 1.000000 MHz
SW1 = 24038.46 Hz
AT1 = 1.36 sec
Hz per Pt 1stD = 0.73 Hz
SW2 = 1.00 Hz
Hz per Pt 2ndD = 1.00 Hz
O1 = 11067.4053 Hz
O2 = -1.0000 Hz
LB1 = 1.00 Hz
TP A = 0.00
B = 0.00
C = 0.00
173.434
169.257
154.778
141.812
141.214
134.393
134.348
131.624
130.148
129.442
128.918
128.799
127.965
127.442
125.968
124.954
119.868
114.380
77.420
77.110
76.788
62.241
57.431
55.466
46.203
31.385
29.648
26.372
26.324
25.617
25.313
O
N
O
N
O
OMe
200
150
100
50
PPM

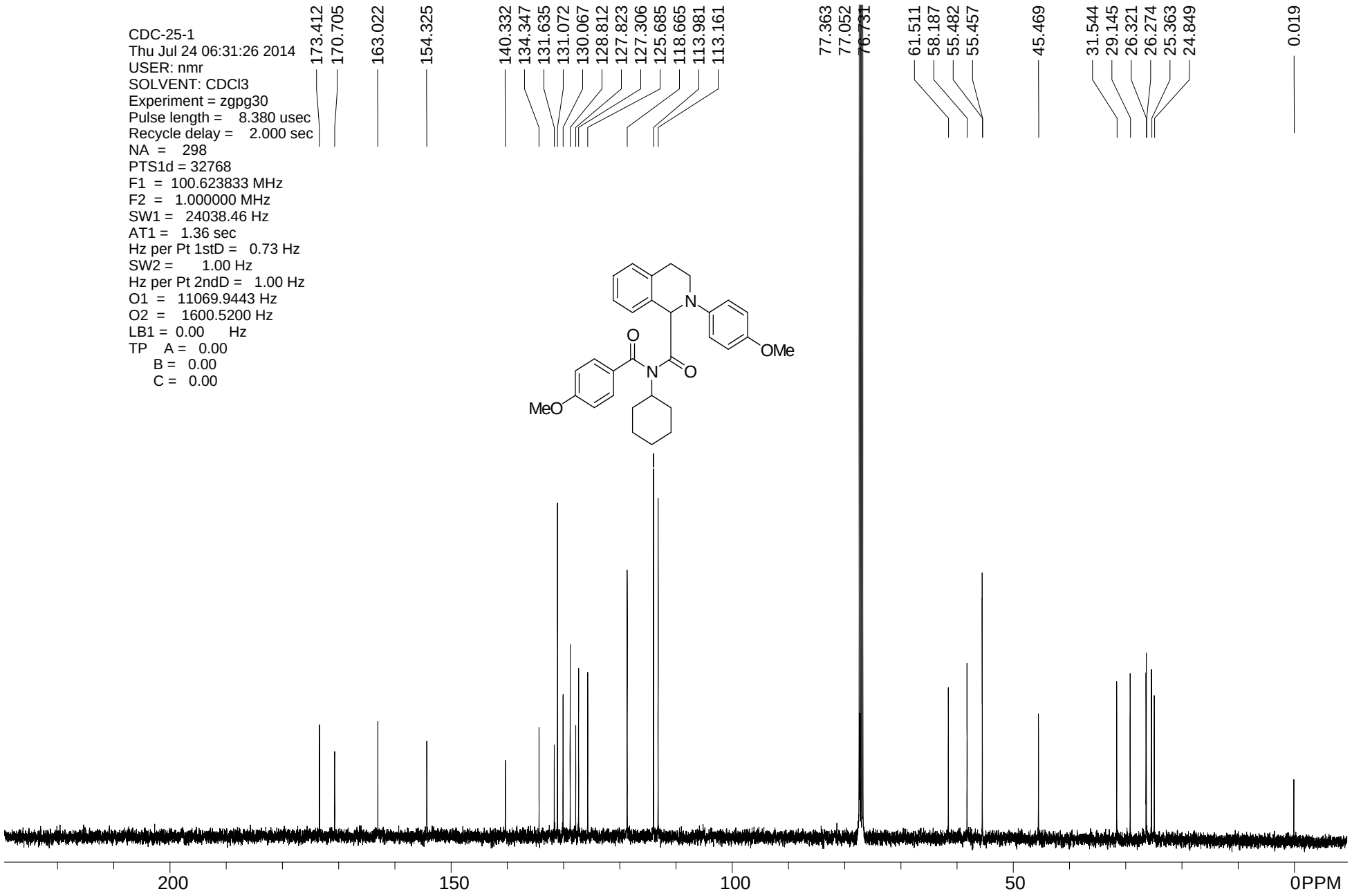

7.858
7.839
7.449
7.436
7.427
7.255
7.234
7.221
7.213
7.202
7.134
7.125
7.112
7.072
7.070
7.053
7.034
7.031
6.868
6.850
6.827
6.804
6.759
6.736
5.954
3.739
3.662
3.644
3.631
3.624
3.610
3.566
3.556
3.541
3.528
3.510
2.864
2.850
2.843
2.823
2.810
2.046
2.028
2.019
1.998
1.989
1.675
1.643
1.600
1.481
1.463
1.275
1.254
1.240
1.048
1.025
1.019
1.005
0.917
0.880
-0.001
CDC-17-1
140423-442
15:48:40.875
SOLVENT: CDCl3
Experiment = zg30
Pulse length = 12.580 usec
Recycle delay = 1.000 sec
NA = 8
Solvent = CDCl3
PTS1d = 32768
F1 = 400.130005 MHz
F2 = 1.000000 MHz
SW1 = 8223.68 Hz
AT1 = 3.98 sec
Hz per Pt 1stD = 0.25 Hz
SW2 = 1.00 Hz
Hz per Pt 2ndD = 1.00 Hz
O1 = 2464.1101 Hz
O2 = -1.0000 Hz
LB1 = 0.30 Hz
TP A = 0.00
B = 0.00
C = 0.00
I
O
N
O
N
OMe
1.00
1.02
3.08
1.10
1.08
2.06
2.10
0.91
0.98
3.00
1.28
1.86
2.03
2.18
4.22
2.08
1.82
10
8
6
4
2
0
PPM

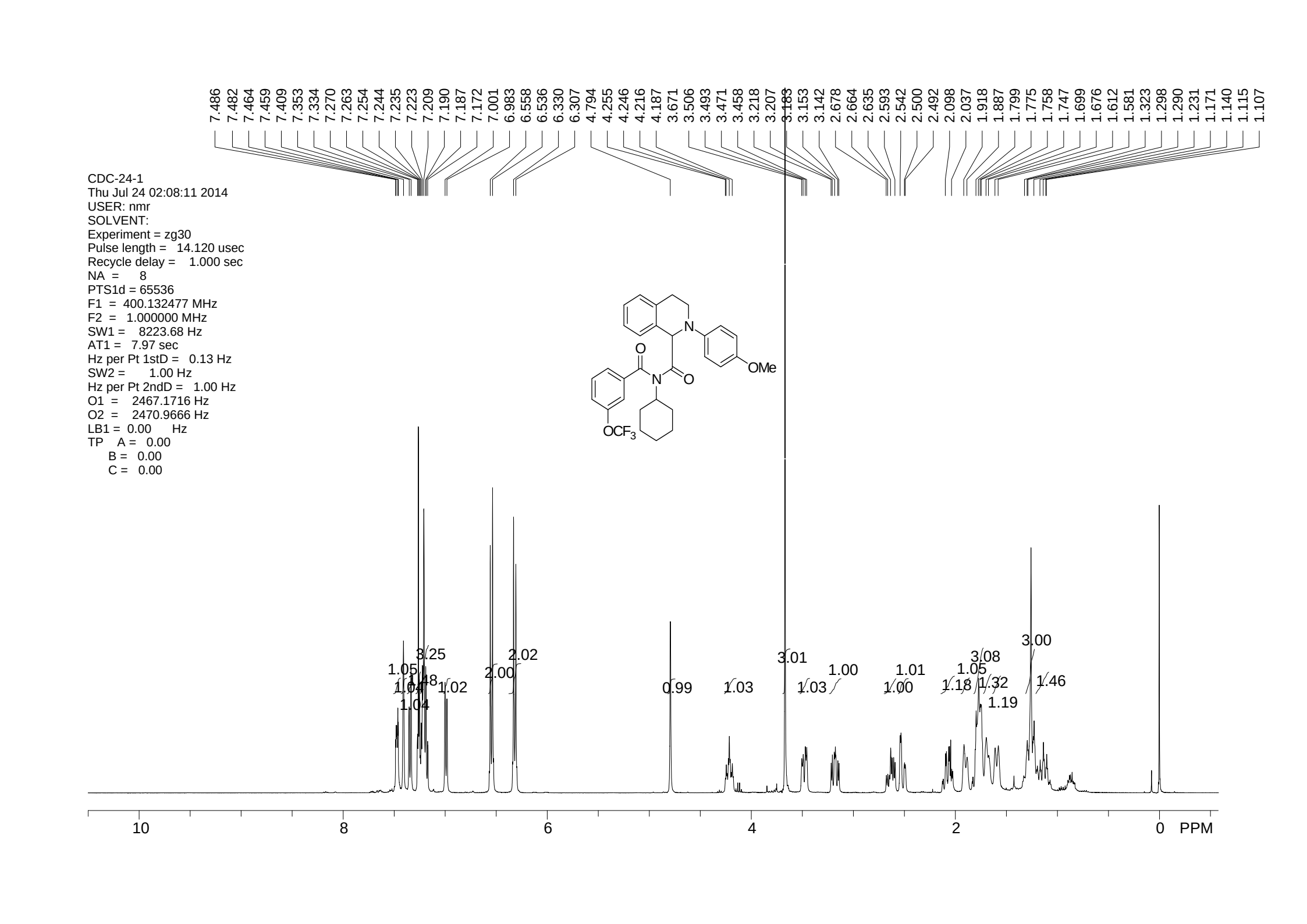

CDC-16-1c
140423-443-CDCl3-13C
15:59:44.06
SOLVENT: CDCl3
Experiment = zgpg30
Pulse length = 8.800 usec
Recycle delay = 2.000 sec
NA = 329
Solvent = CDCl3
PTS1d = 32768
F1 = 100.612770 MHz
F2 = 1.000000 MHz
SW1 = 24038.46 Hz
AT1 = 1.36 sec
Hz per Pt 1stD = 0.73 Hz
SW2 = 1.00 Hz
Hz per Pt 2ndD = 1.00 Hz
O1 = 11067.4053 Hz
O2 = -1.0000 Hz
LB1 = 1.00 Hz
TP A = 0.00
B = 0.00
C = 0.00
176.406
173.615
153.882
143.018
140.849
140.458
135.233
132.303
131.455
128.823
128.331
127.910
127.768
127.532
126.147
119.165
114.552
93.581
77.385
77.266
77.072
76.753
63.361
60.727
55.602
45.907
30.495
29.725
26.394
26.345
26.319
25.039
0.031
I
O
N
O
N
OMe
200
150
100
50
0PPM

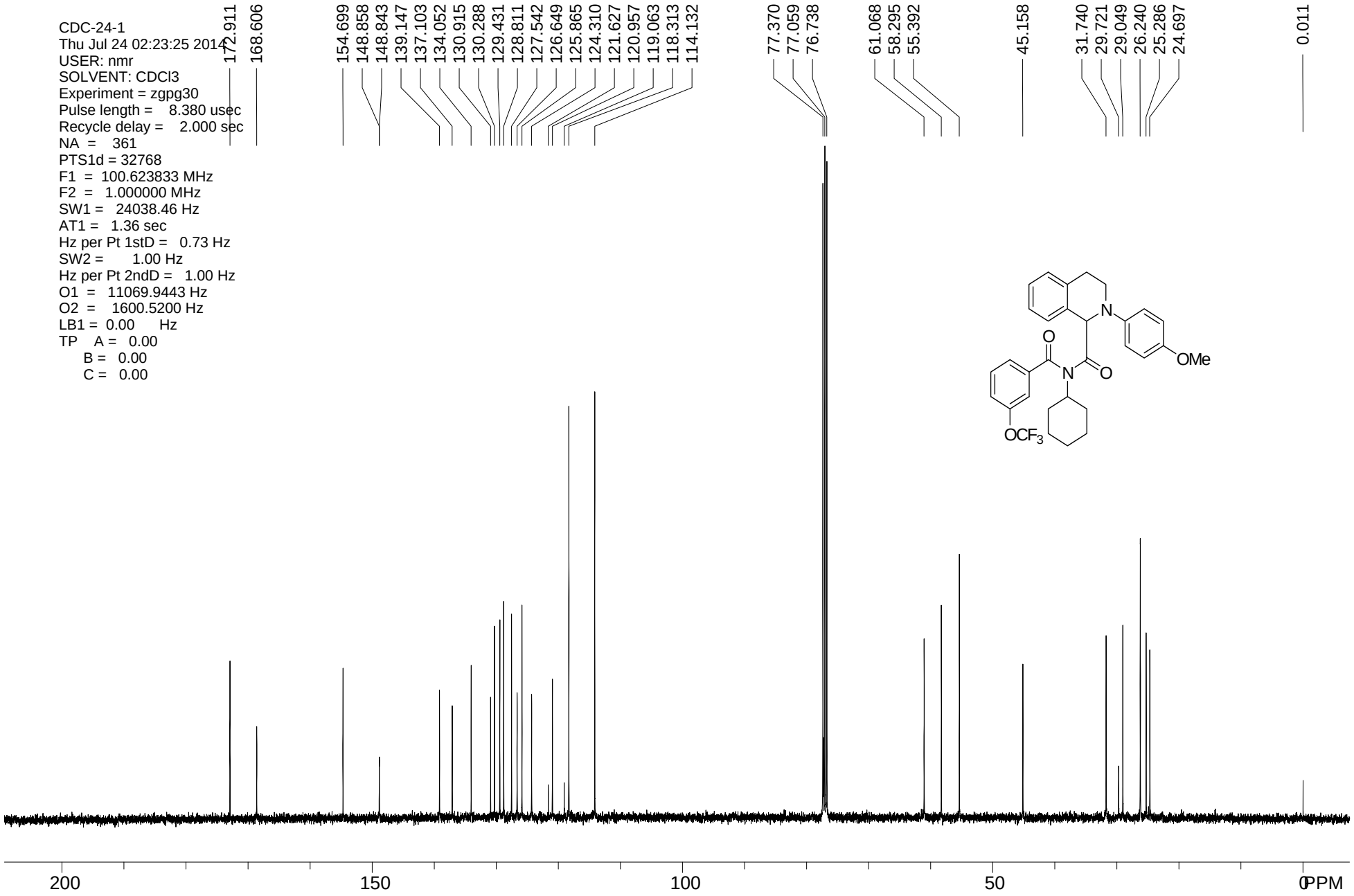

CDC-21-1
140430-630
16:12:27.171
SOLVENT: CDCl3
Experiment = zg30
Pulse length = 14.120 usec
Recycle delay = 1.000 sec
NA = 4
Solvent = CDCl3
PTS1d = 65536
F1 = 400.130005 MHz
F2 = 1.000000 MHz
SW1 = 8223.68 Hz
AT1 = 7.97 sec
Hz per Pt 1stD = 0.13 Hz
SW2 = 1.00 Hz
Hz per Pt 2ndD = 1.00 Hz
O1 = 2463.9941 Hz
O2 = -1.0000 Hz
LB1 = 0.30 Hz
TP A = 0.00
B = 0.00
C = 0.00
7.359 7.355 7.336 7.319 7.315 7.296 7.282 7.255 7.237 7.214 7.197 7.189 7.183 7.175 7.067 7.057 7.053 7.045 6.823 6.802 6.798 6.685 6.662 6.634 6.611 5.532 3.923 3.901 3.892 3.887 3.884 3.863 3.825 3.714 3.710 3.591 3.576 3.562 3.553 3.529 2.807 2.772 2.751 2.744 2.720 2.691 1.985 1.974 1.964 1.955 1.944 1.934 1.679 1.662 1.632 1.601 1.525 1.499 1.070 1.064 1.054 -0.001
OMe
O
N
O
N
OMe
5.99
1.97
2.00
0.99
2.01
1.04
1.04
1.04
1.98
0.99
1.08
2.07
2.01
2.03
3.38
2.15
3.08
10
8
6
4
2
0
PPM

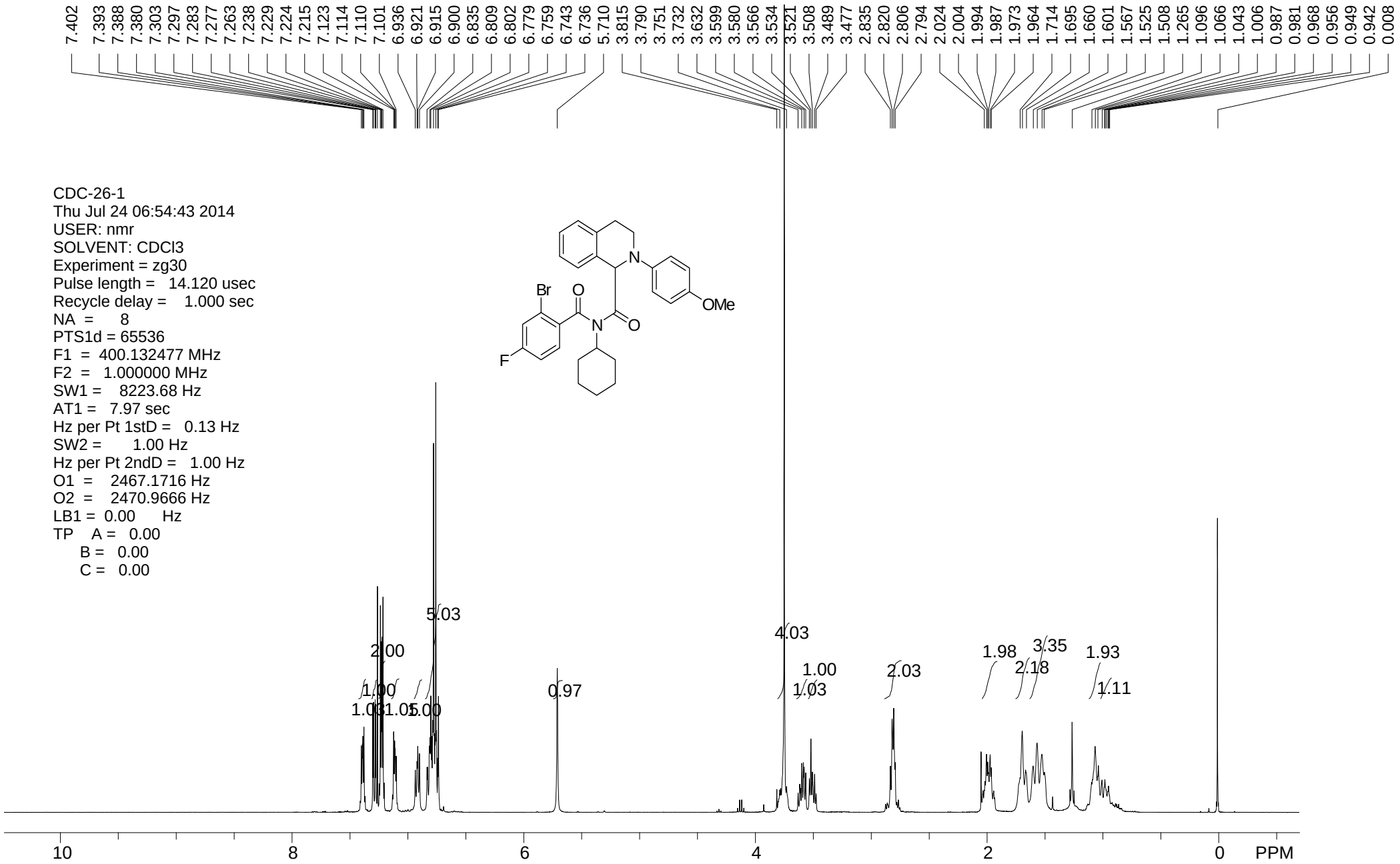

176.147
171.657
157.178
153.244
142.202
135.147
132.709
132.543
130.273
129.117
128.599
127.397
125.814
124.834
120.312
117.679
114.304
111.168
77.399
77.082
76.756
62.984
59.745
55.623
55.394
44.909
30.699
29.729
26.444
26.411
25.686
25.286
CDC-21-1c
140430-631
16:21:54.515
SOLVENT: CDCl3
Experiment = zgpg30
Pulse length = 8.380 usec
Recycle delay = 2.000 sec
NA = 154
Solvent = CDCl3
PTS1d = 32768
F1 = 100.612770 MHz
F2 = 1.000000 MHz
SW1 = 24038.46 Hz
AT1 = 1.36 sec
Hz per Pt 1stD = 0.73 Hz
SW2 = 1.00 Hz
Hz per Pt 2ndD = 1.00 Hz
O1 = 11067.4053 Hz
O2 = -1.0000 Hz
LB1 = 1.00 Hz
TP A = 0.00
B = 0.00
C = 0.00
OMe
O
N
O
N
OMe
26.8 26.6 26.4 26.2 26.0 25.8 25.6 25.4 PPM
134.0 133.5 133.0 132.5 132.0 PPM
200
150
100
50
0 PPM

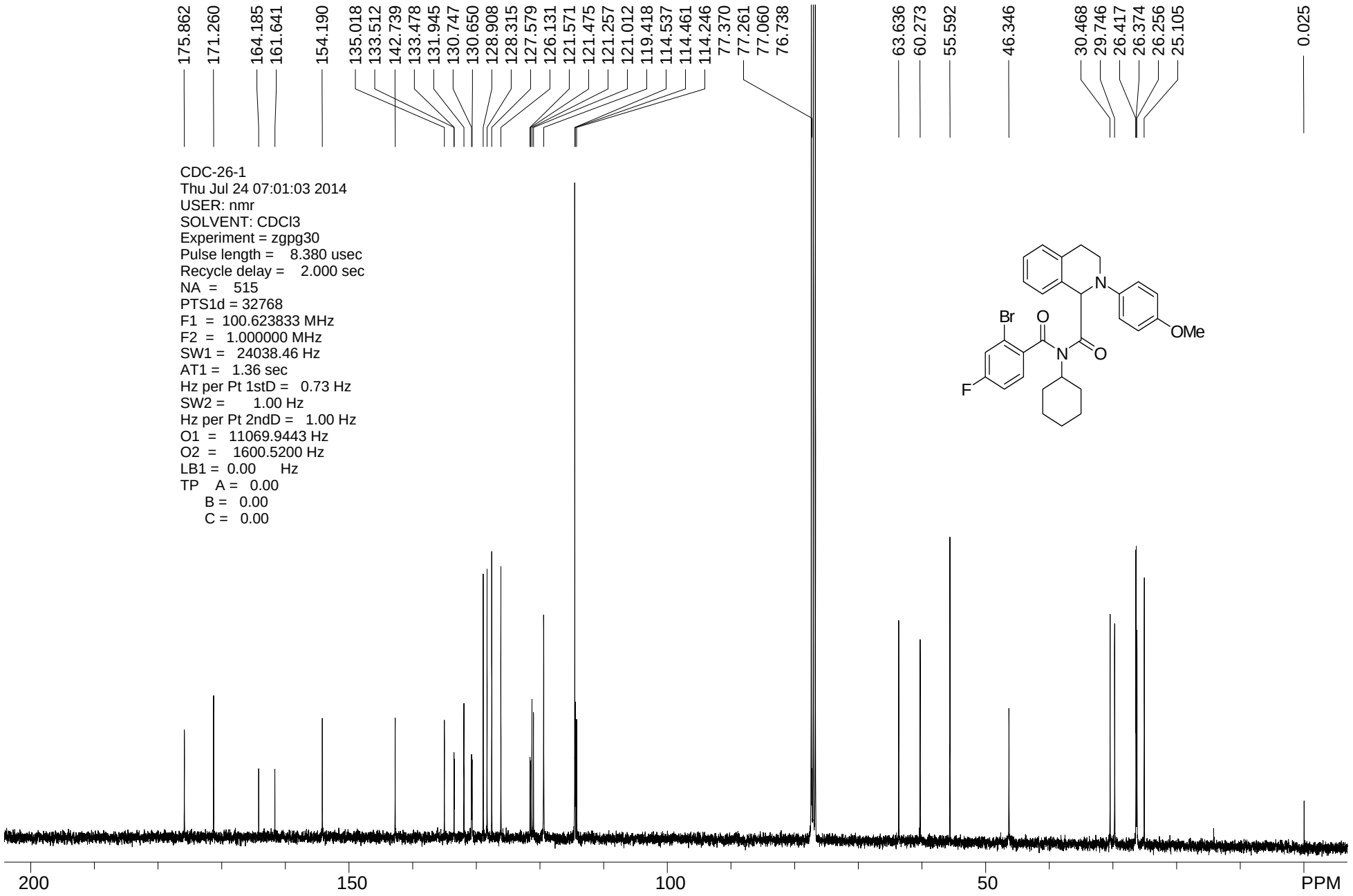

7.518 7.495 7.334 7.316 7.263 7.246 7.230 7.227 7.212 7.208 7.193 7.189 7.174 7.171 7.156 7.152 7.002 6.984 6.703 6.680 6.562 6.539 6.349 6.326 4.863 4.172 4.142 4.133 4.112 3.796 3.680 3.503 3.493 3.468 3.453 3.303 3.292 3.268 3.239 2.674 2.645 2.632 2.617 2.603 2.527 2.479 2.073 2.064 2.042 2.033 1.889 1.843 1.822 1.813 1.783 1.769 1.735 1.593 1.562 1.283 1.275 1.235 1.219 1.203 1.156 1.125 1.092 0.003
CDC-25-1h
Thu Jul 24 06:26:55 2014
USER: nmr
SOLVENT: CDCl3
Experiment = zg30
Pulse length = 14.120 usec
Recycle delay = 1.000 sec
NA = 8
PTS1d = 65536
F1 = 400.132477 MHz
F2 = 1.000000 MHz
SW1 = 8223.68 Hz
AT1 = 7.97 sec
Hz per Pt 1stD = 0.13 Hz
SW2 = 1.00 Hz
Hz per Pt 2ndD = 1.00 Hz
O1 = 2467.1716 Hz
O2 = 2470.9666 Hz
LB1 = 0.00 Hz
TP A = 0.00
B = 0.00
C = 0.00
N
O
N
O
OMe
MeO
2.00
1.09
1.04
1.02
1.04
1.99
1.97
1.96
1.01
1.02
2.98
3.05
1.03
1.02
0.99
1.00
1.08
3.26
1.96
1.26
2.23
1.16
10
8
6
4
2
0
PPM

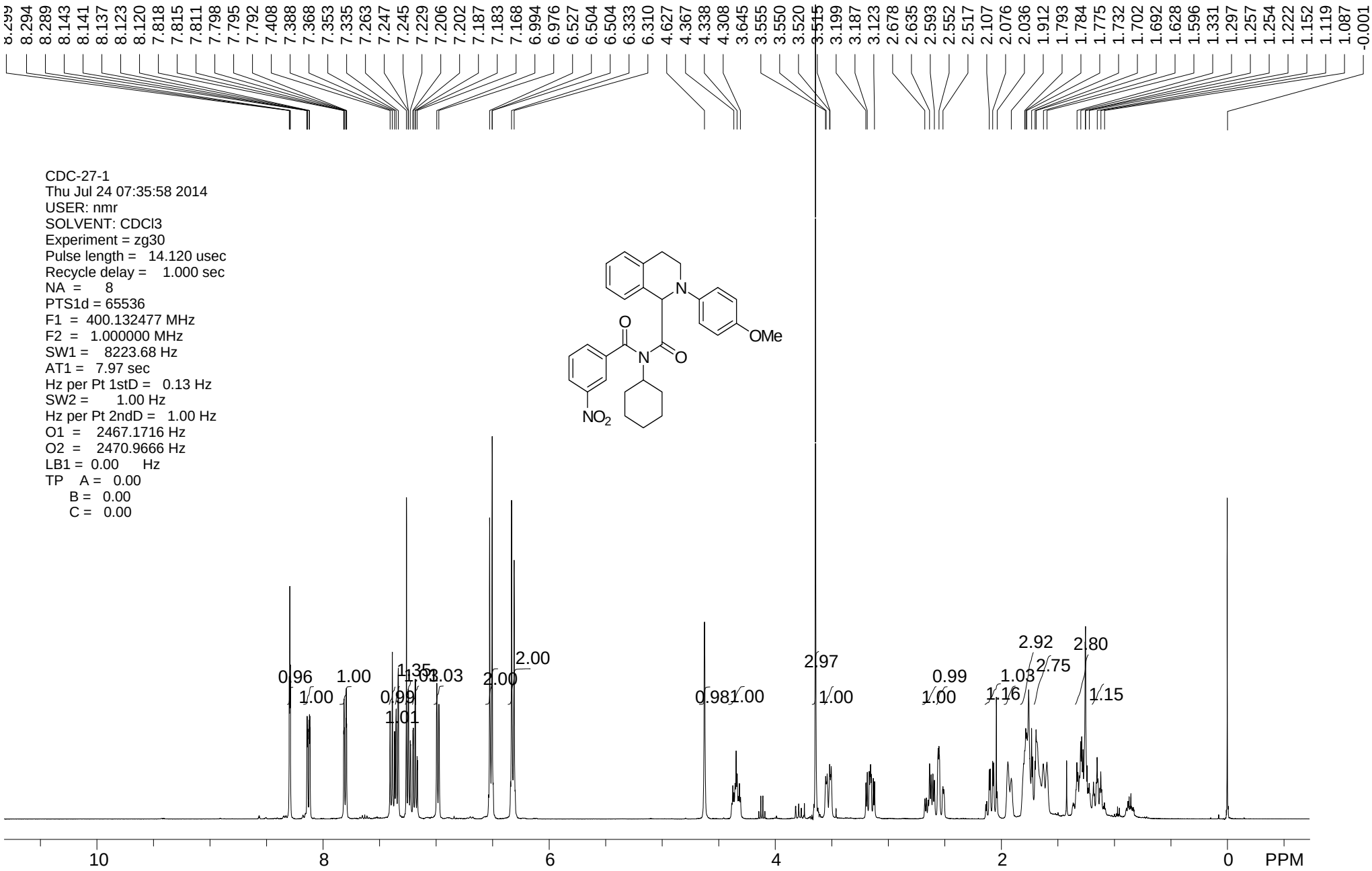

CDC-25-1
Thu Jul 24 06:31:26 2014
USER: nmr
SOLVENT: CDCl3
Experiment = zgpg30
Pulse length = 8.380 usec
Recycle delay = 2.000 sec
NA = 298
PTS1d = 32768
F1 = 100.623833 MHz
F2 = 1.000000 MHz
SW1 = 24038.46 Hz
AT1 = 1.36 sec
Hz per Pt 1stD = 0.73 Hz
SW2 = 1.00 Hz
Hz per Pt 2ndD = 1.00 Hz
O1 = 11069.9443 Hz
O2 = 1600.5200 Hz
LB1 = 0.00 Hz
TP A = 0.00
B = 0.00
C = 0.00
173.412
170.705
163.022
154.325
140.332
134.347
131.635
131.072
130.067
128.812
127.823
127.306
125.685
118.665
113.981
113.161
77.363
77.052
76.731
61.511
58.187
55.482
55.457
45.469
31.544
29.145
26.321
26.274
25.363
24.849
0.019
N
O
OMe
N
O
MeO
200
150
100
50
0PPM

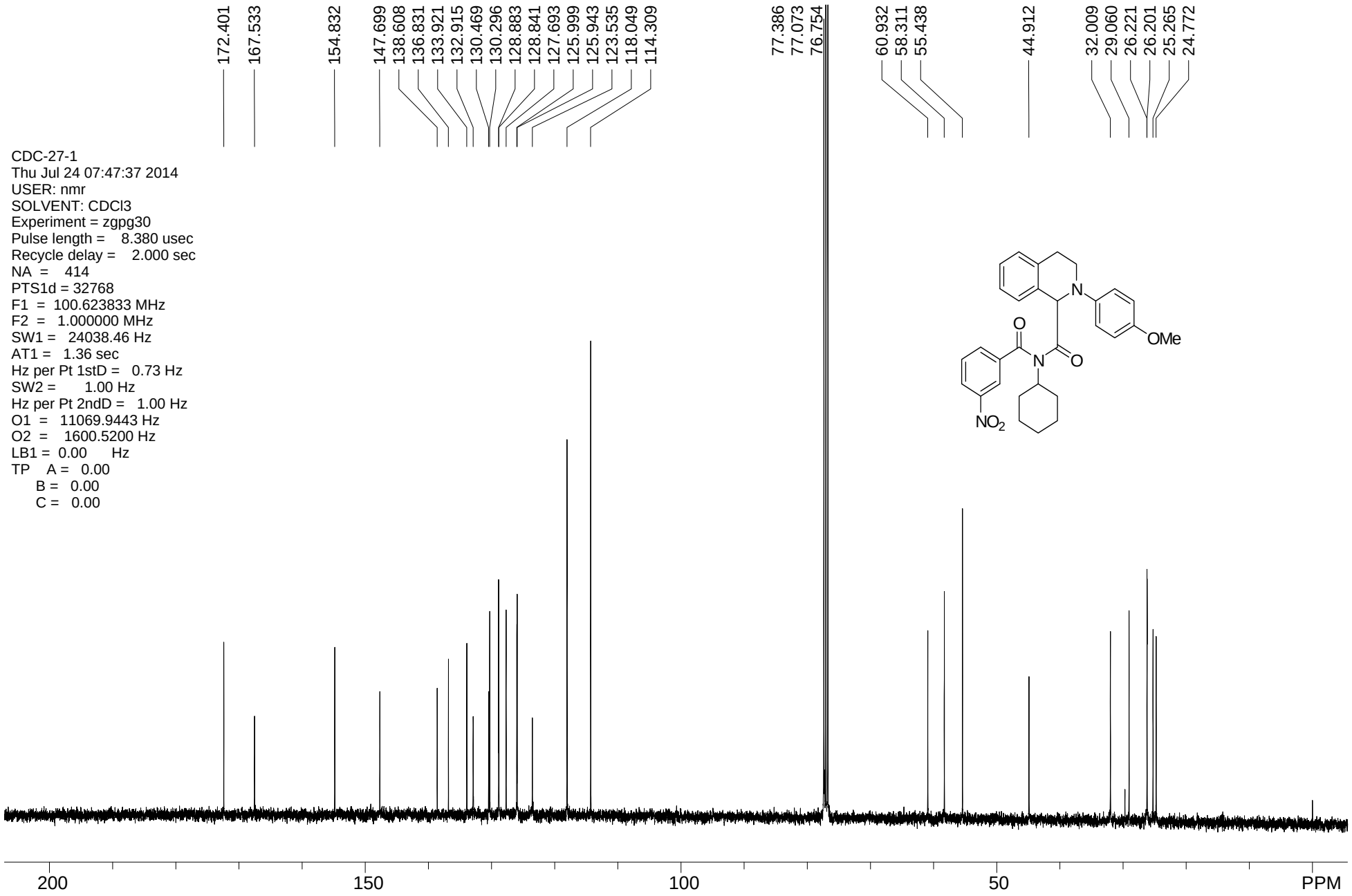

7.486 7.482 7.464 7.459 7.409 7.353 7.334 7.270 7.263 7.254 7.244 7.235 7.223 7.209 7.190 7.187 7.172 7.001 6.983 6.558 6.536 6.330 6.307 4.794 4.255 4.246 4.216 4.187 3.671 3.506 3.493 3.471 3.458 3.218 3.207 3.183 3.153 3.142 2.678 2.664 2.635 2.593 2.542 2.500 2.492 2.098 2.037 1.918 1.887 1.799 1.775 1.758 1.747 1.699 1.676 1.612 1.581 1.323 1.298 1.290 1.231 1.171 1.140 1.115 1.107
CDC-24-1
Thu Jul 24 02:08:11 2014
USER: nmr
SOLVENT:
Experiment = zg30
Pulse length = 14.120 usec
Recycle delay = 1.000 sec
NA = 8
PTS1d = 65536
F1 = 400.132477 MHz
F2 = 1.000000 MHz
SW1 = 8223.68 Hz
AT1 = 7.97 sec
Hz per Pt 1stD = 0.13 Hz
SW2 = 1.00 Hz
Hz per Pt 2ndD = 1.00 Hz
O1 = 2467.1716 Hz
O2 = 2470.9666 Hz
LB1 = 0.00 Hz
TP A = 0.00
B = 0.00
C = 0.00
N
O
N
O
OMe
OCF3
1.05
1.04
1.04
3.25
1.18
1.02
2.00
2.02
0.99
1.03
3.01
1.03
1.00
1.00
1.01
1.18
1.05
3.08
1.32
1.19
3.00
1.46
10
8
6
4
2
0
PPM

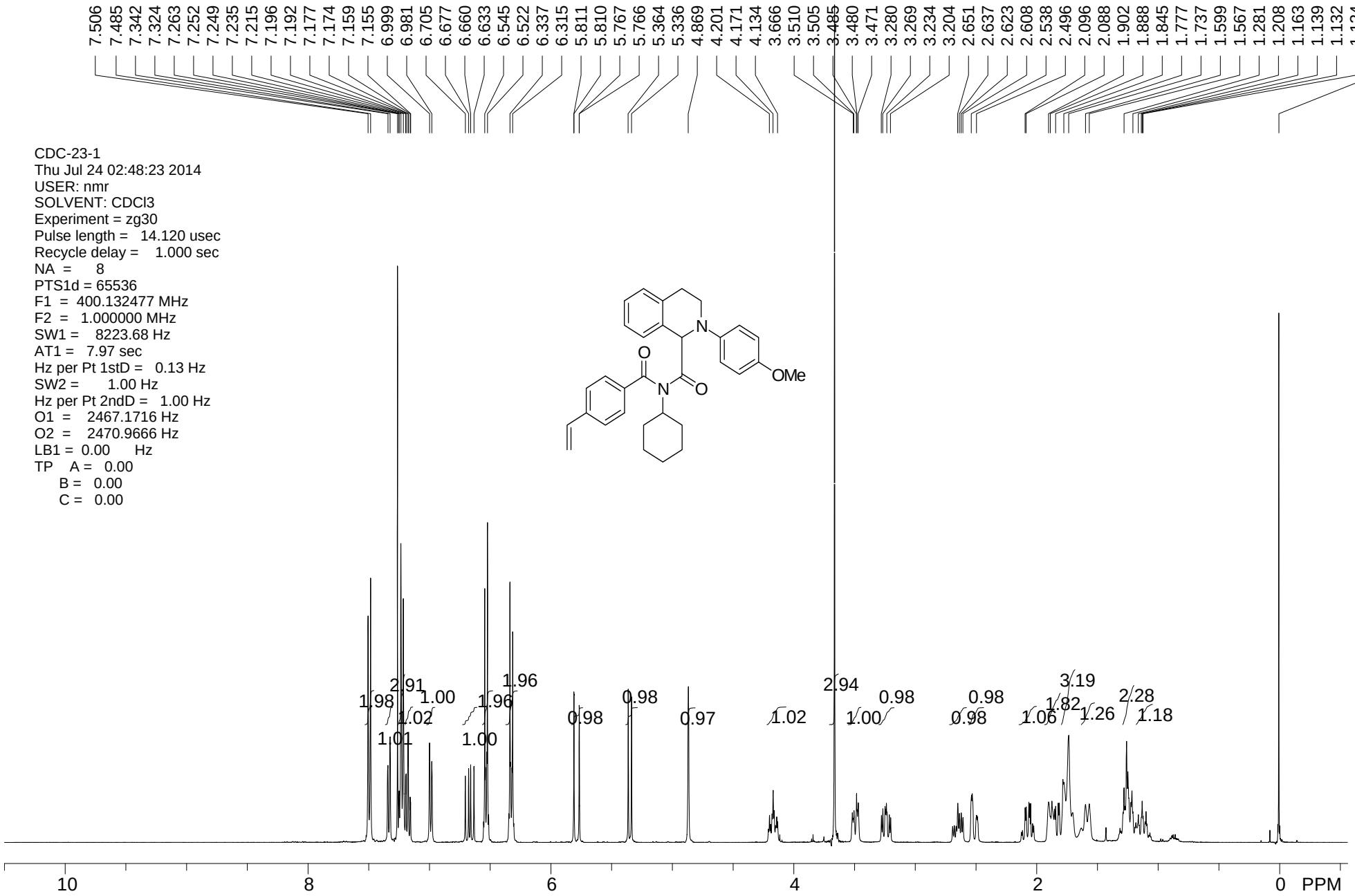

CDC-24-1
Thu Jul 24 02:23:25 2014
USER: nmr
SOLVENT: CDCl3
Experiment = zgpg30
Pulse length = 8.380 usec
Recycle delay = 2.000 sec
NA = 361
PTS1d = 32768
F1 = 100.623833 MHz
F2 = 1.000000 MHz
SW1 = 24038.46 Hz
AT1 = 1.36 sec
Hz per Pt 1stD = 0.73 Hz
SW2 = 1.00 Hz
Hz per Pt 2ndD = 1.00 Hz
O1 = 11069.9443 Hz
O2 = 1600.5200 Hz
LB1 = 0.00 Hz
TP A = 0.00
B = 0.00
C = 0.00
172.911
168.606
154.699
148.858
148.843
139.147
137.103
134.052
130.915
130.288
129.431
128.811
127.542
126.649
125.865
124.310
121.627
120.957
119.063
118.313
114.132
77.370
77.059
76.738
61.068
58.295
55.392
45.158
31.740
29.721
29.049
26.240
25.286
24.697
0.011
O
N
N
O
O
OMe
OCF3
200
150
100
50
0
PPM

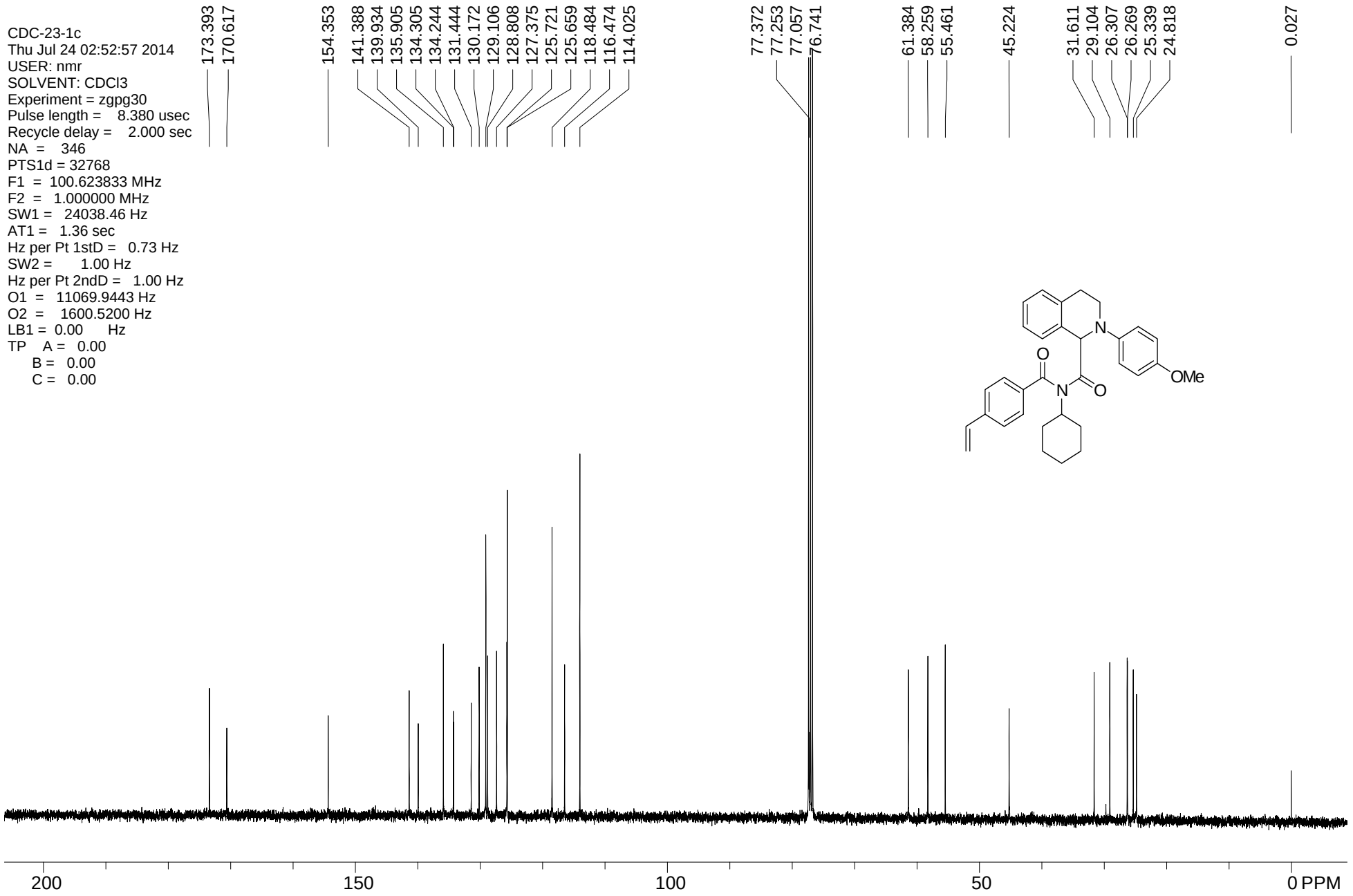

7.402 7.393 7.388 7.380 7.303 7.297 7.283 7.277 7.263 7.238 7.229 7.224 7.215 7.123 7.114 7.110 7.101 6.936 6.921 6.915 6.900 6.835 6.809 6.802 6.779 6.759 6.743 6.736 5.710 3.815 3.790 3.751 3.732 3.632 3.599 3.580 3.566 3.534 3.521 3.508 3.489 3.477 2.835 2.820 2.806 2.794 2.024 2.004 1.994 1.987 1.973 1.964 1.714 1.695 1.660 1.601 1.567 1.525 1.508 1.265 1.096 1.066 1.043 1.006 0.987 0.981 0.968 0.956 0.949 0.942 0.008
CDC-26-1
Thu Jul 24 06:54:43 2014
USER: nmr
SOLVENT: CDCl3
Experiment = zg30
Pulse length = 14.120 usec
Recycle delay = 1.000 sec
NA = 8
PTS1d = 65536
F1 = 400.132477 MHz
F2 = 1.000000 MHz
SW1 = 8223.68 Hz
AT1 = 7.97 sec
Hz per Pt 1stD = 0.13 Hz
SW2 = 1.00 Hz
Hz per Pt 2ndD = 1.00 Hz
O1 = 2467.1716 Hz
O2 = 2470.9666 Hz
LB1 = 0.00 Hz
TP A = 0.00
B = 0.00
C = 0.00
Br
O
N
OMe
N
O
F
5.03
2.00
1.00
1.03
1.05
5.00
0.97
4.03
1.00
1.03
2.03
1.98
3.35
2.18
1.93
1.11
10
8
6
4
2
0
PPM

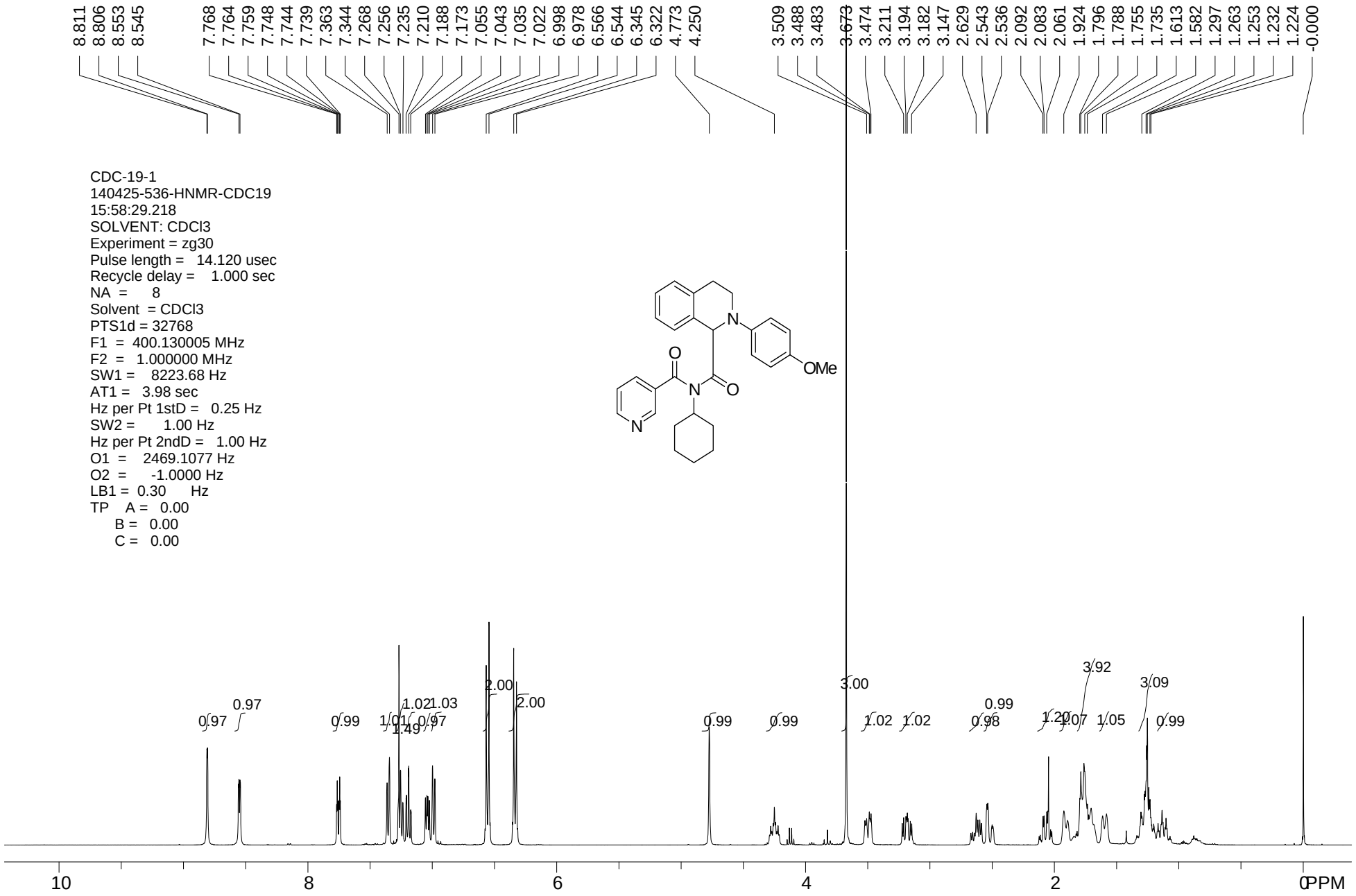

175.862
171.260
164.185
161.641
154.190
135.018
133.512
142.739
133.478
131.945
130.747
130.650
128.908
128.315
127.579
126.131
121.571
121.475
121.257
121.012
119.418
114.537
114.461
114.246
77.370
77.261
77.060
76.738
63.636
60.273
55.592
46.346
30.468
29.746
26.417
26.374
26.256
25.105
0.025
CDC-26-1
Thu Jul 24 07:01:03 2014
USER: nmr
SOLVENT: CDCl3
Experiment = zgpg30
Pulse length = 8.380 usec
Recycle delay = 2.000 sec
NA = 515
PTS1d = 32768
F1 = 100.623833 MHz
F2 = 1.000000 MHz
SW1 = 24038.46 Hz
AT1 = 1.36 sec
Hz per Pt 1stD = 0.73 Hz
SW2 = 1.00 Hz
Hz per Pt 2ndD = 1.00 Hz
O1 = 11069.9443 Hz
O2 = 1600.5200 Hz
LB1 = 0.00 Hz
TP A = 0.00
B = 0.00
C = 0.00
Br
O
N
OMe
N
O
F
200
150
100
50
PPM

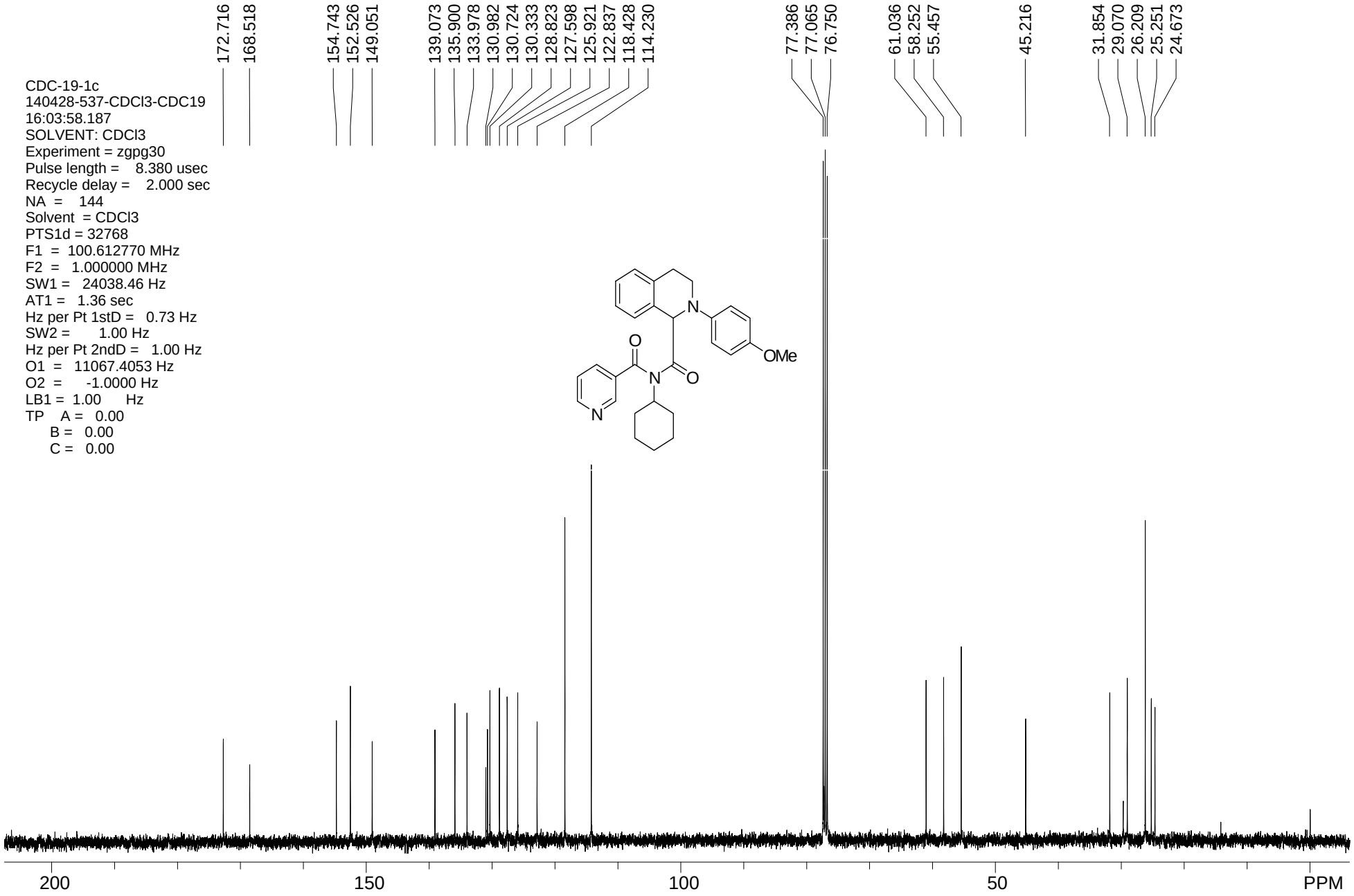

8.299 8.294 8.289 8.143 8.141 8.137 8.123 8.120 7.818 7.815 7.811 7.798 7.795 7.792 7.408 7.388 7.368 7.353 7.335 7.263 7.247 7.245 7.229 7.206 7.202 7.187 7.183 7.168 6.994 6.976 6.527 6.504 6.504 6.333 6.310 4.627 4.367 4.338 4.308 3.645 3.555 3.550 3.520 3.515 3.199 3.187 3.123 2.678 2.635 2.593 2.552 2.517 2.107 2.076 2.036 1.912 1.793 1.784 1.775 1.732 1.702 1.692 1.628 1.596 1.331 1.297 1.257 1.254 1.222 1.152 1.119 1.087 -0.001
CDC-27-1
Thu Jul 24 07:35:58 2014
USER: nmr
SOLVENT: CDCl3
Experiment = zg30
Pulse length = 14.120 usec
Recycle delay = 1.000 sec
NA = 8
PTS1d = 65536
F1 = 400.132477 MHz
F2 = 1.000000 MHz
SW1 = 8223.68 Hz
AT1 = 7.97 sec
Hz per Pt 1stD = 0.13 Hz
SW2 = 1.00 Hz
Hz per Pt 2ndD = 1.00 Hz
O1 = 2467.1716 Hz
O2 = 2470.9666 Hz
LB1 = 0.00 Hz
TP A = 0.00
B = 0.00
C = 0.00
N
OMe
O
N
O
NO2
0.96
1.00
1.00
0.99
1.01
1.35
1.03
1.03
2.00
2.00
0.98
1.00
2.97
1.00
0.99
1.00
1.03
1.16
2.92
2.75
2.80
1.15
10
8
6
4
2
0
PPM

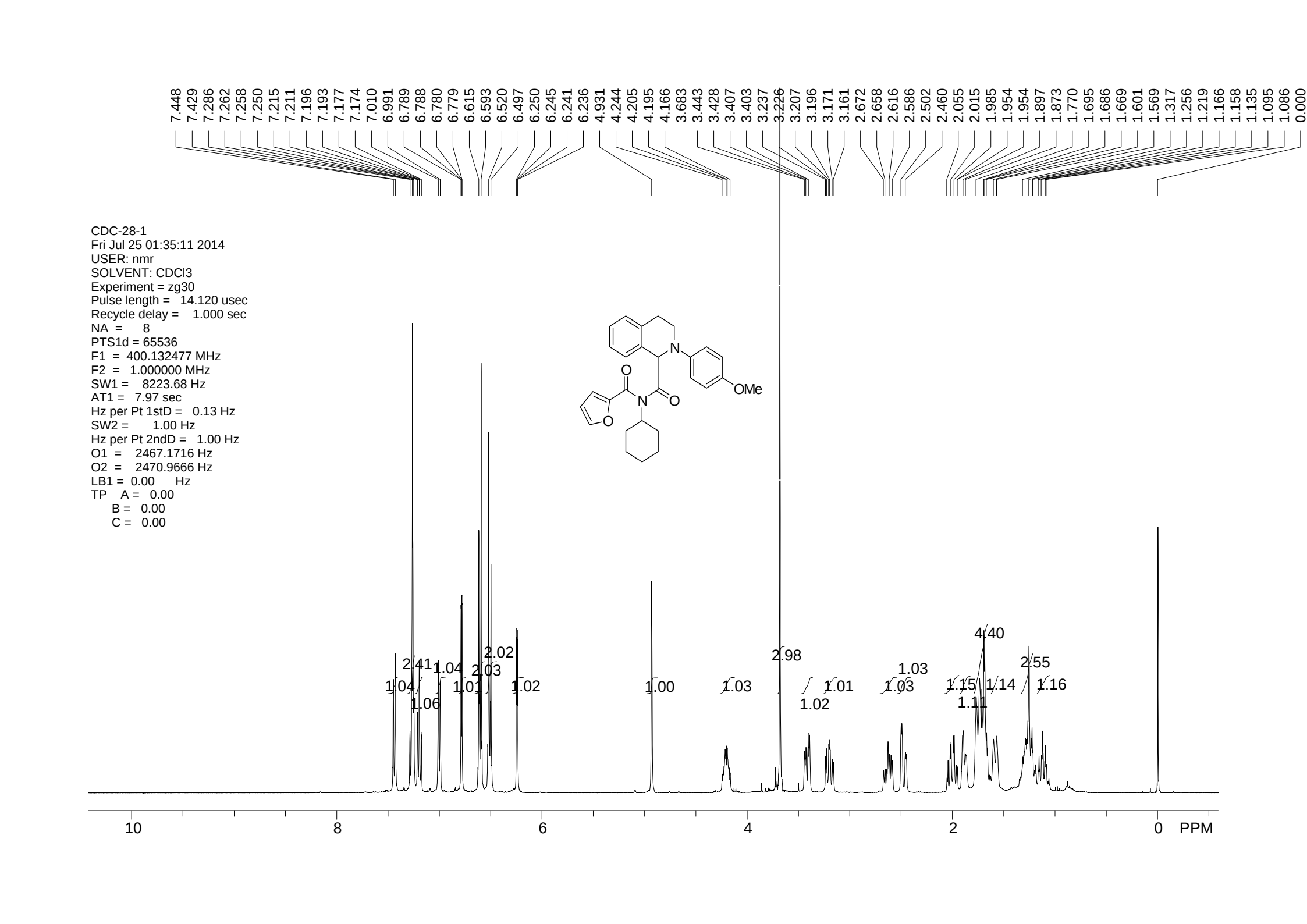

172.401
167.533
154.832
147.699
138.608
136.831
133.921
132.915
130.469
130.296
128.883
128.841
127.693
125.999
125.943
123.535
118.049
114.309
77.386
77.073
76.754
60.932
58.311
55.438
44.912
32.009
29.060
26.221
26.201
25.265
24.772
CDC-27-1
Thu Jul 24 07:47:37 2014
USER: nmr
SOLVENT: CDCl3
Experiment = zgpg30
Pulse length = 8.380 usec
Recycle delay = 2.000 sec
NA = 414
PTS1d = 32768
F1 = 100.623833 MHz
F2 = 1.000000 MHz
SW1 = 24038.46 Hz
AT1 = 1.36 sec
Hz per Pt 1stD = 0.73 Hz
SW2 = 1.00 Hz
Hz per Pt 2ndD = 1.00 Hz
O1 = 11069.9443 Hz
O2 = 1600.5200 Hz
LB1 = 0.00 Hz
TP A = 0.00
B = 0.00
C = 0.00
N
O
N
O
OMe
NO2
200
150
100
50
PPM

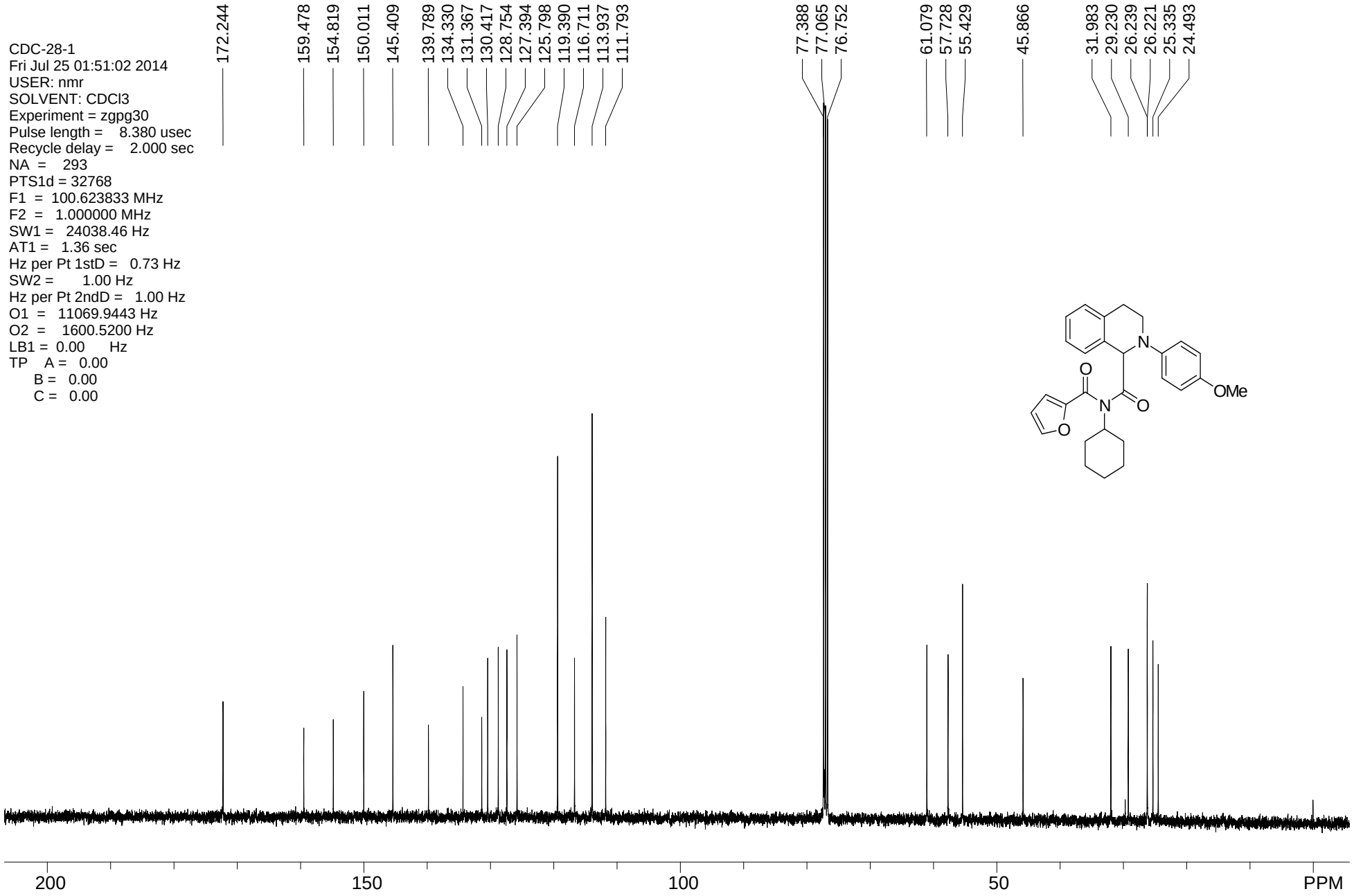

7.506 7.485 7.342 7.324 7.263 7.252 7.249 7.235 7.215 7.196 7.192 7.177 7.174 7.159 7.155 6.999 6.981 6.705 6.677 6.660 6.633 6.545 6.522 6.337 6.315 5.811 5.810 5.767 5.766 5.364 5.336 4.869 4.201 4.171 4.134 3.666 3.510 3.505 3.485 3.480 3.471 3.280 3.269 3.234 3.204 2.651 2.637 2.623 2.608 2.538 2.496 2.096 2.088 1.902 1.888 1.845 1.777 1.737 1.599 1.567 1.281 1.208 1.163 1.139 1.132 1.124 0.006
CDC-23-1
Thu Jul 24 02:48:23 2014
USER: nmr
SOLVENT: CDCl3
Experiment = zg30
Pulse length = 14.120 usec
Recycle delay = 1.000 sec
NA = 8
PTS1d = 65536
F1 = 400.132477 MHz
F2 = 1.000000 MHz
SW1 = 8223.68 Hz
AT1 = 7.97 sec
Hz per Pt 1stD = 0.13 Hz
SW2 = 1.00 Hz
Hz per Pt 2ndD = 1.00 Hz
O1 = 2467.1716 Hz
O2 = 2470.9666 Hz
LB1 = 0.00 Hz
TP A = 0.00
B = 0.00
C = 0.00
N
O
N
O
OMe
1.98
2.91
1.00
1.02
1.01
1.00
1.96
1.96
0.98
0.98
0.97
1.02
2.94
1.00
0.98
0.98
0.98
1.06
3.19
1.82
1.26
2.28
1.18
10
8
6
4
2
0
PPM

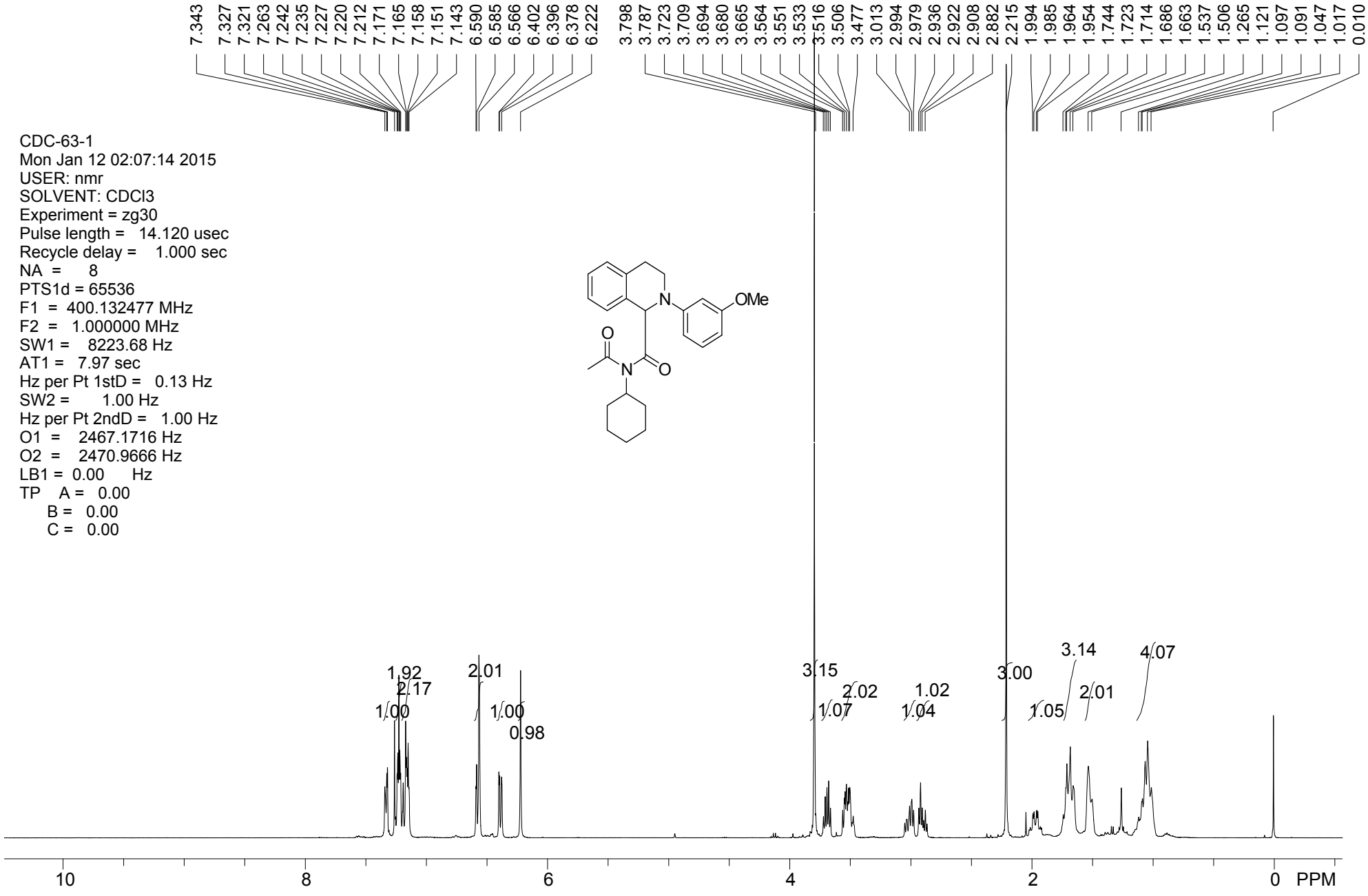

CDC-23-1c
Thu Jul 24 02:52:57 2014
USER: nmr
SOLVENT: CDCl3
Experiment = zgpg30
Pulse length = 8.380 usec
Recycle delay = 2.000 sec
NA = 346
PTS1d = 32768
F1 = 100.623833 MHz
F2 = 1.000000 MHz
SW1 = 24038.46 Hz
AT1 = 1.36 sec
Hz per Pt 1stD = 0.73 Hz
SW2 = 1.00 Hz
Hz per Pt 2ndD = 1.00 Hz
O1 = 11069.9443 Hz
O2 = 1600.5200 Hz
LB1 = 0.00 Hz
TP A = 0.00
B = 0.00
C = 0.00
173.393
170.617
154.353
141.388
139.934
135.905
134.305
134.244
131.444
130.172
129.106
128.808
127.375
125.721
125.659
118.484
116.474
114.025
77.372
77.253
77.057
76.741
61.384
58.259
55.461
45.224
31.611
29.104
26.307
26.269
25.339
24.818
0.027
N
O
N
O
OMe
200
150
100
50
0 PPM

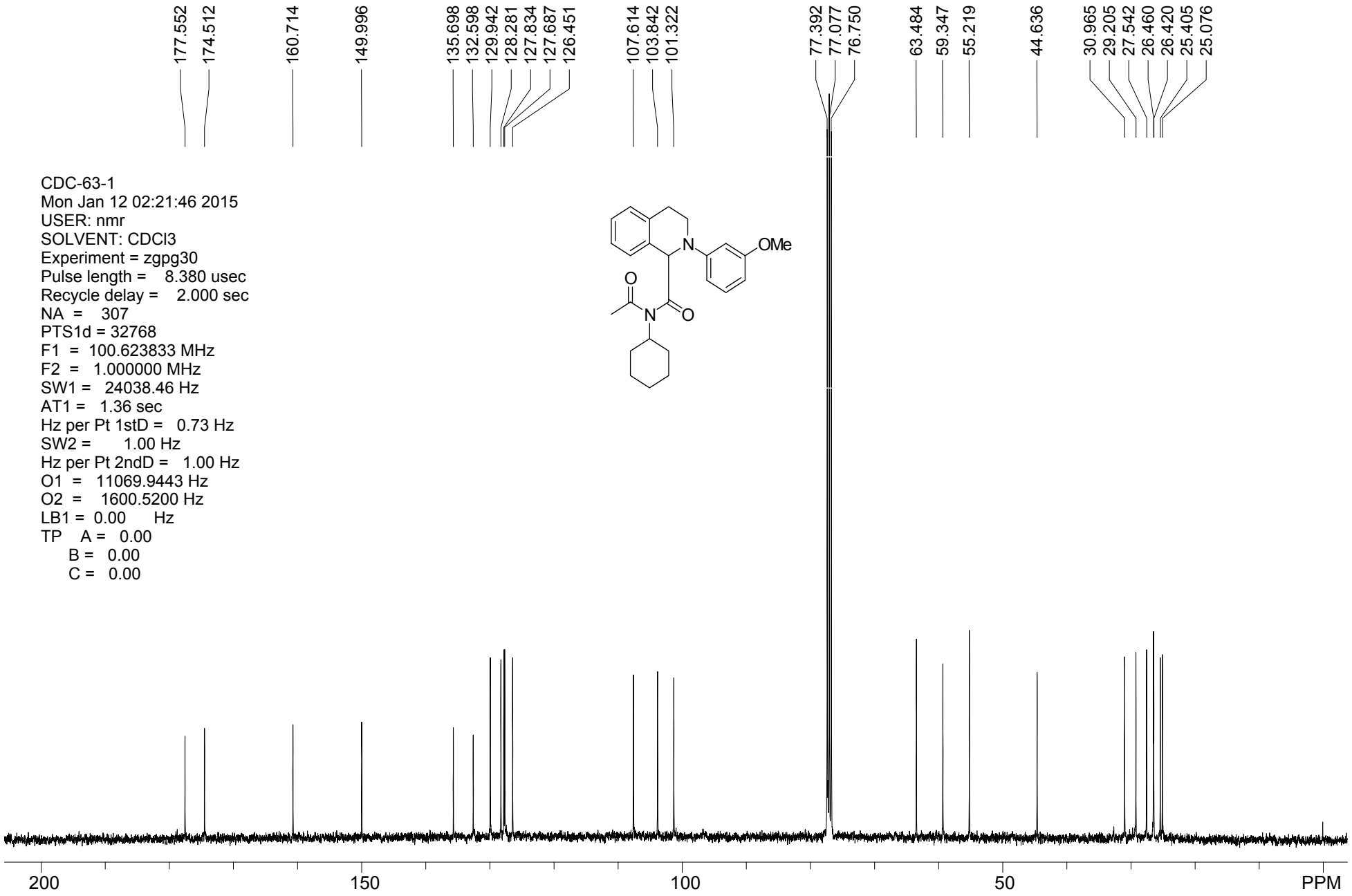

8.811
8.806
8.553
8.545
7.768
7.764
7.759
7.748
7.744
7.739
7.363
7.344
7.268
7.256
7.235
7.210
7.188
7.173
7.055
7.043
7.035
7.022
6.998
6.978
6.566
6.544
6.345
6.322
4.773
4.250
3.509
3.488
3.483
3.473
3.474
3.211
3.194
3.182
3.147
2.629
2.543
2.536
2.092
2.083
2.061
1.924
1.796
1.788
1.755
1.735
1.613
1.582
1.297
1.263
1.253
1.232
1.224
-0.000
CDC-19-1
140425-536-HNMR-CDC19
15:58:29.218
SOLVENT: CDCl3
Experiment = zg30
Pulse length = 14.120 usec
Recycle delay = 1.000 sec
NA = 8
Solvent = CDCl3
PTS1d = 32768
F1 = 400.130005 MHz
F2 = 1.000000 MHz
SW1 = 8223.68 Hz
AT1 = 3.98 sec
Hz per Pt 1stD = 0.25 Hz
SW2 = 1.00 Hz
Hz per Pt 2ndD = 1.00 Hz
O1 = 2469.1077 Hz
O2 = -1.0000 Hz
LB1 = 0.30 Hz
TP A = 0.00
B = 0.00
C = 0.00
N
O
N
O
N
OMe
0.97
0.97
0.99
1.01
1.49
1.02
0.97
1.03
2.00
2.00
0.99
0.99
3.00
1.02
1.02
0.98
0.99
1.20
2.07
1.05
3.92
3.09
0.99
10
8
6
4
2
0
PPM

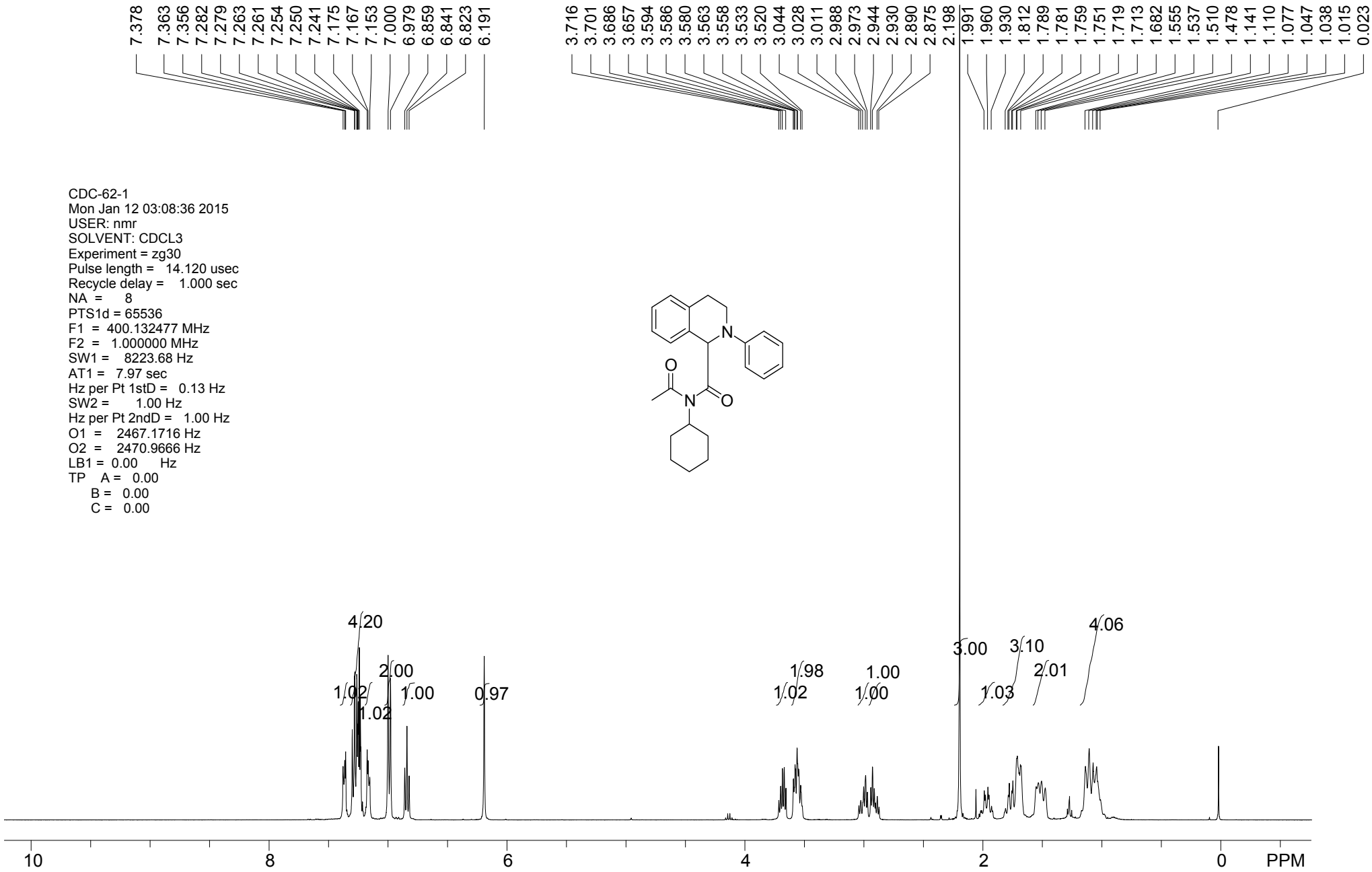

172.716
168.518
154.743
152.526
149.051
139.073
135.900
133.978
130.982
130.724
130.333
128.823
127.598
125.921
122.837
118.428
114.230
77.386
77.065
76.750
61.036
58.252
55.457
45.216
31.854
29.070
26.209
25.251
24.673
CDC-19-1c
140428-537-CDCl3-CDC19
16:03:58.187
SOLVENT: CDCl3
Experiment = zgpg30
Pulse length = 8.380 usec
Recycle delay = 2.000 sec
NA = 144
Solvent = CDCl3
PTS1d = 32768
F1 = 100.612770 MHz
F2 = 1.000000 MHz
SW1 = 24038.46 Hz
AT1 = 1.36 sec
Hz per Pt 1stD = 0.73 Hz
SW2 = 1.00 Hz
Hz per Pt 2ndD = 1.00 Hz
O1 = 11067.4053 Hz
O2 = -1.0000 Hz
LB1 = 1.00 Hz
TP A = 0.00
B = 0.00
C = 0.00
N
O
N
O
N
OMe
200
150
100
50
PPM

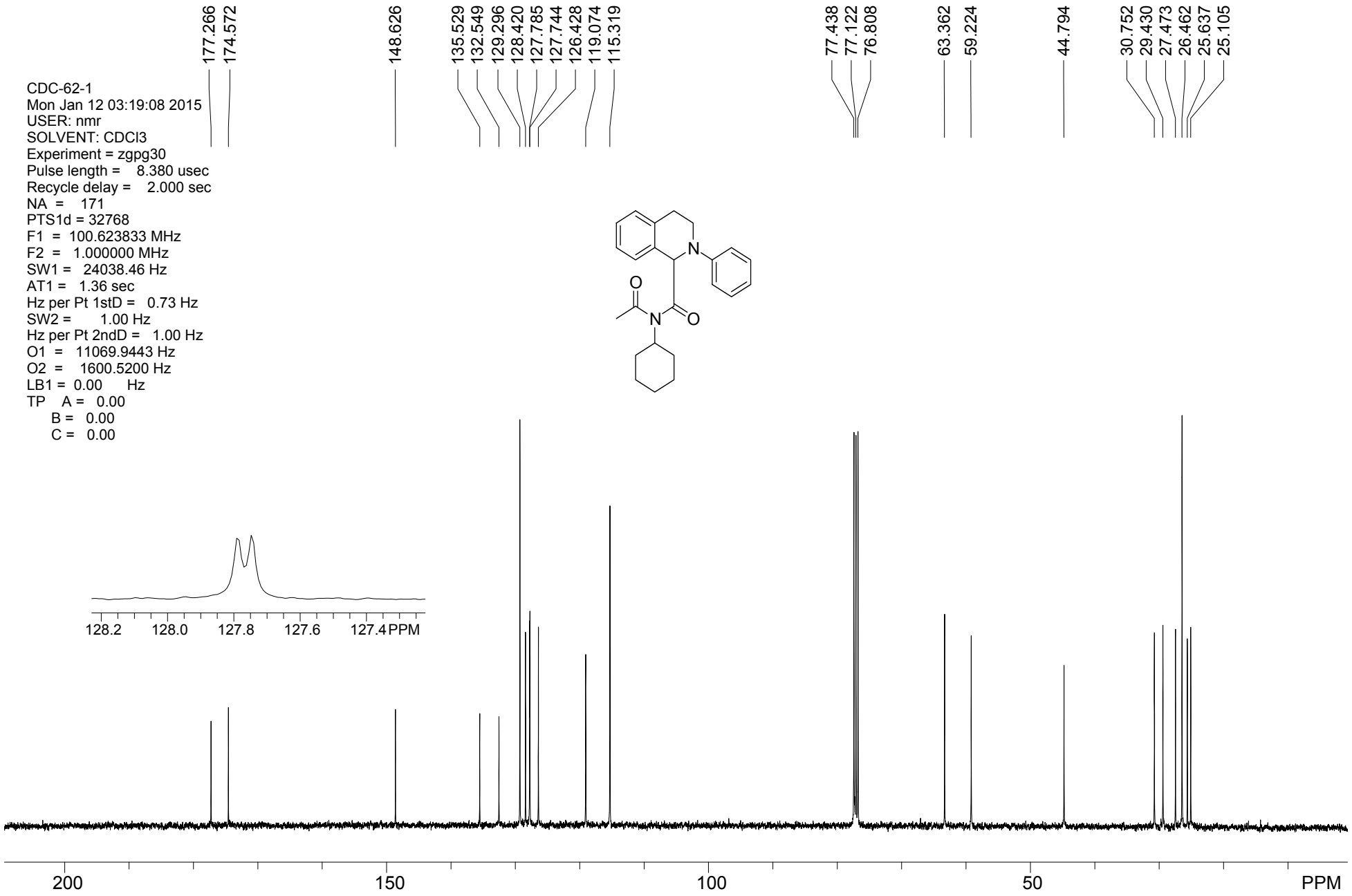

7.448 7.429 7.286 7.262 7.258 7.250 7.215 7.211 7.196 7.193 7.177 7.174 7.010 6.991 6.789 6.788 6.780 6.779 6.615 6.593 6.520 6.497 6.250 6.245 6.241 6.236 4.931 4.244 4.205 4.195 4.166 3.683 3.443 3.428 3.407 3.403 3.237 3.226 3.207 3.196 3.171 3.161 2.672 2.658 2.616 2.586 2.502 2.460 2.055 2.015 1.985 1.954 1.954 1.897 1.873 1.770 1.695 1.686 1.669 1.601 1.569 1.317 1.256 1.219 1.166 1.158 1.135 1.095 1.086 0.000
CDC-28-1
Fri Jul 25 01:35:11 2014
USER: nmr
SOLVENT: CDCl3
Experiment = zg30
Pulse length = 14.120 usec
Recycle delay = 1.000 sec
NA = 8
PTS1d = 65536
F1 = 400.132477 MHz
F2 = 1.000000 MHz
SW1 = 8223.68 Hz
AT1 = 7.97 sec
Hz per Pt 1stD = 0.13 Hz
SW2 = 1.00 Hz
Hz per Pt 2ndD = 1.00 Hz
O1 = 2467.1716 Hz
O2 = 2470.9666 Hz
LB1 = 0.00 Hz
TP A = 0.00
B = 0.00
C = 0.00
N
O
N
O
O
OMe
1.04
2.41
1.06
1.04
1.01
2.03
2.02
1.02
1.00
1.03
2.98
1.02
1.01
1.03
1.03
1.15
1.11
4.40
1.14
2.55
1.16
10
8
6
4
2
0
PPM

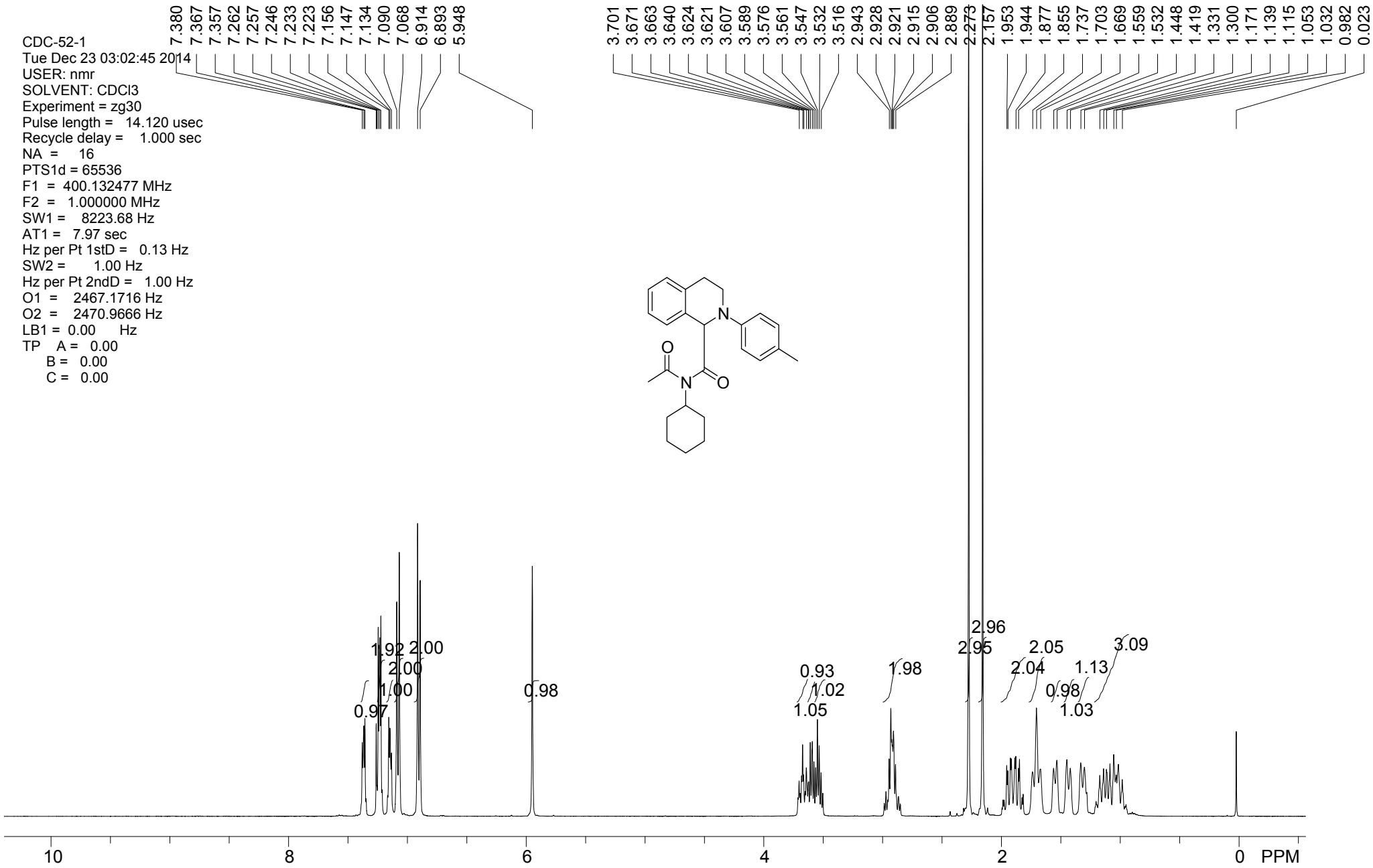

CDC-28-1
Fri Jul 25 01:51:02 2014
USER: nmr
SOLVENT: CDCl3
Experiment = zgpg30
Pulse length = 8.380 usec
Recycle delay = 2.000 sec
NA = 293
PTS1d = 32768
F1 = 100.623833 MHz
F2 = 1.000000 MHz
SW1 = 24038.46 Hz
AT1 = 1.36 sec
Hz per Pt 1stD = 0.73 Hz
SW2 = 1.00 Hz
Hz per Pt 2ndD = 1.00 Hz
O1 = 11069.9443 Hz
O2 = 1600.5200 Hz
LB1 = 0.00 Hz
TP A = 0.00
B = 0.00
C = 0.00
172.244
159.478
154.819
150.011
145.409
139.789
134.330
131.367
130.417
128.754
127.394
125.798
119.390
116.711
113.937
111.793
77.388
77.065
76.752
61.079
57.728
55.429
45.866
31.983
29.230
26.239
26.221
25.335
24.493
N
O
N
O
O
OMe
200
150
100
50
PPM

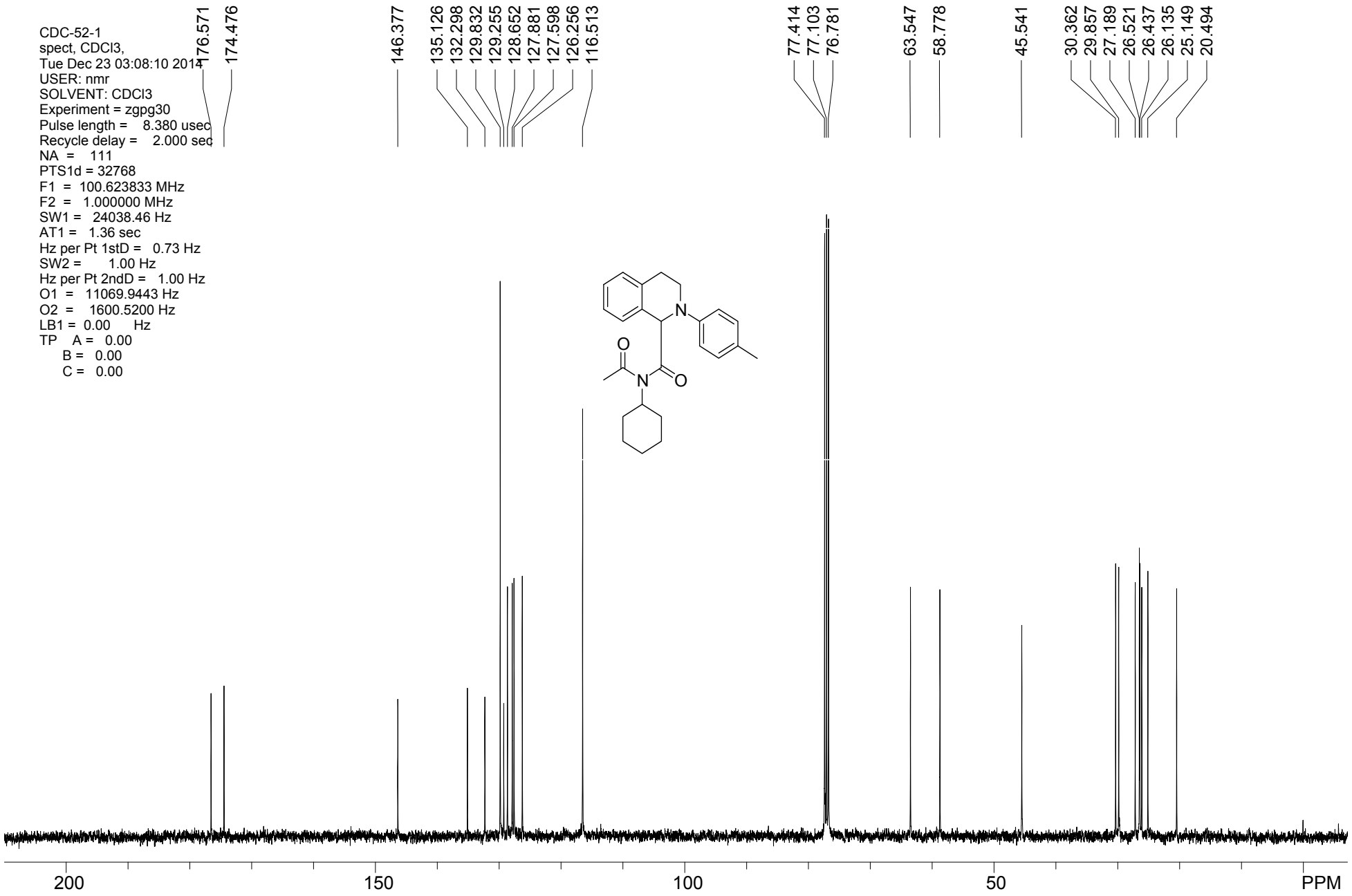

7.343
7.327
7.321
7.263
7.242
7.235
7.227
7.220
7.212
7.171
7.165
7.158
7.151
7.143
6.590
6.585
6.566
6.402
6.396
6.378
6.222
3.798
3.787
3.723
3.709
3.694
3.680
3.665
3.564
3.551
3.533
3.516
3.506
3.477
3.013
2.994
2.979
2.936
2.922
2.908
2.882
2.215
1.994
1.985
1.964
1.954
1.744
1.723
1.714
1.686
1.663
1.537
1.506
1.265
1.121
1.097
1.091
1.047
1.017
0.010
CDC-63-1
Mon Jan 12 02:07:14 2015
USER: nmr
SOLVENT: CDCl3
Experiment = zg30
Pulse length = 14.120 usec
Recycle delay = 1.000 sec
NA = 8
PTS1d = 65536
F1 = 400.132477 MHz
F2 = 1.000000 MHz
SW1 = 8223.68 Hz
AT1 = 7.97 sec
Hz per Pt 1stD = 0.13 Hz
SW2 = 1.00 Hz
Hz per Pt 2ndD = 1.00 Hz
O1 = 2467.1716 Hz
O2 = 2470.9666 Hz
LB1 = 0.00 Hz
TP A = 0.00
B = 0.00
C = 0.00
OMe
O
N
O
N
1.92
2.17
1.00
2.01
1.00
0.98
3.15
1.07
2.02
1.04
1.02
3.00
1.05
3.14
2.01
4.07
10
8
6
4
2
0
PPM

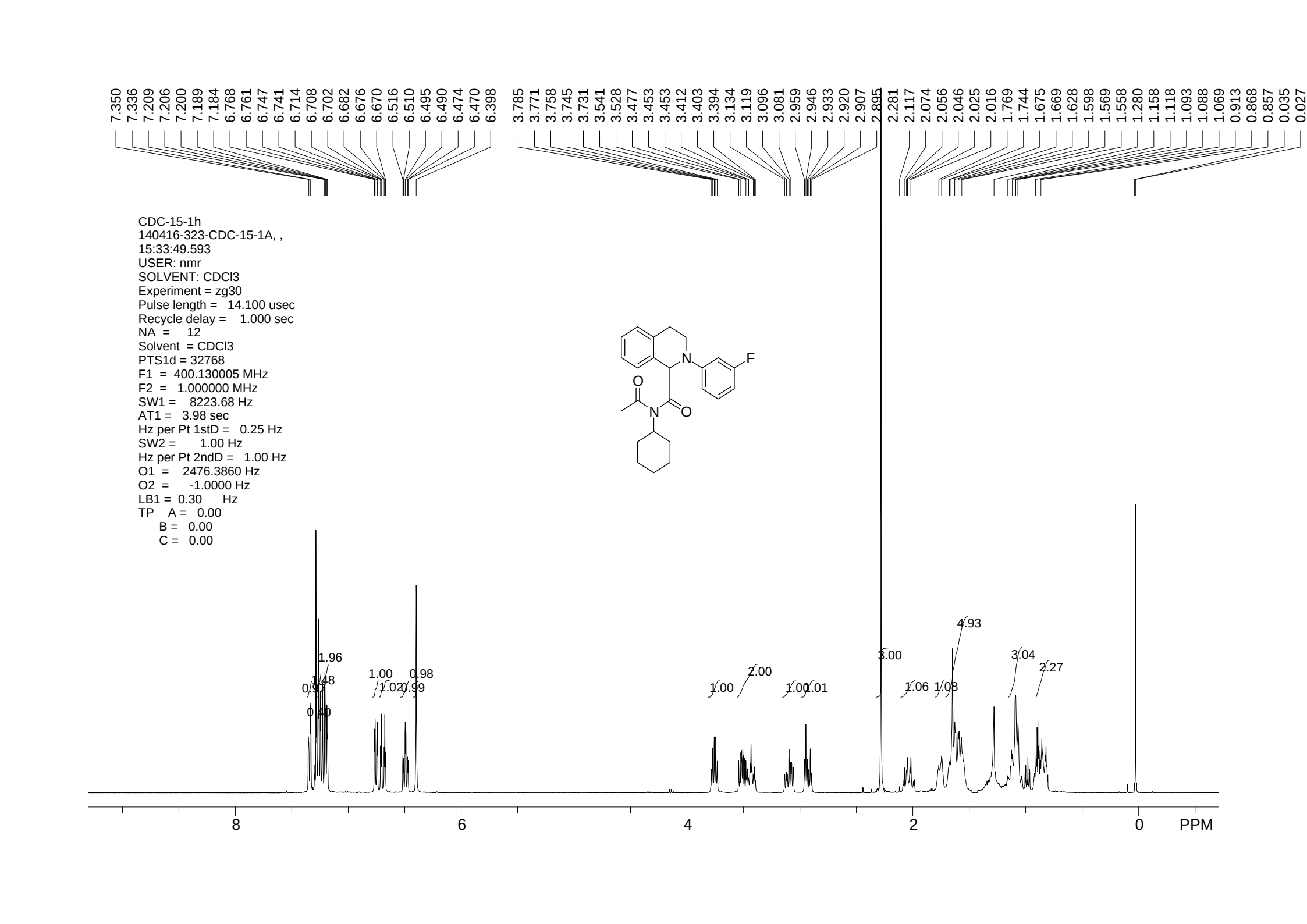

177.552
174.512
160.714
149.996
135.698
132.598
129.942
128.281
127.834
127.687
126.451
107.614
103.842
101.322
77.392
77.077
76.750
63.484
59.347
55.219
44.636
30.965
29.205
27.542
26.460
26.420
25.405
25.076
CDC-63-1
Mon Jan 12 02:21:46 2015
USER: nmr
SOLVENT: CDCl3
Experiment = zgpg30
Pulse length = 8.380 usec
Recycle delay = 2.000 sec
NA = 307
PTS1d = 32768
F1 = 100.623833 MHz
F2 = 1.000000 MHz
SW1 = 24038.46 Hz
AT1 = 1.36 sec
Hz per Pt 1stD = 0.73 Hz
SW2 = 1.00 Hz
Hz per Pt 2ndD = 1.00 Hz
O1 = 11069.9443 Hz
O2 = 1600.5200 Hz
LB1 = 0.00 Hz
TP A = 0.00
B = 0.00
C = 0.00
N
OMe
O
N
O
200
150
100
50
PPM

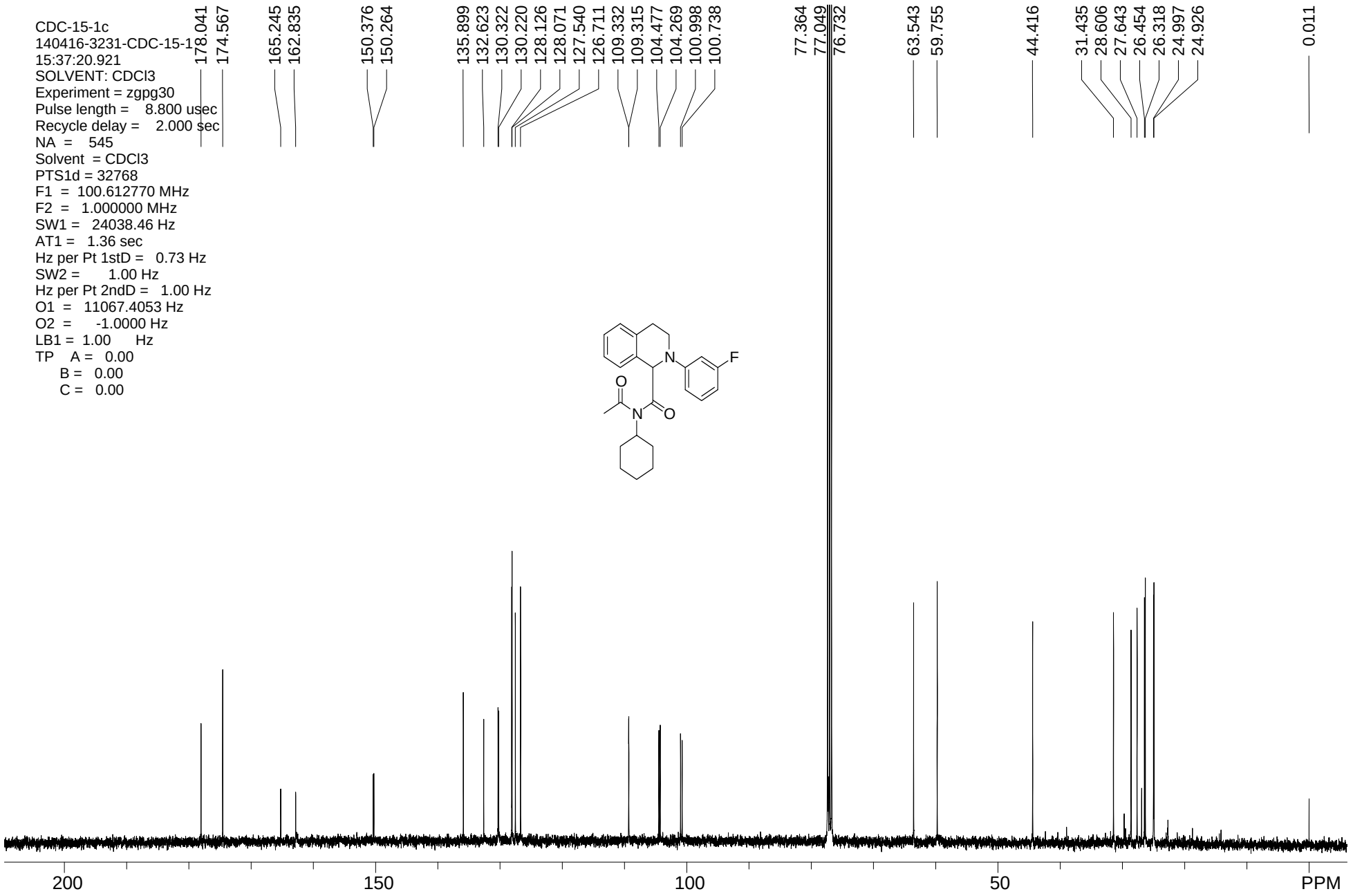

7.378
7.363
7.356
7.282
7.279
7.263
7.261
7.254
7.250
7.241
7.175
7.167
7.153
7.000
6.979
6.859
6.841
6.823
6.191
3.716
3.701
3.686
3.657
3.594
3.586
3.580
3.563
3.558
3.533
3.520
3.044
3.028
3.011
2.988
2.973
2.944
2.930
2.890
2.875
2.198
1.991
1.960
1.930
1.812
1.789
1.781
1.759
1.751
1.719
1.713
1.682
1.555
1.537
1.510
1.478
1.141
1.110
1.077
1.047
1.038
1.015
0.023
CDC-62-1
Mon Jan 12 03:08:36 2015
USER: nmr
SOLVENT: CDCL3
Experiment = zg30
Pulse length = 14.120 usec
Recycle delay = 1.000 sec
NA = 8
PTS1d = 65536
F1 = 400.132477 MHz
F2 = 1.000000 MHz
SW1 = 8223.68 Hz
AT1 = 7.97 sec
Hz per Pt 1stD = 0.13 Hz
SW2 = 1.00 Hz
Hz per Pt 2ndD = 1.00 Hz
O1 = 2467.1716 Hz
O2 = 2470.9666 Hz
LB1 = 0.00 Hz
TP A = 0.00
B = 0.00
C = 0.00
O
N
N
O
4.20
1.02
2.00
1.02
1.00
0.97
1.98
1.02
1.00
1.00
3.00
1.03
3.10
2.01
4.06
10
8
6
4
2
0
PPM

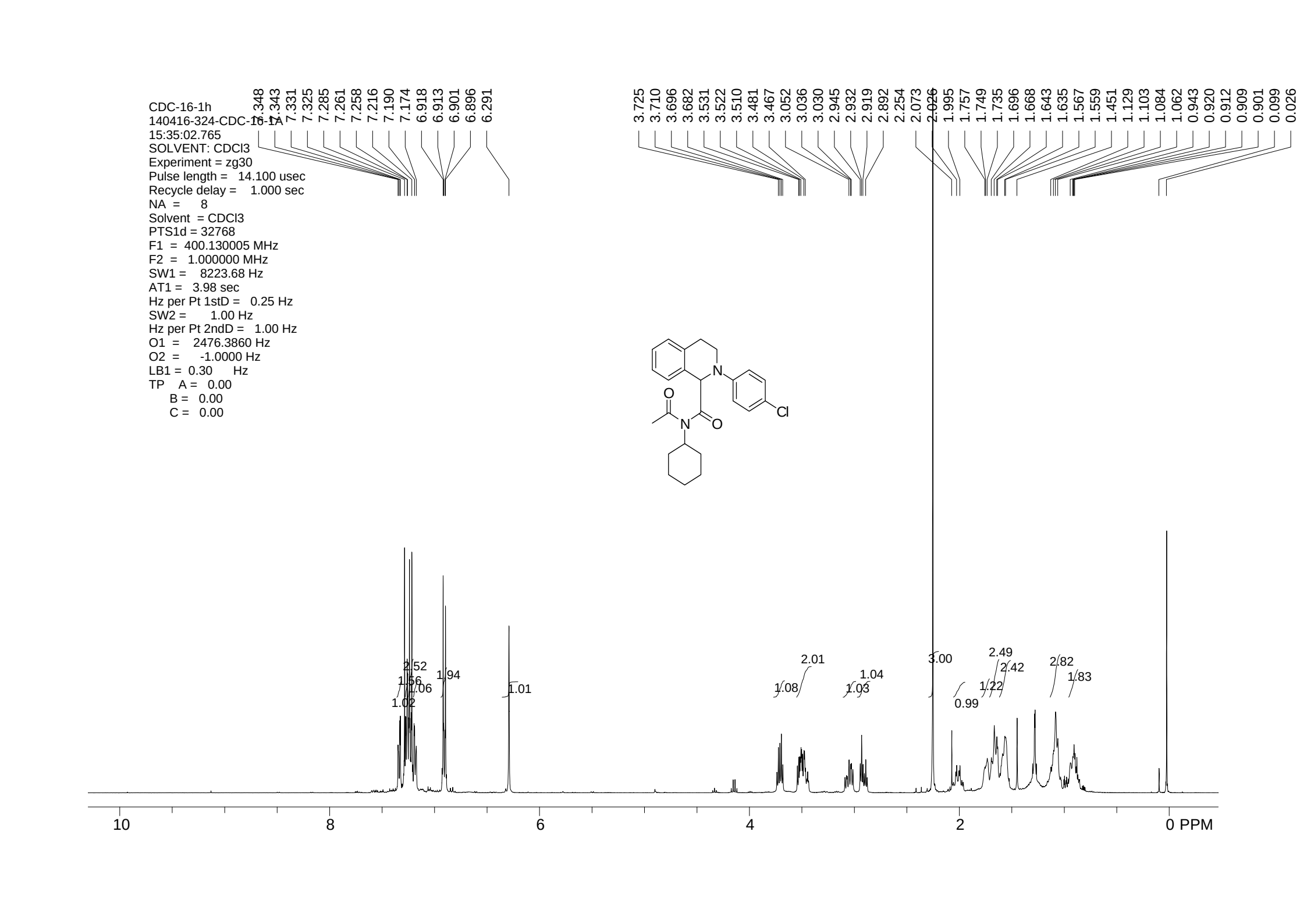

177.266
174.572
148.626
135.529
132.549
129.296
128.420
127.785
127.744
126.428
119.074
115.319
77.438
77.122
76.808
63.362
59.224
44.794
30.752
29.430
27.473
26.462
25.637
25.105
CDC-62-1
Mon Jan 12 03:19:08 2015
USER: nmr
SOLVENT: CDCl3
Experiment = zgpg30
Pulse length = 8.380 usec
Recycle delay = 2.000 sec
NA = 171
PTS1d = 32768
F1 = 100.623833 MHz
F2 = 1.000000 MHz
SW1 = 24038.46 Hz
AT1 = 1.36 sec
Hz per Pt 1stD = 0.73 Hz
SW2 = 1.00 Hz
Hz per Pt 2ndD = 1.00 Hz
O1 = 11069.9443 Hz
O2 = 1600.5200 Hz
LB1 = 0.00 Hz
TP A = 0.00
B = 0.00
C = 0.00
N
O
N
O
128.2
128.0
127.8
127.6
127.4 PPM
200
150
100
50
PPM

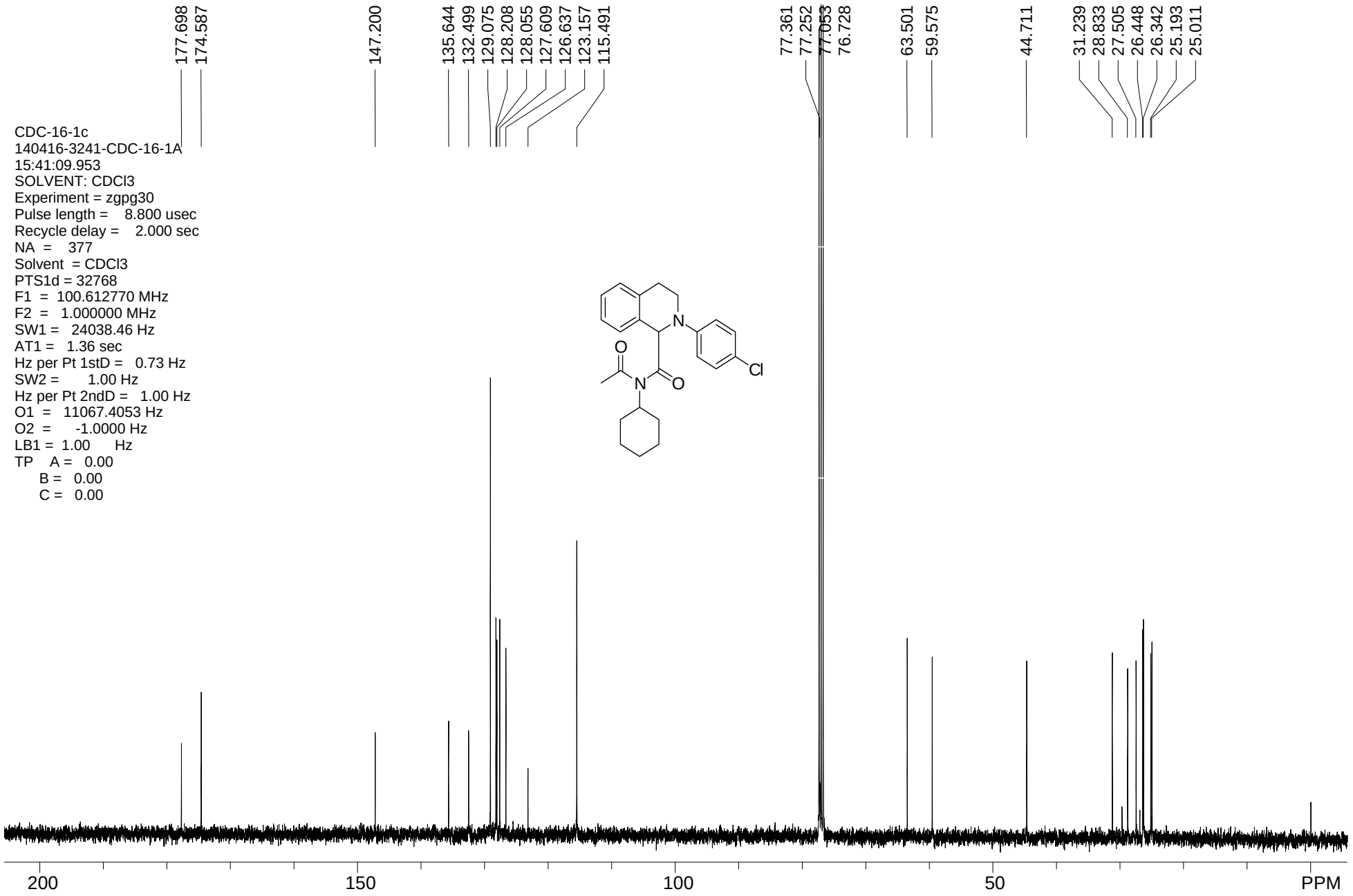

CDC-52-1
Tue Dec 23 03:02:45 2014
USER: nmr
SOLVENT: CDCl3
Experiment = zg30
Pulse length = 14.120 usec
Recycle delay = 1.000 sec
NA = 16
PTS1d = 65536
F1 = 400.132477 MHz
F2 = 1.000000 MHz
SW1 = 8223.68 Hz
AT1 = 7.97 sec
Hz per Pt 1stD = 0.13 Hz
SW2 = 1.00 Hz
Hz per Pt 2ndD = 1.00 Hz
O1 = 2467.1716 Hz
O2 = 2470.9666 Hz
LB1 = 0.00 Hz
TP A = 0.00
B = 0.00
C = 0.00
7.380 7.367 7.357 7.262 7.257 7.246 7.233 7.223 7.156 7.147 7.134 7.090 7.068 6.914 6.893 5.948
3.701 3.671 3.663 3.640 3.624 3.621 3.607 3.589 3.576 3.561 3.547 3.532 3.516 2.943 2.928 2.921 2.915 2.906 2.889 2.273 2.157 1.953 1.944 1.877 1.855 1.737 1.703 1.669 1.559 1.532 1.448 1.419 1.331 1.300 1.171 1.139 1.115 1.053 1.032 0.982 0.023
O
N
N
O
0.97
1.92
2.00
2.00
1.00
0.98
0.93
1.02
1.05
1.98
2.96
2.95
2.05
2.04
0.98
1.03
1.13
3.09
10
8
6
4
2
0
PPM

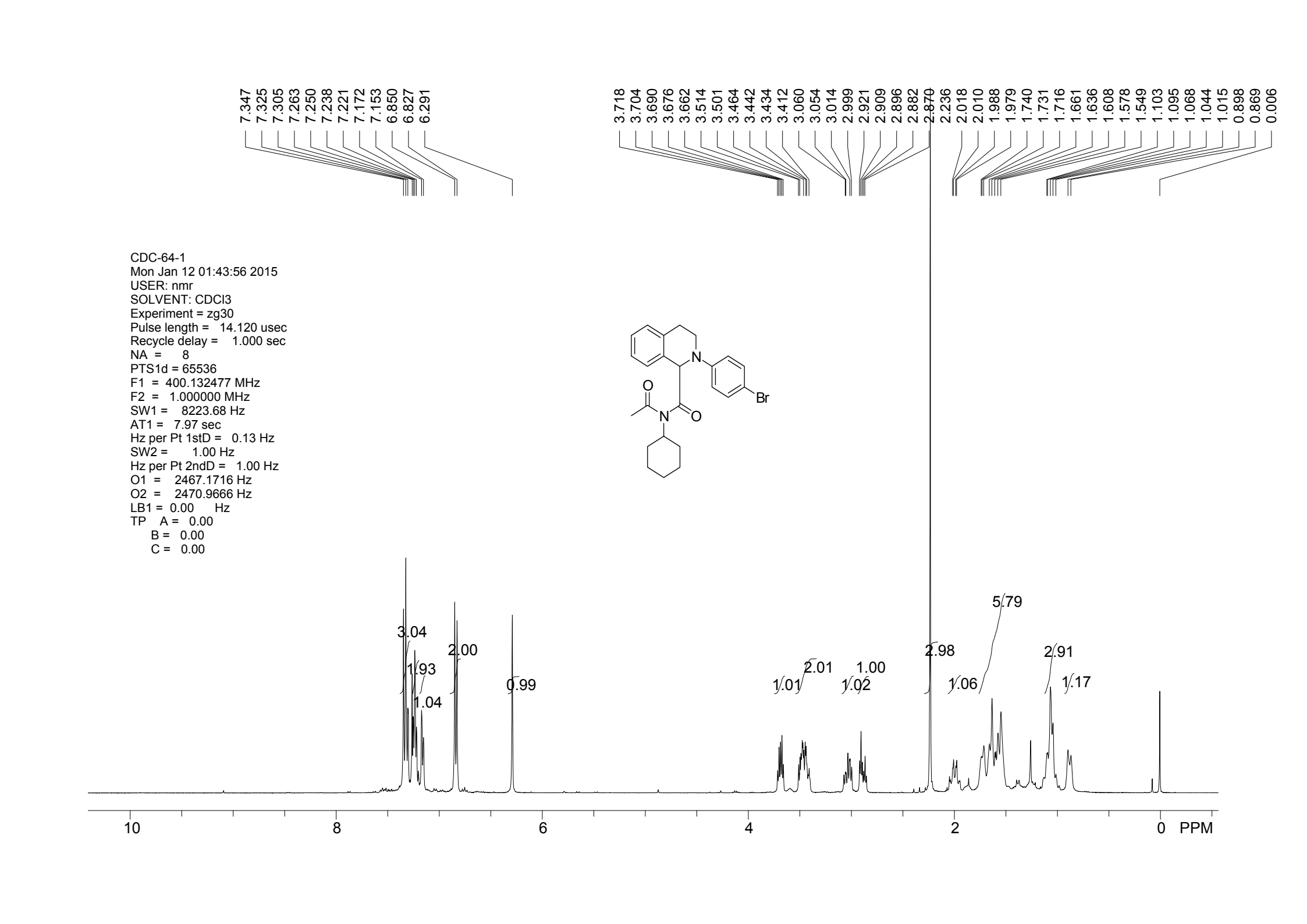

CDC-52-1
spect, CDCl3,
Tue Dec 23 03:08:10 2014
USER: nmr
SOLVENT: CDCl3
Experiment = zgpg30
Pulse length = 8.380 usec
Recycle delay = 2.000 sec
NA = 111
PTS1d = 32768
F1 = 100.623833 MHz
F2 = 1.000000 MHz
SW1 = 24038.46 Hz
AT1 = 1.36 sec
Hz per Pt 1stD = 0.73 Hz
SW2 = 1.00 Hz
Hz per Pt 2ndD = 1.00 Hz
O1 = 11069.9443 Hz
O2 = 1600.5200 Hz
LB1 = 0.00 Hz
TP A = 0.00
B = 0.00
C = 0.00
176.571
174.476
146.377
135.126
132.298
129.832
129.255
128.652
127.881
127.598
126.256
116.513
77.414
77.103
76.781
63.547
58.778
45.541
30.362
29.857
27.189
26.521
26.437
26.135
25.149
20.494
O
N
O
N
200
150
100
50
PPM

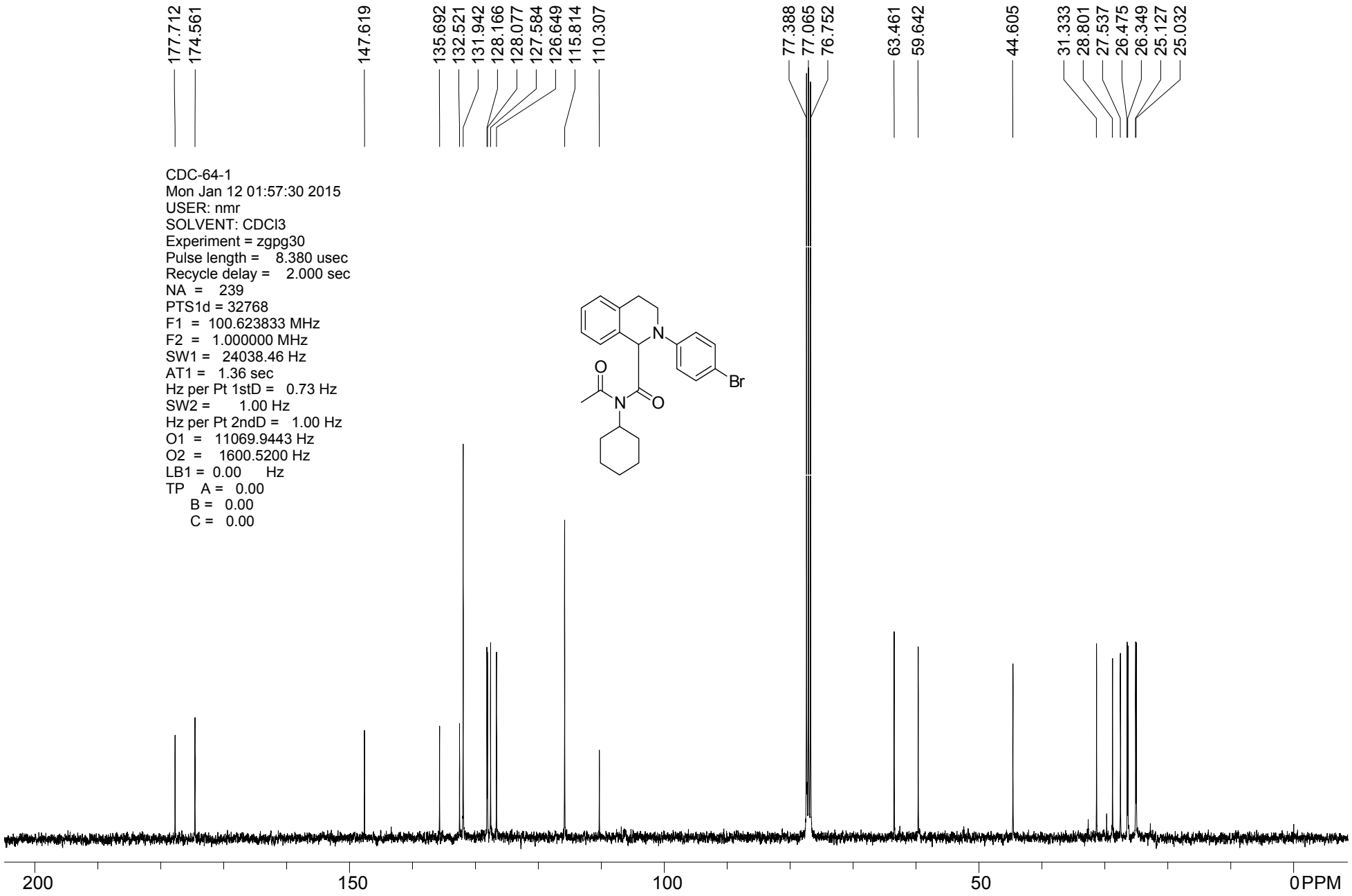

7.350 7.336 7.209 7.206 7.200 7.189 7.184 6.768 6.761 6.747 6.741 6.714 6.708 6.702 6.682 6.676 6.670 6.516 6.510 6.495 6.490 6.474 6.470 6.398
3.785 3.771 3.758 3.745 3.731 3.541 3.528 3.477 3.453 3.453 3.412 3.403 3.394 3.134 3.119 3.096 3.081 2.959 2.946 2.933 2.920 2.907 2.895
2.281 2.117 2.074 2.056 2.046 2.025 2.016 1.769 1.744 1.675 1.669 1.628 1.598 1.569 1.558 1.280 1.158 1.118 1.093 1.088 1.069 0.913 0.868 0.857 0.035 0.027
CDC-15-1h
140416-323-CDC-15-1A, ,
15:33:49.593
USER: nmr
SOLVENT: CDCl3
Experiment = zg30
Pulse length = 14.100 usec
Recycle delay = 1.000 sec
NA = 12
Solvent = CDCl3
PTS1d = 32768
F1 = 400.130005 MHz
F2 = 1.000000 MHz
SW1 = 8223.68 Hz
AT1 = 3.98 sec
Hz per Pt 1stD = 0.25 Hz
SW2 = 1.00 Hz
Hz per Pt 2ndD = 1.00 Hz
O1 = 2476.3860 Hz
O2 = -1.0000 Hz
LB1 = 0.30 Hz
TP A = 0.00
B = 0.00
C = 0.00
N
F
O
N
O
1.96
1.48
0.97
0.40
1.00
1.02
0.98
0.99
1.00
2.00
1.00
1.01
3.00
1.06
1.08
4.93
3.04
2.27
8
6
4
2
0
PPM

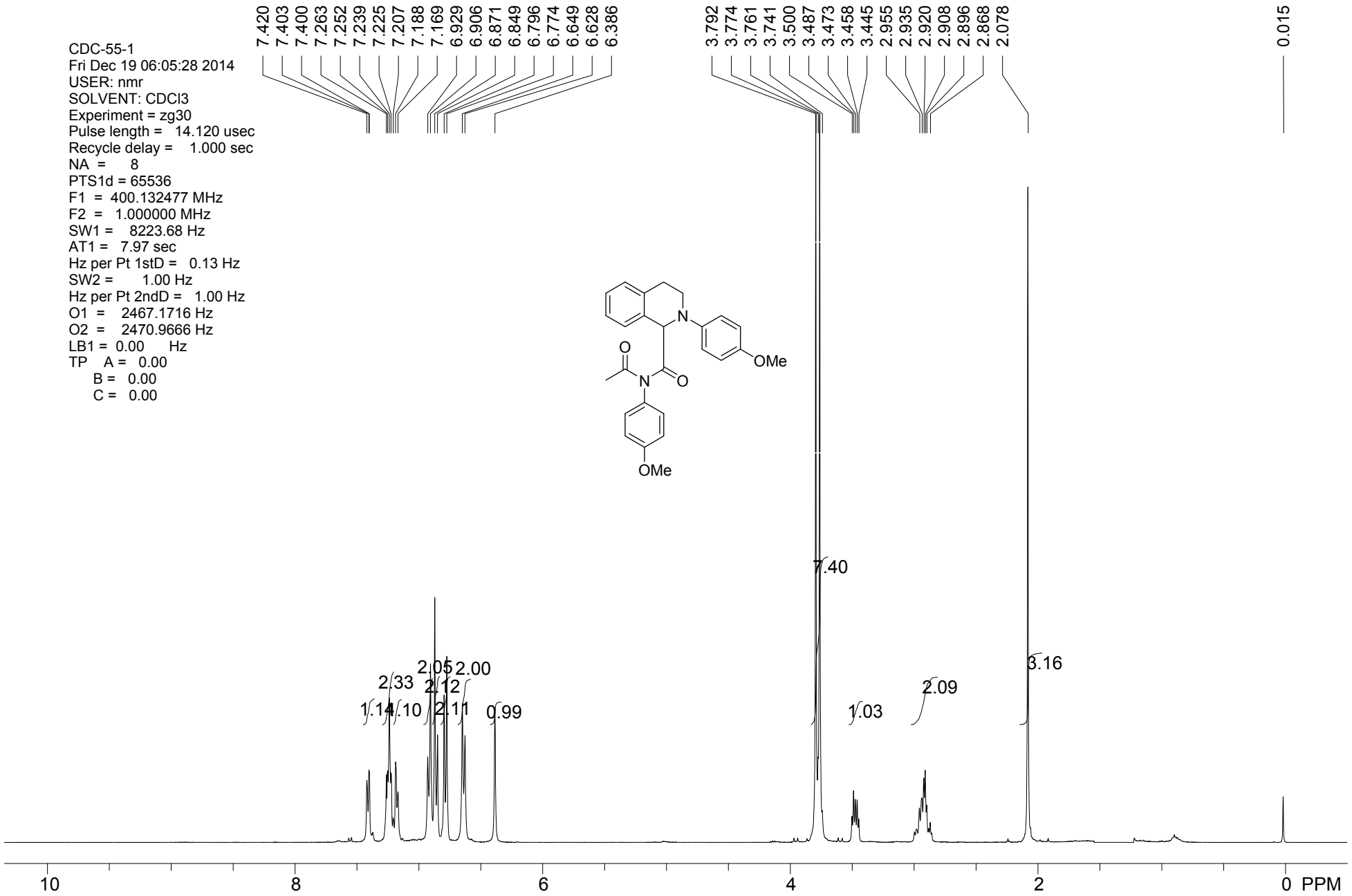

CDC-15-1c
140416-3231-CDC-15-1
15:37:20.921
SOLVENT: CDCl3
Experiment = zgpg30
Pulse length = 8.800 usec
Recycle delay = 2.000 sec
NA = 545
Solvent = CDCl3
PTS1d = 32768
F1 = 100.612770 MHz
F2 = 1.000000 MHz
SW1 = 24038.46 Hz
AT1 = 1.36 sec
Hz per Pt 1stD = 0.73 Hz
SW2 = 1.00 Hz
Hz per Pt 2ndD = 1.00 Hz
O1 = 11067.4053 Hz
O2 = -1.0000 Hz
LB1 = 1.00 Hz
TP A = 0.00
B = 0.00
C = 0.00
178.041
174.567
165.245
162.835
150.376
150.264
135.899
132.623
130.322
130.220
128.126
128.071
127.540
126.711
109.332
109.315
104.477
104.269
100.998
100.738
77.364
77.049
76.732
63.543
59.755
44.416
31.435
28.606
27.643
26.454
26.318
24.997
24.926
0.011
N
F
O
N
O
200
150
100
50
PPM

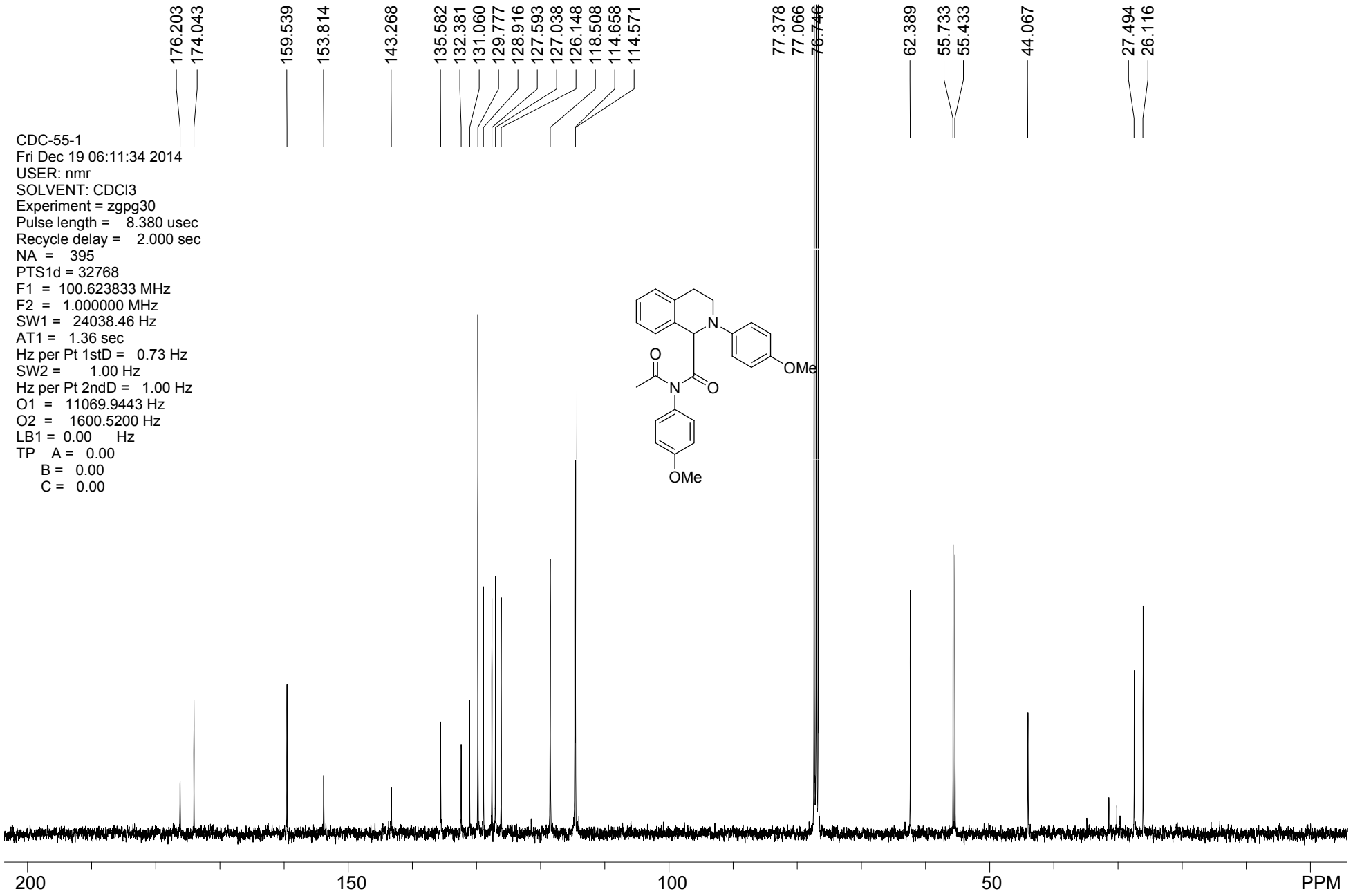

CDC-16-1h
140416-324-CDC-16-1A
15:35:02.765
SOLVENT: CDCl3
Experiment = zg30
Pulse length = 14.100 usec
Recycle delay = 1.000 sec
NA = 8
Solvent = CDCl3
PTS1d = 32768
F1 = 400.130005 MHz
F2 = 1.000000 MHz
SW1 = 8223.68 Hz
AT1 = 3.98 sec
Hz per Pt 1stD = 0.25 Hz
SW2 = 1.00 Hz
Hz per Pt 2ndD = 1.00 Hz
O1 = 2476.3860 Hz
O2 = -1.0000 Hz
LB1 = 0.30 Hz
TP A = 0.00
B = 0.00
C = 0.00
7.348
7.343
7.331
7.325
7.285
7.261
7.258
7.216
7.190
7.174
6.918
6.913
6.901
6.896
6.291
3.725
3.710
3.696
3.682
3.531
3.522
3.510
3.481
3.467
3.052
3.036
3.030
2.945
2.932
2.919
2.892
2.254
2.073
2.026
1.995
1.757
1.749
1.735
1.696
1.668
1.643
1.635
1.567
1.559
1.451
1.129
1.103
1.084
1.062
0.943
0.920
0.912
0.909
0.901
0.099
0.026
N
O
N
O
Cl
2.52
1.56
1.06
1.02
1.94
1.01
2.01
1.08
1.04
1.03
3.00
2.49
2.42
1.22
0.99
2.82
1.83
10
8
6
4
2
0 PPM

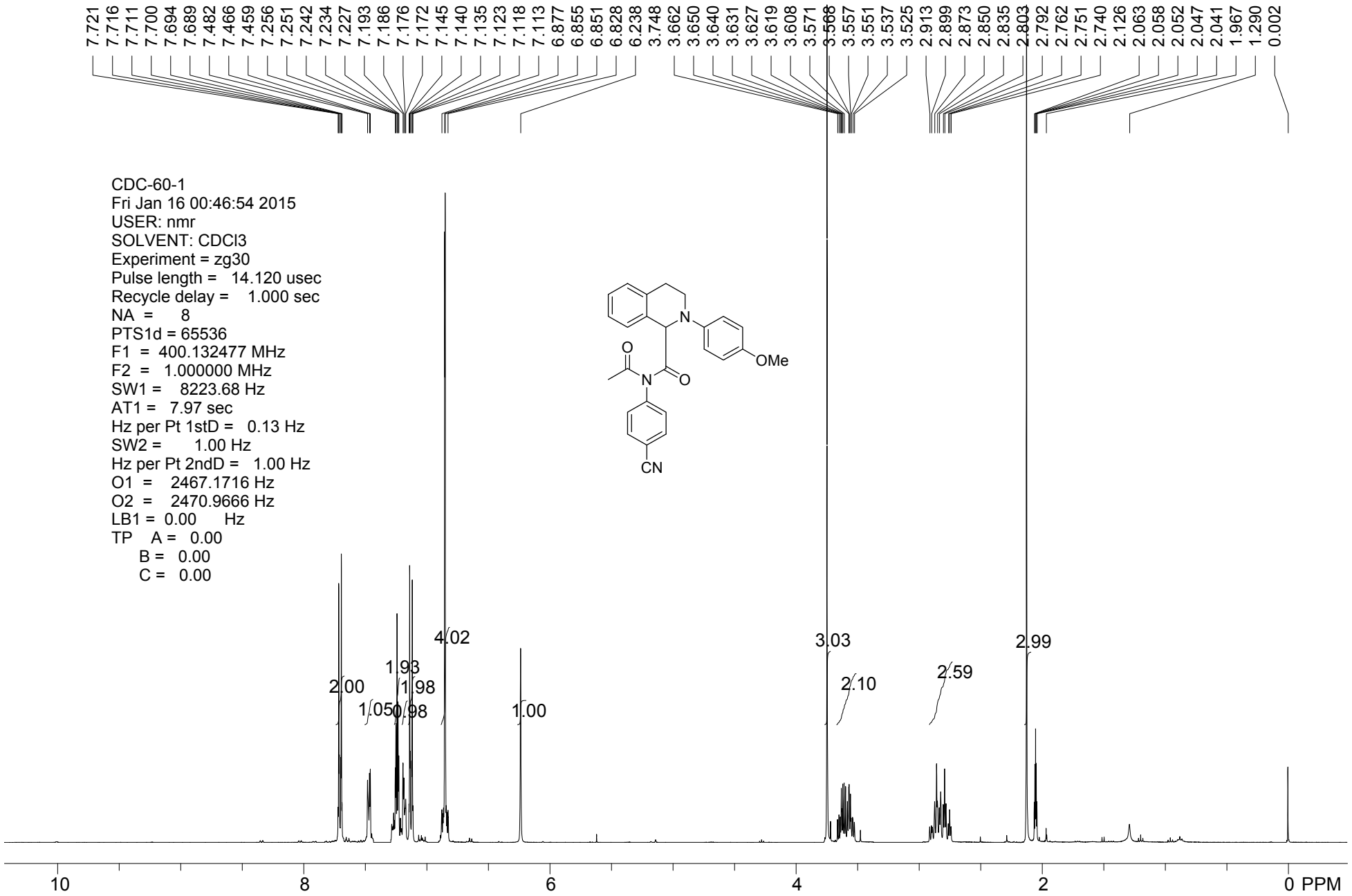

177.698
174.587
147.200
135.644
132.499
129.075
128.208
128.055
127.609
126.637
123.157
115.491
77.361
77.252
77.053
76.728
63.501
59.575
44.711
31.239
28.833
27.505
26.448
26.342
25.193
25.011
CDC-16-1c
140416-3241-CDC-16-1A
15:41:09.953
SOLVENT: CDCl3
Experiment = zgpg30
Pulse length = 8.800 usec
Recycle delay = 2.000 sec
NA = 377
Solvent = CDCl3
PTS1d = 32768
F1 = 100.612770 MHz
F2 = 1.000000 MHz
SW1 = 24038.46 Hz
AT1 = 1.36 sec
Hz per Pt 1stD = 0.73 Hz
SW2 = 1.00 Hz
Hz per Pt 2ndD = 1.00 Hz
O1 = 11067.4053 Hz
O2 = -1.0000 Hz
LB1 = 1.00 Hz
TP A = 0.00
B = 0.00
C = 0.00
N
O
N
O
Cl
200
150
100
50
PPM

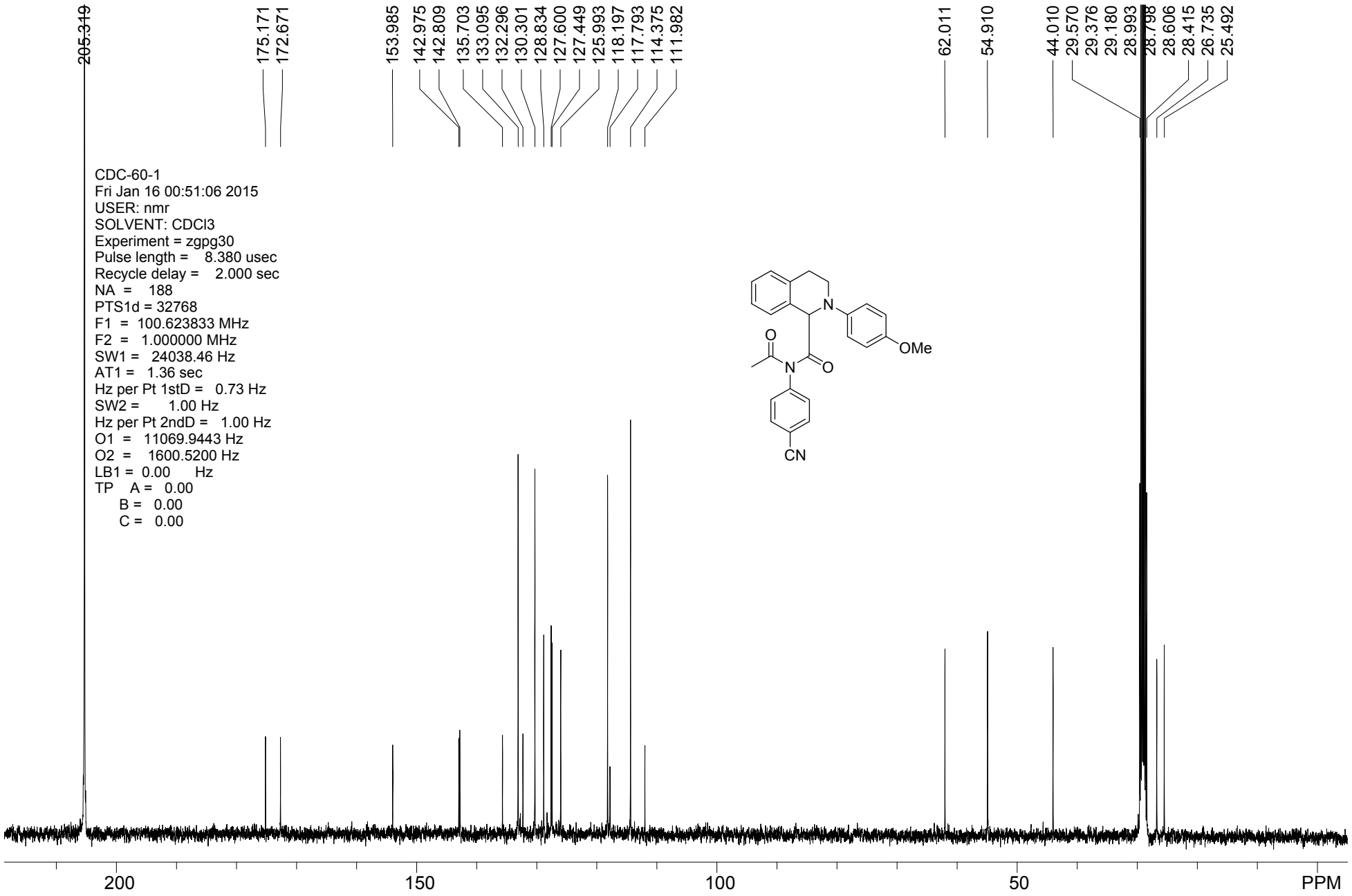

7.347
7.325
7.305
7.263
7.250
7.238
7.221
7.172
7.153
6.850
6.827
6.291
3.718
3.704
3.690
3.676
3.662
3.514
3.501
3.464
3.442
3.434
3.412
3.060
3.054
3.014
2.999
2.921
2.909
2.896
2.882
2.870
2.236
2.018
2.010
1.988
1.979
1.740
1.731
1.716
1.661
1.636
1.608
1.578
1.549
1.103
1.095
1.068
1.044
1.015
0.898
0.869
0.006
CDC-64-1
Mon Jan 12 01:43:56 2015
USER: nmr
SOLVENT: CDCl3
Experiment = zg30
Pulse length = 14.120 usec
Recycle delay = 1.000 sec
NA = 8
PTS1d = 65536
F1 = 400.132477 MHz
F2 = 1.000000 MHz
SW1 = 8223.68 Hz
AT1 = 7.97 sec
Hz per Pt 1stD = 0.13 Hz
SW2 = 1.00 Hz
Hz per Pt 2ndD = 1.00 Hz
O1 = 2467.1716 Hz
O2 = 2470.9666 Hz
LB1 = 0.00 Hz
TP A = 0.00
B = 0.00
C = 0.00
N
O
N
O
Br
3.04
1.93
1.04
2.00
0.99
1.01
2.01
1.02
1.00
2.98
1.06
5.79
2.91
1.17
10
8
6
4
2
0
PPM

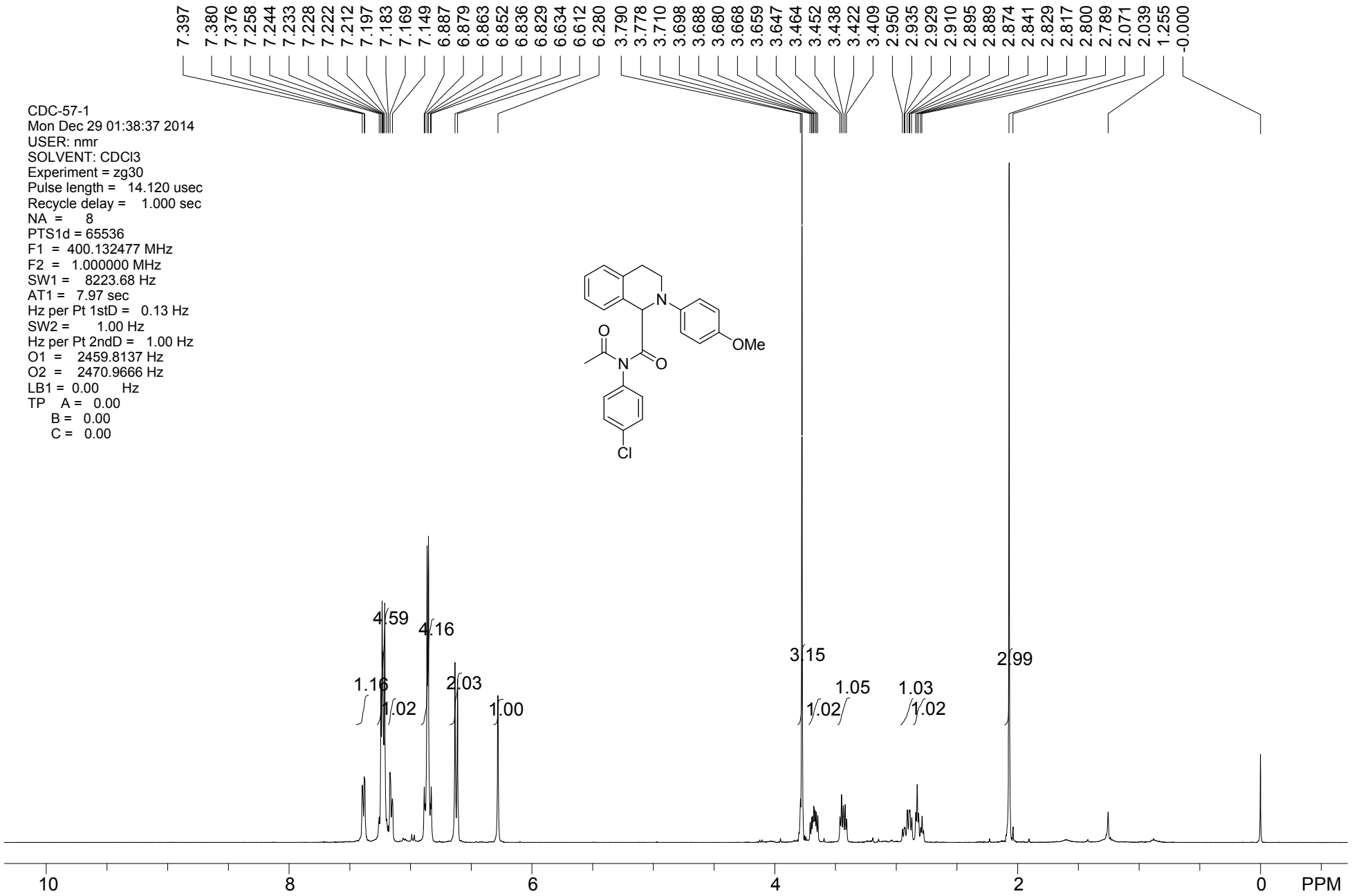

177.712
174.561
147.619
135.692
132.521
131.942
128.166
128.077
127.584
126.649
115.814
110.307
77.388
77.065
76.752
63.461
59.642
44.605
31.333
28.801
27.537
26.475
26.349
25.127
25.032
CDC-64-1
Mon Jan 12 01:57:30 2015
USER: nmr
SOLVENT: CDCl3
Experiment = zgpg30
Pulse length = 8.380 usec
Recycle delay = 2.000 sec
NA = 239
PTS1d = 32768
F1 = 100.623833 MHz
F2 = 1.000000 MHz
SW1 = 24038.46 Hz
AT1 = 1.36 sec
Hz per Pt 1stD = 0.73 Hz
SW2 = 1.00 Hz
Hz per Pt 2ndD = 1.00 Hz
O1 = 11069.9443 Hz
O2 = 1600.5200 Hz
LB1 = 0.00 Hz
TP A = 0.00
B = 0.00
C = 0.00
N
O
N
O
Br
200
150
100
50
0 PPM

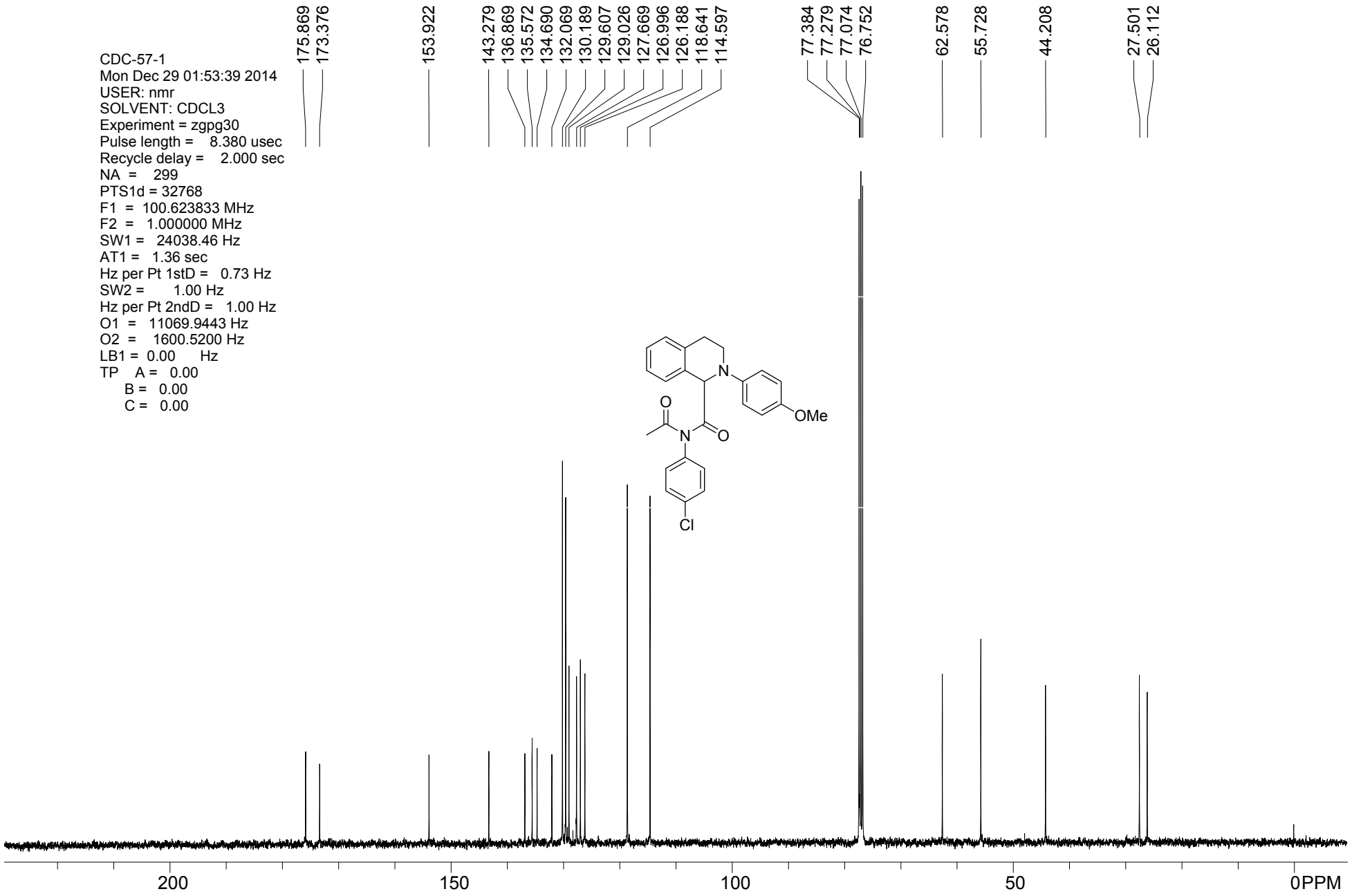

CDC-55-1
Fri Dec 19 06:05:28 2014
USER: nmr
SOLVENT: CDCl3
Experiment = zg30
Pulse length = 14.120 usec
Recycle delay = 1.000 sec
NA = 8
PTS1d = 65536
F1 = 400.132477 MHz
F2 = 1.000000 MHz
SW1 = 8223.68 Hz
AT1 = 7.97 sec
Hz per Pt 1stD = 0.13 Hz
SW2 = 1.00 Hz
Hz per Pt 2ndD = 1.00 Hz
O1 = 2467.1716 Hz
O2 = 2470.9666 Hz
LB1 = 0.00 Hz
TP A = 0.00
B = 0.00
C = 0.00
7.420
7.403
7.400
7.263
7.252
7.239
7.225
7.207
7.188
7.169
6.929
6.906
6.871
6.849
6.796
6.774
6.649
6.628
6.386
3.792
3.774
3.761
3.741
3.500
3.487
3.473
3.458
3.445
2.955
2.935
2.920
2.908
2.896
2.868
2.078
0.015
N
OMe
O
N
O
OMe
7.40
3.16
2.09
1.03
2.33
2.05
2.12
2.00
1.14
1.10
2.11
0.99
10
8
6
4
2
0 PPM

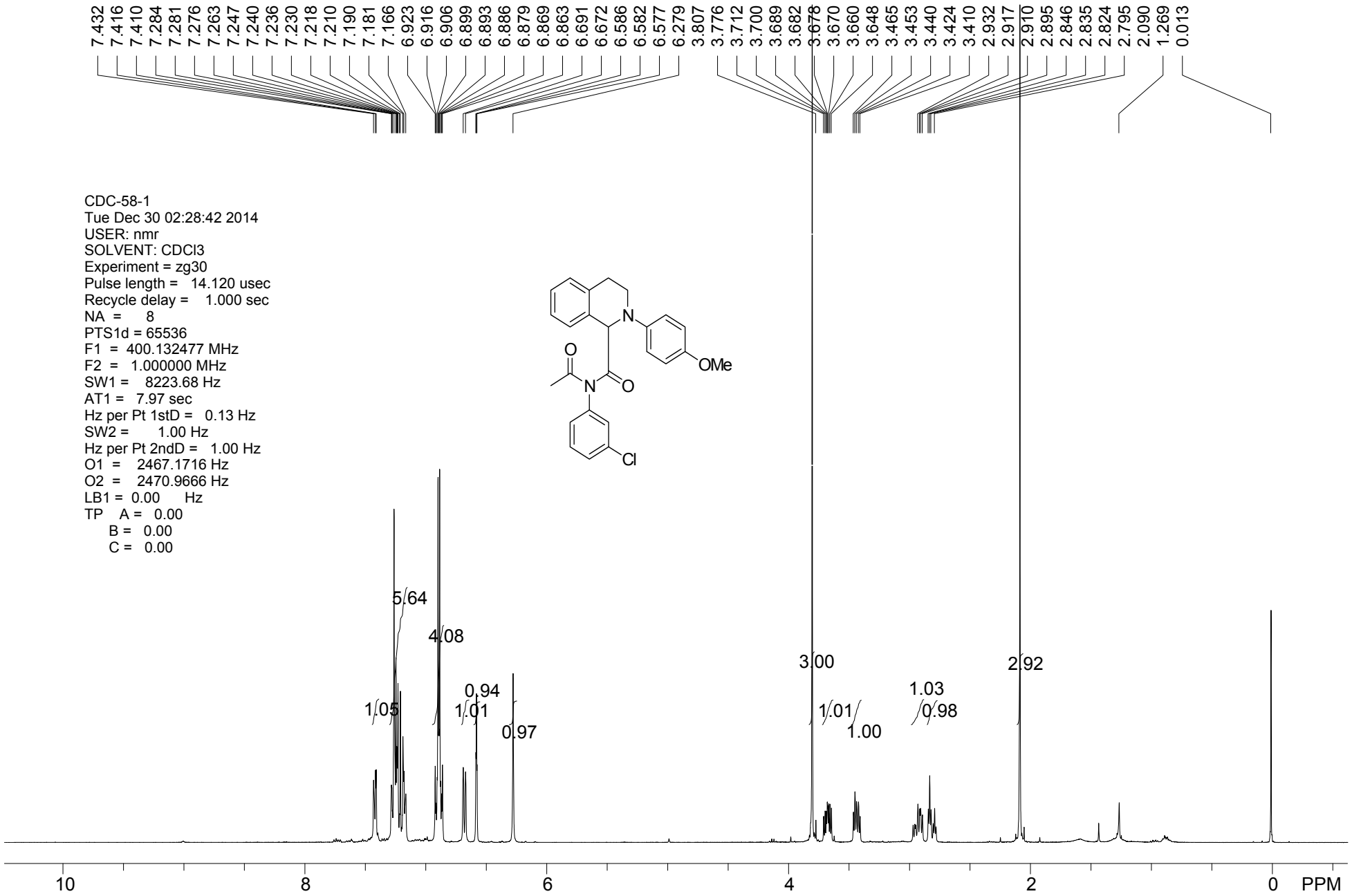

176.203
174.043
159.539
153.814
143.268
135.582
132.381
131.060
129.777
128.916
127.593
127.038
126.148
118.508
114.658
114.571
77.378
77.066
76.746
62.389
55.733
55.433
44.067
27.494
26.116
CDC-55-1
Fri Dec 19 06:11:34 2014
USER: nmr
SOLVENT: CDCl3
Experiment = zgpg30
Pulse length = 8.380 usec
Recycle delay = 2.000 sec
NA = 395
PTS1d = 32768
F1 = 100.623833 MHz
F2 = 1.000000 MHz
SW1 = 24038.46 Hz
AT1 = 1.36 sec
Hz per Pt 1stD = 0.73 Hz
SW2 = 1.00 Hz
Hz per Pt 2ndD = 1.00 Hz
O1 = 11069.9443 Hz
O2 = 1600.5200 Hz
LB1 = 0.00 Hz
TP A = 0.00
B = 0.00
C = 0.00
N
O
N
O
OMe
OMe
200
150
100
50
PPM

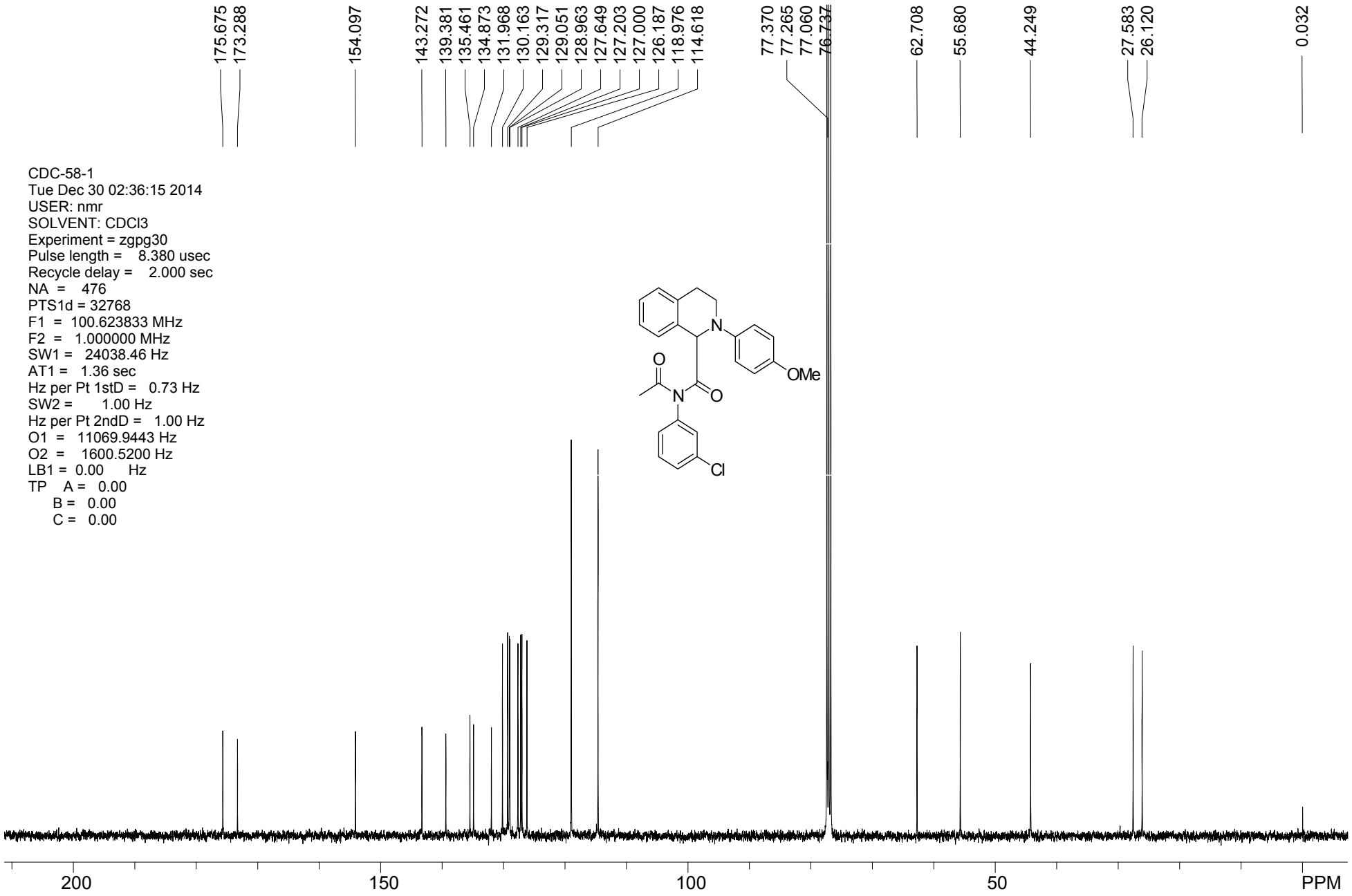

7.721 7.716 7.711 7.700 7.694 7.689 7.482 7.466 7.459 7.256 7.251 7.242 7.234 7.227 7.193 7.186 7.176 7.172 7.145 7.140 7.135 7.123 7.118 7.113 6.877 6.855 6.851 6.828 6.238 3.748 3.662 3.650 3.640 3.631 3.627 3.619 3.608 3.571 3.568 3.557 3.551 3.537 3.525 2.913 2.899 2.873 2.850 2.835 2.803 2.792 2.762 2.751 2.740 2.126 2.063 2.058 2.052 2.047 2.041 1.967 1.290 0.002
CDC-60-1
Fri Jan 16 00:46:54 2015
USER: nmr
SOLVENT: CDCl3
Experiment = zg30
Pulse length = 14.120 usec
Recycle delay = 1.000 sec
NA = 8
PTS1d = 65536
F1 = 400.132477 MHz
F2 = 1.000000 MHz
SW1 = 8223.68 Hz
AT1 = 7.97 sec
Hz per Pt 1stD = 0.13 Hz
SW2 = 1.00 Hz
Hz per Pt 2ndD = 1.00 Hz
O1 = 2467.1716 Hz
O2 = 2470.9666 Hz
LB1 = 0.00 Hz
TP A = 0.00
B = 0.00
C = 0.00
N
OMe
O
N
O
CN
2.00
1.05
1.93
1.98
0.98
4.02
1.00
3.03
2.10
2.59
2.99
10
8
6
4
2
0 PPM

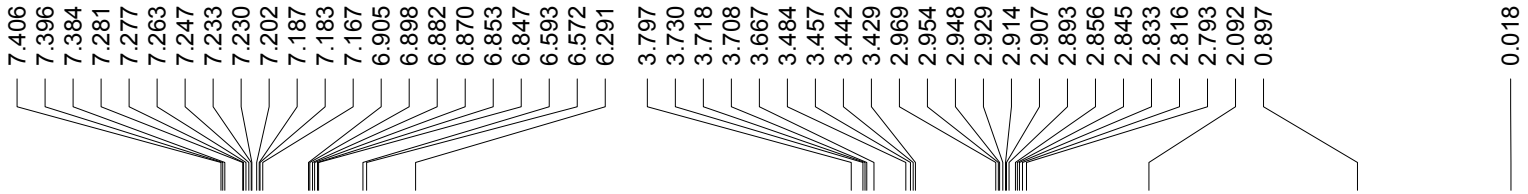

205.319
175.171
172.671
153.985
142.975
142.809
135.703
133.095
132.296
130.301
128.834
127.600
127.449
125.993
118.197
117.793
114.375
111.982
62.011
54.910
44.010
29.570
29.376
29.180
28.993
28.798
28.606
28.415
26.735
25.492
CDC-60-1
Fri Jan 16 00:51:06 2015
USER: nmr
SOLVENT: CDCl3
Experiment = zgpg30
Pulse length = 8.380 usec
Recycle delay = 2.000 sec
NA = 188
PTS1d = 32768
F1 = 100.623833 MHz
F2 = 1.000000 MHz
SW1 = 24038.46 Hz
AT1 = 1.36 sec
Hz per Pt 1stD = 0.73 Hz
SW2 = 1.00 Hz
Hz per Pt 2ndD = 1.00 Hz
O1 = 11069.9443 Hz
O2 = 1600.5200 Hz
LB1 = 0.00 Hz
TP A = 0.00
B = 0.00
C = 0.00
N
OMe
O
N
O
CN
200
150
100
50
PPM


7.397
7.380
7.376
7.258
7.244
7.233
7.228
7.222
7.212
7.197
7.183
7.169
7.149
6.887
6.879
6.863
6.852
6.836
6.829
6.634
6.612
6.280
3.790
3.778
3.710
3.698
3.688
3.680
3.668
3.659
3.647
3.464
3.452
3.438
3.422
3.409
2.950
2.935
2.929
2.910
2.895
2.889
2.874
2.841
2.829
2.817
2.800
2.789
2.071
2.039
1.255
-0.000
CDC-57-1
Mon Dec 29 01:38:37 2014
USER: nmr
SOLVENT: CDCl3
Experiment = zg30
Pulse length = 14.120 usec
Recycle delay = 1.000 sec
NA = 8
PTS1d = 65536
F1 = 400.132477 MHz
F2 = 1.000000 MHz
SW1 = 8223.68 Hz
AT1 = 7.97 sec
Hz per Pt 1stD = 0.13 Hz
SW2 = 1.00 Hz
Hz per Pt 2ndD = 1.00 Hz
O1 = 2459.8137 Hz
O2 = 2470.9666 Hz
LB1 = 0.00 Hz
TP A = 0.00
B = 0.00
C = 0.00
N
OMe
O
N
O
Cl
4.59
4.16
1.16
1.02
2.03
1.00
3.15
1.02
1.05
1.03
1.02
2.99
10
8
6
4
2
0
PPM

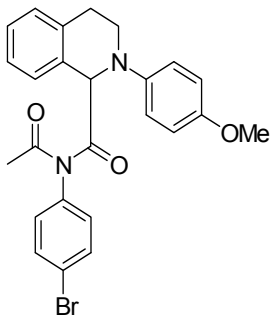

175.869
173.376
153.922
143.279
136.869
135.572
134.690
132.069
130.189
129.607
129.026
127.669
126.996
126.188
118.641
114.597
77.384
77.279
77.074
76.752
62.578
55.728
44.208
27.501
26.112
CDC-57-1
Mon Dec 29 01:53:39 2014
USER: nmr
SOLVENT: CDCL3
Experiment = zgpg30
Pulse length = 8.380 usec
Recycle delay = 2.000 sec
NA = 299
PTS1d = 32768
F1 = 100.623833 MHz
F2 = 1.000000 MHz
SW1 = 24038.46 Hz
AT1 = 1.36 sec
Hz per Pt 1stD = 0.73 Hz
SW2 = 1.00 Hz
Hz per Pt 2ndD = 1.00 Hz
O1 = 11069.9443 Hz
O2 = 1600.5200 Hz
LB1 = 0.00 Hz
TP A = 0.00
B = 0.00
C = 0.00
N
OMe
O
N
O
Cl
200
150
100
50
0PPM

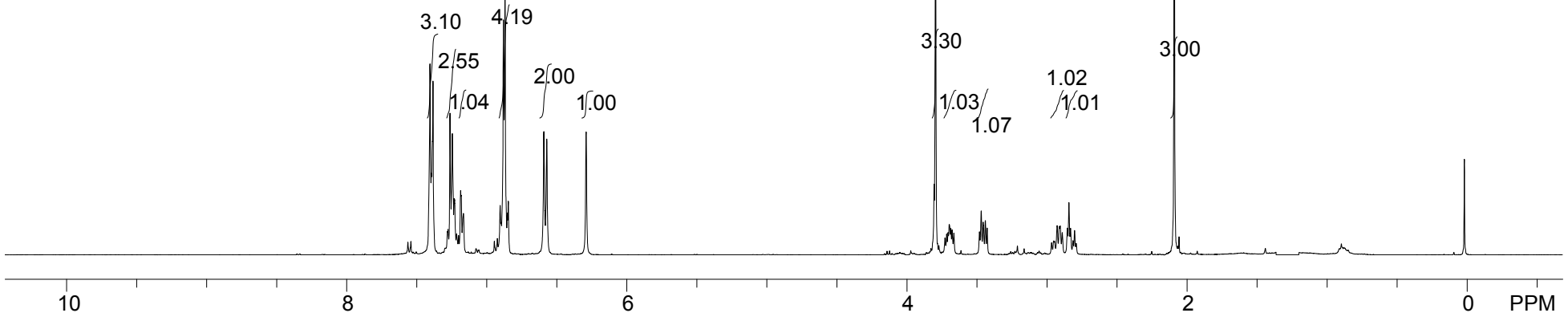

7.432
7.416
7.410
7.284
7.281
7.276
7.263
7.247
7.240
7.236
7.230
7.218
7.210
7.190
7.181
7.166
6.923
6.916
6.906
6.899
6.893
6.886
6.879
6.869
6.863
6.691
6.672
6.586
6.582
6.577
6.279
3.807
3.776
3.712
3.700
3.689
3.682
3.678
3.670
3.660
3.648
3.465
3.453
3.440
3.424
3.410
2.932
2.917
2.910
2.895
2.846
2.835
2.824
2.795
2.090
1.269
0.013
CDC-58-1
Tue Dec 30 02:28:42 2014
USER: nmr
SOLVENT: CDCl3
Experiment = zg30
Pulse length = 14.120 usec
Recycle delay = 1.000 sec
NA = 8
PTS1d = 65536
F1 = 400.132477 MHz
F2 = 1.000000 MHz
SW1 = 8223.68 Hz
AT1 = 7.97 sec
Hz per Pt 1stD = 0.13 Hz
SW2 = 1.00 Hz
Hz per Pt 2ndD = 1.00 Hz
O1 = 2467.1716 Hz
O2 = 2470.9666 Hz
LB1 = 0.00 Hz
TP A = 0.00
B = 0.00
C = 0.00
N
O
OMe
O
N
O
Cl
5.64
4.08
1.05
0.94
1.01
0.97
3.00
1.01
1.00
1.03
0.98
2.92
10
8
6
4
2
0
PPM

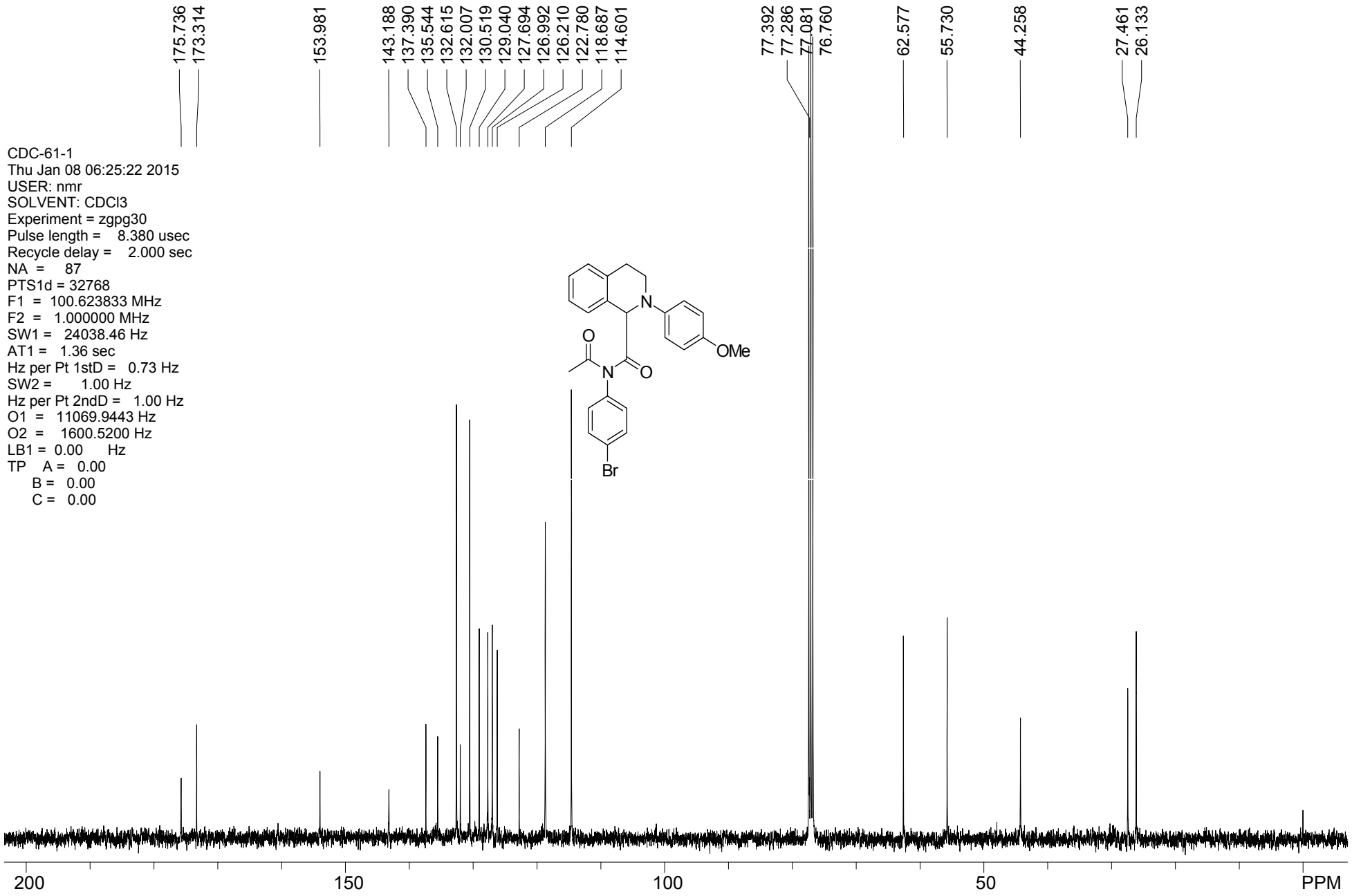

175.675
173.288
154.097
143.272
139.381
135.461
134.873
131.968
130.163
129.317
129.051
128.963
127.649
127.203
127.000
126.187
118.976
114.618
77.370
77.265
77.060
76.737
62.708
55.680
44.249
27.583
26.120
0.032
CDC-58-1
Tue Dec 30 02:36:15 2014
USER: nmr
SOLVENT: CDCl3
Experiment = zgpg30
Pulse length = 8.380 usec
Recycle delay = 2.000 sec
NA = 476
PTS1d = 32768
F1 = 100.623833 MHz
F2 = 1.000000 MHz
SW1 = 24038.46 Hz
AT1 = 1.36 sec
Hz per Pt 1stD = 0.73 Hz
SW2 = 1.00 Hz
Hz per Pt 2ndD = 1.00 Hz
O1 = 11069.9443 Hz
O2 = 1600.5200 Hz
LB1 = 0.00 Hz
TP A = 0.00
B = 0.00
C = 0.00
N
O
N
O
OMe
Cl
200
150
100
50
PPM

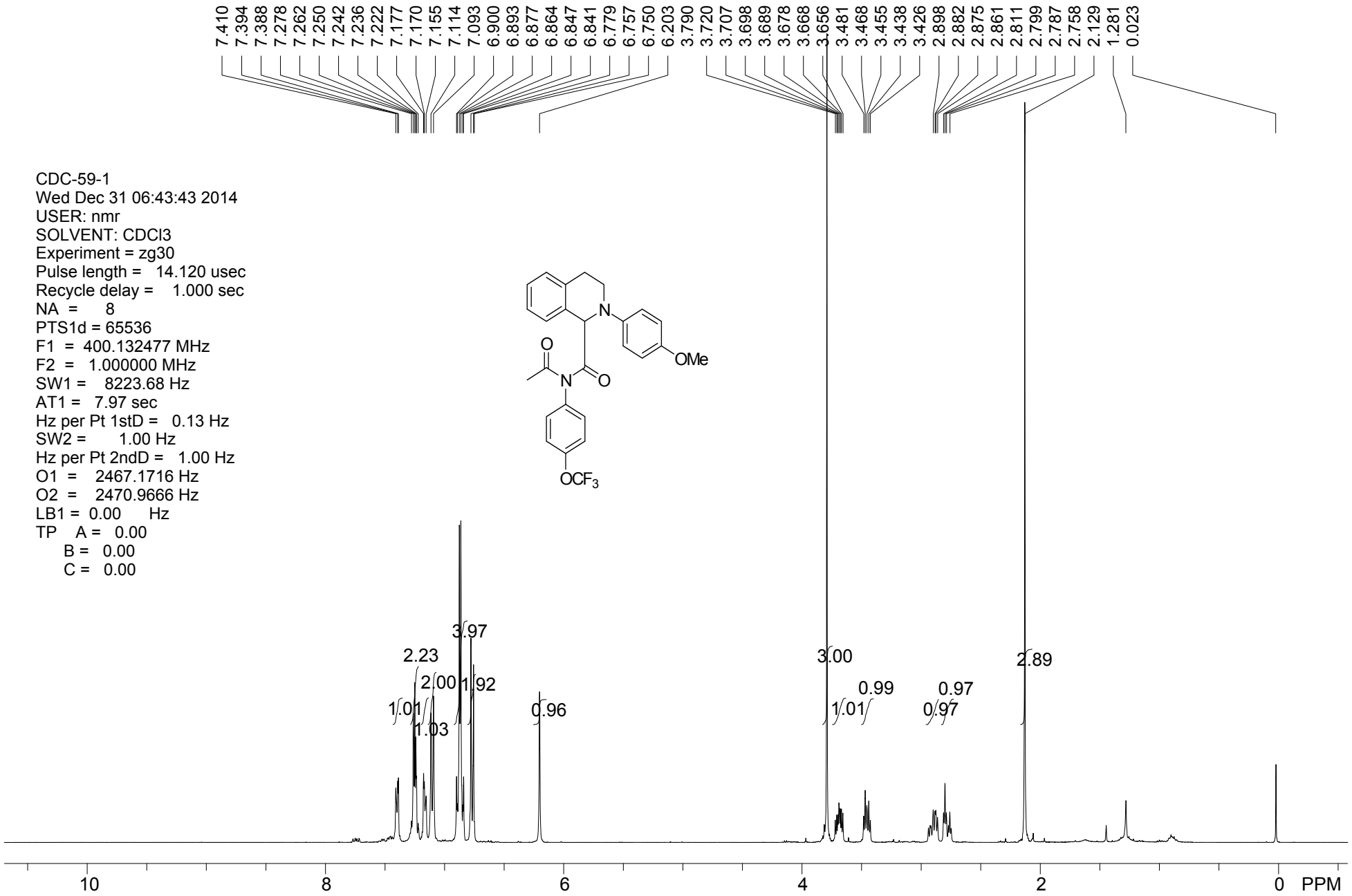


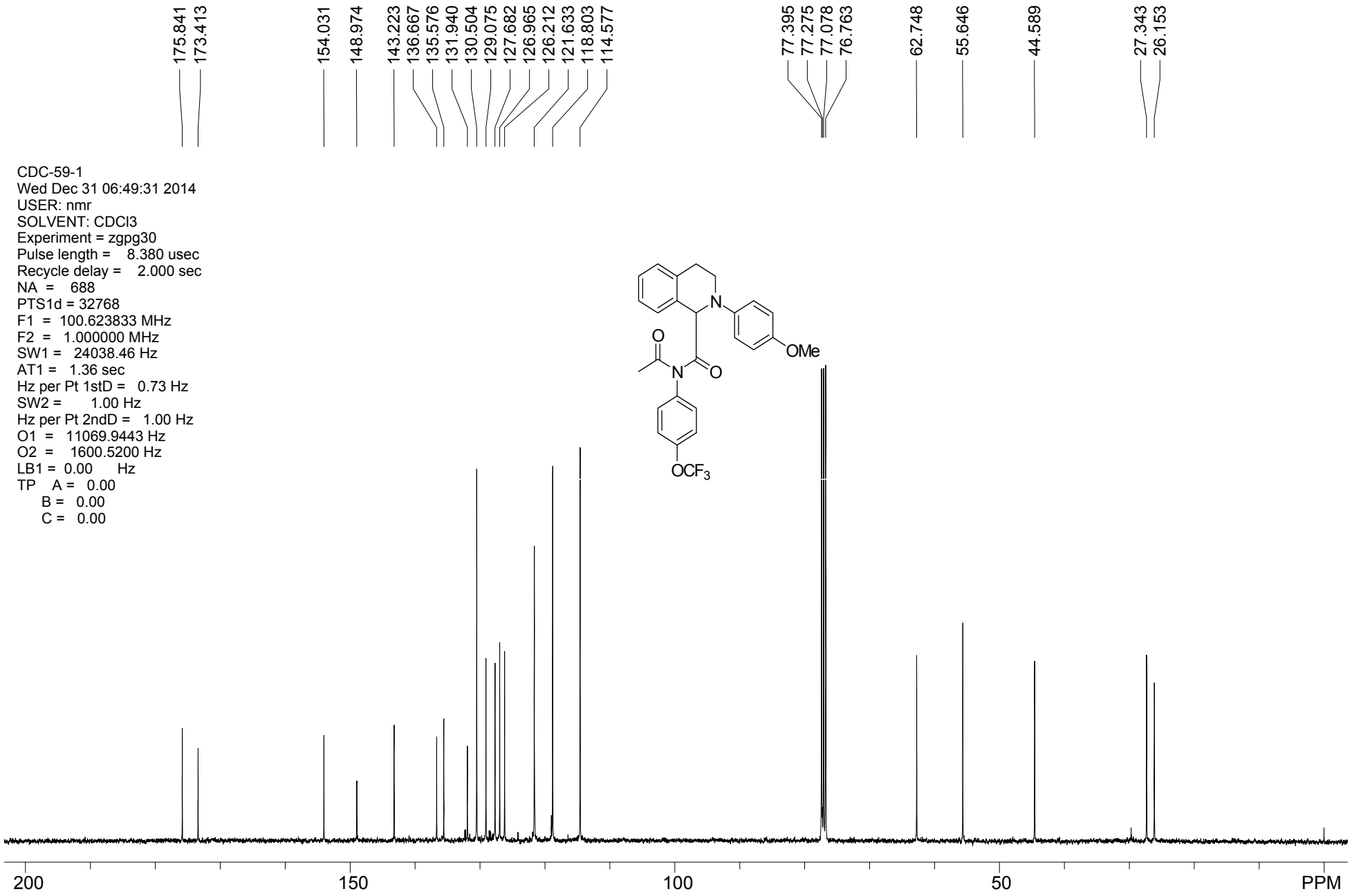
CDC-61-1
Thu Jan 08 06:19:52 2015
USER: nmr
SOLVENT: CDCl3
Experiment = zg30
Pulse length = 14.120 usec
Recycle delay = 1.000 sec
NA = 8
PTS1d = 65536
F1 = 400.132477 MHz
F2 = 1.000000 MHz
SW1 = 8223.68 Hz
AT1 = 7.97 sec
Hz per Pt 1stD = 0.13 Hz
SW2 = 1.00 Hz
Hz per Pt 2ndD = 1.00 Hz
O1 = 2467.1716 Hz
O2 = 2470.9666 Hz
LB1 = 0.00 Hz
TP A = 0.00
B = 0.00
C = 0.00

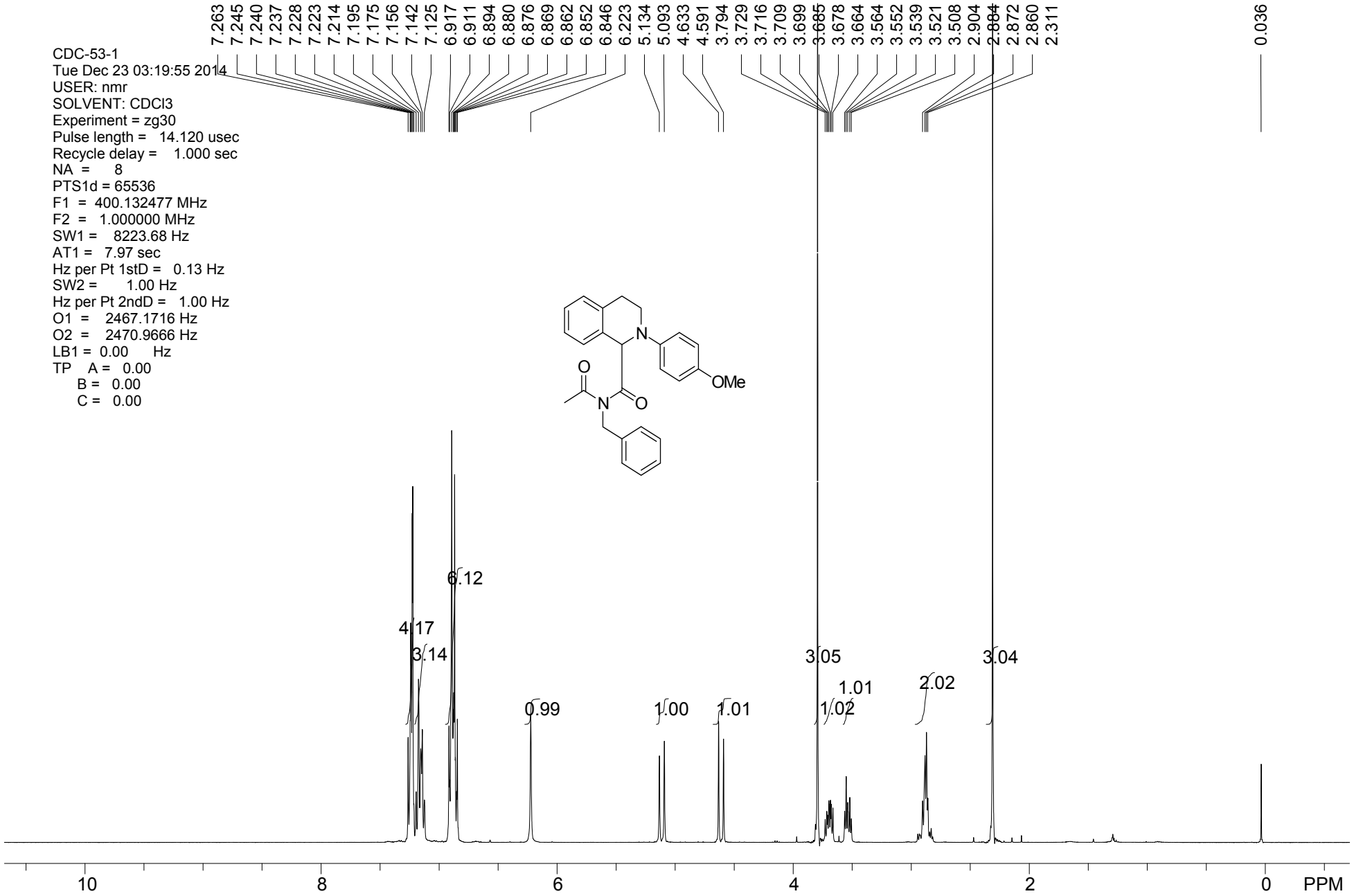


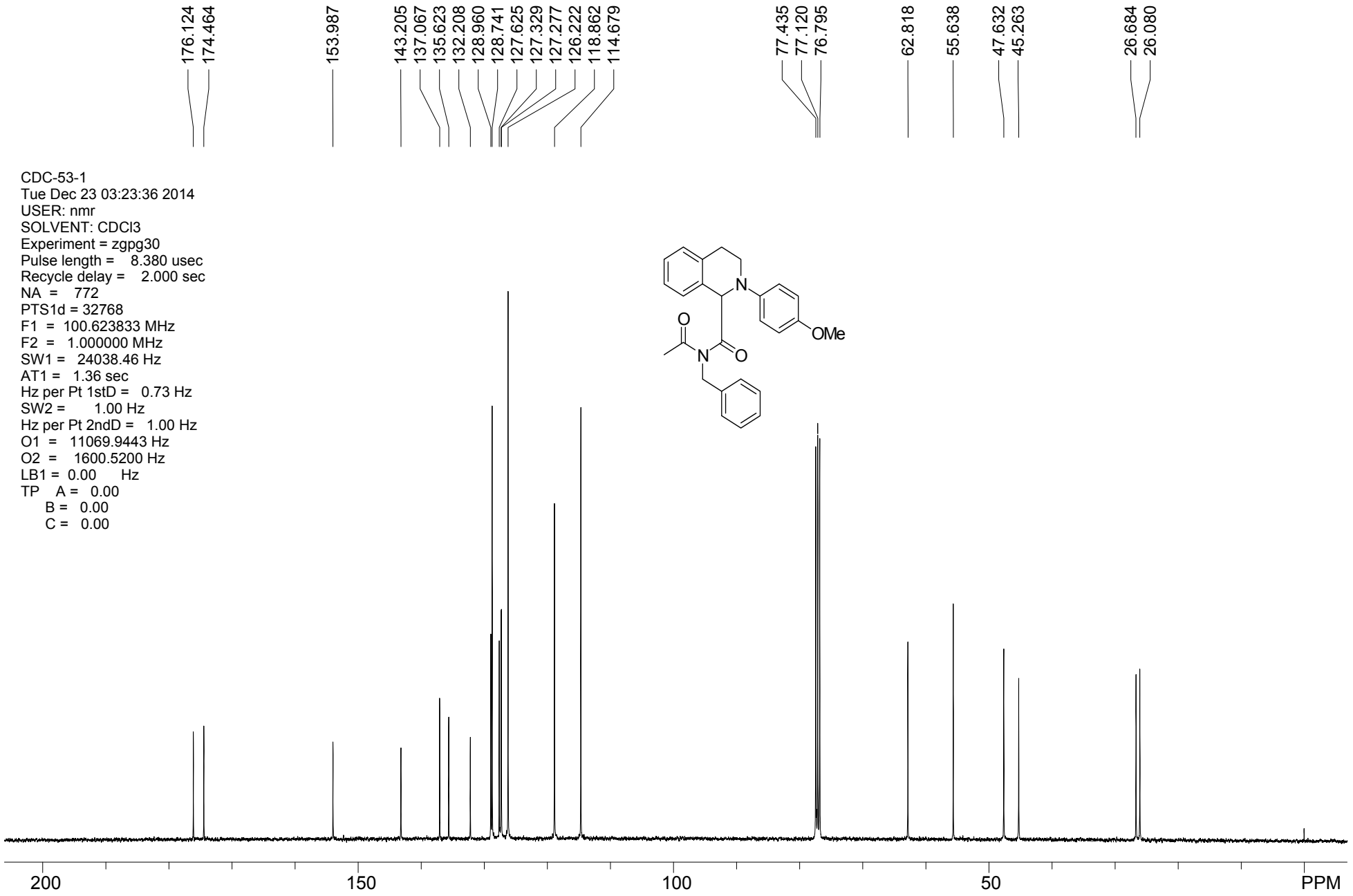



175.736
173.314
153.981
143.188
137.390
135.544
132.615
132.007
130.519
129.040
127.694
126.992
126.210
122.780
118.687
114.601
77.392
77.286
77.081
76.760
62.577
55.730
44.258
27.461
26.133
CDC-61-1
Thu Jan 08 06:25:22 2015
USER: nmr
SOLVENT: CDCl3
Experiment = zgpg30
Pulse length = 8.380 usec
Recycle delay = 2.000 sec
NA = 87
PTS1d = 32768
F1 = 100.623833 MHz
F2 = 1.000000 MHz
SW1 = 24038.46 Hz
AT1 = 1.36 sec
Hz per Pt 1stD = 0.73 Hz
SW2 = 1.00 Hz
Hz per Pt 2ndD = 1.00 Hz
O1 = 11069.9443 Hz
O2 = 1600.5200 Hz
LB1 = 0.00 Hz
TP A = 0.00
B = 0.00
C = 0.00
N
OMe
O
N
O
Br
200
150
100
50
PPM


7.410
7.394
7.388
7.278
7.262
7.250
7.242
7.236
7.222
7.177
7.170
7.155
7.114
7.093
6.900
6.893
6.877
6.864
6.847
6.841
6.779
6.757
6.750
6.203
3.790
3.720
3.707
3.698
3.689
3.678
3.668
3.656
3.481
3.468
3.455
3.438
3.426
2.898
2.882
2.875
2.861
2.811
2.799
2.787
2.758
2.129
1.281
0.023
CDC-59-1
Wed Dec 31 06:43:43 2014
USER: nmr
SOLVENT: CDCl3
Experiment = zg30
Pulse length = 14.120 usec
Recycle delay = 1.000 sec
NA = 8
PTS1d = 65536
F1 = 400.132477 MHz
F2 = 1.000000 MHz
SW1 = 8223.68 Hz
AT1 = 7.97 sec
Hz per Pt 1stD = 0.13 Hz
SW2 = 1.00 Hz
Hz per Pt 2ndD = 1.00 Hz
O1 = 2467.1716 Hz
O2 = 2470.9666 Hz
LB1 = 0.00 Hz
TP A = 0.00
B = 0.00
C = 0.00
N
O
N
O
OMe
OCF3
3.97
2.23
2.00
1.92
1.01
1.03
0.96
3.00
0.99
0.97
1.01
0.97
2.89
10
8
6
4
2
0
PPM


175.841
173.413
154.031
148.974
143.223
136.667
135.576
131.940
130.504
129.075
127.682
126.965
126.212
121.633
118.803
114.577
77.395
77.275
77.078
76.763
62.748
55.646
44.589
27.343
26.153
CDC-59-1
Wed Dec 31 06:49:31 2014
USER: nmr
SOLVENT: CDCl3
Experiment = zgpg30
Pulse length = 8.380 usec
Recycle delay = 2.000 sec
NA = 688
PTS1d = 32768
F1 = 100.623833 MHz
F2 = 1.000000 MHz
SW1 = 24038.46 Hz
AT1 = 1.36 sec
Hz per Pt 1stD = 0.73 Hz
SW2 = 1.00 Hz
Hz per Pt 2ndD = 1.00 Hz
O1 = 11069.9443 Hz
O2 = 1600.5200 Hz
LB1 = 0.00 Hz
TP A = 0.00
B = 0.00
C = 0.00
N
O
OMe
N
O
O
OCF3
200
150
100
50
PPM


7.263
7.245
7.240
7.237
7.228
7.223
7.214
7.195
7.175
7.156
7.142
7.125
6.917
6.911
6.894
6.880
6.876
6.869
6.862
6.852
6.846
6.223
5.134
5.093
4.633
4.591
3.794
3.729
3.716
3.709
3.699
3.685
3.678
3.664
3.564
3.552
3.539
3.521
3.508
2.904
2.884
2.872
2.860
2.311
0.036
CDC-53-1
Tue Dec 23 03:19:55 2014
USER: nmr
SOLVENT: CDCl3
Experiment = zg30
Pulse length = 14.120 usec
Recycle delay = 1.000 sec
NA = 8
PTS1d = 65536
F1 = 400.132477 MHz
F2 = 1.000000 MHz
SW1 = 8223.68 Hz
AT1 = 7.97 sec
Hz per Pt 1stD = 0.13 Hz
SW2 = 1.00 Hz
Hz per Pt 2ndD = 1.00 Hz
O1 = 2467.1716 Hz
O2 = 2470.9666 Hz
LB1 = 0.00 Hz
TP A = 0.00
B = 0.00
C = 0.00
N
OMe
O
N
O
6.12
4.17
3.14
0.99
1.00
1.01
3.05
1.01
1.02
2.02
3.04
10
8
6
4
2
0
PPM


176.124
174.464
153.987
143.205
137.067
135.623
132.208
128.960
128.741
127.625
127.329
127.277
126.222
118.862
114.679
77.435
77.120
76.795
62.818
55.638
47.632
45.263
26.684
26.080
CDC-53-1
Tue Dec 23 03:23:36 2014
USER: nmr
SOLVENT: CDCl3
Experiment = zgpg30
Pulse length = 8.380 usec
Recycle delay = 2.000 sec
NA = 772
PTS1d = 32768
F1 = 100.623833 MHz
F2 = 1.000000 MHz
SW1 = 24038.46 Hz
AT1 = 1.36 sec
Hz per Pt 1stD = 0.73 Hz
SW2 = 1.00 Hz
Hz per Pt 2ndD = 1.00 Hz
O1 = 11069.9443 Hz
O2 = 1600.5200 Hz
LB1 = 0.00 Hz
TP A = 0.00
B = 0.00
C = 0.00
N
O
N
O
OMe
200
150
100
50
PPM