General Procedures

All reactions were carried out under an argon atmosphere. Toluene was purchased from J.T. Baker in a CYCLE-TAINER solvent-deliver keg and vigorously purged with argon for 1 hour. The solvent was further purified by passing through successive alumina and Q5 reactant-packed columns on a solvent purification system. The anhydrous DMF was purchased from Aldrich Chemical Co. in Sure-Seal bottles and was used as received. $Pd_2(dba)_3$ and **L2** were purchased from Strem Chemicals Inc. and $TMSN_3$, CuI, alkynes, aryl halides, aryl triflates, benzotriazole and 1,2,3-triazole were purchased from Aldrich Chemical Co., Alfa Aesar, or TCI America and were used without further purification. Anhydrous tribasic potassium phosphate was purchased from Alfa Aesar, and stored in a glovebox. Small portions were removed and stored in a desiccator for up to 2 weeks (All reactions were set-up outside of the glovebox). **L1**, **L3** and **L4** were prepared by literature procedure.[1,2]

Reactions were monitored by GC and thin-layer chromatography (TLC) carried out on 0.25 mm E. Merck silica gel plates (60F-254) using UV light (N^2-arylated 1,2,3-triazoles are more volatile and less polar than corresponding N^1-arylated products). Flash silica gel chromatography was performed using Silicycle SiliaFlashP60 (230-400 mesh) silica gel. All compounds were characterized by ^{1}H NMR, ^{13}C NMR, IR spectroscopy. Copies of the ^{1}H and ^{13}C NMR spectra can be found at the end of the Supporting Information. Nuclear Magnetic Resonance spectra were recorded on a Bruker 400 MHz instrument. All ^{1}H NMR experiments are reported in δ units, parts per million (ppm), and were measured relative to the signals for residual chloroform (7.26 ppm) or dimethylsulfoxide (2.50 ppm) in the deuterated solvent. All ^{13}C NMR spectra are reported in ppm relative to deuterochloroform (77.23 ppm) or dimethylsulfoxide-*d6* (39.52 ppm), and all were obtained with 1H decoupling. All IR spectra were taken on a Perkin – Elmer 2000 FTIR. All GC analyses were performed on a Agilent 6890 gas chromatograph with an FID detectorusing a J & W DB-1 column (10 m, 0.1 mm I.D.). Elemental analyses were performed by Atlantic Microlabs Inc., Norcross, GA. The pure compounds are estimated to be ≥ 95% pure as determined by ^{1}H NMR and GC analysis

Computational Methods

All calculations were carried out with Gaussian03 suite of computational programs.[3] Ground state geometry optimizations were evaluated using B3LYP[4] density functional method. For C, H, and N atoms, the 6-31G(d) basis set was used; while LANL2DZ effective core potentials of Hay and Wadt[5] with double-ζ basis sets were used for Pd and P atoms. Frequency calculations were performed on all optimized structures to verify that they have no negative frequencies. The Gibbs free energies were calculated at 298.15 K and 1 atm. Single point energy calculations were done with the 6-311+G(2d,p) basis set to obtain higher accuracy electronic energies.

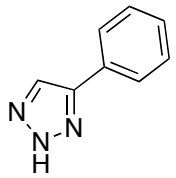
General Procedure for the synthesis of 4-substituted 1,2,3-triazoles[6]

Caution: This reaction produces explosive and toxic hydrogen azide (HN_3) in situ. The reaction should be conducted behind a safety shield in a hood.

An oven-dried vial was equipped with a magnetic stir bar and charged with CuI (95 mg, 0.5 mmol) (alkynes that were solid at room temperature were added at this point). The vial was sealed with a screw-cap septum, and then evacuated and backfilled with argon (this process was repeated a total of 3 times). $TMSN_3$ (2.0 mL, 15 mmol) and alkyne (10 mmol) were added via syringe, followed by addition of DMF/MeOH (4:1, 10 mL). The reaction mixture was stirred at 100 °C for 6-24 h. The reaction mixture was cooled to room temperature, diluted with EtOAc, washed with 30% aqueous NH_4OH, dried over $MgSO_4$, concentrated in vacuo and purified via flash chromatography.

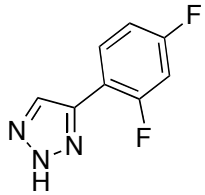
Note: A safer two-step preparation of 4-substituted 1,2,3-triazoles is also available.[7]

4-Phenyl-1,2,3-triazole (CAS:1680-44-0)



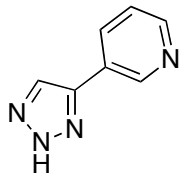
Following general procedure for the synthesis of 4-substituted-1,2,3-triazoles, a mixture of phenylacetylene (1.1 mL, 10 mmol), $TMSN_3$ (2.0 mL, 1.2 mmol), CuI (95 mg, 0.5 mmol), in DMF/MeOH (4:1, 10 mL) was heated to 100 °C for 6 h. The crude product was purified via flash chromatography (Hexanes/EtOAc, 1:1) to provide the title compound as a white solid (1.26 g, 86%), mp 144-145 °C. ^{1}H NMR (400 MHz, DMSO-*d6*) δ 15.20 (s, 1H), 8.34 (s, 1H), 7.88 (d, *J* = 7.6 Hz, 2H), 7.48-7.38 (m, 2H), 7.37-7.27 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 145.3, 130.4, 129.0, 128.4, 128.2, 125.6; IR (film) νmax 3854, 3746, 3115, 2852, 2335, 1699, 1652, 1558, 1456, 1385, 1081, 976, 874, 765, 692, 514 cm^{-1}; Anal. Calcd. For $C_8H_7N_3$: C, 66.19; H, 4.86. Found: C, 66.31; H, 4.81.

4-(2,4-Difluorophenyl)-1,2,3-triazole (CAS:1043553-13-4)



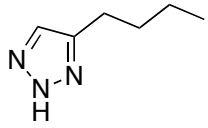
Following general procedure for the synthesis of 4-substituted-1,2,3-triazoles, a mixture of 2,4-difluorophenylacetylene (1.38 g, 10 mmol), $TMSN_3$ (2.0 mL, 1.2 mmol), CuI (95 mg, 0.5 mmol), in DMF/MeOH (4:1, 10 mL) was heated to 100 °C for 6 h. The crude product was purified via flash chromatography (Hexanes/EtOAc, 3:2) to provide the title compound as a white solid (1.47 g, 81%). mp 110-112 °C ^{1}H NMR (400 MHz, DMSO-*d6*) δ 15.34 (s, 1H), 8.13 (s, 1H), 8.01 (dd, *J* = 8.4, 15.6 Hz, 1H), 7.33-7.24 (m, 1H), 7.17-7.08 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 161.9 (dd, *J* = 13, 247 Hz), 159.1 (dd, *J* = 12, 250 Hz), 139.0, 129.2 (dd, *J* = 5, 10 Hz), 128.0, 115.1 (dd, *J* = 5, 14 Hz), 112.2 (dd, *J* = 4, 21 Hz), 104.6 (t, *J* = 26 Hz); IR (film) νmax 3853, 3745, 3127, 2858, 2335, 1697, 1652, 1538, 1471, 1385, 1270, 1137, 1072, 982, 844, 772, 668, 612 cm^{-1}; Anal. Calcd. For $C_8H_5N_3F_2$: C, 53.04; H, 2.78. Found: C, 53.49; H, 2.78.

3-(1,2,3-Triazol-4-yl)pyridine (CAS:120241-79-4)



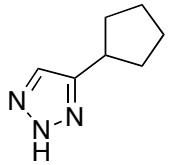
Following general procedure for the synthesis of 4-substituted-1,2,3-triazoles, a mixture of 3-ethynylpyridine (1.03 g, 10 mmol), $TMSN_3$ (2.0 mL, 1.2 mmol), CuI (95 mg, 0.5 mmol), in DMF/MeOH (4:1, 10 mL) was heated to 100 °C for 18 h. The crude product was recrystalized from EtOAc/Et_2O to give the title compound as a off-white solid (1.19 g, 83%) mp 180-182 °C. ^{1}H NMR (400 MHz, DMSO-*d6*) δ 15.36 (s, 1H), 9.10 (s, 1H), 8.54 (d, *J* = 3.6 Hz, 1H), 8.47 (s, 1H), 8.21 (d, *J* = 8.0 Hz, 1H), 7.45 (dd, *J* = 3.6, 7.6 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 148.7, 146.4, 142.6, 132.5, 126.9, 126.1, 123.6; IR (film) νmax 3854, 3746, 2362, 1652, 1507, 1457, 1358, 1124, 953, 895, 806, 694 cm^{-1}; Anal. Calcd. For $C_7H_6N_4$: C, 57.53; H, 4.14. Found: C, 57.55; H, 4.09.

4-Butyl-1,2,3-triazole (CAS: 152066-45-0)



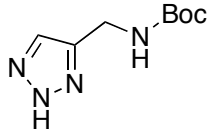
Following general procedure for the synthesis of 4-substituted-1,2,3-triazoles, a mixture of 1-hexyne (1.5 mL, 10 mmol), $TMSN_3$ (2.0 mL, 1.2 mmol), CuI (95 mg, 0.5 mmol), in DMF/MeOH (4:1, 10 mL) was heated to 100 °C for 24 h. The crude product was purified via flash chromatography (Hexanes/EtOAc, 3:2) to provide the title compound as pale yellow oil (1.06 g, 84%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 15.02 (s, 1H), 7.49 (s, 1H), 2.67 (t, J = 7.8 Hz, 2H), 1.64-1.53 (m, 2H), 1.34-1.22 (m, 2H), 0.83 (t, J = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) 145.0, 129.3, 31.3, 24.3, 22.2, 13.7; IR (film) νmax 3747, 3137, 2957, 2865, 2362, 1558, 1460, 1383, 1219, 1111, 975, 849, 668 cm^{-1}.

4-Cyclopentyl-1,2,3-triazole (CAS:1231244-99-7)



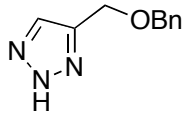
Following general procedure for the synthesis of 4-substituted-1,2,3-triazoles, a mixture of ethynylcyclopentane (500 mg, 5.3 mmol), $TMSN_3$ (1.07 mL, 7.95 mmol), CuI (42 mg, 0.22 mmol), in DMF/MeOH (4:1, 5 mL) was heated to 100 °C for 18 h. The crude product was purified via flash chromatography (Hexanes/EtOAc, 3:2) to provide the title compound as pale yellow oil (582 mg, 80%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 15.17 (s, 1H), 7.46 (s, 1H), 3.18-3.06 (m, 1H), 2.08-1.93 (m, 2H), 1.71-1.46 (m, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) 148.8, 127.9, 35.6, 33.0, 25.0; IR (film) νmax 3747, 3137, 2957, 2865, 2362, 1558, 1460, 1383, 1219, 1111, 975, 849, 668 cm^{-1}.

***tert*-Butyl ((1,2,3-triazol-4-yl)methyl)carbamate** (CAS:1009101-68-1)



Following general procedure for the synthesis of 4-substituted-1,2,3-triazoles, a mixture of *N*-Boc-propargylamine (1.59 g, 10 mmol), $TMSN_3$ (2.0 mL, 15 mmol), CuI (95 mg, 0.5 mmol), in DMF/MeOH (4:1, 10 mL) was heated to 100 °C for 18 h. The crude product was purified via flash chromatography (Hexanes/EtOAc, 1:1) to provide the title compound as a white solid (1.38 g, 69%). mp 80-81 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 14.41 (s, 1H), 7.62 (s, 1H), 5.76 (br, 1H), 4.40 (d, J = 5.2 Hz, 2H), 1.37 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$) 156.5, 144.8, 131.6, 80.2, 35.7, 28.5; IR (film) νmax 3747, 3145, 2934, 2869, 2361, 1686, 1521, 1456, 1367, 1280, 1170, 1020, 932, 860, 772, 667 cm^{-1}; Anal. Calcd. For $C_8H_{14}N_4O_2$: C, 48.47; H, 7.12. Found: C, 48.66; H, 6.96.

4-((Benzyloxy)methyl)-1,2,3-triazole (CAS:796034-32-7)



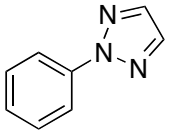
Following general procedure for the synthesis of 4-substituted-1,2,3-triazoles, a mixture of benzyl 2-propynyl ether (1.44 mL, 10 mmol), $TMSN_3$ (2.0 mL, 15 mmol), CuI (95 mg, 0.5 mmol), in DMF/MeOH (4:1, 10 mL) was heated to 100 °C for 18 h. The crude product was purified via flash chromatography (Hexanes/EtOAc, 1:1) to provide the title compound as a white solid (1.5 g, 79%). mp 51-53 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 14.87 (s, 1H), 7.73 (s, 1H), 7.41-7.22 (m, 5H), 4.73 (s, 2H), 4.59 (s, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) 143.1, 137.3, 128.4, 127.9, 127.8, 127.7, 72.4, 62.7; IR (film) νmax 3754, 3145, 2865, 2362, 1651, 1559, 1496, 1454, 1362, 1212, 1099, 1027, 742, 698, 603 cm^{-1}; Anal. Calcd. For $C_{10}H_{11}N_3O$: C, 63.48; H, 5.86. Found: C, 63.51; H, 6.01.

General Procedure for *N*-arylation of 1,2,3-triazoles

An oven-dried vial was equipped with a magnetic stir bar and charged with $Pd_2(dba)_3$ and **L1**. The vial was sealed with a screw-cap septum, and then evacuated and backfilled with argon (this process was

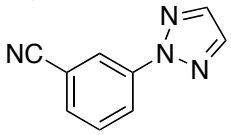
repeated a total of 3 times). Toluene (0.5 mL) was added to the vial via syringe. The resulting dark purple mixture was stirred at 120 °C for 3 min, at this point the color of the mixture turned to dark brown. A second oven-dried vial, which was equipped with stir bar, was charged with K_3PO_4 (424 mg, 2.0 mmol) (aryl halides and 1,2,3-triazoles that were solid at room temperature were added at this point). The vial was sealed with a screw-cap septum, and then evacuated and backfilled with argon (this process was repeated a total of 3 times) and then 1,2,3-triazole (1.2 mmol) and aryl halide (1.0 mmol) were added by syringe and the premixed catalyst solution and toluene (0.5 mL) was added by syringe to the second vial (total 1.0 mL toluene). The reaction mixture was heated at 120 °C for 5 h. The reaction was cooled to room temperature, diluted with EtOAc, washed with brine, dried over $MgSO_4$, concentrated in vacuo and purified via flash chromatography.

2-Phenyl-2*H*-1,2,3-triazole (CAS:51039-49-7)



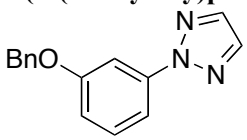
Following general procedure for *N*-arylation of 1,2,3-triazoles, a mixture of bromobenzene (116 μL, 1.0 mmol), 1,2,3-triazole (70 μL, 1.2 mmol), K_3PO_4 (424 mg, 2.0 mmol), $Pd_2(dba)_3$ (6.9 mg, 0.0075 mmol), **L1** (8.6 mg, 0.018 mmol) in toluene (1.0 mL) was heated to 120 °C for 5 h. The crude product was purified via flash chromatography (Hexanes/EtOAc, 9:1) to provide the title compound as colorless oil (130 mg, 90%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.12-8.06 (m, 2H), 7.81 (s, 2H), 7.51-7.44 (m, 2H), 7.38-7.32 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 140.0, 135.7, 129.5, 127.7, 119.1; IR (film) νmax 3128, 3059, 2362, 1745, 1598, 1500, 1410, 1376, 1259, 1152, 1069, 953, 820, 757, 692, 668, 510, 455 cm^{-1}; Anal. Calcd. For $C_8H_7N_3$: C, 66.19; H, 4.86. Found: C, 66.44; H, 5.03.

3-(2*H*-1,2,3-Triazol-2-yl)benzonitrile



Following general procedure for *N*-arylation of 1,2,3-triazoles, a mixture of 3-bromobenzonitrile (182 mg, 1.0 mmol), 1,2,3-triazole (70 μL, 1.2 mmol), K_3PO_4 (424 mg, 2.0 mmol), $Pd_2(dba)_3$ (4.6 mg, 0.005 mmol), **L1** (4.8 mg, 0.01 mmol) in toluene (1.0 mL) was heated to 120 °C for 5 h. The crude product was purified via flash chromatography (Hexanes/EtOAc, 8:1) to provide the title compound as a white solid (1st run: 153 mg, 90%; 2nd run: 148 mg, 87%), mp 100-101 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.32 (s, 1H), 8.29-8.24 (m, 1H), 7.80 (s, 2H), 7.59-7.51 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 140.1, 136.5, 130.8, 130.4, 122.9, 122.2, 118.0, 113.6; IR (film) νmax 3853, 3744, 3122, 2361, 2232, 1696, 1582, 1478, 1406, 1376, 1259, 1162, 1082, 953, 886, 844, 798, 667, 602, 472 cm^{-1}; Anal. Calcd. For $C_9H_6N_4$: C, 63.52; H, 3.55. Found: C, 63.52; H, 3.51.

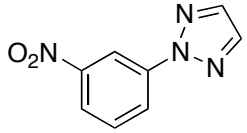
2-(3-(Benzyloxy)phenyl)-2*H*-1,2,3-triazole



Following general procedure for *N*-arylation of 1,2,3-triazoles, a mixture of 1-(benzyloxy)-3-bromobenzene (263 mg, 1.0 mmol), 1,2,3-triazole (70 μL, 1.2 mmol), K_3PO_4 (424 mg, 2.0 mmol), $Pd_2(dba)_3$ (4.6 mg, 0.005 mmol), **L1** (4.8 mg, 0.01 mmol) in toluene (1.0 mL) was heated to 120 °C for 5 h. The crude product was purified via flash chromatography (Hexanes/EtOAc, 10:1) to provide the title compound as a white solid (1st run: 225 mg, 90%; 2nd run: 226 mg, 90%), mp 70-71 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.85 (t, *J* = 2.2 Hz, 1H), 7.82 (s, 2H), 7.80-7.76 (m, 1H), 7.53-7.48 (m, 2H), 7.47-7.35 (m, 4H), 7.03-6.98 (m, 1H), 5.16 (s, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 159.6, 141.0, 136.6, 135.6, 130.2, 128.7, 128.1, 127.6, 114.5, 111.5, 105.5, 70.2; IR (film) νmax 3845, 3746,

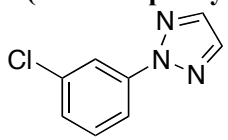
3142, 3066, 2936, 2875, 2362, 1773, 1620, 1495, 1407, 1375, 1295, 1246, 1219, 1168, 1085, 1013, 950, 882, 827, 777, 750, 699, 665, 530 cm^{-1}; Anal. Calcd. For $C_{15}H_{13}N_3O$: C, 71.70; H, 5.21. Found: C, 71.90; H, 5.15.

2-(3-Nitrophenyl)-2*H*-1,2,3-triazole (CAS:342623-98-7)



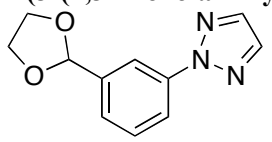
Following general procedure for *N*-arylation of 1,2,3-triazoles, a mixture of 1-bromo-3-nitrobenzene (202 mg, 1.0 mmol), 1,2,3-triazole (70 μL, 1.2 mmol), K_3PO_4 (424 mg, 2.0 mmol), $Pd_2(dba)_3$ (2.3 mg, 0.0025 mmol), **L1** (2.4 mg, 0.005 mmol) in toluene (1.0 mL) was heated to 120 °C for 5 h. The crude product was purified via flash chromatography (Hexanes/EtOAc, 9:1) to provide the title compound as a pale yellow solid (1st run: 167 mg, 88%; 2nd run: 164 mg, 86%), mp 126-127 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.91 (t, *J* = 2.0 Hz, 1H), 8.43-8.37 (m, 1H), 8.19-815 (m, 1H), 7.86 (s, 2H), 7.65 (t, *J* = 8.0 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 149.0, 140.6, 136.7, 130.5, 124.4, 122.0, 114.2; IR (film) νmax 3854, 375, 3128, 2362, 1698, 1652, 1520, 1406, 1381, 1348, 1069, 954, 893, 839, 808, 736, 658, 466 cm^{-1}.

2-(3-Chlorophenyl)-2*H*-1,2,3-triazole (CAS:59067-28-6)



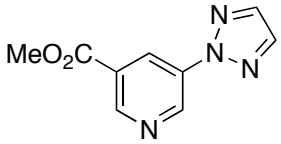
Following general procedure for *N*-arylation of 1,2,3-triazoles, a mixture of 1-bromo-3-chlorobenzene (191 mg, 1.0 mmol), 1,2,3-triazole (70 μL, 1.2 mmol), K_3PO_4 (424 mg, 2.0 mmol), $Pd_2(dba)_3$ (2.3 mg, 0.0025 mmol), **L1** (2.4 mg, 0.005 mmol) in toluene (1.0 mL) was heated to 120 °C for 5 h. The crude product was purified via flash chromatography (Hexanes/EtOAc, 5:1) to provide the title compound as a white solid (1st run: 163 mg, 91%; 2nd run: 161 mg, 90%), mp 38-40 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.11 (t, *J* = 2.0 Hz, 1H), 7.99-7.94 (m, 1H), 7.80 (s, 2H), 7.41-7.35 (m, 1H), 7.33-7.27 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 140.8, 136.1, 135.3, 130.5, 127.7, 119.4, 117.1; IR (film) νmax 3747, 3081, 2361, 1594, 1486, 1438, 1408, 1373, 1261, 1153, 1105, 1074, 953, 869, 826, 778, 666, 488 cm^{-1}; Anal. Calcd. For $C_8H_6N_2Cl$: C, 53.50; H, 3.37. Found: C, 53.79; H, 3.40.

2-(3-(1,3-Dioxolan-2-yl)phenyl)-2*H*-1,2,3-triazole



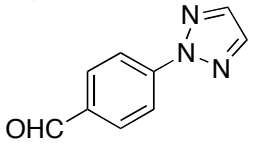
Following general procedure for *N*-arylation of 1,2,3-triazoles, a mixture of 2-(3-bromophenyl)-1,3-dioxolane (151 μL, 1.0 mmol), 1,2,3-triazole (70 μL, 1.2 mmol), K_3PO_4 (424 mg, 2.0 mmol), $Pd_2(dba)_3$ (4.6 mg, 0.005 mmol), **L1** (4.8 mg, 0.01 mmol) in toluene (1.0 mL) was heated to 120 °C for 5 h. The crude product was purified via flash chromatography (Hexanes/EtOAc, 6:1) to provide the title compound colorless oil (1st run: 189 mg, 88%; 2nd run 184 mg, 85%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.23-8.21 (m, 1H), 8.10-8.05 (m, 1H), 7.79 (s, 2H), 7.51-7.43 (m, 2H), 5.88 (s, 1H), 4.15-3.99 (m, 4H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 140.1, 139.9, 135.8, 129.6, 125.8, 119.7, 117.2, 103.2, 65.5; IR (film) νmax 3745, 3132, 2960, 2888, 2362, 1597, 1478, 1406, 1260, 1209, 1081, 960, 889, 825, 797, 701, 671, 477 cm^{-1}; Anal. Calcd. For $C_{11}H_{11}N_3O_2$: C, 60.82; H, 5.10. Found: C, 61.08; H, 5.14.

Methyl 5-(2*H*-1,2,3-triazol-2-yl)nicotinate



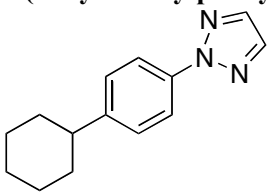
Following general procedure for *N*-arylation of 1,2,3-triazoles, a mixture of methyl 5-bromonicotinate (216 mg, 1.0 mmol), 1,2,3-triazole (70 μL, 1.2 mmol), K_3PO_4 (424 mg, 2.0 mmol), $Pd_2(dba)_3$ (4.6 mg, 0.005 mmol), **L1** (4.8 mg, 0.01 mmol) in toluene (1.0 mL) was heated to 120 °C for 5 h. The crude product was purified via flash chromatography (Hexanes/EtOAc, 5:1) to provide the title compound as a white solid (1st run: 172 mg, 84%; 2nd run: 168 mg, 82%), mp 99-100 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.48-9.45 (m, 1H), 9.14-9.11 (m, 1H), 8.88-8.84 (m, 1H), 7.84 (s, 2H), 3.95 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 165.0, 149.3, 144.0, 136.8, 136.1, 126.8, 126.6, 52.8; IR (film) νmax 3745, 2361, 1721, 1569, 1459, 1384, 1315, 1276, 1105, 946, 842, 758, 666 cm^{-1}; Anal. Calcd. For $C_9H_8N_4O_2$: C, 52.94; H, 3.95. Found: C, 53.11; H, 3.93.

4-(2*H*-1,2,3-Triazol-2-yl)benzaldehyde



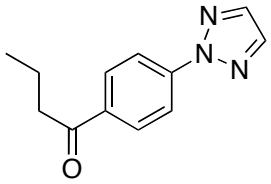
Following general procedure for *N*-arylation of 1,2,3-triazoles, a mixture of 4-bromobenzaldehyde (185 mg, 1.0 mmol), 1,2,3-triazole (70 μL, 1.2 mmol), K_3PO_4 (424 mg, 2.0 mmol), $Pd_2(dba)_3$ (4.6 mg, 0.005 mmol), **L1** (4.8 mg, 0.01 mmol) in toluene (1.0 mL) was heated to 120 °C for 5 h. The crude product was purified via flash chromatography (Hexanes/EtOAc, 6:1) to provide the title compound as a white solid (1sr Run: 132 mg, 77%; 2nd run: 141 mg, 81%), mp 100-102 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.99 (s, 1H), 8.21 (d, J = 8.8 Hz, 2H), 7.95 (d, J = 8.4 Hz, 2H), 7.83 (s, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 191.1, 143.7, 136.7, 135.1, 131.2, 119.2; IR (film) νmax 3853, 3745, 2361, 1694, 1601, 1508, 1383, 1206, 1154, 1103, 949, 830, 666, 505, 461, cm^{-1}; Anal. Calcd. For $C_9H_7N_3O$: C, 62.42; H, 4.07. Found: C, 62.66; H, 4.04.

2-(4-Cyclohexylphenyl)-2*H*-1,2,3-triazole



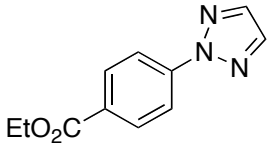
Following general procedure for *N*-arylation of 1,2,3-triazoles, a mixture of 1-bromo-4-cyclohexylbenzene (239 mg, 1.0 mmol), 1,2,3-triazole (70 μL, 1.2 mmol), K_3PO_4 (424 mg, 2.0 mmol), $Pd_2(dba)_3$ (6.9 mg, 0.0075 mmol), **L1** (8.6 mg, 0.018 mmol) in toluene (1.0 mL) was heated to 120 °C for 5 h. The crude product was purified via flash chromatography (Hexanes/EtOAc, 10:1) to provide the title compound as a white solid (1st run: 177 mg, 78%; 2nd run: 174mg, 77%), mp 46-48 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.01 (d, J = 8.8 Hz, 2H), 7.78 (s, 2H), 7.31 (d, J = 8.4 Hz, 2H), 2.60-2.50 (m, 1H), 1.96-1.71 (m, 5H), 1.50-1.20 (m, 5H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 147.7, 138.0, 135.3, 127.7, 119.0, 44.2, 34.5, 26.9, 26.2; IR (film) νmax 3745, 2925, 2853, 2361, 1514, 1448, 1412, 1382, 1259, 1151, 953, 830, 673, 543, cm^{-1}; Anal. Calcd. For $C_{14}H_{17}N_3$: C, 73.98; H, 7.54. Found: C, 74.17; H, 7.47.

1-(4-(2*H*-1,2,3-Triazol-2-yl)phenyl)butan-1-one



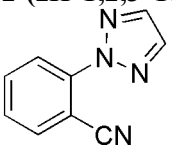
Following general procedure for *N*-arylation of 1,2,3-triazoles, a mixture of 1-(4-chlorophenyl)butan-1-one (183 mg, 1.0 mmol), 1,2,3-triazole (70 μL, 1.2 mmol), K_3PO_4 (424 mg, 2.0 mmol), $Pd_2(dba)_3$ (2.3 mg, 0.0025 mmol), **L1** (2.4 mg, 0.005 mmol) in toluene (1.0 mL) was heated to 120 °C for 5 h. The crude product was purified via flash chromatography (Hexanes/EtOAc, 8:1) to provide the title compound as a white solid (1st run: 180 mg, 84%; 2nd run: 181mg, 84%), mp 64-66 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.10 (d, *J* = 9.2 Hz, 2H), 8.01 (d, *J* = 9.2 Hz, 2H), 7.78 (s, 2H), 2.90 (t, *J* = 7.2 Hz, 2H), 1.79-1.66 (m, 2H), 0.96 (t, *J* = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 199.0, 142.6, 136.3, 135.8, 129.5, 118.6, 40.6, 17.7, 13.9; IR (film) νmax 3745, 3122, 2959, 2359, 1937, 1675, 1600, 1511, 1457, 1386, 1308, 1213, 1170, 1107, 1052, 949, 906, 832, 738, 665, 569, 468 cm^{-1}; Anal. Calcd. For $C_{12}H_{13}N_3O$: C, 66.96; H, 6.09. Found: C, 67.25; H, 6.05.

Ethyl 4-(2*H*-1,2,3-triazol-2-yl)benzoate



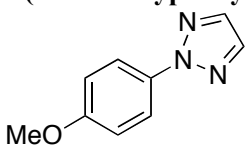
Following general procedure for *N*-arylation of 1,2,3-triazoles, a mixture of ethyl 4-chlorobenzoate (156 μL, 1.0 mmol), 1,2,3-triazole (70 μL, 1.2 mmol), K_3PO_4 (424 mg, 2.0 mmol), $Pd_2(dba)_3$ (3.2 mg, 0.0035 mmol), **L1** (3.4 mg, 0.007 mmol) in toluene (1.0 mL) was heated to 120 °C for 5 h. The crude product was purified via flash chromatography (Hexanes/EtOAc, 8:1) to provide the title compound as a white solid (1st run: 180 mg, 83%; 2nd run: 177 mg, 82%), mp 49-51 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.11-8.08 (s, 4H), 7.78 (s, 2H), 4.34 (q, *J* = 7.2 Hz, 2H), 1.35 (t, *J* = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 165.8, 142.7, 136.3, 130.9, 129.4, 118.5, 61.2, 14.4; IR (film) νmax 3117, 2973, 2360, 1713, 1608, 1508, 1466, 1410, 1281, 1104, 1019, 951, 852, 815, 763, 681, 503, 451 cm^{-1}; Anal. Calcd. For $C_{11}H_{11}N_3O_2$: C, 60.82; H, 5.10. Found: C, 61.10; H, 5.08.

2-(2*H*-1,2,3-Triazol-2-yl)benzonitrile



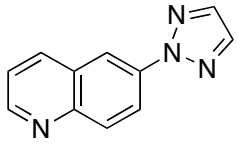
Following general procedure for *N*-arylation of 1,2,3-triazoles, a mixture of 2-chlorobenzonitrile (138 mg , 1.0 mmol), 1,2,3-triazole (70 μL, 1.2 mmol), K_3PO_4 (424 mg, 2.0 mmol), $Pd_2(dba)_3$ (9.2 mg, 0.01 mmol), **L1** (9.7 mg, 0.02 mmol) in toluene (1.0 mL) was heated to 120 °C for 5 h. The crude product was purified via flash chromatography (Hexanes/EtOAc, 7:1) to provide the title compound as a white solid (1st run: 78 mg, 46%; 2nd run: 76 mg, 45%), mp 125-126 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.10-8.05 (m, 1H), 7.92 (s, 2H), 7.84-7.79 (m, 1H), 7.74-7.67 (m, 1H), 7.49-7.43 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 140.5, 136.9, 135.3, 133.9, 128.1, 122.8, 117.0, 104.9; IR (film) νmax 2960, 2361, 1696, 1651, 1559, 1499, 1457, 1383, 1261, 1073, 950, 821, 759, 667, 555, 498 cm^{-1}.

2-(4-Methoxyphenyl)-2*H*-1,2,3-triazole (CAS:68535-51-3)



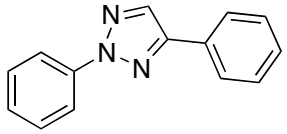
Following general procedure for *N*-arylation of 1,2,3-triazoles, a mixture of 4-methoxyphenyl trifluoromethanesulfonate (256 mg, 1.0 mmol), 1,2,3-triazole (70 μL, 1.2 mmol), K_3PO_4 (424 mg, 2.0 mmol), $Pd_2(dba)_3$ (6.9 mg, 0.0075 mmol), **L1** (8.6 mg, 0.018 mmol) in toluene (1.0 mL) was heated to 120 °C for 5 h. The crude product was purified via flash chromatography (Hexanes/EtOAc, 8:1) to provide the title compound as colorless oil (1st run: 158 mg, 90%; 2nd run: 155 mg, 89%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.98 (d, *J* = 9.2 Hz, 2H), 7.75 (s, 2H), 6.97 (d, *J* = 9.2 Hz, 2H), 3.81 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 159.1, 135.2, 133.9, 120.5, 114.5, 55.6; IR (film) νmax 3745, 2955, 2838, 2360, 1609, 1512, 1459, 1412, 1302, 1249, 1171, 1096, 1029, 953, 829, 671, 622, 526 cm^{-1}; Anal. Calcd. For $C_9H_9N_3O$: C, 61.70; H, 5.18. Found: C, 61.89; H, 5.21.

6-(2*H*-1,2,3-Triazol-2-yl)quinoline



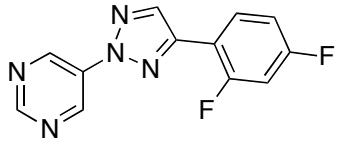
Following general procedure for *N*-arylation of 1,2,3-triazoles, a mixture of quinolin-6-yl trifluoromethanesulfonate (277 mg, 1.0 mmol), 1,2,3-triazole (70 μL, 1.2 mmol), K_3PO_4 (424 mg, 2.0 mmol), $Pd_2(dba)_3$ (2.3 mg, 0.0025 mmol), **L1** (2.4 mg, 0.005 mmol) in toluene (1.0 mL) was heated to 120 °C for 5 h. The crude product was purified via flash chromatography (Hexanes/EtOAc, 3:2) to provide the title compound as a white solid (1st run: 183 mg, 91%; 2nd run: 177 mg, 90%), mp 75-76 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.89-8.85 (m, 1H), 8.49-8.36 (m, 2H), 8.20-8.12 (m, 2H), 7.80 (s, 2H), 7.40-7.33 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 150.7, 147.2, 137.6, 136.5, 136.1, 130.9, 128.4, 122.1, 121.5, 116.2; IR (film) νmax 3745, 3123, 2361, 1696, 1625, 1560, 1505, 1377, 1308, 1259, 1116, 1074, 954, 872, 826, 790, 667, 469 cm^{-1}.

2,4-Diphenyl-2*H*-1,2,3-triazole (CAS:20034-95-1)



Following general procedure for *N*-arylation of 1,2,3-triazoles, a mixture of bromobenzene (106 μL, 1.0 mmol), 4-phenyl-1,2,3-triazole (174 mg, 1.2 mmol), K_3PO_4 (424 mg, 2.0 mmol), $Pd_2(dba)_3$ (6.9 mg, 0.0075 mmol), **L1** (8.6 mg, 0.018 mmol) in toluene (1.0 mL) was heated to 120 °C for 5 h. The crude product was purified via flash chromatography (Hexanes/EtOAc, 20:1) to provide the title compound as a white solid (1st run: 200 mg, 90%; 2nd run: 196 mg, 89%), mp 41-42 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.25-8.20 (m, 2H), 8.09 (s, 1H), 7.98-7.94 (m, 2H), 7.56-7.47 (m, 4H), 7.46-7.35 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 148.9, 140.0, 132.6, 130.1, 129.3, 129.0, 128.9, 127.4, 126.2, 118.8; IR (film) νmax 3853, 3746, 3067, 2335, 1950, 1698, 1597, 1498, 458, 1389, 1343, 1072, 971, 912, 845, 761, 690, 661, 500 cm^{-1}; Anal. Calcd. For $C_{14}H_{11}N_3$: C, 76.00; H, 5.01. Found: C, 75.73; H, 5.11.

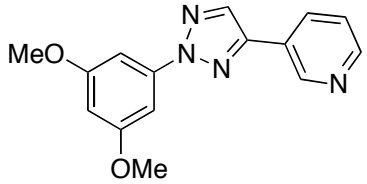
5-(4-(2,4-Difluorophenyl)-2*H*-1,2,3-triazol-2-yl)pyrimidine



Following general procedure for *N*-arylation of 1,2,3-triazoles, a mixture of 5-bromopyrimidine (159 mg , 1.0 mmol), 4-(2,4-difluorophenyl)-1,2,3-triazole (217 mg, 1.2 mmol), K_3PO_4 (424 mg, 2.0 mmol), $Pd_2(dba)_3$ (4.6 mg, 0.005 mmol), **L1** (4.8 mg, 0.01 mmol) in toluene (1.0 mL) was heated to 120 °C for 5 h. The crude product was purified via flash chromatography (Hexanes/EtOAc, 3:1) to provide the title compound as a white solid (1st run: 233 mg, 90%; 2nd run: 230 mg, 89%), mp 118-120 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.42 (s, 2H), 9.17 (s, 1H), 8.16 (d, *J* = 4.0 Hz, 1H), 8.09-8.00

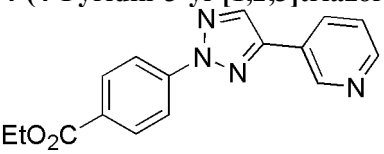
(m, 1H), 7.00-6.87 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 163.5 (dd, *J* = 12, 251 Hz), 160.5 (dd, *J* = 12, 252 Hz), 157.2, 146.9, 144.4, 136.3 (d, *J* = 12 Hz), 134.3, 129.7 (dd, *J* = 4, 9 Hz), 113.7 (dd, *J* = 4, 13 Hz), 112.5 (dd, *J* = 3, 21 Hz), 104.7 (t, *J* = 25 Hz); IR (film) νmax 3745, 3030, 2362, 1565, 1420, 1385, 1267, 1080, 960, 850, 713, 656, 621, 487 cm^{-1}; Anal. Calcd. For $C_{12}H_7F_2N_5$: C, 55.60; H, 2.72. Found: C, 55.74; H, 2.66.

3-(2-(3,5-Dimethoxyphenyl)-2*H*-1,2,3-triazol-4-yl)pyridine



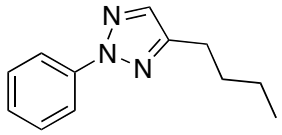
Following general procedure for *N*-arylation of 1,2,3-triazoles, a mixture of 3,5-dimethoxybromobenzene (217 mg, 1.0 mmol), 3-(1,2,3-triazol-4-yl)pyridine (175 mg, 1.2 mmol), K_3PO_4 (424 mg, 2.0 mmol), $Pd_2(dba)_3$ (6.9 mg, 0.0075 mmol), **L1** (8.6 mg, 0.018 mmol) in toluene (1.0 mL) was heated to 120 °C for 5 h. The crude product was purified via flash chromatography (Hexanes/EtOAc, 1:2) to provide the title compound as a white solid (1st run: 242 mg, 86%; 2nd run: 245 mg, 87%), mp 119-121 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.06 (d, *J* = 3.6 Hz, 1H), 8.59-8.55 (m, 1H), 8.16-8.08 (m, 1H), 8.04-8.00 (m, 1H), 7.38-7.22 (m, 3H), 6.43-6.38 (m, 1H), 3.82 (s, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 161.4, 150.0, 147.5, 145.9, 141.2, 133.4, 132.6, 126.2, 123.8, 100.2, 97.3, 55.7; IR (film) νmax 3676, 3364, 2958, 2361, 1602, 1481, 1424, 1385, 1264, 1208, 1154, 1065, 1039, 978, 818, 702, 664, 533 cm^{-1}; Anal. Calcd. For $C_{15}H_{14}N_4O_2$: C, 63.82; H, 5.00. Found: C, 63.95; H, 5.02.

4-(4-Pyridin-3-yl-[1,2,3]triazol-2-yl)-benzoic acid ethyl ester



Following general procedure for *N*-arylation of 1,2,3-triazoles, a mixture of ethyl 4-bromobenzoate (163 μL, 1.0 mmol), 3-(1,2,3-triazol-4-yl)pyridine (175 mg, 1.2 mmol), K_3PO_4 (424 mg, 2.0 mmol), $Pd_2(dba)_3$ (2.3 mg, 0.0025 mmol), **L1** (2.4 mg, 0.005 mmol) in toluene (1.0 mL) was heated to 120 °C for 5 h. The crude product was purified via flash chromatography (Hexanes/EtOAc, 3:1) to provide the title compound as a white solid (1st run: 253 mg, 86%; 2nd run: 246 mg, 84%), mp 110-112 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.01 (t, *J* = 1.2 Hz, 1H), 8.57-8.52 (m, 1H), 8.08-8.00 (m, 6H), 7.28 (dd, *J* = 4.8, 8.0 Hz, 1H), 4.30 (q, *J* = 7.2, 3H), 1.33 (t, , *J* = 7.2, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 165.6, 150.1, 147.4, 146.6, 142.3, 133.3, 133.3, 130.9, 129.4, 125.7 123.8, 118.3, 61.2, 14.3; IR (film) νmax 3414, 2976, 2362, 1715, 1607, 1511, 1424, 1394, 1279, 1105, 1023, 1105, 1023, 964, 855, 813, 764, 702, 492 cm^{-1}.

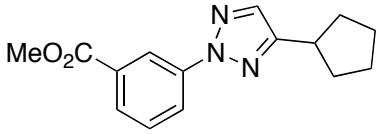
4-Butyl-2-phenyl-2*H*-1,2,3-triazole



Following general procedure for *N*-arylation of 1,2,3-triazoles, a mixture of bromobenzene (106 μL, 1.0 mmol), 4-butyl-1,2,3-triazole (150 mg, 1.2 mmol), K_3PO_4 (424 mg, 2.0 mmol), $Pd_2(dba)_3$ (6.9 mg, 0.0075 mmol), **L1** (8.6 mg, 0.018 mmol) in toluene (1.0 mL) was heated to 120 °C for 5 h. The crude product was purified via flash chromatography (Hexanes/EtOAc, 40:1) to provide the title compound as colorless oil (1st run: 185 mg, 92%; 2nd run: 180 mg, 90%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.08-8.02 (m, 2H), 7.57 (s, 1H), 7.48-7.41 (m, 2H), 7.33-7.26 (m, 1H), 2.76 (t, J = 8.0 Hz, 2H), 1.76-1.66 (m, 2H), 1.48-1.36 (m, 2H), 0.96 (t, *J* = 7.4 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 150.3, 140.1, 134.4, 129.3, 127.1, 118.7, 31.4, 25.4, 22.5, 14.0; IR (film) νmax 3055, 2956, 2931,

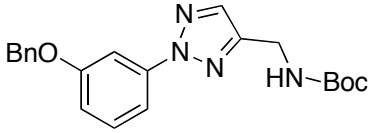
2362, 1598, 1500, 1462, 1341, 1236, 1161, 1070, 1030, 964, 843, 756, 691, 663, 508 cm^{-1}; Anal. Calcd. For $C_{12}H_{15}N_3$: C, 71.61; H, 7.51. Found: C, 71.48; H, 7.49.

Methyl 3-(4-cyclopentyl-2*H*-1,2,3-triazol-2-yl)benzoate



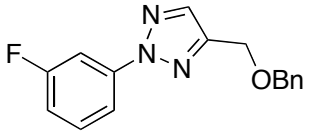
Following general procedure for *N*-arylation of 1,2,3-triazoles, a mixture of methyl 3-bromobenzoate (215 mg, 1.0 mmol), 4-cyclopentyl-1,2,3-triazole (164 mg, 1.2 mmol), K_3PO_4 (424 mg, 2.0 mmol), $Pd_2(dba)_3$ (4.3 mg, 0.005 mmol), **L1** (4.8 mg, 0.01 mmol) in toluene (1.0 mL) was heated to 120 °C for 5 h. The crude product was purified via flash chromatography (Hexanes/EtOAc, 30:1) to provide the title compound as colorless oil (1st run: 260 mg, 95%; 2nd run: 249 mg, 92%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.63 (t, *J* = 2.0 Hz, 1H), 8.18-8.14 (m, 1H), 7.92-7.88 (m, 1H), 7.54 (s, 1H), 7.48-7.42 (m, 1H), 3.89 (s, 3H), 3.21-3.11 (m, 1H), 2.12-2.00 (m, 2H), 1.79-1.58 (m, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 166.3, 154.8, 140.1, 133.7, 131.4, 129.3, 127.8, 122.6, 119.5, 52.3, 36.7, 33.1, 25.3; IR (film) νmax 3436, 3087, 2954, 2361, 1723, 1595, 1458, 1364, 1268, 1078, 1035, 964, 908, 845, 751, 662, 539 cm^{-1}; Anal. Calcd. For $C_{15}H_{17}N_3O_2$: C, 66.40; H, 6.32. Found: C, 66.62; H, 6.23.

***tert*-Butyl ((2-(3-(benzyloxy)phenyl)-2*H*-1,2,3-triazol-4-yl)methyl)carbamate**



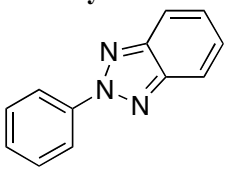
Following general procedure for *N*-arylation of 1,2,3-triazoles, a mixture of 3-benzyloxybromobenzene (261 mg, 1.0 mmol), *tert*-butyl ((1,2,3-triazol-4-yl)methyl)carbamate (238 mg, 1.2 mmol), K_3PO_4 (424 mg, 2.0 mmol), $Pd_2(dba)_3$ (6.9 mg, 0.0075 mmol), **L1** (8.6 mg, 0.018 mmol) in toluene (1.0 mL) was heated to 120 °C for 5 h. The crude product was purified via flash chromatography (Hexanes/EtOAc, 6:1) to provide the title compound as a white solid (1st run: 342 mg, 90%; 2nd run: 345 mg, 91%), mp 90-91 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.74-7.68 (m, 2H), 7.65-7.61 (m, 1H), 7.47-7.29 (m, 6H), 6.92 (dd, J = 2.0, 8.0 Hz, 1H), 5.43 (br, 1H), 5.08 (s, 2H), 4.45 (d, *J* = 5.6 Hz, 2H), 1.48 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 159.5, 155.9, 147.4, 140.8, 136.5, 134.3, 130.1, 128.6, 128.1, 127.5, 114.2, 111.2, 79.8, 70.2, 36.2, 28.4; IR (film) νmax 3349, 2977, 2932, 2362, 1706, 1605, 1497, 1458, 1368, 1244, 1167, 1024, 972, 858, 755, 696, 666, 458 cm^{-1}; Anal. Calcd. For $C_{21}H_{24}N_4O_3$: C, 66.30; H, 6.36. Found: C, 66.21; H, 6.30.

***tert*-Butyl ((2-(3-(benzyloxy)phenyl)-2*H*-1,2,3-triazol-4-yl)methyl)carbamate**



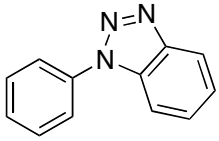
Following general procedure for *N*-arylation of 1,2,3-triazoles, a mixture of 3-bromofluorobenzene (112 μL, 1.0 mmol), 4-((benzyloxy)methyl)-1,2,3-triazole (227 mg, 1.2 mmol), K_3PO_4 (424 mg, 2.0 mmol), $Pd_2(dba)_3$ (6.9 mg, 0.0075 mmol), **L1** (8.6 mg, 0.018 mmol) in toluene (1.0 mL) was heated to 120 °C for 5 h. The crude product was purified via flash chromatography (Hexanes/EtOAc, 10:1) to provide the title compound as colorless oil (1st run: 252 mg, 94%; 2nd run: 279 mg, 93%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.93-7.89 (m, 1H), 7.89-7.83 (m, 2H), 7.46-7.32 (m, 6H), 7.08-7.02 (m, 1H), 4.75 (s, 2H), 4.66 (s, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 163.1 (d, *J* = 245 Hz), 147.3, 141.0 (d, *J* = 10 Hz), 137.7, 135.5, 130.7 (d, *J* = 9 Hz), 128.6, 128.0, 128.0, 114.3 (d, *J* = 4 Hz), 114.2 (d, *J* = 22 Hz), 106.6 (d, *J* = 27 Hz), 72.7, 63.3; IR (film) νmax 3086, 3032, 2860, 2361, 1609, 1494, 1464, 1357, 1316, 1234, 1205, 1095, 1037, 972, 873, 780, 741, 697, 603, 534, 455 cm^{-1}; Anal. Calcd. For $C_{16}H_{14}FN_3O$: C, 67.83; H, 4.98. Found: C, 67.87; H, 4.97.

2-Phenyl-2*H*-benzo[*d*][1,2,3]triazole (CAS: 1916-72-9)



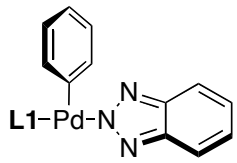
Following general procedure for *N*-arylation of 1,2,3-triazoles, a mixture of bromobenzene (106 μL, 1.0 mmol), benzotriazole (143 mg, 1.2 mmol), K_3PO_4 (424 mg, 2.0 mmol), $Pd_2(dba)_3$ (6.9 mg, 0.0075 mmol), **L1** (8.6 mg, 0.018 mmol) in toluene (2.5 mL) was heated to 120 °C for 5 h. GC analysis of the crude reaction mixture indicated N^2:N^1 ratio of 47:53. The crude product was purified via flash chromatography (Hexanes/EtOAc, 10:1 to 3:1) to provide the title compound as a white solid (84 mg, 43%) mp 103-105 °C, followed by 1-phenyl-2*H*-benzo[*d*][1,2,3]triazole. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.39-8.33 (m, 2H), 7.94 (dd, *J* = 3.2, 6.4 Hz, 2H), 7.58-7.52 (m, 2H), 7.48-7.38 (m, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 145.2, 140.5, 129.6, 129.1, 127.3, 120.8, 118.6; IR (film) νmax 3065, 2361, 1594, 1563, 1492, 1461, 1384, 1338, 1289, 1221, 964, 918, 748, 680 cm^{-1}; , 573, 517 cm^{-1}; Anal. Calcd. For $C_{12}H_9N_3$: C, 73.83; H, 4.65. Found: C, 74.09; H, 4.63.

1-Phenyl-2*H*-benzo[*d*][1,2,3]triazole (CAS: 883-39-6)



White solid (86 mg, 44%), mp 84-85 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.15-8.09 (m, 1H), 7.78-7.70 (m, 3H), 7.62-7.55 (m, 2H), 7.55-7.45 (m, 2H), 7.44-7.36 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 146.6, 137.1, 132.4, 130.0, 128.8, 128.4, 124.5, 122.9, 120.4, 110.5; IR (film) νmax 3061, 2362, 1597, 1501, 1456, 1279, 1188, 1086, 1054, 752, 694, 573, 517 cm^{-1}; Anal. Calcd. For $C_{12}H_9N_3$: C, 73.83; H, 4.65. Found: C, 73.93; H, 4.60.

Cartersian Coordinates for all Calculated Complexes:



Complex A

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C	-0.605052	-1.508476	-0.087473
C	0.063306	-1.878451	1.124768
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H	1.786703	-2.586186	-2.282086
C	-2.123784	-1.404787	-0.076447
C	-2.896669	-0.219590	0.084831
C	-2.780813	-2.659767	-0.201999
C	-4.304524	-0.332011	0.193516
C	-4.187918	-2.732903	-0.220452
C	-4.944182	-1.578708	0.025231
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C	-0.586930	-1.737035	2.501040
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C	3.272733	-3.548862	-0.141858
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C	4.008937	-3.554942	-1.488066
H	3.461085	-4.129643	-2.245936
H	4.160528	-2.539178	-1.864039
H	4.992568	-4.023072	-1.371159
C	3.072736	-4.993130	0.366853
H	4.036471	-5.510121	0.443549
H	2.598053	-5.015633	1.353692
H	2.437336	-5.562467	-0.323153
C	-0.555819	-1.398879	-2.681515
H	-1.419806	-0.762023	-2.481685
C	0.428305	-0.602342	-3.563486
H	-0.102343	-0.163919	-4.417383
H	0.922319	0.195571	-3.001940
H	1.217388	-1.246794	-3.967406
C	-1.067511	-2.625172	-3.465121
H	-1.425464	-2.314668	-4.454423
H	-0.269737	-3.362119	-3.616048
H	-1.896574	-3.119864	-2.952879
C	0.291263	-0.931648	3.479085
H	-0.260088	-0.736608	4.407506
H	1.200445	-1.480806	3.746935
H	0.613775	0.020353	3.048003
C	-0.940488	-3.107201	3.116797
H	-0.043984	-3.720725	3.262737
H	-1.412730	-2.968625	4.096983
H	-1.634563	-3.670223	2.485859
Pd	0.478636	0.853711	0.011817
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C	-2.346200	2.400921	1.907785
C	-4.044565	2.849828	-1.565078
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H	-4.492718	3.395020	-0.731230
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H	-1.987649	4.511072	-2.225349
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H	-2.228234	2.513362	-3.527216
H	-0.981011	1.650106	-2.614081
H	-2.596385	0.938812	-2.811128
C	-3.394257	3.530284	1.886056
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C	-4.880655	-4.060249	-0.470471
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H	-4.228487	-4.775613	-0.971661
H	-5.216875	-4.529888	0.464615
C	1.311537	2.675010	-0.332433
C	1.829802	3.464235	0.698838
C	1.517661	3.071576	-1.659021
C	2.477070	4.670930	0.408365
H	1.762393	3.136252	1.729990
C	2.167243	4.277638	-1.946781
H	1.183435	2.447537	-2.481909
C	2.639211	5.087857	-0.913499
H	2.870149	5.274299	1.223732
H	2.311291	4.572438	-2.983897
H	3.147526	6.022405	-1.136513

C	4.363193	0.145706	1.113149
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C	6.706279	-0.198126	1.411489
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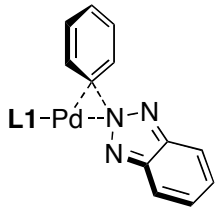

Complex A-TS

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C	0.210330	-1.985290	-0.962270
C	-0.587613	-1.572422	0.144538
C	-0.030919	-1.678885	1.456771
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C	-2.099872	-1.496128	-0.015306
C	-2.890577	-0.317615	-0.163029
C	-2.734678	-2.769576	0.013291
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P	-1.974585	1.396944	-0.163642
C	-0.819148	-1.313403	2.714589
H	-1.764158	-0.868400	2.393692
C	3.322176	-3.427450	0.824702
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C	4.162105	-3.717460	-0.426144
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H	2.518860	-4.558535	2.534117
H	2.486131	-5.440319	0.999521
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H	-1.176234	-1.295051	-2.424055
C	0.763910	-1.280884	-3.347850
H	0.302215	-1.037676	-4.312530
H	1.196484	-0.370359	-2.924154
H	1.591081	-1.971236	-3.551895
C	-0.687955	-3.300099	-2.970971
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H	0.187466	0.607904	2.993258
C	-1.173005	-2.553781	3.561376
H	-0.270517	-3.062519	3.920337
H	-1.760444	-2.258823	4.439530
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Pd	0.492152	0.952103	0.042479
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C	-2.716780	2.572708	1.302047
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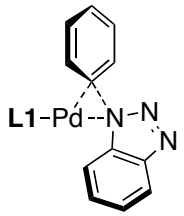
H	-1.030877	3.974816	1.078258
H	-1.815225	3.987721	2.667297
C	-1.961141	-4.055891	0.276038
H	-2.421820	-4.614298	1.099448
H	-1.965111	-4.722158	-0.594529
H	-0.920931	-3.884401	0.539672
C	-5.236526	0.726499	-0.329377
H	-5.902758	0.666748	-1.198010
H	-5.884398	0.767519	0.556441
H	-4.706206	1.664369	-0.391118
C	-6.418220	-1.811238	-0.382852
H	-6.790191	-2.819377	-0.201920
H	-6.910871	-1.154307	0.342445
H	-6.775351	-1.503277	-1.375405
C	-4.790536	-4.246559	-0.226528
H	-5.536747	-4.291669	-1.025638
H	-4.076226	-5.047561	-0.414321
H	-5.308448	-4.488780	0.711998

C	1.788123	2.643108	0.262563
C	1.932364	3.086679	1.588391
C	1.906891	3.556443	-0.797729
C	2.067597	4.450177	1.846553
H	1.954827	2.366650	2.398441
C	2.043208	4.917215	-0.520907
H	1.911542	3.194502	-1.819690
C	2.111453	5.375332	0.798540
H	2.154448	4.788335	2.876500
H	2.112107	5.621327	-1.346920
H	2.232308	6.434802	1.006176
C	4.482719	0.146524	0.309519
C	4.302267	0.325604	-1.096233
C	5.672469	-0.420112	0.822961
C	5.303163	-0.068328	-2.013975
C	6.642064	-0.789053	-0.088642
H	5.813228	-0.544900	1.892449
C	6.458521	-0.616879	-1.492337
H	5.164420	0.068445	-3.082163
H	7.574566	-1.220403	0.265763
H	7.256103	-0.924348	-2.163583
N	2.607276	1.061200	-0.055686
N	3.389918	0.624838	0.943217
N	3.105902	0.919458	-1.297204

Complex A'

C	1.265054	-2.575961	1.035925
C	1.819080	-2.976436	-0.182645
C	1.156804	-2.587519	-1.349122
C	-0.041848	-1.869932	-1.331498
C	-0.636466	-1.519645	-0.076375
C	0.053216	-1.883390	1.125435
H	1.780694	-2.847934	1.953669
H	1.586529	-2.847154	-2.309063
C	-2.142382	-1.308561	-0.015494
C	-2.826552	-0.066064	0.111786
C	-2.887439	-2.519762	-0.064841
C	-4.238458	-0.073995	0.231987
C	-4.295953	-2.496155	-0.048860
C	-4.965855	-1.279182	0.137198
P	-1.766538	1.563054	0.153277
C	-0.549101	-1.671529	2.516044
H	-1.494715	-1.138449	2.389560
C	3.083981	-3.830023	-0.185149
H	3.773261	-3.368361	0.535574
C	3.810121	-3.894867	-1.536303
H	3.207835	-4.412850	-2.293751
H	4.061179	-2.896558	-1.907033
H	4.742279	-4.460533	-1.424720
C	2.763562	-5.252998	0.323769
H	3.679778	-5.851173	0.393939
H	2.293575	-5.237249	1.313438
H	2.078582	-5.764579	-0.364045
C	-0.698269	-1.536337	-2.672913
H	-1.501146	-0.823768	-2.472618
C	0.293756	-0.874335	-3.652957
H	-0.254664	-0.423547	-4.489080
H	0.906502	-0.111724	-3.166407
H	0.986665	-1.609739	-4.077786
C	-1.343714	-2.761504	-3.353288
H	-1.722243	-2.481019	-4.343844
H	-0.614300	-3.568186	-3.492360
H	-2.184313	-3.154540	-2.776171
C	0.360774	-0.820295	3.420807
H	-0.115539	-0.652400	4.394695
H	1.322849	-1.311718	3.601834
H	0.569565	0.153240	2.965500
C	-0.879789	-3.007503	3.214274
H	0.023787	-3.603447	3.385618
H	-1.343181	-2.817635	4.190011
H	-1.573829	-3.612838	2.624324
Pd	0.631149	0.815814	-0.067002
C	-2.248597	2.703589	-1.425434
C	-2.130993	2.535882	1.891585
C	-3.734505	3.015817	-1.654445
H	-4.330300	2.114079	-1.814791
H	-4.183102	3.604088	-0.850038
H	-3.807080	3.618605	-2.569987
C	-1.481192	4.033293	-1.308352
H	-0.416923	3.890465	-1.127565
H	-1.585865	4.572087	-2.259608
H	-1.885347	4.683736	-0.528948
C	-1.745069	1.931030	-2.653636
H	-1.846735	2.570027	-3.540922
H	-0.695704	1.645583	-2.561808
H	-2.339730	1.029226	-2.827105
C	-3.122550	3.715169	1.850162
H	-4.160149	3.422767	1.686173
H	-3.089606	4.203737	2.833131
H	-2.853330	4.472588	1.112725
C	-2.601604	1.520420	2.943293
H	-2.729331	2.044101	3.900378
H	-3.555383	1.053464	2.689671
H	-1.865700	0.730281	3.100692
C	-0.772062	3.102997	2.330431
H	-0.021318	2.315063	2.424088
H	-0.388986	3.847283	1.628381
H	-0.886446	3.586464	3.310286
C	-2.214995	-3.885910	-0.096418
H	-2.627068	-4.529456	0.689441
H	-2.385398	-4.404480	-1.046847
H	-1.139340	-3.839391	0.050239
C	-5.059263	1.159690	0.512149

H	-5.859616	1.294977	-0.223997
H	-5.548859	1.089717	1.492660
H	-4.460726	2.057555	0.509645
C	-6.476283	-1.237453	0.271865
H	-6.783015	-0.698491	1.175533
H	-6.948138	-0.720182	-0.574722
H	-6.916822	-2.232065	0.332241
C	-5.087286	-3.782512	-0.202591
H	-5.464843	-4.147478	0.762789
H	-5.954209	-3.640187	-0.854280
H	-4.492025	-4.584701	-0.637974
C	1.556734	2.585779	-0.427490
C	2.048092	3.409661	0.589764
C	1.830346	2.918938	-1.760393
C	2.736510	4.588639	0.276258
H	1.918183	3.143356	1.632492
C	2.516200	4.097903	-2.070183
H	1.531235	2.257017	-2.566522
C	2.962759	4.943673	-1.053232
H	3.106248	5.219452	1.081674
H	2.714072	4.341583	-3.111499
H	3.501530	5.856292	-1.294333
C	3.625342	0.129342	0.629010
C	4.748979	-0.246516	-0.143852
C	3.738316	0.359256	2.012519
C	6.012139	-0.418962	0.450309
C	4.991076	0.192396	2.583899
H	2.883116	0.659089	2.609592
C	6.117252	-0.196107	1.814068
H	6.868889	-0.712662	-0.149500
H	5.117532	0.365489	3.649963
H	7.077704	-0.315775	2.308718
N	2.583877	0.175573	-0.254223
N	3.059516	-0.110898	-1.486358
N	4.342239	-0.381036	-1.449532



Complex A'-TS

C	-1.130441	2.707670	0.836313
C	-1.620636	3.081295	-0.417710
C	-0.906087	2.645338	-1.534526
C	0.283461	1.913246	-1.432757
C	0.806420	1.597342	-0.145750
C	0.066004	2.001001	1.004143
H	-1.682038	3.016971	1.721341
H	-1.275734	2.890430	-2.523698
C	2.278925	1.241422	-0.000428
C	2.834979	-0.064357	0.164861
C	3.140341	2.373822	-0.015156
C	4.234907	-0.187644	0.337857
C	4.537685	2.217861	0.083178
C	5.078535	0.941997	0.288103
P	1.625683	-1.587738	0.202420
C	0.574029	1.792965	2.431924
H	1.496645	1.209000	2.375214
C	-2.851618	3.979725	-0.504792
H	-3.583039	3.585705	0.214852
C	-3.531258	4.004195	-1.880753
H	-2.879349	4.443588	-2.646383
H	-3.825682	2.999563	-2.196617
H	-4.435485	4.622513	-1.835091
C	-2.489904	5.413496	-0.057566
H	-3.381349	6.052397	-0.048317
H	-2.052489	5.427460	0.946842
H	-1.760982	5.860400	-0.745179
C	0.998392	1.535716	-2.732366
H	1.779702	0.813803	-2.481793
C	0.043179	0.868707	-3.743403
H	0.616044	0.420515	-4.564116
H	-0.563102	0.090930	-3.272042
H	-0.646325	1.596063	-4.187062
C	1.690523	2.738482	-3.407335
H	2.127100	2.433255	-4.366405
H	0.974449	3.544287	-3.607960
H	2.495557	3.145130	-2.790406
C	-0.435090	1.009548	3.292621
H	-0.019447	0.809635	4.288217
H	-1.367673	1.567967	3.428948
H	-0.692782	0.054956	2.822719
C	0.928143	3.125612	3.124580
H	0.045417	3.767228	3.228219
H	1.321812	2.936579	4.130906
H	1.684511	3.685443	2.567013
Pd	-0.731001	-0.815981	-0.078146
C	2.016742	-2.837686	-1.315479
C	1.832998	-2.564043	1.960138
C	3.444904	-3.374698	-1.490924
H	4.166212	-2.578384	-1.691703
H	3.796343	-3.966570	-0.641715
H	3.446056	-4.039731	-2.365724
C	1.049512	-4.026385	-1.164530
H	0.017381	-3.704673	-1.022686
H	1.086772	-4.624508	-2.084870
H	1.322984	-4.690237	-0.339773
C	1.649770	-2.060114	-2.586909
H	1.744829	-2.726753	-3.454939
H	0.620999	-1.696541	-2.550412
H	2.319989	-1.209902	-2.747309
C	2.749711	-3.802563	1.999451
H	3.811428	-3.566942	1.917226
H	2.612782	-4.287619	2.975583
H	2.498782	-4.545603	1.240204
C	2.306830	-1.564923	3.025284
H	2.332672	-2.070605	4.000401

H	3.309055	-1.178845	2.823244
H	1.627547	-0.715767	3.114816
C	0.411571	-3.038084	2.319247
H	-0.289830	-2.200640	2.361997
H	0.020006	-3.757375	1.594683
H	0.433798	-3.524205	3.304743
C	2.603848	3.797351	-0.099135
H	2.994950	4.401569	0.728017
H	2.915126	4.296186	-1.024336
H	1.519118	3.850128	-0.059070
C	4.918621	-1.501096	0.620644
H	5.729979	-1.699797	-0.089115
H	5.372667	-1.503493	1.620711
H	4.232364	-2.332198	0.570963
C	6.570790	0.752790	0.484446
H	6.784993	0.165654	1.384607
H	7.027083	0.211567	-0.355916
H	7.101050	1.698891	0.588270
C	5.458671	3.421660	-0.008130
H	5.857628	3.703566	0.976168
H	6.317363	3.217239	-0.655334
H	4.957061	4.299493	-0.413479
C	-2.214605	-2.244871	-0.631474
C	-2.550919	-3.258749	0.285054
C	-2.258175	-2.527282	-2.012785
C	-2.830100	-4.547716	-0.174433
H	-2.576490	-3.056827	1.348503
C	-2.535855	-3.820165	-2.450092
H	-2.097863	-1.730846	-2.729293
C	-2.817109	-4.843965	-1.538913
H	-3.062839	-5.324508	0.550541
H	-2.544431	-4.023280	-3.518481
H	-3.044600	-5.846929	-1.888093
C	-3.672784	-0.297845	0.808216
C	-4.661486	0.546853	0.264288
C	-3.689756	-0.652910	2.165771
C	-5.701643	1.057983	1.055953
C	-4.726348	-0.146820	2.939528
H	-2.918597	-1.275341	2.604998
C	-5.722361	0.698630	2.395070
H	-6.455150	1.708753	0.622850
H	-4.771032	-0.402010	3.994988
H	-6.510733	1.071535	3.042896
N	-2.832565	-0.583843	-0.252183
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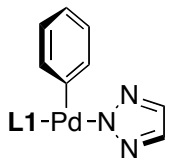
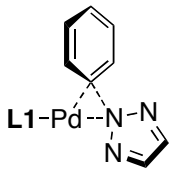
N	-4.391125	0.726808	-1.076958



Complex B

C	-1.401808	2.645057	1.230404
C	-2.056595	3.045635	0.064673
C	-1.521081	2.620704	-1.153035
C	-0.353311	1.859793	-1.235954
C	0.348345	1.506018	-0.037335
C	-0.212700	1.909293	1.216995
H	-1.823840	2.933848	2.189024
H	-2.031024	2.880477	-2.073071
C	1.844335	1.236344	-0.119344
C	2.489102	-0.030896	-0.034892
C	2.627730	2.415055	-0.263001
C	3.904789	-0.078227	-0.037712
C	4.029518	2.333763	-0.380832
C	4.666314	1.094129	-0.230214
P	1.368398	-1.609418	0.106215
C	0.491931	1.670912	2.552161
H	1.374043	1.057615	2.353999
C	-3.303009	3.918516	0.169438
H	-3.945034	3.448717	0.927559
C	-4.119636	4.013405	-1.126153
H	-3.570282	4.546630	-1.912523
H	-4.385806	3.020745	-1.501074
H	-5.045535	4.570259	-0.942691
C	-2.933823	5.329339	0.676635
H	-3.836320	5.935629	0.820022
H	-2.397338	5.291525	1.630852
H	-2.291863	5.845930	-0.047918
C	0.149539	1.469735	-2.626197
H	0.956677	0.747308	-2.488298
C	-0.958138	0.794370	-3.462091
H	-0.523665	0.324038	-4.352606
H	-1.498130	0.037941	-2.885747
H	-1.699276	1.523816	-3.807767
C	0.734409	2.658179	-3.416837
H	1.009618	2.335726	-4.428555
H	0.003221	3.469475	-3.513719
H	1.631879	3.063302	-2.942368
C	-0.402629	0.917976	3.556076
H	0.171878	0.659214	4.454451
H	-1.253488	1.530163	3.874082
H	-0.816464	0.002916	3.123153
C	0.997290	2.986294	3.180946
H	0.166881	3.668936	3.395524
H	1.510973	2.778521	4.127527
H	1.699879	3.507788	2.524239
Pd	-0.987264	-0.741831	0.115619
C	1.691825	-2.787039	-1.486796
C	1.806372	-2.582888	1.826365
C	3.140777	-3.180465	-1.807272
H	3.769922	-2.314715	-2.026220
H	3.610392	-3.777318	-1.022002
H	3.120607	-3.802559	-2.712611
C	0.864649	-4.073275	-1.307459
H	-0.164734	-3.876050	-1.012389
H	0.836609	-4.599819	-2.271044
H	1.312480	-4.759382	-0.584725
C	1.152951	-1.995382	-2.687322

H	1.184815	-2.635684	-3.579040
H	0.121184	-1.673185	-2.539083
H	1.769080	-1.114275	-2.891420
C	2.703304	-3.830653	1.712838
H	3.726492	-3.623344	1.396491
H	2.771396	-4.276152	2.714366
H	2.284398	-4.594382	1.056405
C	2.438790	-1.598218	2.821175
H	2.606024	-2.125162	3.770238
H	3.400381	-1.203855	2.487026
H	1.776879	-0.756852	3.030028
C	0.453379	-3.043686	2.391264
H	-0.223945	-2.201244	2.550035
H	-0.048872	-3.754676	1.731513
H	0.621070	-3.536683	3.358771
C	2.007498	3.806145	-0.260790
H	2.519644	4.449616	0.463841
H	2.100460	4.297305	-1.236491
H	0.951331	3.804707	-0.005054
C	4.699203	-1.336849	0.209735
H	5.414100	-1.538082	-0.596042
H	5.289154	-1.248429	1.131647
H	4.068304	-2.207187	0.310107
C	6.179575	0.990901	-0.236349
H	6.665338	1.965240	-0.275402
H	6.549114	0.486441	0.664051
H	6.545161	0.407357	-1.092087
C	4.852131	3.583731	-0.636997
H	5.641184	3.397088	-1.371463
H	4.248190	4.404507	-1.022946
H	5.341760	3.944771	0.278172
C	-2.029157	-2.460559	-0.172963
C	-2.532983	-3.211477	0.893823
C	-2.380855	-2.820810	-1.479779
C	-3.312238	-4.349341	0.653029
H	-2.348810	-2.905501	1.917540
C	-3.161522	-3.957606	-1.717784
H	-2.060001	-2.220444	-2.325444
C	-3.620907	-4.733383	-0.652609
H	-3.690938	-4.924173	1.495502
H	-3.417482	-4.224984	-2.740756
H	-4.230435	-5.614367	-0.837101
N	-3.475418	0.010538	1.527200
N	-2.909080	-0.040580	0.319753
N	-3.754817	0.198313	-0.682342
C	-4.759848	0.334194	1.294488
C	-4.934740	0.449836	-0.087212
H	-5.461971	0.458148	2.107675
H	-5.814543	0.688960	-0.668854



Complex B-TS

C	-0.976418	2.671247	1.475996
C	-1.512195	3.326635	0.362795
C	-0.978868	3.004393	-0.883702
C	0.093052	2.113304	-1.040862
C	0.672493	1.503600	0.109204
C	0.099737	1.785318	1.386923
H	-1.399084	2.881855	2.455327
H	-1.388535	3.472060	-1.771933
C	2.093891	0.965395	0.035365
C	2.487911	-0.402016	-0.078949
C	3.088169	1.980797	0.114760
C	3.870134	-0.708748	-0.100422
C	4.456612	1.654978	0.028422
C	4.843966	0.311307	-0.058184
P	1.092020	-1.757804	-0.128818
C	0.675879	1.230550	2.690166
H	1.470079	0.526402	2.430087
C	-2.607642	4.369721	0.564413
H	-3.359020	3.913968	1.224989
C	-3.323251	4.797017	-0.724290
H	-2.647369	5.334593	-1.400942
H	-3.732445	3.936408	-1.262684
H	-4.151190	5.474822	-0.486559
C	-2.044565	5.609951	1.292107
H	-2.843103	6.332168	1.501524
H	-1.572601	5.343155	2.243627
H	-1.289408	6.110616	0.673513
C	0.632885	1.901119	-2.457488
H	1.313357	1.047507	-2.425248
C	-0.491417	1.577523	-3.464391
H	-0.058751	1.206401	-4.401331
H	-1.189018	0.829441	-3.078511
H	-1.074551	2.472651	-3.712164
C	1.443796	3.106561	-2.977526
H	1.740841	2.937434	-4.019976
H	0.848318	4.026921	-2.945554
H	2.353917	3.269573	-2.395384
C	-0.382792	0.467985	3.510073
H	0.079390	-0.009459	4.383153
H	-1.166982	1.138986	3.879399
H	-0.867077	-0.304623	2.904462
C	1.319854	2.332898	3.556706
H	0.583300	3.091268	3.846991
H	1.733287	1.900405	4.476136
H	2.132678	2.840504	3.029003
Pd	-1.143499	-0.615938	-0.069391
C	1.143559	-2.712733	-1.889662

C	1.375924	-3.079629	1.372039
C	2.462560	-3.351557	-2.346649
H	3.258595	-2.613140	-2.470900
H	2.814587	-4.144900	-1.682700
H	2.290521	-3.810512	-3.330265
C	0.049063	-3.793612	-1.841673
H	-0.909334	-3.391586	-1.509747
H	-0.086262	-4.198630	-2.854105
H	0.307199	-4.634400	-1.192258
C	0.744904	-1.664856	-2.937890
H	0.619642	-2.159467	-3.910912
H	-0.198683	-1.176379	-2.679827
H	1.517462	-0.898822	-3.054207
C	2.097818	-4.402656	1.047794
H	3.164396	-4.290407	0.849027
H	2.011820	-5.051217	1.930193
H	1.644596	-4.943069	0.214708
C	2.112807	-2.377784	2.522739
H	2.158429	-3.062163	3.381038
H	3.137974	-2.099433	2.265119
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C	2.732396	3.446596	0.332659
H	3.257646	3.840436	1.210790
H	3.033755	4.069572	-0.517357
H	1.669584	3.612654	0.487239
C	4.404776	-2.118231	-0.138345
H	5.091609	-2.269925	-0.979370
H	4.973408	-2.350898	0.771826
H	3.615995	-2.849033	-0.228128
C	6.310792	-0.074258	-0.083612
H	6.970473	0.777874	0.077385
H	6.545135	-0.811707	0.692974
H	6.594662	-0.531041	-1.041470
C	5.516535	2.742317	0.048177
H	6.253132	2.592923	-0.748154
H	5.098113	3.738228	-0.089372
H	6.068621	2.752327	0.997904
C	-2.888615	-1.823731	0.136748
C	-3.234501	-2.093235	1.472457
C	-3.236764	-2.737901	-0.871570
C	-3.802555	-3.323606	1.801963
H	-3.066599	-1.342206	2.236255
C	-3.805908	-3.963388	-0.522938
H	-3.074611	-2.478926	-1.911882
C	-4.080587	-4.272316	0.812909
H	-4.041103	-3.534307	2.842032
H	-4.048885	-4.675621	-1.308382
H	-4.535196	-5.223491	1.075153
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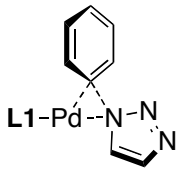
C	-4.706914	1.375086	-0.214117
C	-4.497157	1.041722	-1.562987
H	-5.408106	2.064644	0.234878
H	-4.986054	1.400310	-2.458203

Complex B'

C	1.492782	-2.528232	1.365896
C	2.154593	-2.987381	0.224180
C	1.617742	-2.633855	-1.015301
C	0.431745	-1.905986	-1.142229
C	-0.278319	-1.497940	0.033845
C	0.294589	-1.810763	1.309880
H	1.913524	-2.767675	2.339692
H	2.137435	-2.931419	-1.917902
C	-1.783939	-1.295728	-0.071931
C	-2.481011	-0.054245	-0.094669
C	-2.515222	-2.514124	-0.150490
C	-3.895161	-0.064969	-0.178228
C	-3.914073	-2.500395	-0.319760
C	-4.601859	-1.278944	-0.309024
P	-1.435635	1.573474	0.056920
C	-0.415262	-1.497844	2.626592
H	-1.310355	-0.920420	2.385016
C	3.396477	-3.859464	0.379009
H	4.004616	-3.394211	1.167123
C	4.271783	-3.953021	-0.878395
H	3.753200	-4.474206	-1.693326
H	4.575355	-2.961652	-1.227798
H	5.177114	-4.528862	-0.653519
C	2.995890	-5.268459	0.869247
H	3.888113	-5.879640	1.050310
H	2.417910	-5.227894	1.799375
H	2.383511	-5.780875	0.116747
C	-0.084933	-1.622823	-2.554148
H	-0.903979	-0.905326	-2.464318
C	1.007287	-0.997471	-3.448767
H	0.550876	-0.567744	-4.348854
H	1.578671	-0.226300	-2.926244
H	1.729548	-1.752574	-3.779661
C	-0.657780	-2.875958	-3.248542
H	-0.931805	-2.636716	-4.283298
H	0.082315	-3.684293	-3.278435
H	-1.553134	-3.250006	-2.745335
C	0.460135	-0.650006	3.569726
H	-0.110037	-0.353432	4.458785
H	1.337239	-1.209734	3.914438
H	0.820032	0.255212	3.069175
C	-0.889435	-2.773906	3.352368
H	-0.044398	-3.419076	3.619376
H	-1.412508	-2.509247	4.279426

H	-1.576161	-3.359284	2.734228
Pd	0.960012	0.804183	0.135880
C	-1.666671	2.695922	-1.594555
C	-2.052468	2.572101	1.707452
C	-3.095483	3.011597	-2.058780
H	-3.664637	2.110997	-2.301095
H	-3.661298	3.612959	-1.342864
H	-3.018509	3.603299	-2.981223
C	-0.916850	4.023199	-1.379550
H	0.081677	3.883293	-0.967956
H	-0.804388	4.514803	-2.355144
H	-1.468928	4.714544	-0.738393
C	-0.984507	1.896715	-2.715378
H	-0.961383	2.510493	-3.625682
H	0.042454	1.624341	-2.464778
H	-1.540061	0.983273	-2.947624
C	-2.991386	3.772866	1.481279
H	-3.981616	3.504383	1.111214
H	-3.143424	4.260209	2.453844
H	-2.563143	4.523235	0.815809
C	-2.720020	1.591236	2.683204
H	-2.977975	2.138570	3.599857
H	-3.637948	1.149522	2.291167
H	-2.047206	0.780401	2.967959
C	-0.772088	3.113800	2.359604
H	-0.074994	2.308776	2.602367
H	-0.250165	3.825100	1.715985
H	-1.036896	3.629471	3.292825
C	-1.839734	-3.874172	-0.029855
H	-2.337007	-4.478567	0.737574
H	-1.898979	-4.442496	-0.965147
H	-0.788263	-3.811759	0.236600
C	-4.746982	1.177427	-0.097546
H	-5.401847	1.280067	-0.970529
H	-5.405165	1.146530	0.780655
H	-4.154806	2.077322	-0.029755
C	-6.114927	-1.239018	-0.406787
H	-6.555811	-0.675797	0.423995
H	-6.450002	-0.745886	-1.329275
H	-6.560895	-2.232599	-0.388797
C	-4.683268	-3.798066	-0.493449
H	-5.247059	-4.060702	0.412240
H	-5.406727	-3.723798	-1.311396
H	-4.031842	-4.640562	-0.721658
C	1.942479	2.576043	-0.026004
C	2.290100	3.348511	1.087207
C	2.417894	2.957787	-1.287161
C	3.035849	4.524151	0.932053
H	1.997671	3.044334	2.086476
C	3.159264	4.133667	-1.440281
H	2.235270	2.333524	-2.155675
C	3.462881	4.927829	-0.332789
H	3.289433	5.114860	1.809791
H	3.514426	4.415117	-2.429025
H	4.045047	5.837913	-0.452056
N	3.526481	-0.139182	-1.015587
N	2.909394	0.145558	0.143770
C	4.988028	-0.347831	0.575426
H	5.951143	-0.551435	1.023080
N	4.786751	-0.452050	-0.765190
C	3.797918	0.041503	1.161634
H	3.526022	0.244305	2.186490



Complex B'-TS

C	1.041857	2.827742	-1.147814
C	1.657428	3.255084	0.030706
C	1.138170	2.769077	1.231395
C	0.022356	1.926033	1.287384
C	-0.628311	1.540100	0.078674
C	-0.089749	2.002918	-1.158619
H	1.439889	3.181497	-2.096283
H	1.611407	3.059641	2.162507
C	-2.063254	1.035702	0.128616
C	-2.496453	-0.322920	0.043212
C	-3.029371	2.072573	0.254980
C	-3.886121	-0.595287	0.057175
C	-4.402539	1.769626	0.348398
C	-4.829190	0.441425	0.218223
P	-1.145271	-1.712217	-0.133536
C	-0.759617	1.733540	-2.508295
H	-1.599043	1.054078	-2.336690
C	2.804271	4.258571	-0.038969
H	3.446747	3.944482	-0.872051
C	3.685630	4.307044	1.216008
H	3.134270	4.685922	2.086103
H	4.089789	3.319121	1.451137
H	4.529360	4.986365	1.048194
C	2.256910	5.664067	-0.371152
H	3.078735	6.381117	-0.487113
H	1.673097	5.663354	-1.298528
H	1.604312	6.025989	0.433336
C	-0.481223	1.505938	2.670759
H	-1.207400	0.701850	2.528691
C	0.653836	0.966784	3.565099
H	0.235067	0.495703	4.462497
H	1.268225	0.229889	3.041313
H	1.319073	1.770539	3.900265
C	-1.206464	2.647140	3.414553
H	-1.486909	2.321339	4.423906
H	-0.559401	3.526773	3.514907
H	-2.119292	2.953683	2.898700
C	0.200539	1.060040	-3.507601
H	-0.328752	0.797064	-4.431918
H	1.028292	1.725110	-3.779039

H	0.636052	0.150176	-3.082407
C	-1.343154	3.017356	-3.134839
H	-0.555855	3.750833	-3.345014
H	-1.841572	2.783167	-4.083630
H	-2.076624	3.493555	-2.478305
Pd	1.122739	-0.671530	-0.232931
C	-1.210829	-2.949535	1.438504
C	-1.472965	-2.746766	-1.840947
C	-2.529687	-3.664151	1.767948
H	-3.320458	-2.963338	2.046460
H	-2.891804	-4.306588	0.961673
H	-2.351561	-4.311230	2.637978
C	-0.109843	-4.001798	1.211144
H	0.858054	-3.543112	1.006958
H	-0.009085	-4.602946	2.124643
H	-0.346046	-4.691787	0.396261
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H	-0.731792	-2.748077	3.533305
H	0.129647	-1.591619	2.504746
H	-1.592070	-1.346468	2.879296
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H	-3.281966	-3.987414	-1.503058
H	-2.162912	-4.582456	-2.716076
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C	-2.209414	-1.835351	-2.832812
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H	-1.657144	-0.911872	-3.016976
C	-0.070454	-3.053217	-2.399247
H	0.516559	-2.139964	-2.530505
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H	-6.575494	-0.543248	-0.619643
H	-6.593302	-0.448802	1.135895
H	-6.940029	0.983244	0.167530
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H	3.008521	-1.140011	2.167497
C	3.856472	-4.297099	1.191838
H	3.790976	-5.002834	-0.847861
H	3.848173	-3.273932	3.093331
H	4.259756	-5.222982	1.591560
N	3.805501	0.612183	0.339866
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C	4.603531	0.951689	-1.654356
H	5.230932	1.412506	-2.404049
N	4.652352	1.336900	-0.345160
C	3.684444	-0.062801	-1.776303
H	3.365240	-0.657435	-2.617146

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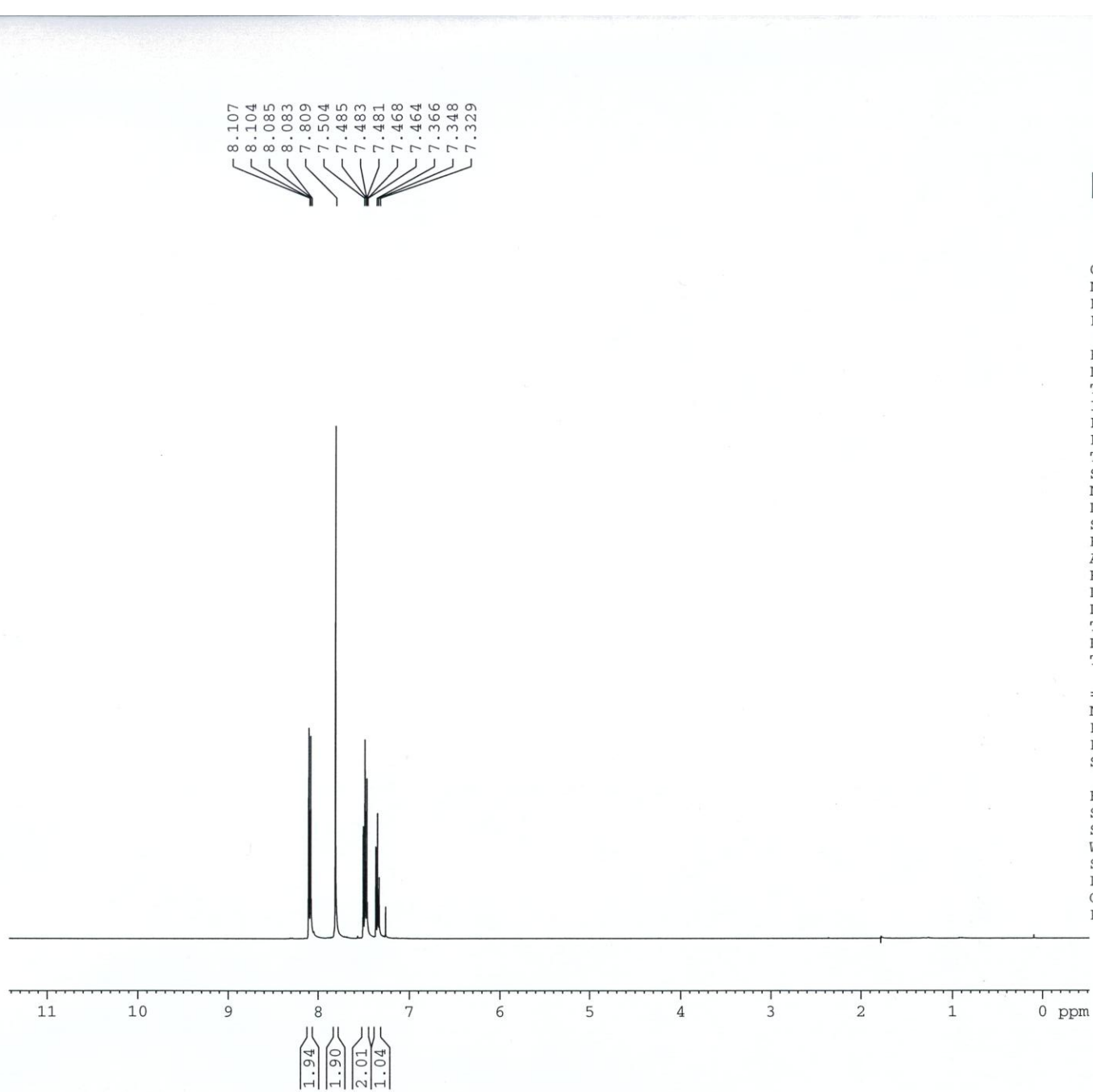

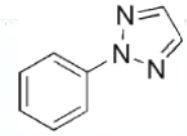

Current Data Parameters
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EXPNO 99
PROCNO 99

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FIDRES 0.126314 Hz
AQ 3.9584243 sec
RG 287.4
DW 60.400 usec
DE 6.00 usec
TE 295.2 K
D1 1.00000000 sec
TD0 1

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PL1 0.00 dB
SFO1 400.1324710 MHz

F2 - Processing parameters
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SF 400.1300092 MHz
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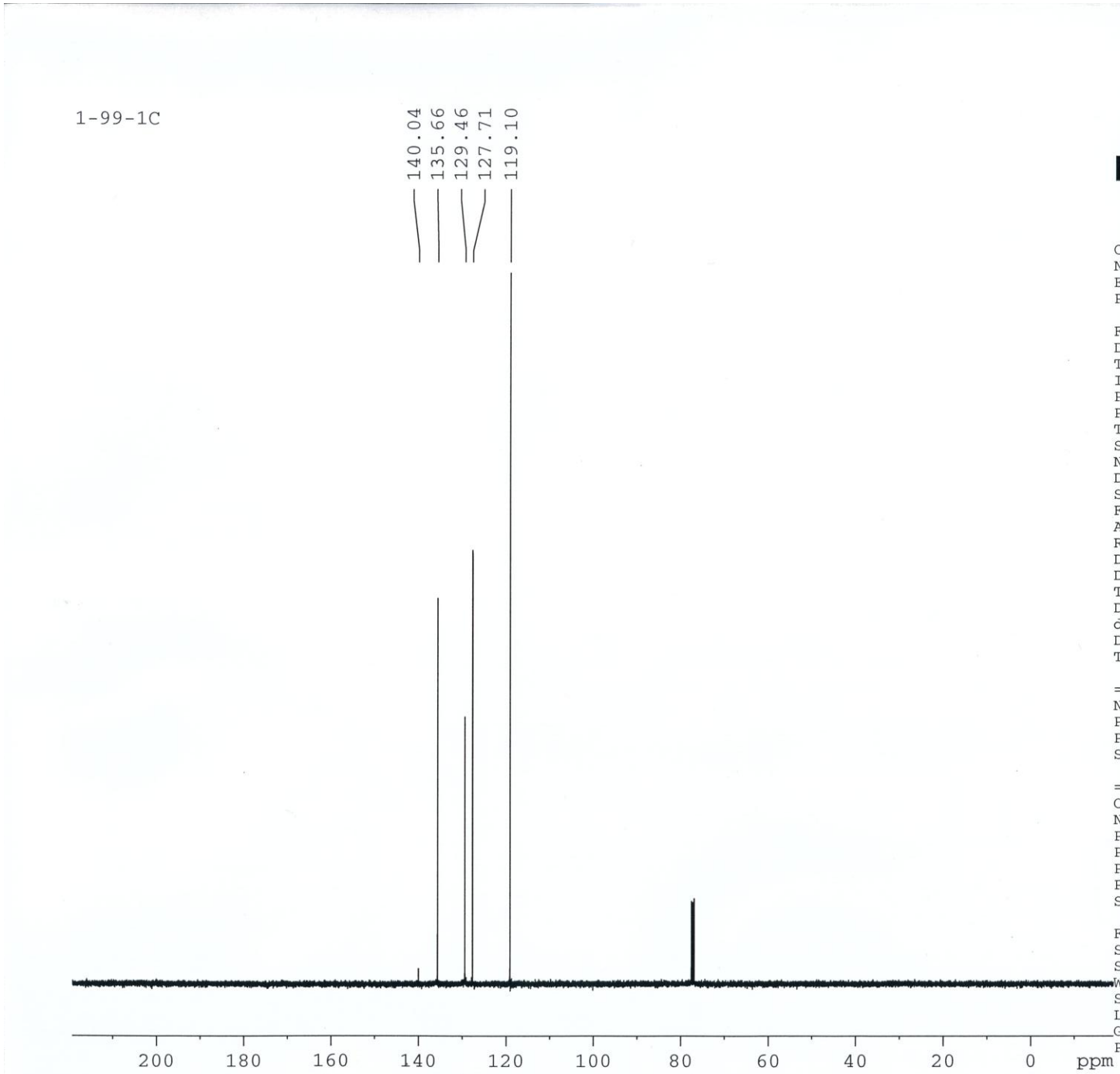
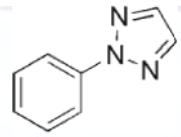
GB 0
PC 1.00





BRUKER

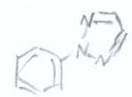
Current Data Parameters
NAME 1-99-1C
EXPNO 99
PROCNO 99

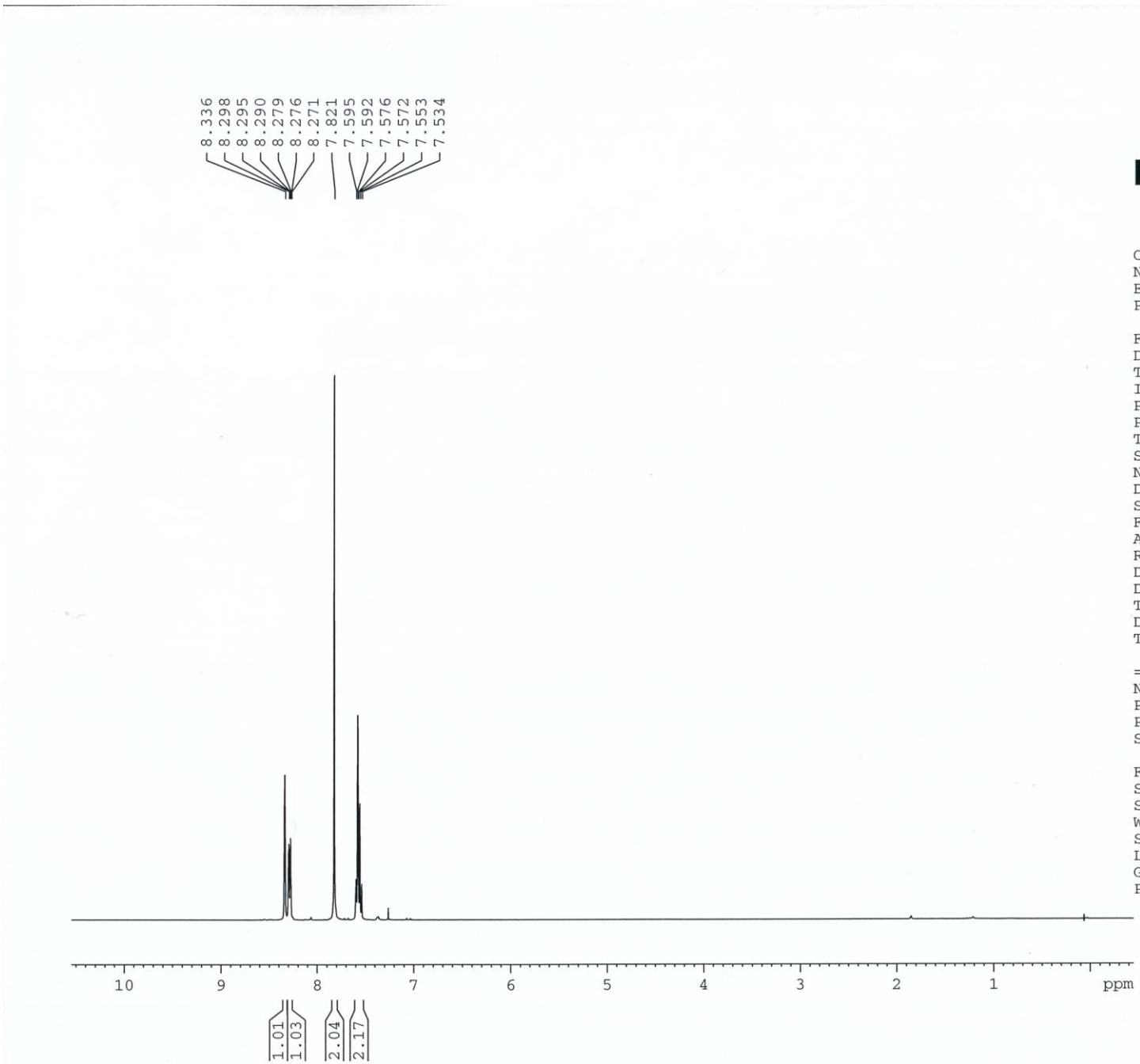
F2 - Acquisition Parameters
Date_ 20100804
Time 7.38
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 128
DS 4
SWH 23980.814 Hz
FIDRES 0.365918 Hz
AQ 1.3664756 sec
RG 1448.2
DW 20.850 usec
DE 6.00 usec
TE 295.2 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1

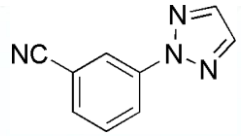
======== CHANNEL f1 ========
NUC1 13C
P1 9.38 usec
PL1 0.00 dB
SFO1 100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 0.00 dB
PL12 16.10 dB
PL13 19.00 dB
SFO2 400.1316005 MHz

F2 - Processing parameters
SI 32768
SF 100.6127544 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.40

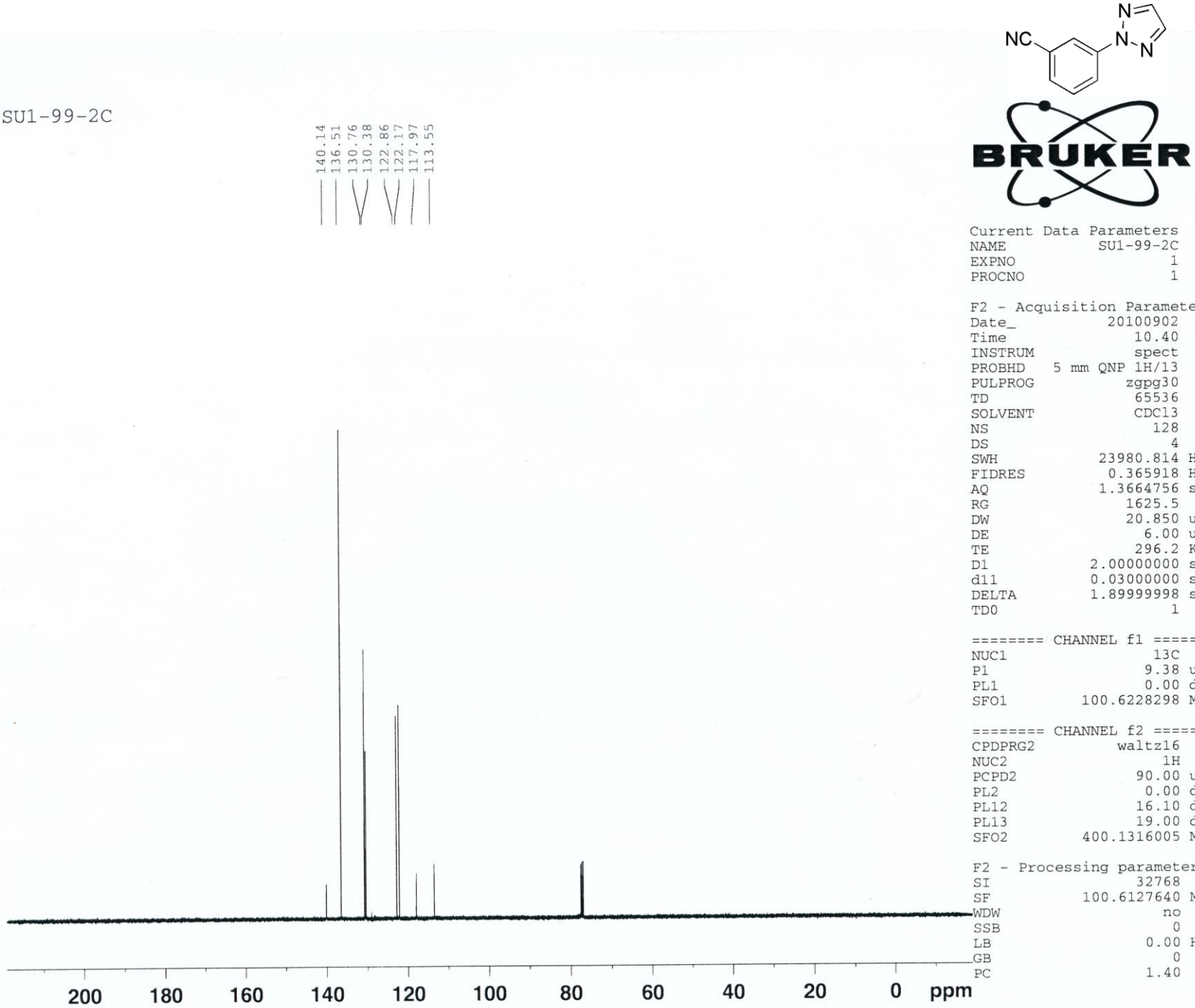


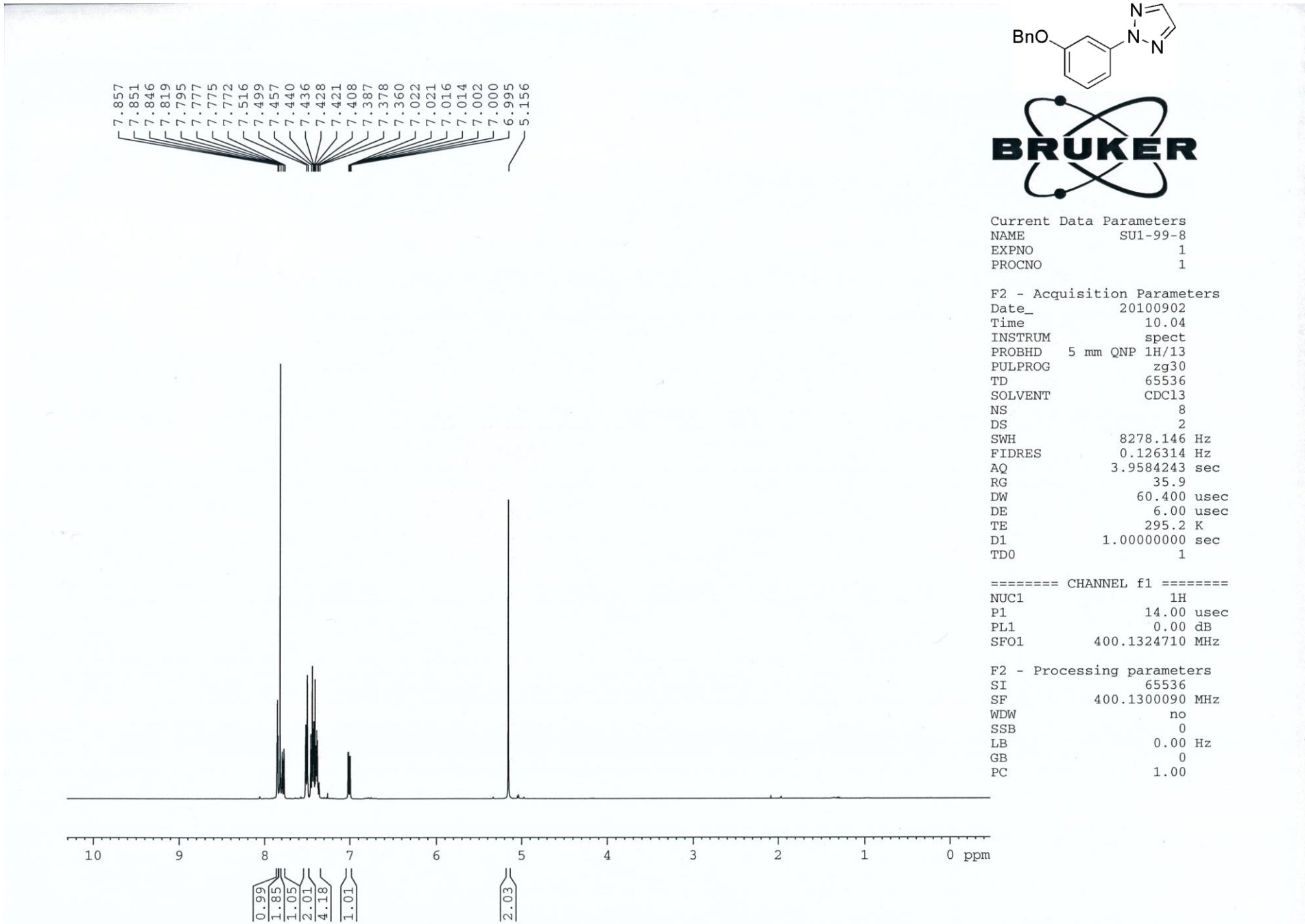


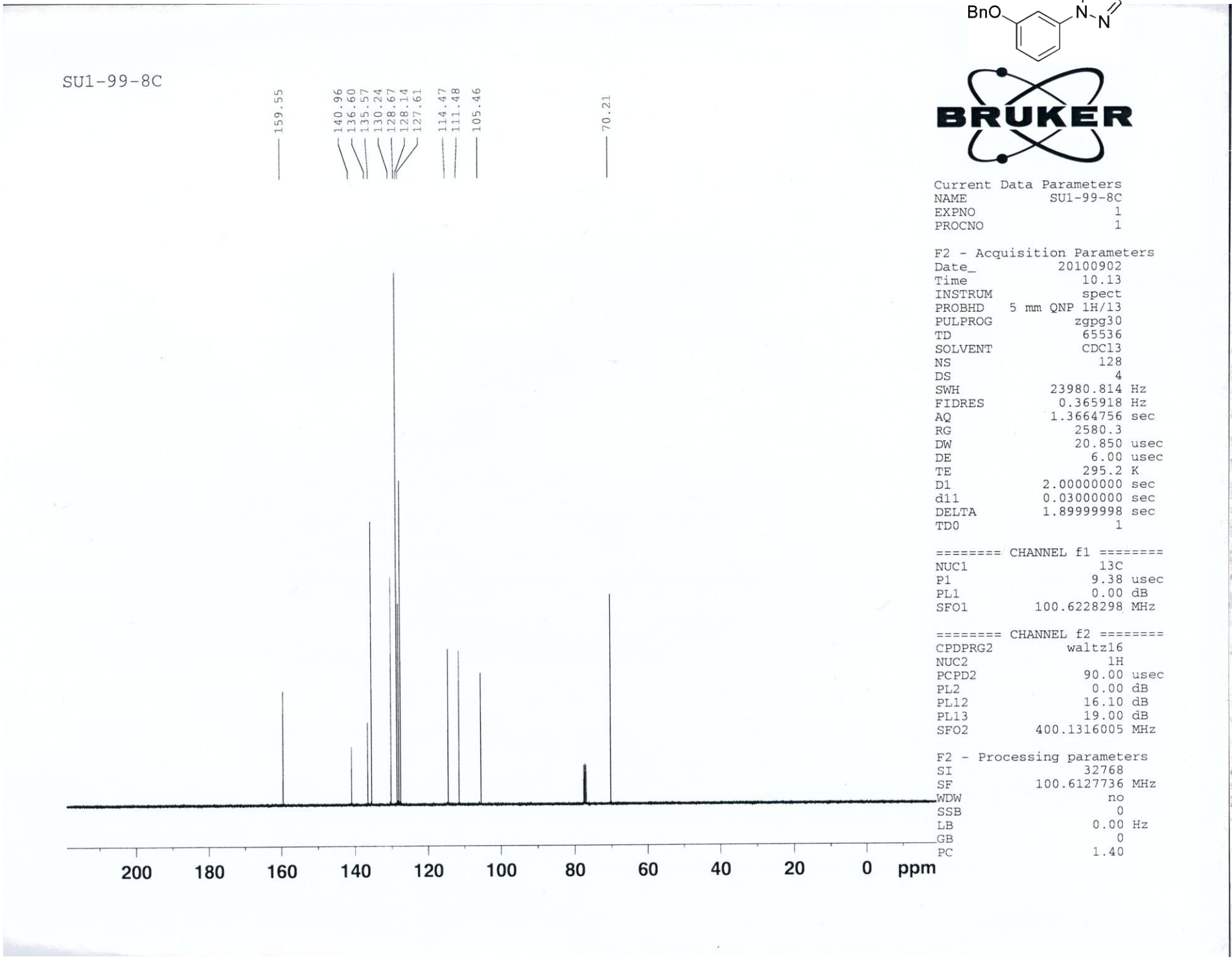


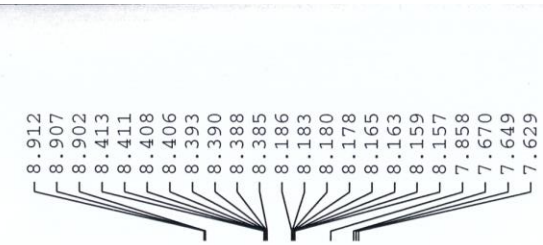
BRUKER

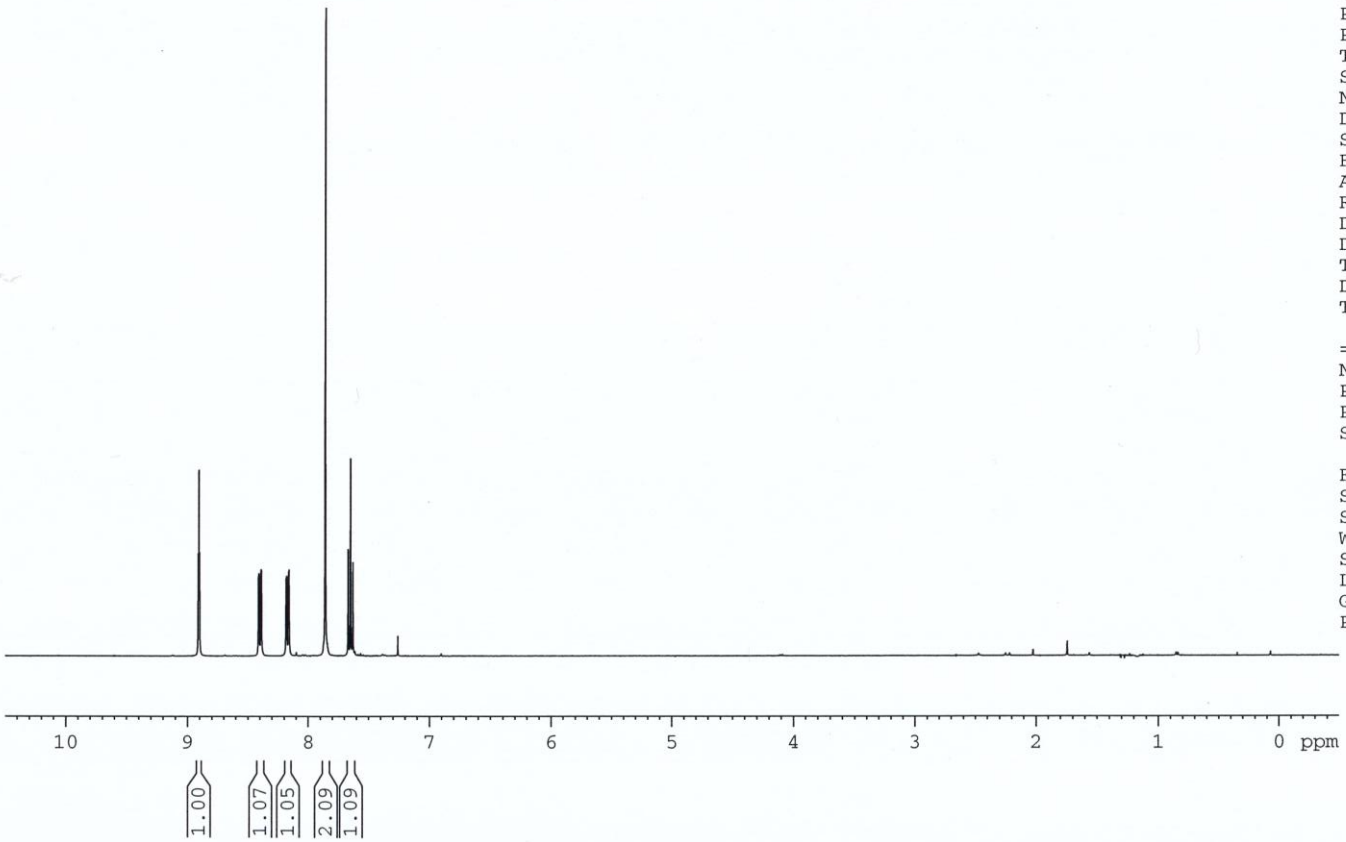
```
Current Data Parameters
NAME                  SU1-99-2
EXPNO                        1
PROCNO                       1

F2 - Acquisition Parameters
Date_                 20100902
Time                     10.32
INSTRUM                  spect
PROBHD    5 mm QNP 1H/13
PULPROG                   zg30
TD                       65536
SOLVENT                  CDCl3
NS                           9
DS                           2
SWH                 8278.146 Hz
FIDRES               0.126314 Hz
AQ                  3.9584243 sec
RG                       101.6
DW                    60.400 usec
DE                     6.00 usec
TE                     295.2 K
D1                 1.00000000 sec
TD0                          1

======== CHANNEL f1 ========
NUC1                        1H
P1                     14.00 usec
PL1                     0.00 dB
SFO1           400.1324710 MHz

F2 - Processing parameters
SI                       65536
SF             400.1300094 MHz
WDW                         no
SSB                          0
LB                      0.00 Hz
GB                           0
PC                        1.00
```

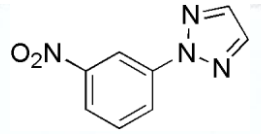

SU1-99-2C
140.14
136.51
130.76
130.38
122.86
122.17
117.97
113.55
NC
N
N
N
BRUKER
Current Data Parameters
NAME SU1-99-2C
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20100902
Time 10.40
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 128
DS 4
SWH 23980.814 Hz
FIDRES 0.365918 Hz
AQ 1.3664756 sec
RG 1625.5
DW 20.850 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 9.38 usec
PL1 0.00 dB
SFO1 100.6228298 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 0.00 dB
PL12 16.10 dB
PL13 19.00 dB
SFO2 400.1316005 MHz
F2 - Processing parameters
SI 32768
SF 100.6127640 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.40
200
180
160
140
120
100
80
60
40
20
0
ppm


7.857
7.851
7.846
7.819
7.795
7.777
7.775
7.772
7.516
7.499
7.457
7.440
7.436
7.428
7.421
7.408
7.387
7.378
7.360
7.022
7.021
7.016
7.014
7.002
7.000
6.995
5.156
BnO
N
N
N
BRUKER
Current Data Parameters
NAME SU1-99-8
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20100902
Time 10.04
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 8
DS 2
SWH 8278.146 Hz
FIDRES 0.126314 Hz
AQ 3.9584243 sec
RG 35.9
DW 60.400 usec
DE 6.00 usec
TE 295.2 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 14.00 usec
PL1 0.00 dB
SFO1 400.1324710 MHz
F2 - Processing parameters
SI 65536
SF 400.1300090 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
10
9
8
7
6
5
4
3
2
1
0 ppm
0.99
1.85
1.05
2.01
4.18
1.01
2.03

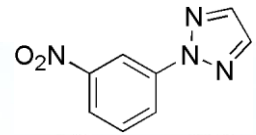

SU1-99-8C
159.55
140.96
136.60
135.57
130.24
128.67
128.14
127.61
114.47
111.48
105.46
70.21
BnO
N
N
N
BRUKER
Current Data Parameters
NAME SU1-99-8C
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20100902
Time 10.13
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 128
DS 4
SWH 23980.814 Hz
FIDRES 0.365918 Hz
AQ 1.3664756 sec
RG 2580.3
DW 20.850 usec
DE 6.00 usec
TE 295.2 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 9.38 usec
PL1 0.00 dB
SFO1 100.6228298 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 0.00 dB
PL12 16.10 dB
PL13 19.00 dB
SFO2 400.1316005 MHz
F2 - Processing parameters
SI 32768
SF 100.6127736 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.40
200
180
160
140
120
100
80
60
40
20
0
ppm





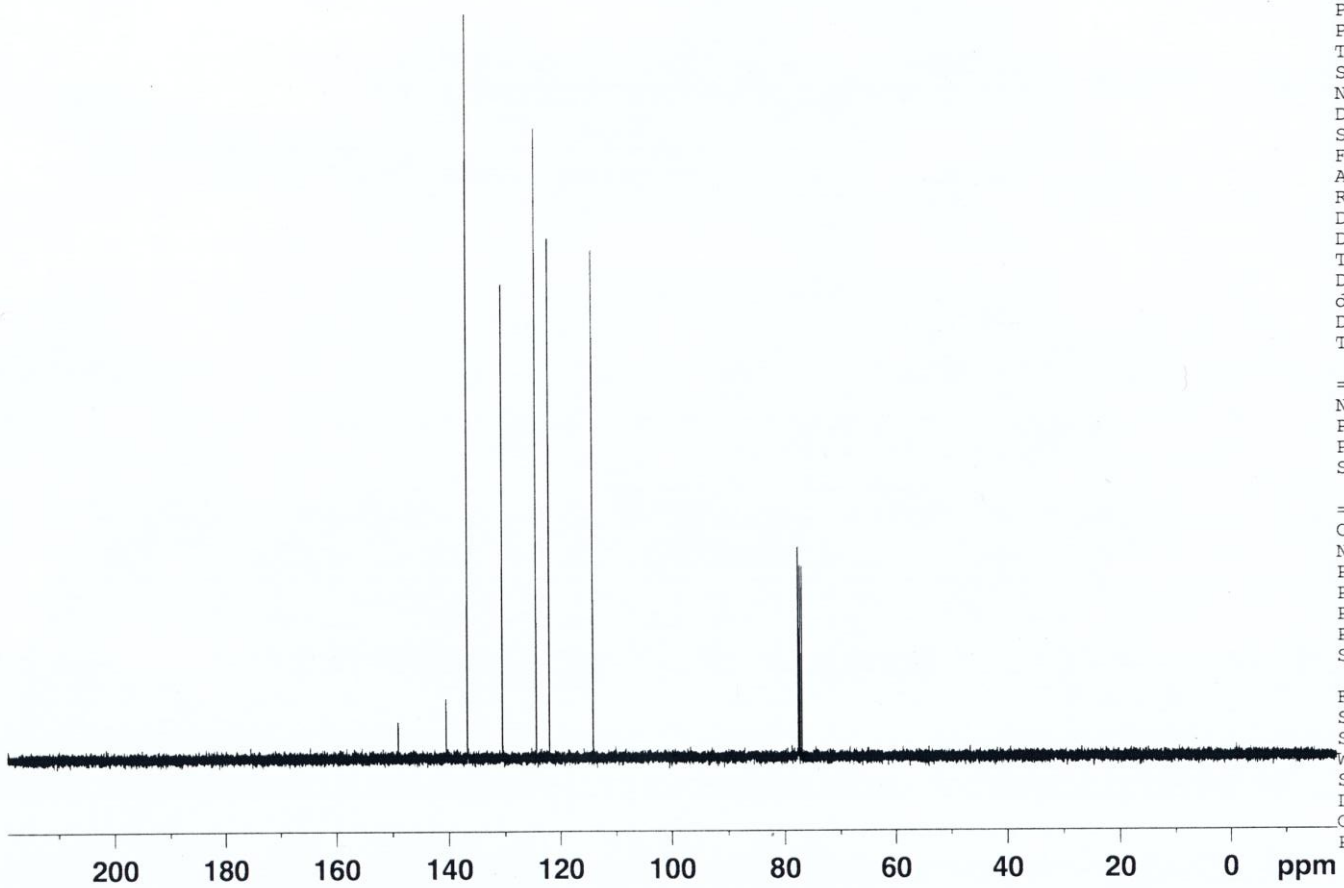



```
Current Data Parameters
NAME                  SU1-99-7
EXPNO                        1
PROCNO                       1

F2 - Acquisition Parameters
Date_                 20100829
Time                     14.26
INSTRUM                  spect
PROBHD     5 mm QNP 1H/13
PULPROG                   zg30
TD                       65536
SOLVENT                  CDCl3
NS                           8
DS                           2
SWH                 8278.146 Hz
FIDRES              0.126314 Hz
AQ                  3.9584243 sec
RG                       161.3
DW                    60.400 usec
DE                     6.00 usec
TE                     300.0 K
D1                 1.00000000 sec
TD0                          1

======== CHANNEL f1 ========
NUC1                        1H
P1                      14.00 usec
PL1                      0.00 dB
SFO1             400.1324710 MHz

F2 - Processing parameters
SI                       65536
SF               400.1300096 MHz
WDW                         no
SSB                          0
LB                       0.00 Hz
GB                           0
PC                        1.00
```



SU1-99-7C

149.02
140.55
136.71
130.49
124.40
122.02
114.16



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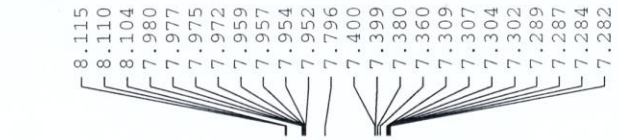
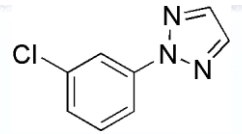
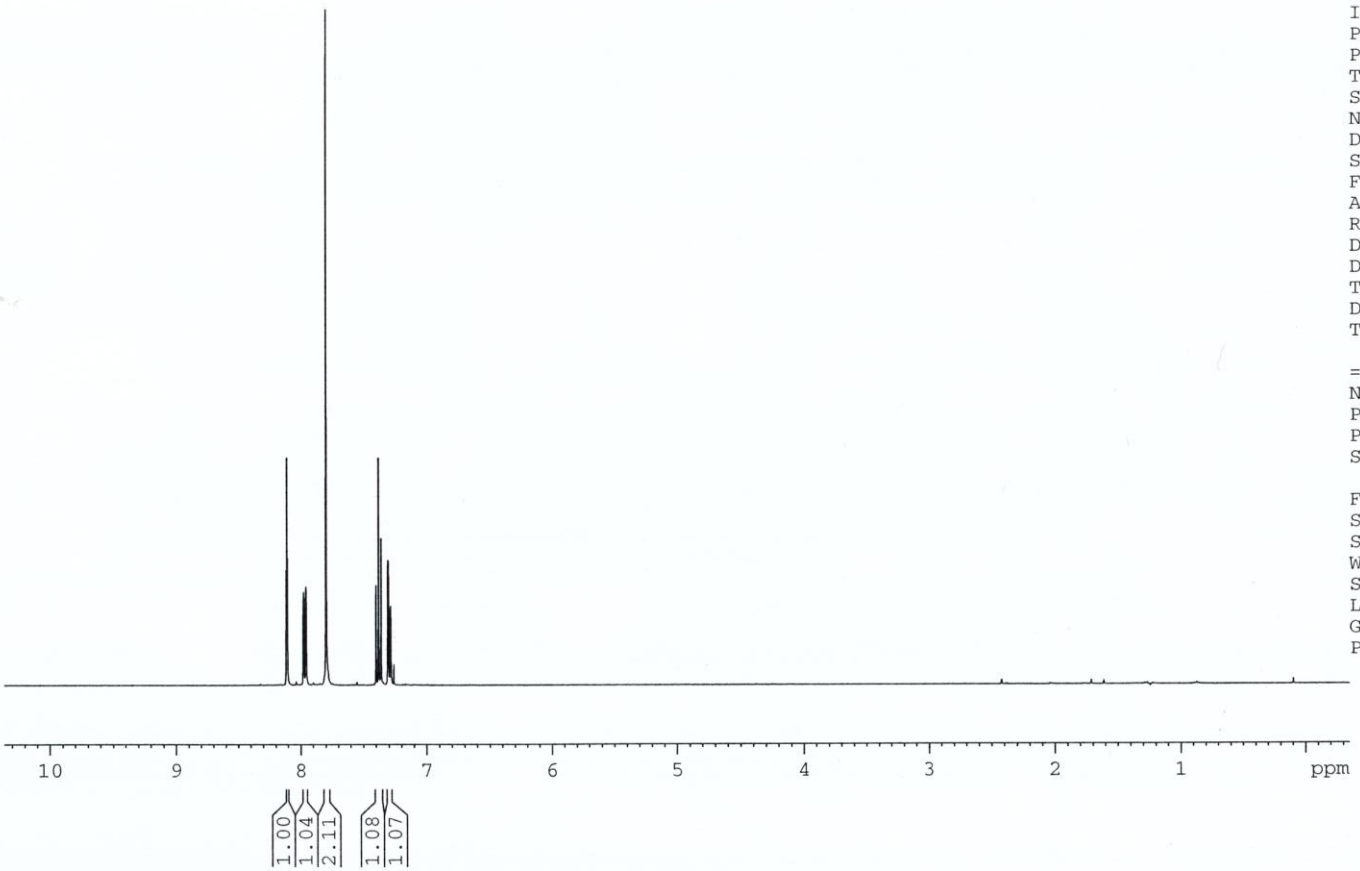
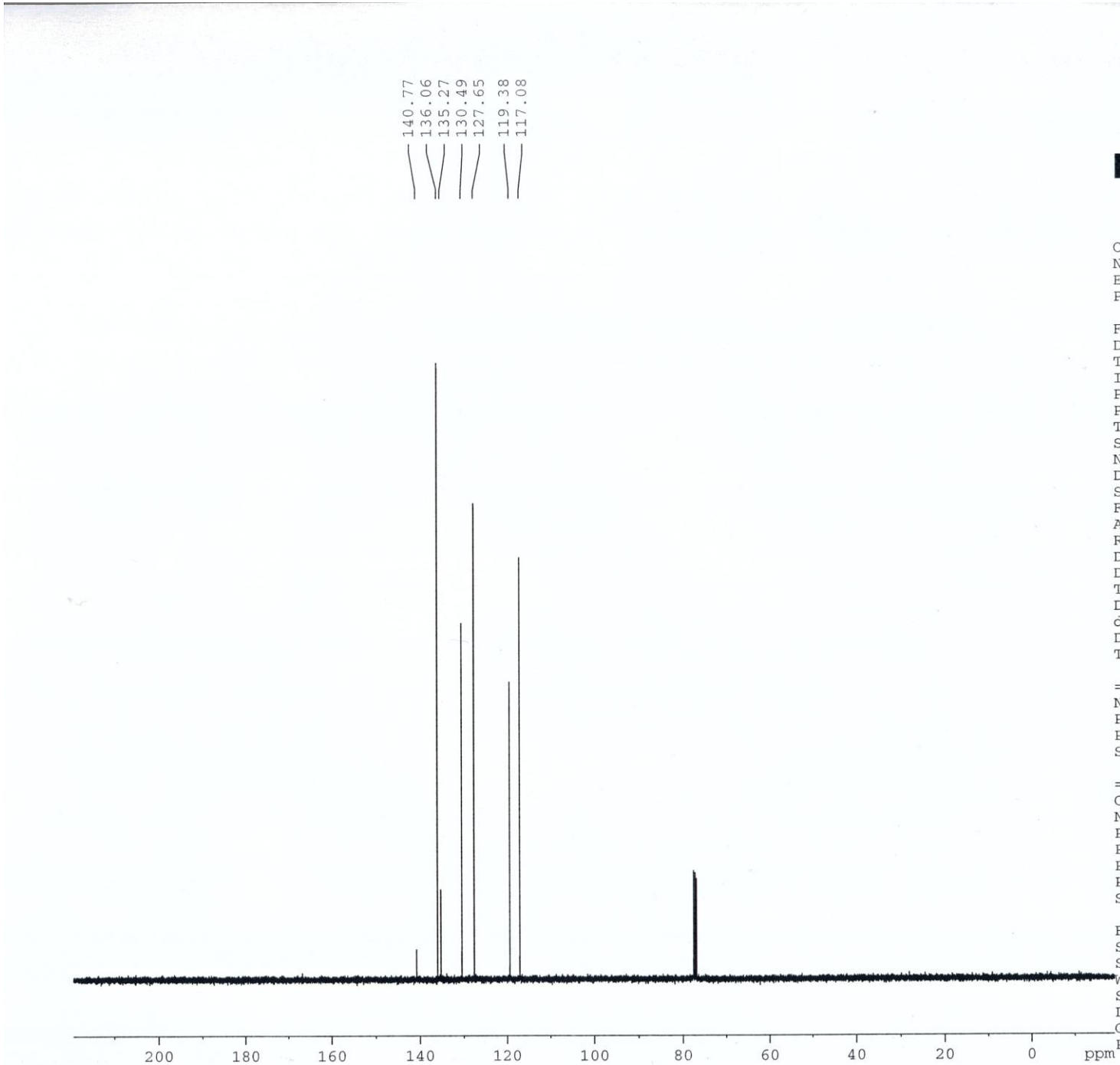
```
Current Data Parameters
NAME                  SU1-99-7C
EXPNO                         1
PROCNO                        1

F2 - Acquisition Parameters
Date_                  20100829
Time                      14.35
INSTRUM                   spect
PROBHD    5 mm QNP 1H/13
PULPROG                 zgpg30
TD                        65536
SOLVENT                   CDCl3
NS                          128
DS                            4
SWH                 23980.814 Hz
FIDRES               0.365918 Hz
AQ                   1.3664756 sec
RG                         4096
DW                       20.850 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                        9.38 usec
PL1                       0.00 dB
SFO1               100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG2                waltz16
NUC2                        1H
PCPD2                    90.00 usec
PL2                       0.00 dB
PL12                     16.10 dB
PL13                     19.00 dB
SFO2               400.1316005 MHz

F2 - Processing parameters
SI                        32768
SF                 100.6127544 MHz
WDW                          no
SSB                           0
LB                        0.00 Hz
GB                            0
PC                         1.40
```

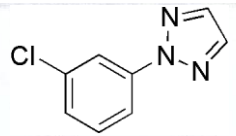







```
Current Data Parameters
NAME                  SU1-30-38
EXPNO                         1
PROCNO                        1

F2 - Acquisition Parameters
Date_                  20110107
Time                      10.25
INSTRUM                   spect
PROBHD    5 mm QNP 1H/13
PULPROG                   zg30
TD                       65536
SOLVENT                  CDCl3
NS                           8
DS                           2
SWH                 8278.146 Hz
FIDRES              0.126314 Hz
AQ                  3.9584243 sec
RG                         114
DW                    60.400 usec
DE                     6.00 usec
TE                     296.2 K
D1                 1.00000000 sec
TD0                          1

======== CHANNEL f1 ========
NUC1                        1H
P1                     14.00 usec
PL1                     0.00 dB
SFO1             400.1324710 MHz

F2 - Processing parameters
SI                       65536
SF               400.1300096 MHz
WDW                         no
SSB                          0
LB                      0.00 Hz
GB                           0
PC                        1.00
```





BRUKER

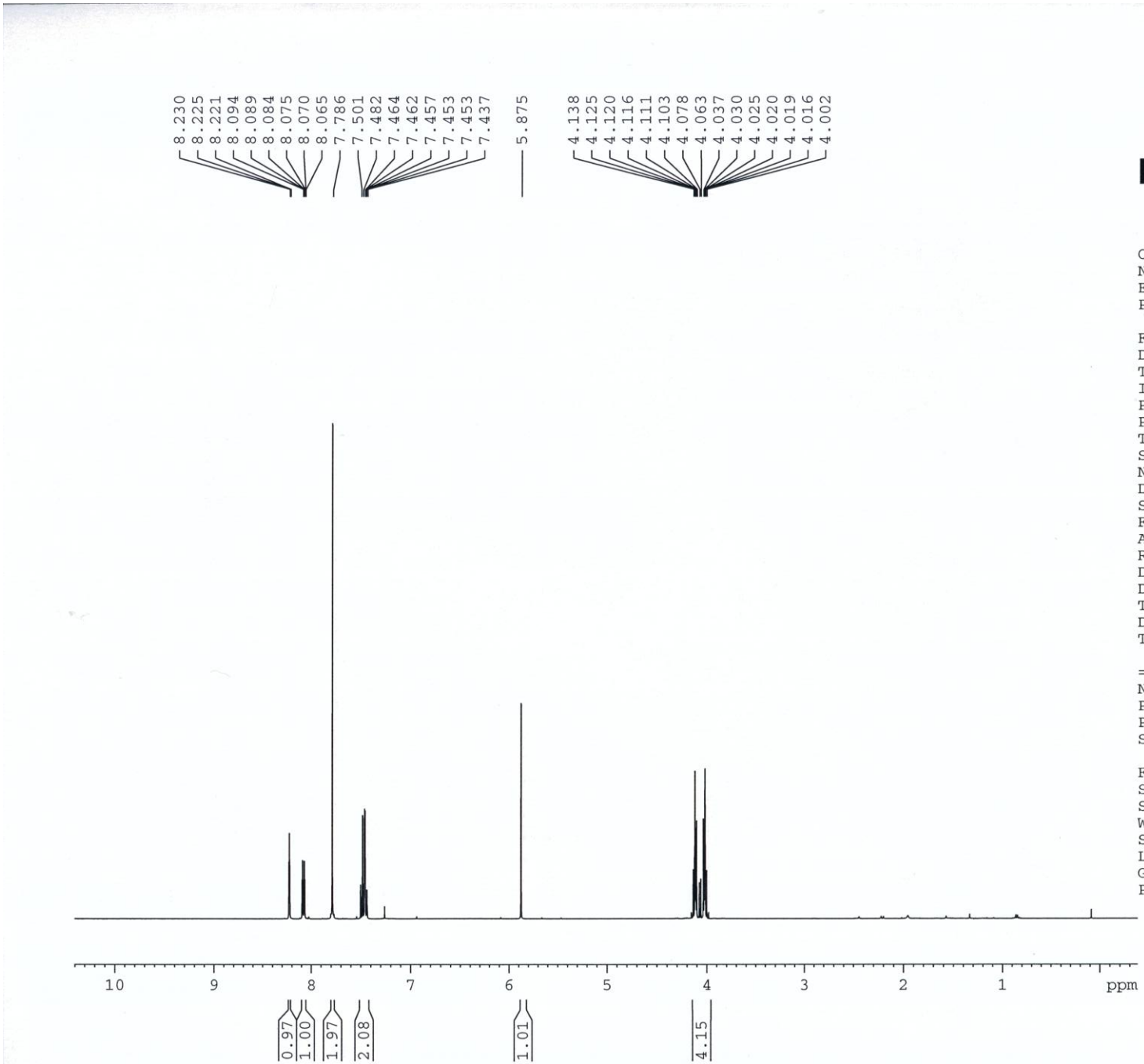
Current Data Parameters
NAME SU1-30-38C
EXPNO 1
PROCNO 1

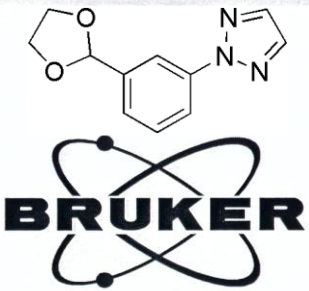
F2 - Acquisition Parameters
Date_ 20110107
Time 10.34
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 128
DS 4
SWH 23980.814 Hz
FIDRES 0.365918 Hz
AQ 1.3664756 sec
RG 1625.5
DW 20.850 usec
DE 6.00 usec
TE 296.2 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1

======== CHANNEL f1 ========
NUC1 13C
P1 9.38 usec
PL1 0.00 dB
SFO1 100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 0.00 dB
PL12 16.10 dB
PL13 19.00 dB
SFO2 400.1316005 MHz

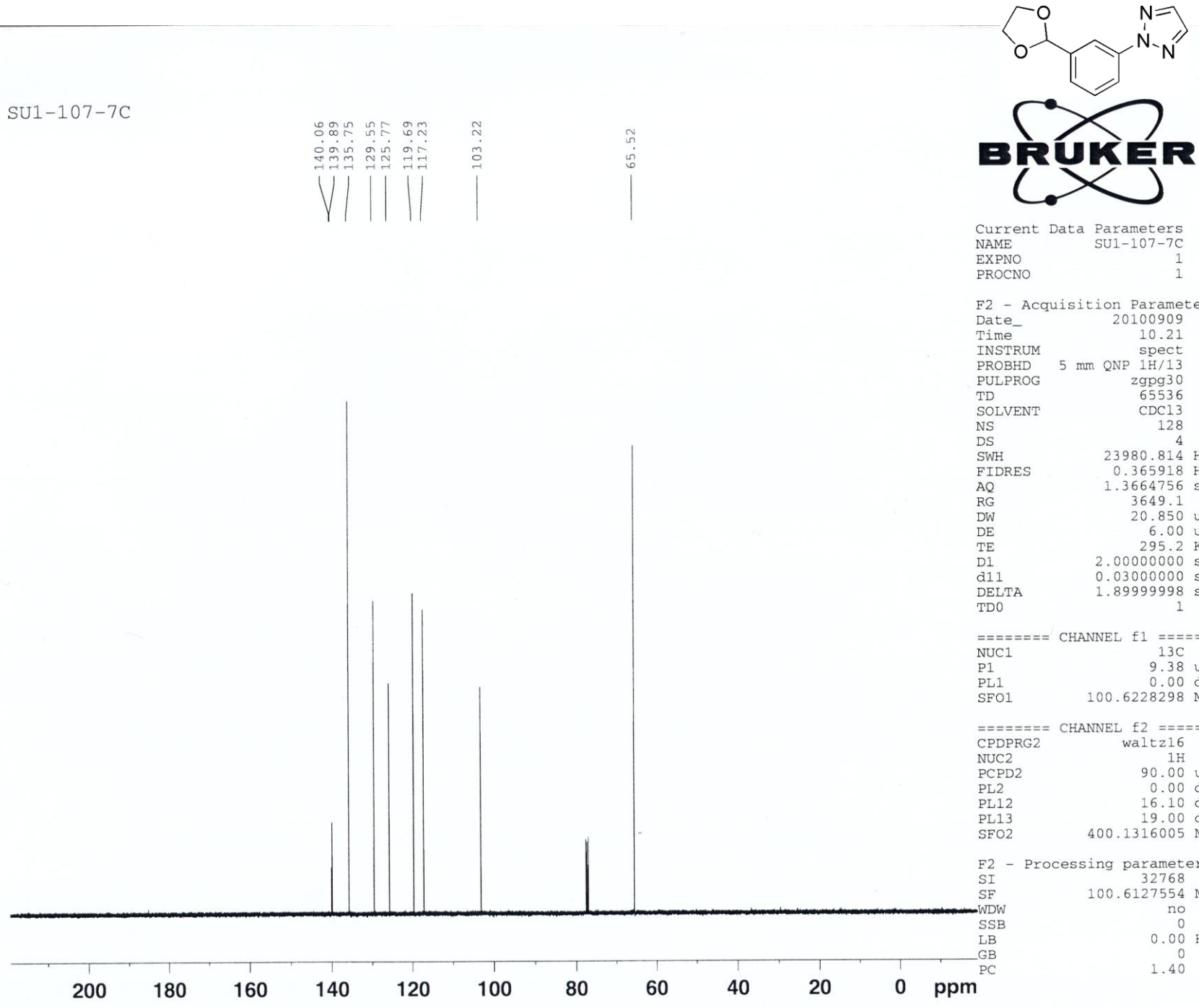
F2 - Processing parameters
SI 32768
SF 100.6127541 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.40





BRUKER

```
Current Data Parameters
NAME                  SU1-107-7
EXPNO                         1
PROCNO                        1

F2 - Acquisition Parameters
Date_                  20100909
Time                      10.12
INSTRUM                   spect
PROBHD    5 mm QNP 1H/13
PULPROG                   zg30
TD                       65536
SOLVENT                  CDCl3
NS                            8
DS                            2
SWH                    8278.146 Hz
FIDRES                 0.126314 Hz
AQ                     3.9584243 sec
RG                           57
DW                        60.400 usec
DE                         6.00 usec
TE                        295.2 K
D1                     1.00000000 sec
TD0                           1

======== CHANNEL f1 ========
NUC1                         1H
P1                        14.00 usec
PL1                        0.00 dB
SFO1                400.1324710 MHz

F2 - Processing parameters
SI                       65536
SF                  400.1300094 MHz
WDW                         no
SSB                          0
LB                        0.00 Hz
GB                           0
PC                        1.00
```



BRUKER

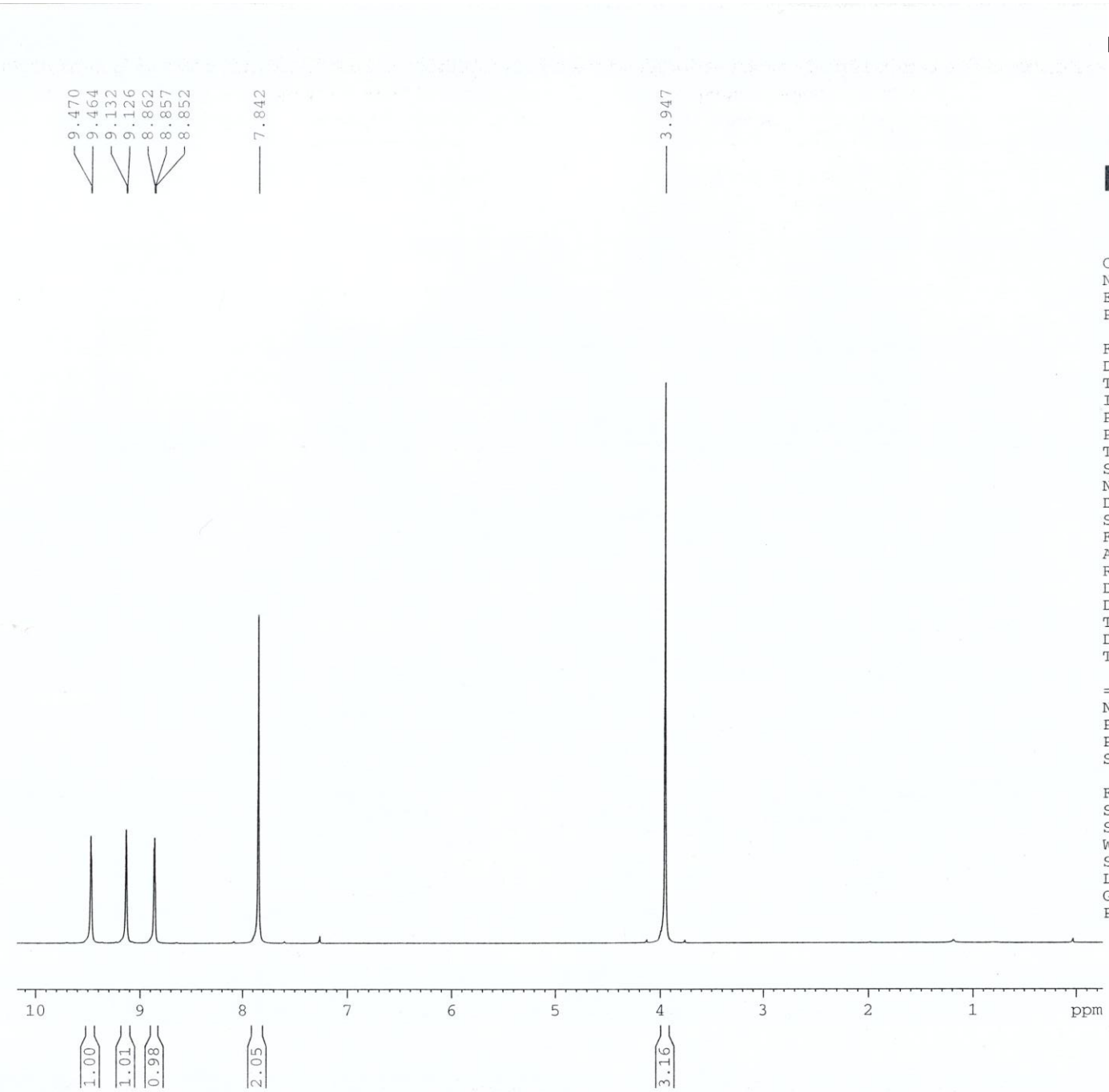
Current Data Parameters
NAME SU1-107-7C
EXPNO 1
PROCNO 1

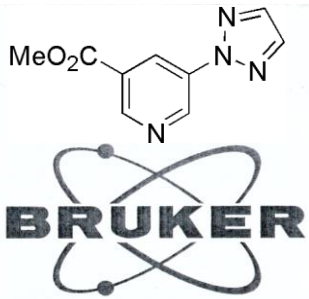
F2 - Acquisition Parameters
Date_ 20100909
Time 10.21
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 128
DS 4
SWH 23980.814 Hz
FIDRES 0.365918 Hz
AQ 1.3664756 sec
RG 3649.1
DW 20.850 usec
DE 6.00 usec
TE 295.2 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1

======== CHANNEL f1 ========
NUC1 13C
P1 9.38 usec
PL1 0.00 dB
SFO1 100.6228298 MHz

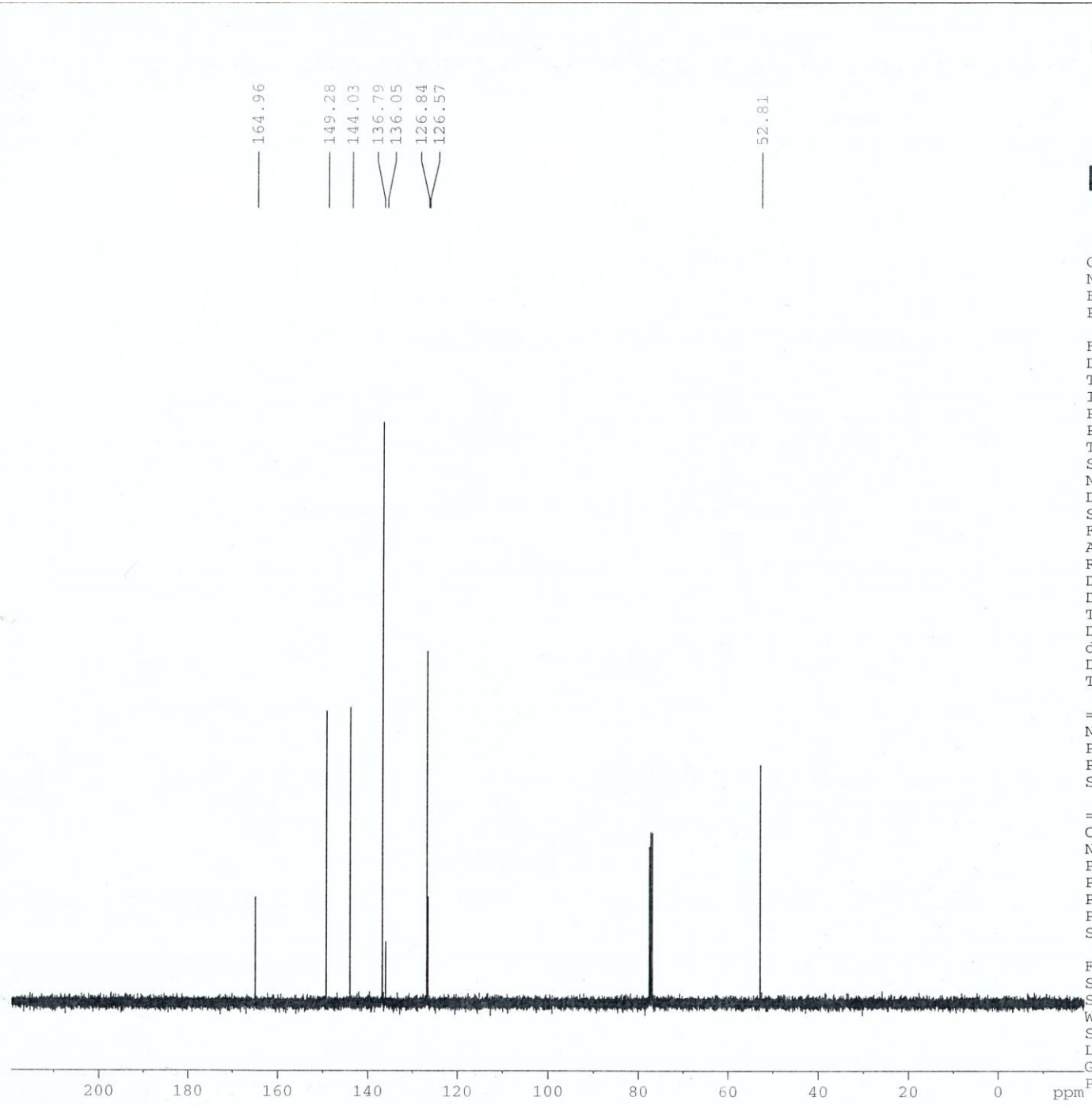
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 0.00 dB
PL12 16.10 dB
PL13 19.00 dB
SFO2 400.1316005 MHz

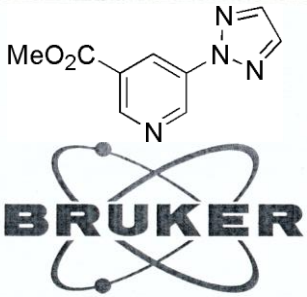
F2 - Processing parameters
SI 32768
SF 100.6127554 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.40






```
Current Data Parameters
NAME                  SU1-111-1
EXPNO                         1
PROCNO                        1

F2 - Acquisition Parameters
Date_                  20110302
Time                       8.52
INSTRUM                   spect
PROBHD    5 mm QNP 1H/13
PULPROG                    zg30
TD                        65536
SOLVENT                   CDCl3
NS                            8
DS                            2
SWH                    8278.146 Hz
FIDRES                 0.126314 Hz
AQ                     3.9584243 sec
RG                         161.3
DW                        60.400 usec
DE                         6.00 usec
TE                        295.2 K
D1                    1.00000000 sec
TD0                           1

======== CHANNEL f1 ========
NUC1                         1H
P1                        14.00 usec
PL1                        0.00 dB
SFO1                400.1324710 MHz

F2 - Processing parameters
SI                        65536
SF                  400.1300090 MHz
WDW                          no
SSB                           0
LB                         0.00 Hz
GB                            0
PC                         1.00
```





Current Data Parameters
NAME SU1-111-1C
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters

Date_	20110302
Time	9.00
INSTRUM	spect
PROBHD	5 mm QNP 1H/13
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	128
DS	4
SWH	23980.814 Hz
FIDRES	0.365918 Hz
AQ	1.3664756 sec
RG	1625.5
DW	20.850 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 ========

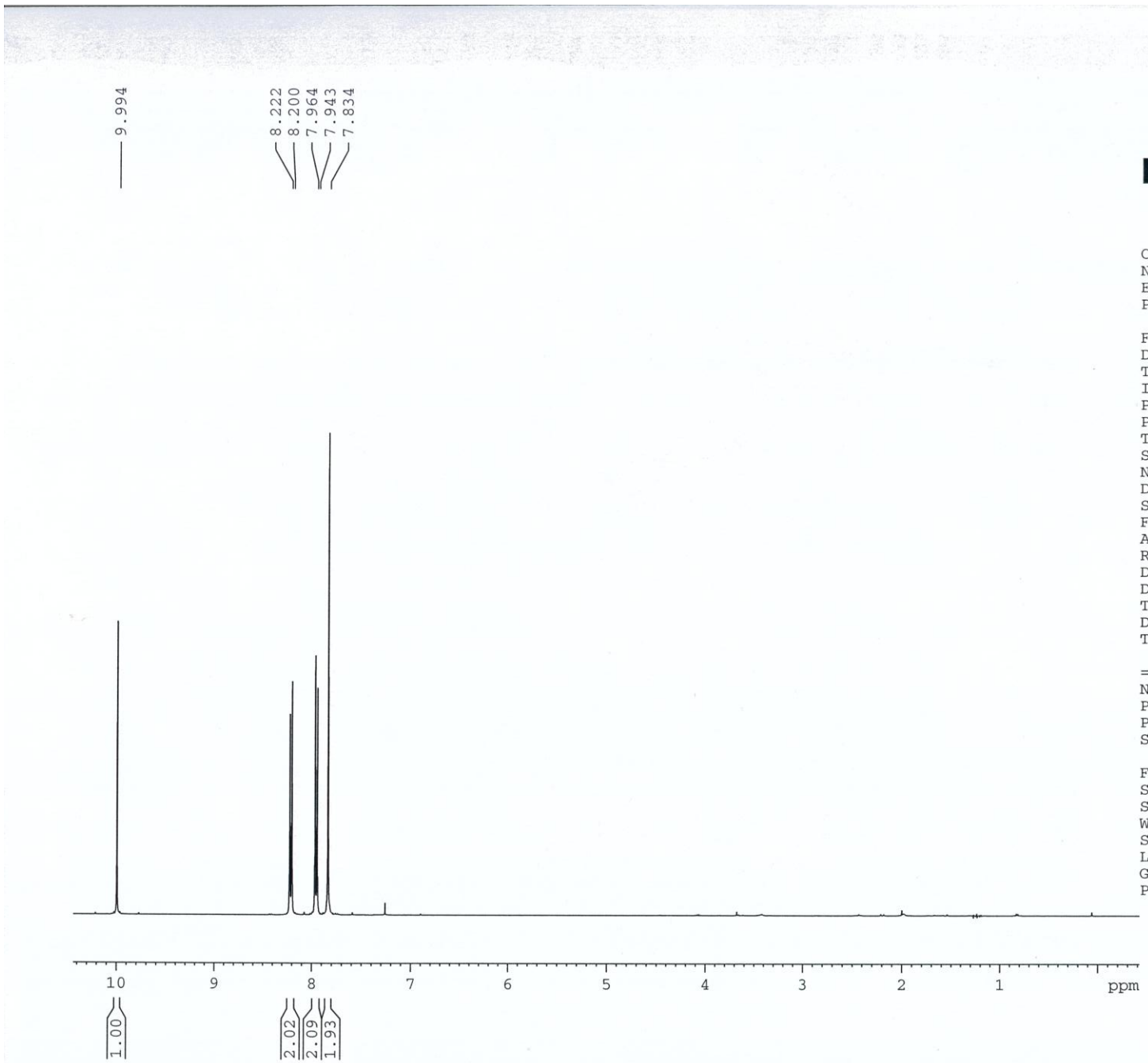
NUC1	13C
P1	9.38 usec
PL1	0.00 dB
SFO1	100.6228298 MHz

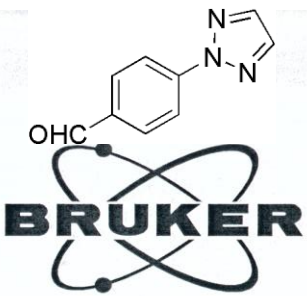
======== CHANNEL f2 ========

CPDPRG2	waltz16
NUC2	1H
PCPD2	90.00 usec
PL2	0.00 dB
PL12	16.10 dB
PL13	19.00 dB
SFO2	400.1316005 MHz

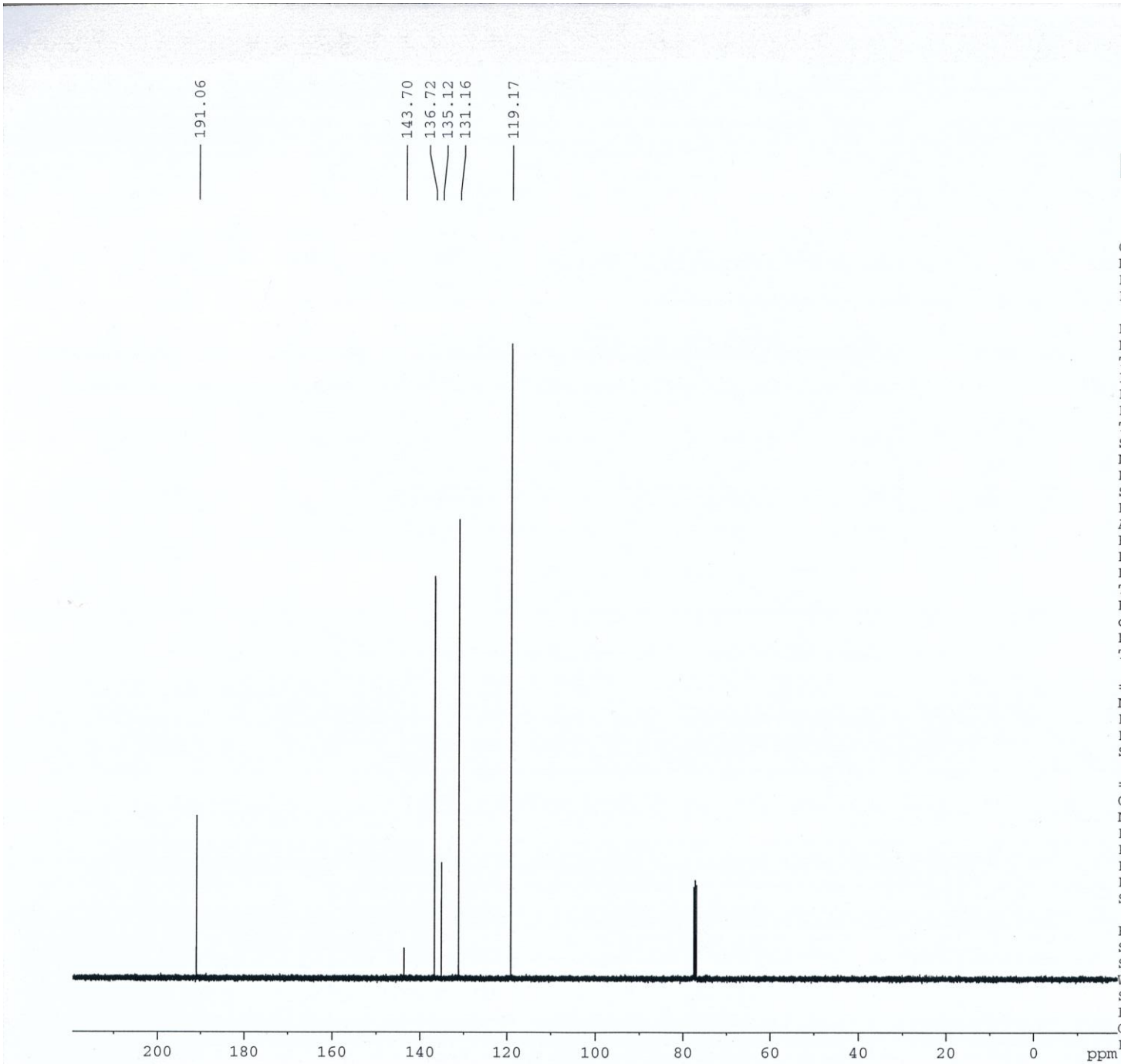
F2 - Processing parameters

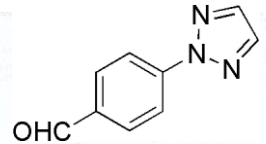
SI	32768
SF	100.6127560 MHz
WDW	no
SSB	0
LB	0.00 Hz
GB	0
PC	1.40





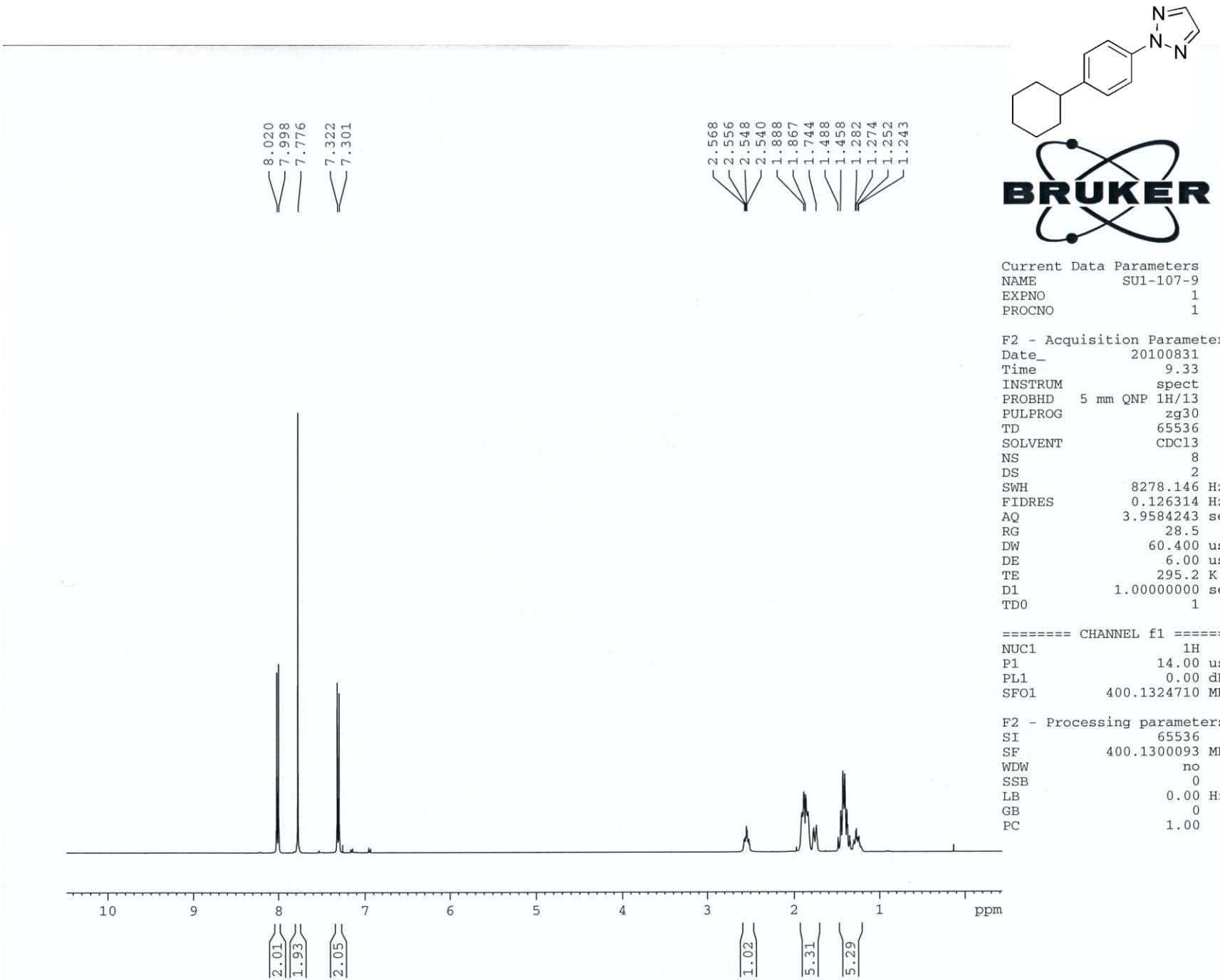

```
Current Data Parameters
NAME                  SU1-149
EXPNO                       2
PROCNO                      2

F2 - Acquisition Parameters
Date_               20101005
Time                    9.00
INSTRUM                spect
PROBHD    5 mm BBO BB-1H
PULPROG                 zg30
TD                     65536
SOLVENT                CDCl3
NS                        16
DS                         2
SWH                 8278.146 Hz
FIDRES              0.126314 Hz
AQ                  3.9584243 sec
RG                        57
DW                    60.400 usec
DE                     6.00 usec
TE                     296.2 K
D1                1.00000000 sec
TD0                        1

======== CHANNEL f1 ========
NUC1                      1H
P1                     15.07 usec
PL1                     0.00 dB
SFO1            400.1324710 MHz

F2 - Processing parameters
SI                     65536
SF              400.1300086 MHz
WDW                       no
SSB                        0
LB                      0.00 Hz
GB                         0
PC                      1.00
```





BRUKER

```
Current Data Parameters
NAME                  SU1-149C
EXPNO                        2
PROCNO                       2

F2 - Acquisition Parameters
Date_                 20101005
Time                      9.08
INSTRUM                  spect
PROBHD     5 mm BBO BB-1H
PULPROG                 zgpg30
TD                       65536
SOLVENT                  CDCl3
NS                         128
DS                           2
SWH                23980.814 Hz
FIDRES              0.365918 Hz
AQ                  1.3664756 sec
RG                        8192
DW                      20.850 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                        8.75 usec
PL1                      -3.00 dB
SFO1              100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG2                waltz16
NUC2                       1H
PCPD2                    90.00 usec
PL2                      -1.00 dB
PL12                     14.52 dB
PL13                     18.00 dB
SFO2              400.1316005 MHz

F2 - Processing parameters
SI                       65536
SF                100.6127576 MHz
WDW                         no
SSB                          0
LB                        0.00 Hz
GB                           0
PC                        1.40
```



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Current Data Parameters
NAME SU1-107-9
EXPNO 1
PROCNO 1

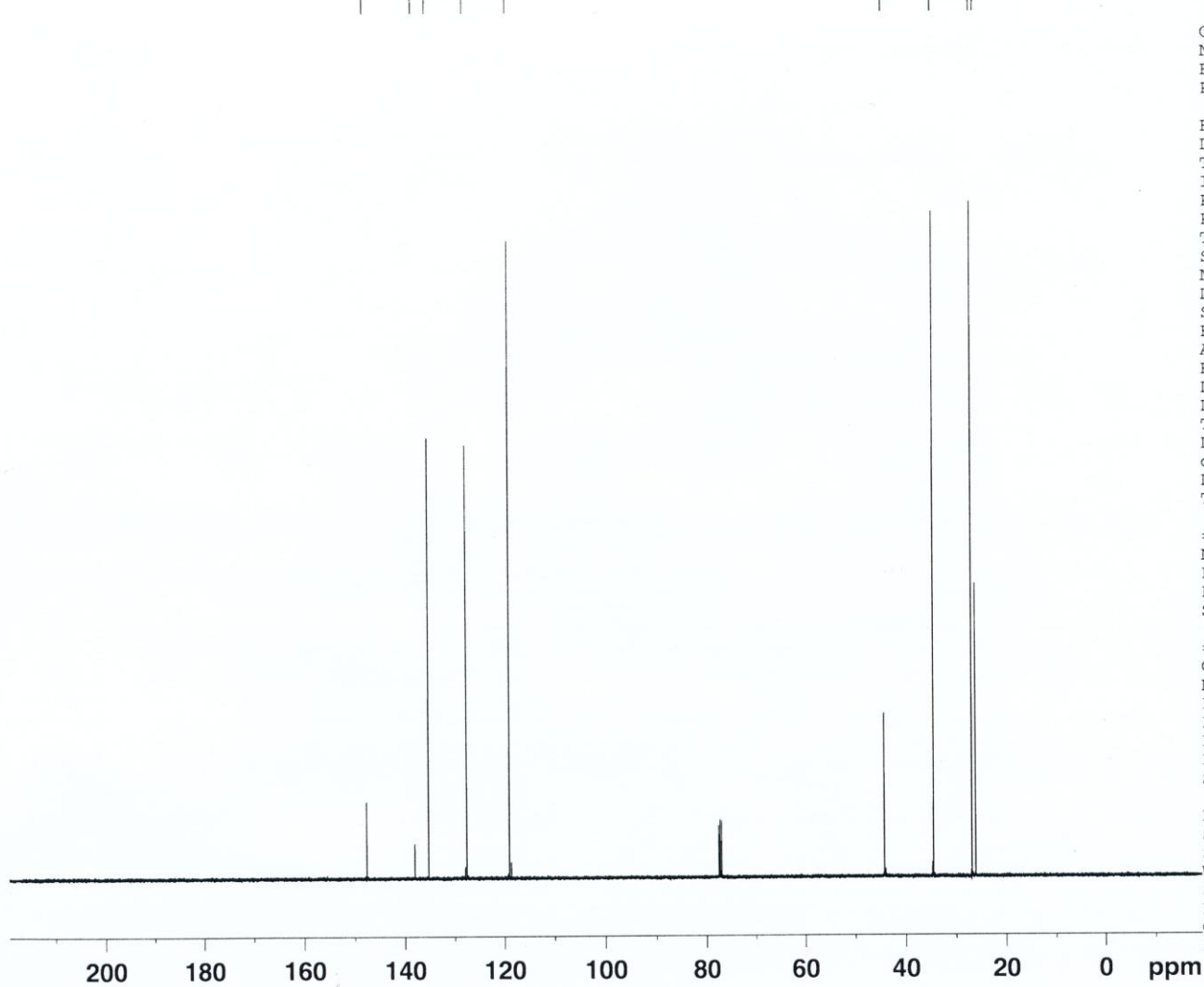
F2 - Acquisition Parameters
Date_ 20100831
Time 9.33
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 8
DS 2
SWH 8278.146 Hz
FIDRES 0.126314 Hz
AQ 3.9584243 sec
RG 28.5
DW 60.400 usec
DE 6.00 usec
TE 295.2 K
D1 1.00000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 1H
P1 14.00 usec
PL1 0.00 dB
SFO1 400.1324710 MHz

F2 - Processing parameters
SI 65536
SF 400.1300093 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00

SU1-107-9C

147.70
138.04
135.28
127.68
118.99
44.23
34.49
26.92
26.19



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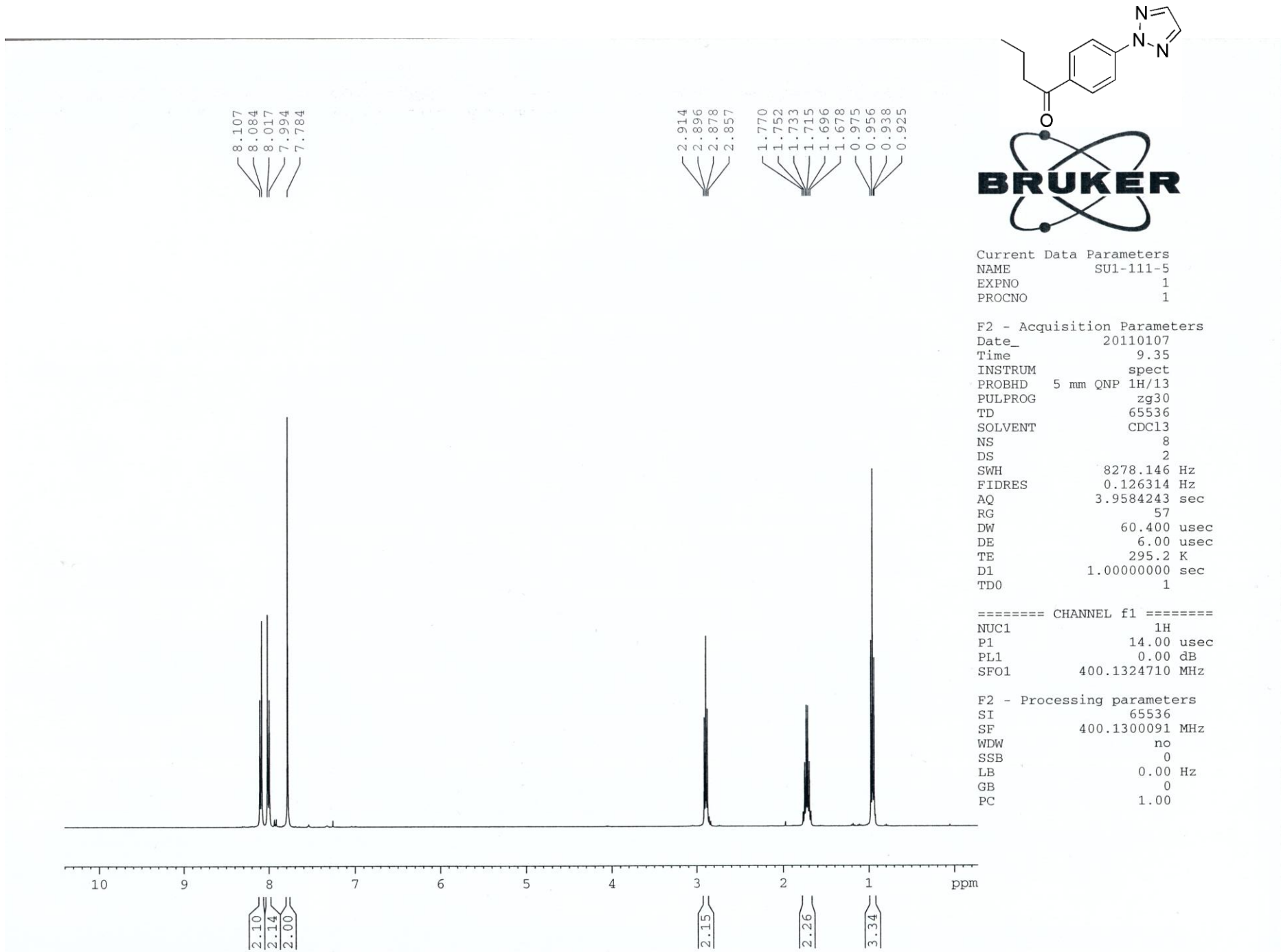
Current Data Parameters
NAME SU1-107-9C
EXPNO 1
PROCNO 1

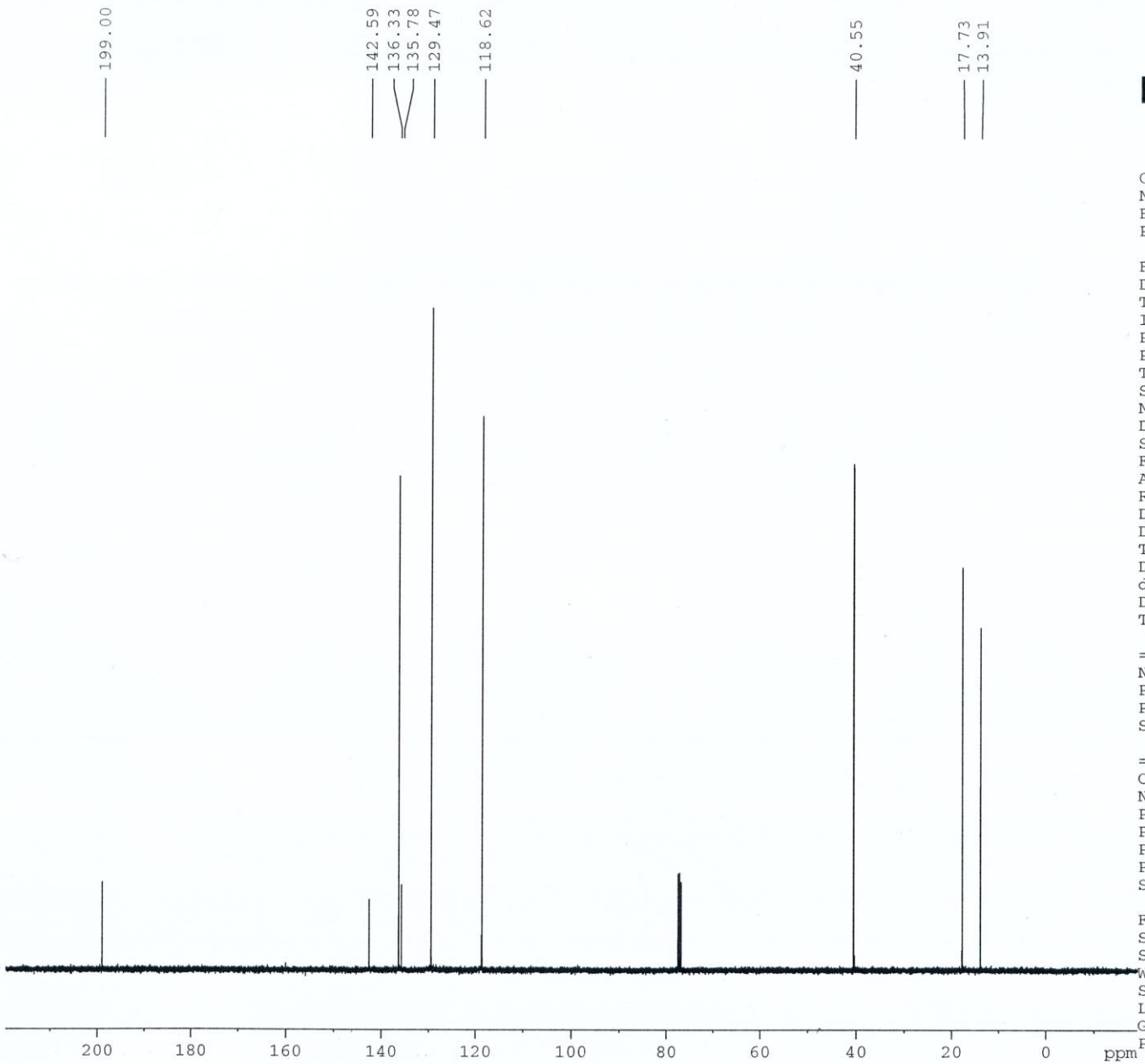
F2 - Acquisition Parameters
Date_ 20100831
Time 9.41
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 128
DS 4
SWH 23980.814 Hz
FIDRES 0.365918 Hz
AQ 1.3664756 sec
RG 5160.6
DW 20.850 usec
DE 6.00 usec
TE 296.2 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1

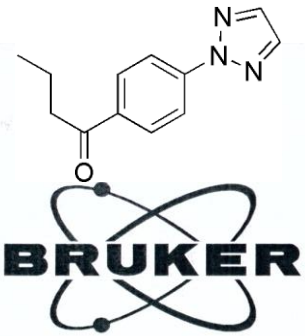
======== CHANNEL f1 ========
NUC1 13C
P1 9.38 usec
PL1 0.00 dB
SFO1 100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 0.00 dB
PL12 16.10 dB
PL13 19.00 dB
SFO2 400.1316005 MHz

F2 - Processing parameters
SI 32768
SF 100.6127617 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.40


8.107
8.084
8.017
7.994
7.784
2.914
2.896
2.878
2.857
1.770
1.752
1.733
1.715
1.696
1.678
0.975
0.956
0.938
0.925
10
9
8
7
6
5
4
3
2
1
ppm
2.10
2.14
2.00
2.15
2.26
3.34
N
N
N
O
BRUKER
Current Data Parameters
NAME SU1-111-5
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20110107
Time 9.35
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 8
DS 2
SWH 8278.146 Hz
FIDRES 0.126314 Hz
AQ 3.9584243 sec
RG 57
DW 60.400 usec
DE 6.00 usec
TE 295.2 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 14.00 usec
PL1 0.00 dB
SFO1 400.1324710 MHz
F2 - Processing parameters
SI 65536
SF 400.1300091 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00





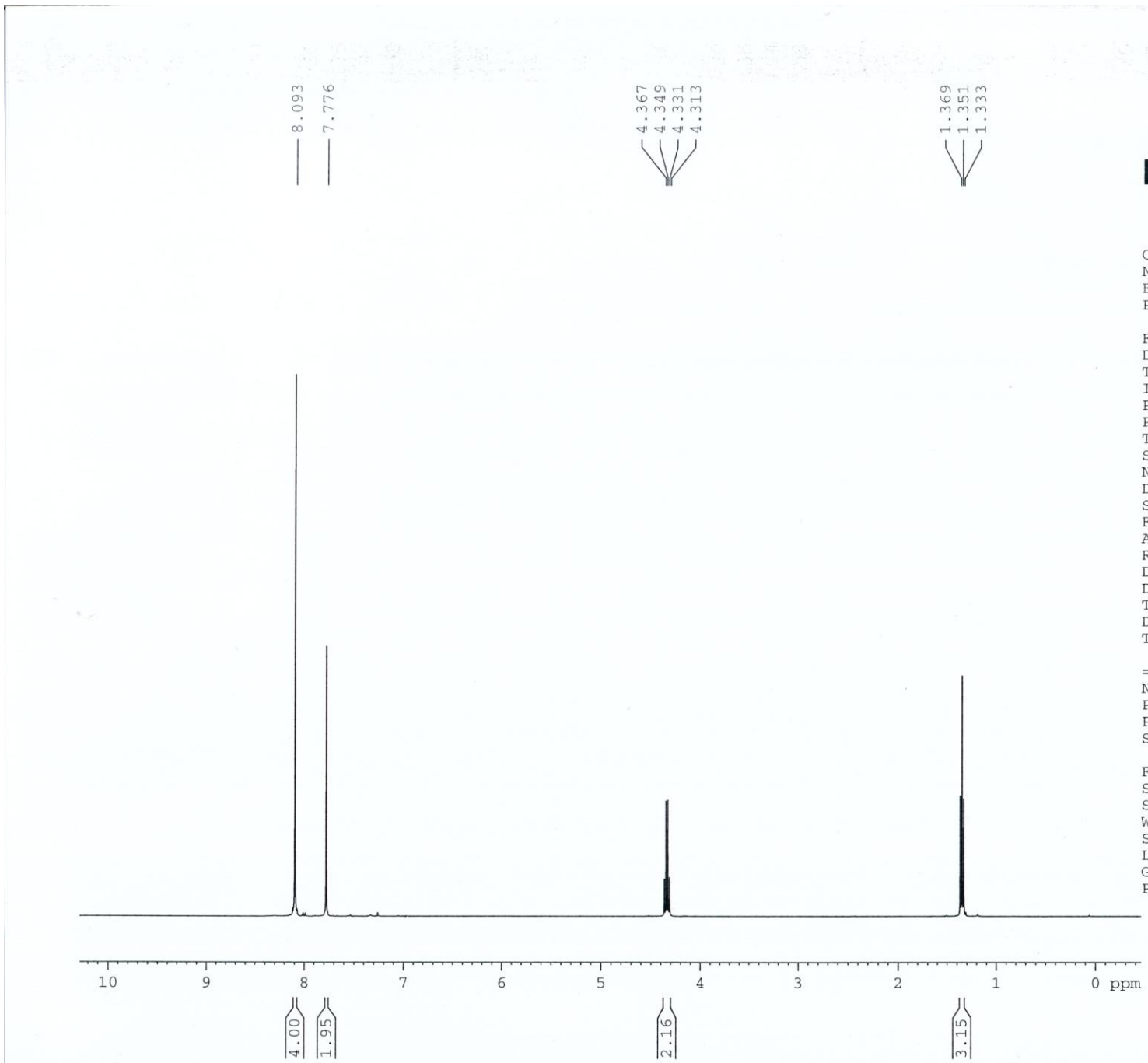
Current Data Parameters
NAME SU1-111-5C
EXPNO 1
PROCNO 1

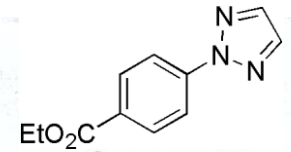
F2 - Acquisition Parameters
Date_ 20110107
Time 9.43
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 128
DS 4
SWH 23980.814 Hz
FIDRES 0.365918 Hz
AQ 1.3664756 sec
RG 1625.5
DW 20.850 usec
DE 6.00 usec
TE 296.2 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1

======== CHANNEL f1 ========
NUC1 13C
P1 9.38 usec
PL1 0.00 dB
SFO1 100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 0.00 dB
PL12 16.10 dB
PL13 19.00 dB
SFO2 400.1316005 MHz

F2 - Processing parameters
SI 32768
SF 100.6127618 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.40





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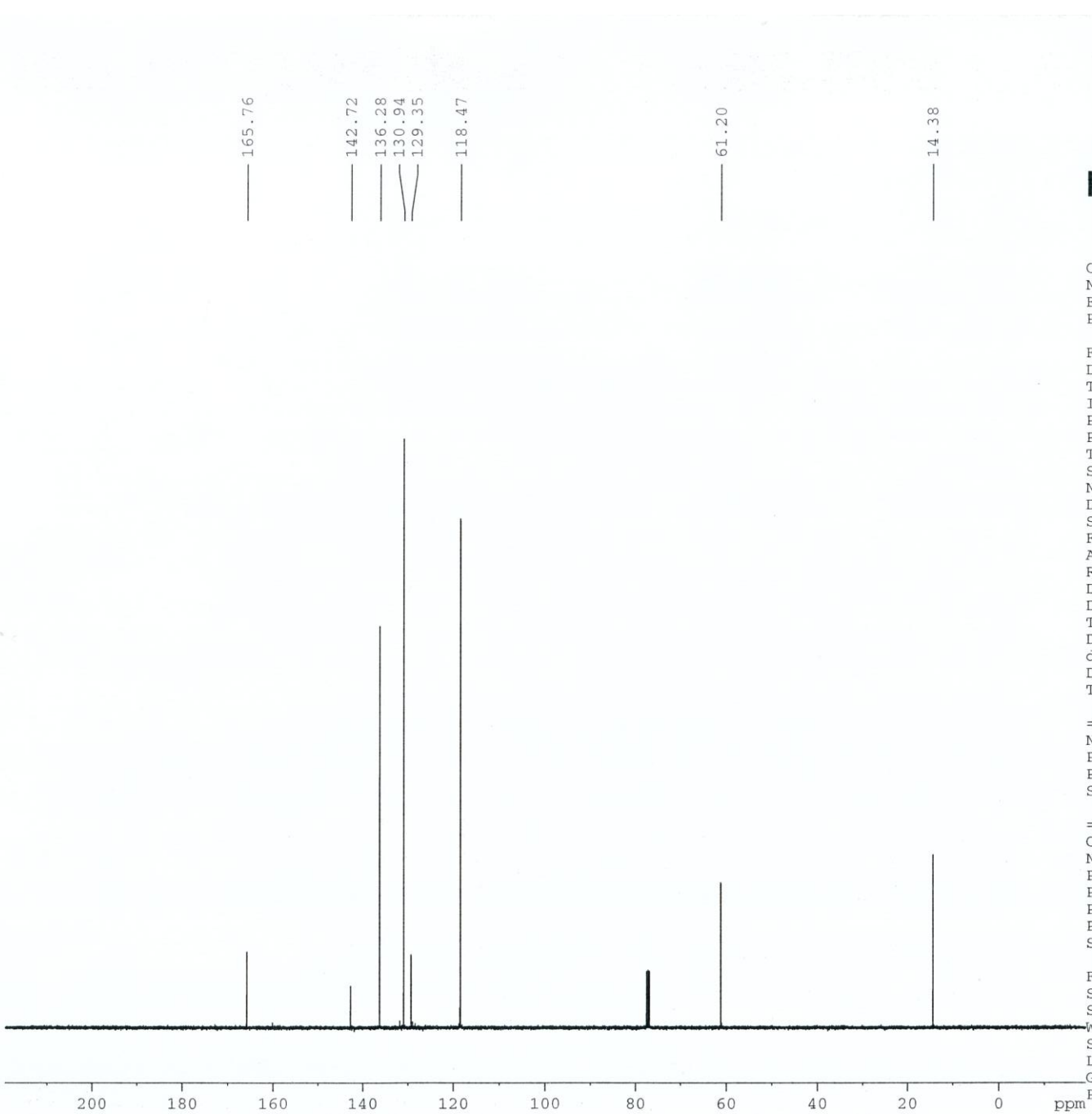
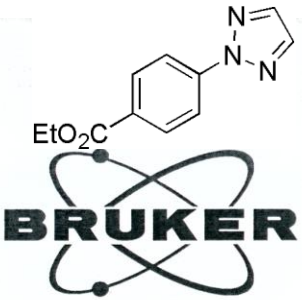
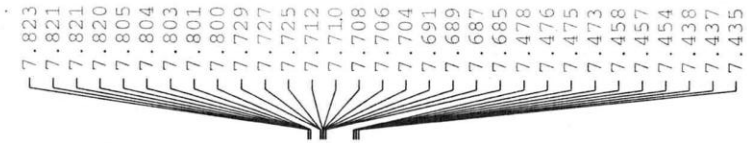
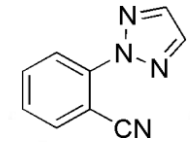
```
Current Data Parameters
NAME          SU1-198-12
EXPNO                  3
PROCNO                 3

F2 - Acquisition Parameters
Date_           20110113
Time               12.59
INSTRUM            spect
PROBHD   5 mm QNP 1H/13
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                     8
DS                     2
SWH             8278.146 Hz
FIDRES          0.126314 Hz
AQ              3.9584243 sec
RG                    57
DW                60.400 usec
DE                 6.00 usec
TE                295.2 K
D1             1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  1H
P1                14.00 usec
PL1                0.00 dB
SFO1         400.1324710 MHz

F2 - Processing parameters
SI                 65536
SF           400.1300093 MHz
WDW                   no
SSB                    0
LB                 0.00 Hz
GB                     0
PC                  1.00
```





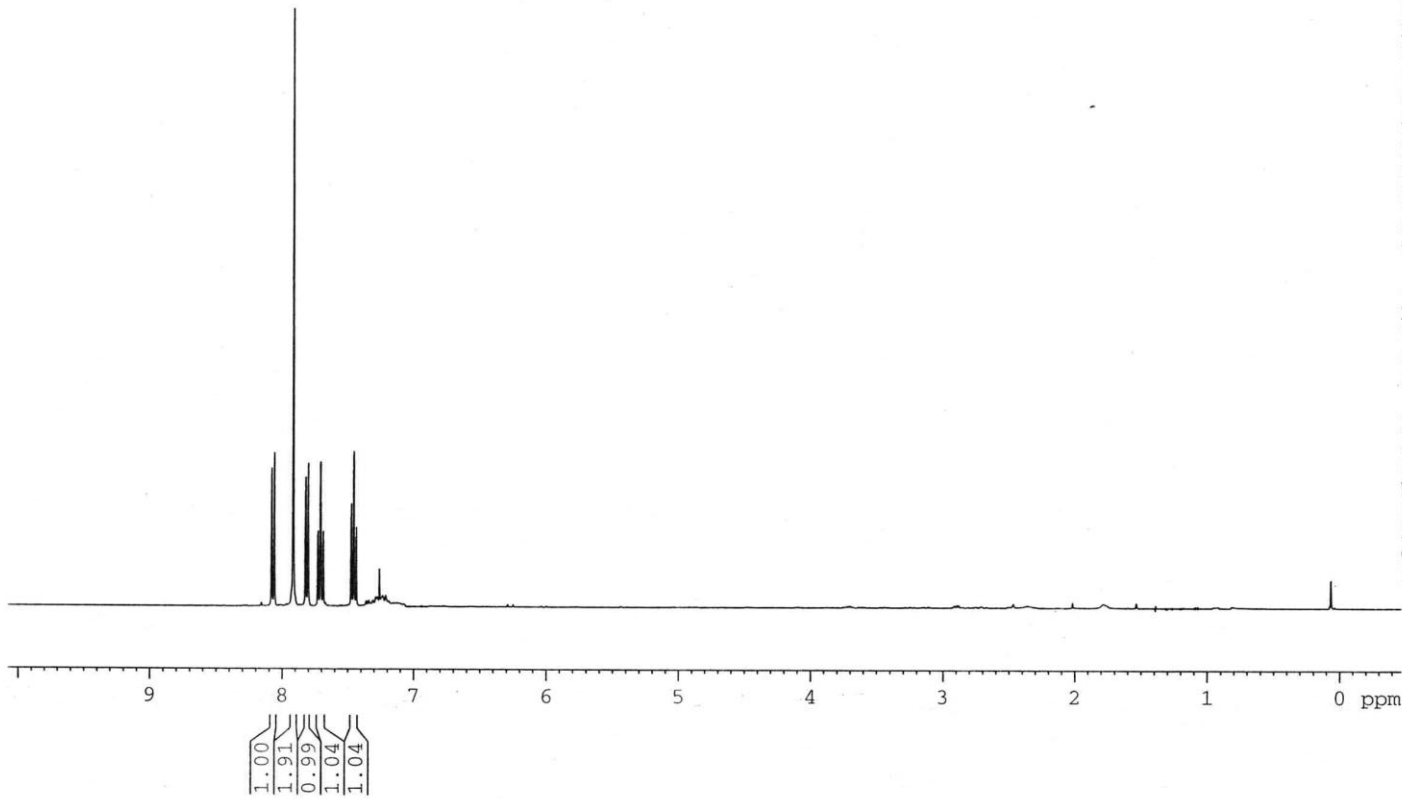

```
Current Data Parameters
NAME          SU1-198-12C
EXPNO                   3
PROCNO                  3

F2 - Acquisition Parameters
Date_            20110113
Time                13.09
INSTRUM             spect
PROBHD   5 mm QNP 1H/13
PULPROG           zgpg30
TD                 65536
SOLVENT            CDCl3
NS                   128
DS                     4
SWH           23980.814 Hz
FIDRES         0.365918 Hz
AQ             1.3664756 sec
RG                5792.6
DW                20.850 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                 9.38 usec
PL1                0.00 dB
SFO1        100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                  1H
PCPD2             90.00 usec
PL2                0.00 dB
PL12              16.10 dB
PL13              19.00 dB
SFO2        400.1316005 MHz

F2 - Processing parameters
SI                 32768
SF          100.6127597 MHz
WDW                   no
SSB                    0
LB                0.00 Hz
GB                     0
PC                 1.40
```

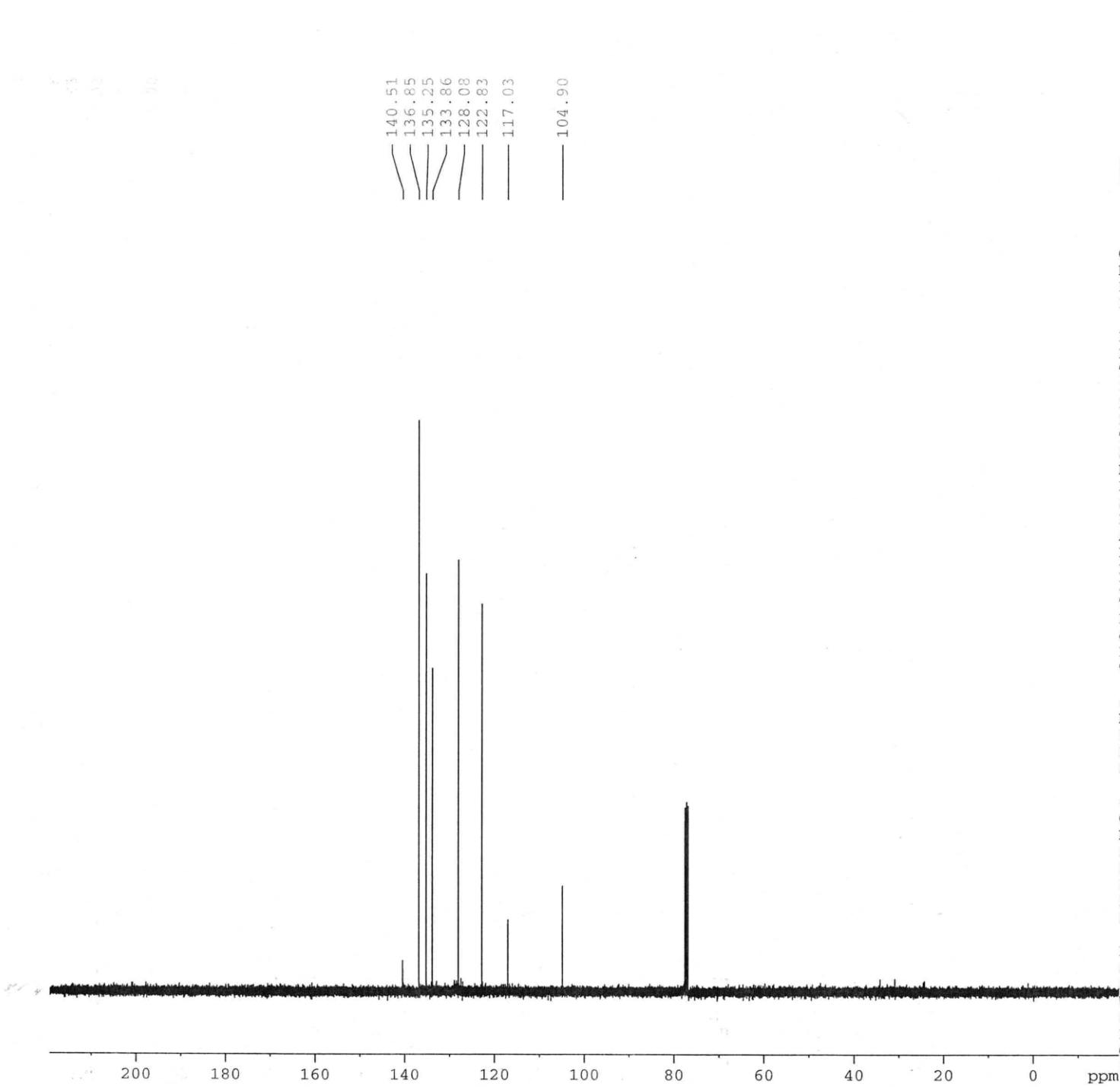


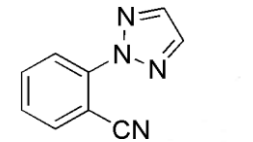


BRUKER

```
Current Data Parameters
NAME                  SU2-115
EXPNO                       1
PROCNO                      1

F2 - Acquisition Parameters
Date_                20110603
Time                     8.54
INSTRUM                 spect
PROBHD   5 mm BBO BB-1H
PULPROG                 zg30
TD                     65536
SOLVENT                CDCl3
NS                         16
DS                          2
SWH                 8278.146 Hz
FIDRES                 0.126314 Hz
AQ                  3.9584243 sec
RG                         57
DW                     60.400 usec
DE                      6.00 usec
TE                     297.2 K
D1                  1.00000000 sec
TD0                         1

======== CHANNEL f1 ========
NUC1                       1H
P1                     15.07 usec
PL1                     0.00 dB
SFO1           400.1324710 MHz

F2 - Processing parameters
SI                     65536
SF             400.1300080 MHz
WDW                       no
SSB                        0
LB                      0.00 Hz
GB                         0
PC                      1.00
```







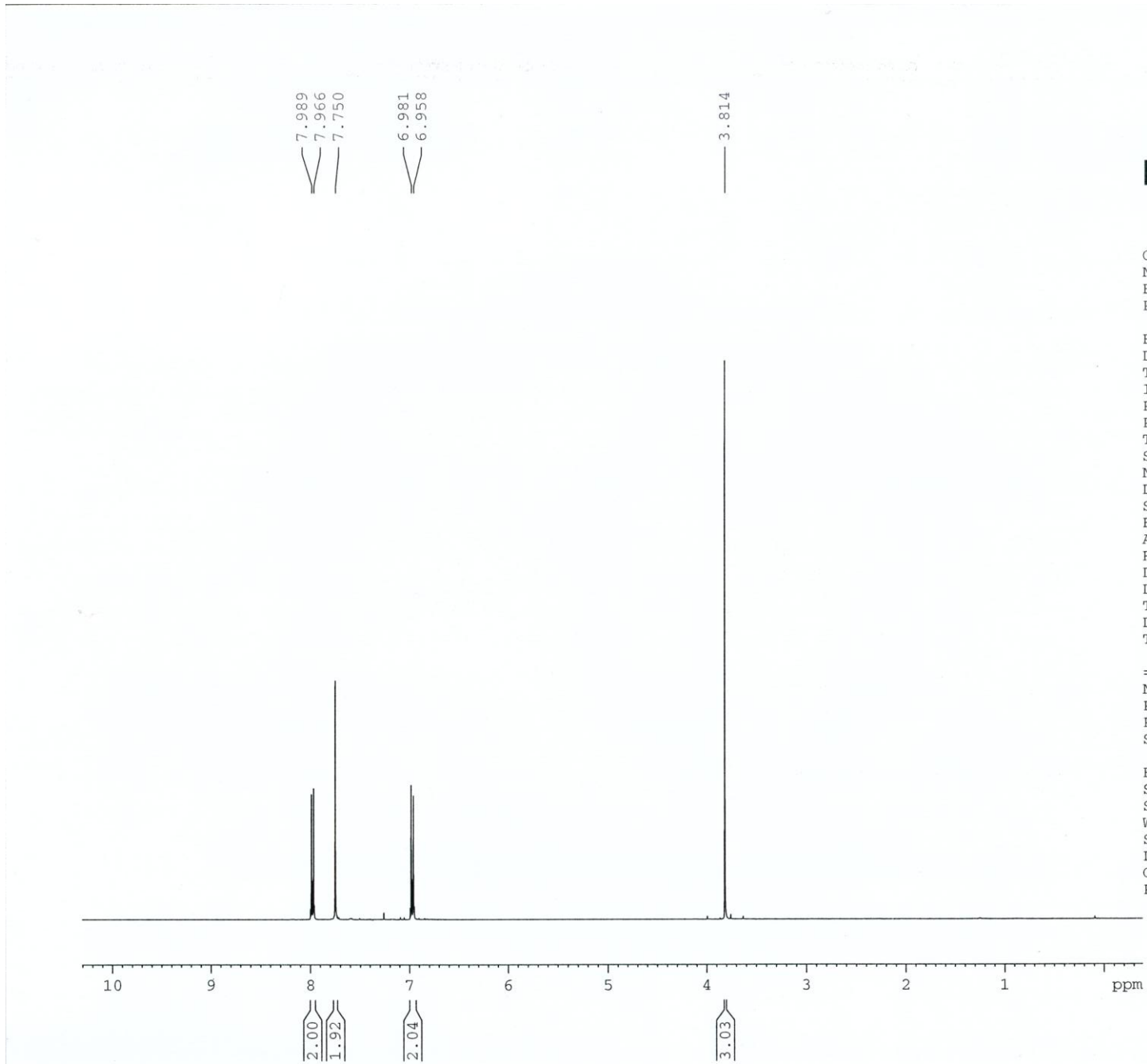
Current Data Parameters
NAME SU2-115C
EXPNO 1
PROCNO 1

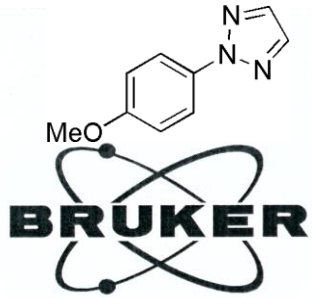
F2 - Acquisition Parameters
Date_ 20110603
Time 9.02
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 128
DS 2
SWH 23980.814 Hz
FIDRES 0.365918 Hz
AQ 1.3664756 sec
RG 16384
DW 20.850 usec
DE 6.00 usec
TE 297.2 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1

======== CHANNEL f1 ========
NUC1 13C
P1 8.75 usec
PL1 -3.00 dB
SFO1 100.6228298 MHz

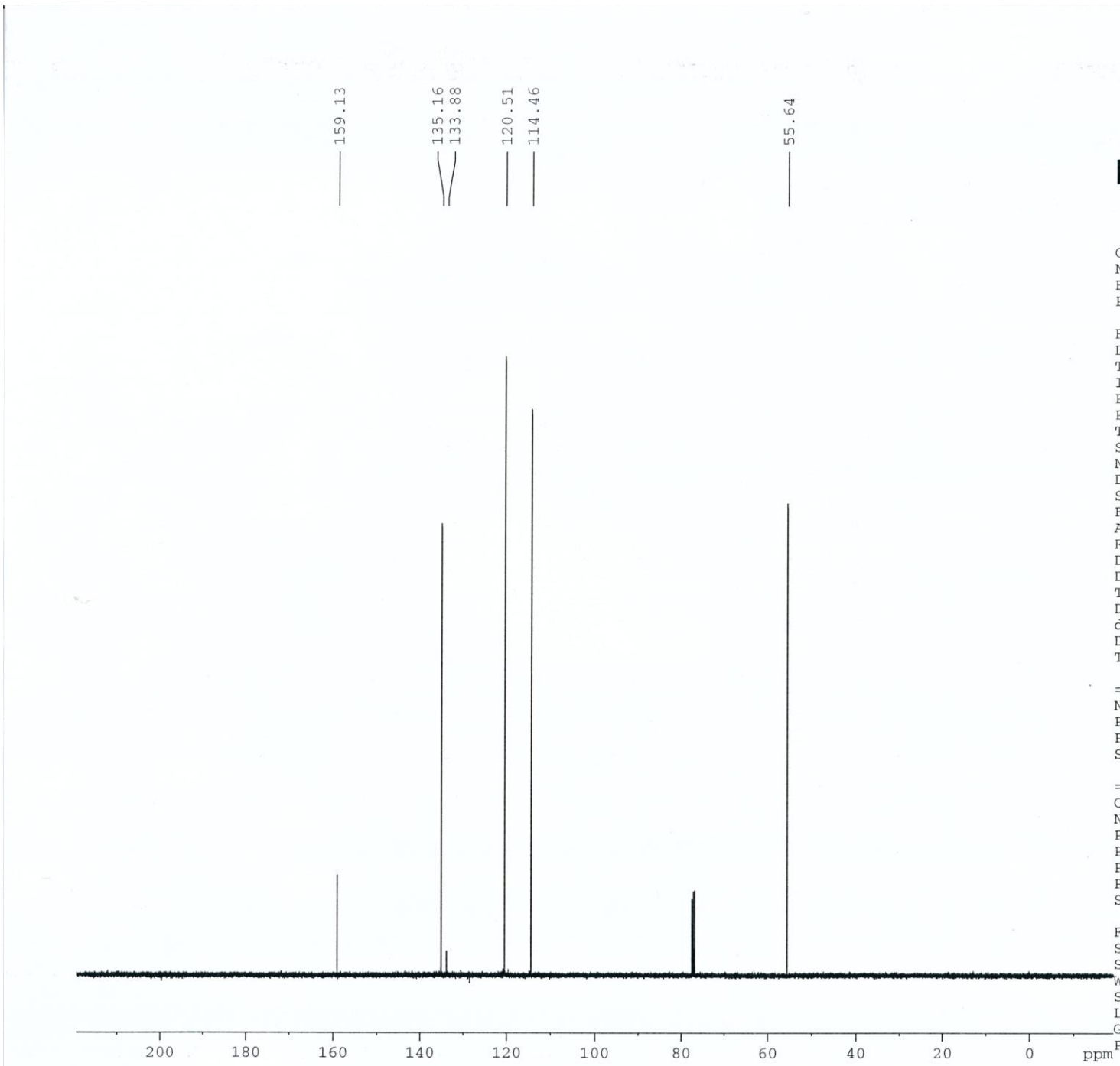
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -1.00 dB
PL12 14.52 dB
PL13 18.00 dB
SFO2 400.1316005 MHz

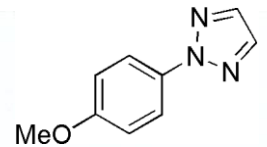
F2 - Processing parameters
SI 65536
SF 100.6127592 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.40






```
Current Data Parameters
NAME                  SU1-107-3
EXPNO                         1
PROCNO                        1

F2 - Acquisition Parameters
Date_                  20110107
Time                      10.13
INSTRUM                   spect
PROBHD    5 mm QNP 1H/13
PULPROG                    zg30
TD                        65536
SOLVENT                   CDCl3
NS                            8
DS                            2
SWH                    8278.146 Hz
FIDRES                 0.126314 Hz
AQ                     3.9584243 sec
RG                           57
DW                        60.400 usec
DE                         6.00 usec
TE                        296.2 K
D1                     1.00000000 sec
TD0                           1

======== CHANNEL f1 ========
NUC1                         1H
P1                        14.00 usec
PL1                        0.00 dB
SFO1                400.1324710 MHz

F2 - Processing parameters
SI                        65536
SF                 400.1300093 MHz
WDW                          no
SSB                           0
LB                         0.00 Hz
GB                            0
PC                         1.00
```





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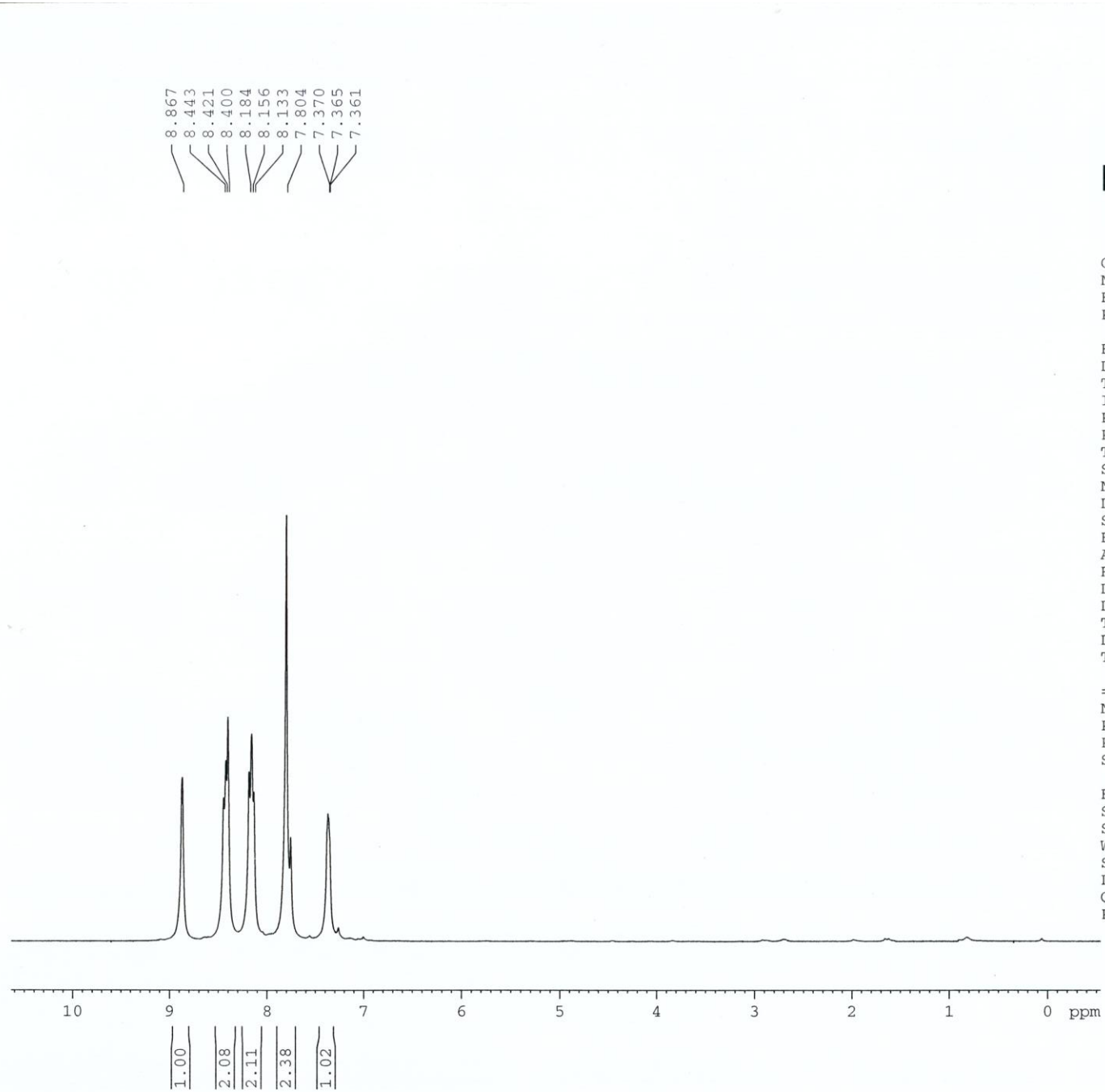
Current Data Parameters
NAME SU1-107-3C
EXPNO 1
PROCNO 1

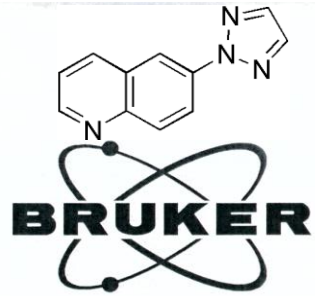
F2 - Acquisition Parameters
Date_ 20110107
Time 10.21
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 128
DS 4
SWH 23980.814 Hz
FIDRES 0.365918 Hz
AQ 1.3664756 sec
RG 5160.6
DW 20.850 usec
DE 6.00 usec
TE 296.2 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1

======== CHANNEL f1 ========
NUC1 13C
P1 9.38 usec
PL1 0.00 dB
SFO1 100.6228298 MHz

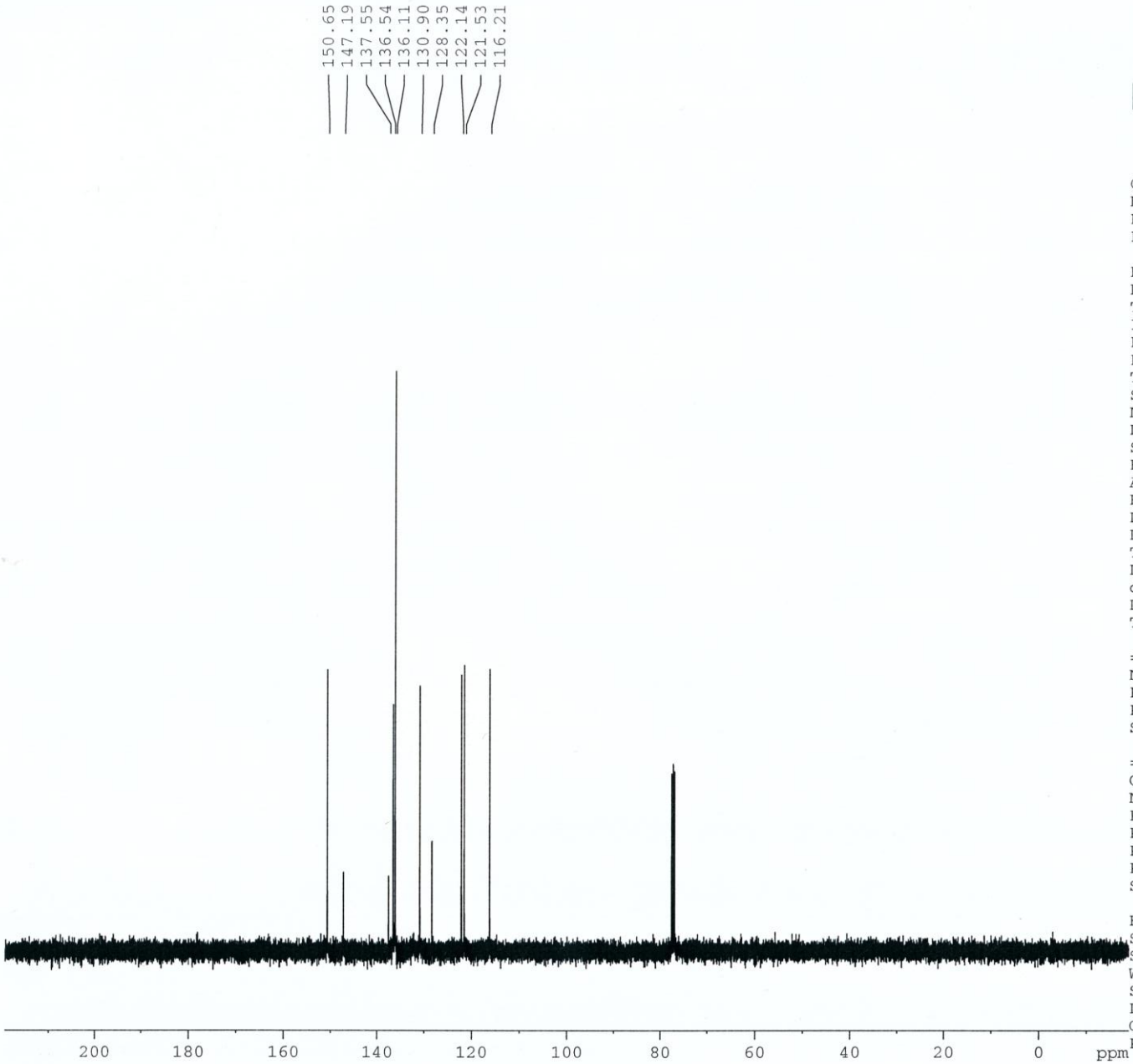
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 0.00 dB
PL12 16.10 dB
PL13 19.00 dB
SFO2 400.1316005 MHz

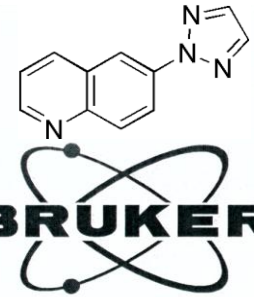
F2 - Processing parameters
SI 32768
SF 100.6127568 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.40






```
Current Data Parameters
NAME                  SU1-38-37
EXPNO                         2
PROCNO                        2

F2 - Acquisition Parameters
Date_                  20110107
Time                      10.00
INSTRUM                   spect
PROBHD    5 mm QNP 1H/13
PULPROG                    zg30
TD                        65536
SOLVENT                   CDCl3
NS                           16
DS                            2
SWH                    8278.146 Hz
FIDRES                 0.126314 Hz
AQ                     3.9584243 sec
RG                         90.5
DW                       60.400 usec
DE                        6.00 usec
TE                       295.2 K
D1                  1.00000000 sec
TD0                           1

======== CHANNEL f1 ========
NUC1                         1H
P1                       14.00 usec
PL1                       0.00 dB
SFO1             400.1324710 MHz

F2 - Processing parameters
SI                        65536
SF               400.1300102 MHz
WDW                          no
SSB                           0
LB                        0.00 Hz
GB                            0
PC                         1.00
```





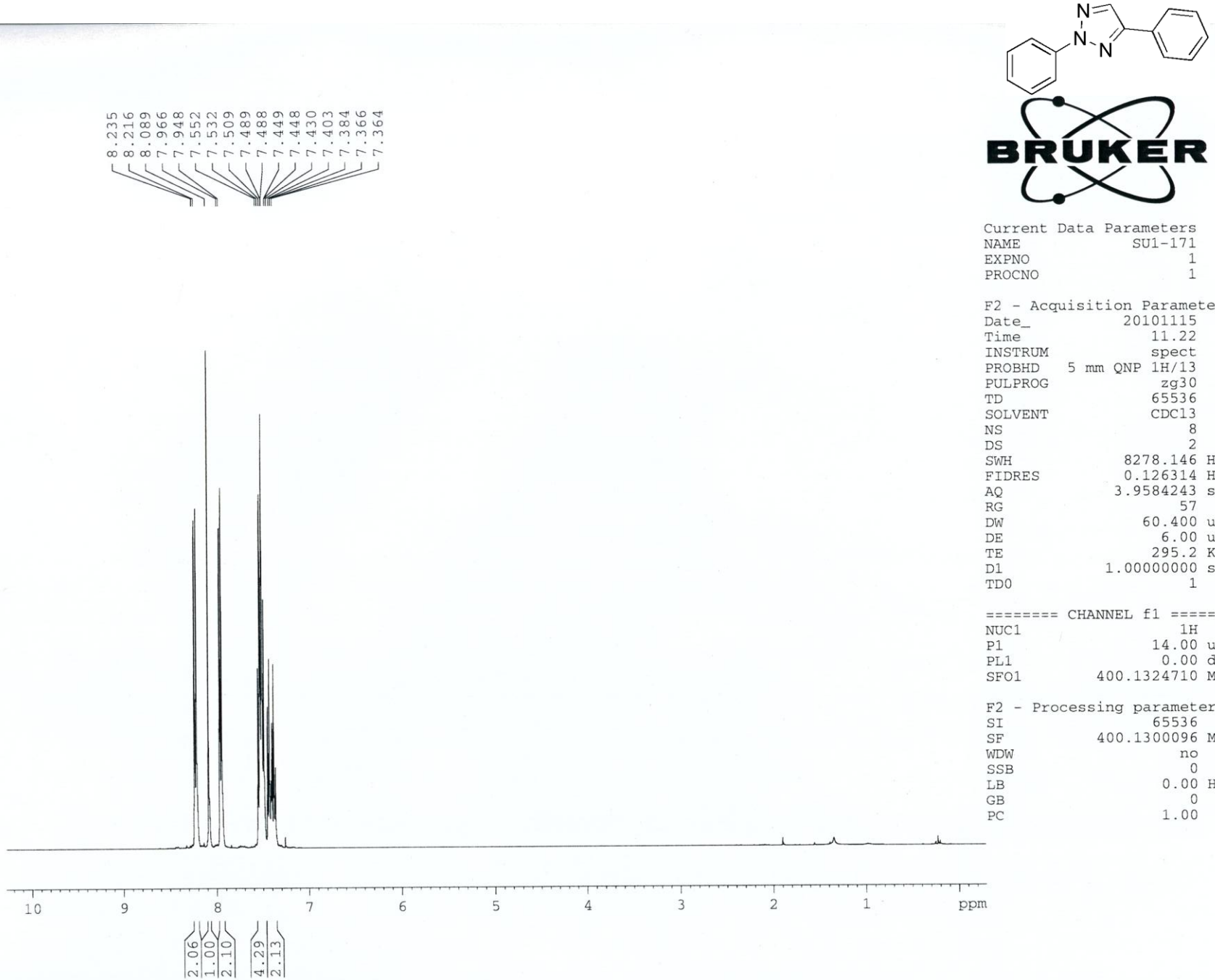
Current Data Parameters
NAME SU1-38-37C
EXPNO 2
PROCNO 2

F2 - Acquisition Parameters
Date_ 20110107
Time 10.09
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 128
DS 4
SWH 23980.814 Hz
FIDRES 0.365918 Hz
AQ 1.3664756 sec
RG 1625.5
DW 20.850 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 9.38 usec
PL1 0.00 dB
SFO1 100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 0.00 dB
PL12 16.10 dB
PL13 19.00 dB
SFO2 400.1316005 MHz

F2 - Processing parameters
SI 32768
SF 100.6127588 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.40

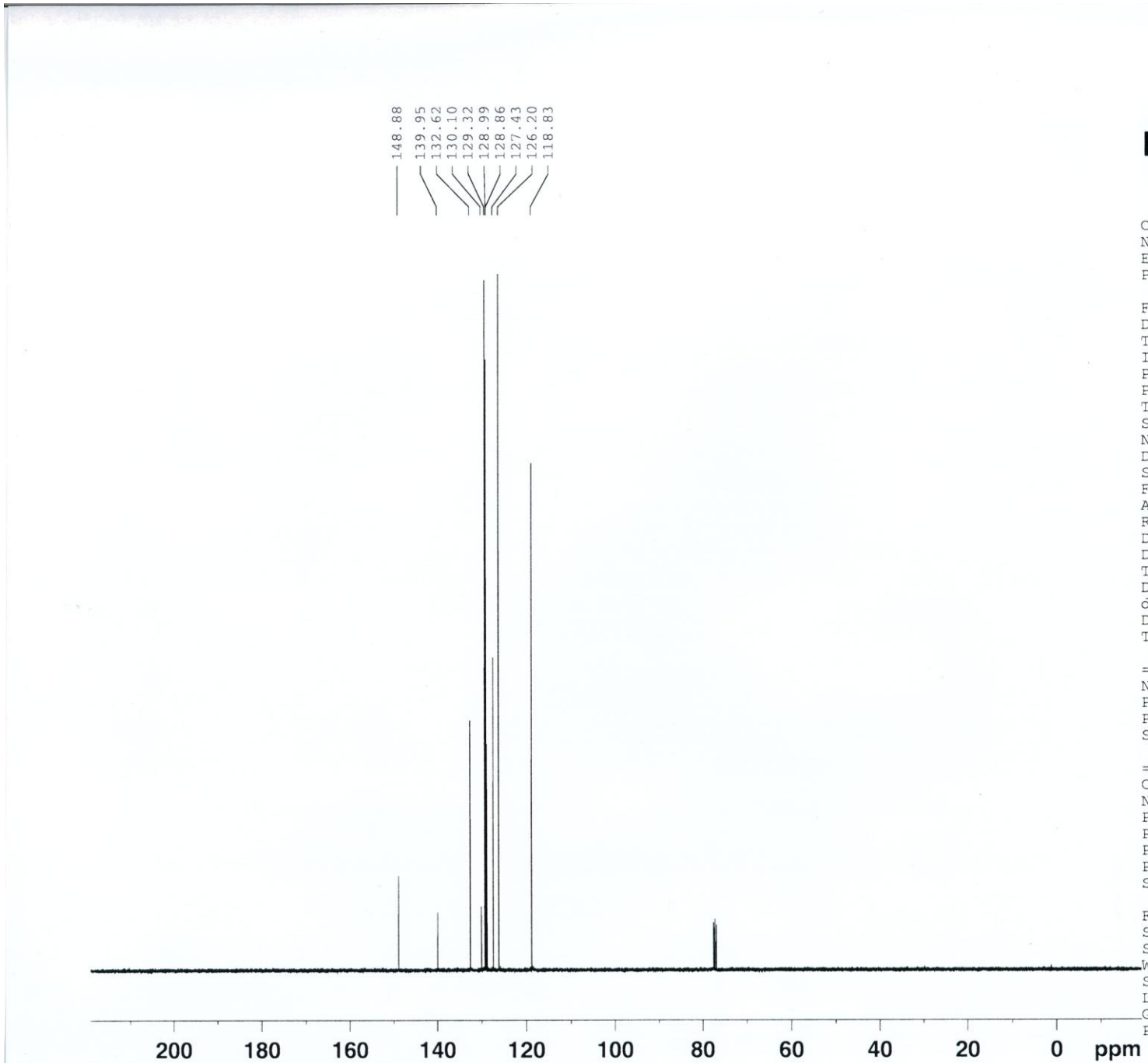


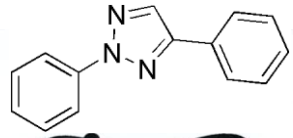
Current Data Parameters
NAME SU1-171
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20101115
Time 11.22
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 8
DS 2
SWH 8278.146 Hz
FIDRES 0.126314 Hz
AQ 3.9584243 sec
RG 57
DW 60.400 usec
DE 6.00 usec
TE 295.2 K
D1 1.00000000 sec
TD0 1

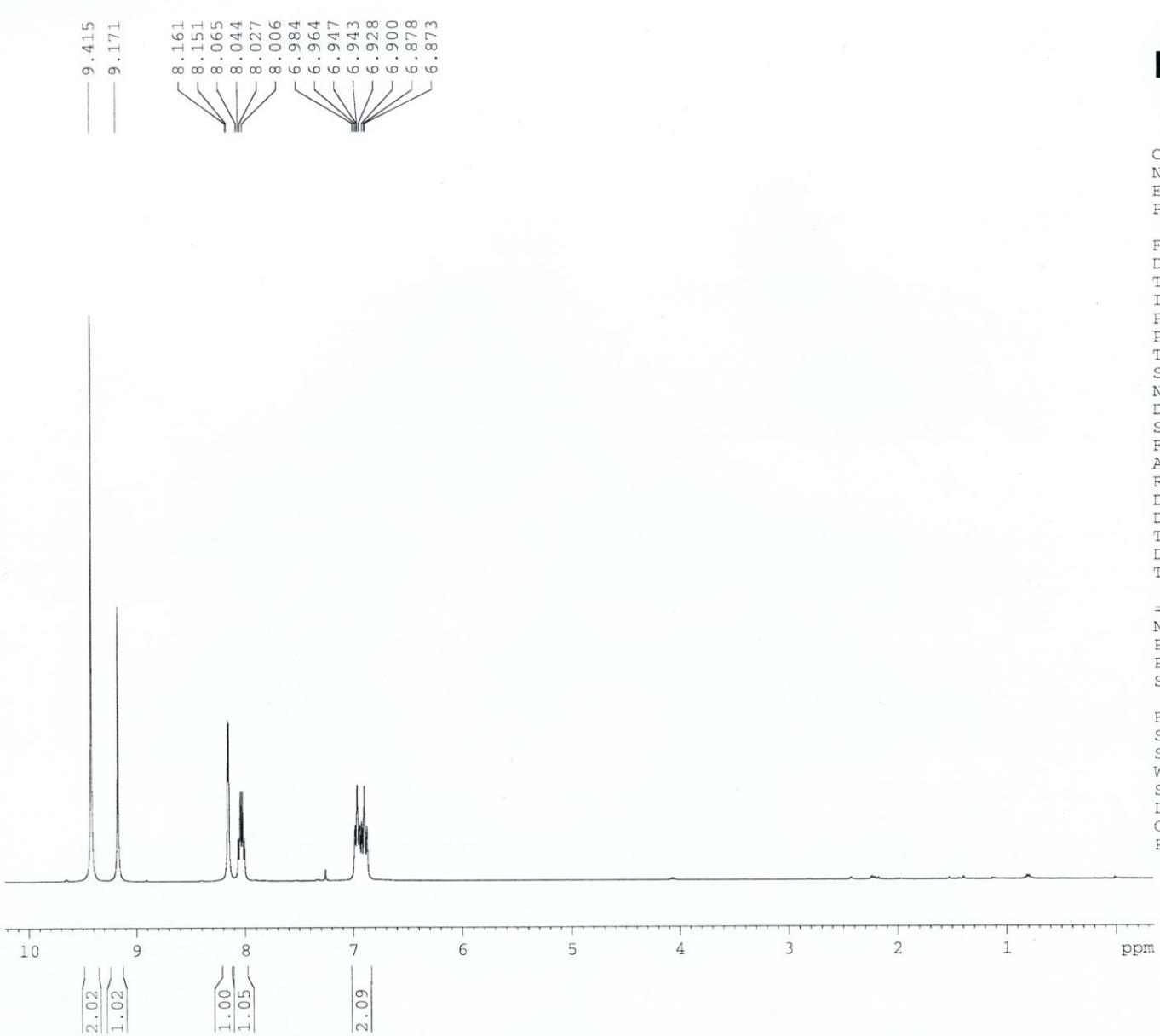
======== CHANNEL f1 ========
NUC1 1H
P1 14.00 usec
PL1 0.00 dB
SFO1 400.1324710 MHz

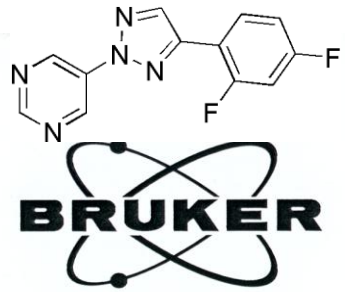
F2 - Processing parameters
SI 65536
SF 400.1300096 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00



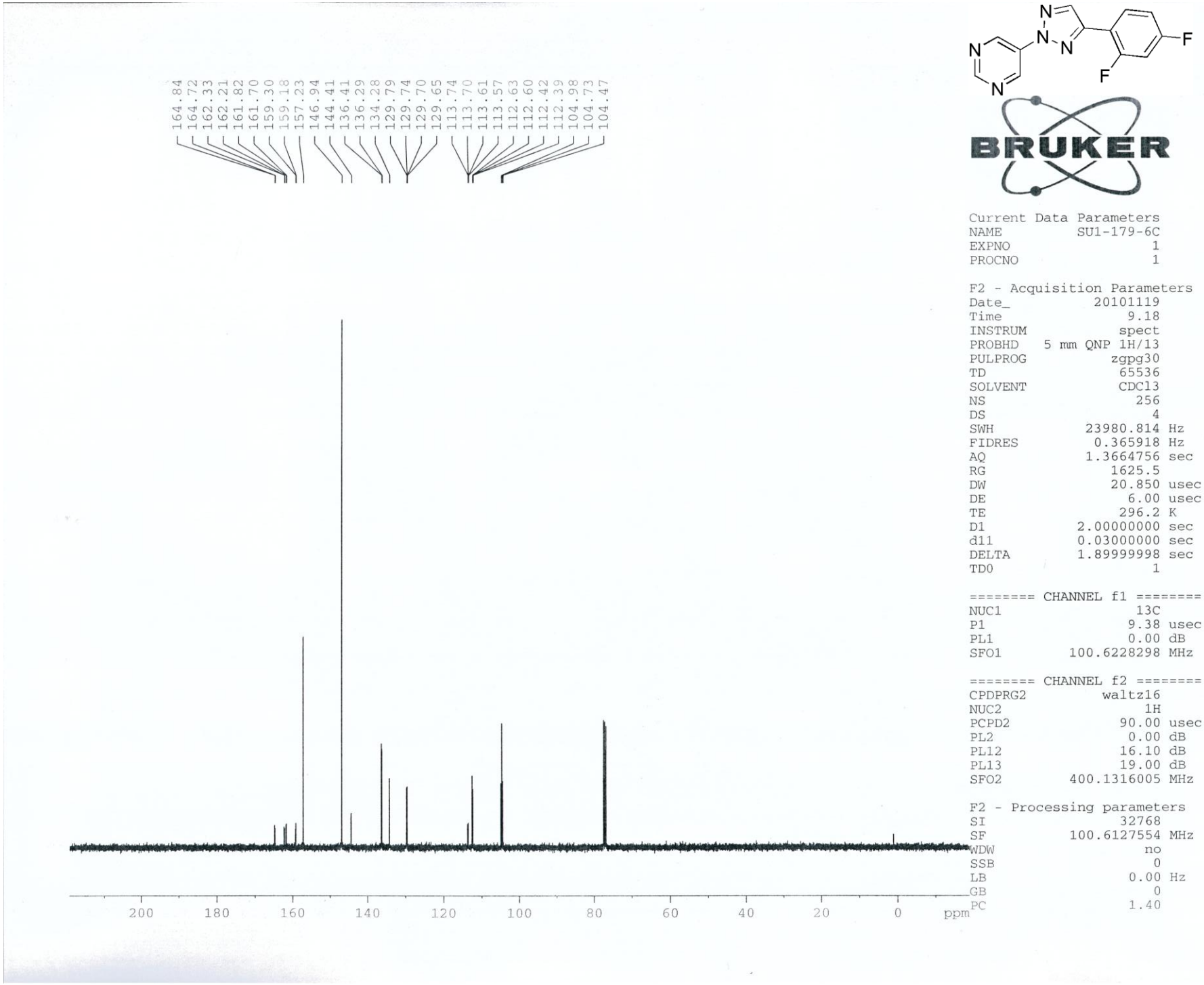


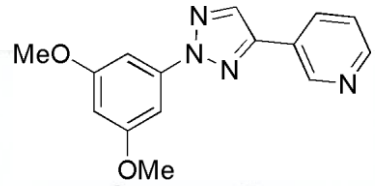

```
Current Data Parameters
NAME                  SU1-171C
EXPNO                        1
PROCNO                       1

F2 - Acquisition Parameters
Date_                 20101115
Time                     11.31
INSTRUM                  spect
PROBHD    5 mm QNP 1H/13
PULPROG                zgpg30
TD                        65536
SOLVENT                  CDCl3
NS                         128
DS                           4
SWH                  23980.814 Hz
FIDRES               0.365918 Hz
AQ                   1.3664756 sec
RG                      5160.6
DW                      20.850 usec
DE                       6.00 usec
TE                      295.2 K
D1                   2.00000000 sec
d11                  0.03000000 sec
DELTA                1.89999998 sec
TD0                          1

======== CHANNEL f1 ========
NUC1                       13C
P1                        9.38 usec
PL1                       0.00 dB
SFO1              100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG2                waltz16
NUC2                       1H
PCPD2                    90.00 usec
PL2                       0.00 dB
PL12                     16.10 dB
PL13                     19.00 dB
SFO2              400.1316005 MHz

F2 - Processing parameters
SI                         32768
SF                100.6127720 MHz
WDW                           no
SSB                            0
LB                        0.00 Hz
GB                             0
PC                         1.40
```

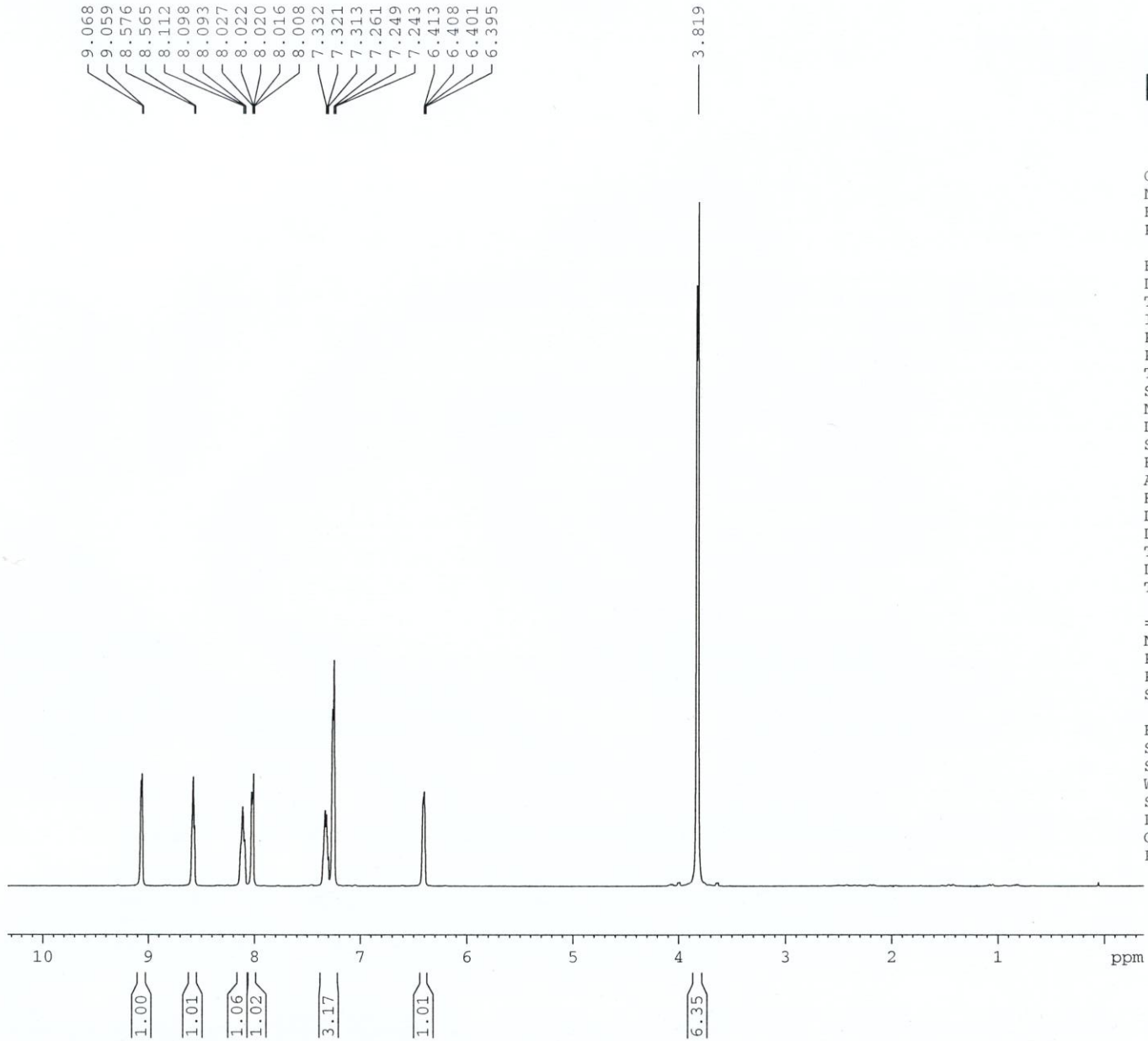





```
Current Data Parameters
NAME                  SU1-179-6
EXPNO                         1
PROCNO                        1

F2 - Acquisition Parameters
Date_                  20101119
Time                       9.03
INSTRUM                   spect
PROBHD    5 mm QNP 1H/13
PULPROG                    zg30
TD                        65536
SOLVENT                   CDCl3
NS                           16
DS                            2
SWH                    8278.146 Hz
FIDRES                 0.126314 Hz
AQ                     3.9584243 sec
RG                          114
DW                       60.400 usec
DE                        6.00 usec
TE                       295.2 K
D1                  1.00000000 sec
TD0                           1

======== CHANNEL f1 ========
NUC1                         1H
P1                       14.00 usec
PL1                       0.00 dB
SFO1               400.1324710 MHz

F2 - Processing parameters
SI                        65536
SF                 400.1300098 MHz
WDW                          no
SSB                           0
LB                        0.00 Hz
GB                            0
PC                         1.00
```

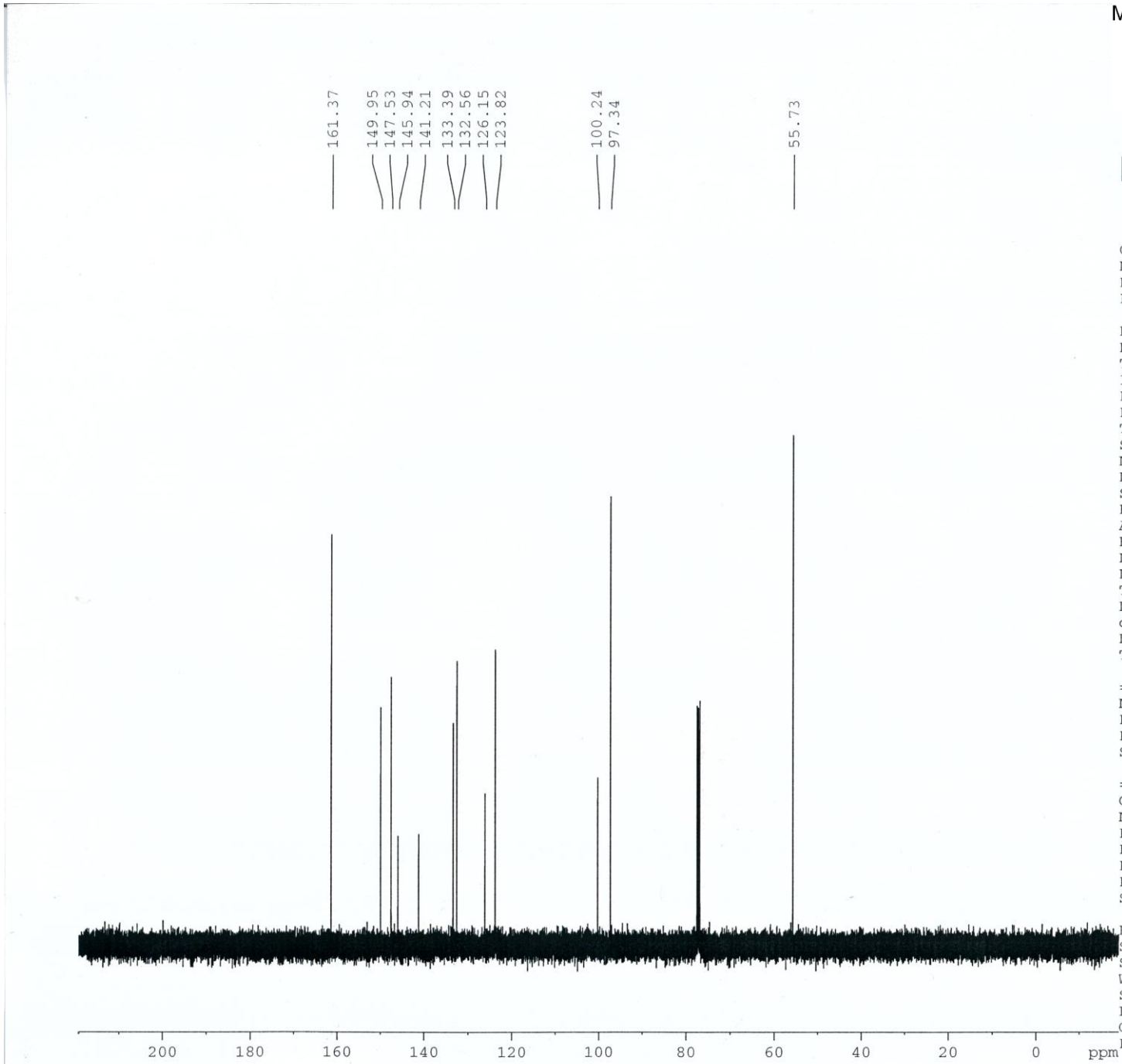

164.84
164.72
162.33
162.21
161.82
161.70
159.30
159.18
157.23
146.94
144.41
136.41
136.29
134.28
129.79
129.74
129.70
129.65
113.74
113.70
113.61
113.57
112.63
112.60
112.42
112.39
104.98
104.73
104.47
200
180
160
140
120
100
80
60
40
20
0
ppm
N
N
N
N
F
F
BRUKER
Current Data Parameters
NAME SU1-179-6C
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20101119
Time 9.18
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 256
DS 4
SWH 23980.814 Hz
FIDRES 0.365918 Hz
AQ 1.3664756 sec
RG 1625.5
DW 20.850 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 9.38 usec
PL1 0.00 dB
SFO1 100.6228298 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 0.00 dB
PL12 16.10 dB
PL13 19.00 dB
SFO2 400.1316005 MHz
F2 - Processing parameters
SI 32768
SF 100.6127554 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.40

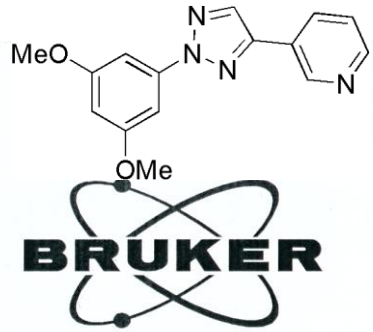




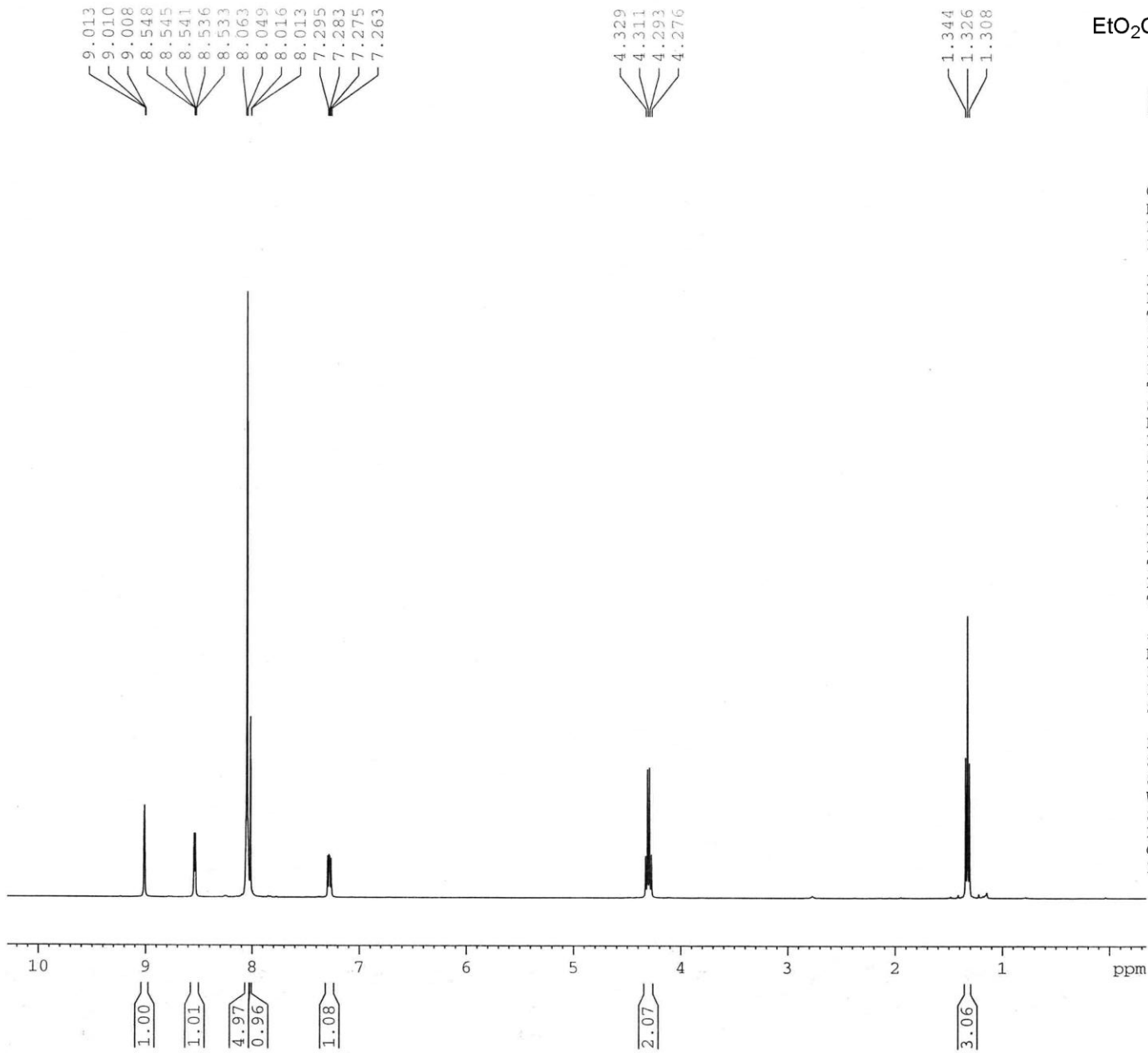
BRUKER

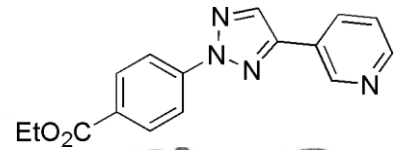
```
Current Data Parameters
NAME                  Su1-209
EXPNO                       1
PROCNO                      1

F2 - Acquisition Parameters
Date_              20101222
Time                  11.44
INSTRUM               spect
PROBHD    5 mm BBO BB-1H
PULPROG                zg30
TD                    65536
SOLVENT               CDCl3
NS                        8
DS                        2
SWH                8278.146 Hz
FIDRES            0.126314 Hz
AQ                3.9584243 sec
RG                     40.3
DW                   60.400 usec
DE                    6.00 usec
TE                   296.2 K
D1              1.00000000 sec
TD0                       1

======== CHANNEL f1 ========
NUC1                     1H
P1                   15.07 usec
PL1                   0.00 dB
SFO1          400.1324710 MHz

F2 - Processing parameters
SI                    65536
SF            400.1300124 MHz
WDW                      no
SSB                       0
LB                    0.00 Hz
GB                        0
PC                     1.00
```






```
Current Data Parameters
NAME                  Su1-209C
EXPNO                        1
PROCNO                       1

F2 - Acquisition Parameters
Date_                 20101222
Time                     11.51
INSTRUM                  spect
PROBHD     5 mm BBO BB-1H
PULPROG                 zgpg30
TD                       65536
SOLVENT                  CDCl3
NS                         128
DS                           2
SWH                23980.814 Hz
FIDRES              0.365918 Hz
AQ                  1.3664756 sec
RG                        8192
DW                     20.850 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                      8.75 usec
PL1                    -3.00 dB
SFO1              100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG2                waltz16
NUC2                       1H
PCPD2                  90.00 usec
PL2                    -1.00 dB
PL12                   14.52 dB
PL13                   18.00 dB
SFO2              400.1316005 MHz

F2 - Processing parameters
SI                       65536
SF                100.6127575 MHz
WDW                         no
SSB                          0
LB                      0.00 Hz
GB                           0
PC                        1.40
```





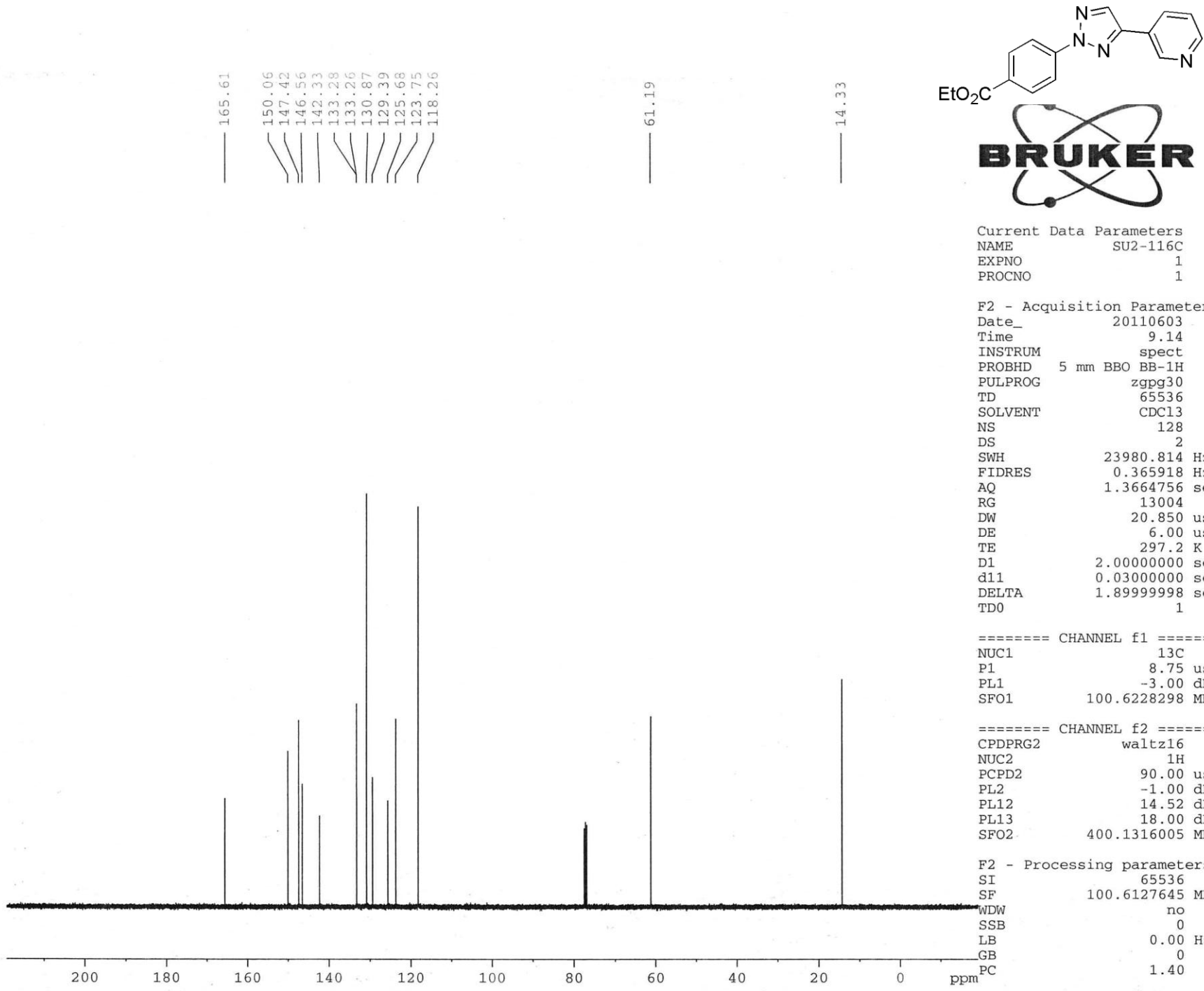
BRUKER

Current Data Parameters
NAME SU2-116
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20110603
Time 9.05
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 8
DS 2
SWH 8278.146 Hz
FIDRES 0.126314 Hz
AQ 3.9584243 sec
RG 28.5
DW 60.400 usec
DE 6.00 usec
TE 297.2 K
D1 1.00000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 1H
P1 15.07 usec
PL1 0.00 dB
SFO1 400.1324710 MHz

F2 - Processing parameters
SI 65536
SF 400.1300087 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00


165.61
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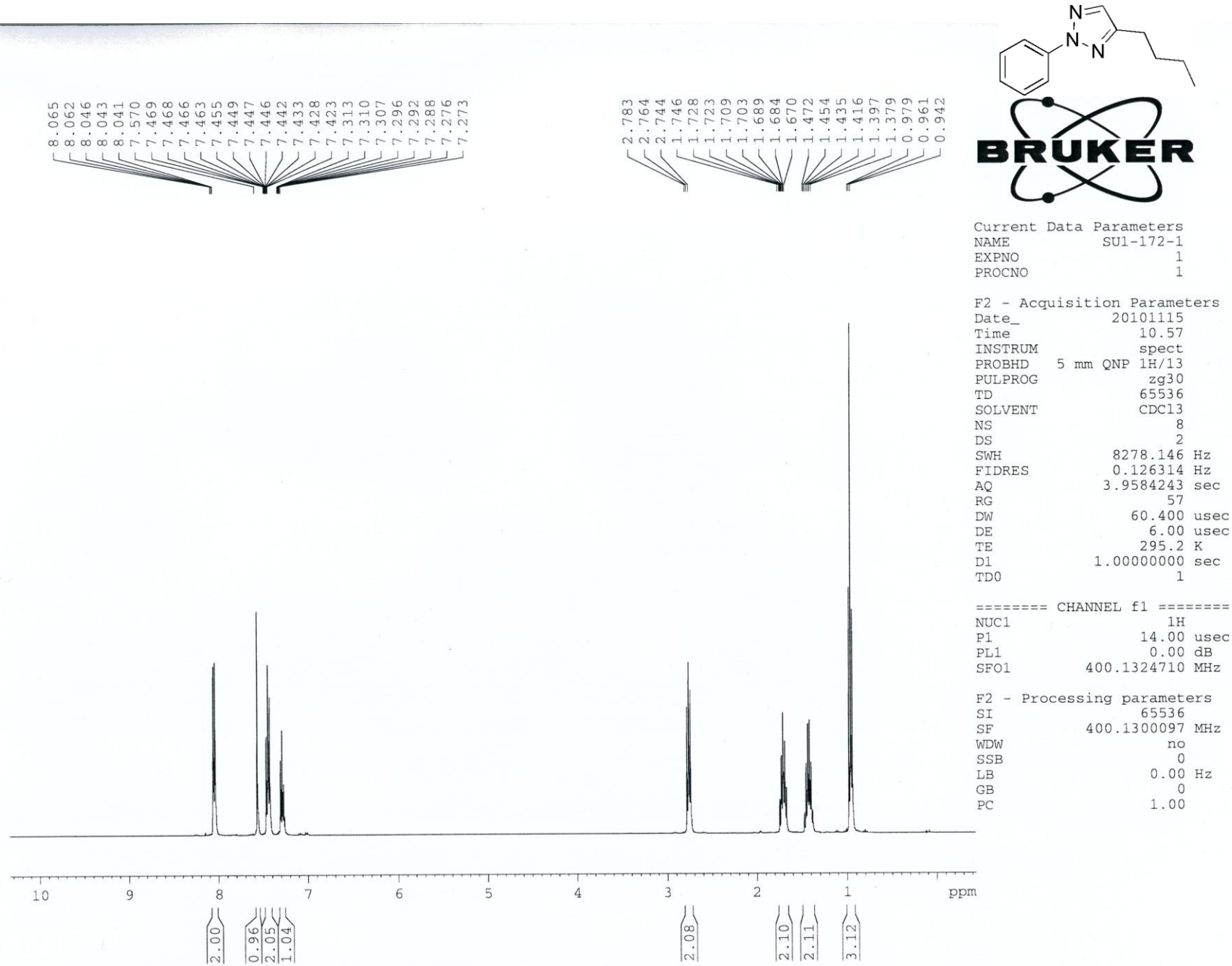
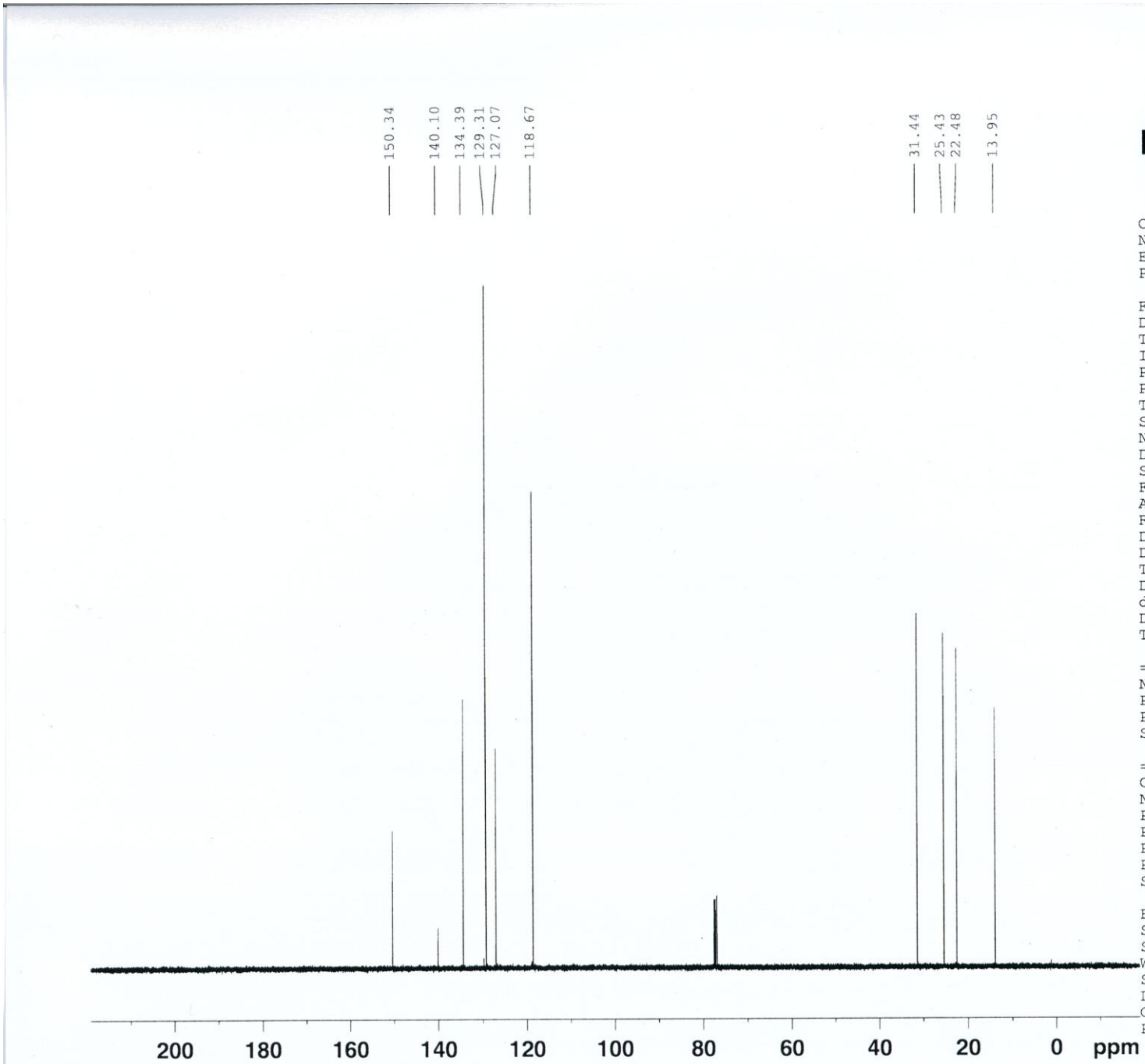
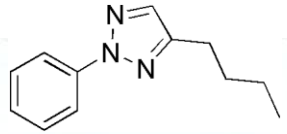
147.42
146.56
142.33
133.28
133.26
130.87
129.39
125.68
123.75
118.26
61.19
14.33
EtO2C
N
N
N
N
BRUKER
Current Data Parameters
NAME SU2-116C
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20110603
Time 9.14
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 128
DS 2
SWH 23980.814 Hz
FIDRES 0.365918 Hz
AQ 1.3664756 sec
RG 13004
DW 20.850 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 8.75 usec
PL1 -3.00 dB
SFO1 100.6228298 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -1.00 dB
PL12 14.52 dB
PL13 18.00 dB
SFO2 400.1316005 MHz
F2 - Processing parameters
SI 65536
SF 100.6127645 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.40
200
180
160
140
120
100
80
60
40
20
0
ppm


8.065
8.062
8.046
8.043
8.041
7.570
7.469
7.468
7.466
7.463
7.455
7.449
7.447
7.446
7.442
7.433
7.428
7.423
7.313
7.310
7.307
7.296
7.292
7.288
7.276
7.273
2.783
2.764
2.744
1.746
1.728
1.723
1.709
1.703
1.689
1.684
1.670
1.472
1.454
1.435
1.416
1.397
1.379
0.979
0.961
0.942
BRUKER
Current Data Parameters
NAME SU1-172-1
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20101115
Time 10.57
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 8
DS 2
SWH 8278.146 Hz
FIDRES 0.126314 Hz
AQ 3.9584243 sec
RG 57
DW 60.400 usec
DE 6.00 usec
TE 295.2 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 14.00 usec
PL1 0.00 dB
SFO1 400.1324710 MHz
F2 - Processing parameters
SI 65536
SF 400.1300097 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
10
9
8
7
6
5
4
3
2
1
ppm
2.00
0.96
2.05
1.04
2.08
2.10
2.11
3.12





BRUKER

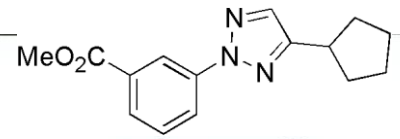
Current Data Parameters
NAME SU1-172-1C
EXPNO 1
PROCNO 1

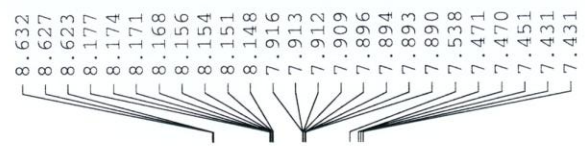
F2 - Acquisition Parameters
Date_ 20101115
Time 11.06
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 128
DS 4
SWH 23980.814 Hz
FIDRES 0.365918 Hz
AQ 1.3664756 sec
RG 5160.6
DW 20.850 usec
DE 6.00 usec
TE 295.2 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1

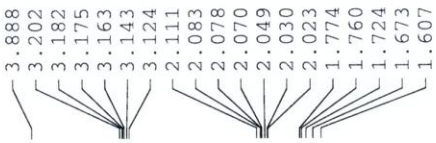
======== CHANNEL f1 ========
NUC1 13C
P1 9.38 usec
PL1 0.00 dB
SFO1 100.6228298 MHz

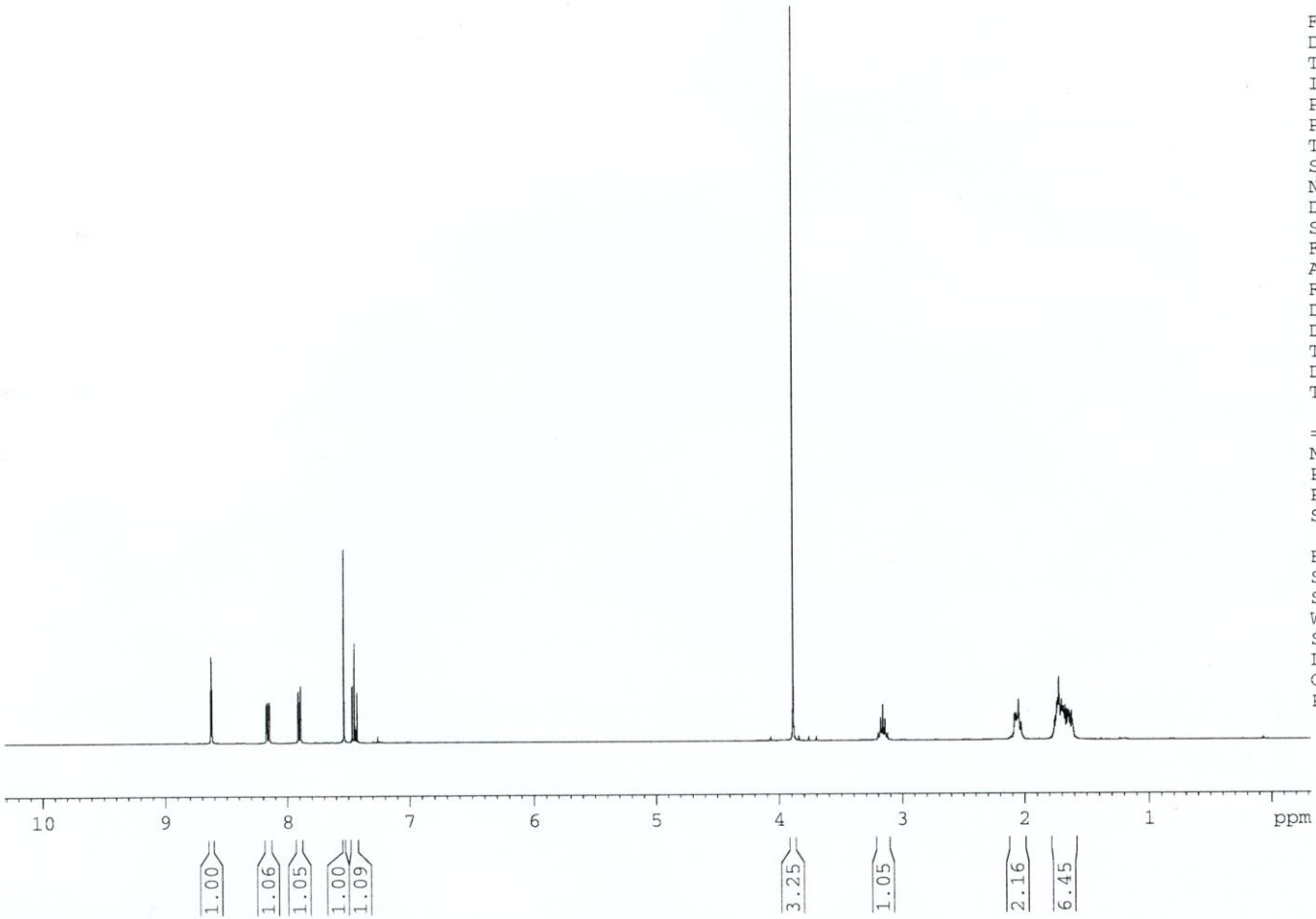
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 0.00 dB
PL12 16.10 dB
PL13 19.00 dB
SFO2 400.1316005 MHz

F2 - Processing parameters
SI 32768
SF 100.6127580 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.40

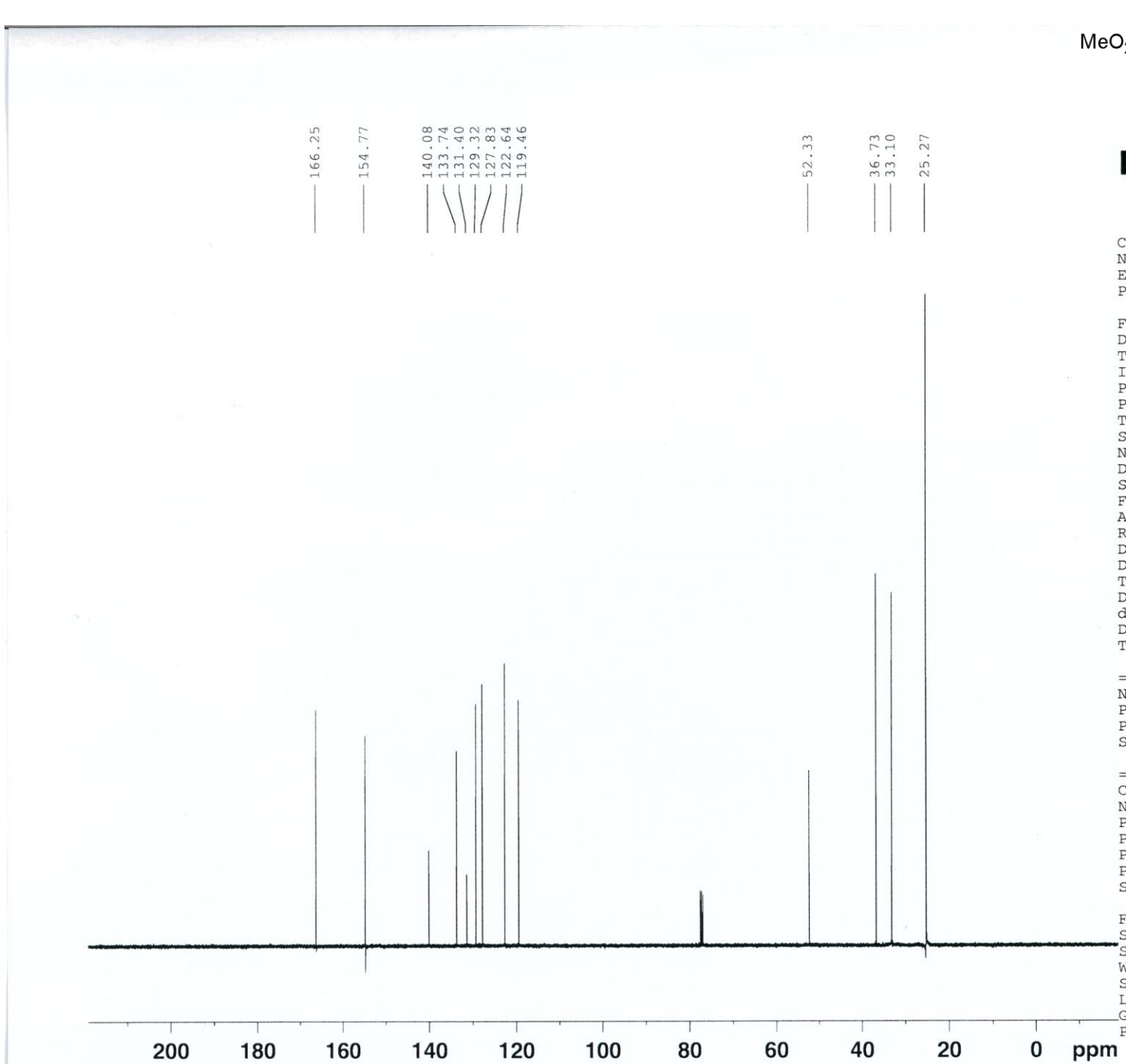




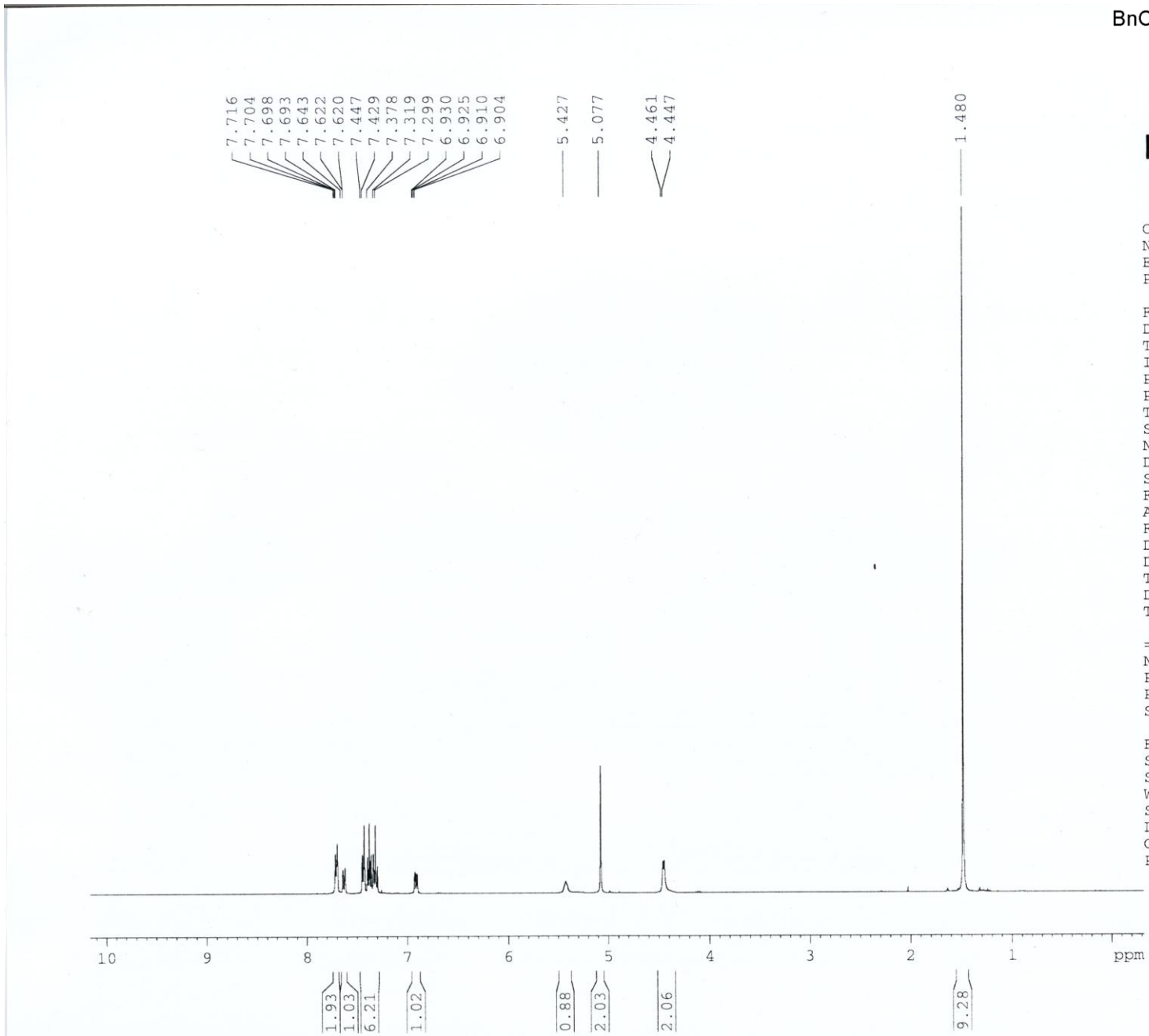


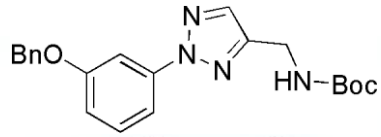



```
Current Data Parameters
NAME                  SU1-179-1
EXPNO                         1
PROCNO                        1

F2 - Acquisition Parameters
Date_                  20101117
Time                       9.00
INSTRUM                   spect
PROBHD    5 mm QNP 1H/13
PULPROG                    zg30
TD                        65536
SOLVENT                   CDCl3
NS                            8
DS                            2
SWH                    8278.146 Hz
FIDRES                 0.126314 Hz
AQ                     3.9584243 sec
RG                         28.5
DW                        60.400 usec
DE                         6.00 usec
TE                        295.2 K
D1                     1.00000000 sec
TD0                           1

======== CHANNEL f1 ========
NUC1                         1H
P1                        14.00 usec
PL1                        0.00 dB
SFO1                400.1324710 MHz

F2 - Processing parameters
SI                        65536
SF                 400.1300091 MHz
WDW                          no
SSB                           0
LB                         0.00 Hz
GB                            0
PC                         1.00
```




```
Current Data Parameters
NAME          SU1-179-1C
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20101117
Time                9.08
INSTRUM            spect
PROBHD   5 mm QNP 1H/13
PULPROG          zgpg30
TD                65536
SOLVENT           CDC13
NS                  128
DS                    4
SWH           23980.814 Hz
FIDRES         0.365918 Hz
AQ             1.3664756 sec
RG                 4096
DW               20.850 usec
DE                6.00 usec
TE                295.2 K
D1            2.00000000 sec
d11           0.03000000 sec
DELTA         1.89999998 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                 13C
P1                 9.38 usec
PL1                0.00 dB
SFO1        100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG2         waltz16
NUC2                 1H
PCPD2             90.00 usec
PL2                0.00 dB
PL12              16.10 dB
PL13              19.00 dB
SFO2        400.1316005 MHz

F2 - Processing parameters
SI                32768
SF          100.6127619 MHz
WDW                  no
SSB                   0
LB                 0.00 Hz
GB                    0
PC                 1.40
```





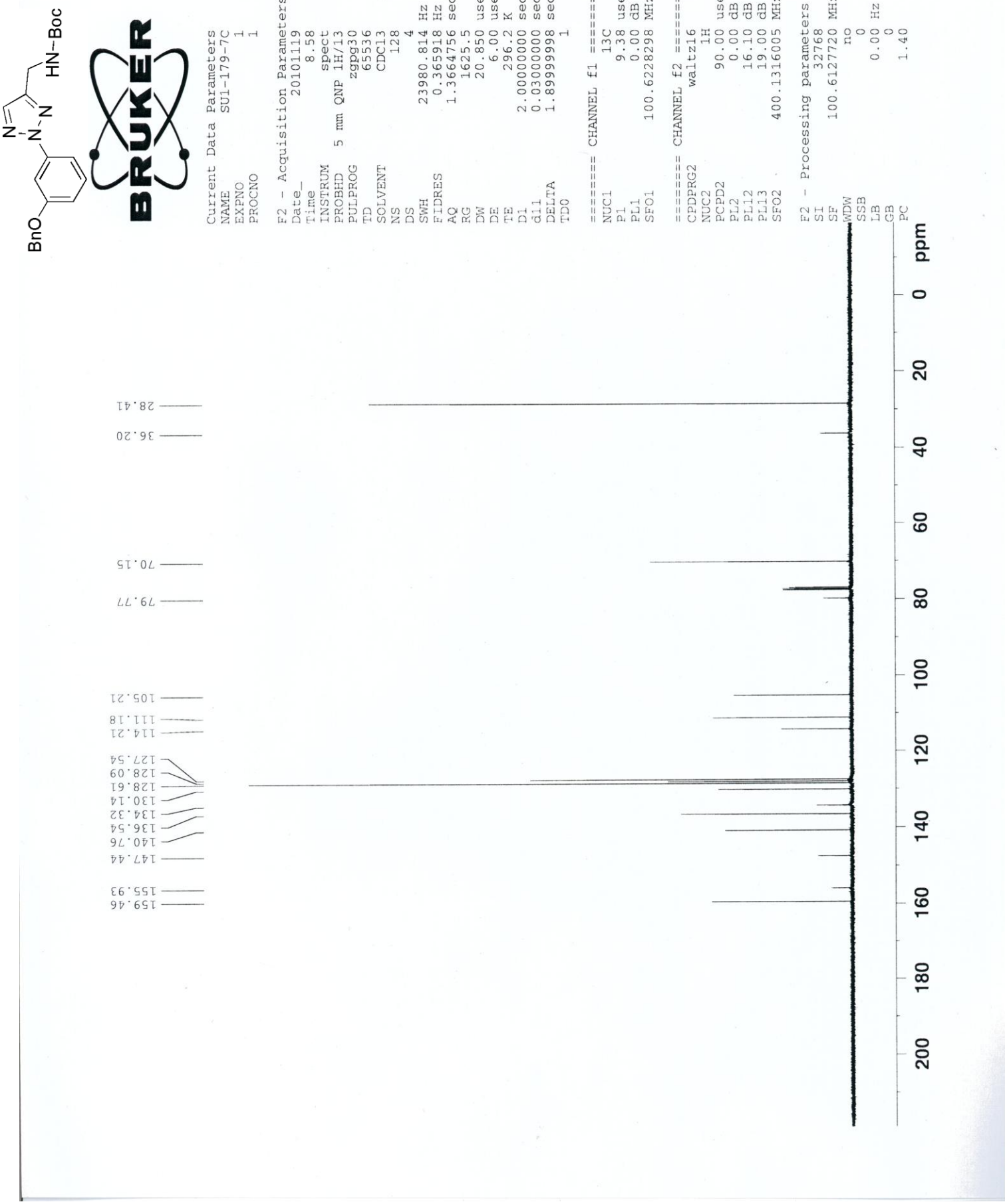
BRUKER

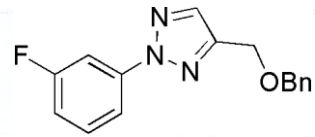
Current Data Parameters
NAME SU1-179-7
EXPNO 1
PROCNO 1

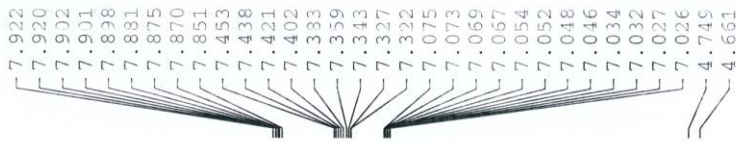
F2 - Acquisition Parameters
Date_ 20101119
Time 8.50
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 8
DS 2
SWH 8278.146 Hz
FIDRES 0.126314 Hz
AQ 3.9584243 sec
RG 25.4
DW 60.400 usec
DE 6.00 usec
TE 295.2 K
D1 1.00000000 sec
TD0 1

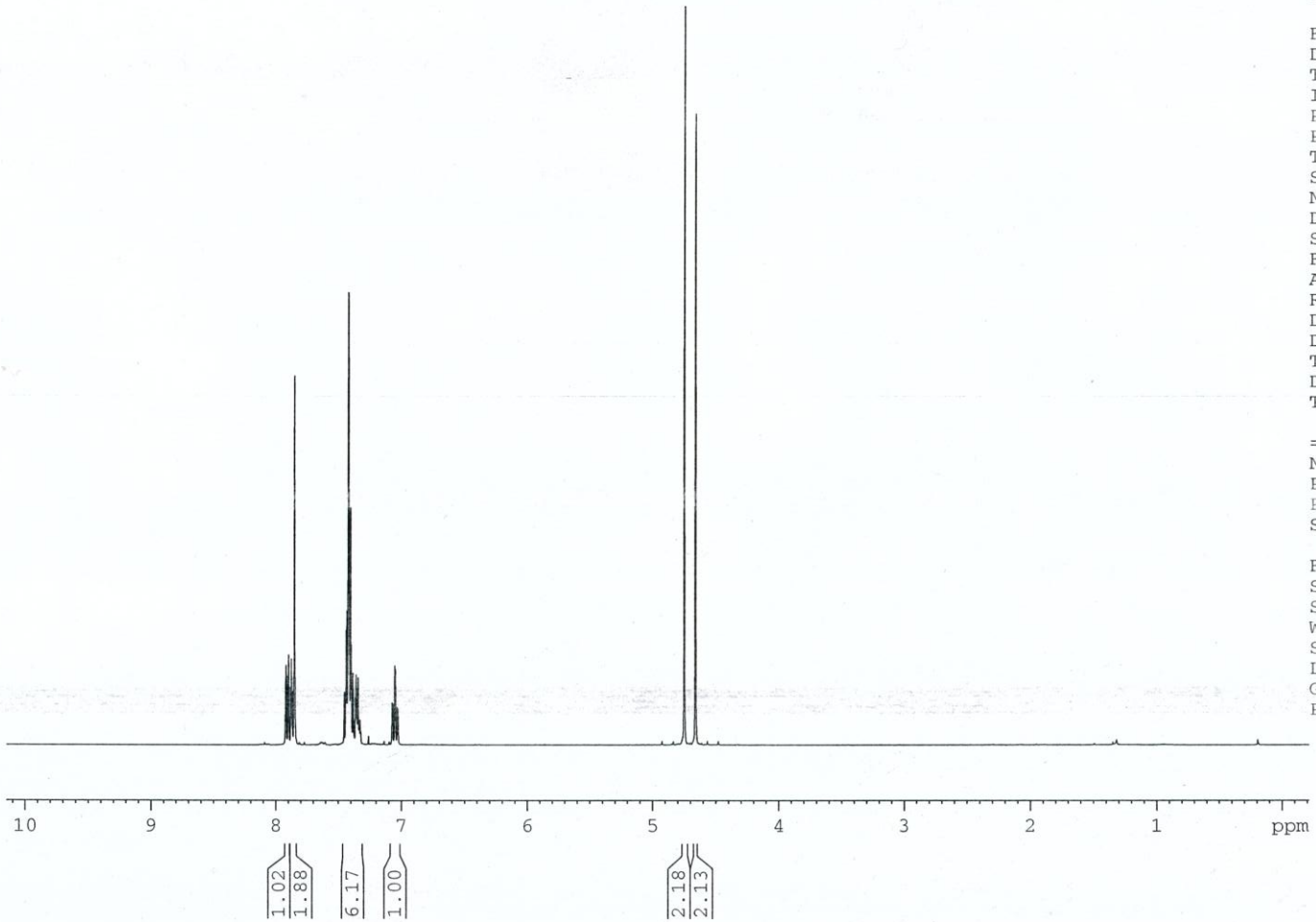
======== CHANNEL f1 ========
NUC1 1H
P1 14.00 usec
PL1 0.00 dB
SFO1 400.1324710 MHz

F2 - Processing parameters
SI 65536
SF 400.1300093 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00

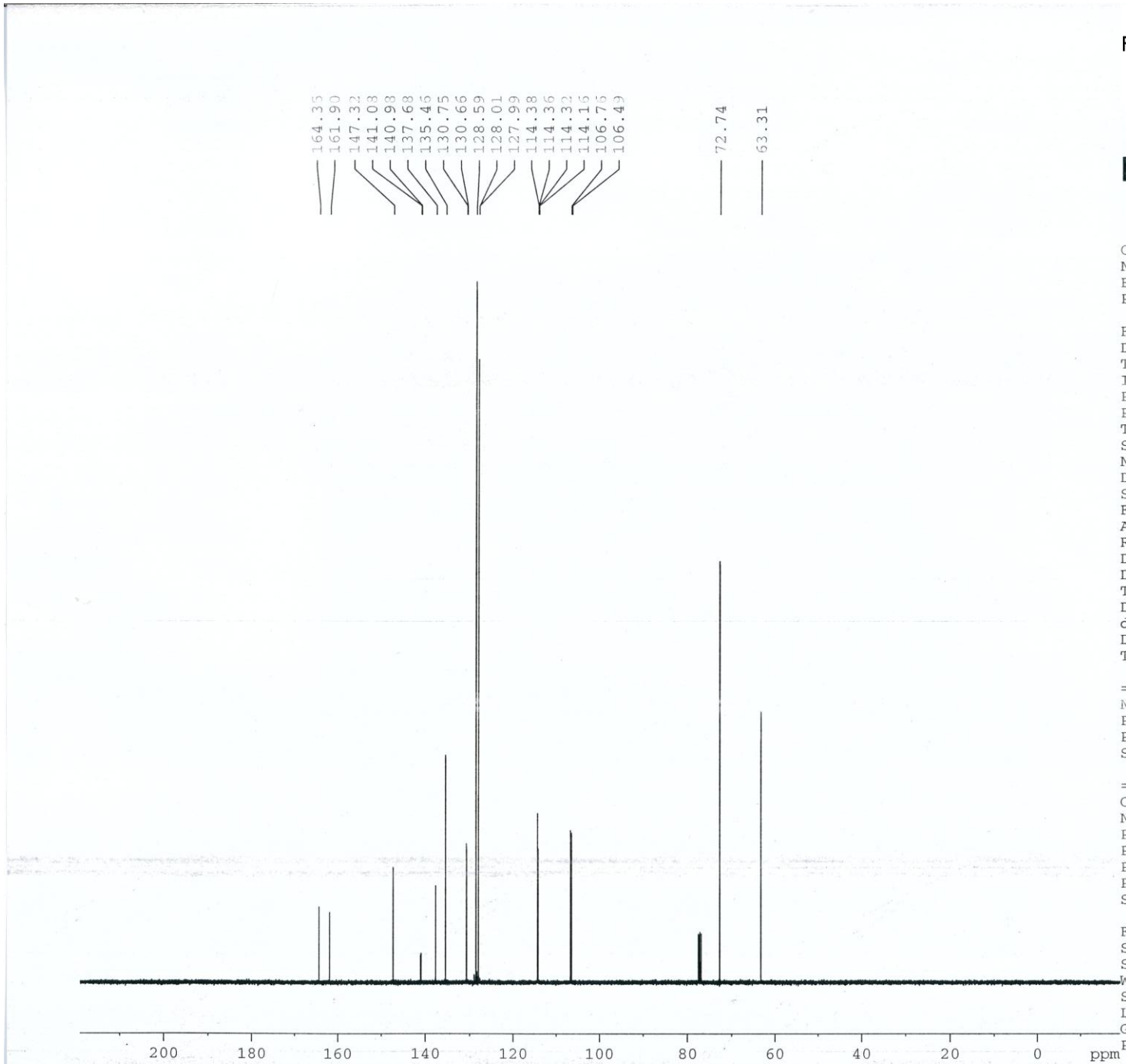

BnO
HN–Boc
BRUKER
Current Data Parameters
NAME SU1-179-7C
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20101119
Time 8.58
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 128
DS 4
SWH 23980.814 Hz
FIDRES 0.365918 Hz
AQ 1.3664756 sec
RG 1625.5
DW 20.850 usec
DE 6.00 usec
TE 296.2 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 9.38 usec
PL1 0.00 dB
SFO1 100.6228298 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 0.00 dB
PL12 16.10 dB
PL13 19.00 dB
SFO2 400.1316005 MHz
F2 - Processing parameters
SI 32768
SF 100.6127720 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.40
28.41
36.20
70.15
79.77
105.21
111.18
114.21
127.54
128.09
128.61
130.14
134.32
136.54
140.76
147.44
155.93
159.46
200
180
160
140
120
100
80
60
40
20
0
ppm

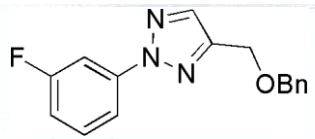







```
Current Data Parameters
NAME                  SU1-186-5
EXPNO                         1
PROCNO                        1

F2 - Acquisition Parameters
Date_                  20101203
Time                      15.02
INSTRUM                   spect
PROBHD    5 mm BBO BB-1H
PULPROG                    zg30
TD                        65536
SOLVENT                   CDCl3
NS                            8
DS                            2
SWH                    8278.146 Hz
FIDRES                 0.126314 Hz
AQ                     3.9584243 sec
RG                         22.6
DW                       60.400 usec
DE                        6.00 usec
TE                        296.2 K
D1                   1.00000000 sec
TD0                           1

======== CHANNEL f1 ========
NUC1                         1H
P1                        15.07 usec
PL1                        0.00 dB
SFO1               400.1324710 MHz

F2 - Processing parameters
SI                        65536
SF                 400.1300075 MHz
WDW                          no
SSB                           0
LB                         0.00 Hz
GB                            0
PC                         1.00
```





BRUKER

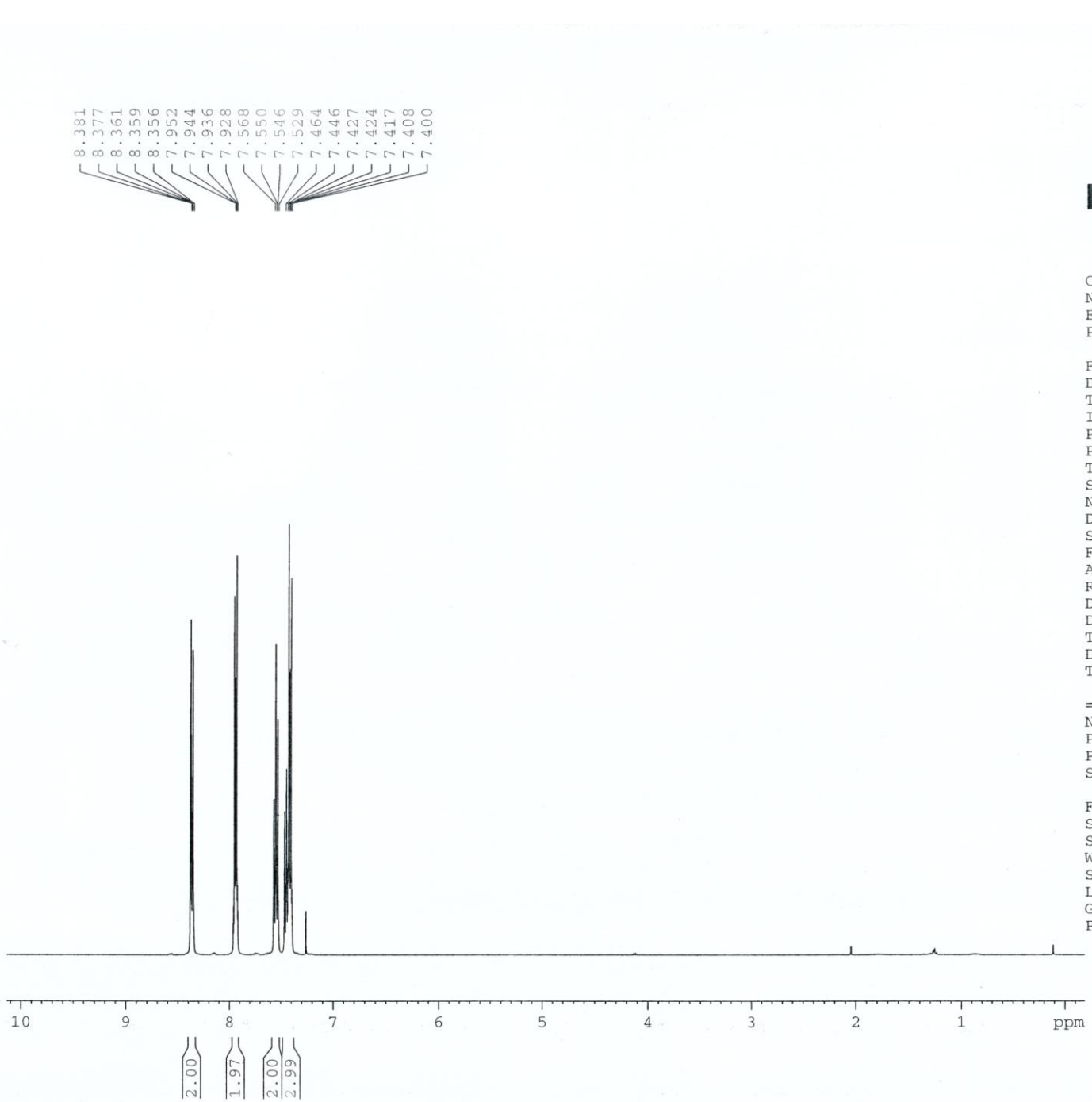
Current Data Parameters
NAME SU1-186-5
EXPNO 4
PROCNO 4

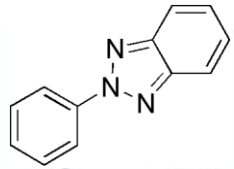
F2 - Acquisition Parameters
Date_ 20101203
Time 15.18
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 128
DS 2
SWH 23980.814 Hz
FIDRES 0.365918 Hz
AQ 1.3664756 sec
RG 8192
DW 20.850 usec
DE 6.00 usec
TE 297.2 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1

======== CHANNEL f1 ========
NUC1 13C
P1 8.75 usec
PL1 -3.00 dB
SFO1 100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -1.00 dB
PL12 14.52 dB
PL13 18.00 dB
SFO2 400.1316005 MHz

F2 - Processing parameters
SI 65536
SF 100.6127671 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.40





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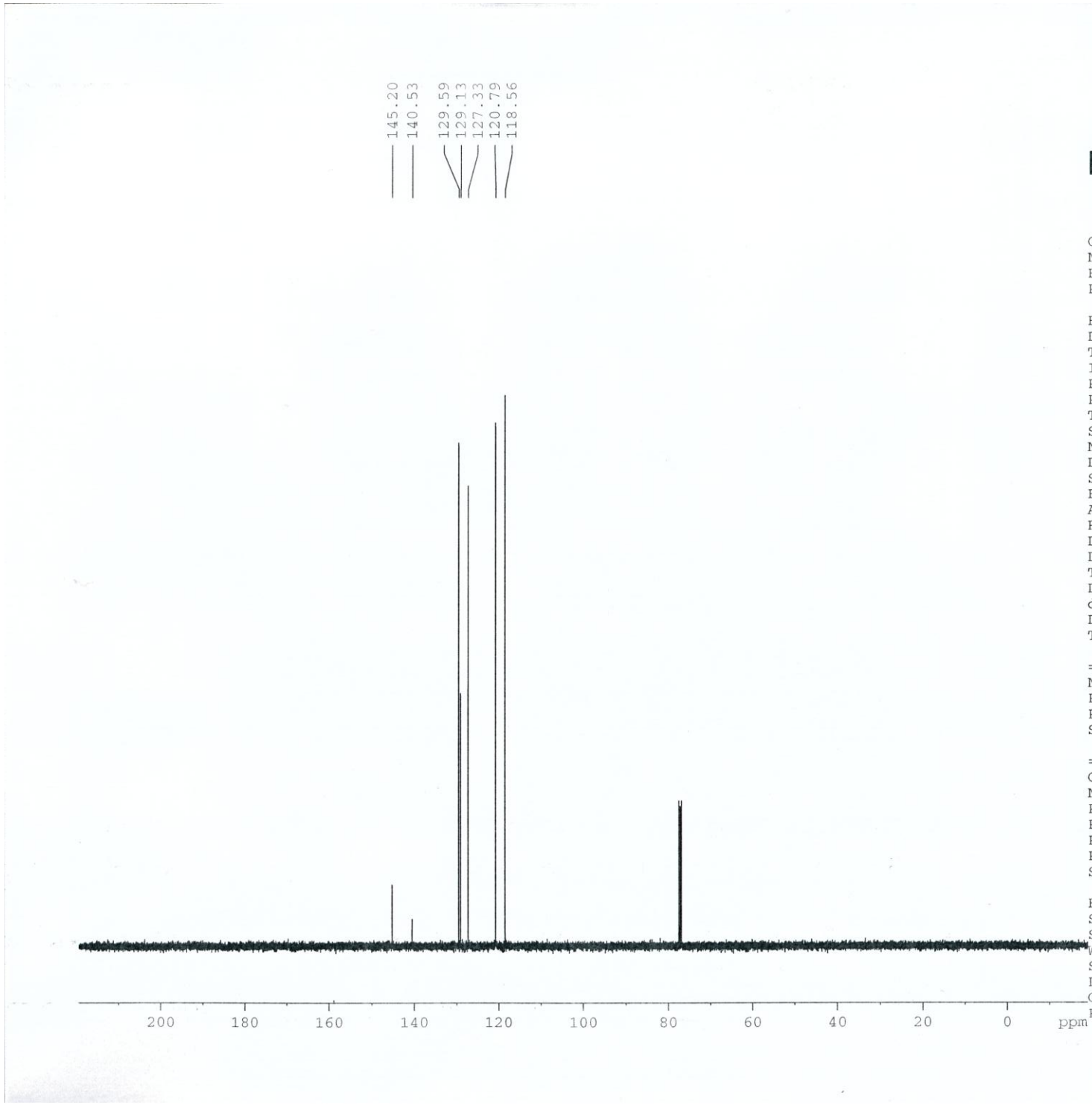
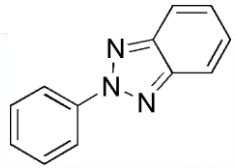
Current Data Parameters
NAME SU1-227 Fr3-10
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20110302
Time 9.33
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8278.146 Hz
FIDRES 0.126314 Hz
AQ 3.9584243 sec
RG 181
DW 60.400 usec
DE 6.00 usec
TE 296.2 K
D1 1.00000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 1H
P1 14.00 usec
PL1 0.00 dB
SFO1 400.1324710 MHz

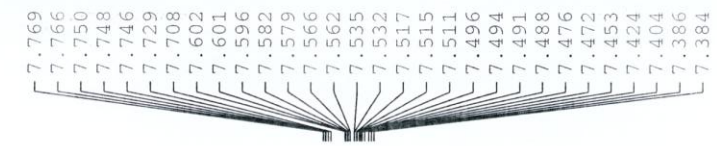
F2 - Processing parameters
SI 65536
SF 400.1300095 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00

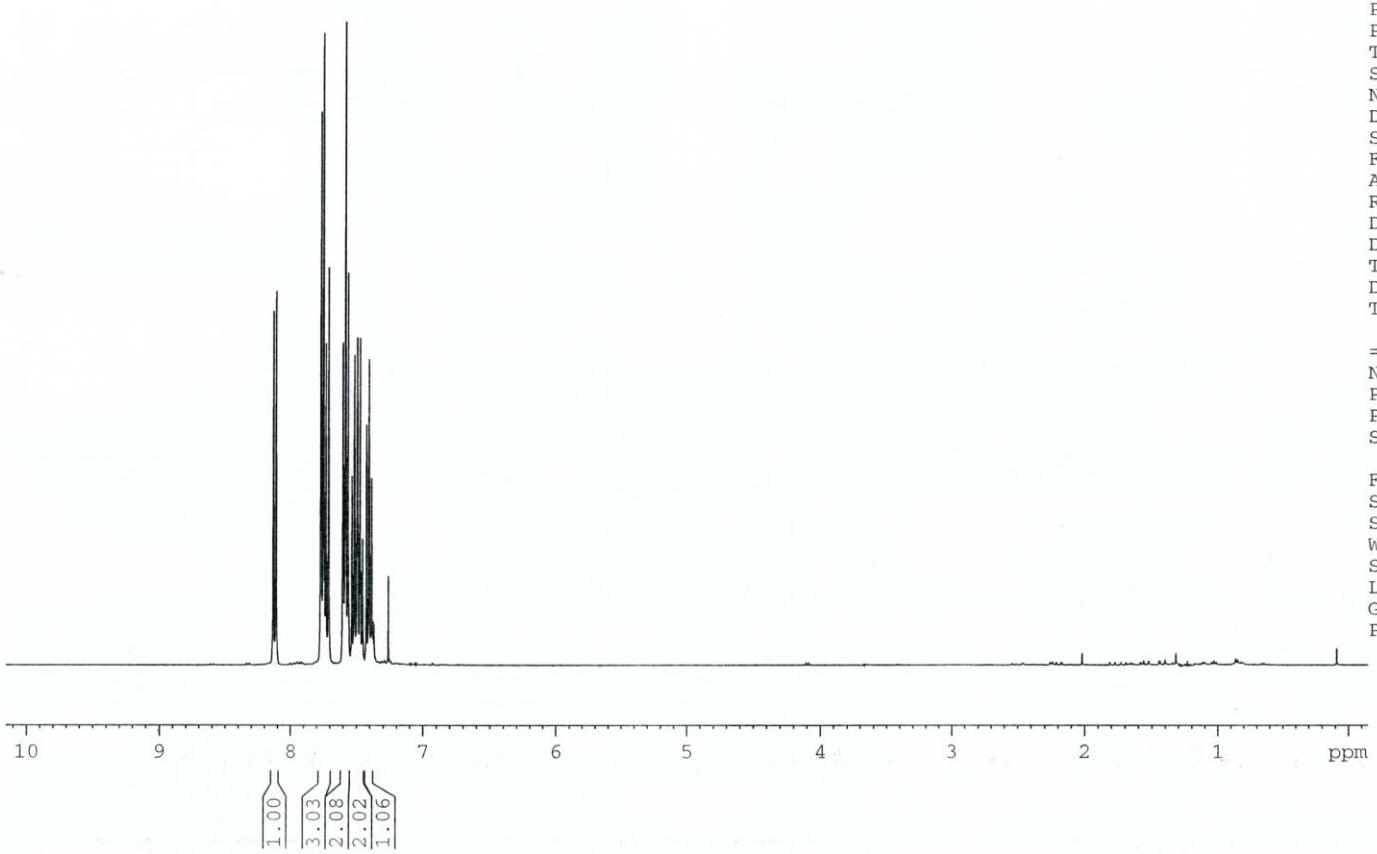


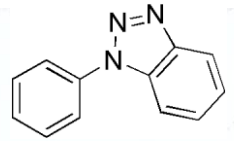


BRUKER

```
Current Data Parameters
NAME      SU1-227 Fr3-10C
EXPNO                   1
PROCNO                  1

F2 - Acquisition Parameters
Date_           20110302
Time                9.41
INSTRUM            spect
PROBHD   5 mm QNP 1H/13
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                  128
DS                    4
SWH           23980.814 Hz
FIDRES         0.365918 Hz
AQ             1.3664756 sec
RG                 4096
DW               20.850 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                9.38 usec
PL1               0.00 dB
SFO1        100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG2         waltz16
NUC2                 1H
PCPD2            90.00 usec
PL2               0.00 dB
PL12             16.10 dB
PL13             19.00 dB
SFO2        400.1316005 MHz

F2 - Processing parameters
SI                32768
SF          100.6127535 MHz
WDW                  no
SSB                   0
LB                0.00 Hz
GB                    0
PC                 1.40
```

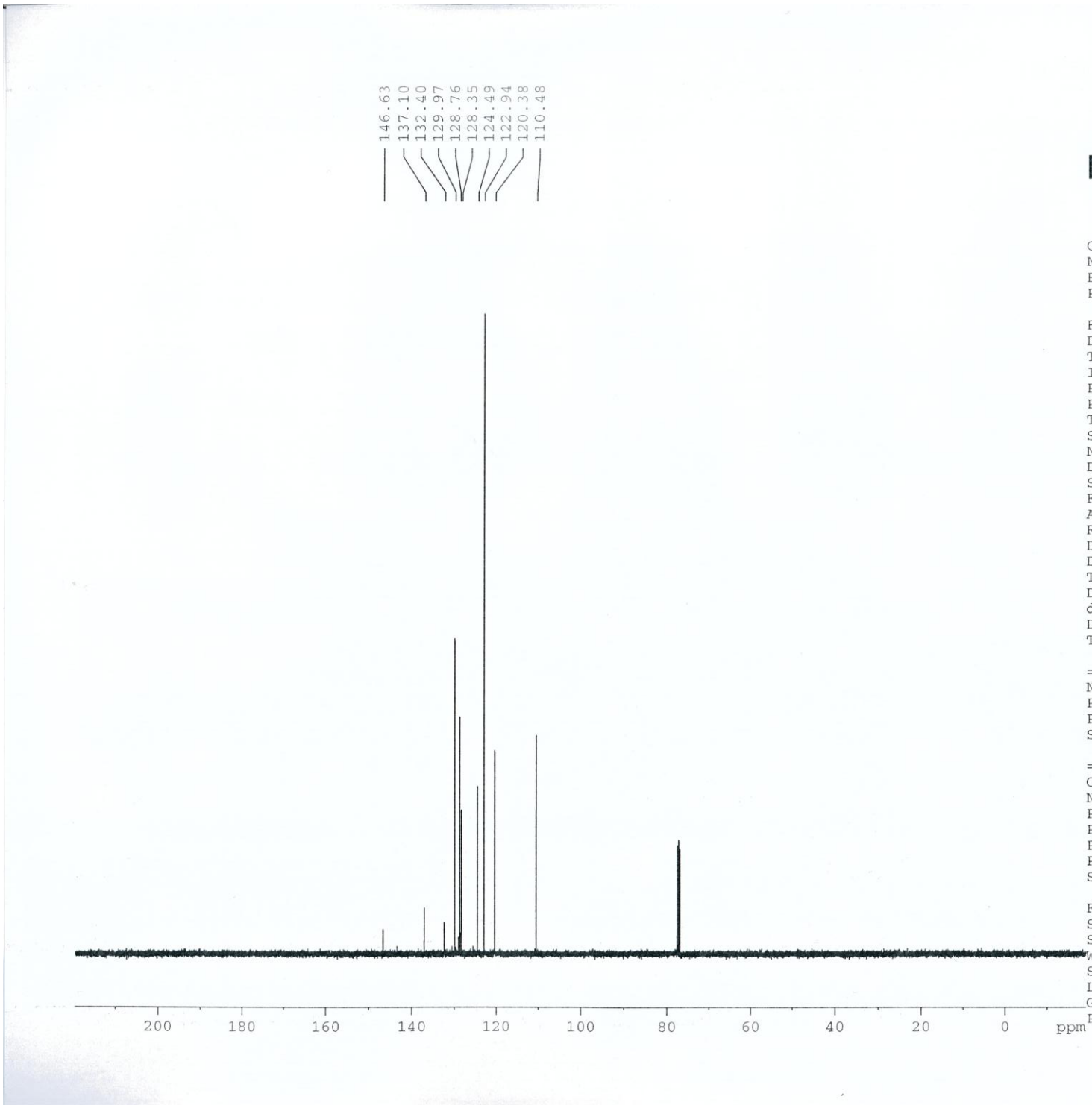


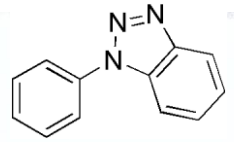




BRUKER

```
Current Data Parameters
NAME      SU1-227 Fr13-20
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20110302
Time                9.45
INSTRUM            spect
PROBHD   5 mm QNP 1H/13
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    16
DS                     2
SWH             8278.146 Hz
FIDRES          0.126314 Hz
AQ              3.9584243 sec
RG                 143.7
DW                60.400 usec
DE                 6.00 usec
TE                296.2 K
D1           1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  1H
P1                14.00 usec
PL1                0.00 dB
SFO1        400.1324710 MHz

F2 - Processing parameters
SI                 65536
SF          400.1300094 MHz
WDW                   no
SSB                    0
LB                 0.00 Hz
GB                     0
PC                  1.00
```





Current Data Parameters
NAME SU1-227 Fr13-20C
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20110302
Time 9.53
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 128
DS 4
SWH 23980.814 Hz
FIDRES 0.365918 Hz
AQ 1.3664756 sec
RG 1625.5
DW 20.850 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 9.38 usec
PL1 0.00 dB
SFO1 100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 0.00 dB
PL12 16.10 dB
PL13 19.00 dB
SFO2 400.1316005 MHz

F2 - Processing parameters
SI 32768
SF 100.6127589 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.40