Supporting Information

for

General Methodology for the Preparation of 2,5-Disubstituted-1,3-Oxazoles

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General Information

Proton nuclear magnetic resonance (^{1}H NMR) spectra were measured on a Vairan INOVA-400 (400 MHz) or Gem-300 (300 MHz). Carbon nuclear magnetic resonance (^{13}C NMR) spectra were measured on a Vairan INOVA-500 (500 MHz), Varian INOVA-400 (400 MHz), or Varian VXR-400 (400 MHz). ^{1}H NMR and ^{13}C NMR spectra were acquired as solutions in $CDCl_3$ and are reported in parts per million (ppm) downfield (δ) from tetramethylsilane using residual chloroform ($CHCl_3$) as an internal standard set to δ 7.27 and δ 77.00, respectively. Proton NMR data are reported in the form: δ (multiplicity, coupling constants, number of protons). Mass spectral data (MS and HRMS) were recorded on a Kratos MS-80 RFA mass spectrometer by use of chemical ionization (CI) with methane or electron impact (EI).

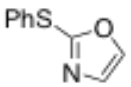
Analytical thin-layer chromatography (TLC) was performed using glass-backed 0.25 mm thickness silica gel 60 (F_{254}) plates (EM Science) which were visualized under UV light and/or staining with ethanolic *p*-anisaldehyde. Flash chromatography was performed using Merck silica gel 60 (Kiesegel 60) (E. M. Science; 230-400 mesh ASTM) or similar products from Whatman Scientific or Sorbent Technologies and pressure was obtained using an airline bleed.

All reagents were used immediately before dried under vacuum, using molecular sieves, or distilled unless noted otherwise. Oxazole was used as received from Sigma Aldrich. All solvents were reagent grade and used as received unless noted otherwise. Bulk grade hexanes and ethyl acetate (EtOAc) for chromatography were distilled before use. Diethyl ether (Et_2O) and tetrahydrofuran (THF) were

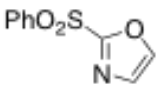
distilled under nitrogen from sodium/benzophenone ketyl immediately before use. Diisopropylamine was distilled from CaH_2 under dry air immediately before use.

Unless otherwise noted, all reactions were conducted in flame or oven-dried glassware under an atmosphere of nitrogen. All non-volatile samples were pumped to a constant weight under high vacuum (0.1-0.2 mmHg) at ambient temperature following removal of solvent by rotary evaporation.

Experimental Procedures



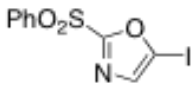
2-(Phenylthio)oxazole. To a stirred solution of oxazole (0.80 g, 11.58 mmol, 1.0 equiv) in THF (120 mL) was added slowly dropwise *n*-BuLi (5.65 mL, 13.90 mmol, 1.2 equiv) at -78 ^{o}C and it was stirred at -78 ^{o}C for 1 h. A solution of phenyl disulfide (3.54 g, 16.21 mmol, 1.4 equiv) in anhydrous THF (50 mL) was added slowly dropwise via syringe. The resulting mixture was allowed to stir at -78 ^{o}C for 1 h, warm to room temperature slowly, and stir at room temperature for 48 h. After the completion of the reaction, it was quenched with saturated aqueous NH_4Cl (30 mL) and extracted with Et_2O (3 x 20 mL). The separated organic extracts were washed with saturated aqueous $NaHCO_3$ (30 mL), brine (30 mL) and dried over Na_2SO_4. Removal of solvent and flash column chromatography over silica gel using hexanes:EtOAc (10:1 & 4:1) to give 2-(phenylthio)oxazole (1.87 g, 10.56 mmol, 91%) as yellowish oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.68 (s, 1H), 7.56-7.61 (m, 2H), 7.38-7.43 (m, 3H), 7.14 (s, 1H); ^{13}C NMR (400 MHz, $CDCl_3$): δ 159.0, 141.1, 133.4, 129.7, 129.3, 129.2, 129.1.



2-(Phenylsulfonyl)oxazole (1). Ammonium Molybdate (2.60 g, 2.02 mmol, 2.2 equiv) in a reaction flask was added 30% hydrogen peroxide (10.30 mL) at 0 ^{o}C, and it was further stirred at 0 ^{o}C for 15 min. The resulting bright yellow solution was added dropwise to a solution of 2-(phenylthio)oxazole (0.16 g, 0.92 mmol, 1.0 equiv) in ethanol (15 mL) at 0 ^{o}C. The reaction was allowed to warm to room temperature overnight. It was then

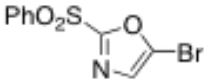
partitioned between H_2O and Et_2O. The aqueous phase was extracted with Et_2O (3 x 30 mL), the combined organic extracts were washed with brine (20 mL), and dried over Na_2SO_4. Removal of solvent and flash column chromatography over silica gel using hexanes:EtOAc (3:1) to give 2-(phenylsulfonyl)oxazole (**1**) (0.19 g, 0.91 mmol, 99%) as a white solid; ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.73-7.86 (m, 2H), 7.51 (s, 1H), 7.37-7.46 (m, 1H), 7.27-7.36 (m, 2H), 6.99 (s, 1H); ^{13}C NMR (400 MHz, $CDCl_3$): δ 158.8, 142.6, 137.9, 135.3, 129.9, 129.5, 129.0; HRMS-CI (calcd. for $C_9H_8O_3NS$ $[M+H]^+$) 210.0219, found 210.0212.

Representative procedure for alkylation of 2-(phenylsulfonyl)oxazole:

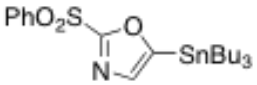


5-Iodo-2-(phenylsulfonyl)oxazole (6). To a stirred solution of (*i*-Pr)$_2$NH (0.40 mL, 2.8 mmol, 1.4 equiv) in THF (50 mL) was slowly added *n*-BuLi (2.46 M in hexanes, 0.90 mL, 2.2 mmol, 1.1 equiv) dropwise at 0 ^{o}C, and it was further stirred at 0 ^{o}C for 0.5 h. It was then cooled to -78 ^{o}C and a solution of 2-(phenylsulfonyl)oxazole (**1**) (0.42 g, 2.0 mmol, 1.0 equiv) in THF (10 mL) was added dropwise. The resulting mixture was stirred at -78 ^{o}C for 1 h and a solution of *N*-iodosuccinic imide (0.50 g, 2.2 mmol, 1.1 equiv) in THF (10 mL) was added slowly. Kept at -78 ^{o}C for 0.5 h, it was then allowed to warm to room temperature slowly, and quenched with saturated NH_4Cl (20 mL). The aqueous layer was extracted with Et_2O (3 x 20 mL), the combined organic extracts were washed with brine (30 mL), and dried over Na_2SO_4. Removal of solvent and flash column chromatography over silica gel using hexanes:EtOAc (4:1) to give **6** (0.58 g,

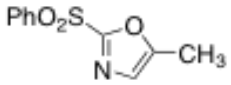
1.7 mmol, 87%) as a yellowish solid; ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.24-8.28 (m, 2H), 7.86-7.94 (m, 1H), 7.74-7.83 (m, 2H), 7.49 (s, 1H); ^{13}C NMR (400 MHz, $CDCl_3$): δ 163.2, 138.0, 137.8, 135.7, 130.2, 129.4, 93.8; HRMS-CI (calcd. for $C_9H_7O_3NIS$ $[M+H]^+$) 335.9186, found 335.9193.



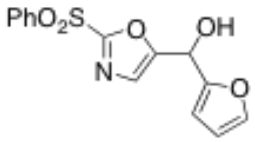
5-Bromo-2-(phenylsulfonyl)oxazole (7). General procedure using 2-(phenylsulfonyl)oxazole (**1**) (1.0 equiv), *n*-BuLi (1.1 equiv), (*i*-Pr)$_2$NH (1.4 equiv), *N*-bromosuccinic imide (1.1 equiv); yield (81%); ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.11 (m, 2H), 7.70-7.79 (m, 1H), 7.56-7.68 (m, 2H), 7.19 (s, 1H); ^{13}C NMR (400 MHz, $CDCl_3$): δ 160.1, 140.9, 137.8, 135.7, 130.2, 130.0, 129.4, 127.1; HRMS-CI (calcd. for $C_9H_7O_3NBrS$ $[M+H]^+$) 287.9325, found 287.9324.



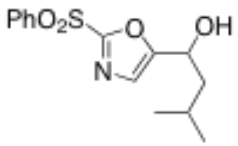
2-(Phenylsulfonyl)-5-(tributylstannyl)oxazole (8). General procedure using 2-(phenylsulfonyl)oxazole (**1**) (1.0 equiv), *n*-BuLi (1.1 equiv), (*i*-Pr)$_2$NH (1.4 equiv), tributyltin chloride (1.1 equiv); yield (86%); ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.10 (d, *J* = 7.3 Hz, 2H), 7.66-7.69 (m, 1H), 7.56-7.61 (m, 2H), 7.25 (s, 1H), 1.47-1.55 (m, 6H), 1.24-1.34 (m, 6H), 1.12-1.16 (t, *J* = 8.0 Hz, 6H), 0.87 (t, *J* = 7.2 Hz, 3H); ^{13}C NMR (400 MHz, $CDCl_3$): δ 162.9, 162.8, 139.1, 138.7, 134.7, 129.6, 128.9, 28.9, 27.2, 13.8, 10.8; HRMS-CI (calcd. for $C_{21}H_{34}O_3NSSn$ $[M+H]^+$) 500.1276, found 500.1254.



5-Methyl-2-(phenylsulfonyl)oxazole (9). General procedure using 2-(phenylsulfonyl)oxazole (**1**) (1.0 equiv), *n*-BuLi (1.1 equiv), (*i*-Pr)$_2$NH (1.4 equiv), iodomethane (1.1 equiv); yield (91%); ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.10 (m, 2H), 7.67-7.73 (m, 1H), 7.56-7.62 (m, 2H), 6.93 (s, 1H), 2.38 (s, 3H); ^{13}C NMR (400 MHz, $CDCl_3$): δ 157.3, 153.8, 138.3, 135.0, 129.7, 128.9, 125.7, 11.4; HRMS-CI (calcd. for $C_{10}H_{10}O_3NS$ $[M+H]^+$) 224.0376, found 224.0375.

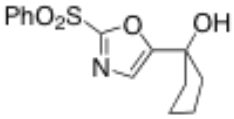


Furan-2-yl(2-(phenylsulfonyl)oxazol-5-yl)methanol (10). General procedure using 2-(phenylsulfonyl)oxazole (**1**) (1.0 equiv), *n*-BuLi (1.1 equiv), (*i*-Pr)$_2$NH (1.4 equiv), furo-2-aldehyde (1.1 equiv); yield (72%); ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.10 (d, *J* = 8.1 Hz, 2H), 7.70-7.75 (m, 1H), 7.58-7.64 (m, 2H), 7.44 (s, 1H), 7.18 (s, 1H), 6.36-6.40 (m, 2H), 5.92 (s, 1H), 2.77 (br s, 1H); ^{13}C NMR (400 MHz, $CDCl_3$): δ 158.5, 154.6, 150.8, 143.6, 137.9, 135.2, 129.8, 129.1, 126.9, 110.9, 109.2, 62.5; HRMS-CI (calcd. for $C_{14}H_{12}O_5NS$ $[M+H]^+$) 306.0431, found 306.0439.

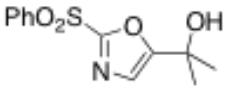


3-Methyl-1-(2-(phenylsulfonyl)oxazol-5-yl)butan-1-ol (11). General procedure using 2-(phenylsulfonyl)oxazole (**1**) (1.0 equiv), *n*-BuLi (1.1 equiv), (*i*-Pr)$_2$NH (1.4 equiv), isovaleraldehyde (1.1 equiv); yield (75%); ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.07-8.11 (m, 2H), 7.69-7.74 (m, 1H), 7.58-7.63 (m, 2H), 7.12 (d, *J* = 0.8 Hz, 1H), 4.82-4.90 (m, 1H), 2.39 (d, *J* = 5.5 Hz, 1H), 1.70-1.84 (m, 2H), 1.58-1.67 (m, 1H), 0.94 (t, *J* = 6.5 Hz, 6H); ^{13}C NMR (400 MHz, $CDCl_3$): δ

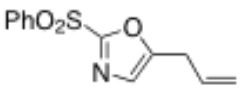
158.5, 157.7, 137.8, 134.9, 129.6, 128.8, 124.9, 64.3, 44.0, 24.3, 23.0, 21.7; HRMS-CI (calcd. for $C_{14}H_{18}O_4NS$ $[M+H]^+$) 296.0951, found 296.0943.



1-(2-(Phenylsulfonyl)oxazol-5-yl)cyclopentanol (12). General procedure using 2-(phenylsulfonyl)oxazole (**1**) (1.0 equiv), *n*-BuLi (1.1 equiv), $(i\text{-Pr})_2NH$ (1.4 equiv), cyclopentanone (1.1 equiv); yield (87%); ^1H NMR (400 MHz, $CDCl_3$): δ 8.08 (d, *J* = 7.7 Hz, 2H), 7.67-7.74 (m, 1H), 7.56-7.63 (m, 2H), 7.11 (s, 1H), 2.28 (br s, 1H), 1.70-2.02 (m, 8H); ^{13}C NMR (400 MHz, $CDCl_3$): δ 160.7, 157.7, 138.1, 135.1, 129.8, 128.9, 124.2, 78.5, 77.6, 77.2, 76.9, 40.2, 23.7; HRMS-CI (calcd. for $C_{14}H_{16}O_4NS$ $[M+H]^+$) 294.0795, found 294.0785.

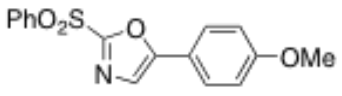


2-(2-(Phenylsulfonyl)oxazol-5-yl)propan-2-ol (13). General procedure using 2-(phenylsulfonyl)oxazole (**1**) (1.0 equiv), *n*-BuLi (1.1 equiv), $(i\text{-Pr})_2NH$ (1.4 equiv), acetone (1.1 equiv); yield (81%); ^1H NMR (400 MHz, $CDCl_3$): δ 8.07 (d, *J* = 7.6 Hz, 2H), 7.65-7.73 (m, 1H), 7.53-7.64 (m, 2H), 7.08 (s, 1H), 2.59 (br s, 1H), 1.59 (s, 6H); ^{13}C NMR (400 MHz, $CDCl_3$): δ 161.9, 157.9, 138.3, 135.4, 130.0, 129.2, 123.9, 68.5, 29.0; HRMS-CI (calcd. for $C_{12}H_{14}O_4NS$ $[M+H]^+$) 268.0638, found 268.0634.



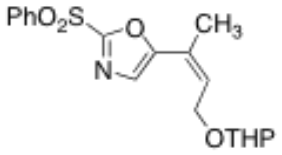
5-Allyl-2-(phenylsulfonyl)oxazole (14). To a stirred solution of $(i\text{-Pr})_2NH$ (0.06 mL, 0.38 mmol, 1.5 equiv) in THF (10 mL) was slowly added *n*-BuLi (2.46 M in hexanes, 0.12 mL, 0.30 mmol, 1.2 equiv) dropwise at 0 °C and it was stirred at 0 °C for further 0.5 h. It was then cooled

to -78 °C and a solution of 2-(phenylsulfonyl)oxazole (**1**) (53.0 mg, 0.25 mmol, 1.0 equiv) in THF (5 mL) was slowly added dropwise. It was stirred at -78 °C for 1 h and a solution of $ZnBr_2$ (45.0 mg, 0.20 mmol, 0.8 equiv) in THF (5 mL) was slowly added. After staying at -78 °C for 0.5 h, it was allowed to warm to room temperature and stirred at room temperature for 1 h. A solution of $Pd(PPh_3)_4$ (28.9 mg, 0.025 mmol, 10% equiv) and allyl bromide (60.5 mg, 0.50 mmol, 2.0 equiv) in THF (5 mL) was slowly added and it was heated to 60 °C. After the completion of the reaction, it was cooled to room temperature and quenched with saturated aqueous NH_4Cl (20 mL). The separated aqueous layer was extracted with Et_2O (2 x 20 mL), the combined organic extracts were washed with saturated aqueous $NaHCO_3$ (20 mL), brine (20 mL), and dried over Na_2SO_4. Removal of solvent and flash column chromatography over silica gel using hexanes:EtOAc (5:1) to give **14** (56.0 mg, 0.23 mmol, 90%) as yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.10 (m, 2H), 7.57-7.75 (m, 3H), 6.96 (s, 1H), 5.80-5.90 (m, 1H), 5.20 (m, 2H), 3.47 (dd, J_1 = 6.6 Hz, J_2 = 1.1 Hz, 2H); ^{13}C NMR (400 MHz, $CDCl_3$): δ 157.7, 155.5, 138.3, 135.0, 130.7, 129.7, 129.0, 125.6, 119.5, 30.3; HRMS-CI (calcd. for $C_{12}H_{12}O_3NS$ $[M+H]^+$) 250.0532, found 250.0535.



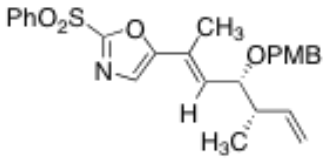
5-(4-Methoxyphenyl)-2-(phenylsulfonyl)oxazole (15). To a stirred solution of 5-iodo-2-phenylsulfonyloxazole (**6**) (52.1 mg, 0.16 mmol, 1.0 equiv), palladium tetrakis(triphenylphosphine) (18.5 mg, 0.016 mmol, 0.1 equiv), phenyl boronic acid (39.0 mg, 0.32 mmol, 2.0 equiv) in THF (2 mL) and toluene (2 mL) was added aqueous Na_2CO_3 (1 mL, 2.0 M), and the resulting mixture was degassed by blowing

in with nitrogen for 5 min. The reaction mixture was then sealed and heated to 70 °C for 18 h. It was cooled to rt, diluted with ether (50 mL), washed with saturated aqueous $NaHCO_3$ (10 mL), brine (10 mL), and dried over Na_2SO_4. Removal of solvent and flash column chromatography over silica gel with hexanes:EtOAc (4:1) to give 5-phenyl-2-phenylsulfonyloxazole (**15**) (41.7 mg, 0.14 mmol, 94%); ^1H NMR (400 MHz, $CDCl_3$): δ 8.12-8.16 (m, 2H), 7.65-7.75 (m, 1H), 7.58-7.65 (m, 4H), 7.35 (s, 1H), 6.76 (d, *J* = 8.8 Hz, 2H), 3.86 (s, 3H); ^{13}C NMR (400 MHz, $CDCl_3$): δ 171.1, 161.5, 157.1, 155.6, 138.7, 135.2, 130.0, 129.2, 127.2, 122.6, 119.2, 115.0, 55.9; HRMS-CI (calcd. for $C_{16}H_{14}O_4NS$ $[M+H]^+$) 316.0638, found 316.0639.



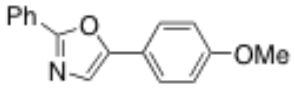
(*Z*)-2-(Phenylsulfonyl)-5-(4-(tetrehydro-2*H*-pyran-2-yloxy)but-2-en-2-yl)oxazole (17). To a stirred solution of 5-tributylstannyl-2-phenylsulfonyloxazole (**8**) (40.0 mg, 0.08 mmol, 1.0 equiv) in anhydrous DMSO (4.0 mL) was added anhydrous LiCl (21.0 mg, 0.48 mmol, 6.0 equiv), CuCl (40.0 mg, 0.40 mmol, 5.0 equiv), $Pd(PPh_3)_4$ (9.3 mg, 10% equiv), and iodide **16** (28.2 mg, 0.10 mmol, 1.2 equiv). It was degassed by blowing in with nitrogen for 5 min, the reaction mixture was then sealed and heated to 60 °C for 4 h. After the completion of the reaction, it was cooled to room temperature, diluted with Et_2O (50 mL), and washed with a mixture of brine (20 mL) and saturated aqueous NH_4Cl (10 mL). The aqueous layer was further extracted with Et_2O (2 x 20 mL), and the combined organic extracts were washed with brine (2 x 20 mL), dried over Na_2SO_4. Removal of solvent and flash column chromatography over silica gel with hexanes:EtOAc (4:1) to give **17** (26.1 mg, 0.072 mmol, 90%) as yellowish oil;

^{1}H NMR (400 MHz, $CDCl_3$): δ 8.08-8.15 (m, 2H), 7.57-7.75 (m, 3H), 7.16 (s, 1H), 5.90 (m, 1H), 4.65 (m, 1H), 4.26 (m, 2H), 3.87 (m, 1H), 3.52 (m, 1H), 2.06 (d, *J* = 1.5 Hz, 3H), 1.70-1.90 (m, 2H), 1.50-1.68 (m, 4H); ^{13}C NMR (400 MHz, $CDCl_3$): δ 157.5, 154.5, 138.2, 135.1, 131.8, 129.8, 129.0, 126.8, 122.6, 98.9, 77.5, 77.2, 76.9, 64.6, 62.7, 30.8, 25.6, 20.7, 19.7; HRMS-CI (calcd. for $C_{18}H_{22}O_5NS$ $[M+H]^+$) 364.1213, found 364.1211.

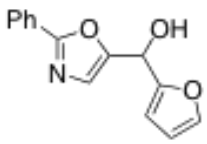


5-((4*R*,5*S*,*E*)-4-(4-Methoxybenzyloxy)-5-methyl-hepta-2,6-dien-2-yl)-2-(phenylsulfonyl)oxazole (18). The same procedure as described for compound **17** using 5-tributylstannyl-2-phenylsulfonyloxazole (**8**) (1.0 equiv), LiCl (6.0 equiv), CuCl (5.0 equiv), $Pd(PPh_3)_4$ (0.1 equiv), and 1-(((3*S*,4*R*,*E*)-6-iodo-3-methylhepta-1,5-dien-4-yloxy)methyl)-4-methoxybenzene (1.1 equiv); yield (92%); ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.13 (m, 2H), 7.58-7.76 (m, 3H), 7.23 (d, *J* = 8.6 Hz, 2H), 7.10 (s, 1H), 6.87 (d, *J* = 8.8 Hz, 2H), 6.15 (dd, J_1 = 9.4 Hz, J_2 = 1.2 Hz, 1H), 5.71-5.85 (m, 1H), 5.94-5.07 (m, 2H), 4.25-4.55 (dd, J_1 = 93.6 Hz, J_2 = 11.7 Hz, 2H), 3.98 (dd, J_1 = 9.5 Hz, J_2 = 6.8 Hz, 1H), 3.81 (s, 3H), 2.44-2.54 (m, 1H), 1.89 (d, *J* = 1.1 Hz, 3H), 1.09 (d, *J* = 6.8 Hz, 3H); ^{13}C NMR (400 MHz, $CDCl_3$): δ 159.4, 157.4, 156.1, 139.7, 138.3, 135.0, 131.8, 130.6, 129.8, 129.4, 129.1, 124.5, 124.2, 115.4, 114.0, 77.8, 70.4, 55.5, 42.8, 15.8, 14.0; HRMS-CI (calcd. for $C_{25}H_{28}O_5NS$ $[M+H]^+$) 454.1683, found, 454.1684.

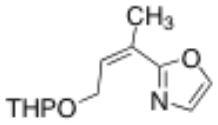
Representative Procedure for the displacement of sulfone:



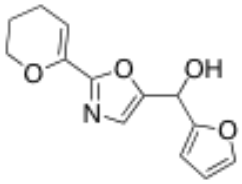
5-(4-Methoxyphenyl)-2-phenyloxazole (19). To a stirred solution of 5-(4-Methoxyphenyl)-2-(phenyl-sulfonyl)oxazole (**15**) (16.6 mg, 0.053 mmol, 1.0 equiv) in THF (2 mL) was slowly added PhLi (1.8 M in butyl ether, 0.04 mL, 0.063 mmol, 1.2 equiv) dropwise. And it was allowed to warm to room temperature and quenched with H_2O (1 mL). The separated aqueous layer was extracted with Et_2O (2 x 5 mL), the combined organic extracts were washed with brine (2 mL), and dried over Na_2SO_4. Removal of solvent and flash column chromatography over silica gel using hexanes:EtOAc (8:1) to give **19** (11.8 mg, 0.047 mmol, 90%) as yellowish oil; ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.09-8.14 (m, 2H), 7.67 (d, *J* = 8.9 Hz, 2H), 7.45-7.52 (m, 3H), 7.34 (s, 1H), 6.99 (d, *J* = 8.9 Hz, 2H), 3.87 (s, 3H); ^{13}C NMR (400 MHz, $CDCl_3$): δ 160.8, 160.1, 151.6, 130.4, 129.9, 129.0, 127.8, 126.4, 126.0, 122.2, 121.1, 115.6, 114.6, 55.6; HRMS-CI (calcd. for $C_{16}H_{14}O_2N$ $[M+H]^+$) 252.1019, found, 252.1022.



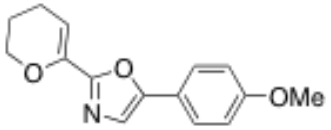
Furan-2-yl(2-phenyloxazol-5-yl)methanol (20). General procedure using sulfone (1.0 equiv) and phenyl lithium (2.2 equiv); yield (85%); ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.01-8.09 (m, 2H), 7.44-7.50 (m, 3H), 7.13 (s, 1H), 6.42 (s, 2H), 5.98 (d, *J* = 5.1 Hz, 1H), 2.64 (d, *J* = 5.7 Hz, 1H); ^{13}C NMR (400 MHz, $CDCl_3$): δ 162.3, 152.3, 150.5, 143.2, 130.8, 129.0, 127.5, 126.7, 126.4, 110.8, 108.5, 62.8; HRMS-CI (calcd. for $C_{14}H_{12}O_3N$ $[M+H]^+$) 242.0812, found, 242.0800.



(*Z*)-2-(4-(Tetrahydro-2*H*-pyran-2-yloxy)but-2-en-2-yl)oxazole (21). General procedure using sulfone (1.0 equiv) and the corresponding alkenyl lithium (generated by treating the corresponding alkenyl iodide (1.5 equiv) with *t*-BuLi (3.0 equiv) at -78 °C); yield (78%); ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.65 (s, 1H), 7.19 (s, 1H), 6.01-6.07 (m, 1H), 4.57-4.82 (m, 3H), 3.86-3.95 (m, 1H), 3.50-3.59 (m, 1H), 2.18 (d, *J* = 1.5 Hz, 3H), 1.49-1.94 (m, 6H); ^{13}C NMR (400 MHz, $CDCl_3$): δ 162.4, 138.3, 134.1, 128.2, 122.7, 98.9, 66.0, 62.6, 31.0, 25.7, 20.8, 19.8; HRMS-CI (calcd. for $C_{12}H_{18}O_3N$ $[M+H]^+$) 224.1281, found, 224.1282.

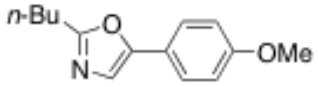


(2-(3,4-Dihydro-2*H*-pyran-6-yl)oxazol-5-yl)(furan-2-yl)-methanol (22). General procedure using sulfone (1.0 equiv) and the corresponding alkenyl lithium (generated by treating the corresponding alkenyl iodide (3.0 equiv) with *t*-BuLi (3.0 equiv) at -50 °C); yield (71%); ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.46 (m, 1H), 7.03 (s, 1H), 6.35-6.42 (m, 2H), 5.85-5.95 (m, 2H), 4.21 (t, *J* = 5.3 Hz, 2H), 2.44 (d, *J* = 6.6 Hz, 1H), 2.20-2.29 (m, 2H), 1.90-1.99 (m, 2H); ^{13}C NMR (500 MHz, $CDCl_3$): δ 158.3, 152.0, 143.0, 142.3, 125.7, 110.6, 110.0, 108.3, 105.0, 66.8, 62.4, 21.9, 20.3; HRMS-CI (calcd. for $C_{13}H_{14}O_4N$ $[M+H]^+$) 248.2546, found, 248.2541.

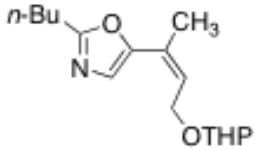


2-(3,4-dihydro-2*H*-pyran-6-yl)-5-(4-methoxy-phenyl)oxazole (23). General procedure using sulfone (1.0 equiv) and the corresponding alkenyl lithium (generated by treating the corresponding alkenyl iodide (1.5 equiv) with *t*-BuLi (1.5 equiv) at -50 °C); yield

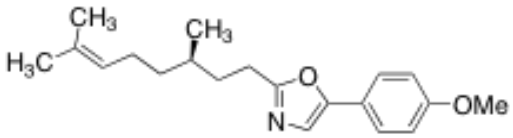
(83%); ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.59 (d, *J* = 9.0 Hz, 2H), 7.23 (s, 1H), 6.95 (d, *J* = 9.0 Hz, 2H), 5.90 (t, *J* = 4.3 Hz, 1H), 4.24 (t, *J* = 5.1 Hz, 2H), 3.85 (s, 3H), 2.25-2.32 (m, 2H), 1.92-2.00 (m, 2H); ^{13}C NMR (500 MHz, $CDCl_3$): δ 159.8, 157.0, 142.5, 125.8, 121.4, 114.3, 104.0, 66.8, 55.4, 22.0, 20.4; HRMS-CI (calcd. for $C_{15}H_{16}O_3N$ $[M+H]^+$) 258.2924, found, 258.2921.



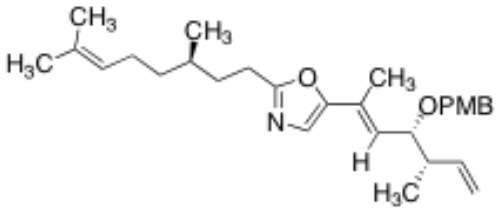
2-Butyl-5-(4-methoxyphenyl)oxazole (24). General procedure using sulfone (1.0 equiv) and *n*-BuLi (1.2 equiv); yield (69%); ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.55 (d, *J* = 9.0 Hz, 2H), 7.09 (s, 1H), 6.94 (d, *J* = 9.0 Hz, 2H), 3.85 (s, 3H), 2.82 (t, *J* = 7.6 Hz, 2H), 1.76-1.86 (m, 2H), 1.41-1.51 (m, 2H), 0.97 (t, *J* = 7.2 Hz, 3H); ^{13}C NMR (500 MHz, $CDCl_3$): δ 159.5, 150.8, 125.5, 121.3, 120.2, 114.3, 55.4, 29.2, 28.0, 22.3, 13.7; HRMS-CI (calcd. for $C_{14}H_{18}O_2N$ $[M+H]^+$) 232.1332, found, 232.1325.



(*Z*)-2-Butyl-5-(4-(tetrahydro-2*H*-pyran-2-yloxy)but-2-en-2-yl)oxazole (25). General procedure using sulfone (1.0 equiv) and *n*-BuLi (1.2 equiv); yield (76%); ^{1}H NMR (400 MHz, $CDCl_3$): δ 6.89 (s, 1H), 5.65 (m, 1H), 4.44 (m, 1H), 4.05-4.17 (m, 1H), 3.70-3.91 (m, 2H), 3.35-3.45 (m, 1H), 2.75 (t, *J* = 7.6 Hz, 2H), 1.99 (s, 3H), 1.38-1.99 (m, 10H), 0.98 (t, *J* = 7.2 Hz, 3H); ^{13}C NMR (500 MHz, $CDCl_3$): δ 149.3, 127.8, 124.7, 123.9, 122.7, 98.5, 65.2, 62.4, 30.7, 29.4, 28.1, 25.4, 22.0, 20.9, 19.6, 13.8; HRMS-CI (calcd. for $C_{16}H_{26}O_3N$ $[M+H]^+$) 280.3825, found, 280.3820.

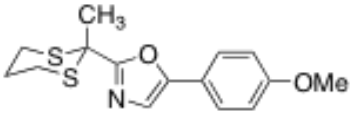


(*R*)-2-(3,7-dimethyloct-6-enyl)-5-(4-methoxyphenyl)oxazole (26). General procedure using sulfone (1.0 equiv) and the corresponding alkyl lithium (generated by treating the corresponding alkyl iodide (1.5 equiv) with *t*-BuLi (3.0 equiv) at -50 ^{o}C); yield (79%); ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.55 (d, *J* = 9.0 Hz, 2H), 7.09 (s, 1H), 6.94 (d, *J* = 9.0 Hz, 2H), 5.02 (m, 1H), 3.85 (s, 3H), 2.65-2.82 (m, 2H), 1.80-2.10 (m, 3H), 1.18-1.72 (m, 10H), 0.96 (d, *J* = 6.7 Hz, 3H); ^{13}C NMR (500 MHz, $CDCl_3$): δ 164.3, 159.5, 150.9, 131.4, 125.7, 124.7, 121.3, 120.4, 114.3,, 55.6, 37.0, 34.2, 32.3, 28.9, 26.2, 25.9, 25.6, 19.4, 17.9; HRMS-CI (calcd. for $C_{20}H_{28}O_2N$ $[M+H]^+$) 314.2115, found, 314.2124.

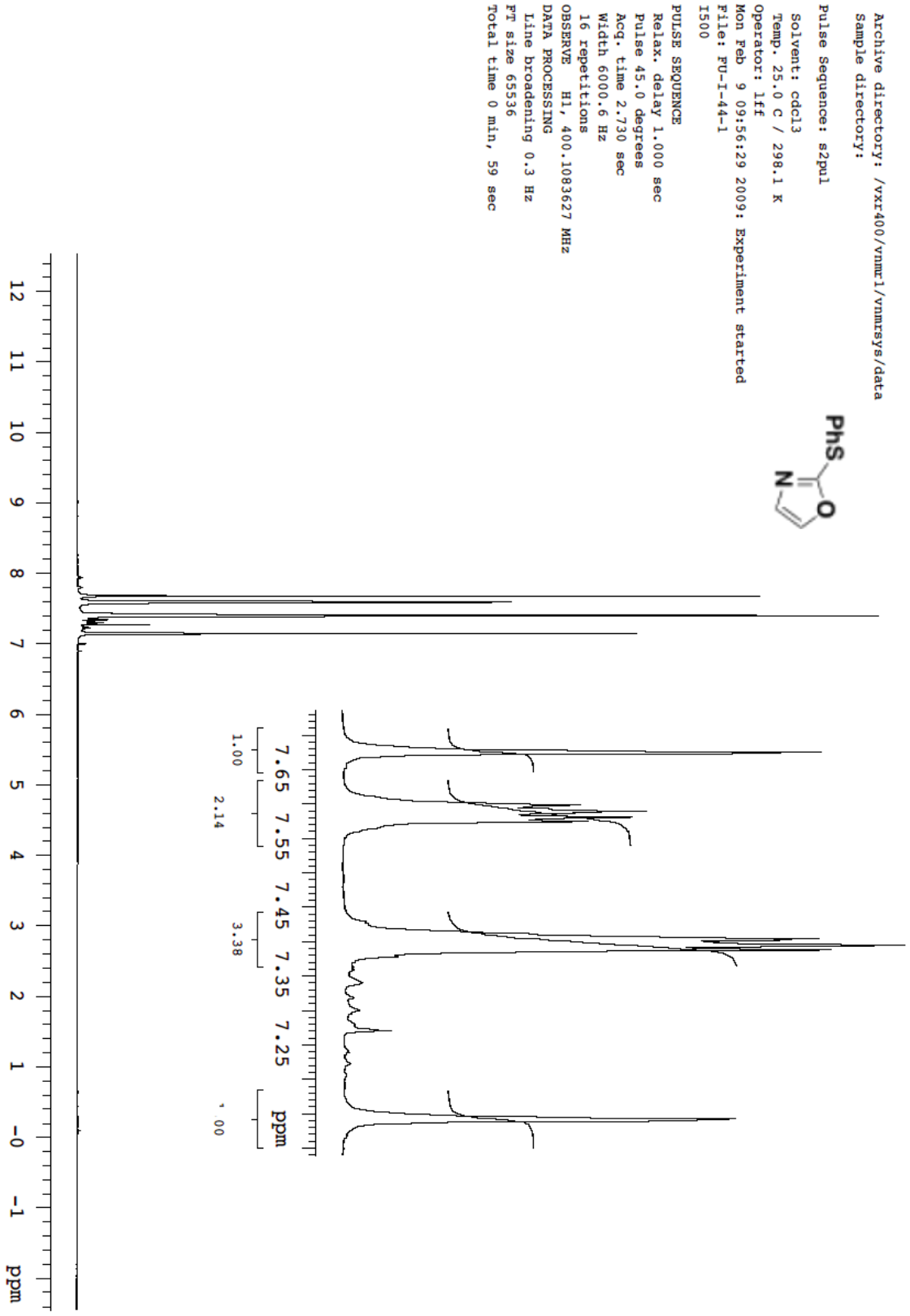


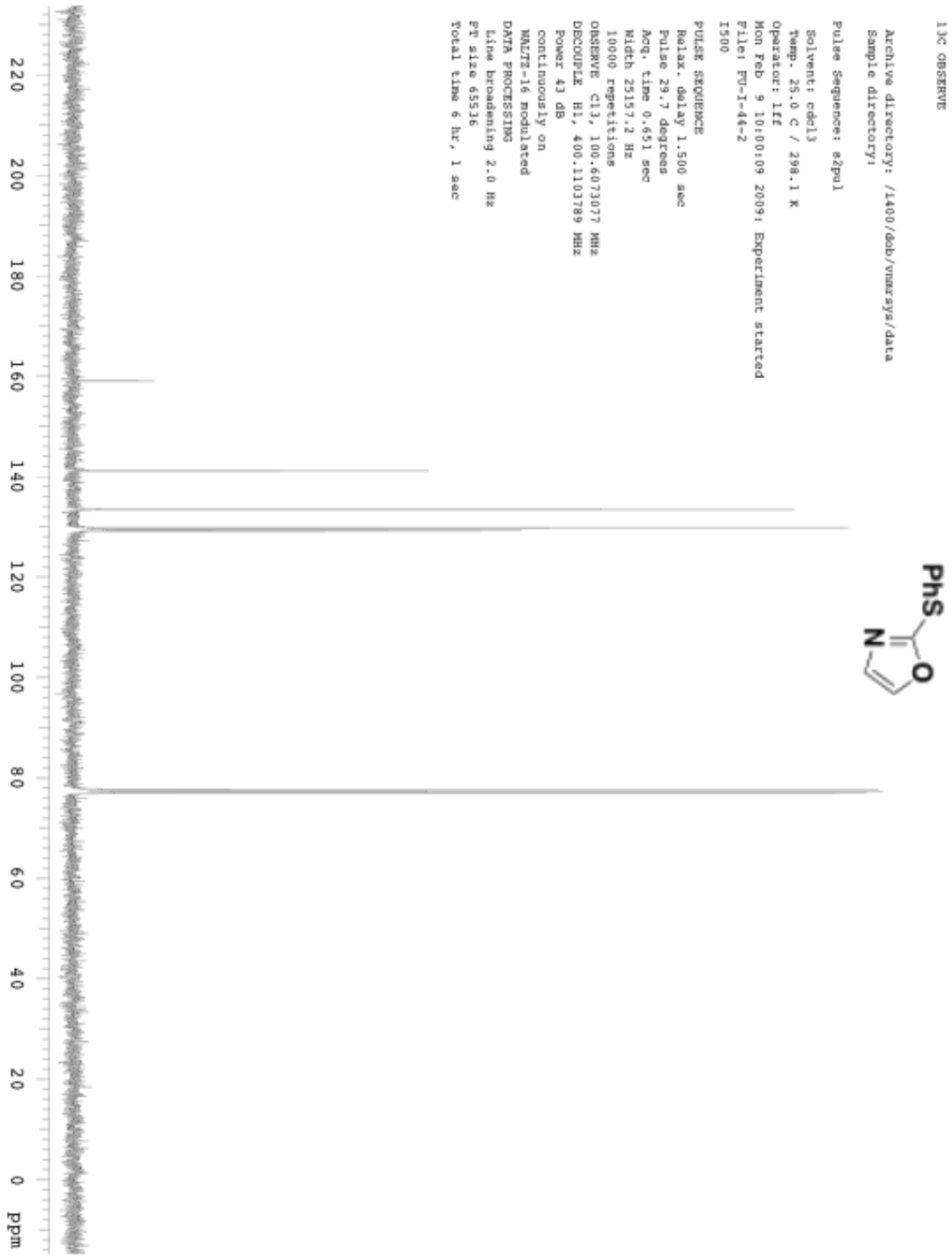
2-((*R*)-3,7-dimethyloct-6-enyl)-5-((4*R*,-5*S*,*E*)-4-(4-methoxybenzyloxy)-5-methylhepta-2,6-dien-2-yl)oxazole (27). General procedure using sulfone (1.0 equiv) and the corresponding alkyl lithium (generated by treating the corresponding alkyl iodide (1.5 equiv) with *t*-BuLi (3.0 equiv) at -50 ^{o}C); yield (81%); ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.25 (d, *J* = 8.6 Hz, 2H), 6.88 (d, *J* = 8.6 Hz, 2H), 6.64 (s, 1H), 5.77-5.88 (m, 2H), 4.96-5.14 (m, 3H), 4.40 (dd, J_1 = 100.5 Hz, J_2 = 16.2 Hz, 2H), 4.36-4.49 (m, 2H), 3.97 (dd, J_1 = 9.4 Hz, J_2 = 6.6 Hz, 1H), 3.81 (s, 3H), 2.42-2.51 (m, 1H), 1.84-2.10 (m, 3H), 1.82 (s, 3H), 1.24-1.74 (m, 10H), 1.08 (d, *J* = 6.6 Hz, 3H), 0.96 (d, J_1 = 6.6 Hz, 3H); ^{13}C NMR (500 MHz, $CDCl_3$): δ 161.6, 159.0, 147.4, 140.1, 131.4, 130.9, 129.2, 128.5, 128.4, 125.3, 124.5, 124.3, 121.7,

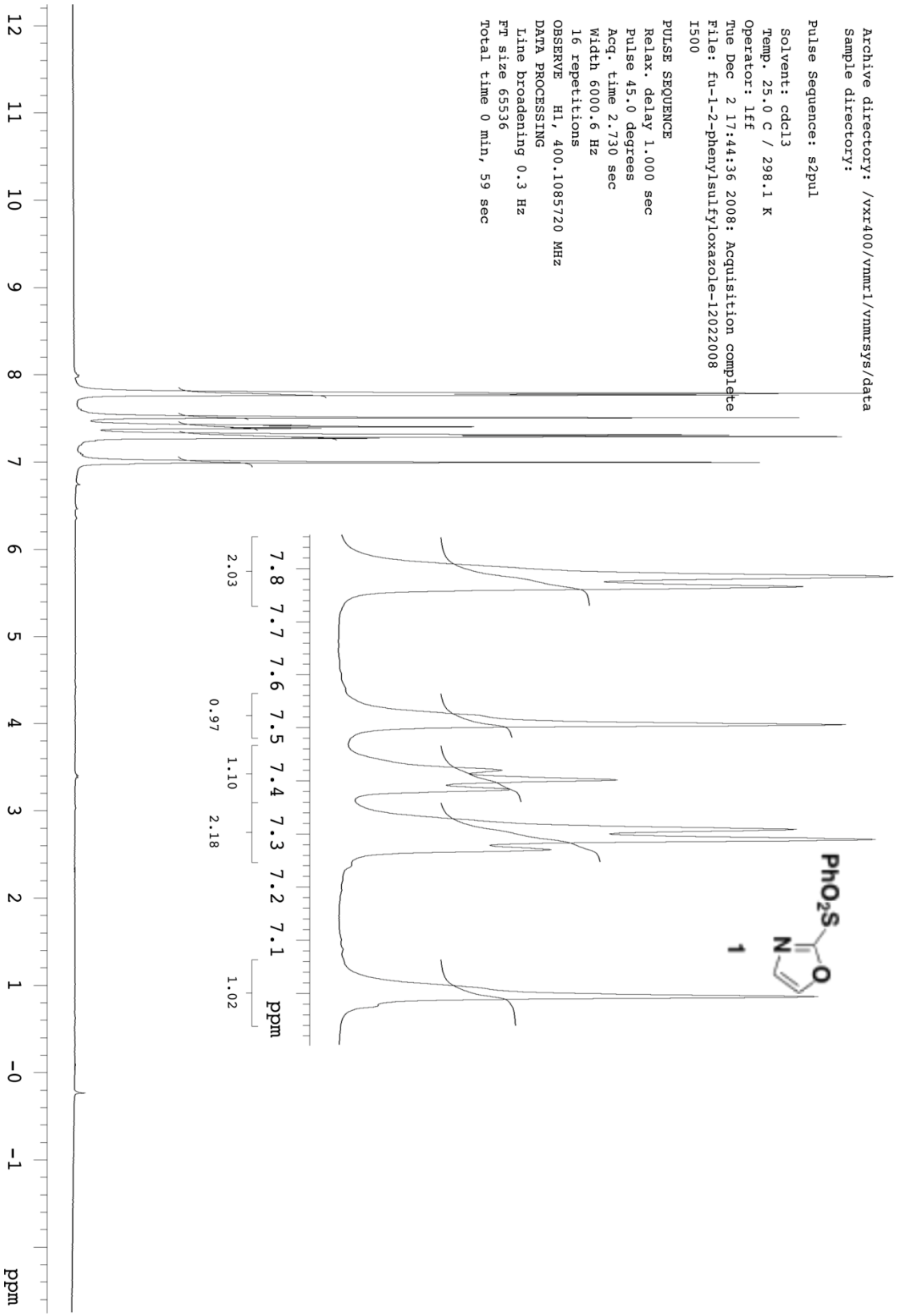
114.7, 113.7, 77.6, 70.0, 69.5, 55.3, 42.7, 37.0, 35.6, 29.2, 25.7, 25.4, 19.4, 17.7, 15.6, 13.1; HRMS-CI (calcd. for $C_{29}H_{42}O_3N$ $[M+H]^+$) 452.3159, found, 452.3178.

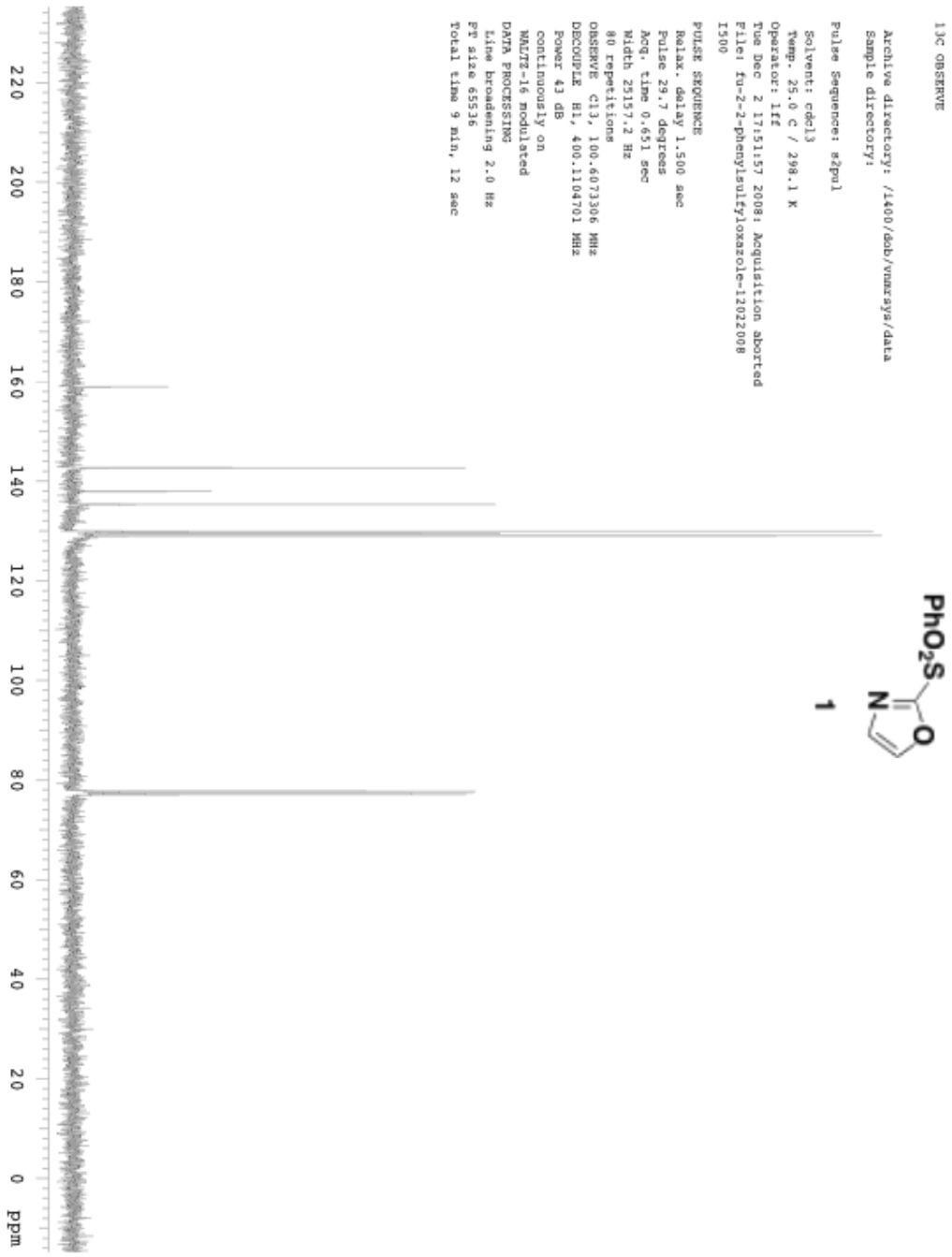


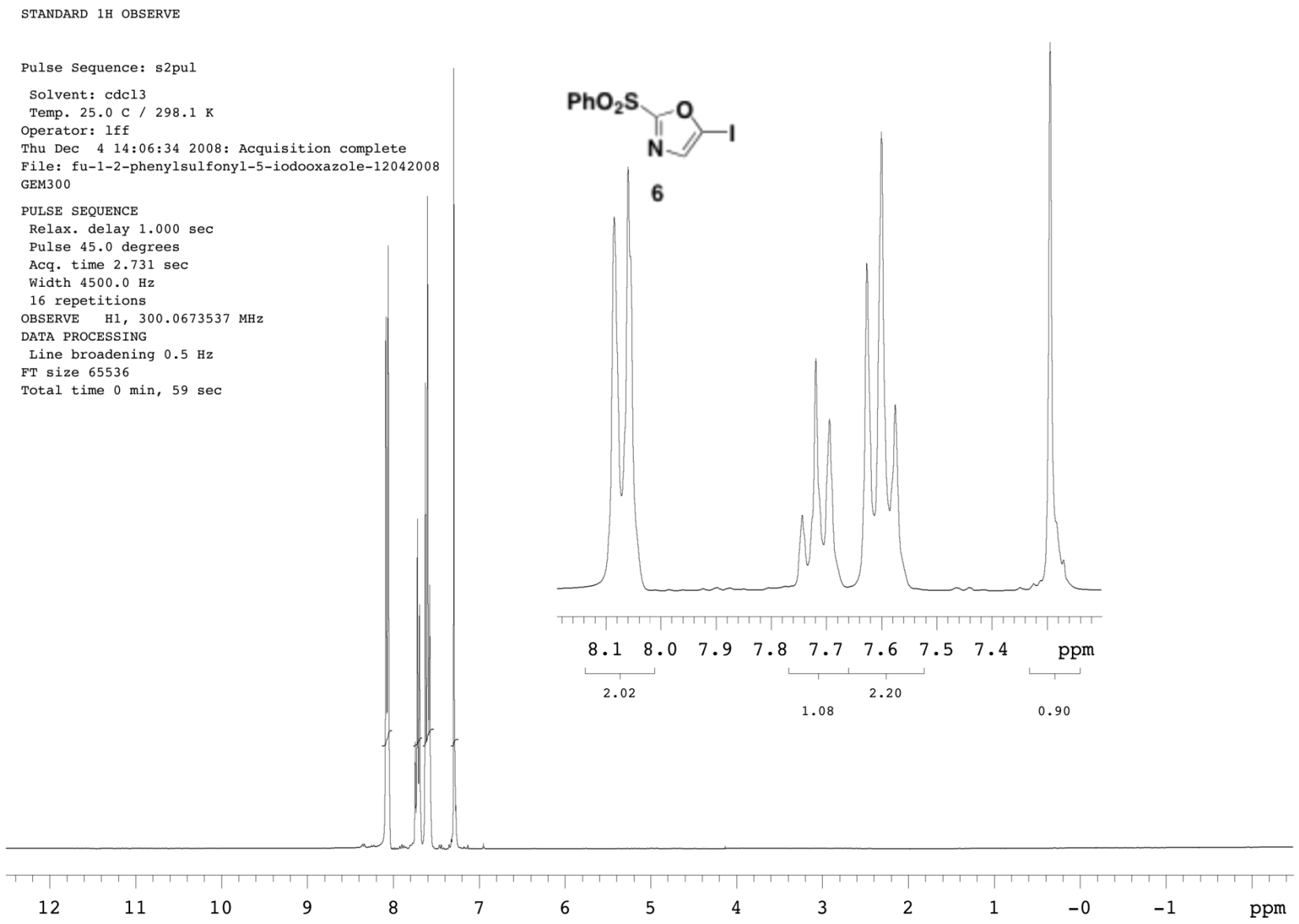
5-(4-Methoxyphenyl)-2-(2-methyl-1,3-dithian-2-yl) oxazole (28). General procedure using sulfone (1.0 equiv) and the corresponding alkyl lithium (generated by treating 2-methyl-1,3-dithiane (1.5 equiv) with *n*-BuLi (1.5 equiv) at -20 °C); yield (82%); ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.56 (d, *J* = 9.0 Hz, 2H), 7.15 (s, 1H), 6.96 (d, *J* = 9.0 Hz, 2H), 3.86 (s, 3H), 3.47 (m, 2H), 2,73 (m, 2H), 2.19 (m, 1H), 1.88-2.08 (m, 4H); ^{13}C NMR (400 MHz, $CDCl_3$): δ 164.6, 159.9, 151.0, 125.8, 120.8, 120.1, 114.4, 55.4, 43.9, 28.4, 27.3, 24.4; HRMS-ESI (calcd. for $C_{15}H_{18}O_2NS_2$ $[M+H]^+$) 308.0779, found, 308.0782.

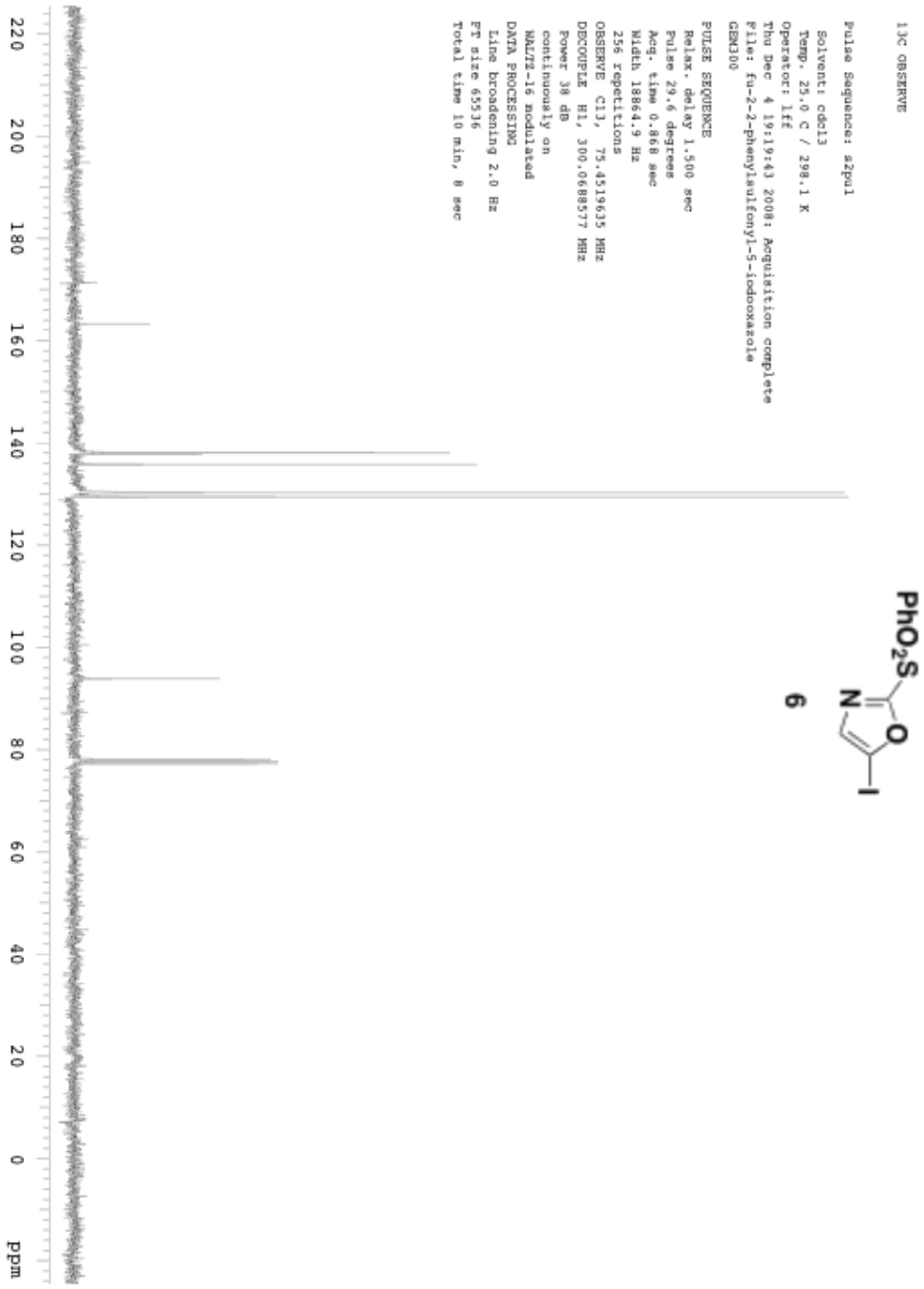

STANDARD 1H OBSERVE
Archive directory: /vxr400/vnmr1/vnmrsys/data
Sample directory:
Pulse Sequence: s2pul
Solvent: cdcl3
Temp. 25.0 C / 298.1 K
Operator: lff
Mon Feb 9 09:56:29 2009: Experiment started
File: FU-I-44-1
I500
PULSE SEQUENCE
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 2.730 sec
Width 6000.6 Hz
16 repetitions
OBSERVE H1, 400.1083627 MHz
DATA PROCESSING
Line broadening 0.3 Hz
FT size 65536
Total time 0 min, 59 sec
PhS
N
O
7.65 7.55 7.45 7.35 7.25 ppm
1.00
2.14
3.38
1.00
12 11 10 9 8 7 6 5 4 3 2 1 -0 -1 ppm

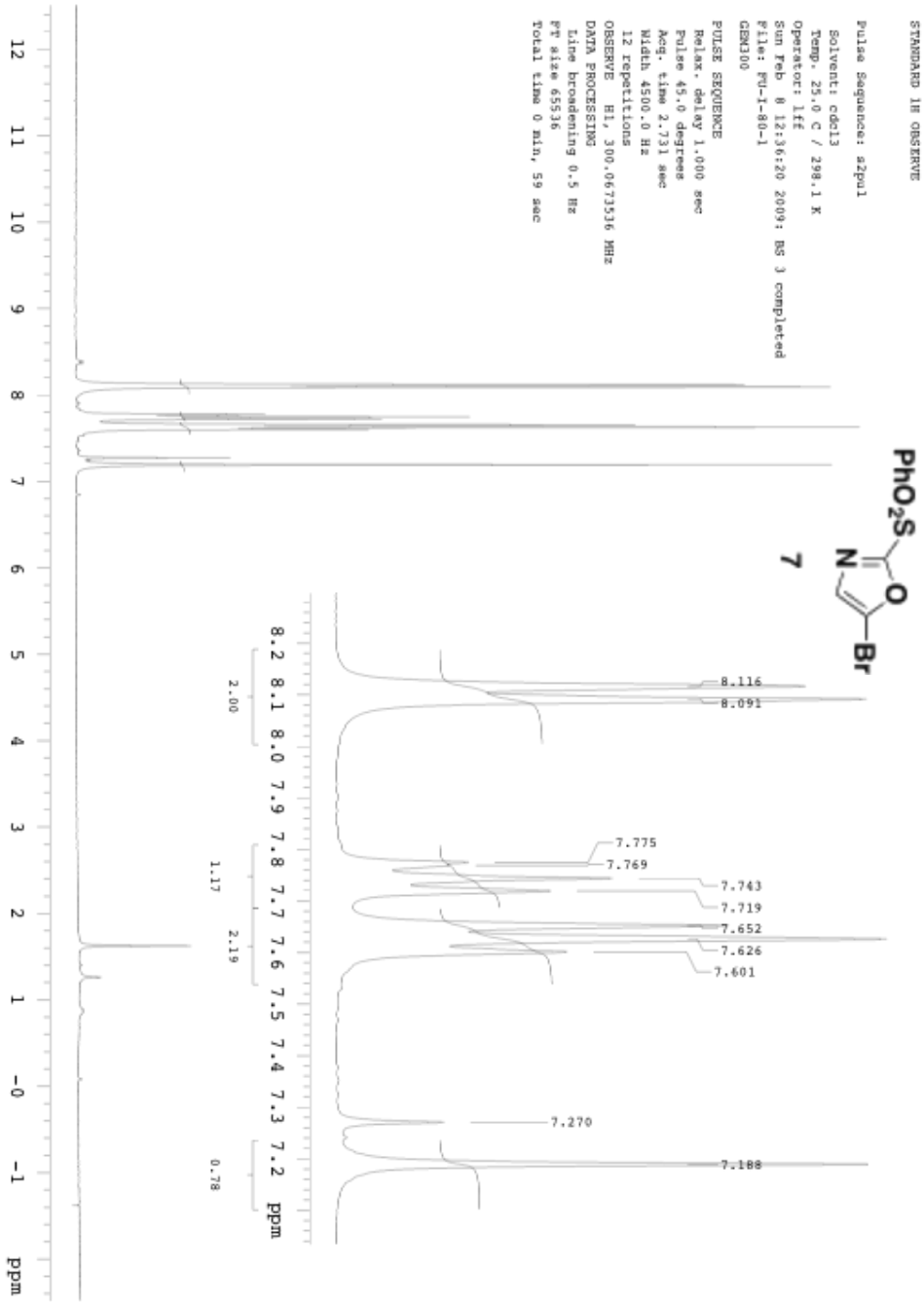

13C OBSERVE
Archive directory: /1400/dob/vnmrsys/data
Sample directory:
Pulse Sequence: s2pul
Solvent: cdcl3
Temp. 25.0 C / 298.1 K
Operator: lfe
Mon Feb 9 10:00:09 2009: Experiment started
File: FU-I-44-2
I500
PULSE SEQUENCE
Relax. delay 1.500 sec
Pulse 29.7 degrees
Acq. time 0.651 sec
Width 25157.2 Hz
10000 repetitions
OBSERVE C13, 100.6073077 MHz
DECOUPLE H1, 400.1103789 MHz
Power 43 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 2.0 Hz
FT size 65536
Total time 6 hr, 1 sec
PhS
N
O
220
200
180
160
140
120
100
80
60
40
20
0
ppm

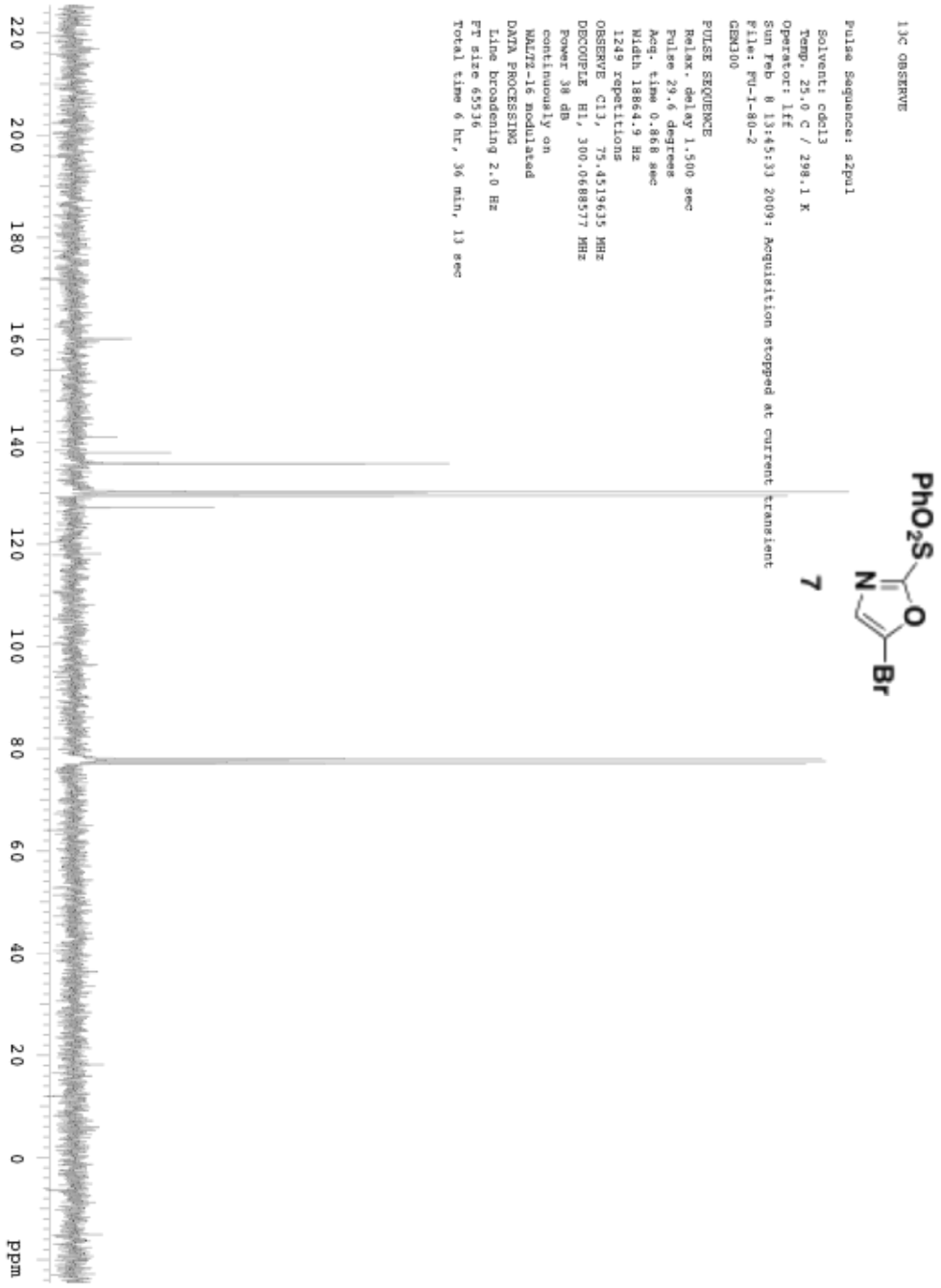

STANDARD 1H OBSERVE
Archive directory: /vxr400/vnmr1/vnmrsys/data
Sample directory:
Pulse Sequence: s2pul
Solvent: cdcl3
Temp. 25.0 C / 298.1 K
Operator: lff
Tue Dec 2 17:44:36 2008: Acquisition complete
File: fu-1-2-phenylsulfyloxazole-12022008
I500
PULSE SEQUENCE
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 2.730 sec
Width 6000.6 Hz
16 repetitions
OBSERVE H1, 400.1085720 MHz
DATA PROCESSING
Line broadening 0.3 Hz
FT size 65536
Total time 0 min, 59 sec
PhO2S
N
O
1
7.8 7.7 7.6 7.5 7.4 7.3 7.2 7.1 ppm
2.03
0.97
1.10
2.18
1.02
12 11 10 9 8 7 6 5 4 3 2 1 -0 -1 ppm

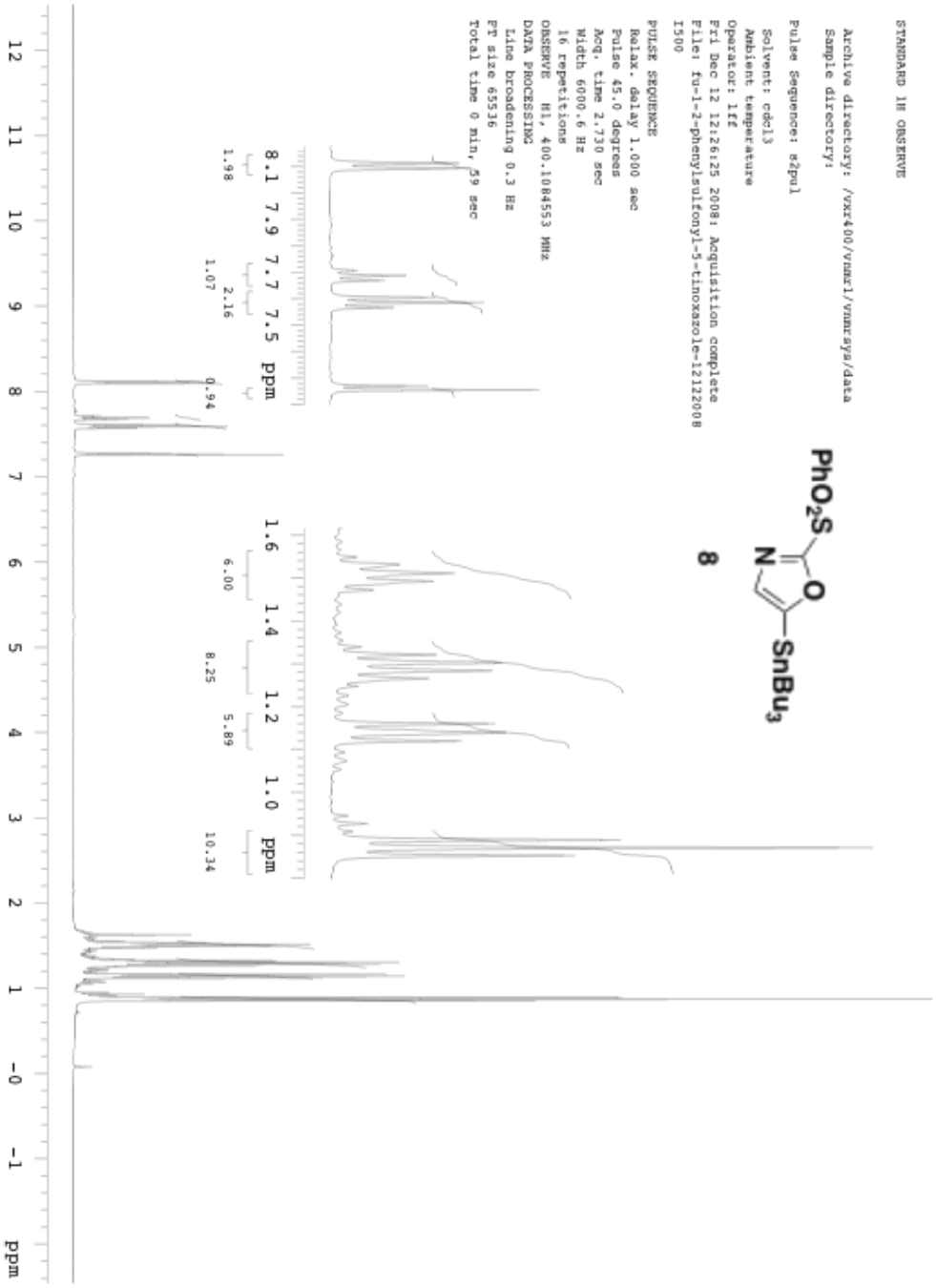

13C OBSERVE
Archive directory: /1400/dob/vnmrsys/data
Sample directory:
Pulse Sequence: s2pul
Solvent: cdcl3
Temp. 25.0 C / 298.1 K
Operator: lfe
Tue Dec 2 17:51:57 2008: Acquisition aborted
File: fu-2-phenylsulfyloxazole-12022008
I500
PULSE SEQUENCE
Relax. delay 1.500 sec
Pulse 29.7 degrees
Acq. time 0.651 sec
Width 25157.2 Hz
80 repetitions
OBSERVE C13, 100.6073306 MHz
DECOUPLE H1, 400.1104701 MHz
Power 43 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 2.0 Hz
FT size 65536
Total time 9 min, 12 sec
PhO2S
N
O
1
220
200
180
160
140
120
100
80
60
40
20
0
ppm

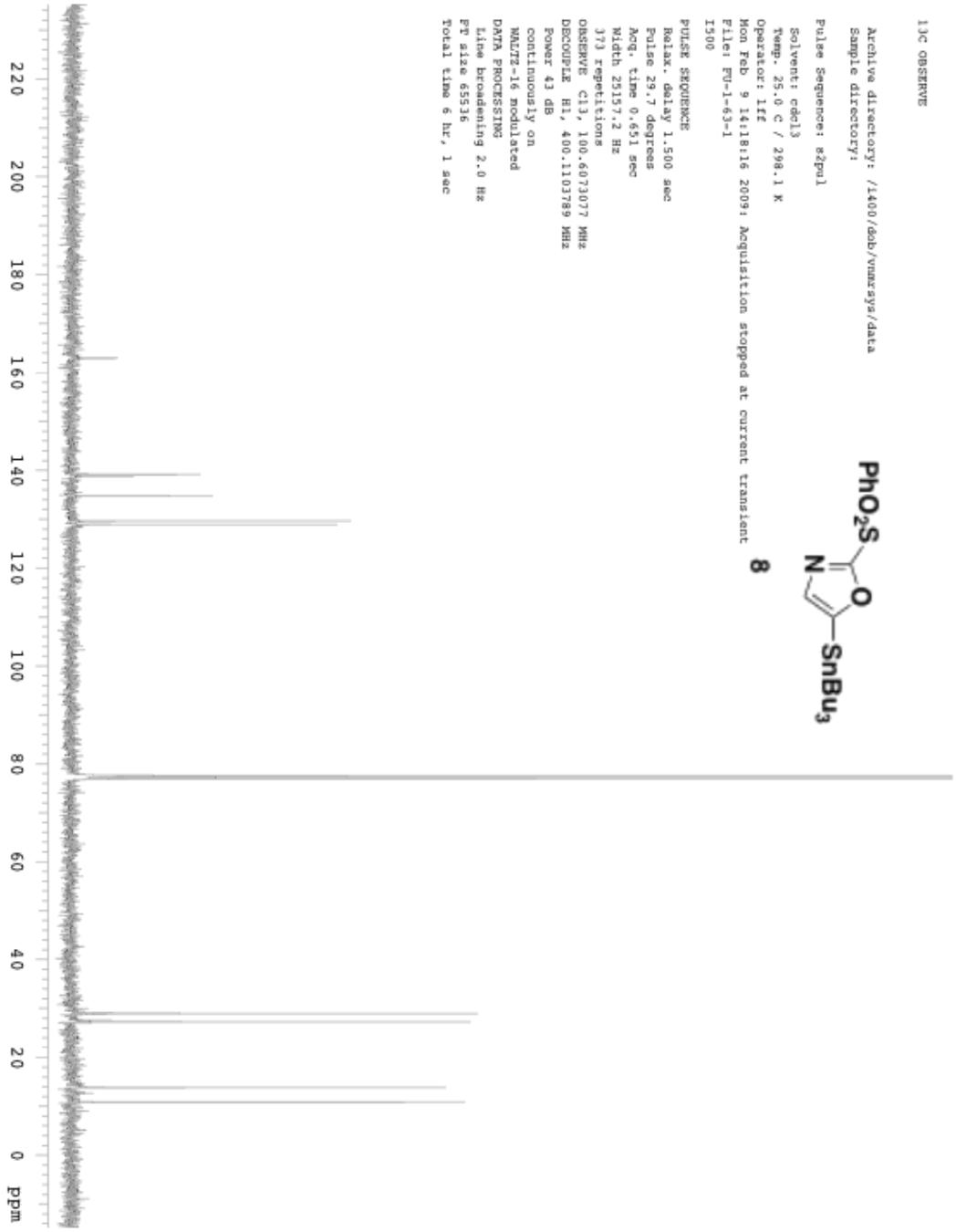

STANDARD 1H OBSERVE
Pulse Sequence: s2pul
Solvent: cdcl3
Temp. 25.0 C / 298.1 K
Operator: lff
Thu Dec 4 14:06:34 2008: Acquisition complete
File: fu-1-2-phenylsulfonyl-5-iodooxazole-12042008
GEM300
PULSE SEQUENCE
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 2.731 sec
Width 4500.0 Hz
16 repetitions
OBSERVE H1, 300.0673537 MHz
DATA PROCESSING
Line broadening 0.5 Hz
FT size 65536
Total time 0 min, 59 sec
PhO2S
O
N
I
6
8.1 8.0 7.9 7.8 7.7 7.6 7.5 7.4 ppm
2.02
2.20
1.08
0.90
12 11 10 9 8 7 6 5 4 3 2 1 -0 -1 ppm

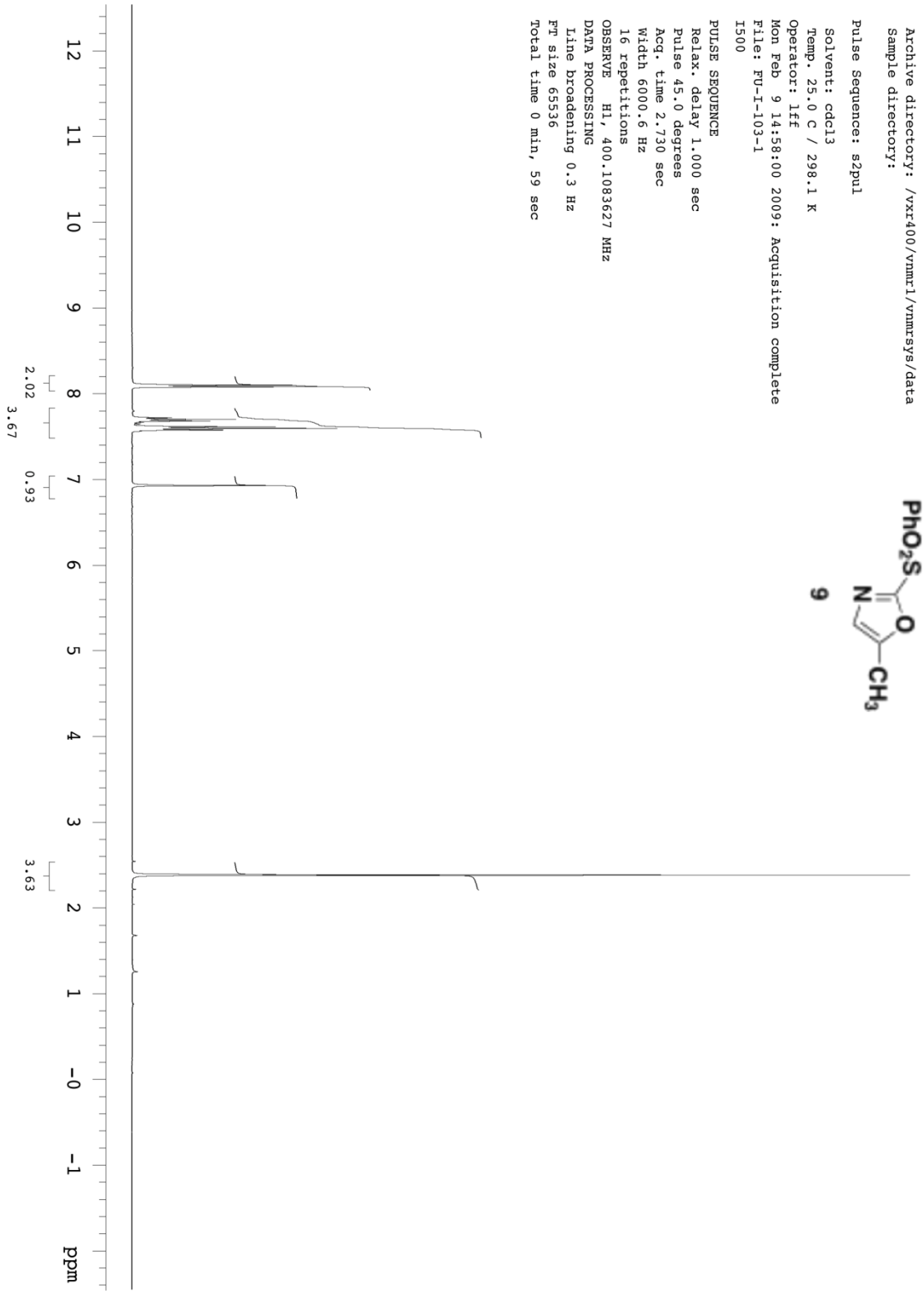

13C OBSERVE
Pulse Sequence: s2pul
Solvent: cdcl3
Temp. 25.0 C / 298.1 K
Operator: lff
Thu Dec 4 19:19:43 2008: Acquisition complete
File: fu-2-2-phenylsulfonyl-5-iodooxazole
GEN300
PULSE SEQUENCE
Relax. delay 1.500 sec
Pulse 29.6 degrees
Acq. time 0.868 sec
Width 18864.9 Hz
256 repetitions
OBSERVE C13, 75.4519635 MHz
DECOUPLE H1, 300.0688577 MHz
Power 38 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 2.0 Hz
FT size 65536
Total time 10 min, 8 sec
PhO2S
N
O
I
6
220
200
180
160
140
120
100
80
60
40
20
0
ppm

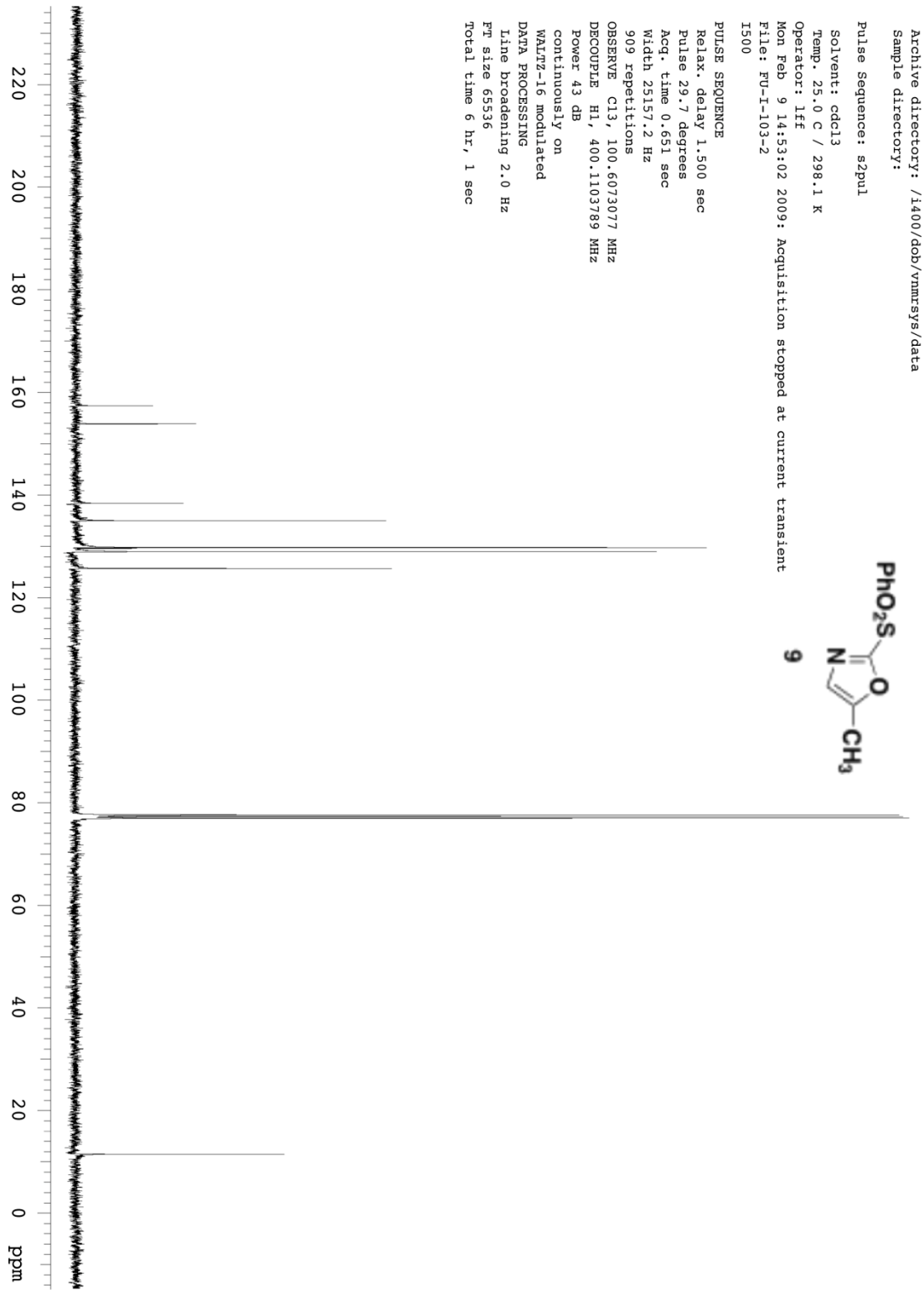

STANDARD 1H OBSERVE
Pulse Sequence: s2pul
Solvent: cdcl3
Temp. 25.0 C / 298.1 K
Operator: lff
Sun Feb 8 12:36:20 2009: RS 3 completed
File: FU-I-80-1
GEM300
PULSE SEQUENCE
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 2.731 sec
Width 4500.0 Hz
12 repetitions
OBSERVE H1, 300.0673536 MHz
DATA PROCESSING
Line broadening 0.5 Hz
FT size 65536
Total time 0 min, 59 sec
PhO2S
N
O
Br
7
8.116
8.091
7.775
7.769
7.743
7.719
7.652
7.626
7.601
7.270
7.188
2.00
1.17
2.19
0.78
ppm
ppm

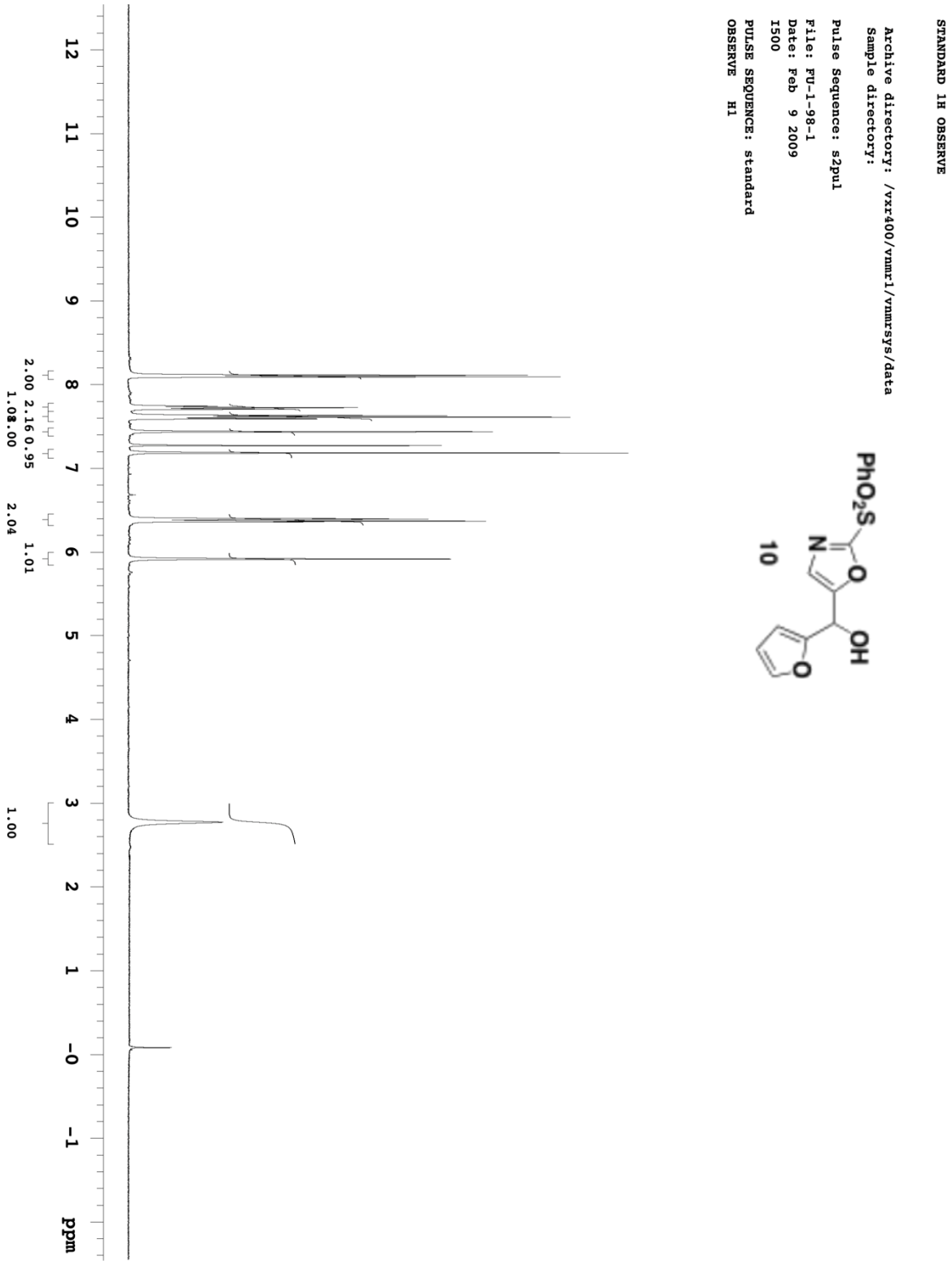

13C OBSERVE
Pulse Sequence: s2pul
Solvent: cdcl3
Temp. 25.0 C / 298.1 K
Operator: lff
Sun Feb 8 13:45:33 2009: Acquisition stopped at current transient
File: FU-I-80-2
GEN300
PULSE SEQUENCE
Relax. delay 1.500 sec
Pulse 29.6 degrees
Acq. time 0.868 sec
Width 1884.9 Hz
1249 repetitions
OBSERVE C13, 75.4519635 MHz
DECOUPLE H1, 300.0688577 MHz
Power 38 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 2.0 Hz
FT size 65536
Total time 6 hr, 36 min, 13 sec
PhO2S
N
O
Br
7
220
200
180
160
140
120
100
80
60
40
20
0
ppm

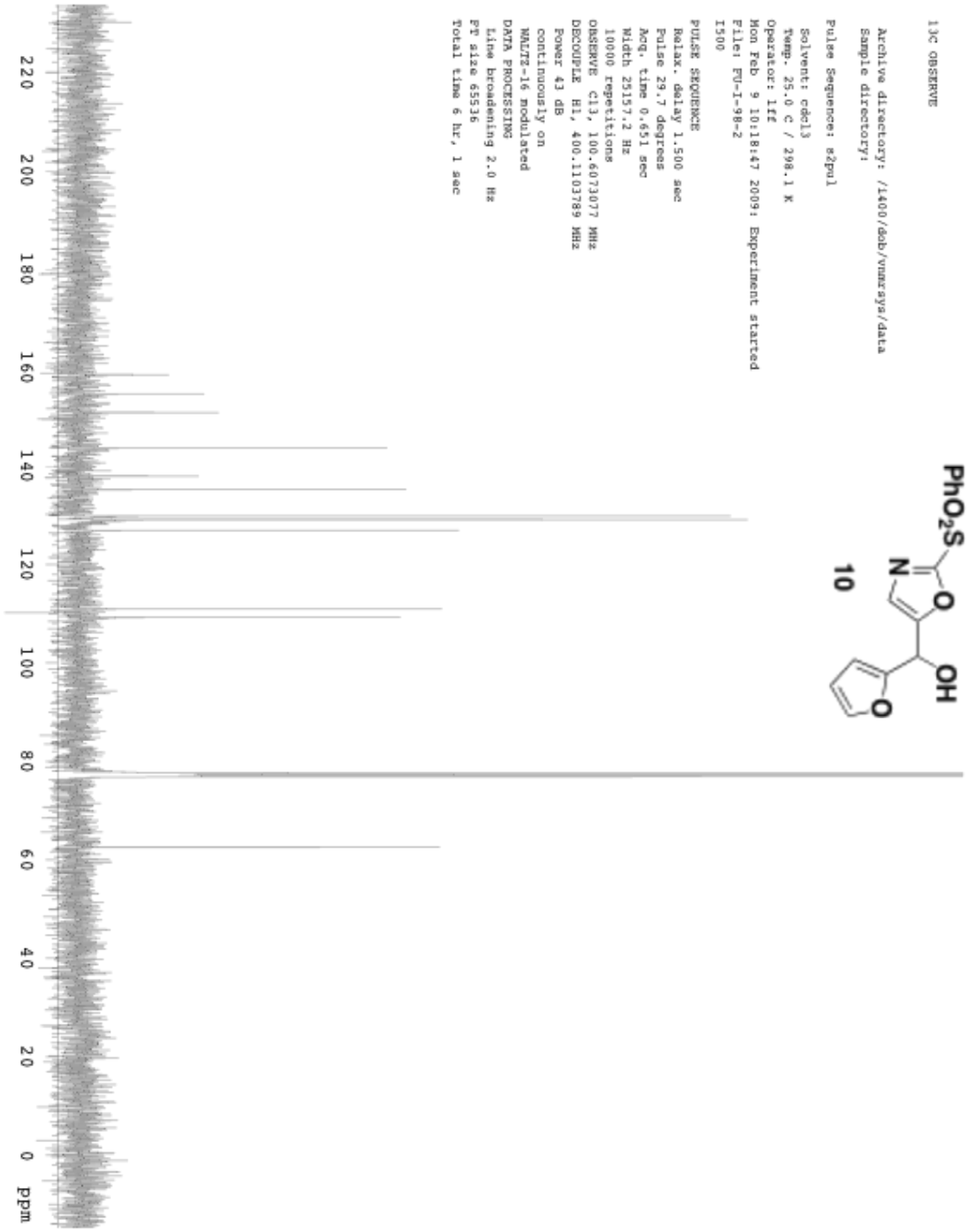

STANDARD 1H OBSERVE
Archive directory: /vxr400/vnmrl/vnmrsys/data
Sample directory:
Pulse Sequence: s2pul
Solvent: cdcl3
Ambient temperature
Operator: lfd
Fri Dec 12 12:26:25 2008: Acquisition complete
File: fu-1-2-phenylsulfonyl-5-tinoxazole-12122008
I500
PULSE SEQUENCE
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 2.730 sec
Width 6000.6 Hz
16 repetitions
OBSERVE H1, 400.1084553 MHz
DATA PROCESSING
Line broadening 0.3 Hz
FT size 65536
Total time 0 min, 59 sec
PhO2S
O
N
SnBu3
8
8.1 7.9 7.7 7.5 ppm
1.98 2.16 1.07 0.94
1.6 1.4 1.2 1.0 ppm
6.00 8.25 5.89 10.34
12 11 10 9 8 7 6 5 4 3 2 1 -0 -1 ppm

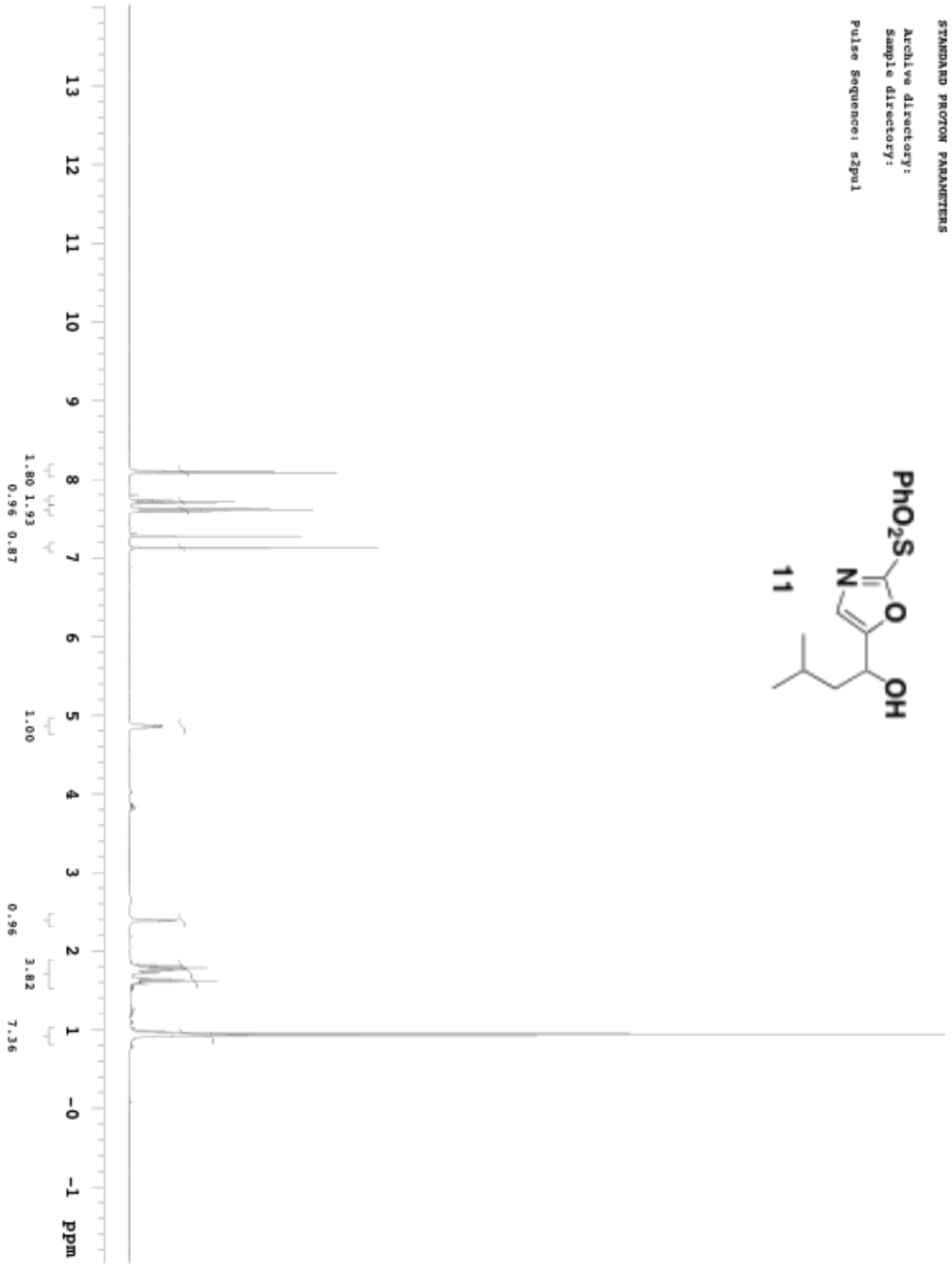

13C OBSERVE
Archive directory: /1400/dob/vnmrsys/data
Sample directory:
Pulse Sequence: s2pul
Solvent: cdcl3
Temp. 25.0 C / 298.1 K
Operator: iff
Mon Feb 9 14:18:16 2009: Acquisition stopped at current transient
File: FU-1-63-1
I500
PULSE SEQUENCE
Relax. delay 1.500 sec
Pulse 29.7 degrees
Acq. time 0.651 sec
Width 25157.2 Hz
373 repetitions
OBSERVE C13, 100.6073077 MHz
DECOUPLE H1, 400.1103789 MHz
Power 43 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 2.0 Hz
FT size 65536
Total time 6 hr, 1 sec
PhO2S
O
N
SnBu3
8
220
200
180
160
140
120
100
80
60
40
20
0
ppm

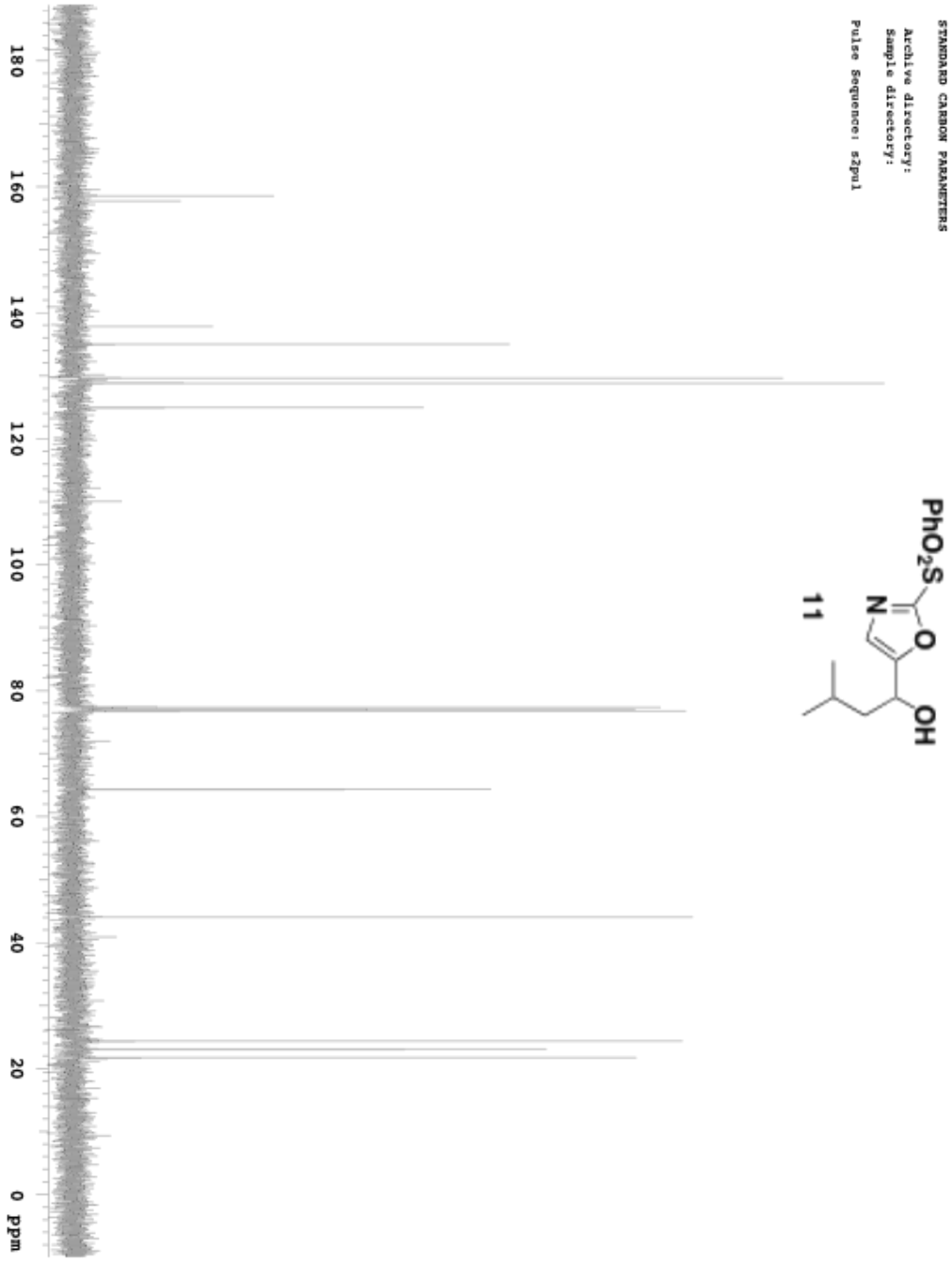

STANDARD 1H OBSERVE
Archive directory: /vxr400/vnmr1/vnmrsys/data
Sample directory:
Pulse Sequence: s2pul
Solvent: cdcl3
Temp. 25.0 C / 298.1 K
Operator: lff
Mon Feb 9 14:58:00 2009: Acquisition complete
File: FU-I-103-1
I500
PULSE SEQUENCE
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 2.730 sec
Width 6000.6 Hz
16 repetitions
OBSERVE H1, 400.1083627 MHz
DATA PROCESSING
Line broadening 0.3 Hz
FT size 65536
Total time 0 min, 59 sec
PhO2S
O
N
CH3
9
12
11
10
9
8
7
6
5
4
3
2
1
-0
-1
ppm
2.02
3.67
0.93
3.63

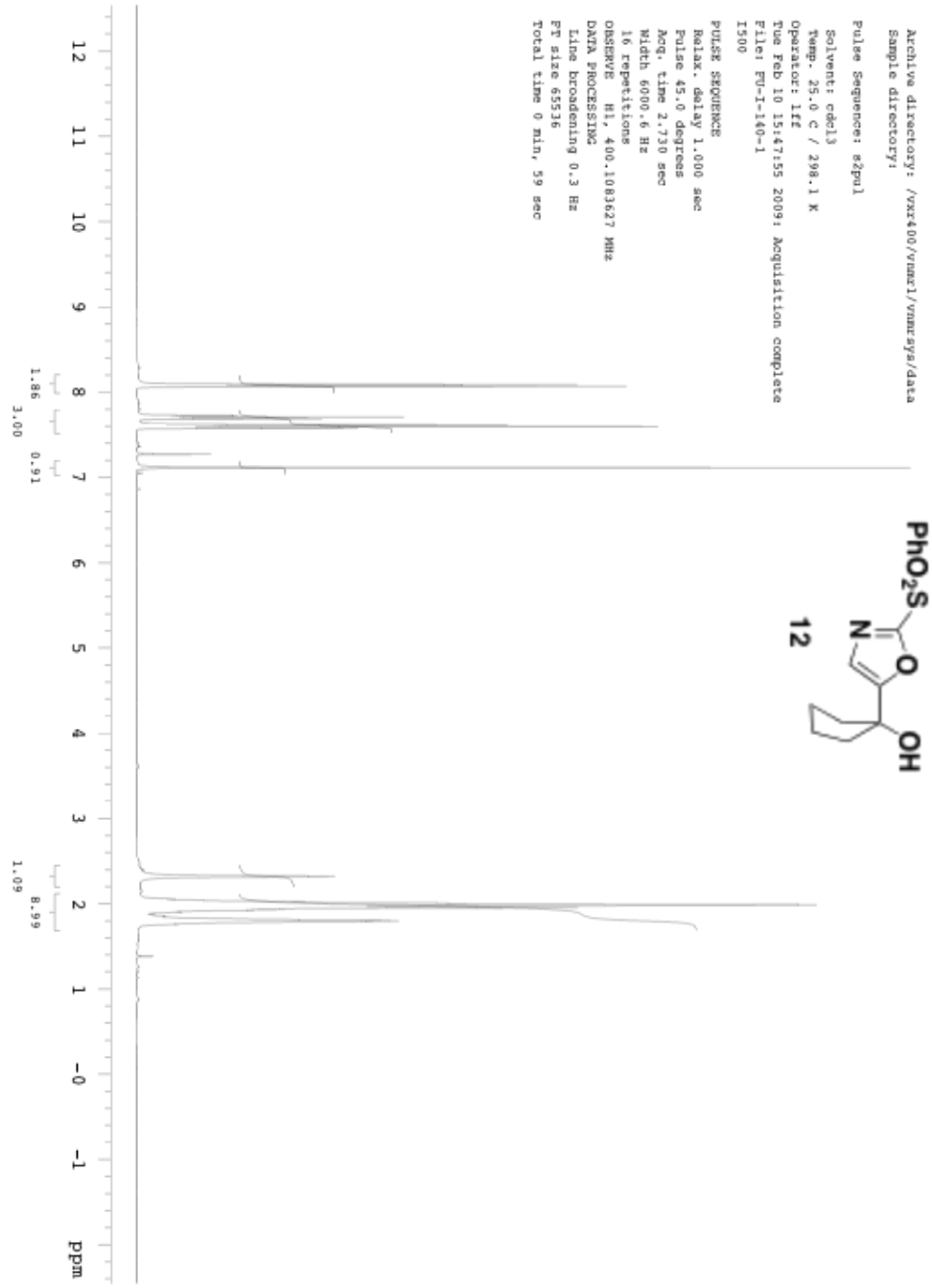

13C OBSERVE
Archive directory: /i400/dob/vnmrsys/data
Sample directory:
Pulse Sequence: s2pul
Solvent: cdcl3
Temp. 25.0 C / 298.1 K
Operator: lff
Mon Feb 9 14:53:02 2009: Acquisition stopped at current transient
File: FU-I-103-2
I500
PULSE SEQUENCE
Relax. delay 1.500 sec
Pulse 29.7 degrees
Acq. time 0.651 sec
Width 25157.2 Hz
909 repetitions
OBSERVE C13, 100.6073077 MHz
DECOUPLE H1, 400.1103789 MHz
Power 43 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 2.0 Hz
FT size 65536
Total time 6 hr, 1 sec
PhO2S
N
O
CH3
9
220
200
180
160
140
120
100
80
60
40
20
0
ppm

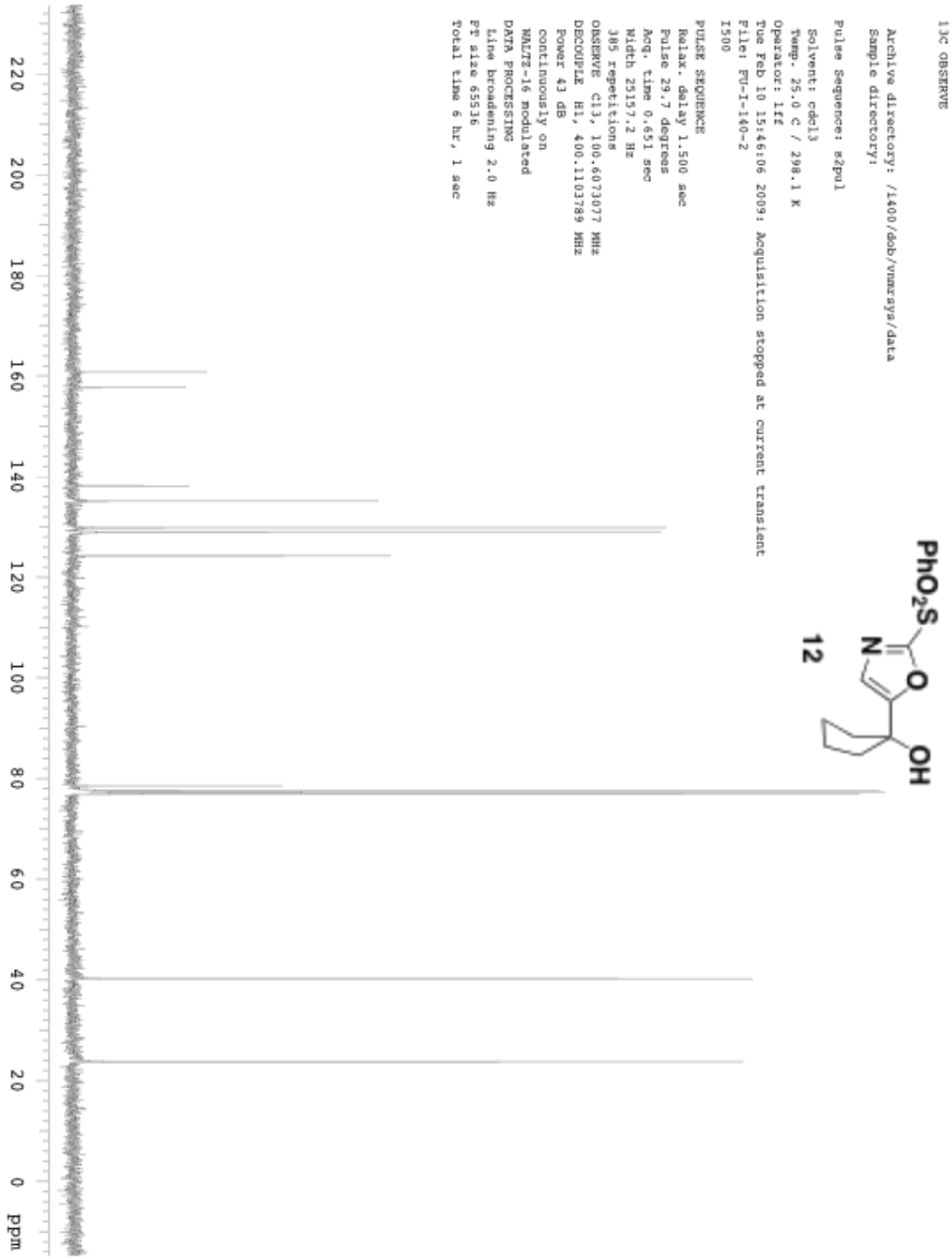

STANDARD 1H OBSERVE
Archive directory: /vxr400/vnmr1/vnmrsys/data
Sample directory:
Pulse Sequence: s2pul
File: FU-1-98-1
Date: Feb 9 2009
I500
PULSE SEQUENCE: standard
OBSERVE H1
PhO2S
N
O
OH
O
10
12
11
10
9
8
7
6
5
4
3
2
1
-0
-1
ppm
2.00 2.16 0.95
1.08 3.00
1.01
2.04
1.00

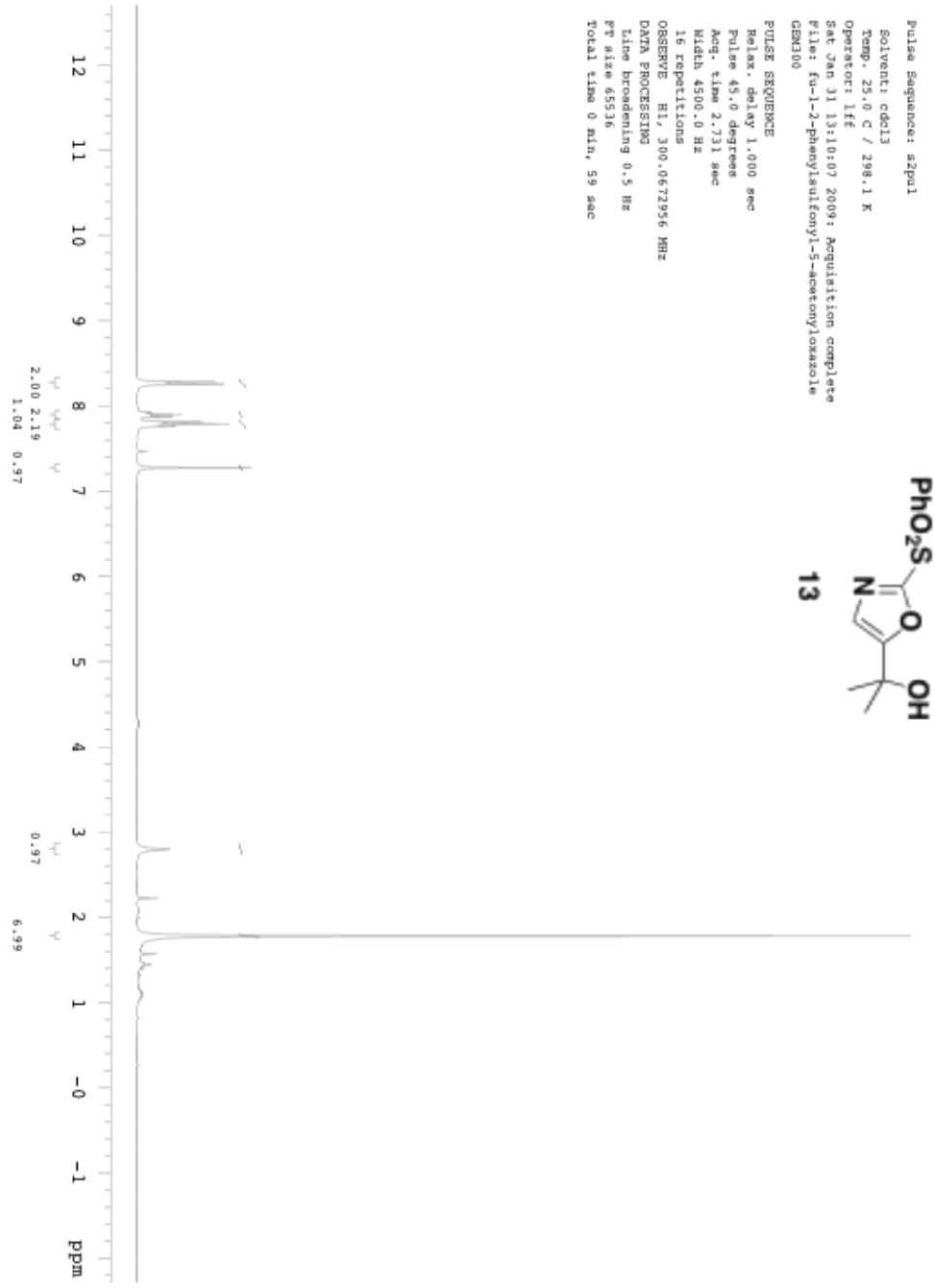

13C OBSERVE
Archive directory: /1400/dob/vnmrsys/data
Sample directory:
Pulse Sequence: s2pul
Solvent: cdcl3
Temp. 25.0 C / 298.1 K
Operator: lfr
Mon Feb 9 10:18:47 2009: Experiment started
File: FU-I-98-2
I500
PULSE SEQUENCE
Relax. delay 1.500 sec
Pulse 29.7 degrees
Acq. time 0.651 sec
Width 25157.2 Hz
10000 repetitions
OBSERVE C13, 100.6073077 MHz
DECOUPLE H1, 400.1103789 MHz
Power 43 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 2.0 Hz
FT size 65536
Total time 6 hr, 1 sec
PhO2S
N
O
OH
O
10
220
200
180
160
140
120
100
80
60
40
20
0
ppm

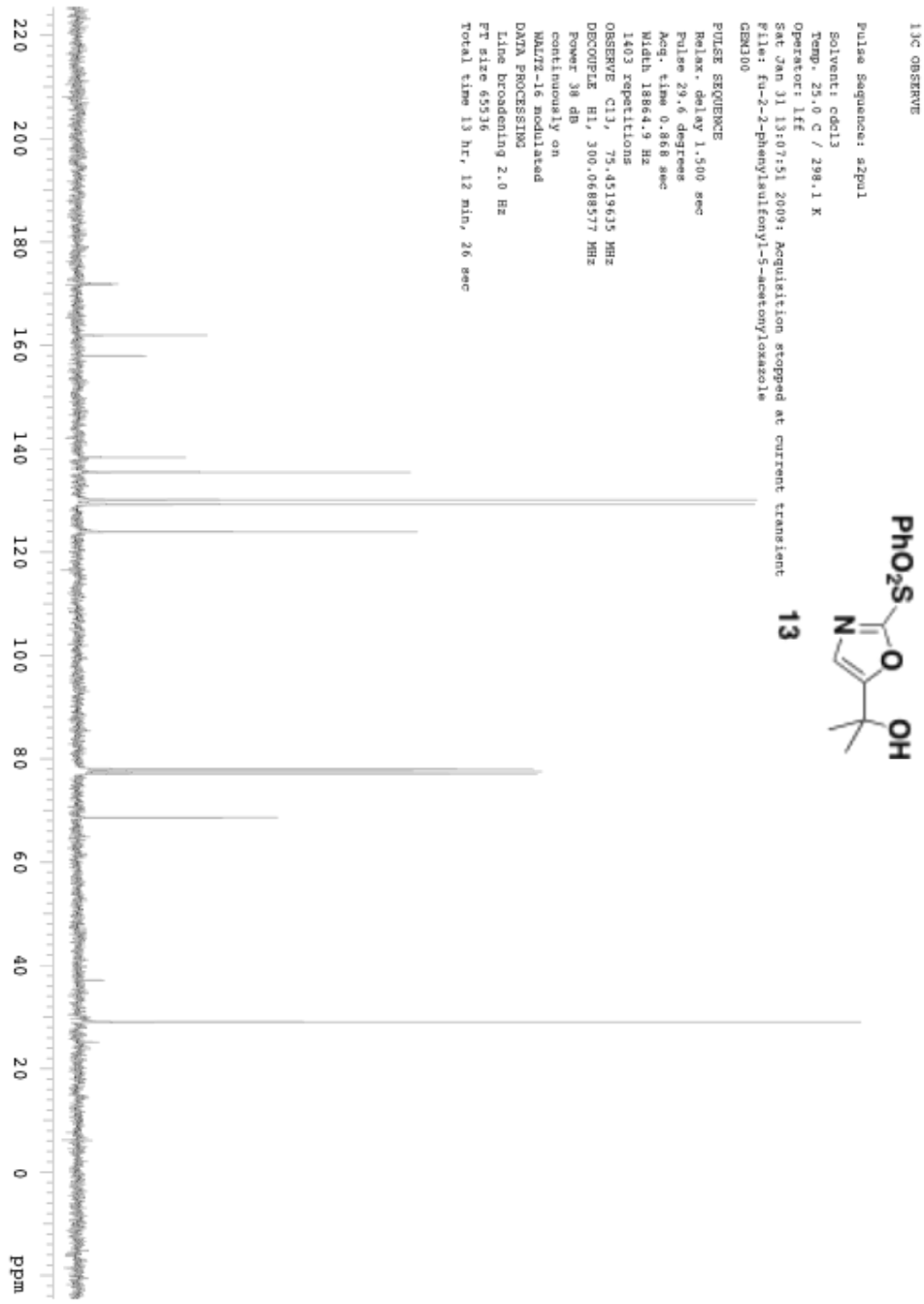

STANDARD PROTON PARAMETERS
Archive directory:
Sample directory:
Pulse Sequence: s2pul
PhO2S
N
O
OH
11
13 12 11 10 9 8 7 6 5 4 3 2 1 -0 -1 ppm
1.80 1.93
0.96 0.87
1.00
0.96
3.82
7.36


STANDARD CARBON PARAMETERS
Archive directory:
Sample directory:
Pulse Sequence: s2pul
11
PhO2S
N
O
OH
180
160
140
120
100
80
60
40
20
0 ppm


STANDARD 1H OBSERVE
Archive directory: /vxr400/vnmr1/vnmrsys/data
Sample directory:
Pulse Sequence: s2pul
Solvent: cdcl3
Temp. 25.0 C / 298.1 K
Operator: lfr
Tue Feb 10 15:47:55 2009: Acquisition complete
File: FU-I-140-1
I500
PULSE SEQUENCE
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 2.730 sec
Width 6000.6 Hz
16 repetitions
OBSERVE H1, 400.1083627 MHz
DATA PROCESSING
Line broadening 0.3 Hz
FT size 65536
Total time 0 min, 59 sec
PhO2S
N
O
OH
12
1.86
3.00
0.91
8.99
1.09
12
11
10
9
8
7
6
5
4
3
2
1
-0
-1
ppm


13C OBSERVE
Archive directory: /1400/dob/vnmrsys/data
Sample directory:
Pulse Sequence: s2pul
Solvent: cdcl3
Temp. 25.0 C / 298.1 K
Operator: lfr
Tue Feb 10 15:46:06 2009: Acquisition stopped at current transient
File: FU-I-140-2
I500
PULSE SEQUENCE
Relax. delay 1.500 sec
Pulse 29.7 degrees
Acq. time 0.651 sec
Width 25157.2 Hz
385 repetitions
OBSERVE C13, 100.6073077 MHz
DECOUPLE H1, 400.1103789 MHz
Power 43 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 2.0 Hz
FT size 65536
Total time 6 hr, 1 sec
PhO2S
O
N
OH
12
220
200
180
160
140
120
100
80
60
40
20
0
ppm


STANDARD 1H OBSERVE
Pulse Sequence: s2pul
Solvent: cdcl3
Temp. 25.0 C / 298.1 K
Operator: lff
Sat Jan 31 13:10:07 2009: Acquisition complete
File: fu-1-2-phenylsulfonyl-5-acetonyloxazole
GEN300
PULSE SEQUENCE
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 2.731 sec
Width 4500.0 Hz
16 repetitions
OBSERVE H1, 300.0672956 MHz
DATA PROCESSING
Line broadening 0.5 Hz
FT size 65536
Total time 0 min, 59 sec
PhO2S
N
O
OH
13
12
11
10
9
8
7
6
5
4
3
2
1
-0
-1
ppm
2.00 2.19
1.04 0.97
0.97
6.99


13C OBSERVE
Pulse Sequence: s2pul
Solvent: cdcl3
Temp. 25.0 C / 298.1 K
Operator: lff
Sat Jan 31 13:07:51 2009: Acquisition stopped at current transient
File: fu-2-phenylsulfonyl-5-acetonyloxazole
GEN300
PULSE SEQUENCE
Relax. delay 1.500 sec
Pulse 29.6 degrees
Acq. time 0.868 sec
Width 1884.9 Hz
1403 repetitions
OBSERVE C13, 75.4519635 MHz
DECOUPLE H1, 300.0688577 MHz
Power 38 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 2.0 Hz
FT size 65536
Total time 13 hr, 12 min, 26 sec
13
PhO2S
N
O
OH
220
200
180
160
140
120
100
80
60
40
20
0
ppm

STANDARD 1H OBSERVE

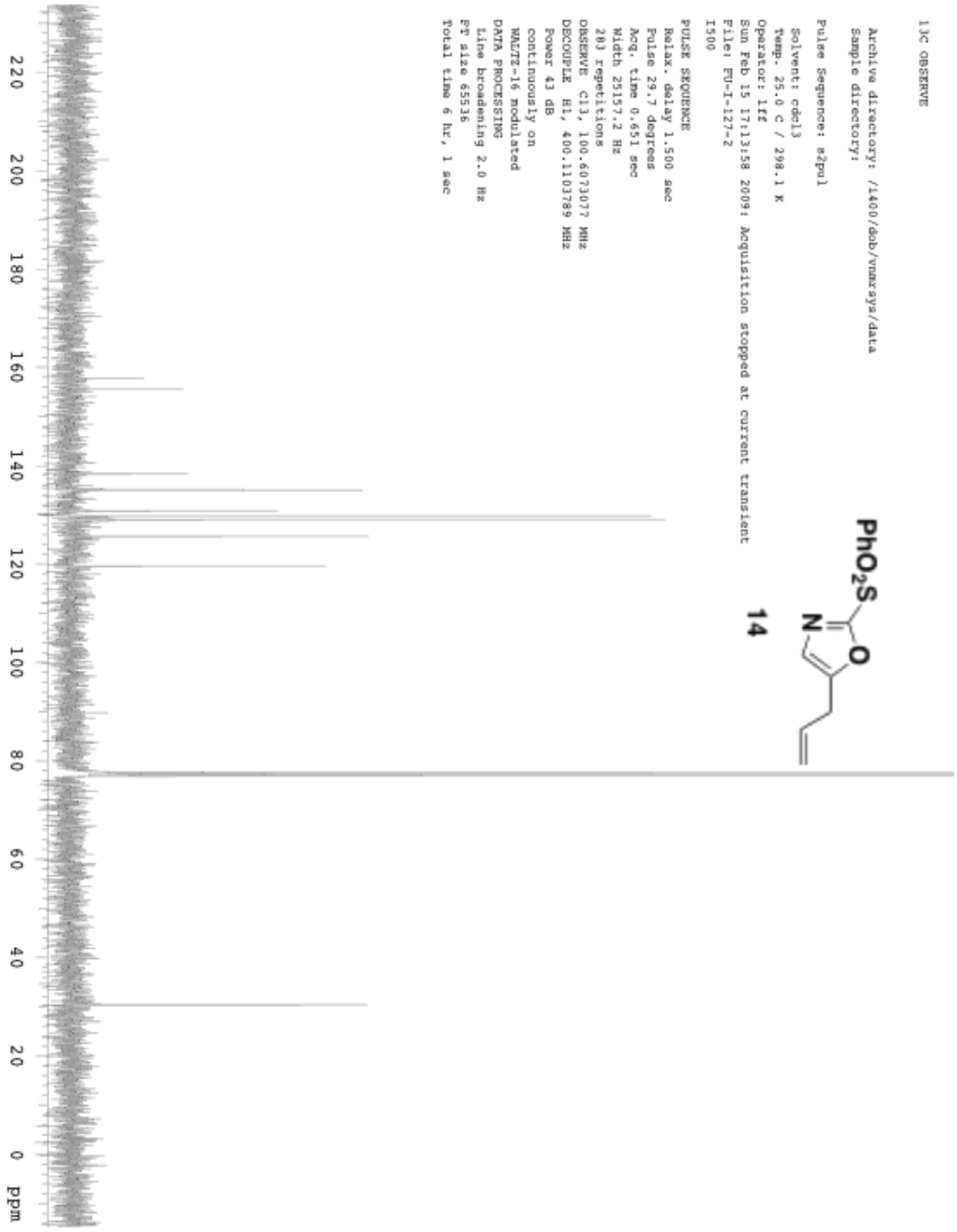
Archive directory: /vxr400/vnmr1/vnmrsys/data
Sample directory:

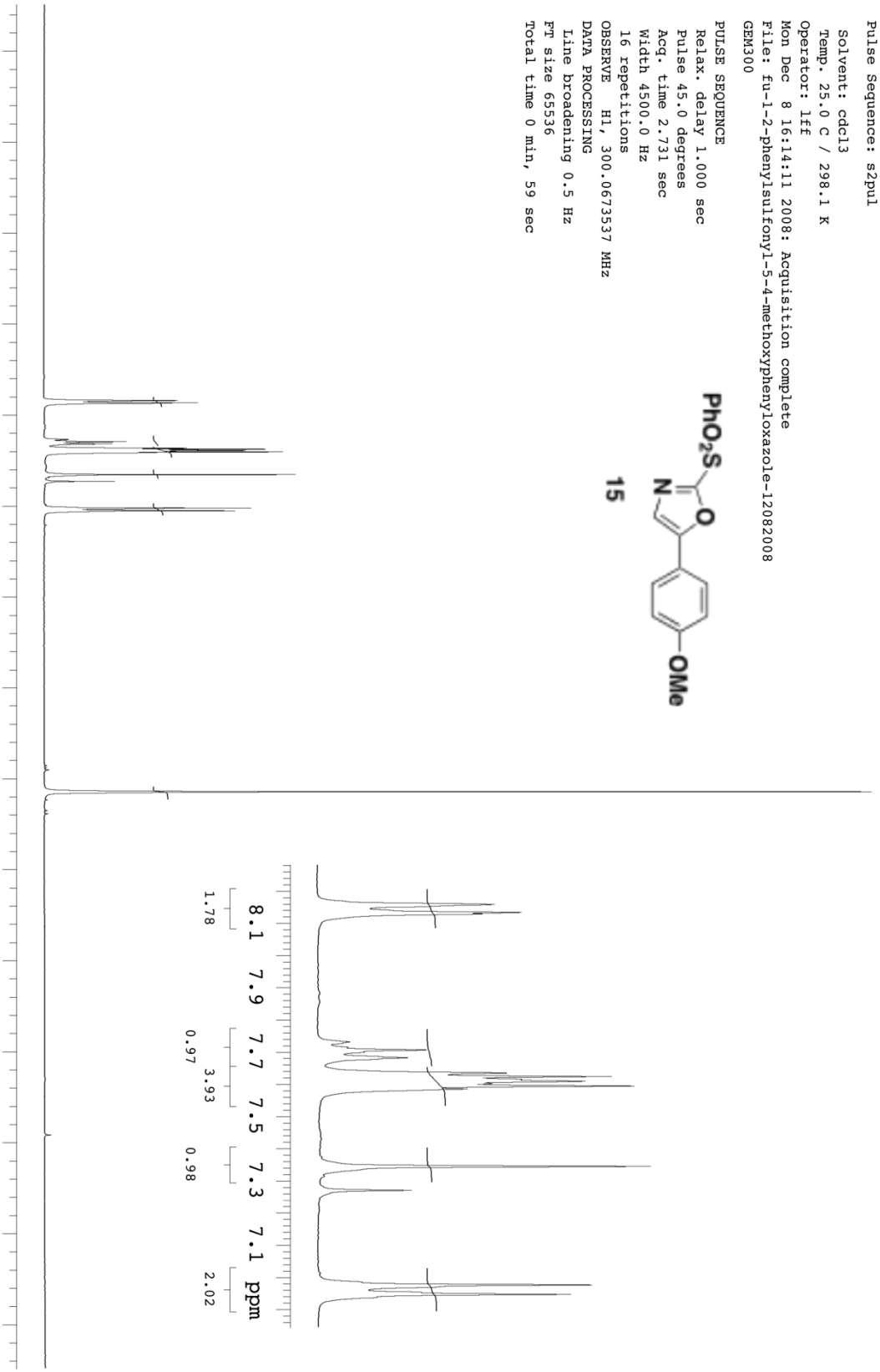
Pulse Sequence: s2pul

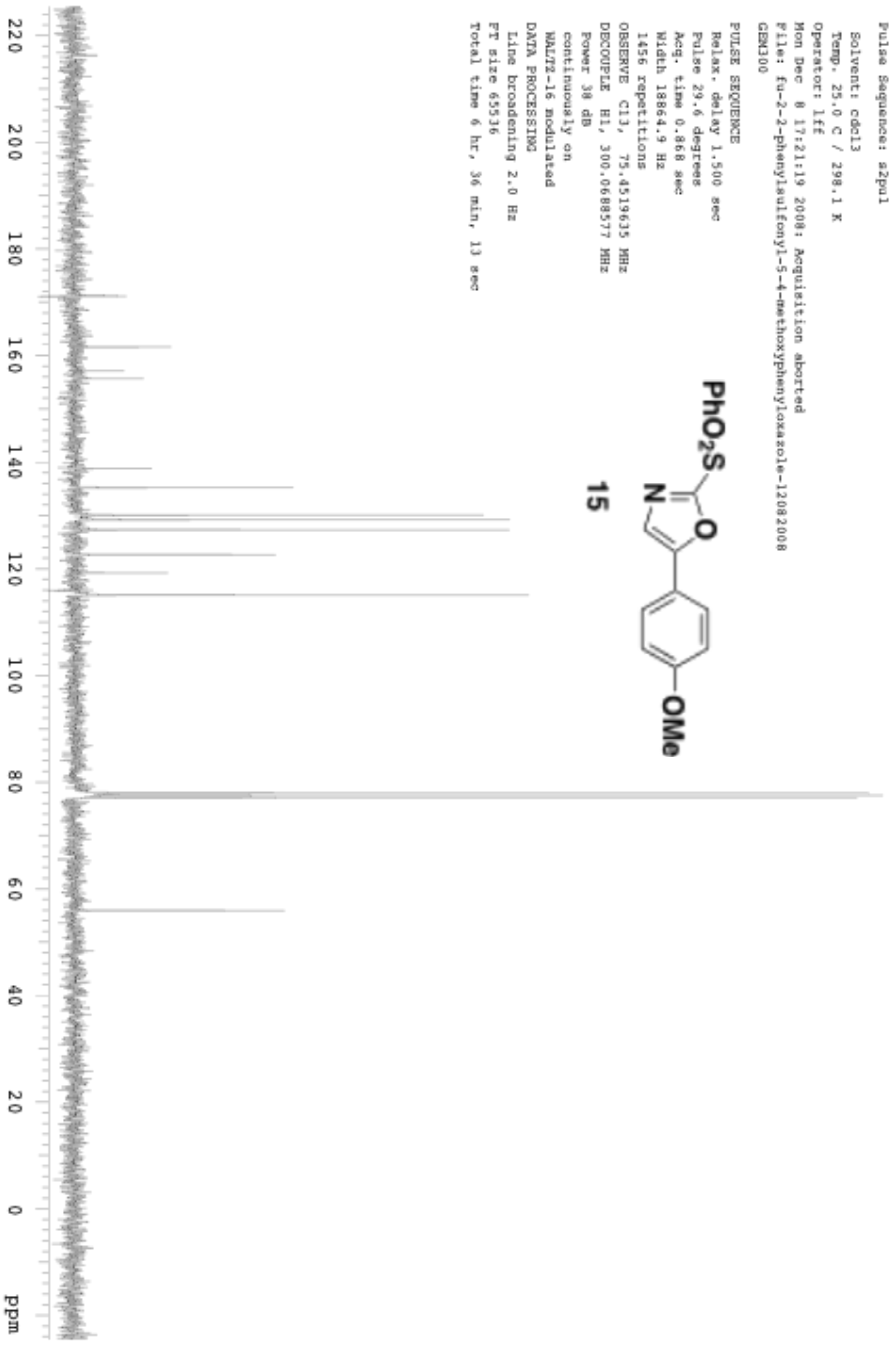
File: FU-I-144-1
Date: Feb 17 2009
I500

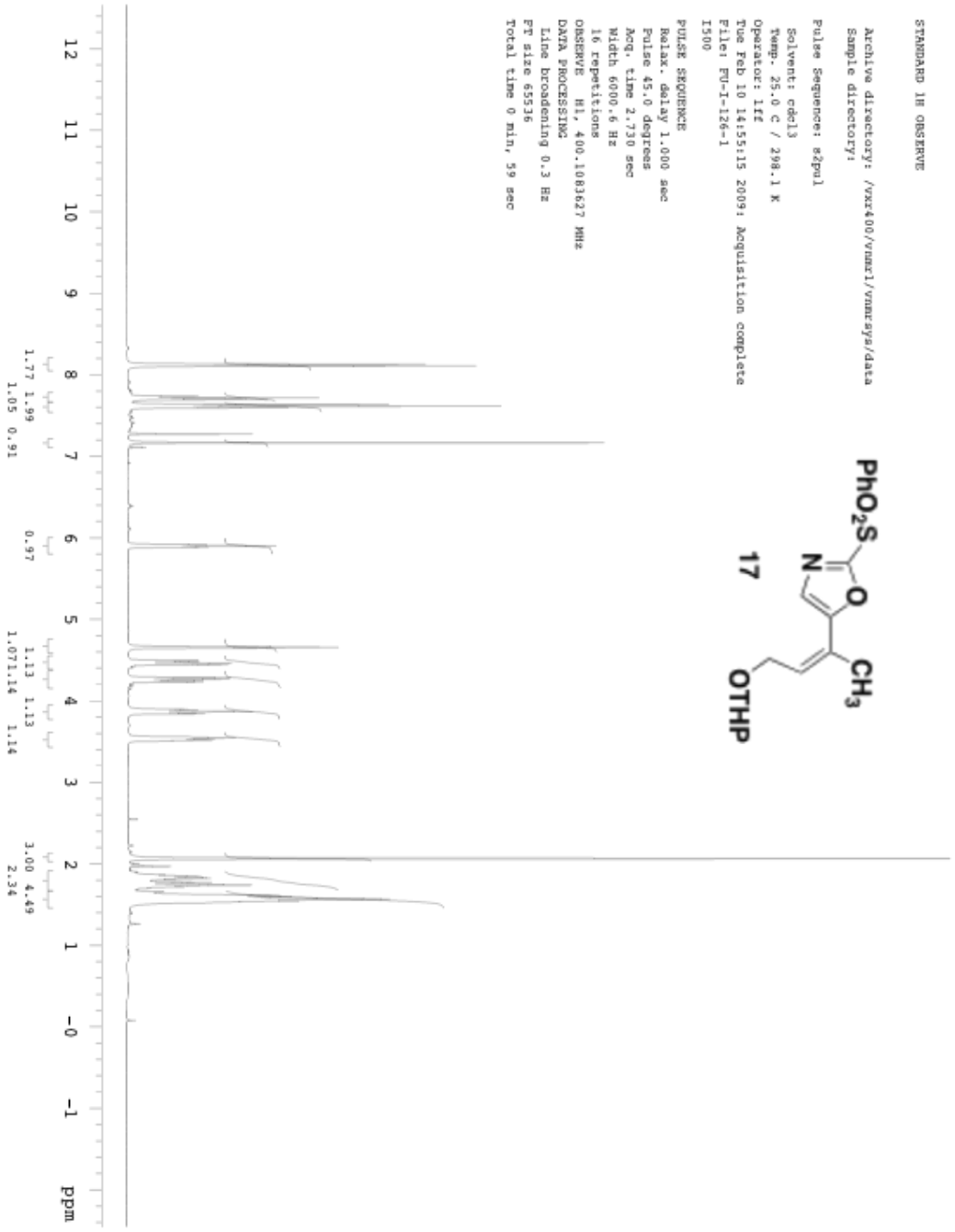
PULSE SEQUENCE: standard
OBSERVE H1

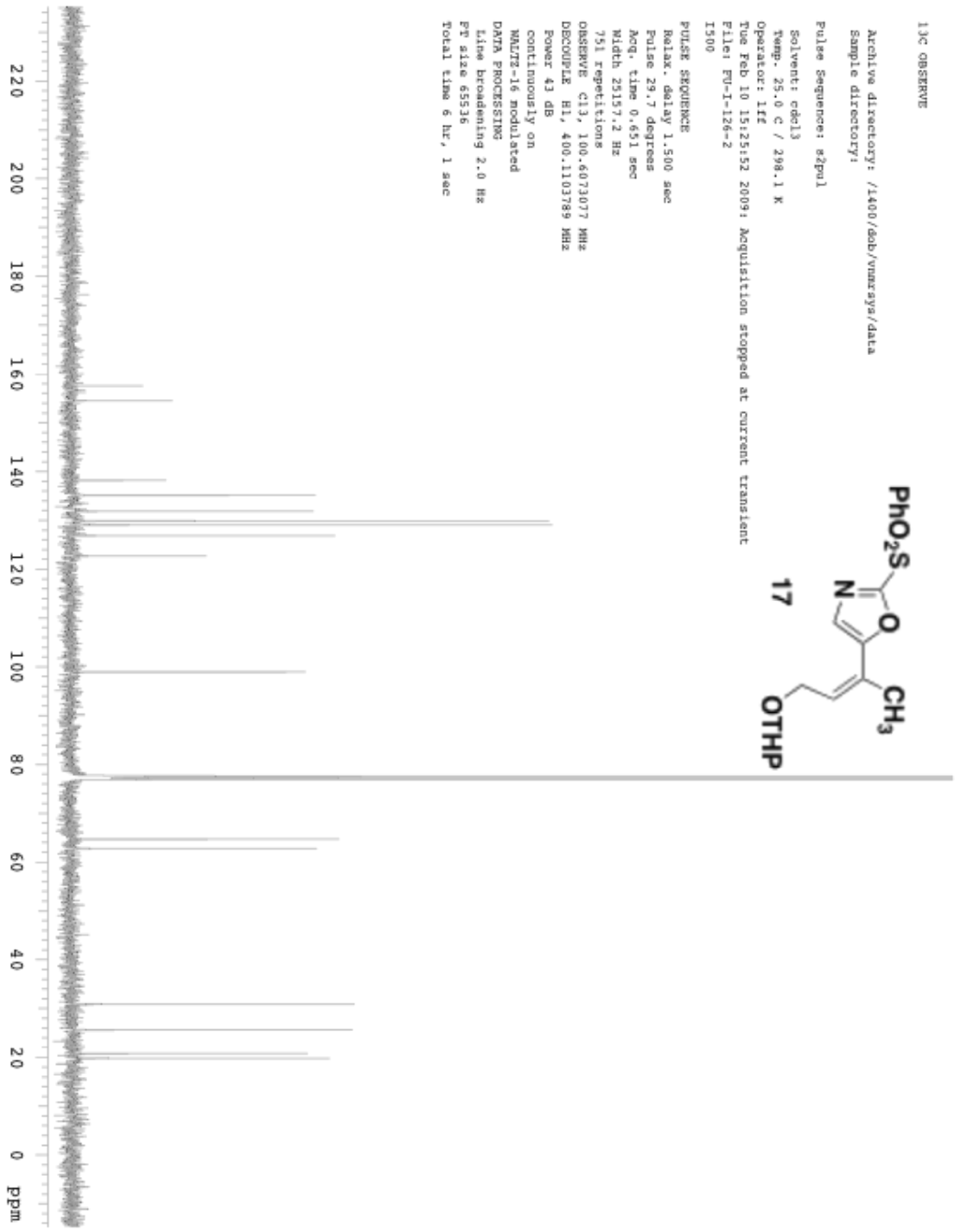
14

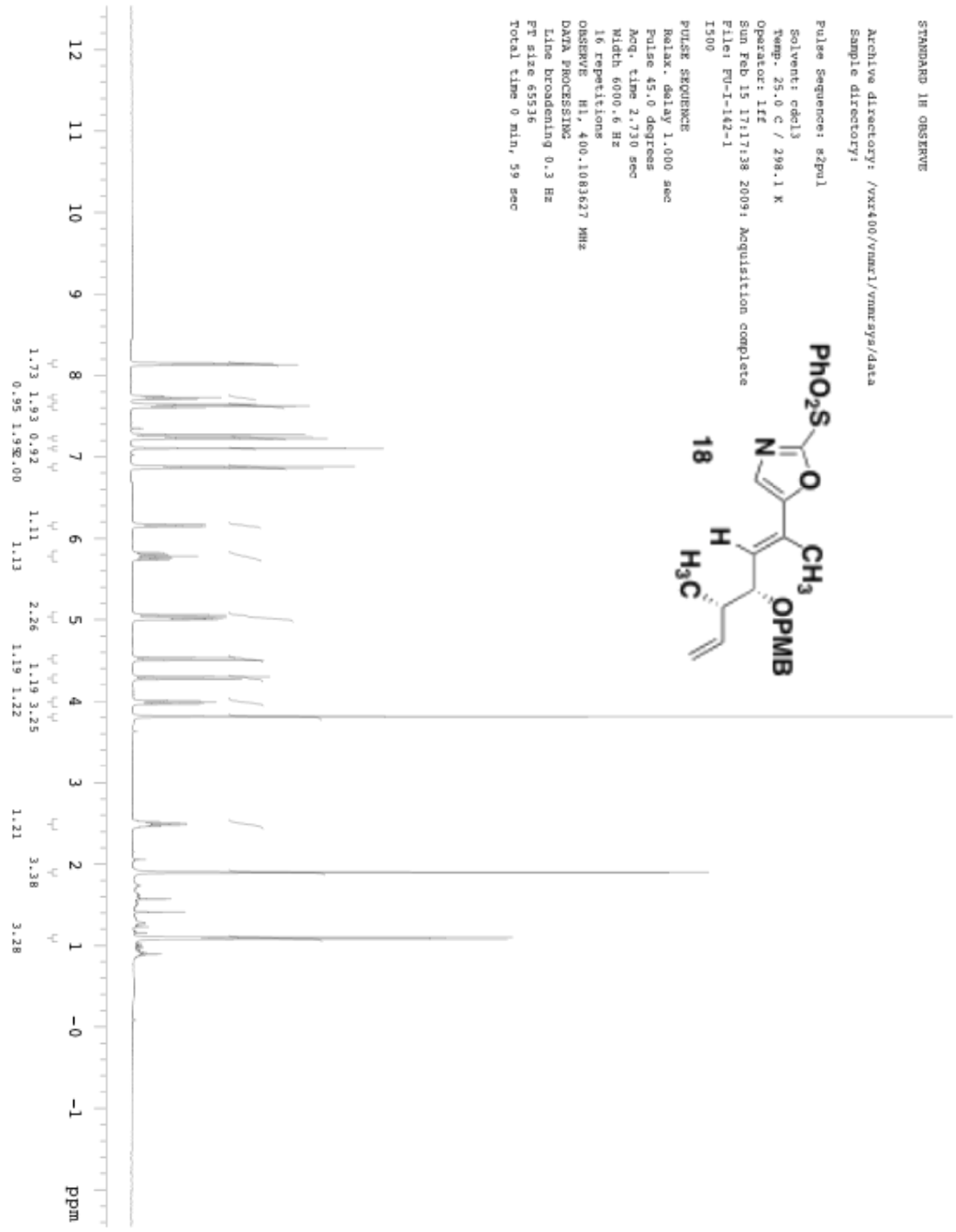

13C OBSERVE
Archive directory: /i400/dob/vnmrsys/data
Sample directory:
Pulse Sequence: s2pul
Solvent: cdcl3
Temp. 25.0 C / 298.1 K
Operator: lfe
Sun Feb 15 17:13:58 2009: Acquisition stopped at current transient
File: FU-I-127-2
I500
PULSE SEQUENCE
Relax. delay 1.500 sec
Pulse 29.7 degrees
Acq. time 0.651 sec
Width 25157.2 Hz
280 repetitions
OBSERVE C13, 100.607307 MHz
DECOUPLE H1, 400.110789 MHz
Power 43 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 2.0 Hz
FT size 65536
Total time 6 hr, 1 sec
PhO2S
O
N
14
220
200
180
160
140
120
100
80
60
40
20
0
ppm

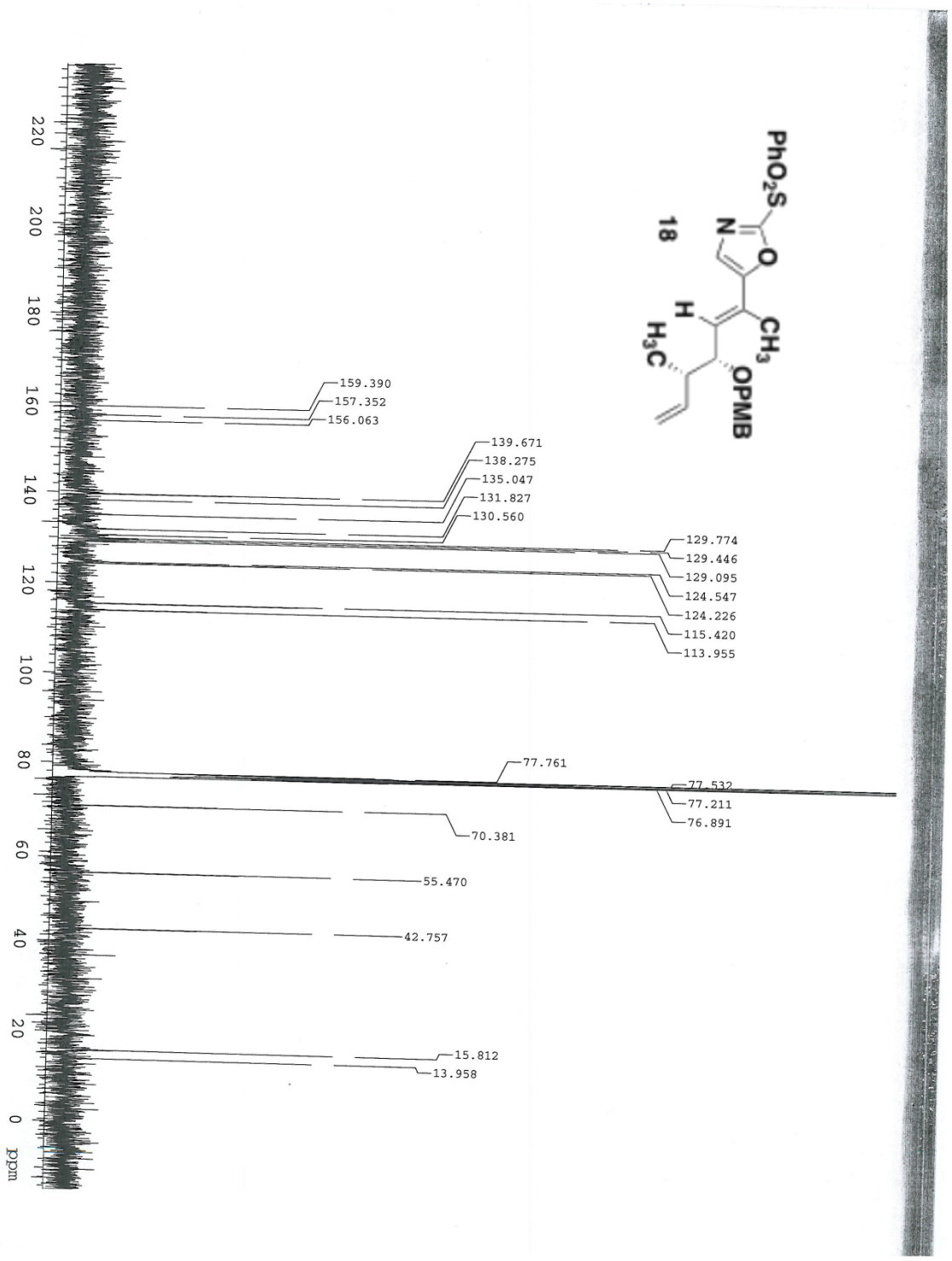

STANDARD 1H OBSERVE
Pulse Sequence: s2pul
Solvent: cdcl3
Temp. 25.0 C / 298.1 K
Operator: lff
Mon Dec 8 16:14:11 2008: Acquisition complete
File: fu-1-2-phenylsulfonyl-5-4-methoxyphenyloxazole-12082008
GEM300
PULSE SEQUENCE
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 2.731 sec
Width 4500.0 Hz
16 repetitions
OBSERVE H1, 300.0673537 MHz
DATA PROCESSING
Line broadening 0.5 Hz
FT size 65536
Total time 0 min, 59 sec
PhO2S
O
N
OMe
15
8.1 7.9 7.7 7.5 7.3 7.1 ppm
1.78
0.97
3.93
0.98
2.02
12 11 10 9 8 7 6 5 4 3 2 1 -0 -1 ppm


13C OBSERVE
Pulse Sequence: s2pul
Solvent: cdcl3
Temp. 25.0 C / 298.1 K
Operator: lff
Mon Dec 8 17:21:19 2008: Acquisition aborted
File: fu-2-2-phenylsulfonyl-5-4-methoxyphenyloxazole-12082008
GEM300
PULSE SEQUENCE
Relax. delay 1.500 sec
Pulse 29.6 degrees
Acq. time 0.868 sec
Width 18864.9 Hz
1456 repetitions
OBSERVE C13, 75.4519635 MHz
DECOUPLE H1, 300.0688577 MHz
Power 38 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 2.0 Hz
FT size 65536
Total time 6 hr, 36 min, 13 sec
PhO2S
N
O
OMe
15
220
200
180
160
140
120
100
80
60
40
20
0
ppm


STANDARD 1H OBSERVE
Archive directory: /vxr400/vnmr1/vnmrsys/data
Sample directory:
Pulse Sequence: s2pul
Solvent: cdcl3
Temp. 25.0 C / 298.1 K
Operator: lfr
Tue Feb 10 14:55:15 2009: Acquisition complete
File: FU-I-126-1
I500
PULSE SEQUENCE
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 2.730 sec
Width 6000.6 Hz
16 repetitions
OBSERVE H1, 400.1083627 MHz
DATA PROCESSING
Line broadening 0.3 Hz
FT size 65536
Total time 0 min, 59 sec
PhO2S
N
O
CH3
17
OTHP
12
11
10
9
8
7
6
5
4
3
2
1
-0
-1
ppm
1.77 1.99
1.05 0.91
0.97
1.13 1.13
1.07 1.14 1.14
3.00 4.49
2.34


13C OBSERVE
Archive directory: /1400/dob/vnmrsys/data
Sample directory:
Pulse Sequence: s2pul
Solvent: cdcl3
Temp. 25.0 C / 298.1 K
Operator: lfr
Tue Feb 10 15:25:52 2009: Acquisition stopped at current transient
File: FU-I-126-2
I500
PULSE SEQUENCE
Relax. delay 1.500 sec
Pulse 29.7 degrees
Acq. time 0.651 sec
Width 29157.2 Hz
751 repetitions
OBSERVE C13, 100.6073077 MHz
DECOUPLE H1, 400.1103789 MHz
Power 43 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 2.0 Hz
FT size 65536
Total time 6 hr, 1 sec
PhO2S
N
O
CH3
17
OTHP
220
200
180
160
140
120
100
80
60
40
20
0
ppm


STANDARD 1H OBSERVE
Archive directory: /vxr400/vnmrl/vnmrsys/data
Sample directory:
Pulse Sequence: s2pul
Solvent: cdcl3
Temp. 25.0 C / 298.1 K
Operator: lfr
Sun Feb 15 17:17:38 2009: Acquisition complete
File: FU-I-142-1
I500
PULSE SEQUENCE
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 2.730 sec
Width 6000.6 Hz
16 repetitions
OBSERVE H1, 400.1083627 MHz
DATA PROCESSING
Line broadening 0.3 Hz
FT size 65536
Total time 0 min, 59 sec
PhO2S
N
O
CH3
H
H3C
OPMB
18
12 11 10 9 8 7 6 5 4 3 2 1 -0 -1 ppm
0.95 1.93 0.92 2.00 1.11 2.26 1.19 3.25 3.38
1.73 1.92 1.13 1.19 1.22 1.21 3.28


PhO2S
N
O
18
H
CH3
H3C
OPMB
159.390
157.352
156.063
139.671
138.275
135.047
131.827
130.560
129.774
129.446
129.095
124.547
124.226
115.420
113.955
77.761
77.532
77.211
76.891
70.381
55.470
42.757
15.812
13.958
220
200
180
160
140
120
100
80
60
40
20
0
ppm

STANDARD 1H OBSERVE

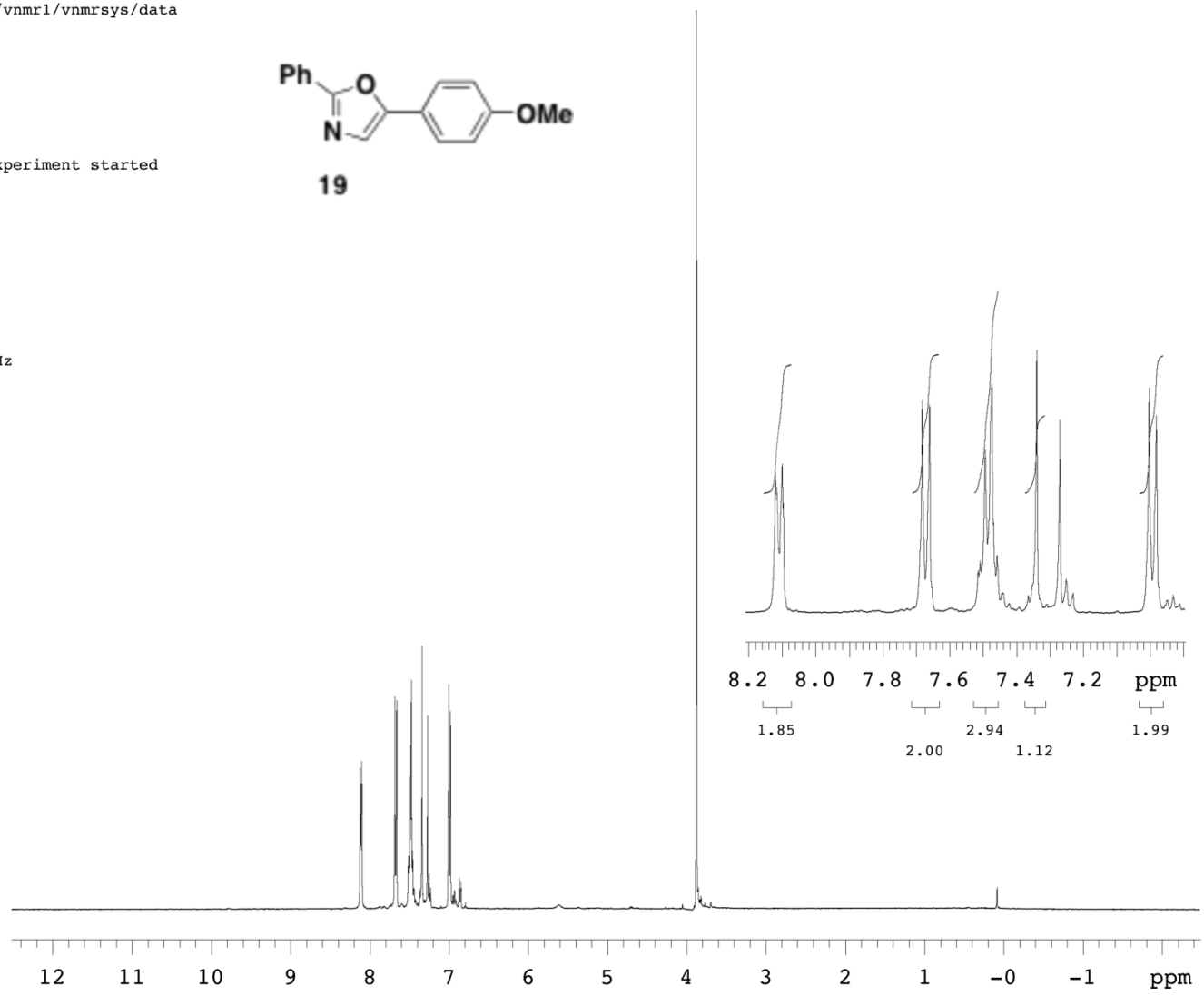
Archive directory: /vxr400/vnmr1/vnmrsys/data
Sample directory:

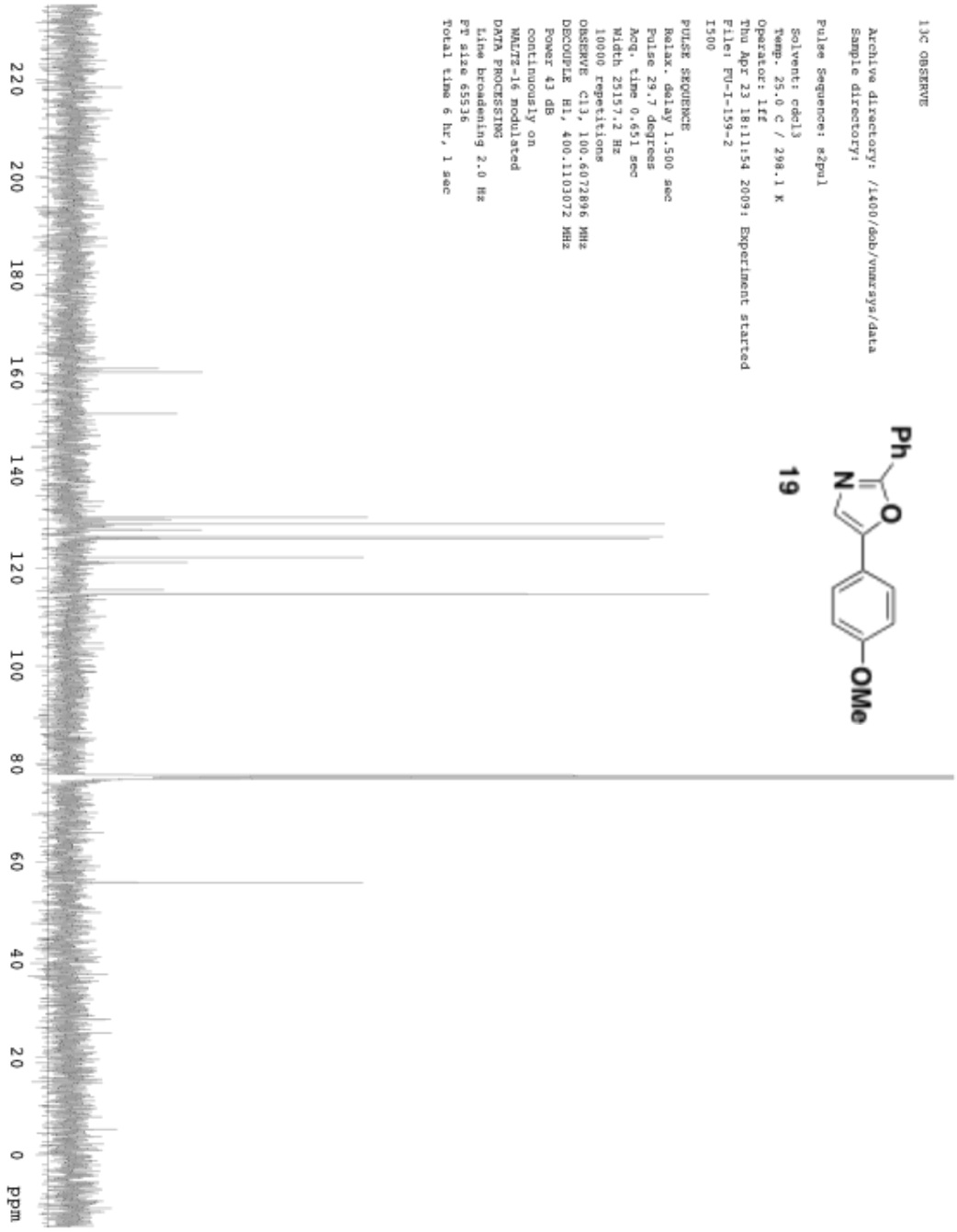
Pulse Sequence: s2pul

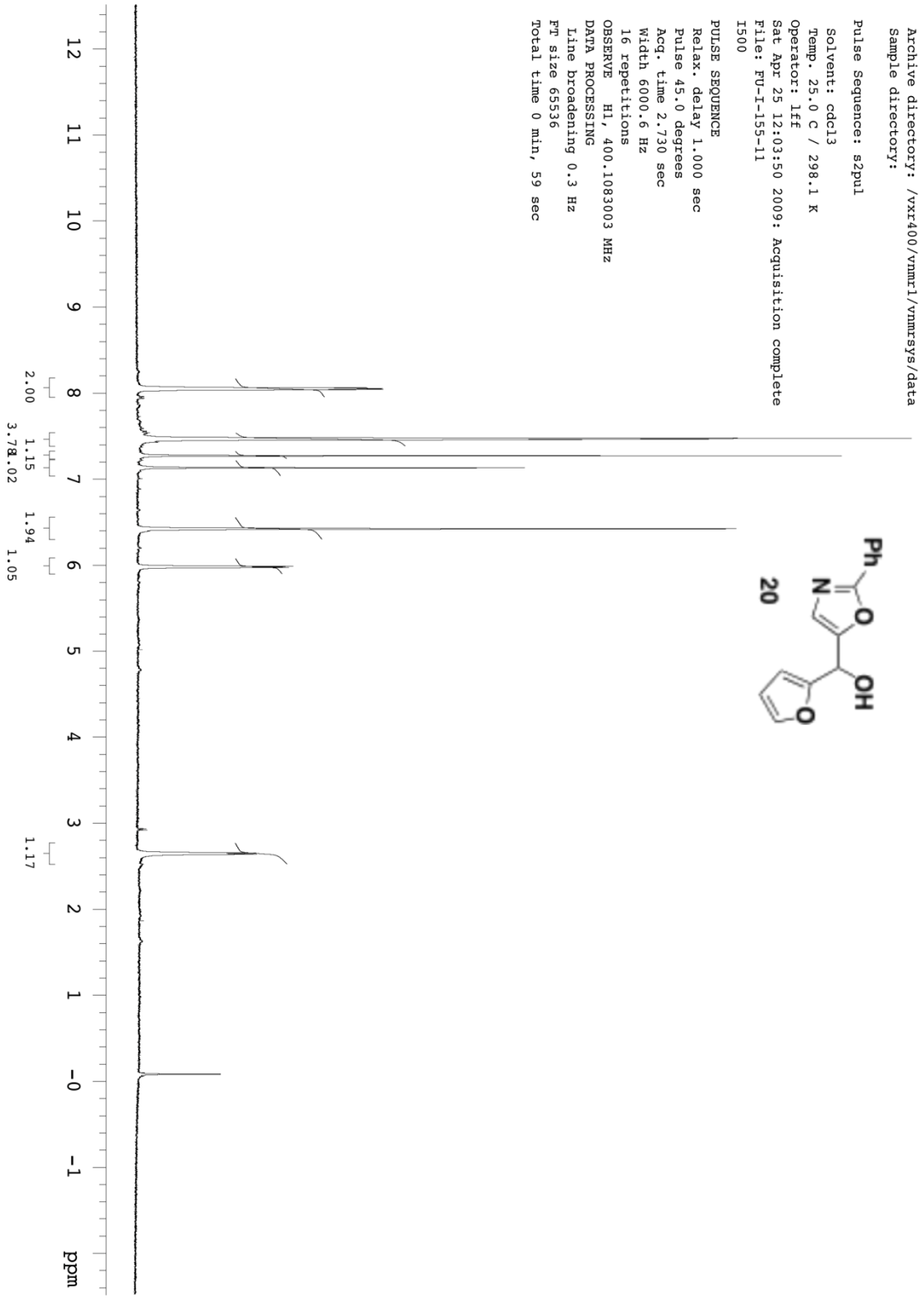
Solvent: cdcl3
Temp. 25.0 C / 298.1 K
Operator: lff
Thu Apr 23 18:10:48 2009: Experiment started
File: FU-I-159-1
I500

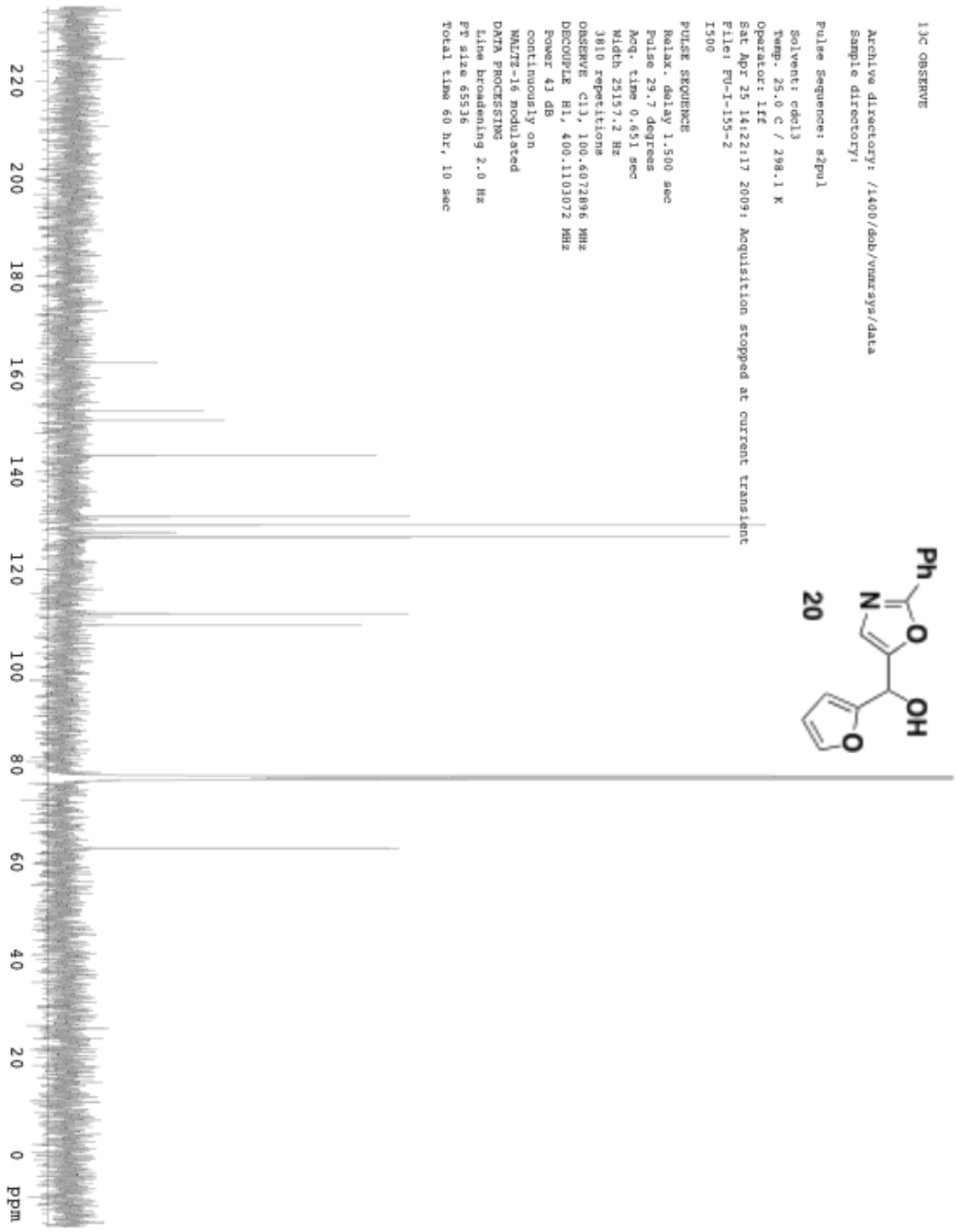
PULSE SEQUENCE
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 2.730 sec
Width 6000.6 Hz
16 repetitions
OBSERVE H1, 400.1083001 MHz
DATA PROCESSING
Line broadening 0.3 Hz
FT size 65536
Total time 0 min, 59 sec

19

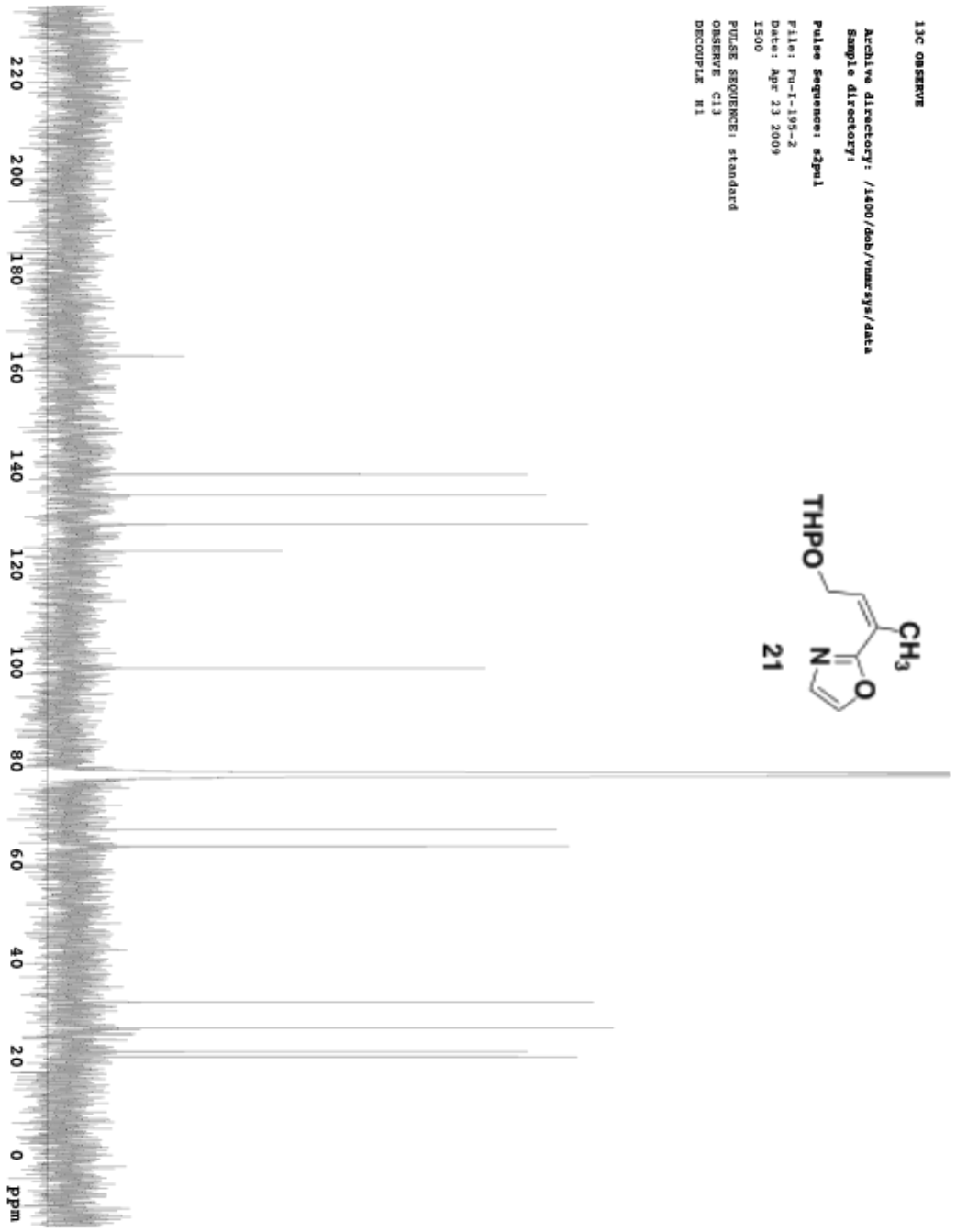


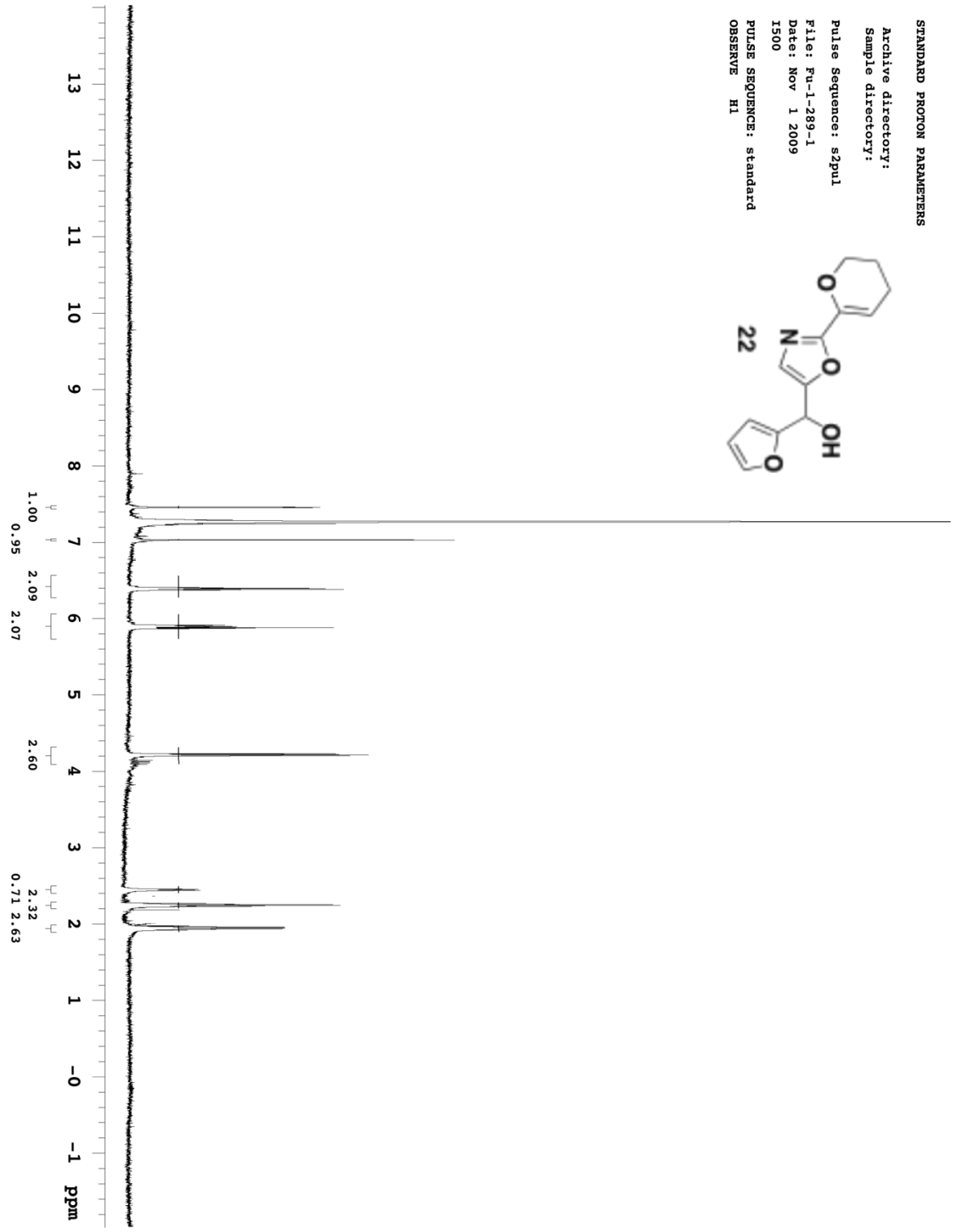

13C OBSERVE
Archive directory: /i400/dob/vnmrsys/data
Sample directory:
Pulse Sequence: s2pul
Solvent: cdcl3
Temp. 25.0 C / 298.1 K
Operator: lfe
Thu Apr 23 18:11:54 2009: Experiment started
File: FU-I-159-2
I500
PULSE SEQUENCE
Relax. delay 1.500 sec
Pulse 29.7 degrees
Acq. time 0.651 sec
Width 25157.2 Hz
10000 repetitions
OBSERVE C13, 100.6072896 MHz
DECOUPLE H1, 400.1103072 MHz
Power 43 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 2.0 Hz
FT size 65536
Total time 6 hr, 1 sec
Ph
O
N
OMe
19
220
200
180
160
140
120
100
80
60
40
20
0
ppm

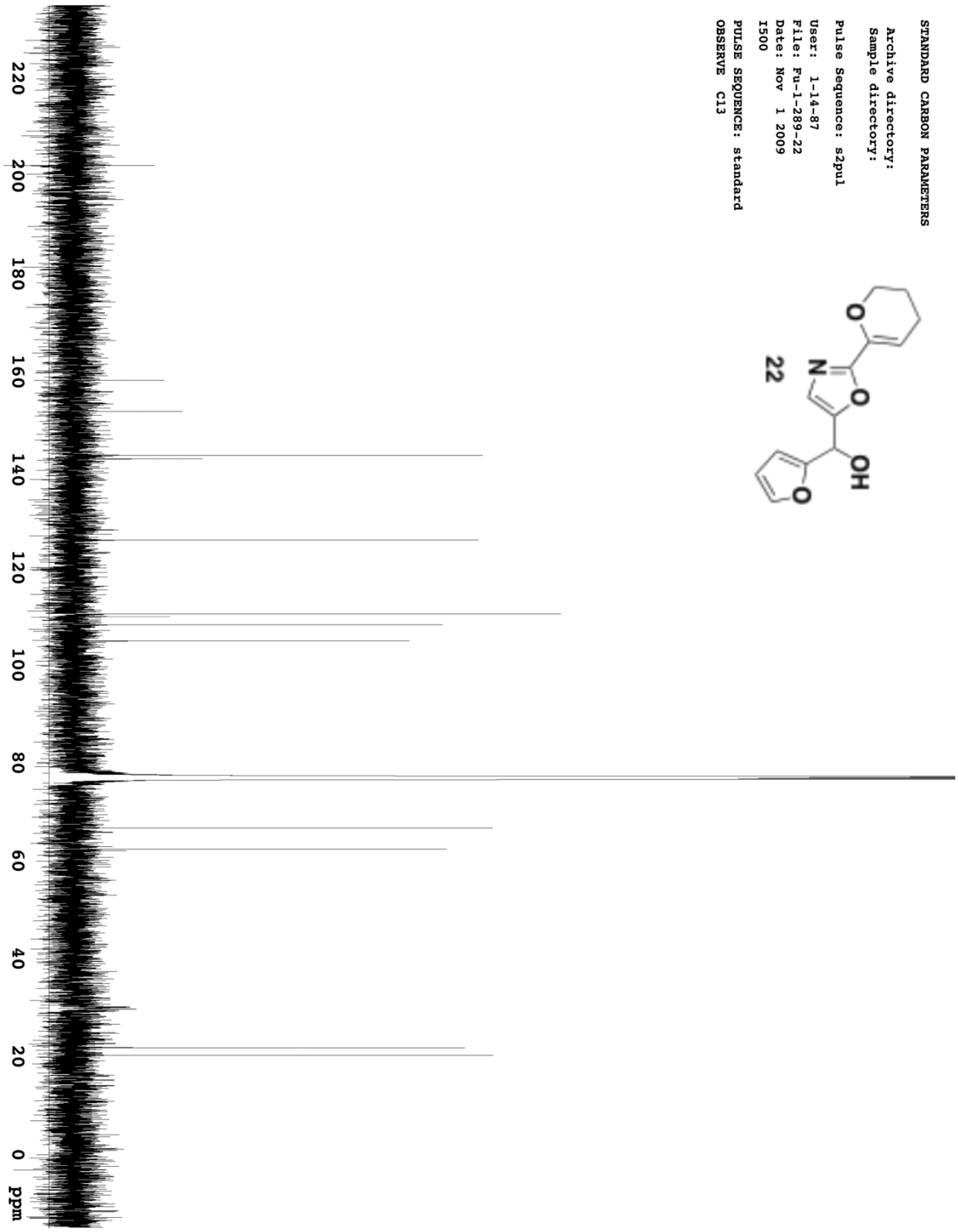

STANDARD 1H OBSERVE
Archive directory: /vxr400/vnmr1/vnmrsys/data
Sample directory:
Pulse Sequence: s2pul
Solvent: cdcl3
Temp. 25.0 C / 298.1 K
Operator: lff
Sat Apr 25 12:03:50 2009: Acquisition complete
File: FU-I-155-11
I500
PULSE SEQUENCE
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 2.730 sec
Width 6000.6 Hz
16 repetitions
OBSERVE H1, 400.1083003 MHz
DATA PROCESSING
Line broadening 0.3 Hz
FT size 65536
Total time 0 min, 59 sec
Ph
O
N
OH
O
20
12
11
10
9
8
7
6
5
4
3
2
1
-0
-1
ppm
2.00
1.15
3.78
1.02
1.94
1.05
1.17

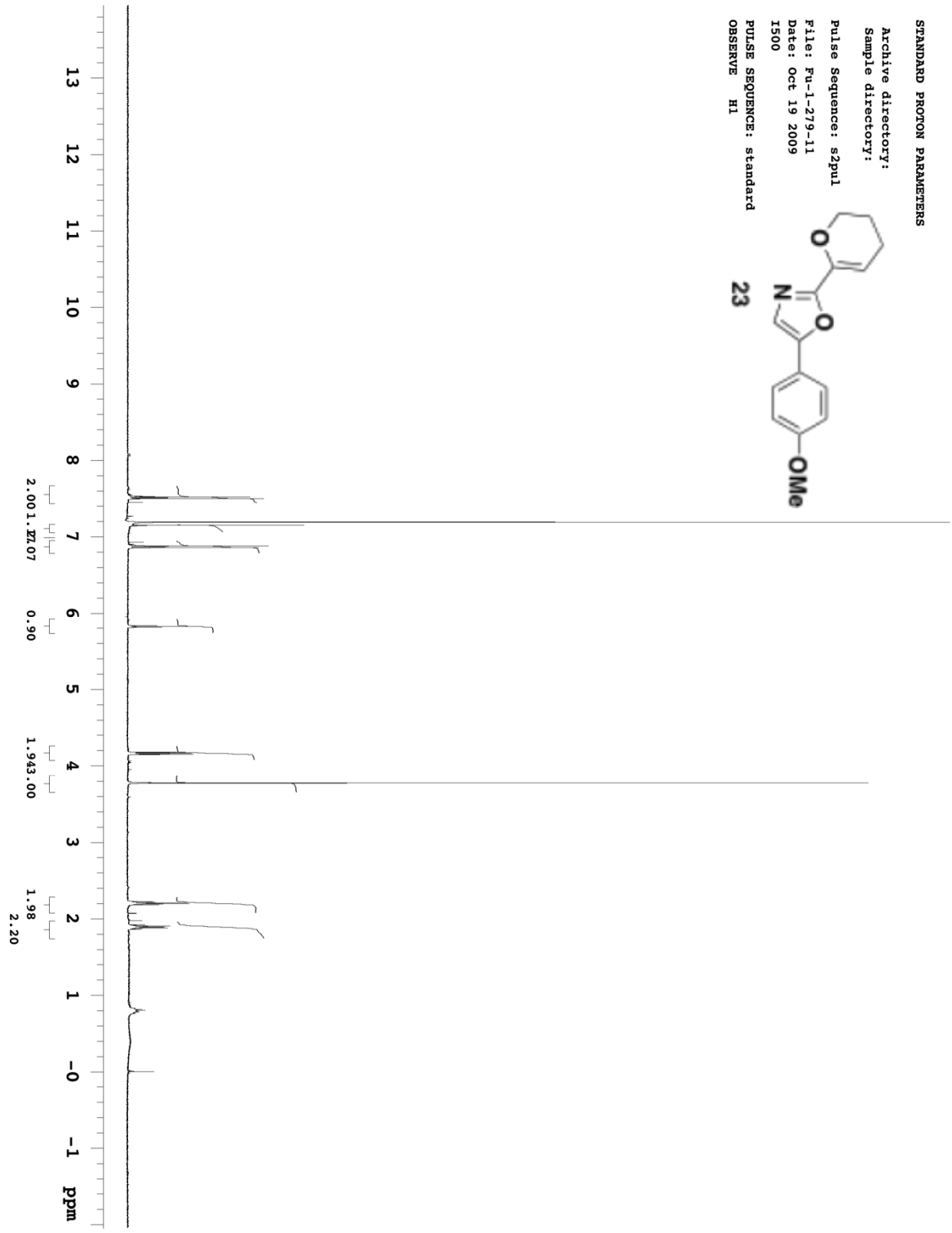

13C OBSERVE
Archive directory: /i400/dob/vnmrsys/data
Sample directory:
Pulse Sequence: s2pul
Solvent: cdcl3
Temp. 25.0 C / 298.1 K
Operator: lfe
Sat Apr 25 14:12:17 2009: Acquisition stopped at current transient
File: FU-I-159-2
I500
PULSE SEQUENCE
Relax. delay 1.500 sec
Pulse 29.7 degrees
Acq. time 0.651 sec
Width 25157.2 Hz
3810 repetitions
OBSERVE C13, 100.6072896 MHz
DECOUPLE H1, 400.1103072 MHz
Power 43 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 2.0 Hz
FT size 65536
Total time 60 hr, 10 sec
Ph
N
O
OH
O
20
220
200
180
160
140
120
100
80
60
40
20
0
ppm

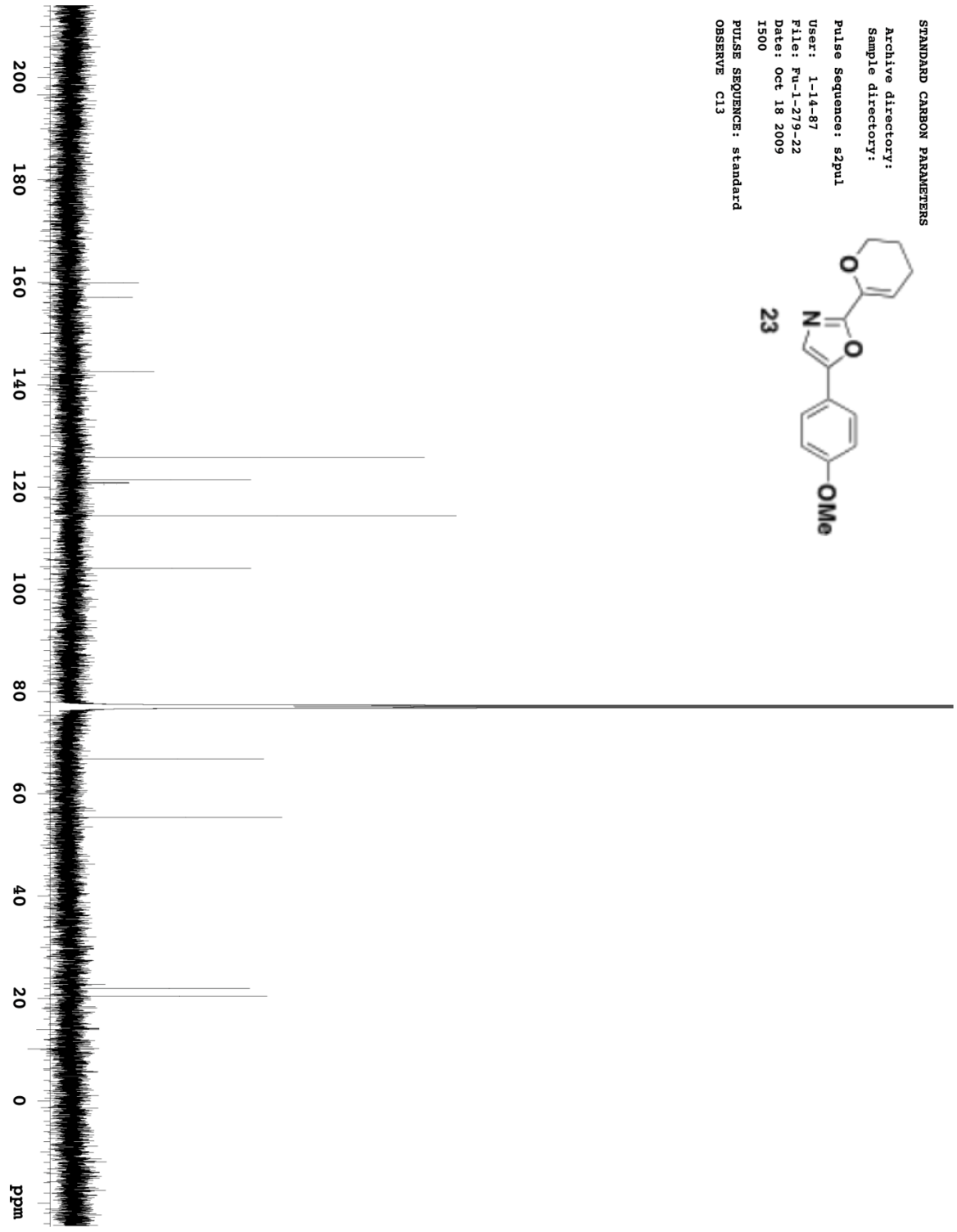
Archive directory: /vxr400/vnmr1/vnmrsys/data
Sample directory:
Pulse Sequence: s2pul
Solvent: cdcl3
Temp. 25.0 C / 298.1 K
Operator: lff
Thu Apr 23 23:03:19 2009: Experiment started
File: FU-I-195-1
I500
PULSE SEQUENCE
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 2.730 sec
Width 6000.6 Hz
16 repetitions
OBSERVE H1, 400.1083003 MHz
DATA PROCESSING
Line broadening 0.3 Hz
FT size 65536
Total time 0 min, 59 sec
THPO
CH3
N
O
21
0.85
1.05
0.95
2.97
1.27
1.37
2.88
3.73
3.30
12
11
10
9
8
7
6
5
4
3
2
1
-0
-1
ppm

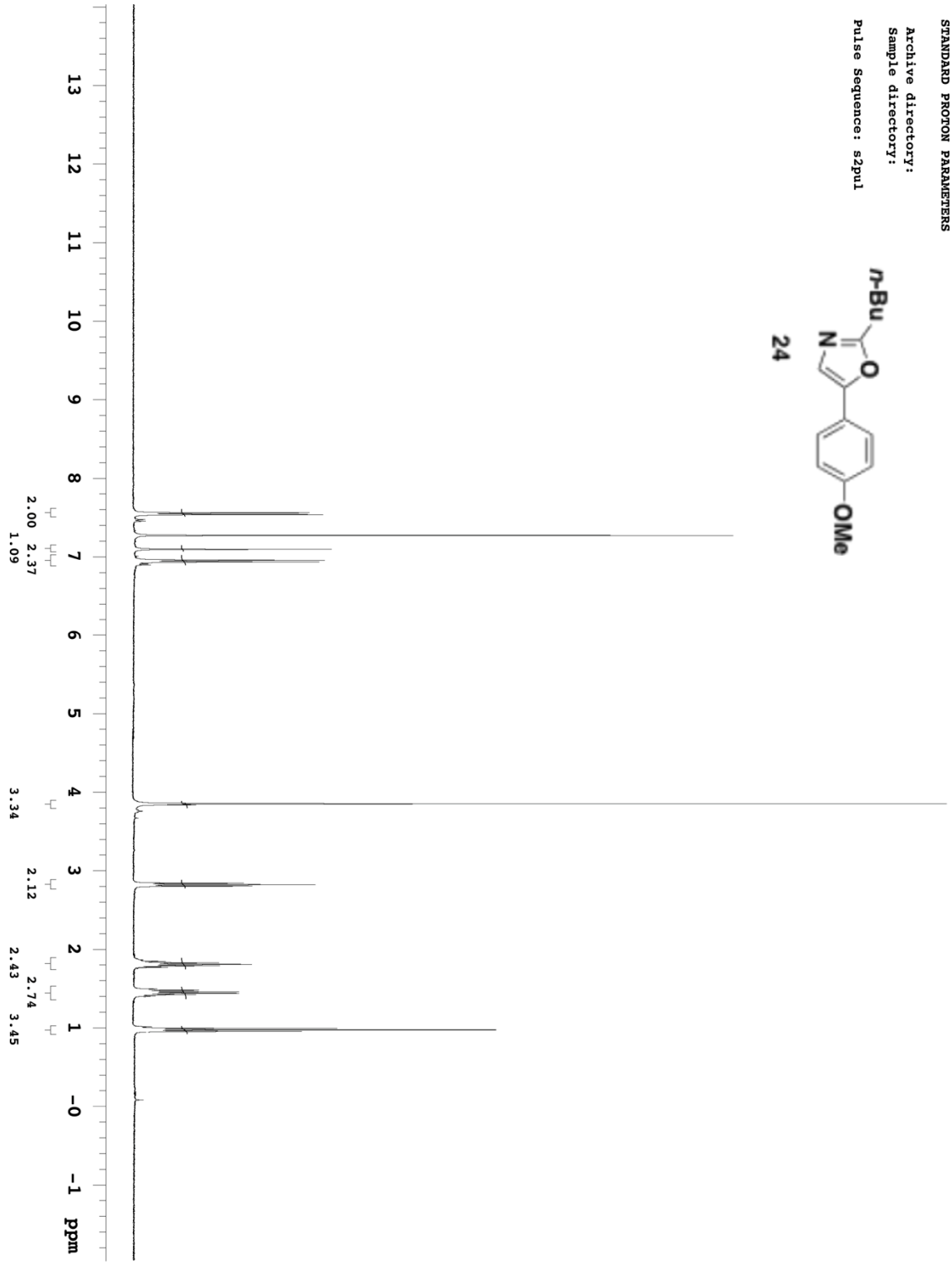

13C OBSERVE
Archive directory: /1400/dob/vnmrsys/data
Sample directory:
Pulse Sequence: s2pul
File: Fu-I-199-2
Date: Apr 23 2009
1500
PULSE SEQUENCE: standard
OBSERVE C13
DECOUPLE H1
THPO
CH3
N
O
21
220
200
180
160
140
120
100
80
60
40
20
0
ppm

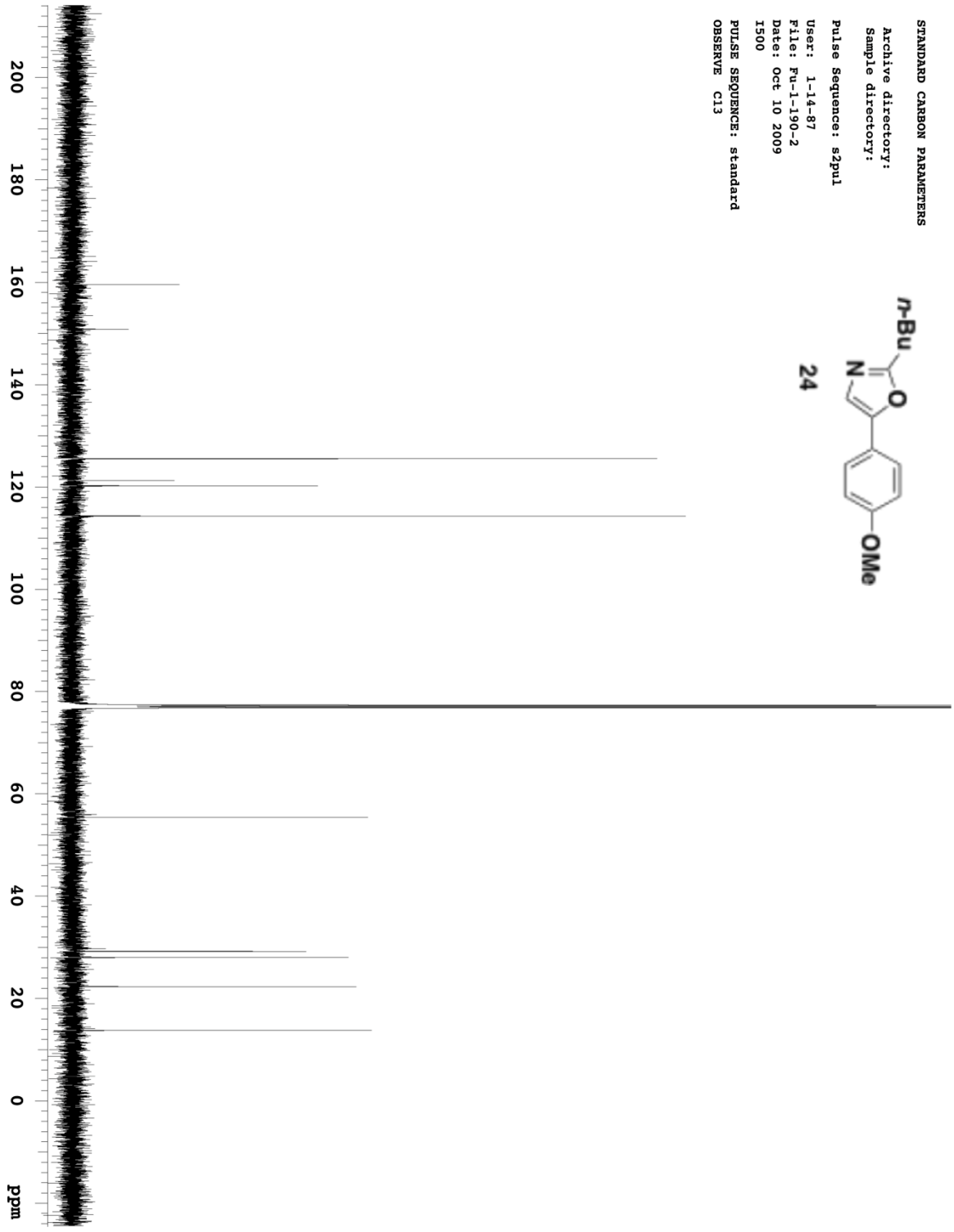

STANDARD PROTON PARAMETERS
Archive directory:
Sample directory:
Pulse Sequence: s2pul
File: Fu-1-289-1
Date: Nov 1 2009
I500
PULSE SEQUENCE: standard
OBSERVE H1
22
O
N
O
OH
O
13
12
11
10
9
8
7
6
5
4
3
2
1
-0
-1
ppm
1.00
0.95
2.09
2.07
2.60
2.32
0.71
2.63

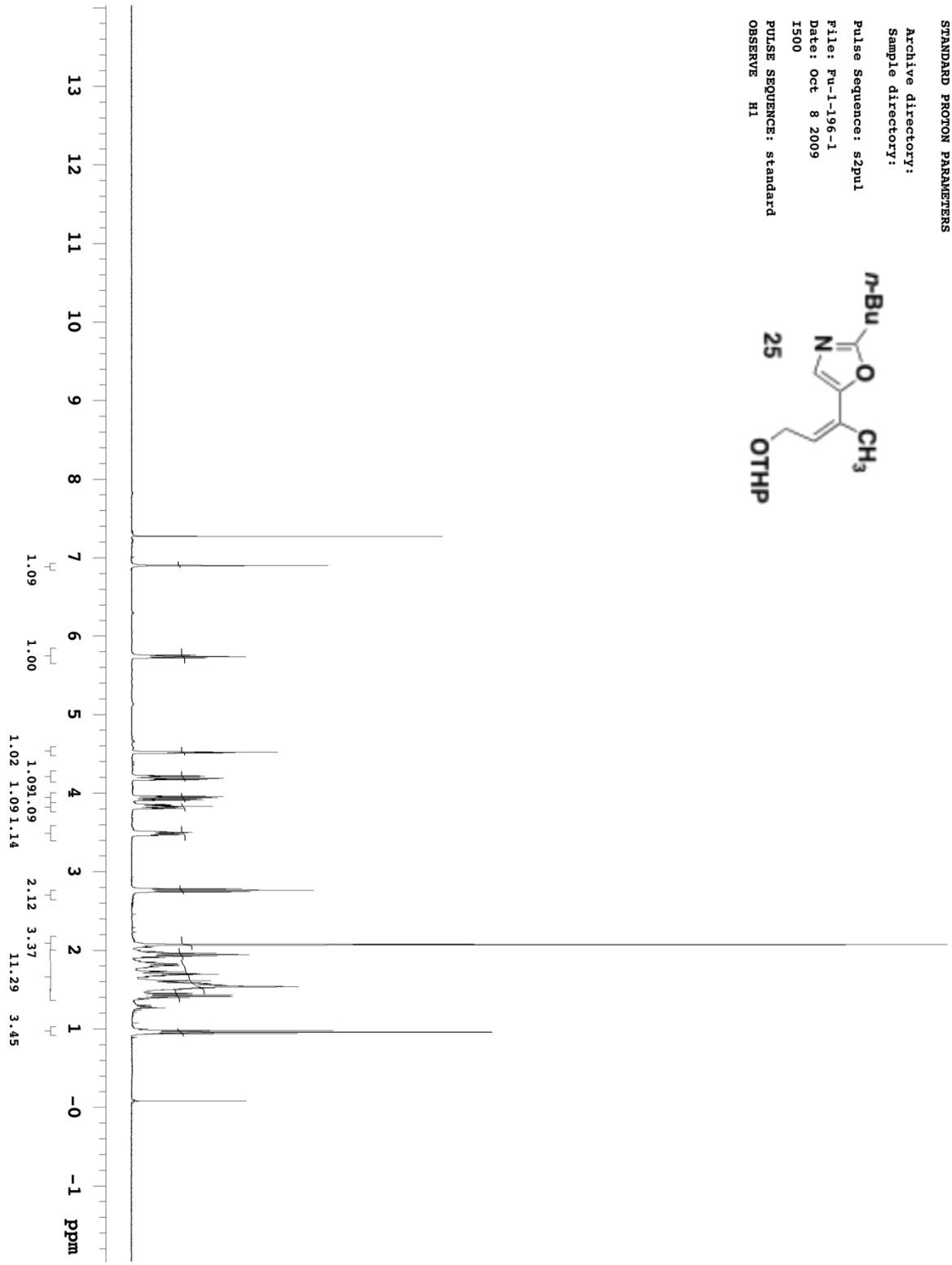

STANDARD CARBON PARAMETERS
Archive directory:
Sample directory:
Pulse Sequence: s2pul
User: l-14-87
File: Fu-l-289-22
Date: Nov 1 2009
I500
PULSE SEQUENCE: standard
OBSERVE C13
O
N
O
OH
O
22
220
200
180
160
140
120
100
80
60
40
20
0
ppm

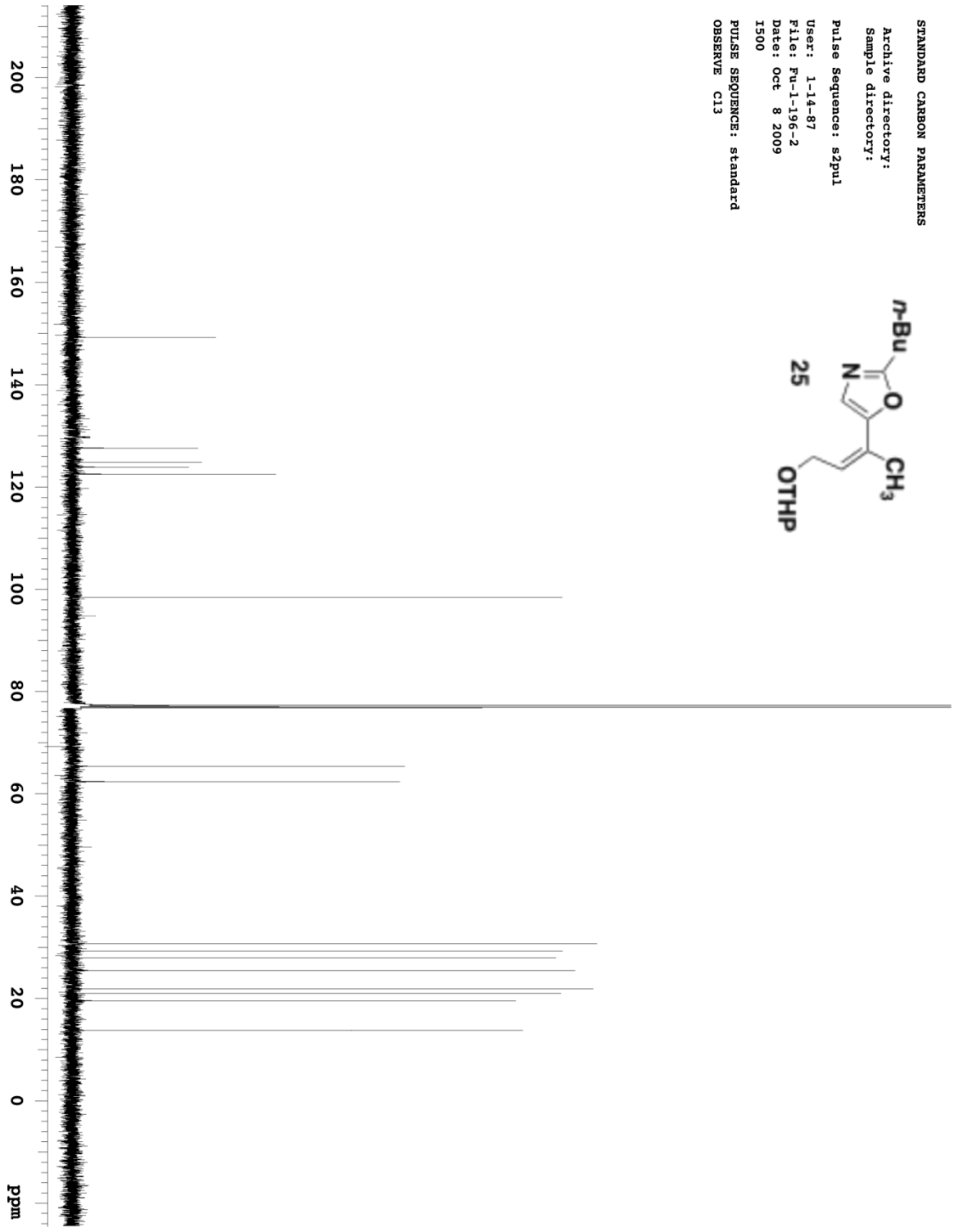

STANDARD PROTON PARAMETERS
Archive directory:
Sample directory:
Pulse Sequence: s2pul
File: Fu-1-279-11
Date: Oct 19 2009
I500
PULSE SEQUENCE: standard
OBSERVE H1
23
O
N
O
OMe
2.00
1.97
0.90
1.94
3.00
1.98
2.20
13
12
11
10
9
8
7
6
5
4
3
2
1
-0
-1
ppm

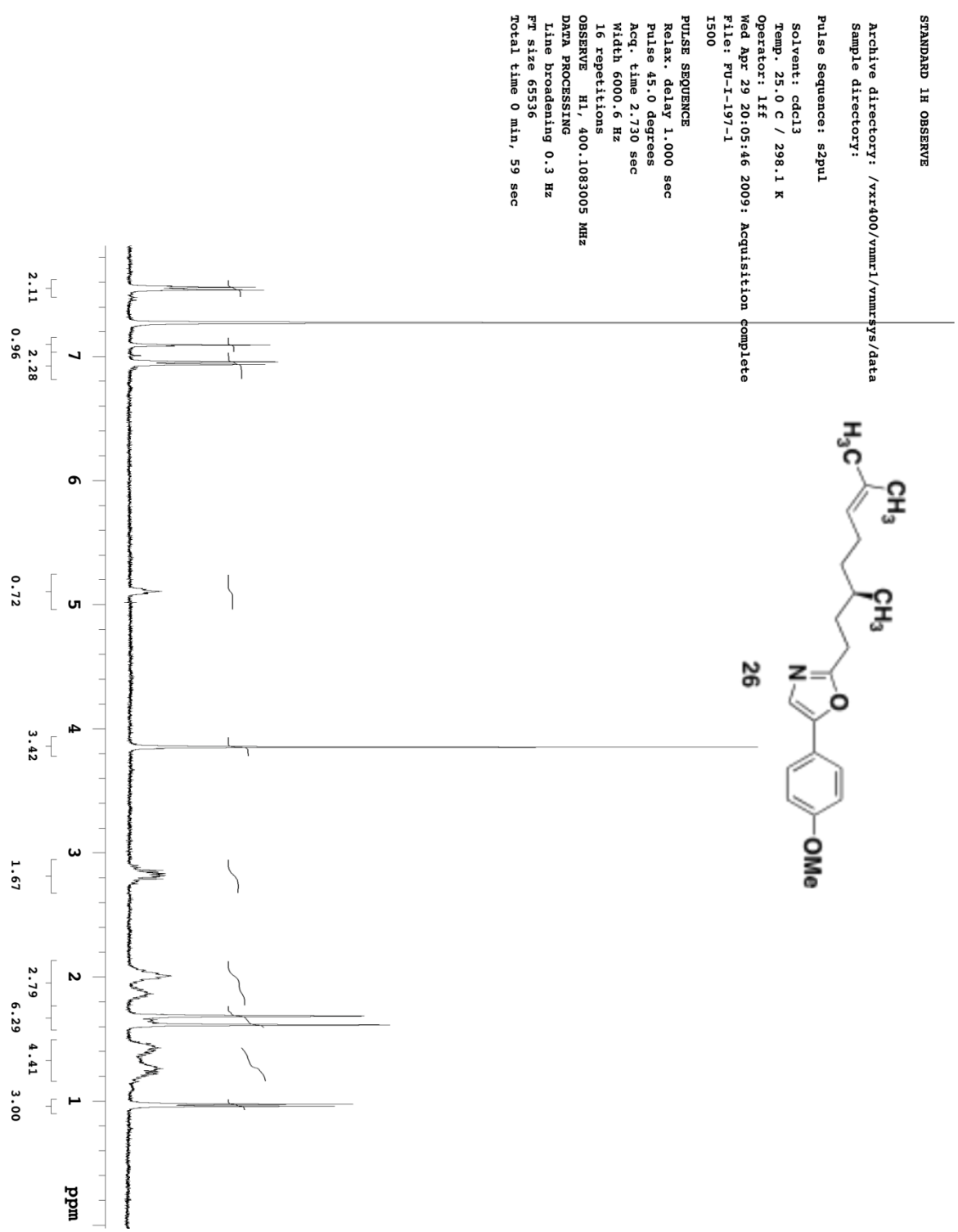

STANDARD CARBON PARAMETERS
Archive directory:
Sample directory:
Pulse Sequence: s2pul
User: l-14-87
File: Fu-l-279-22
Date: Oct 18 2009
I500
PULSE SEQUENCE: standard
OBSERVE C13
O
N
O
OMe
23
200
180
160
140
120
100
80
60
40
20
0
ppm

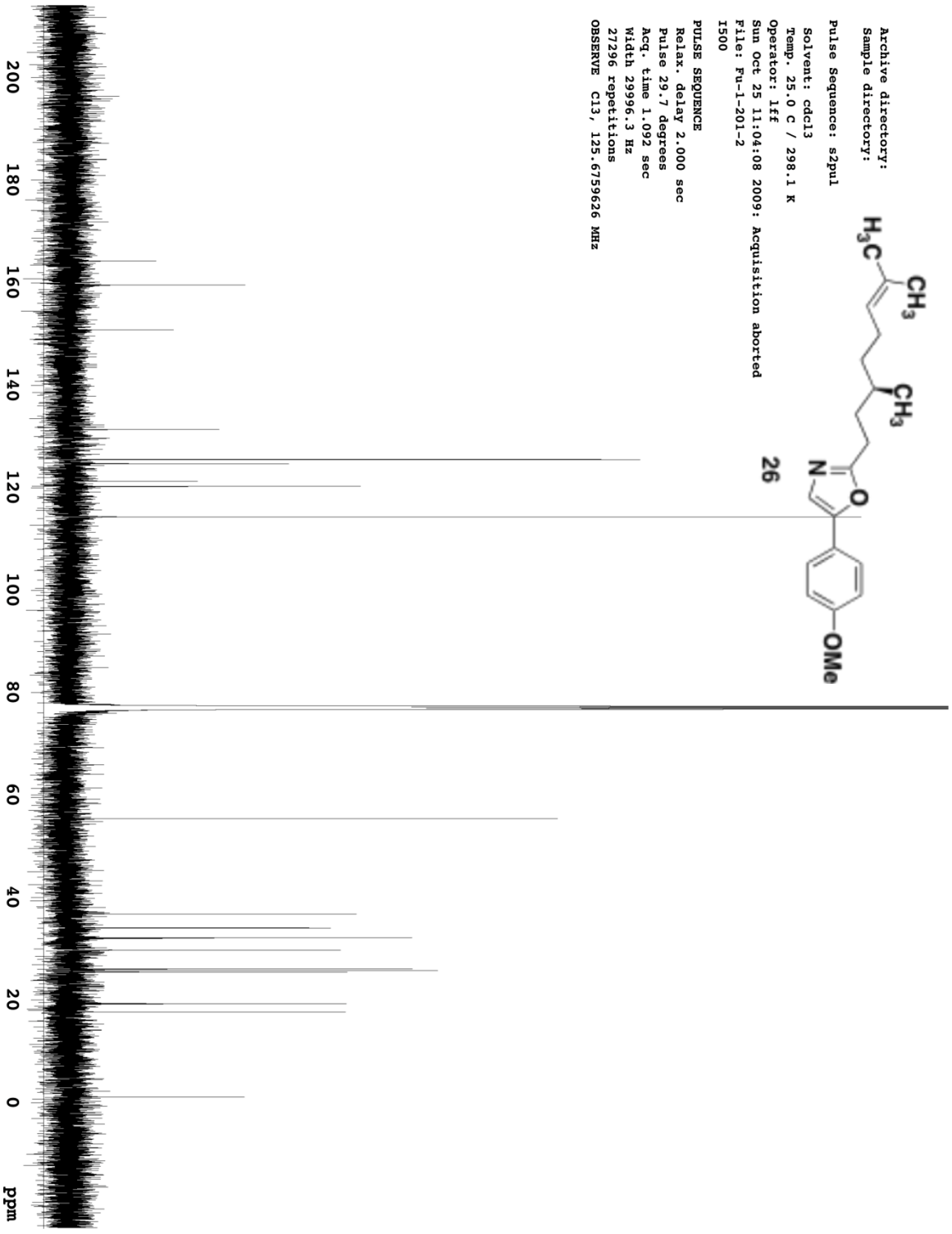

STANDARD PROTON PARAMETERS
Archive directory:
Sample directory:
Pulse Sequence: s2pul
n-Bu
N
O
OMe
24
13 12 11 10 9 8 7 6 5 4 3 2 1 -0 -1 ppm
2.00 2.37
1.09
3.34
2.12
2.43 2.74
3.45

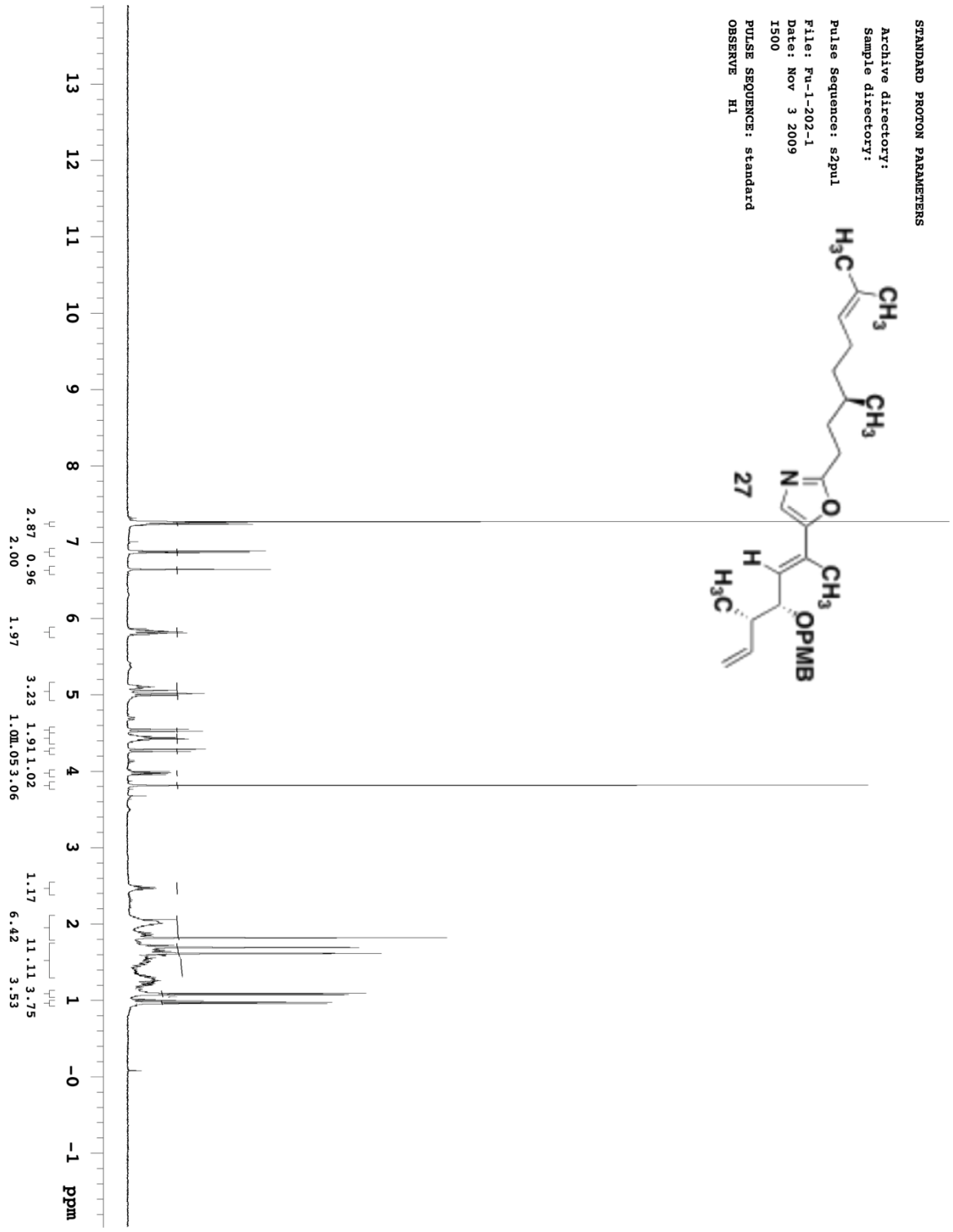

STANDARD CARBON PARAMETERS
Archive directory:
Sample directory:
Pulse Sequence: s2pul
User: l-14-87
File: Fu-l-190-2
Date: Oct 10 2009
I500
PULSE SEQUENCE: standard
OBSERVE C13
n-Bu
N
O
OMe
24
200
180
160
140
120
100
80
60
40
20
0
ppm

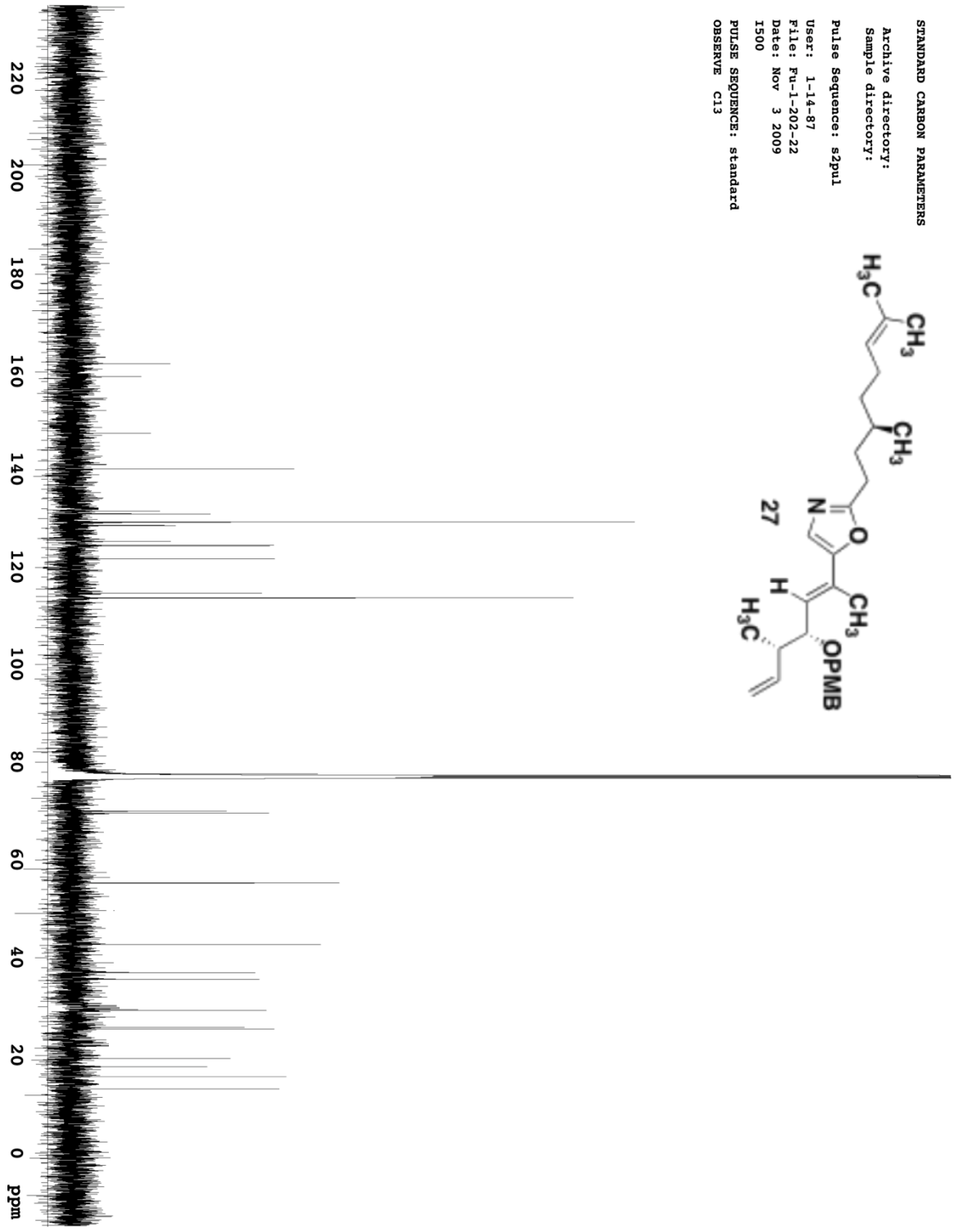

STANDARD PROTON PARAMETERS
Archive directory:
Sample directory:
Pulse Sequence: s2pul
File: Fu-1-196-1
Date: Oct 8 2009
I500
PULSE SEQUENCE: standard
OBSERVE H1
n-Bu
N
O
CH3
25
OTHP
13 12 11 10 9 8 7 6 5 4 3 2 1 -0 -1 ppm
1.09 1.00 1.09 1.09 2.12 3.37
1.02 1.09 1.14 11.29 3.45

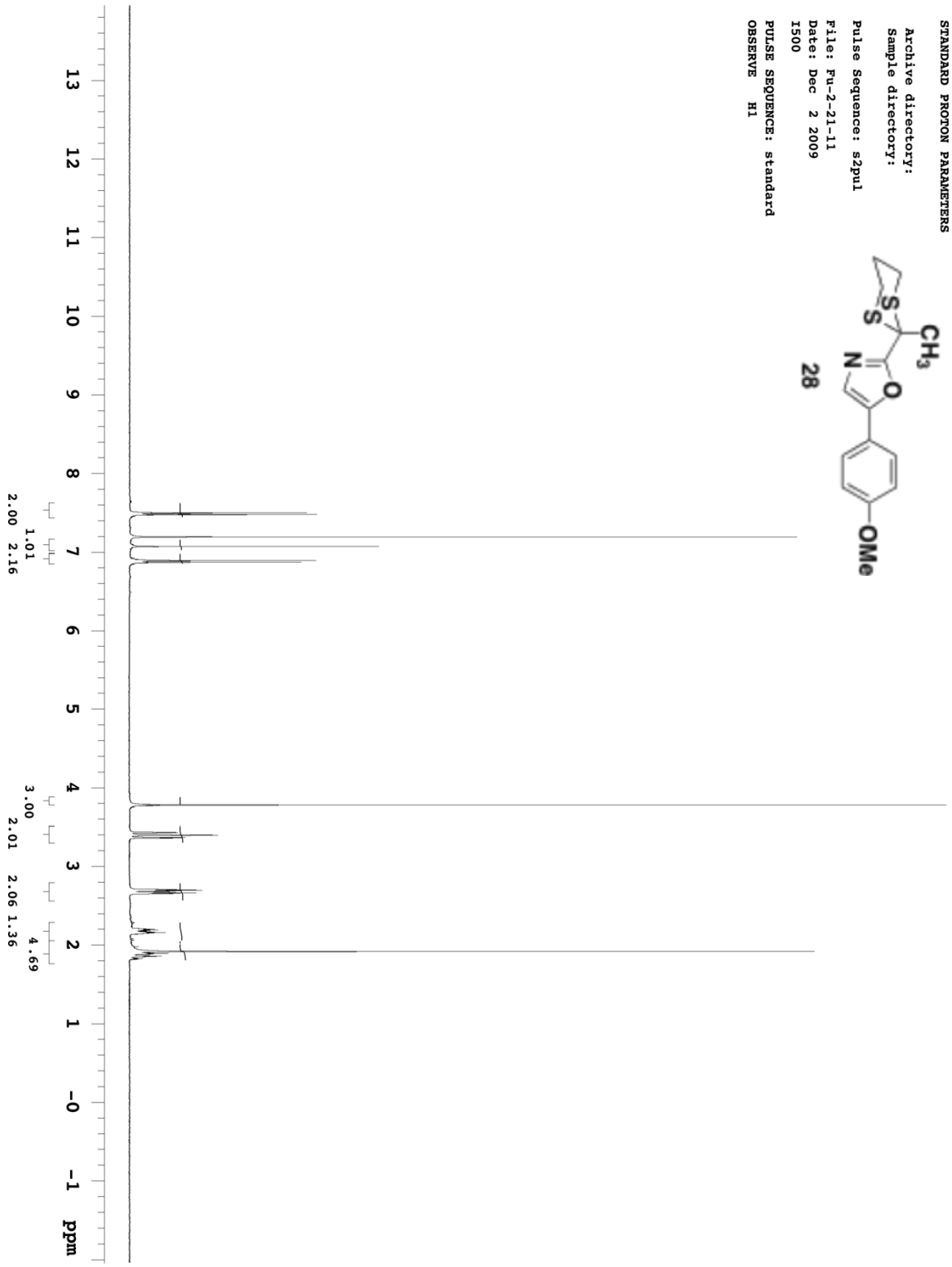

STANDARD CARBON PARAMETERS
Archive directory:
Sample directory:
Pulse Sequence: s2pul
User: l-14-87
File: Fu-l-196-2
Date: Oct 8 2009
I500
PULSE SEQUENCE: standard
OBSERVE C13
n-Bu
N
O
CH3
25
OTHP
200
180
160
140
120
100
80
60
40
20
0
ppm

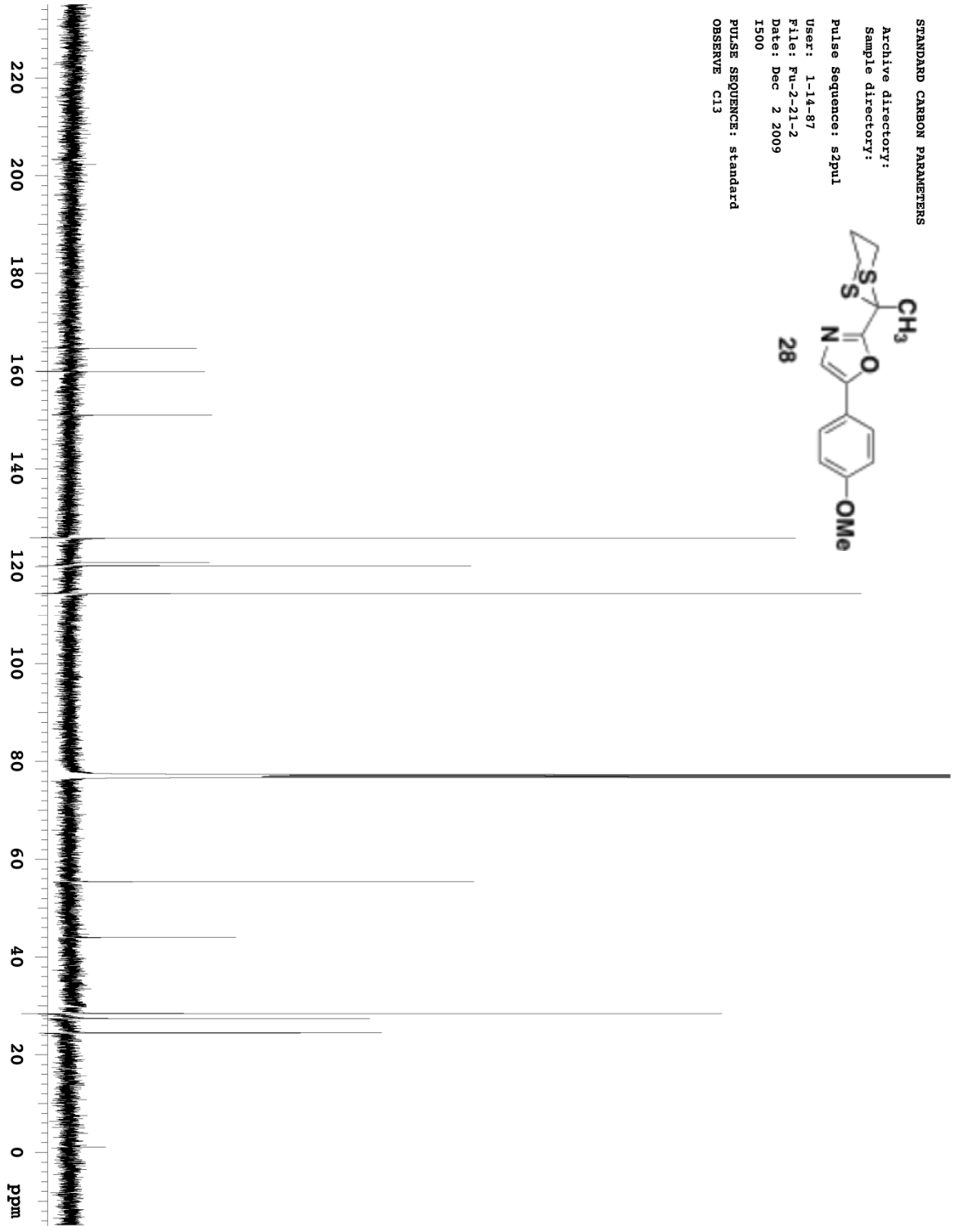

STANDARD 1H OBSERVE
Archive directory: /vxr400/vnmr1/vnmrsys/data
Sample directory:
Pulse Sequence: s2pul
Solvent: cdcl3
Temp. 25.0 C / 298.1 K
Operator: lff
Wed Apr 29 20:05:46 2009: Acquisition complete
File: FU-I-197-1
I500
PULSE SEQUENCE
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 2.730 sec
Width 6000.6 Hz
16 repetitions
OBSERVE H1, 400.1083005 MHz
DATA PROCESSING
Line broadening 0.3 Hz
FT size 65536
Total time 0 min, 59 sec
H3C
CH3
CH3
N
O
OMe
26
7
6
5
4
3
2
1
ppm
2.11
2.28
0.96
0.72
3.42
1.67
2.79
6.29
4.41
3.00


Archive directory:
Sample directory:
Pulse Sequence: s2pul
Solvent: cdcl3
Temp. 25.0 C / 298.1 K
Operator: lff
Sun Oct 25 11:04:08 2009: Acquisition aborted
File: Fu-1-201-2
I500
PULSE SEQUENCE
Relax. delay 2.000 sec
Pulse 29.7 degrees
Acq. time 1.092 sec
Width 29996.3 Hz
27296 repetitions
OBSERVE C13, 125.6759626 MHz
26
H3C
CH3
CH3
N
O
OMe
200
180
160
140
120
100
80
60
40
20
0
ppm


STANDARD PROTON PARAMETERS
Archive directory:
Sample directory:
Pulse Sequence: s2pul
File: Fu-1-202-1
Date: Nov 3 2009
I500
PULSE SEQUENCE: standard
OBSERVE H1
27
OPMB
ppm
2.87 0.96
2.00
1.97
3.23 1.91 1.02
1.00 1.05 3.06
1.17
6.42
11.11 3.75
3.53


STANDARD CARBON PARAMETERS
Archive directory:
Sample directory:
Pulse Sequence: s2pul
User: l-14-87
File: Fu-l-202-22
Date: Nov 3 2009
I500
PULSE SEQUENCE: standard
OBSERVE C13
H3C
CH3
CH3
N
O
27
H
CH3
H3C
OPMB
220
200
180
160
140
120
100
80
60
40
20
0
ppm


STANDARD PROTON PARAMETERS
Archive directory:
Sample directory:
Pulse Sequence: s2pul
File: Fu-2-21-11
Date: Dec 2 2009
I500
PULSE SEQUENCE: standard
OBSERVE H1
28
CH3
S
S
N
O
OMe
13
12
11
10
9
8
7
6
5
4
3
2
1
0
-1
ppm
2.00 2.16
1.01
3.00
2.01 2.06 1.36
4.69


STANDARD CARBON PARAMETERS
Archive directory:
Sample directory:
Pulse Sequence: s2pul
User: 1-14-87
File: Fu-2-21-2
Date: Dec 2 2009
I500
PULSE SEQUENCE: standard
OBSERVE C13
28
220
200
180
160
140
120
100
80
60
40
20
0
ppm