

Synthesis of Dithiocarbamate by Markovnikov Addition Reaction

Azim Ziyaei Halimehjani^{*}, Katayoun Marjani^{*}, Akram Ashoori

*Faculty of Chemistry, Tarbiat Moallem Universit, P. O. Box 11465- 9516
Tehran, 11365, Iran. Fax +98(21)66012983*

ziyaei@tmu.ac.ir

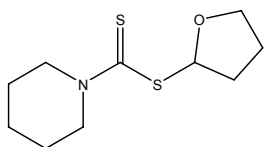
Contents	Pages
General experimental procedures	2
Characterization data	3-8
Copies of ¹H NMR and ¹³C NMR spectra	9-38

Experimental

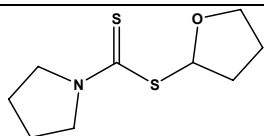
General Procedure for the Markovnikov Addition Reaction. To a mixture of an amine (5 mmol) and carbon disulfide (6 mmol) in water (10 mL) was added an electrophile (6 mmol). The reaction mixture was stirred vigorously at room temperature for 16h. Then, the products were extracted with ethyl acetate (2×20) and the combined organic layers were washed with water and dried over anhydrous Na_2SO_4 . The solvent was evaporated under reduced pressure to give the products with high purity in most of the cases. If needed, the products were purified by flash column chromatography (silica gel, ethyl acetate/ petroleum ether; 2/8). The products were characterized by their IR, ^1H and ^{13}C NMR spectra and CHN analyses.

Typical Procedure for Large Scale Synthesis of 1-ethoxyethyldiethylcarbamoithioate: In a 500 mL round bottom flask, diethyl amine (35 g, 50 mL, 0.48 mol), water (300 mL) and CS_2 (41.8 g, 33.2 mL, 0.55 mol) were added respectively. To this vigorously stirred reaction mixture, ethyl vinyl ether (39.6 g, 52.5 mL, 0.55 mol) was added slowly and stirred at room temperature for 16h. In completion, the organic phase was decanted and washed three times with water. Then, the organic phase was evaporated under reduce pressure to remove excess unreacted materials (CS_2 : b.p. 46.3°C ; ethyl vinyl ether: b.p. $34\text{--}36^\circ\text{C}$) to prepare 1-ethoxyethyldiethylcarbamoithioate with excellent purity and yields (82.7 g, 78%).

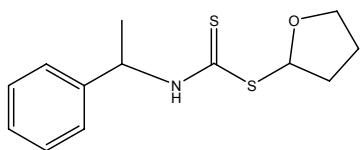
Experimental Procedure for Synthesis of Iodocyclization Product 7. To a stirred solution of α -(ethoxyethyl)-diallyl dithiocarbamate **6** (1 mmol) in THF (5 mL) was added I_2 (2.5 mmol) and the reaction mixture stirred for 48h at room temperature. The resulted yellow precipitate was filtered off and washed with THF to give the product **7** in 65% yields. IR (KBr) ν_{max} 2921, 1634, 1578, 1418, 1286, 1209, 1070, 825, 563 cm^{-1} . ^1H NMR (500 MHz, DMSO-d_6) δ 4.84 (m, 2H), 4.24 (dd, $J = 8.9, 13.4$ Hz, 2H), 3.97 (dd, $J = 3.8, 13.5$ Hz, 2H), 3.69 (m, 4H); ^{13}C NMR (500 MHz, DMSO-d_6) δ 192.1, 58.8, 56.6, 10.6; Anal. Calcd for $\text{C}_7\text{H}_{10}\text{I}_3\text{NS}_2$: C, 15.19; H, 1.80; N, 2.53. Found: C, 15.33; H, 1.84; N, 2.54.



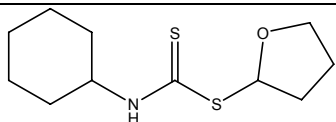
Tetrahydrofuran-2-yl piperidine-1-carbodithioate: IR (neat) $\nu_{\max}$ 2936, 2854, 1471, 1427, 1229, 1130, 1114, 1056, 743, 654 cm^{-1} ; ^1H NMR (300 MHz, CDCl_3) δ 6.35 (dd, J = 3.8, 7.2 Hz, 1H), 4.23 (br, 2H), 3.87 (m, 2H), 3.80 (br, 2H), 2.43 (m, 1H), 2.21 (m, 1H), 1.96 (m, 2H), 1.65 (m, 6H); ^{13}C NMR (300 MHz, CDCl_3) δ 193.7, 90.5, 68.4, 51.8, 51.4, 32.0, 25.9, 25.2, 24.7, 24.1; Anal. Calcd for $\text{C}_{10}\text{H}_{17}\text{NOS}_2$: C, 51.95; H, 7.36; N, 6.06. Found: C, 51.77; H, 7.46; N, 6.10.



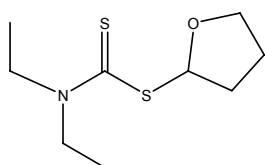
Tetrahydrofuran-2-yl pyrrolidine-1-carbodithioate: m.p. 43-45 $^{\circ}\text{C}$, IR (neat) $\nu_{\max}$ 2970, 2868, 1464, 1436, 1250, 1185, 1161, 1053, 692 cm^{-1} ; ^1H NMR (300MHz, CDCl_3) δ 6.35 (dd, J = 3.9, 7.2 Hz, 1H), 3.83-3.94 (m, 4H), 3.51 -3.83 (m, 2H), 2.38 (m, 1H), 2.12 (m, 1H), 1.89 -2.02 (m, 6H); ^{13}C NMR (300 MHz, CDCl_3) δ 191.0, 98.6, 68.3, 53.8, 50.6, 31.8, 25.8, 24.4, 24.0; Anal. Calcd for $\text{C}_9\text{H}_{15}\text{NOS}_2$: C, 49.77; H, 6.91; N, 6.45. Found: C, 49.65; H, 6.73; N, 6.48.



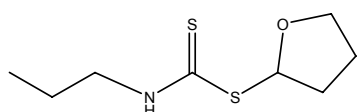
Tetrahydrofuran-2-yl-1-phenylethylcarbamdithioate: IR (neat) $\nu_{\max}$ 3274, 2977, 1516, 1494, 1435, 1377, 1136, 1094, 735, 692 cm^{-1} ; ^1H NMR (300 MHz, CDCl_3) δ 8.79 (br, 1H, NH), 7.26-7.39 (m, 5H), 5.95-6.04 (m, 1H), 5.75 (m, 1H), 3.94 (m, 2H), 2.29 (m, 1H), 2.04 (m, 1H), 1.87-1.95 (m, 2H), 1.60 (dd, J = 2.5, 6.8 Hz, 3H); ^{13}C NMR (300 MHz, CDCl_3) δ 195.2, 141.5, 128.7, 127.5, 125.8, 86.6, 67.9, 54.9, 31.1, 24.3, 20.9; Anal. Calcd for $\text{C}_{13}\text{H}_{17}\text{NOS}_2$: C, 58.43; H, 6.37; N, 5.24. Found: C, 58.55; H, 6.43; N, 5.36.



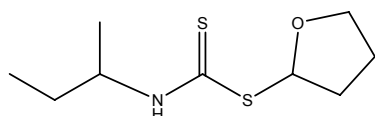
Tetrahydrofuran-2-yl cyclohexanecarbamdithioate: m.p. 40-42 $^{\circ}\text{C}$, IR (neat) $\nu_{\max}$ 3242, 2930, 2855, 1515, 1447, 1387, 1246, 1151, 1041, 986, 932, 886, 675 cm^{-1} ; ^1H NMR (300 MHz, CDCl_3) δ 8.45 (br, 1H, NH), 5.94 (dd, J = 3.2, 7.2 Hz, 1H), 4.39 (m, 1H), 4.01 (m, 2H), 2.28 (m, 1H), 1.90-2.08 (m, 5H), 1.66-1.69 (m, 2H), 1.31-1.41 (m, 6H); ^{13}C NMR (300 MHz, CDCl_3): δ 194.6, 86.4, 68.3, 54.4, 33.1, 32.5, 32.4, 25.3, 24.3; Anal. Calcd for $\text{C}_{11}\text{H}_{19}\text{NOS}_2$: C, 53.88; H, 7.76; N, 5.71. Found: C, 54.04; H, 8.04; N 5.79.



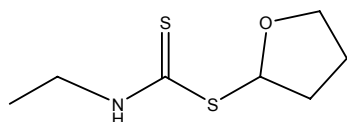
Tetrahydrofuran-2-yl diethylcarbamodithioate: IR (neat) $\nu_{\max}$ 2975, 2933, 1486, 1410, 1141, 1268, 1056, 918, 831 cm^{-1} ; ^1H NMR (300 MHz, CDCl_3) δ 6.36 (dd, $J=3.9, 7.3$ Hz, 1H), 3.90-4.03 (m, 4H), 3.65 (m, 2H), 2.42 (m, 1H), 2.21 (m, 1H), 1.96 (m, 2H), 1.23 (t, $J=7.1$ Hz, 6H); ^{13}C NMR (300 MHz, CDCl_3) δ 194.0, 99.5, 68.4, 48.6, 46.8, 32.0, 24.8, 12.4, 11.4; Anal. Calcd for $\text{C}_9\text{H}_{17}\text{NOS}_2$: C, 49.32; H, 7.76; N, 6.39. Found: C, 49.41; H, 8.04; N, 6.81.



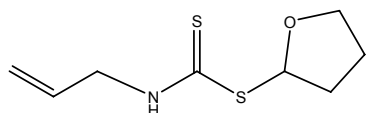
Tetrahydrofuran-2-yl butylcarbamodithioate: ^1H NMR (300 MHz, CDCl_3) δ 8.54 (br, 1H, NH), 5.94 (m, 1H), 3.98-4.03 (m, 2H), 3.61 (m, 2H), 2.33 (m, 1H), 1.76-2.1 (m, 3H), 1.66 (m, 2H), 0.92 (m, 3H). ^{13}C NMR (300 MHz, CDCl_3) δ 196.0, 86.2, 67.8, 47.9, 30.9, 23.9, 21.3, 11.2.



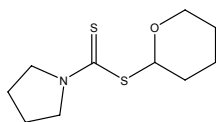
Tetrahydrofuran-2-yl sec-butylcarbamodithioate: ^1H NMR (300 MHz, CDCl_3) δ 8.63 (br, 1H, NH), 5.94 (dd, $J=3.0, 7.4$ Hz, 1H), 4.00 (m, 2H), 3.49 (m, 2H), 2.25 (m, 1H), 1.88-1.97 (m, 4H), 0.94-1.00 (m, 6H); ^{13}C NMR (300 MHz, CDCl_3) δ 196.1, 86.2, 68.2, 53.5, 31.0, 28.1, 25.2, 20.0, 19.5.



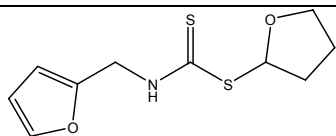
Tetrahydrofuran-2-yl ethylcarbamodithioate: ^1H NMR (300 MHz, CDCl_3) δ 8.42 (br, 1H, NH), 5.97 (dd, dd, $J=3.2, 7.2$ Hz, 1H), 4.01 (dd, $J=6.2, 7.2$ Hz, 2H), 3.37-3.76 (m, 2H), 2.31 (m, 1H), 1.87-2.05 (m, 3H), 1.25-1.30 (t, $J=7.3$ Hz, 3H); ^{13}C NMR (300 MHz, CDCl_3) δ 196.2, 86.4, 67.9, 41.3, 31.1, 24.6, 13.3.



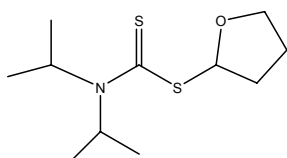
Tetrahydrofuran-2-yl allylcarbamodithioate: ^1H NMR (300 MHz, CDCl_3) δ 8.56 (br, 1H, NH), 5.96 (dd, $J=3.2, 7.2$ Hz, 1H), 5.75 (m, 1H), 5.17 (m, 2H), 4.29 (m, 2H), 3.97 (m, 2H), 2.20 (m, 1H), 1.81 (m, 3H); ^{13}C NMR (300 MHz, CDCl_3) δ 196.3, 134.0, 117.6, 90.0, 68.2, 48.4, 31.9, 24.8.



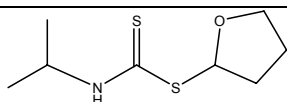
Tetrahydro-2H-pyran-2-yl pyrrolidine-1-carbodithioate: m.p. 60-63 °C, ^1H NMR (500 MHz CDCl_3) δ 6.15-6.17 (dd, $J=3.7, 6.6$ Hz, 1H), 3.94-3.99 (m, 3H), 3.75 (m, 2H), 3.65 (m, 1H), 2.11-1.97 (m, 6H), 1.65-1.80 (m, 4H); ^{13}C NMR (500 MHz, CDCl_3) δ 190.8, 87.6, 66.9, 55.2, 51.3, 31.5, 26.3, 25.7, 24.6, 22.9; Anal. Calcd for $\text{C}_{10}\text{H}_{17}\text{NOS}_2$: C, 51.95; H, 7.36; N, 6.06. Found: C, 52.45, H, 7.64, N 6.33



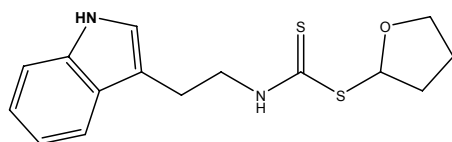
Tetrahydrofuran-2-yl (furan-2-yl)methylcarbomodithioate: IR (neat) ν_{max} 3279, 2979, 1504, 1376, 1321, 1192, 1047, 932, 742, 599 cm^{-1} ; ^1H NMR (500 MHz, CDCl_3) δ 8.69(br, 1H, NH), 7.34 (1H, s, CH), 6.29-6.30 (m, 2H), 5.96 (dd, $J=3.2, 7.2$ Hz, 1H), 4.78-4.90 (m, 2H), 3.94 (m, 2H), 2.24 (m, 1H), 1.97 (m, 1H), 1.82-1.88(m, 2H); ^{13}C NMR (500 MHz, CDCl_3): δ 197.1, 149.6, 143.0, 111.0, 109.0, 87.1, 68.5, 43.5, 31.6, 24.7.



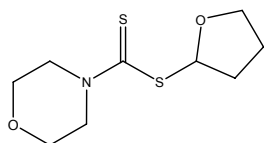
Tetrahydrofuran-2-yl diisopropylcarbomodithioate: ^1H NMR (300 MHz, CDCl_3) δ 6.45-6.46 (br, 1H), 4.85 (br, 1H), 3.91-3.99 (m, 3H), 2.45-2.50 (m, 1H), 2.41 (m, 1H), 1.94-2.02 (m, 2H), 1.25-1.42 (m, 12H); ^{13}C NMR (300 MHz, CDCl_3) δ 196.4, 89.9, 68.4, 55.1 (2C), 31.9, 24.9, 19.6 (4C).



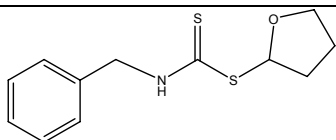
Tetrahydrofuran-2-yl isopropylcarbomodithioate: ^1H NMR (300 MHz, CDCl_3) δ 8.30 (1H, b, NH), 5.92 (dd, $J=3.2, 7.4$ Hz, 1H), 4.63 (m, 1H), 3.97 (m, 2H), 2.26 (m, 1H), 1.83-2.00 (m, 3H), 1.23-1.27 (m, 6H); ^{13}C NMR (300 MHz, CDCl_3) δ 194.7, 86.3, 68.6, 47.9, 30.9, 24.2, 22.2, 21.2.



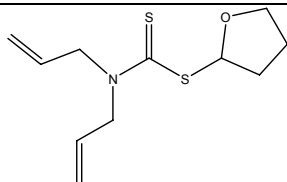
Tetrahydrofuran-2-yl 2-(1H-indol-3-yl)ethylcarbomodithioate: ^1H NMR (300 MHz, CDCl_3) δ 8.53 (br, 1H, NH), 8.20 (br, 1H, NH), 7.66 (d, $J=7.8$ Hz, 1H), 7.39-7.11 (m, 4H), 5.77 (dd, $J=3.2, 7.4$ Hz, 1H), 4.03 (m, 2H), 3.78 (m, 2H), 3.13 (m, 2H), 2.18 (m, 1H), 1.96-1.70 (m, 3H); ^{13}C NMR (300 MHz, CDCl_3) δ 196.2, 136.2, 127.1, 122.4, 122.2, 119.4, 118.3, 112.1, 111.1, 86.2, 67.6, 46.7, 30.9, 24.6, 24.1.



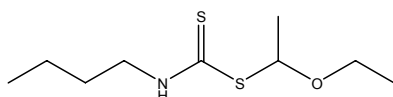
Tetrahydrofuran-2-yl morpholine-4-carbodithioate: m.p. 55-57 °C, ^1H NMR (300 MHz, CDCl_3) δ 6.40 (dd, J = 3.3, 7.2 Hz, 1H), 4.30 (br, 2H), 3.89-4.00 (m, 4H), 3.74 (br, 4H), 2.45 (m, 1H), 2.24 (m, 1H), 1.96 (m, 2H); ^{13}C NMR (300 MHz, CDCl_3): δ 195.8, 90.7, 68.6, 66.1 (2C), 50.4 (2C), 32.2, 24.7.



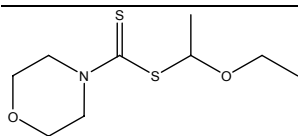
Tetrahydrofuran-2-yl benzylcarbomodithioate: IR (neat) ν_{max} 3275, 2975, 1516, 1383, 1336, 1237, 1048, 932, 734, 698 cm^{-1} ; ^1H NMR (500 MHz, CDCl_3) δ 8.71 (br, 1H, NH), 7.35 (m, 5H), 6.02 (br, 1H), 4.87-4.97-4.87 (m, 2H), 3.99 (m, 2H), 2.44 (m, 1H), 1.97 (m, 1H), 1.79 (m, 2H); ^{13}C NMR (500 MHz, CDCl_3): δ 197.1, 136.6, 129.3, 128.3, 128.2, 86.9, 68.9, 50.7, 31.6, 24.7.



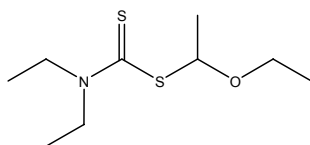
Tetrahydrofuran-2-yl diallylcarbomodithioate: IR (neat) ν_{max} 3081, 2978, 1641, 1467, 1399, 1228, 1172, 1056, 995, 930, 656 cm^{-1} ; ^1H NMR (500 MHz, CDCl_3): δ 6.34 (dd, J = 3.5, 7 Hz, 1H), 5.80-5.95 (m, 2H), 5.16-5.25 (m, 4H), 4.66 (d, J =5.0 Hz, 1H), 4.58 (d, J = 5.7, 1H), 4.29 (d, J = 4.6, 1H), 4.23 (d, J = 5.7, 1H), 3.90-3.97 (m, 2H), 2.44-2.47 (m, 1H), 2.22 (m, 1H), 1.94 (m, 2H); ^{13}C NMR (500 MHz, CDCl_3) δ 196.9, 131.4, 130.8, 119.0, 118.9, 91.6, 69.0, 56.0, 54.2, 32.7, 25.2.



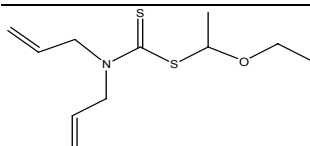
1-ethoxyethyldiallylcarbomodithioate: ^1H NMR (500 MHz CDCl_3) δ 8.13 (br, 1H, NH), 5.38 (q, J = 6.5 Hz, 1H), 3.63-3.79 (m, 4H), 1.63-1.69 (m, 5H), 1.38 (m, 2H), 1.21 (t, J = 7 Hz, 3H), 0.94 (t, J = 7.3 Hz, 3H); ^{13}C NMR (500 MHz, CDCl_3) δ 196.4, 86.8, 63.5, 46.5, 30.7, 22.6, 20.5, 15.3, 14.1.



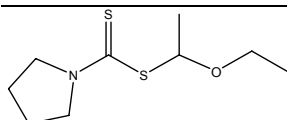
1-ethoxyethyl morpholine-4-carbodithioate: IR (neat) ν_{max} 2971, 1586, 1460, 1418, 1276, 1225, 1112, 870, 643 cm^{-1} ; ^1H NMR (300 MHz, CDCl_3) δ 5.89 (q, J = 6.3 Hz, 1H), 3.92-4.28 (br, 4H), 3.53-3.76 (m, 6H), 1.67 (d, J =6.3 Hz, 3H), 1.13 (t, J = 7 Hz, 3H); ^{13}C NMR (300 MHz, CDCl_3) δ 196.4, 90.9, 66.0 (2C), 64.7, 50.3 (2C), 23.5, 14.7.



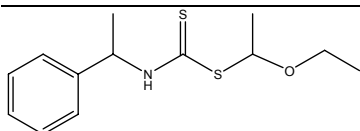
1-ethoxyethyldiethylcarbamodithioate: IR (neat) $\nu_{\max}$ 2976, 1484, 1415, 3789, 1268, 1206, 1113, 916, 830, 647 cm^{-1} ; ^1H NMR (300 MHz, CDCl_3) δ 5.87 (q, $J=6.3$ Hz, 1H), 3.56-4.02 (m, 6H), 1.63 (d, $J=6.3$ Hz, 3H), 1.23 (t, $J=6.9$ Hz, 6H), 1.15 (t, $J=7.0$ Hz, 3H); ^{13}C NMR (300 MHz, CDCl_3) δ 194.6, 90.8, 64.5, 48.6, 46.6, 23.3, 14.8, 12.4, 11.4.



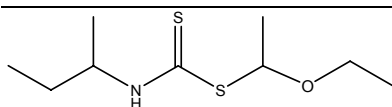
1-ethoxyethyldiallylcarbamodithioate: IR (neat) $\nu_{\max}$ 3083, 2975, 1641, 1469, 1399, 1226, 1113, 931, 845, 651 cm^{-1} ; ^1H NMR (500 MHz, CDCl_3) δ 5.91-5.95 (q, $J=6.3$ Hz, 1H), 5.85 (m, 2H), 5.18-5.29 (m, 4H), 4.63 (dd, $J=13.8, 5.5$ Hz, 2H), 4.32 (dd, $J=4., 13.2$ Hz, 2H), 3.78-3.60 (m, 2H), 1.73 (d, $J=6.3$ Hz, 3H), 1.20 (t, $J=7$ Hz, 3H); ^{13}C NMR (500 MHz, CDCl_3) δ 197.0, 149.5, 143.0, 111.0, 109.2, 86.7, 63.6, 43.4 (2C), 22.4, 15.0.



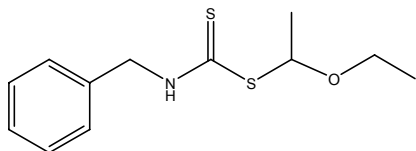
1-ethoxyethyl pyrrolidine-1-carbodithioate: IR (neat) $\nu_{\max}$ 2979, 1428, 1328, 1250, 1162, 1112, 955, 845, 647 cm^{-1} ; ^1H NMR (300 MHz, CDCl_3) δ 5.82 (q, $J=6.3$ Hz, 1H), 3.78 (m, 2H), 3.48-3.67 (m, 4H), 1.85-1.99 (m, 4H), 1.59 (t, $J=6.3$ Hz, 3H), 1.06 (t, $J=7.0$ Hz, 3H); ^{13}C NMR (300 MHz, CDCl_3) δ 191.5, 89.4, 63.8, 53.4, 49.9, 25.5, 24.5, 23.1, 13.2.



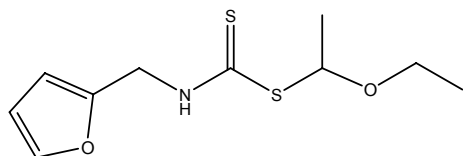
1-ethoxyethyl 1-phenylethylcarbamodithioate: IR (neat) $\nu_{\max}$ 3264, 2986, 1545, 1493, 1451, 1373, 1117, 953, 766, 698 cm^{-1} ; ^1H NMR (300 MHz, CDCl_3): δ 8.61-8.64 (br s, 1H, NH), 7.38-7.25 (m, 5H), 5.57 (m, 1H), 5.21-5.34 (m, 2H), 3.57-3.78 (m, 2H), 1.69 (d, $J=6.5$ Hz, 3H), 1.71-1.58 (m, 6H), 1.15-1.05 (m, 3H); ^{13}C NMR (300 MHz, CDCl_3) δ 194.9, 141.1, 128.5, 127.5, 125.4, 85.7, 64.6, 54.7, 23.3, 23.1, 14.6.



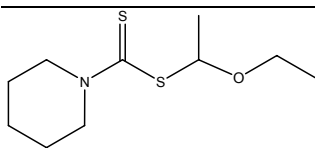
1-ethoxyethyl sec-butylcarbamodithioate: IR (neat) $\nu_{\max}$ 3252, 2966, 1519, 1454, 1377, 1150, 1110, 985, 896, 680 cm^{-1} ; ^1H NMR (500 MHz, CDCl_3) δ 8.18 (br s, 1H, NH), 5.20 (q, $J=6.5$ Hz, 1H), 4.48 (m, 1H), 3.54-3.73 (m, 2H), 1.51-1.62 (m, 5H), 1.12-1.17 (m, 6H), 0.84-0.90 (m, 3H); ^{13}C NMR (500 MHz, CDCl_3) δ 194.7, 85.6, 62.7, 52.9, 29.2, 21.7, 18.6, 14.5, 10.0.



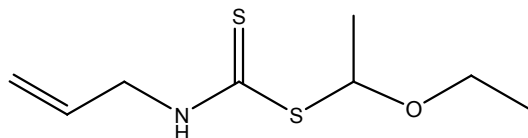
1-ethoxyethylbenzylcarbamodithioate: IR (neat) $\nu_{\max}$ 3267, 2972, 1492, 1452, 1376, 1054, 955, 698 cm^{-1} ; ^1H NMR (300 MHz, CDCl_3) δ 8.49 (br s, 1H, NH), 7.25-7.36 (m, 5H), 5.34 (q, J = 6.5 Hz, 1H), 4.88 (d, J = 5.2 Hz, 2H), 3.75-3.55 (m, 2H), 1.63 (d, J = 6.5 Hz, 3H), 1.03-1.06 (t, J =7 Hz, 3H); ^{13}C NMR (300 MHz, CDCl_3) δ 196.2, 135.7, 128.5, 127.7, 127.2, 86.0, 62.8, 49.9, 21.7, 14.6



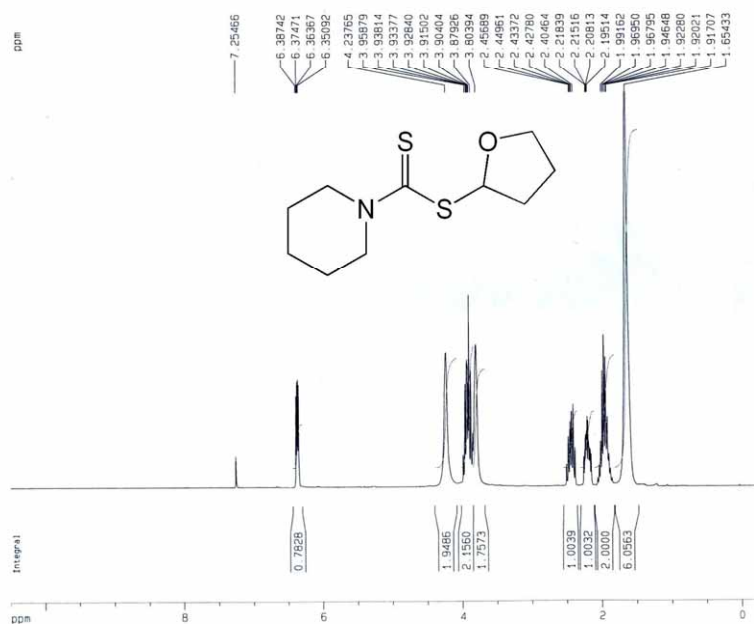
1-ethoxyethyl (furan-2-yl)methylcarbamodithioate: IR (neat) $\nu_{\max}$ 3256, 2974, 1517, 1504, 1373, 1321, 1190, 1147, 1081, 1081, 1011, 937, 744 cm^{-1} ; ^1H NMR (500 MHz, CDCl_3) δ 8.55 (br s, 1H, NH), 7.37 (s, 1H), 6.32-6.34 (m, 2H), 5.34 (q, J = 6.5 Hz, 1H), 4.86 (m, 2H), 3.58-3.77 (m, 2H), 1.65 (d, J = 6.5 Hz, 3H), 1.12-1.15 (t, J = 7.0 Hz, 3H).



1-ethoxyethyl piperidine-1-carbodithioate: IR (neat) $\nu_{\max}$ 2939, 1473, 1427, 1280, 1244, 1227, 1131, 1110, 1004, 892, 852, 800, 648 cm^{-1} ; ^1H NMR (300 MHz, CDCl_3) δ 5.85 (q, J = 6.2 Hz, 1H), 3.84-4.25 (br s, 4H), 3.49-3.74 (m, 2H), 1.64-1.66 (m, 9H), 1.11-1.18 (m, 3H); ^{13}C NMR (300 MHz, CDCl_3) δ 194.2, 90.6, 64.3, 52.3, 51.7, 25.7, 25.1, 24.1, 22.7, 14.6
Anal. Calcd for $\text{C}_{10}\text{H}_{19}\text{NOS}_2$: C, 51.50; H, 8.15; N, 6.01. Found: C, 51.08; H, 8.17; N, 6.36.



1-ethoxyethyl allylcarbamodithioate: ^1H NMR (500 MHz, CDCl_3) δ 8.31 (br s, 1H, NH), 5.88 (m, 1H), 5.36 (dd, J = 6.5, 13.0 Hz, 1H), 5.27-5.19 (m, 2H), 4.34 (br, 2H), 3.76 (m, 1H), 3.59 (m, 1H), 1.65 (d, J = 6.2 Hz, 3H), 1.16 (t, J = 7.0, 3H); ^{13}C NMR (500 MHz, CDCl_3) δ 197.1, 132.2, 118.6, 86.7, 63.6, 48.9, 22.5, 15.3.



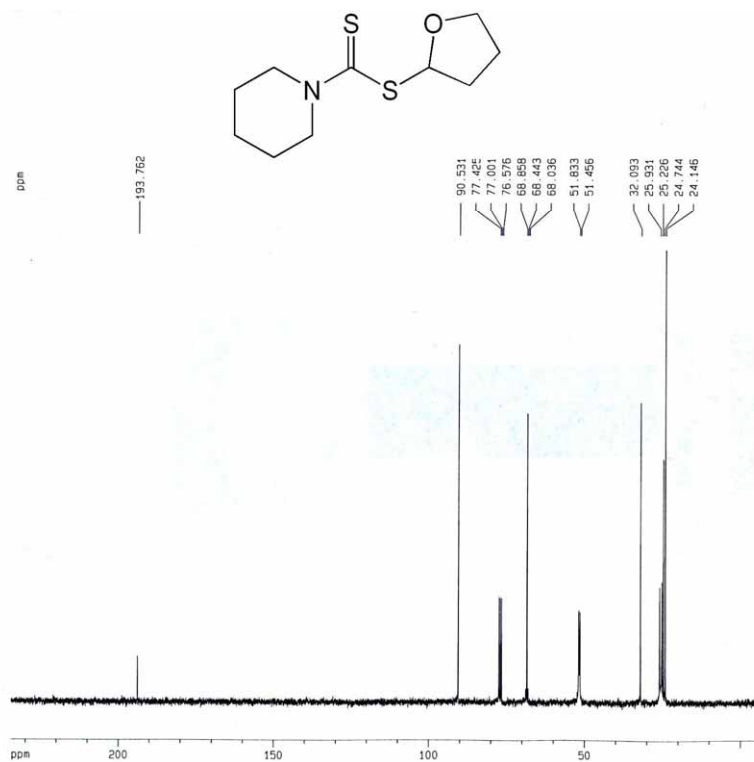
Current Data Parameters
NAME ashr1
EXPNO 105
PROCNO 1

F2 - Acquisition Parameters
Date_ 20091114
Time 9.51
INSTRUM spect
PROBHD 5 mm Multinuc1
PULPROG zg
TD 16384
SOLVENT CDCl3
NS 8
DS 2
SWH 6172.839 Hz
FIDRES 0.376760 Hz
AQ 1.3271540 sec
RG 57
DM 81.000 usec
DE 6.00 usec
TE 300.0 K
D1 6.00000000 sec

***** CHANNEL f1 *****
NUC1 1H
P1 10.00 usec
PL1 0.00 dB
SFO1 300.1315007 MHz

F2 - Processing parameters
SI 32768
SF 300.130070 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

1D NMR plot parameters
CX 20.00 cm
CY 12.50 cm
FIP 10.500 ppm
F1 3151.36 Hz
F2P -0.300 ppm
F2 -90.04 Hz
PPMCM 0.54000 ppm/cm
HZCM 162.07021 Hz/cm



Current Data Parameters
NAME ashr1
EXPNO 106
PROCNO 1

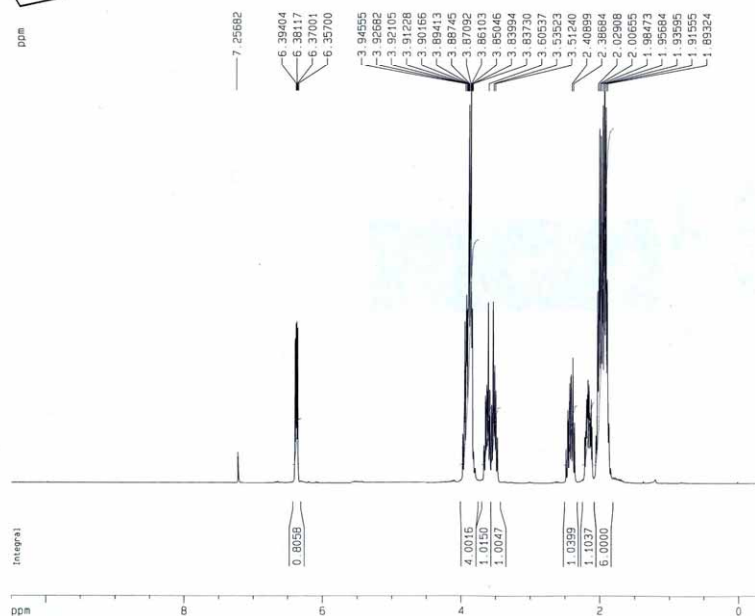
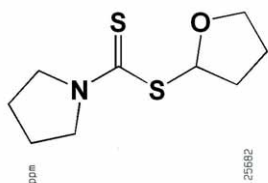
F2 - Acquisition Parameters
Date_ 20091114
Time 10.03
INSTRUM spect
PROBHD 5 mm Multinuc1
PULPROG zgpg
TD 32768
SOLVENT CDCl3
NS 504
DS 0
SWH 18832.393 Hz
FIDRES 0.574719 Hz
AQ 0.8700404 sec
RG 9195.2
DM 26.550 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
D11 0.03000000 sec
D12 0.00000000 sec

***** CHANNEL f1 *****
NUC1 13C
P1 7.00 usec
PL1 -4.00 dB
SFO1 75.4765995 MHz

***** CHANNEL f2 *****
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 0.00 dB
PL12 21.00 dB
PL13 21.00 dB
SFO2 300.1312005 MHz

F2 - Processing parameters
SI 32768
SF 75.4677595 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

1D NMR plot parameters
CX 20.00 cm
CY 12.50 cm
FIP 235.000 ppm
F1 17734.92 Hz
F2P -5.000 ppm
F2 -377.34 Hz
PPMCM 12.00000 ppm/cm
HZCM 395.61288 Hz/cm



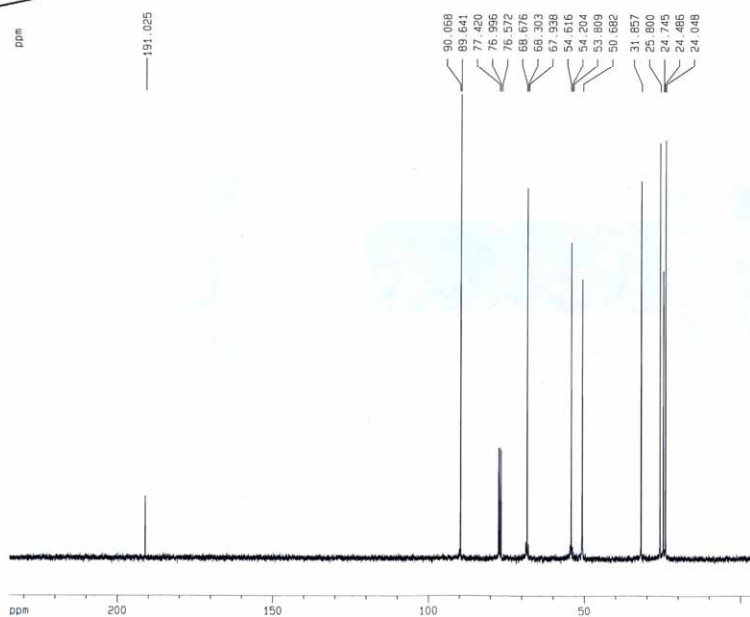
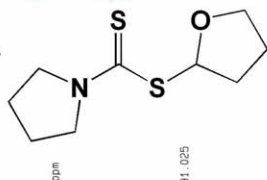
Current Data Parameters
 NAME ashon1
 EXPNO 107
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20091114
 Time 10.22
 INSTRUM spect
 PROBHD 5 mm Multinuc1
 PULPROG zg
 TD 16384
 SOLVENT CDCl3
 NS 8
 DS 2
 SWH 6172.839 Hz
 FIDRES 0.376760 Hz
 AQ 1.3271540 sec
 RG 57
 DW 81.000 usec
 DE 6.00 usec
 TE 300.0 K
 D1 6.00000000 sec

***** CHANNEL f1 *****
 NUC1 1H
 P1 10.00 usec
 PL1 0.00 dB
 SF01 300.1315007 MHz

F2 - Processing parameters
 SI 32768
 SF 300.1300070 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

ID NMR plot parameters
 CX 20.00 cm
 CY 12.50 cm
 F1P 10.500 ppm
 F1 3151.36 Hz
 F2P -0.300 ppm
 F2 -90.04 Hz
 PPMCM 0.54000 ppm/cm
 HZCM 162.07021 Hz/cm



Current Data Parameters
 NAME ashon1
 EXPNO 108
 PROCNO 1

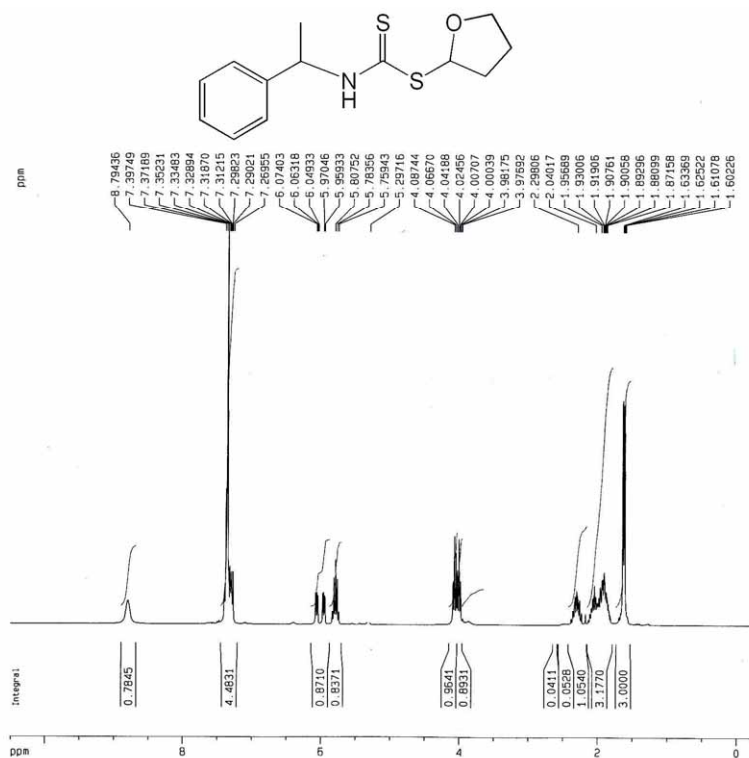
F2 - Acquisition Parameters
 Date_ 20091114
 Time 10.14
 INSTRUM spect
 PROBHD 5 mm Multinuc1
 PULPROG zgpg30
 TD 32768
 SOLVENT CDCl3
 NS 600
 DS 0
 SWH 18832.393 Hz
 FIDRES 0.574719 Hz
 AQ 0.8700404 sec
 RG 9195.2
 DW 26.550 usec
 DE 6.00 usec
 TE 300.0 K
 D1 2.00000000 sec
 d11 0.03000000 sec
 d12 0.00020000 sec

***** CHANNEL f1 *****
 NUC1 13C
 P1 7.00 usec
 PL1 -4.00 dB
 SF01 75.4760505 MHz

***** CHANNEL f2 *****
 CPDPRG2 waltz16
 NUC2 1H
 P2P02 80.00 usec
 PL2 0.00 dB
 PL12 21.00 dB
 PL13 21.00 dB
 SF02 300.1312005 MHz

F2 - Processing parameters
 SI 32768
 SF 75.4677630 MHz
 WDW FM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

ID NMR plot parameters
 CX 20.00 cm
 CY 12.50 cm
 F1P 235.000 ppm
 F1 17734.93 Hz
 F2P -5.000 ppm
 F2 -377.34 Hz
 PPMCM 12.00000 ppm/cm
 HZCM 905.61310 Hz/cm



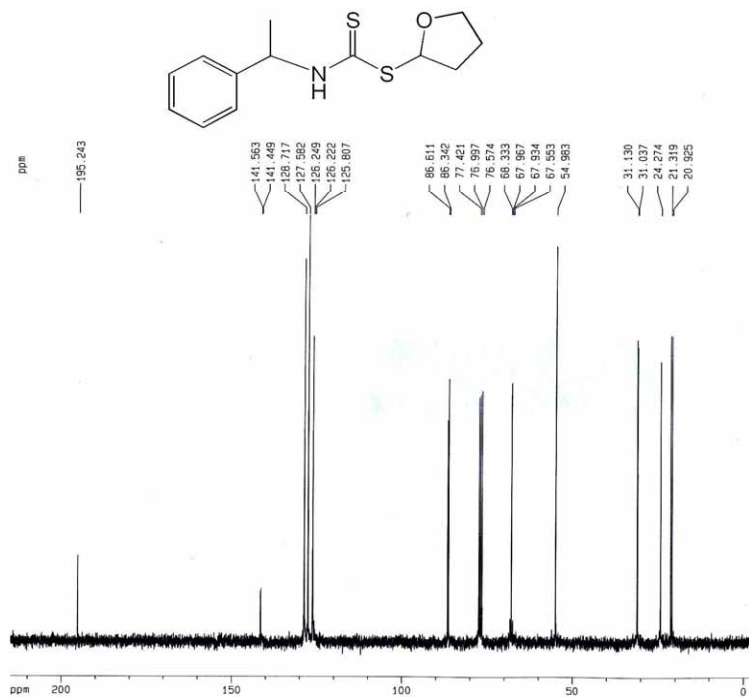
Current Data Parameters
NAME Zi111
EXPNO 127
PROCNO 1

F2 - Acquisition Parameters
Date_ 20091117
Time 10.18
INSTRUM spect
PROBHD 5 mm Multinucl
PULPROG zg
TD 16384
FIDRES 0.370760 Hz
AQ 1.3271540 sec
RG 90.5
DM 81.000 usec
DE 6.00 usec
TE 300.0 K
D1 6.00000000 sec

***** CHANNEL f1 *****
NUC1 1H
P1 10.00 usec
PL1 0.00 dB
SFO1 300.1315007 MHz

F2 - Processing parameters
SI 32768
SF 300.1300036 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

1D NMR plot parameters
CX 20.00 cm
CY 12.50 cm
F1P 10.500 ppm
F1 3151.37 Hz
F2P -0.300 ppm
F2 -90.04 Hz
PPHMC 0.54000 ppm/cm
H2CM 162.07019 Hz/cm



Current Data Parameters
NAME Zi111
EXPNO 128
PROCNO 1

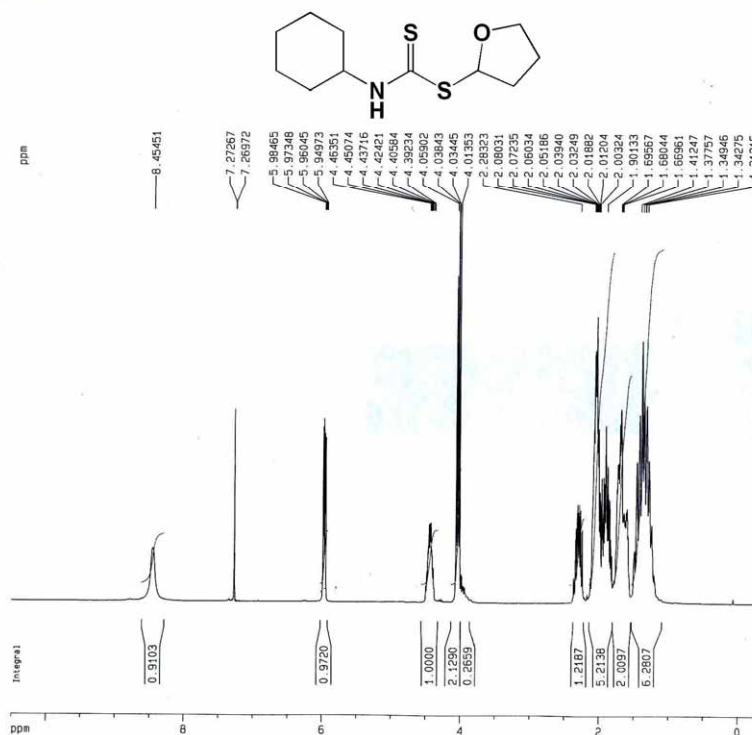
F2 - Acquisition Parameters
Date_ 20091117
Time 10.42
INSTRUM spect
PROBHD 5 mm Multinucl
PULPROG zgpg
TD 32768
FIDRES 0.8702404 Hz
AQ 0.0702404 sec
RG 11585.2
DM 26.500 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
D11 0.03000000 sec
D12 0.00002000 sec

***** CHANNEL f1 *****
NUC1 13C
P1 7.00 usec
PL1 -4.00 dB
SFO1 75.4780503 MHz

***** CHANNEL f2 *****
CPDPRG2 waltz16
NUC2 1H
P2 80.00 usec
PL2 0.00 dB
PL12 21.00 dB
PL13 21.00 dB
SFO2 300.1312005 MHz

F2 - Processing parameters
SI 32768
SF 75.4677567 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

1D NMR plot parameters
CX 20.00 cm
CY 12.50 cm
F1P 215.000 ppm
F1 16225.57 Hz
F2P -5.000 ppm
F2 -377.30 Hz
PPHMC 11.00000 ppm/cm
H2CM 830.14532 Hz/cm



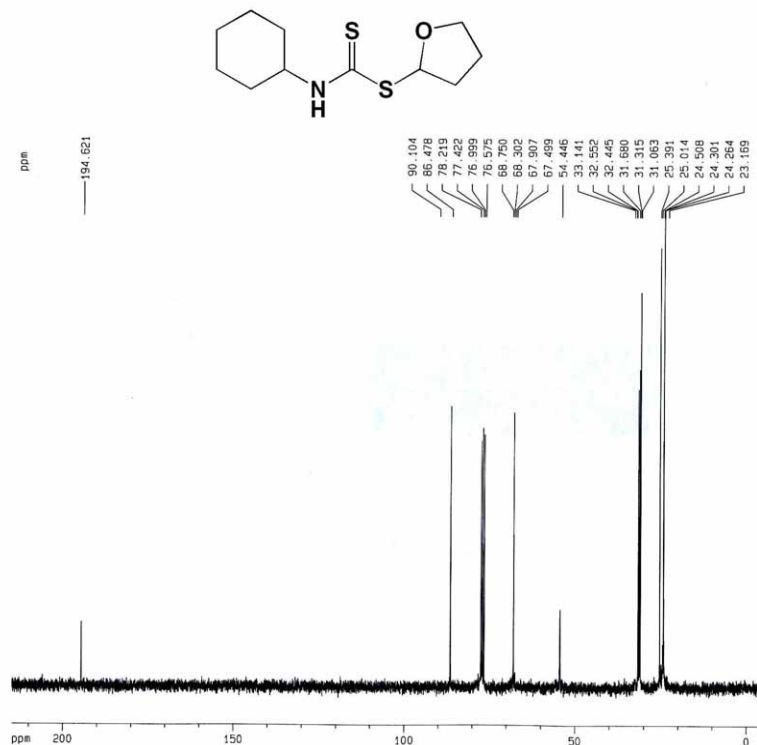
Current Data Parameters
NAME Z1911
EXPNO 125
PROCNO 1

F2 - Acquisition Parameters
Date_ 20091117
Time 9.22
INSTRUM spect
PROBHD 5 mm Multinucl
PULPROG zg
TD 16384
SOLVENT CDCl3
NS 8
DS 2
SWH 6172.839 Hz
FIDRES 0.376760 Hz
AQ 1.3271540 sec
RG 114
DM 81.000 usec
DE 6.00 usec
TE 300.0 K
D1 6.00000000 sec

***** CHANNEL f1 *****
NUC1 1H
P1 10.00 usec
PL1 0.00 dB
SF01 300.1315007 MHz

F2 - Processing parameters
SI 32768
SF 300.1300036 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

1D NMR plot parameters
CX 20.00 cm
CY 12.50 cm
F1P 10.500 ppm
F1 3151.37 Hz
F2P -0.300 ppm
F2 -90.04 Hz
PPMCH 0.54000 ppm/cm
HZCM 162.07019 Hz/cm



Current Data Parameters
NAME Z1911
EXPNO 126
PROCNO 1

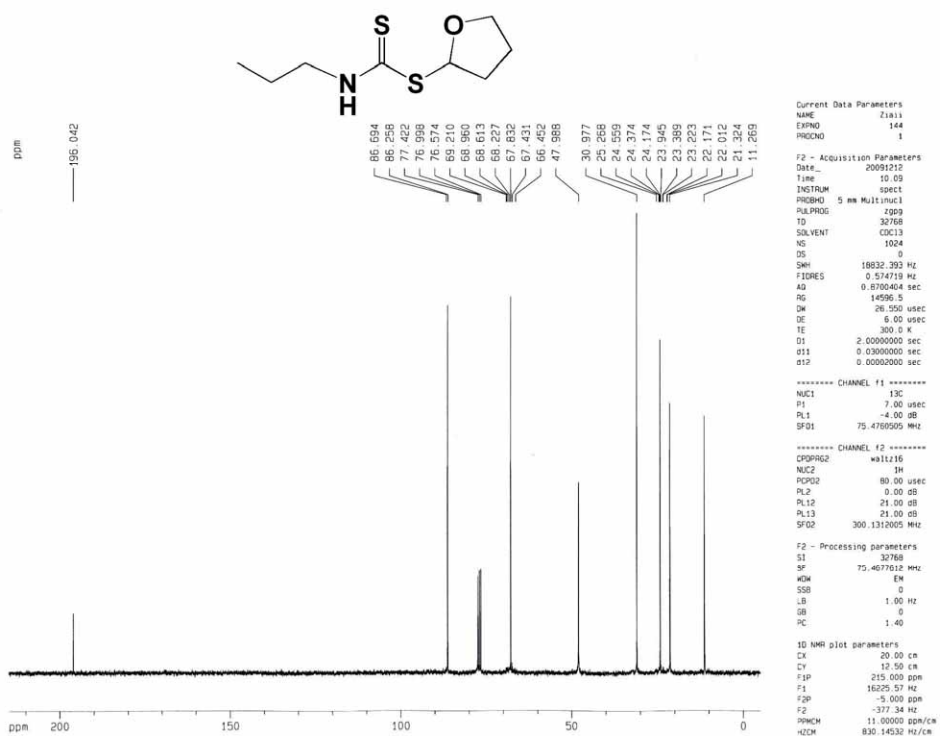
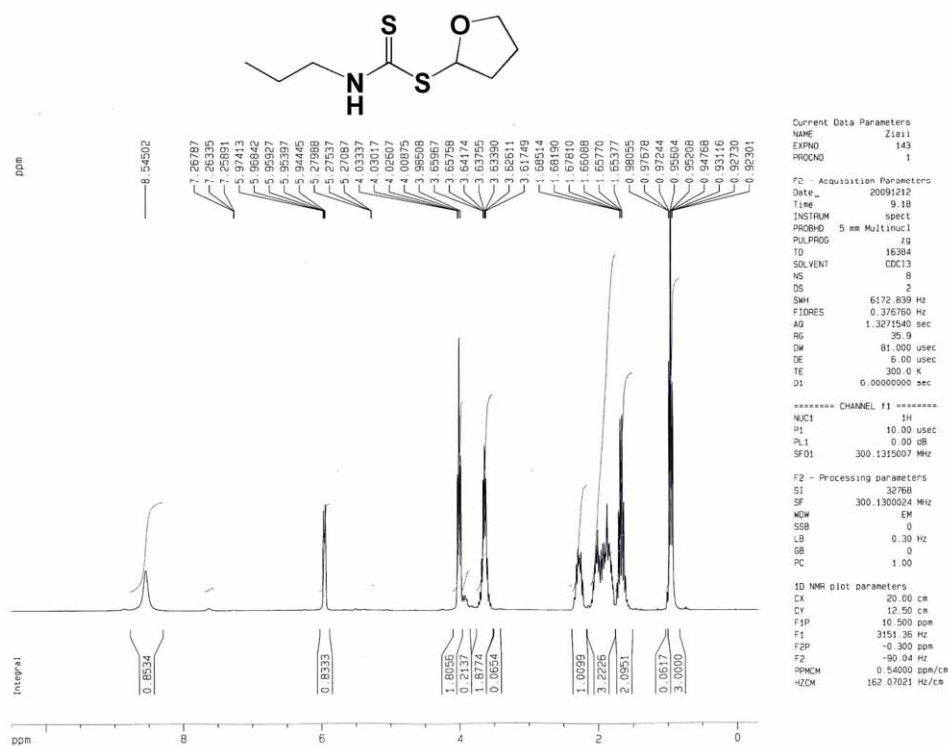
F2 - Acquisition Parameters
Date_ 20091117
Time 9.58
INSTRUM spect
PROBHD 5 mm Multinucl
PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 1024
DS 0
SWH 18832.393 Hz
FIDRES 0.514719 Hz
AQ 0.8700404 sec
RG 11585.2
DM 26.550 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
d11 0.03000000 sec
d12 0.00002000 sec

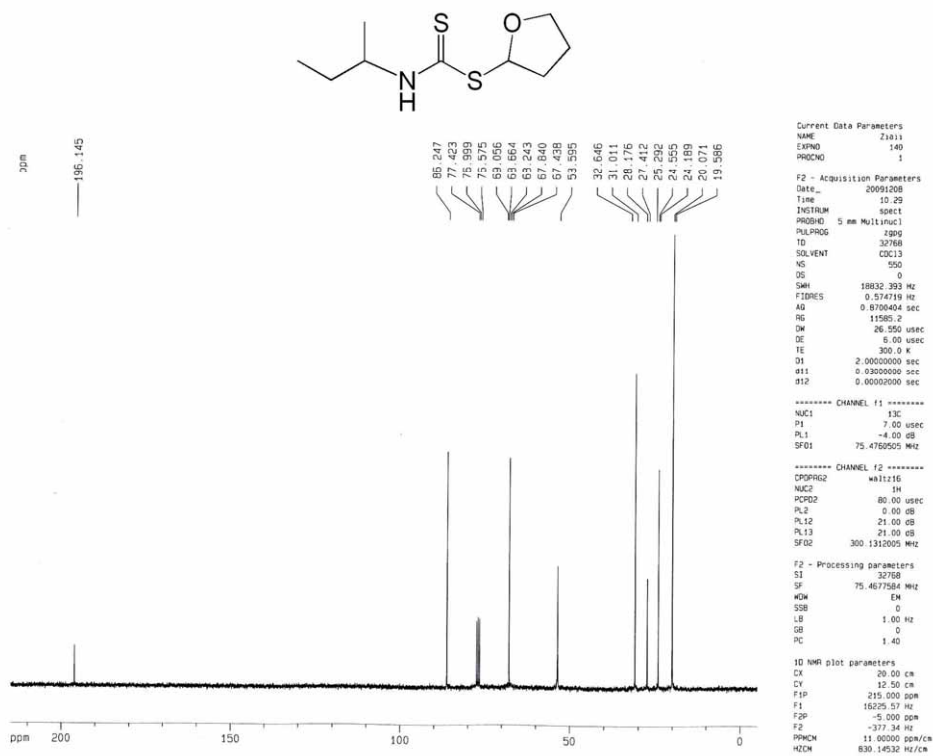
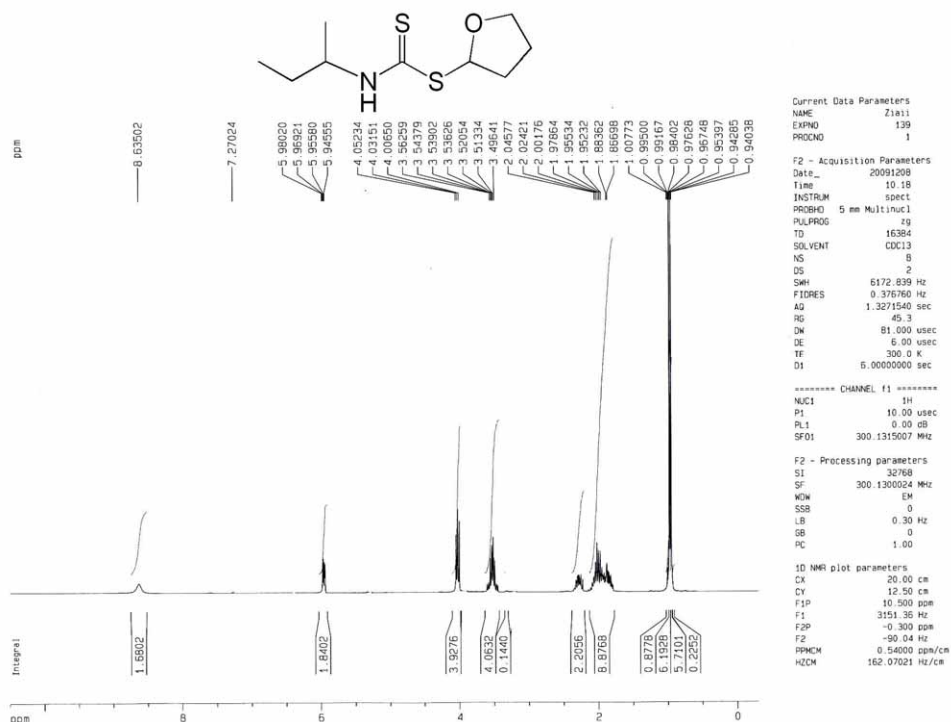
***** CHANNEL f1 *****
NUC1 13C
P1 7.00 usec
PL1 -4.00 dB
SF01 75.4760505 MHz

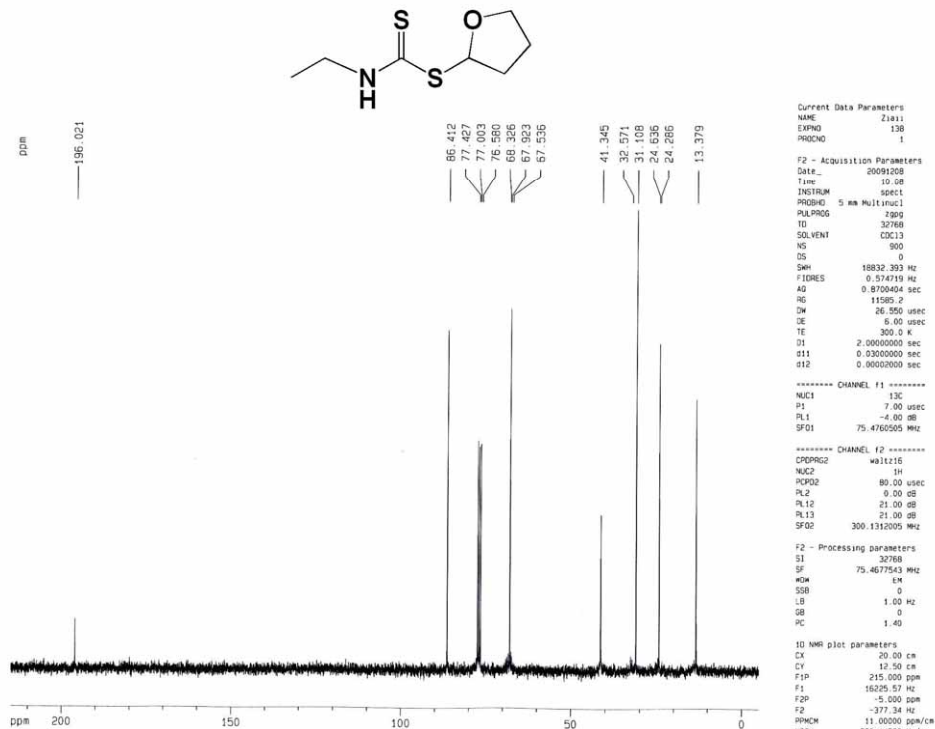
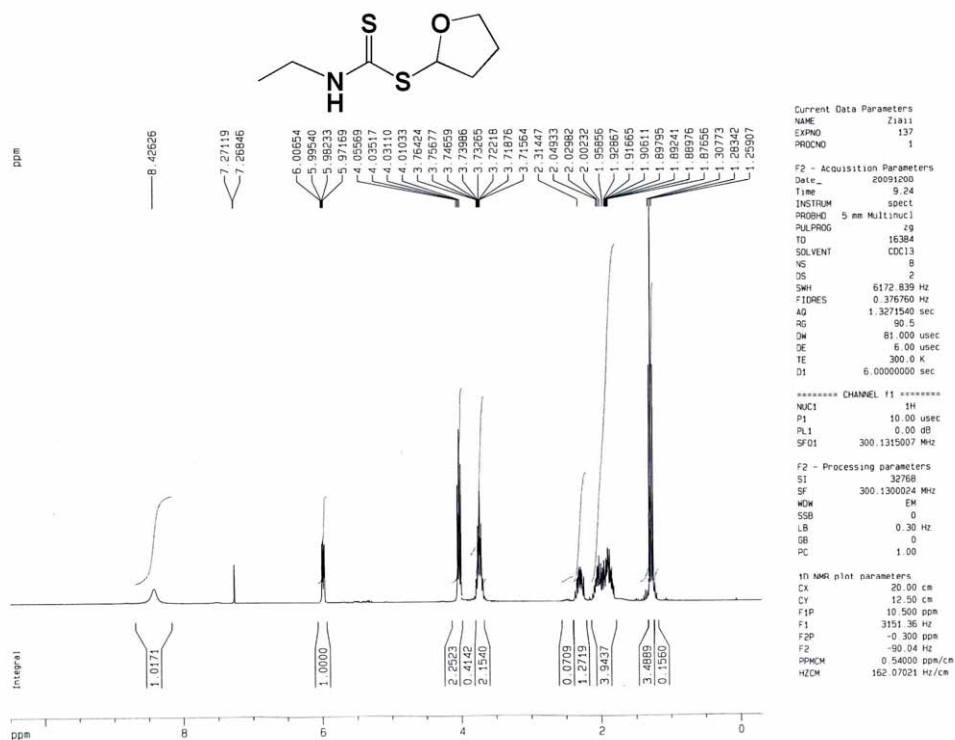
***** CHANNEL f2 *****
CPOPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 0.00 dB
PL12 21.00 dB
PL13 21.00 dB
SF02 300.1312005 MHz

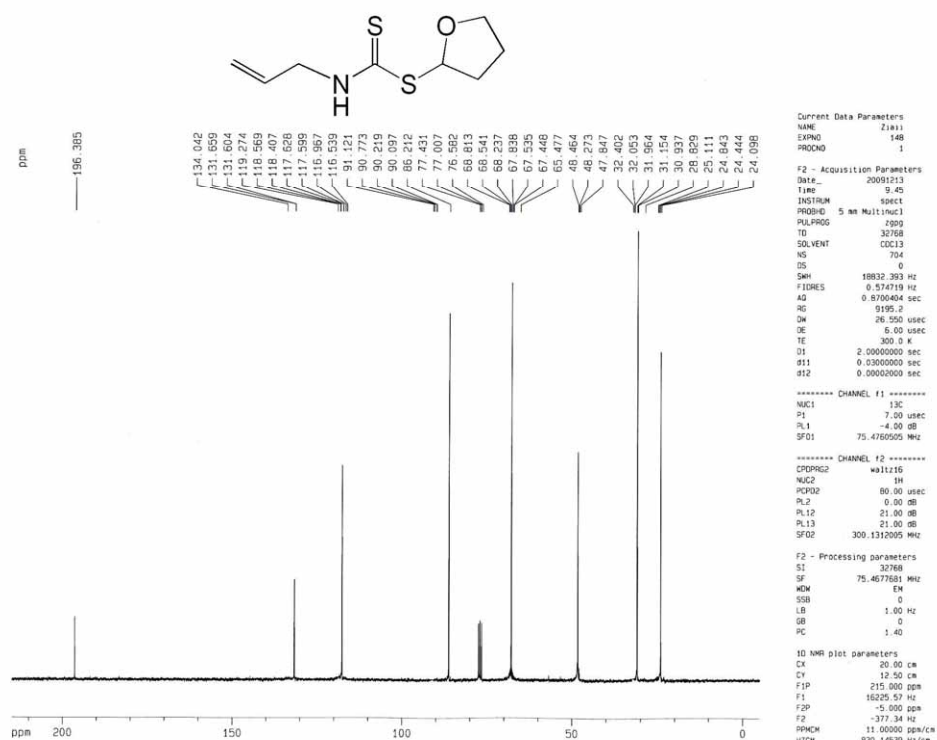
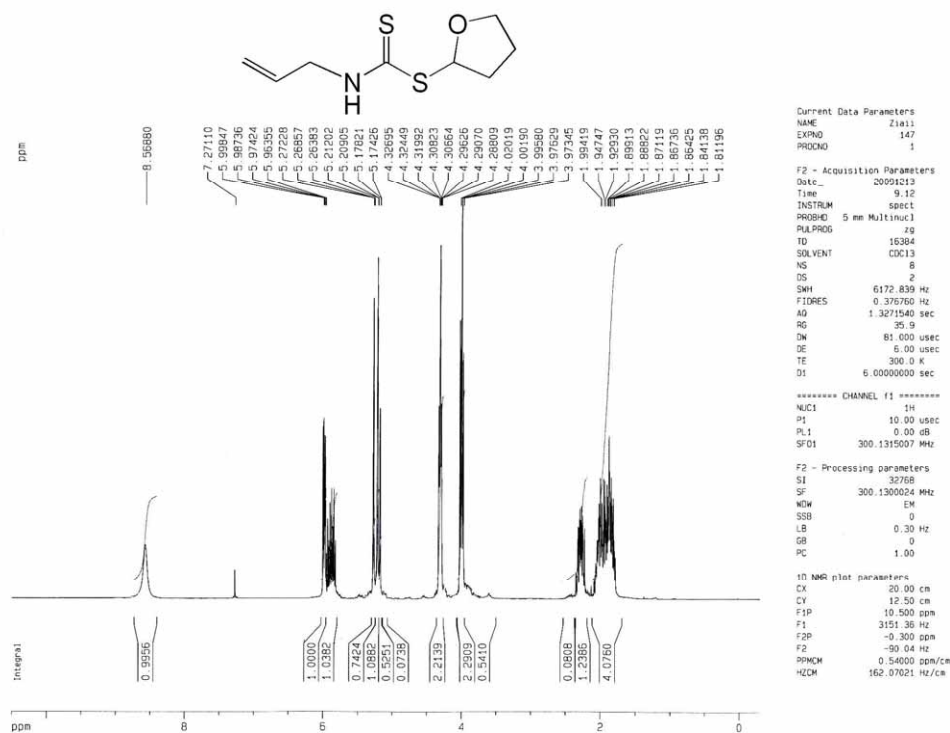
F2 - Processing parameters
SI 32768
SF 75.4677538 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

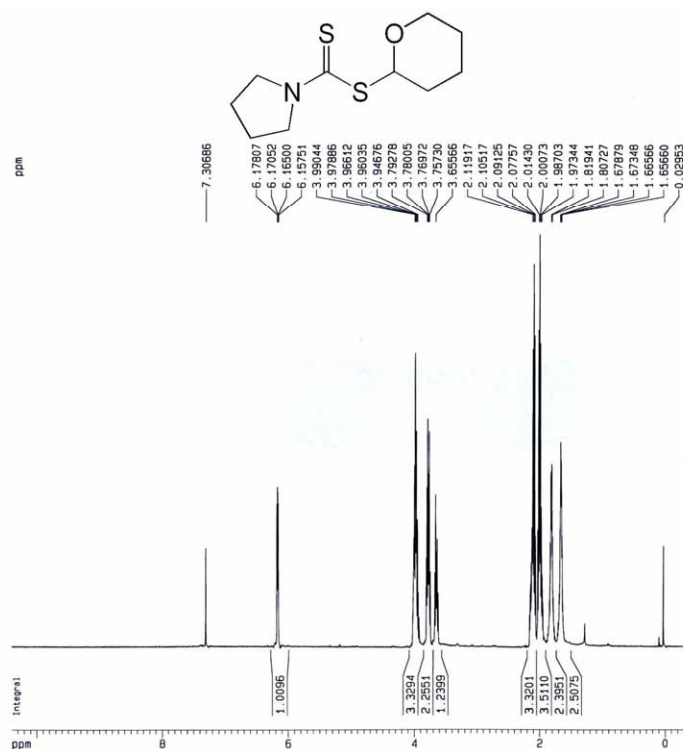
1D NMR plot parameters
CX 20.00 cm
CY 12.50 cm
F1P 215.000 ppm
F1 16225.57 Hz
F2P -5.000 ppm
F2 -377.34 Hz
PPMCH 11.00000 ppm/cm
HZCM 830.14520 Hz/cm











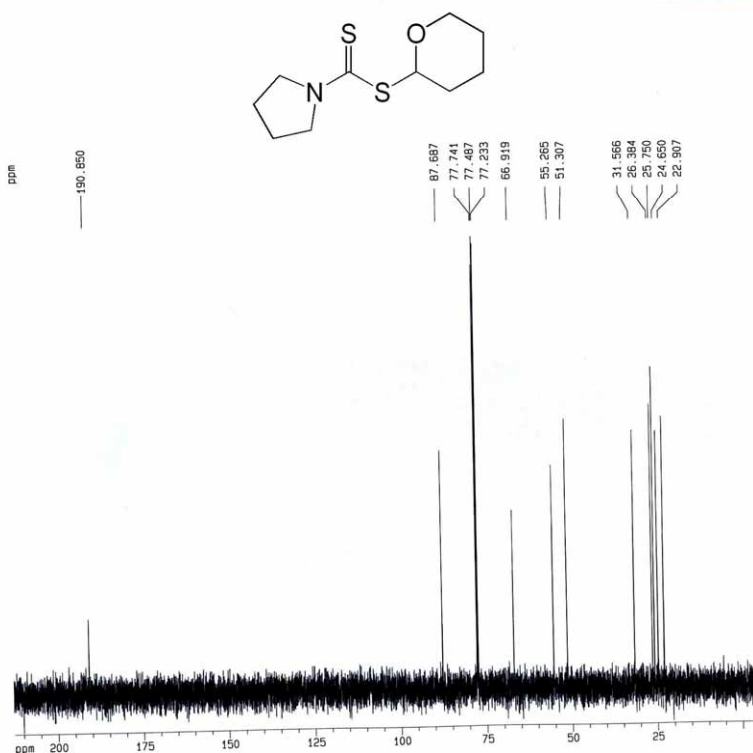
Current Data Parameters
NAME Azim
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20090727
Time 13.28
INSTRUM spect
PROBHD 5 mm GNP 1H/13
PULPROG zg30
TO 32768
SOLVENT CDCl3
NS 1
DS 0
SWH 10330.578 Hz
FIDRES 0.315264 Hz
AQ 1.5860696 sec
RG 161.3
DM 48.400 usec
DE 6.50 usec
TE 298.0 K
D1 1.00000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

***** CHANNEL f1 *****
NUC1 1H
P1 10.50 usec
PL1 -3.00 dB
SFO1 500.1300895 MHz

F2 - Processing parameters
SI 32768
SF 500.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

1D NMR plot parameters
CX 16.00 cm
CY 11.00 cm
F1P 10.396 ppm
F1 5199.54 Hz
F2P -0.313 ppm
F2 -156.64 Hz
PPMCH 0.59498 ppm/cm
HZCH 297.56558 Hz/cm



Current Data Parameters
NAME Azim
EXPNO 3
PROCNO 1

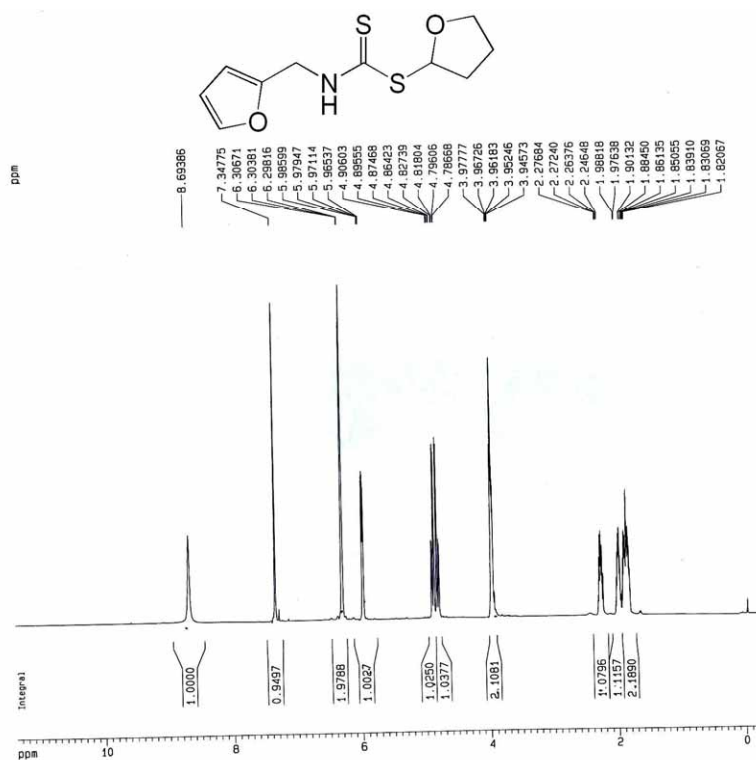
F2 - Acquisition Parameters
Date_ 20090727
Time 13.30
INSTRUM spect
PROBHD 5 mm GNP 1H/13
PULPROG zgpg30
TO 85536
SOLVENT DMSO
NS 29
DS 4
SWH 30030.028 Hz
FIDRES 0.458292 Hz
AQ 1.0912419 sec
RG 14596.5
DM 16.650 usec
DE 6.50 usec
TE 298.0 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

***** CHANNEL f1 *****
NUC1 13C
P1 9.10 usec
PL1 3.00 dB
SFO1 125.7703643 MHz

***** CHANNEL f2 *****
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 0.00 dB
PL12 15.00 dB
PL13 15.50 dB
SFO2 500.1320025 MHz

F2 - Processing parameters
SI 32768
SF 125.7577390 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

1D NMR plot parameters
CX 20.00 cm
CY 12.50 cm
F1P 212.782 ppm
F1 26759.00 Hz
F2P -4.467 ppm
F2 -561.80 Hz
PPMCH 10.86247 ppm/cm
HZCH 1366.03952 Hz/cm



Current Data Parameters

NAME Azin
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters

Date_ 20091122
Time 13.24
INSTRUM spect
PROBHD 5 mm GNP 1H/13
PULPROG zgpg30
TD 32768
SOLVENT CDCl₃
NS 1
DS 0
SWH 10330.579 Hz
FIDRES 0.315264 Hz
AQ 1.5860696 sec
RG 40.3
DM 48.400 usec
DE 6.50 usec
TE 298.0 K
D1 1.00000000 sec
WDECT 0.00000000 sec
HWDK 0.01500000 sec

===== CHANNEL f1 =====

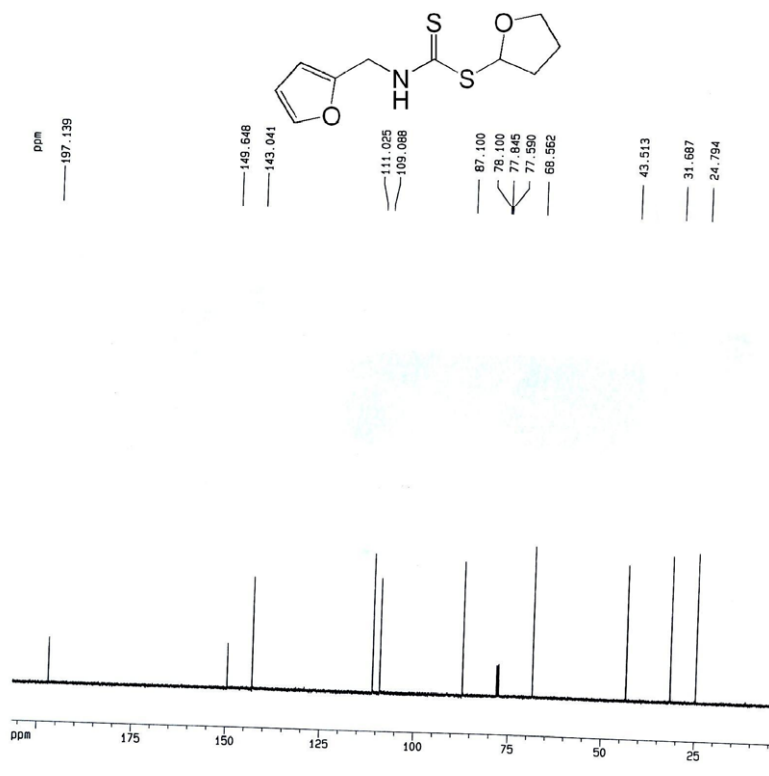
NUC1 1H
P1 10.50 usec
PL1 -3.00 dB
SFO1 500.1330895 MHz

F2 - Processing parameters

SI 32768
SF 500.1300950 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

1D NMR plot parameters

CX 20.00 cm
CY 0.51 cm
F1P 11.389 ppm
F1 5695.86 Hz
F2P -0.309 ppm
F2 -154.39 Hz
PQCM 0.58487 Hz/cm
HZCM 292.51257 Hz/cm



Current Data Parameters

NAME Azin
EXPNO 4
PROCNO 1

F2 - Acquisition Parameters

Date_ 20091122
Time 13.24
INSTRUM spect
PROBHD 5 mm GNP 1H/13
PULPROG zgpg30
TD 32768
SOLVENT Aceton
NS 27
DS 4
SWH 30030.029 Hz
FIDRES 0.916444 Hz
AQ 0.5456039 sec
RG 4096
DM 16.650 usec
DE 6.50 usec
TE 298.0 K
D1 1.00000000 sec
S11 0.03000000 sec
DELTA 0.00000000 sec
WDECT 0.00000000 sec
HWDK 0.01500000 sec

===== CHANNEL f1 =====

NUC1 13C
P1 9.10 usec
PL1 3.00 dB
SFO1 125.7703643 MHz

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

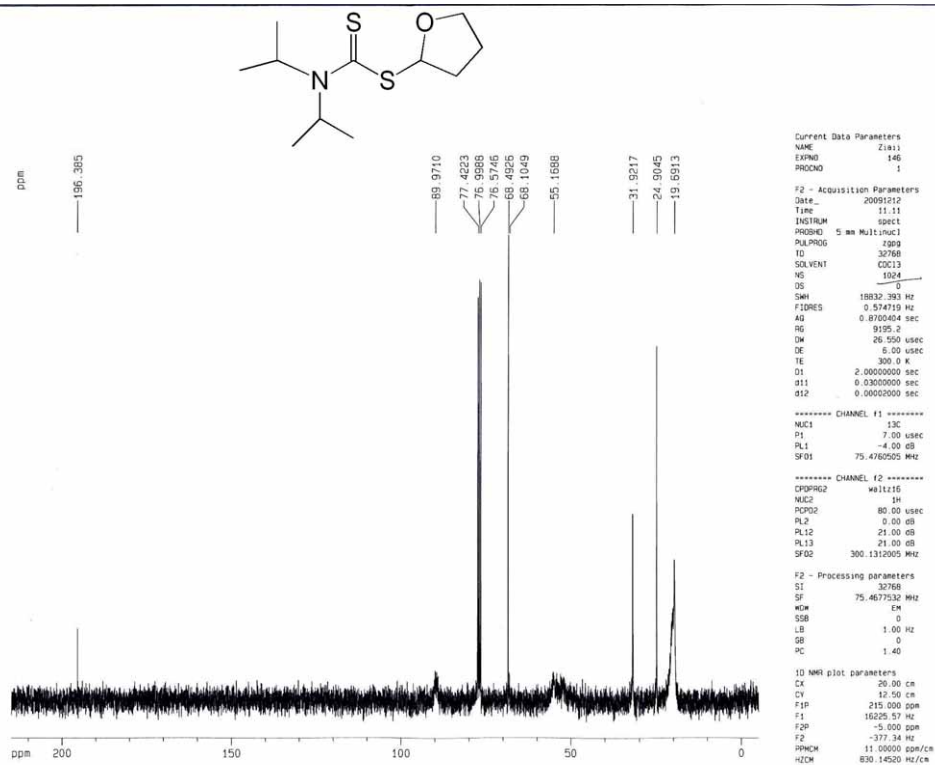
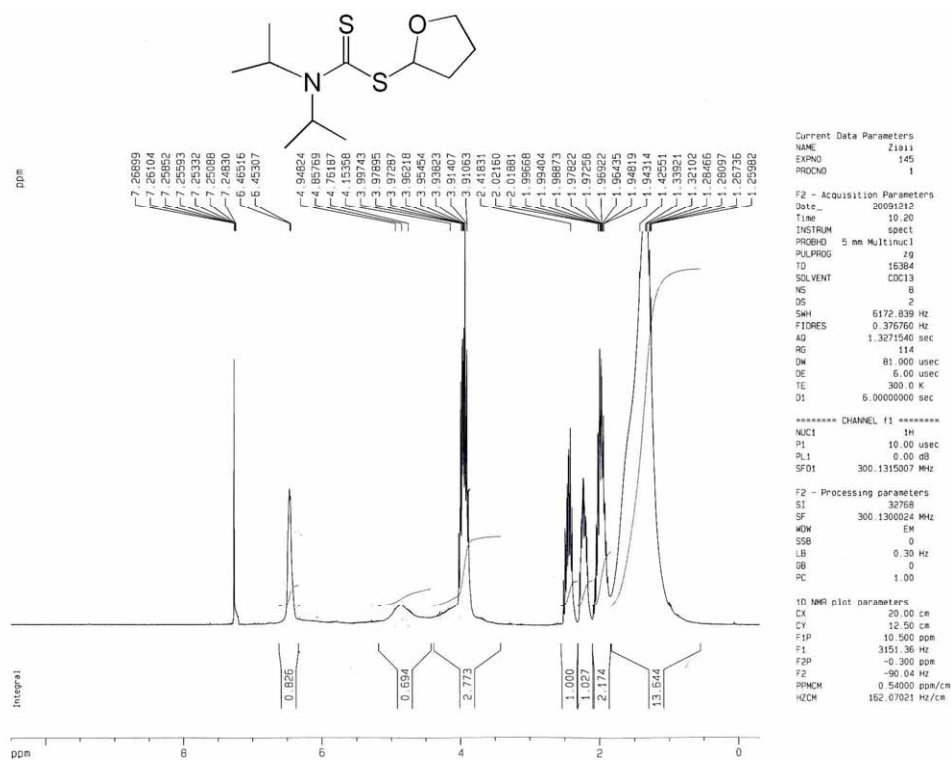
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 0.00 dB
PL12 15.50 dB
PL13 15.50 dB
SFO2 500.1300005 MHz

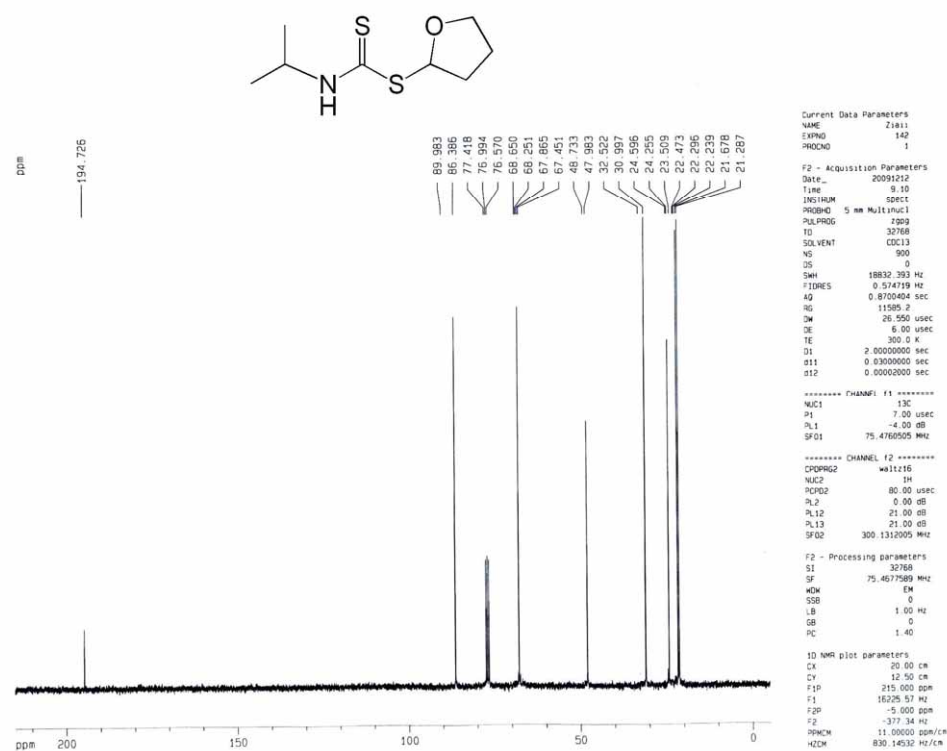
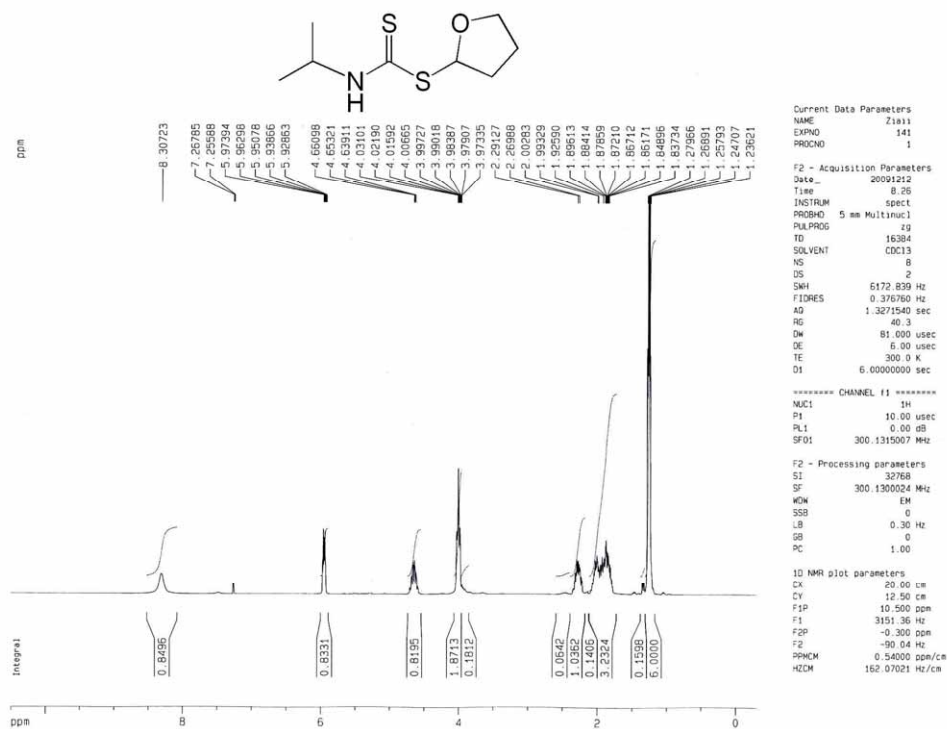
F2 - Processing parameters

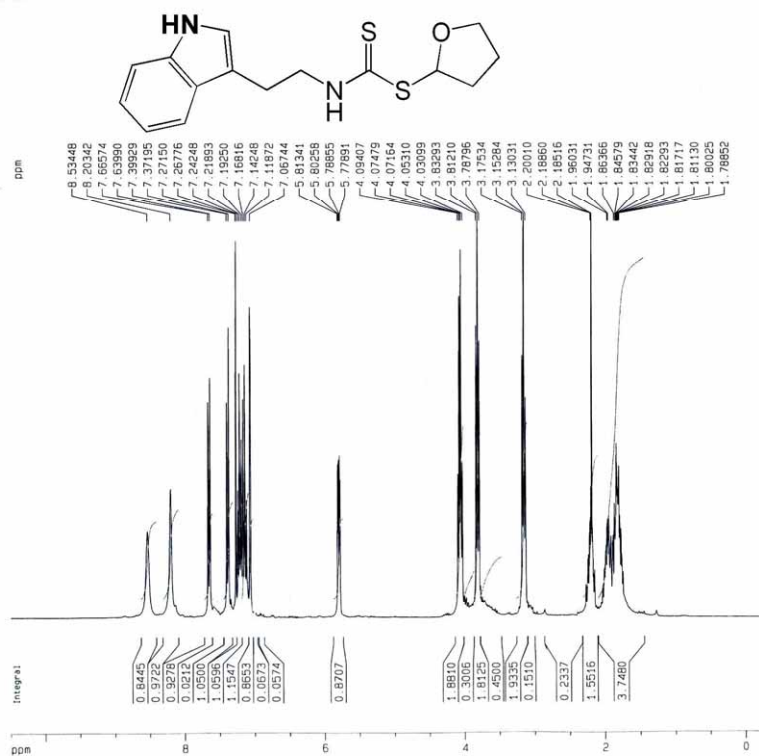
SI 32768
SF 125.7677390 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

1D NMR plot parameters

CX 20.00 cm
CY 3.51 cm
F1P 206.553 ppm
F1 25975.61 Hz
F2P 2.025 ppm
F2 254.24 Hz
PQCM 10.2896 ppm/cm
HZCM 1286.06873 Hz/cm







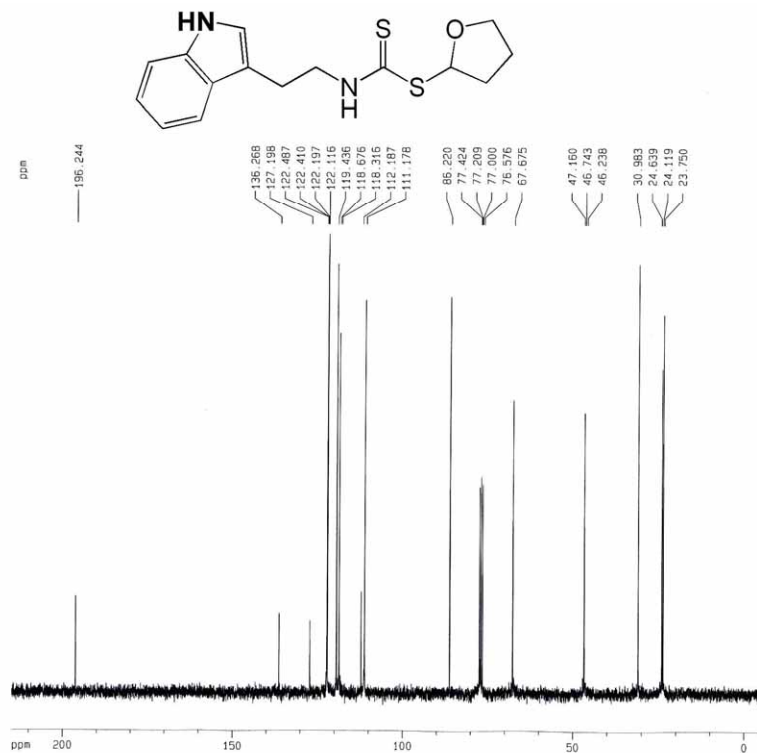
Current Data Parameters
NAME Ziail
EXPNO 135
PROCNO 1

F2 - Acquisition Parameters
Date_ 20091208
Time 8.39
INSTRUM spect
PROBHD 5 mm Multinuc1
PULPROG zgpg
TD 16384
SOLVENT CDCl3
NS 8
DS 2
SWH 6172.839 Hz
FIDRES 0.376760 Hz
AQ 1.3271540 sec
RG 90.5
DQ 81.000 usec
DE 6.00 usec
TE 300.0 K
D1 6.0000000 sec

***** CHANNEL f1 *****
NUC1 1H
P1 10.00 usec
PL1 0.00 dB
SFO1 300.1315007 MHz

F2 - Processing parameters
SI 32768
SF 300.1300024 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

ID NMR plot parameters
CX 20.00 cm
CY 12.50 cm
F1P 3151.36 Hz
F1 3151.36 Hz
F2P -0.300 ppm
F2 -90.04 Hz
PPMCM 0.54000 ppm/cm
HZCM 162.07021 Hz/cm



Current Data Parameters
NAME Ziail
EXPNO 136
PROCNO 1

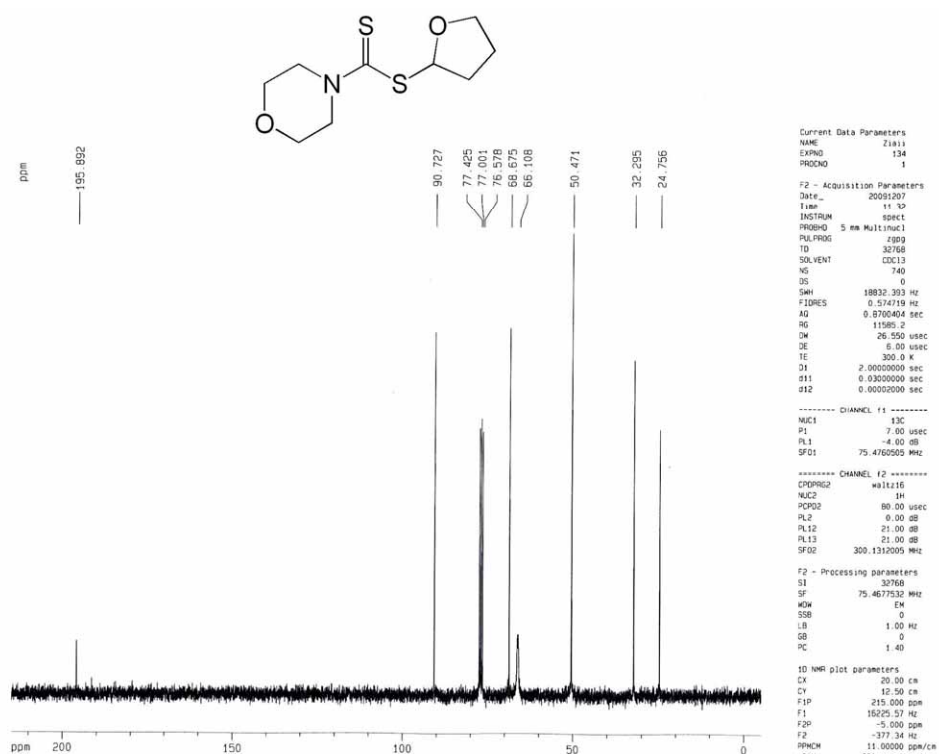
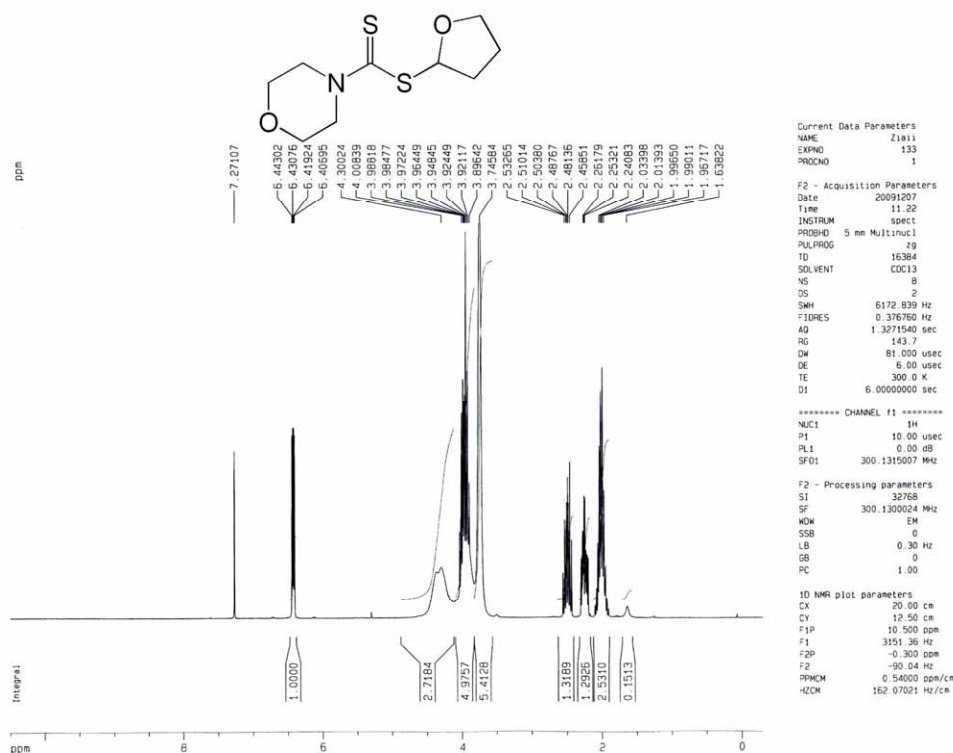
F2 - Acquisition Parameters
Date_ 20091208
Time 9.07
INSTRUM spect
PROBHD 5 mm Multinuc1
PULPROG zgpg
TD 32768
SOLVENT CDCl3
NS 850
DS 0
SWH 18832.393 Hz
FIDRES 0.574719 Hz
AQ 0.8709044 sec
RG 11585.2
DQ 26.550 usec
DE 6.00 usec
TE 300.0 K
D1 2.0000000 sec
D11 0.0300000 sec
D12 0.00002000 sec

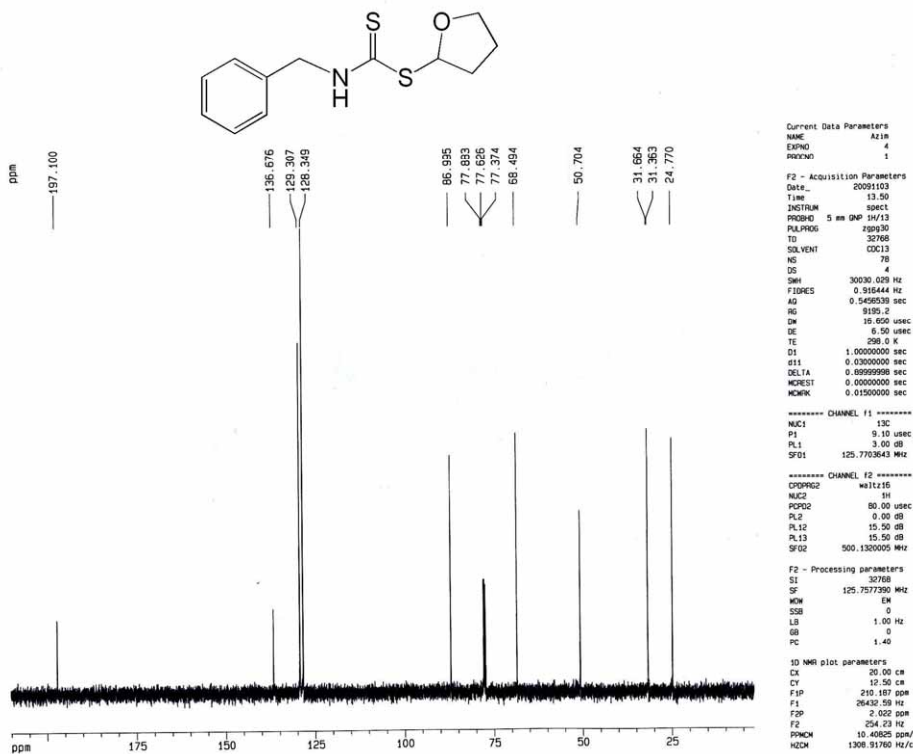
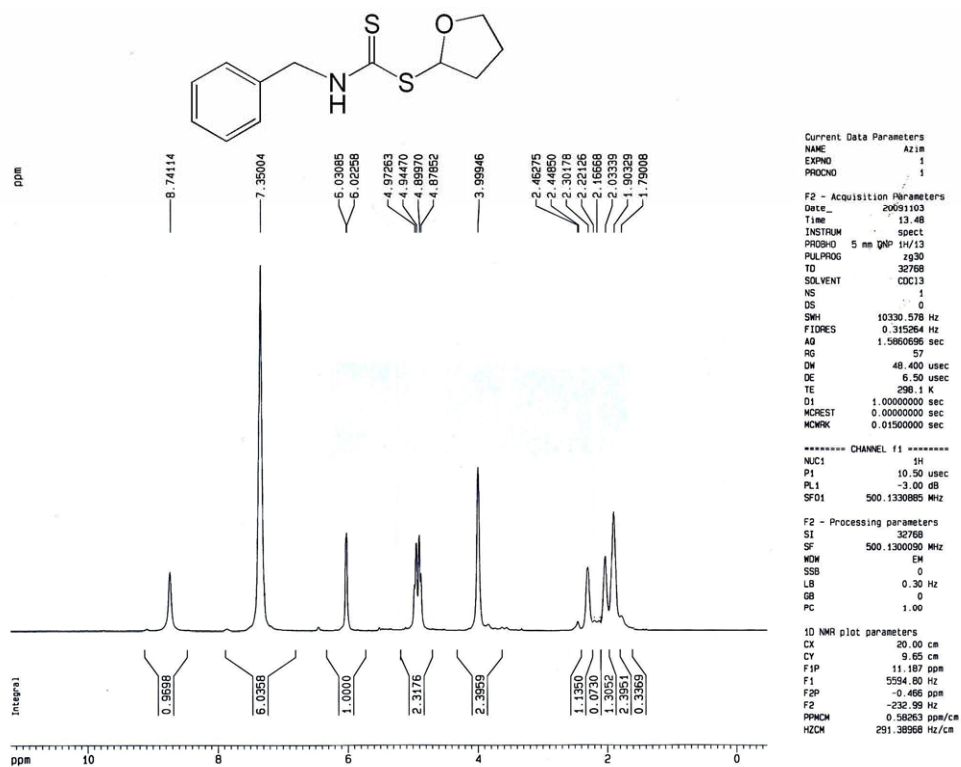
***** CHANNEL f1 *****
NUC1 13C
P1 7.00 usec
PL1 -4.00 dB
SFO1 75.4760505 MHz

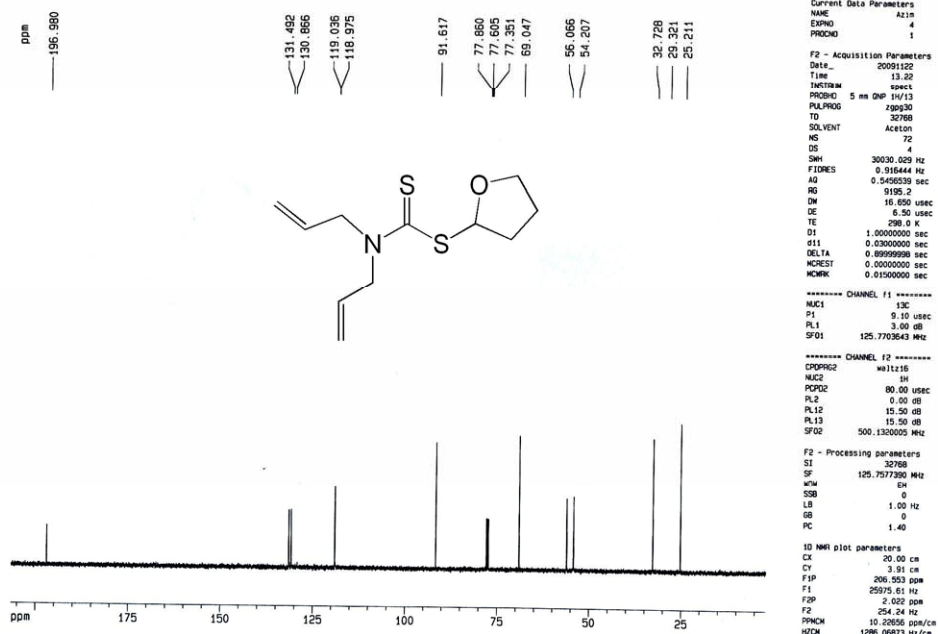
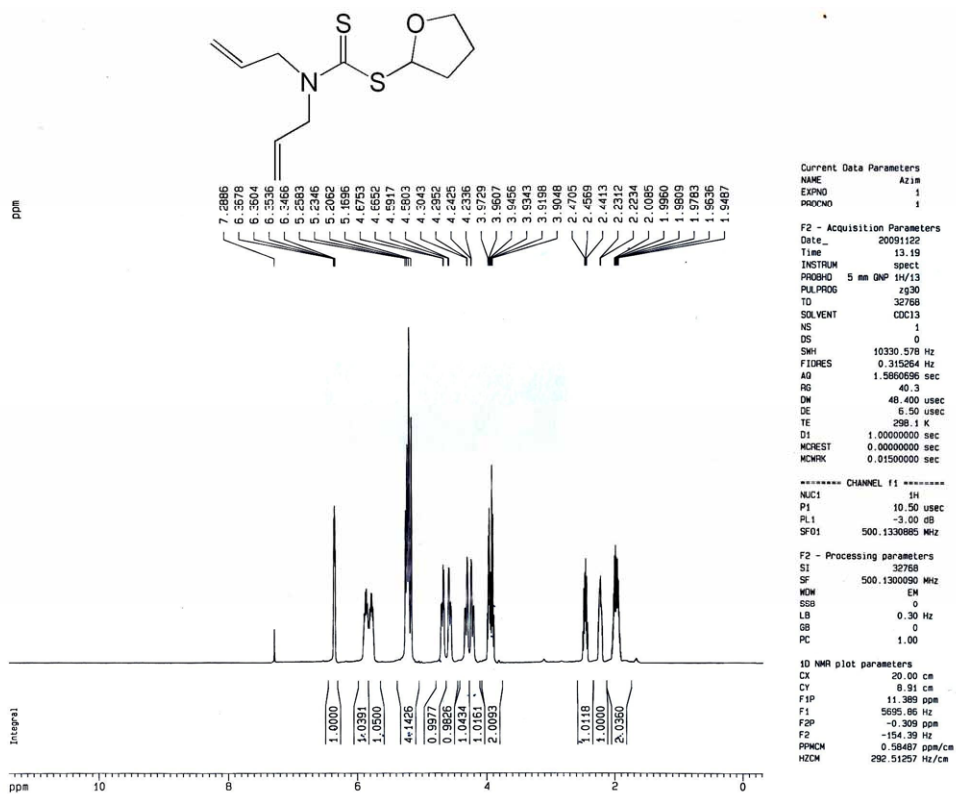
***** CHANNEL f2 *****
CPDPRG2 waltz16
NUC2 1H
P2PRG2 80.00 usec
PL2 0.00 dB
PL12 21.00 dB
PL13 21.00 dB
SFO2 300.1312005 MHz

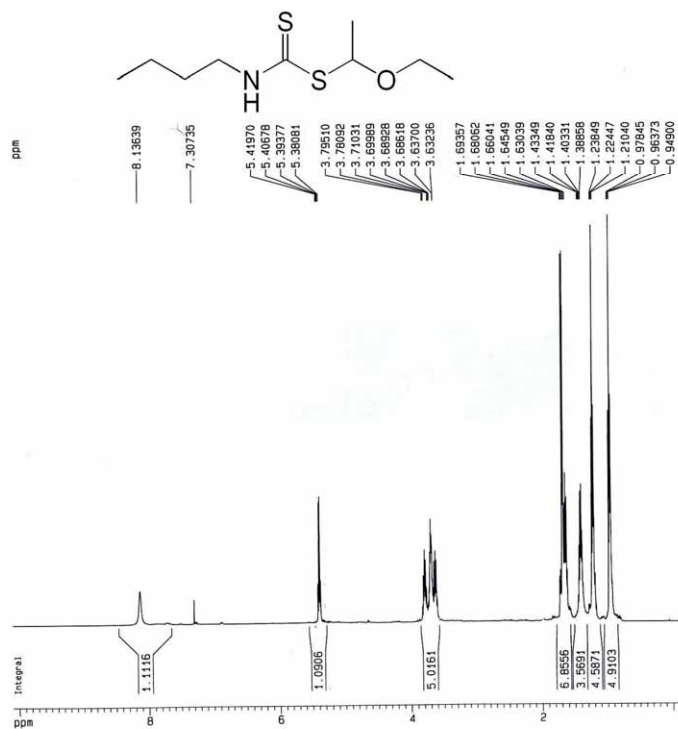
F2 - Processing parameters
SI 32768
SF 75.4677572 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

ID NMR plot parameters
CX 20.00 cm
CY 12.50 cm
F1P 215.000 ppm
F1 16225.57 Hz
F2P -5.000 ppm
F2 -377.34 Hz
PPMCM 11.00000 ppm/cm
HZCM 830.14532 Hz/cm









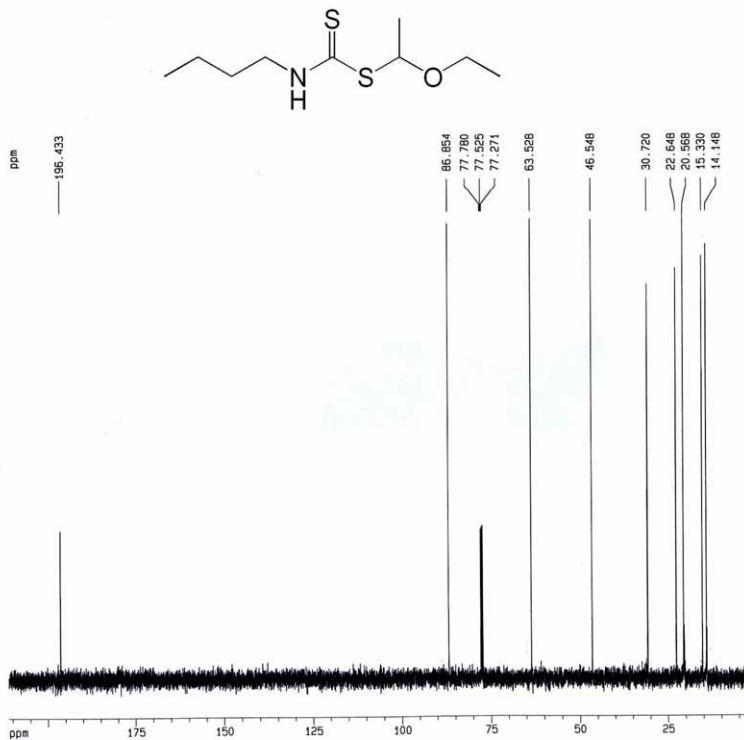
Current Data Parameters
 NAME Azim
 EXPNO 31
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20090520
 Time 13.05
 INSTRUM spect
 PROBHD 5 mm QNP 1H/13
 PULPROG zg30
 TD 32768
 SOLVENT CDCl3
 NS 1
 DS 0
 SWH 10330.578 Hz
 FIDRES 0.315264 Hz
 AQ 1.5860696 sec
 RG 35.9
 DW 40.400 usec
 DE 6.50 usec
 TE 298.0 K
 D1 1.0000000 sec
 MPROST 0.0000000 sec
 MCWRR 0.0150000 sec

***** CHANNEL f1 *****
 NUC1 1H
 P1 10.50 usec
 PL1 -3.00 dB
 SFO1 500.1330885 MHz

F2 - Processing parameters
 SI 32768
 SF 500.1330000 MHz
 WCN CN
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

1D NMR plot parameters
 CX 18.00 cm
 CY 11.00 cm
 F1P 10.095 ppm
 F1 5048.97 Hz
 F2P -0.115 ppm
 F2 -57.82 Hz
 PPMCM 0.56725 ppm/cm
 HZCM 283.69958 Hz/cm



Current Data Parameters
 NAME Azim
 EXPNO 3
 PROCNO 1

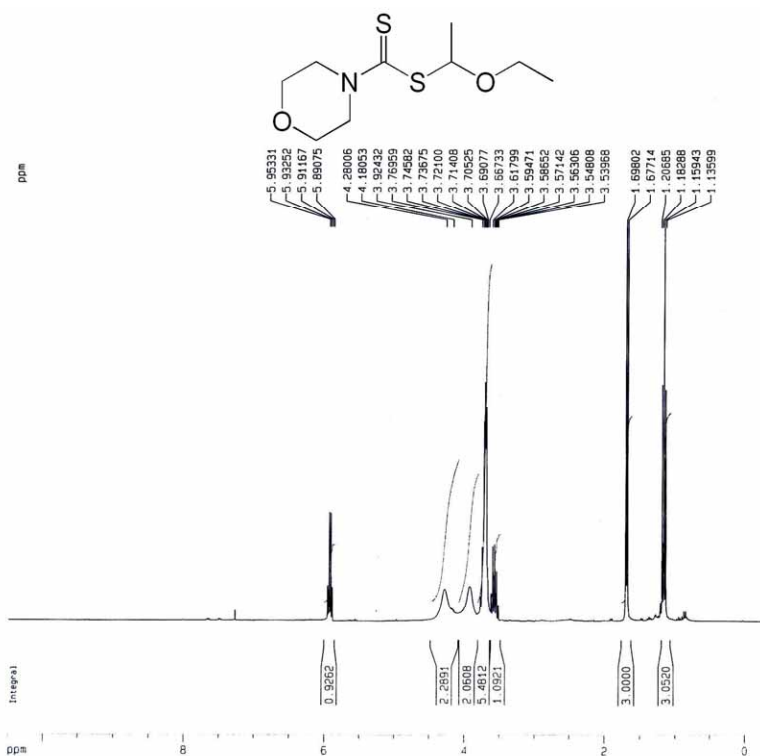
F2 - Acquisition Parameters
 Date_ 20090520
 Time 13.08
 INSTRUM spect
 PROBHD 5 mm QNP 1H/13
 PULPROG zgpg30
 TD 65536
 SOLVENT DMSO
 NS 50
 DS 4
 SWH 30030.029 Hz
 FIDRES 0.458202 Hz
 AQ 1.5515410 sec
 RG 5792.6
 DW 10.650 usec
 DE 6.50 usec
 TE 298.1 K
 D1 2.0000000 sec
 d11 0.0300000 sec
 DELTA 1.8999999 sec
 MPROST 0.0000000 sec
 MCWRR 0.0150000 sec

***** CHANNEL f1 *****
 NUC1 13C
 P1 9.10 usec
 PL1 3.00 dB
 SFO1 125.7703643 MHz

***** CHANNEL f2 *****
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 80.00 usec
 PL2 0.00 dB
 PL12 15.50 dB
 PL13 15.50 dB
 SFO2 500.1320005 MHz

F2 - Processing parameters
 SI 32768
 SF 125.7777390 MHz
 WCN fw
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

1D NMR plot parameters
 CX 20.00 cm
 CY 12.50 cm
 F1P 211.107 ppm
 F1 26545.32 Hz
 F2P 1.620 ppm
 F2 203.79 Hz
 PPMCM 10.47432 ppm/cm
 HZCM 1317.22644 Hz/cm



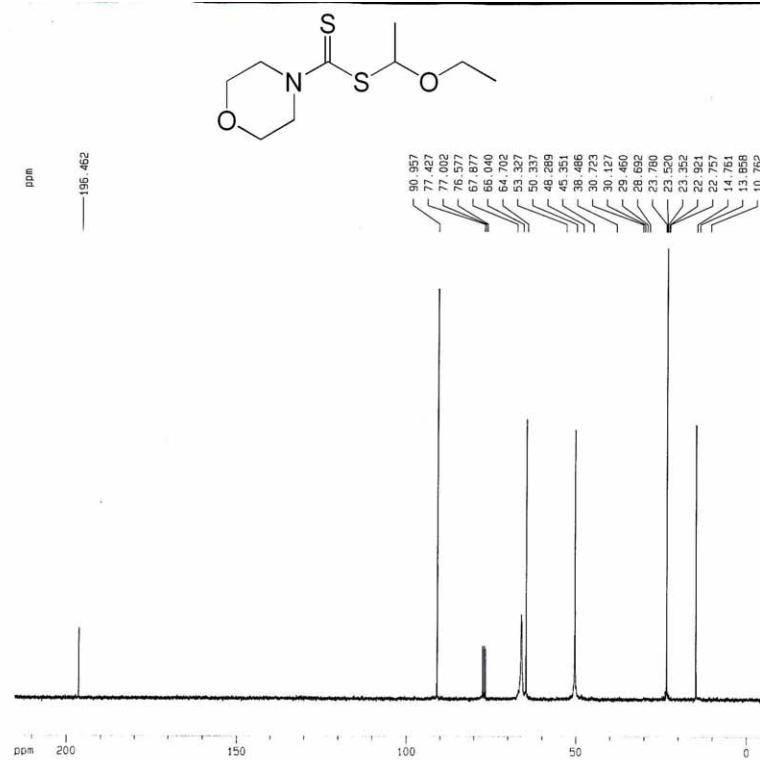
Current Data Parameters
NAME Zi111
EXPNO 85
PROCNO 1

F2 - Acquisition Parameters
Date_ 20090511
Time 11:29
INSTRUM spect
PROBHD 5 mm Multinucl
PULPROG zg
TD 16384
SOLVENT CDCl3
NS 8
DS 2
SWH 6172.839 Hz
FIDRES 0.376760 Hz
AQ 1.3271540 sec
RG 25.4
DW 81.000 usec
DE 6.00 usec
TE 300.0 K
D1 6.00000000 sec

***** CHANNEL f1 *****
NUC1 1H
P1 10.00 usec
PL1 0.00 dB
SFO1 300.1315007 MHz

F2 - Processing parameters
SI 32768
SF 300.1300035 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

1D NMR plot parameters
CX 20.00 cm
CY 12.50 cm
F1 3151.36 Hz
F2P -0.300 ppm
F2 -90.04 Hz
-NUC1 0.54000 ppm/cm
-KZCM 162.07021 Hz/cm



Current Data Parameters
NAME Zi111
EXPNO 86
PROCNO 1

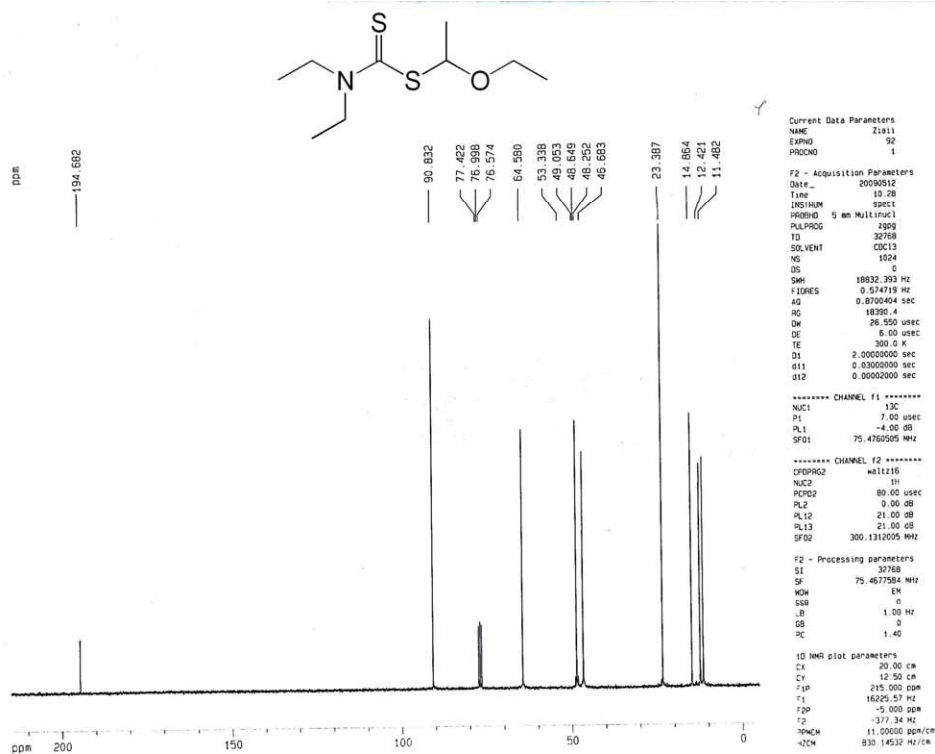
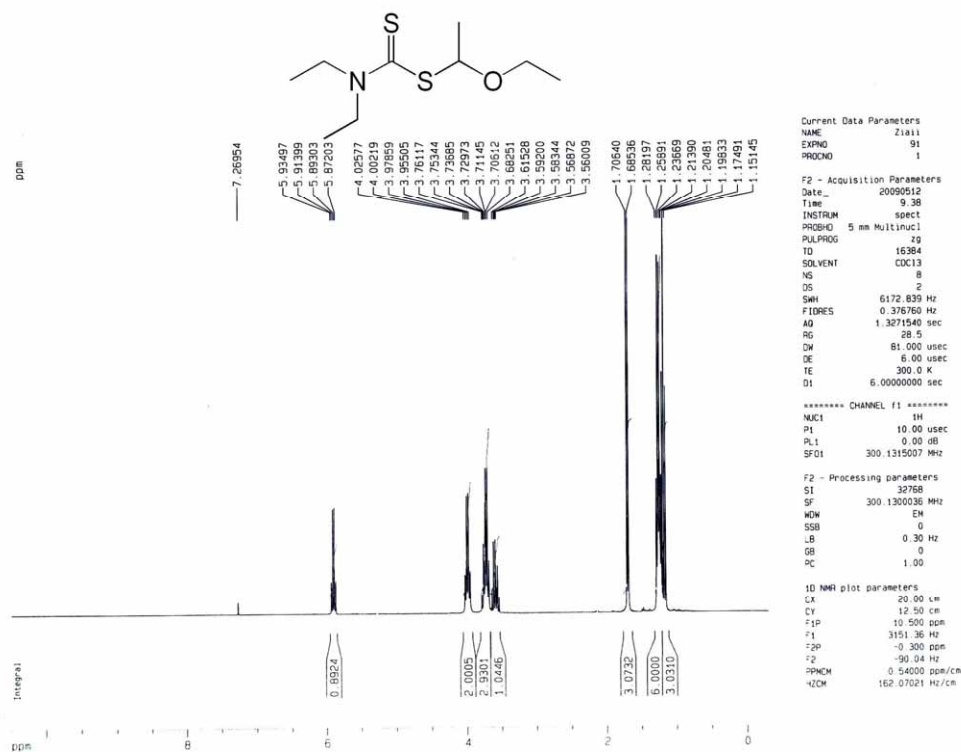
F2 - Acquisition Parameters
Date_ 20090511
Time 11:43
INSTRUM spect
PROBHD 5 mm Multinucl
PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 510
DS 0
SWH 18832.393 Hz
FIDRES 0.574719 Hz
AQ 0.5700404 sec
RG 18390.4
DW 26.550 usec
DE 5.00 usec
TE 300.0 K
D1 2.00000000 sec
d11 0.03000000 sec
d12 0.00020000 sec

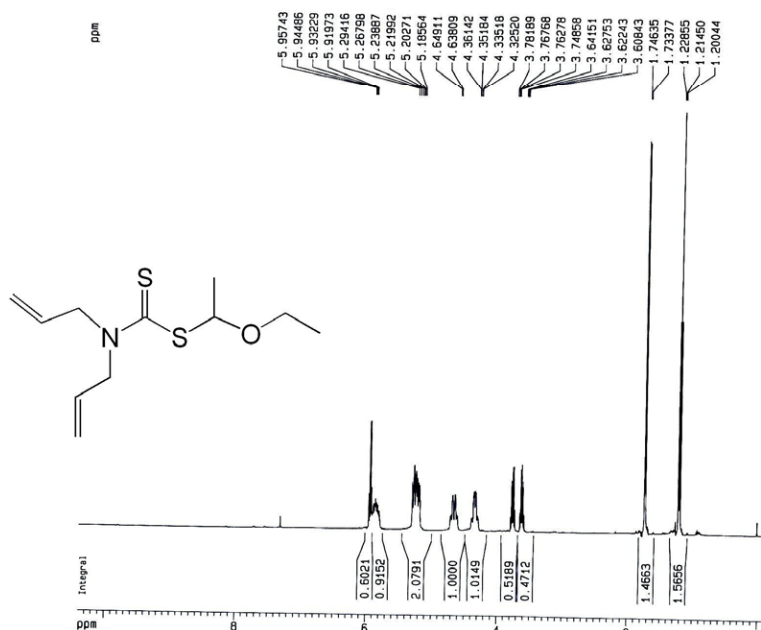
***** CHANNEL f1 *****
NUC1 13C
P1 7.00 usec
PL1 -4.00 dB
SFO1 75.4760505 MHz

***** CHANNEL f2 *****
CPDPRG2 waltz16
NUC2 1H
PCPD2 60.00 usec
PL2 0.00 dB
PL12 21.00 dB
PL13 21.00 dB
SFO2 300.1312605 MHz

F2 - Processing parameters
SI 32768
SF 75.4677630 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

1D NMR plot parameters
CX 20.00 cm
CY 12.50 cm
F1 215.000 ppm
F2 16025.57 Hz
F2P -5.000 ppm
F2 -377.34 Hz
-NUC1 11.00000 ppm/cm
-KZCM 830.14535 Hz/cm





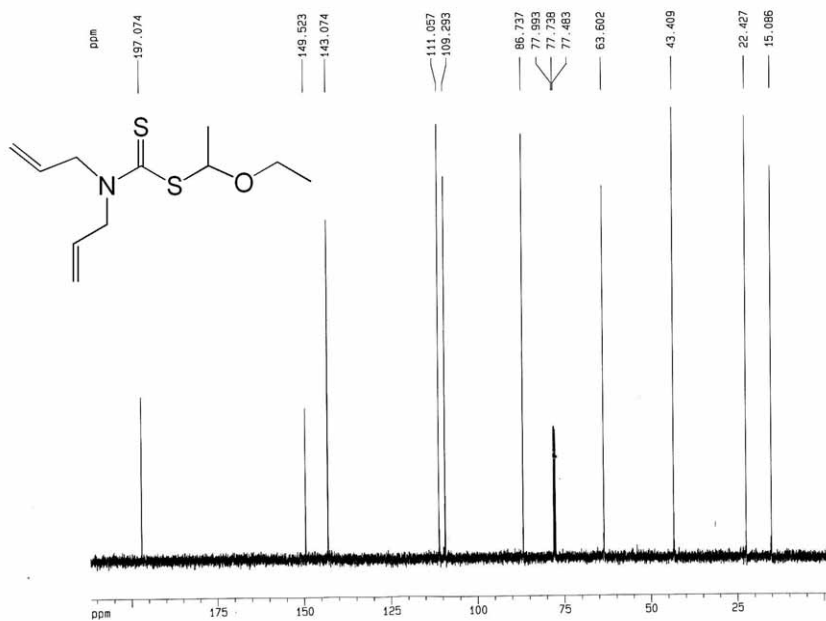
Current Data Parameters
NAME Azim
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20090802
Time 10.54
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 1
DS 0
SWH 10330.578 Hz
FIDRES 0.315264 Hz
AQ 1.5860696 sec
RG 40.3
DW 48.400 usec
DE 6.50 usec
TE 298.1 K
D1 1.00000000 sec
MCREST 0.00000000 sec
MCMRK 0.01500000 sec

----- CHANNEL f1 -----
NUC1 1H
P1 10.50 usec
PL1 -3.00 dB
SFO1 500.1330885 MHz

F2 - Processing parameters
SI 32768
SF 500.1330000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

1D NMR plot parameters
CX 18.00 cm
CY 11.00 cm
F1P 10.396 ppm
F1 5199.54 Hz
F2P -0.156 ppm
F2 -78.04 Hz
PPMCM 0.58625 ppm/cm
HZCM 293.19879 Hz/cm



Current Data Parameters
NAME Azim
EXPNO 3
PROCNO 1

F2 - Acquisition Parameters
Date_ 20090804
Time 10.56
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 30
DS 4
SWH 30030.025 Hz
FIDRES 0.458222 Hz
AQ 1.0512410 sec
RG 5792.6
DW 16.650 usec
DE 6.50 usec
TE 298.0 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.69999999 sec
MCREST 0.00000000 sec
MCMRK 0.01500000 sec

----- CHANNEL f1 -----
NUC1 13C
P1 9.10 usec
PL1 3.00 dB
SFO1 125.7703643 MHz

----- CHANNEL f2 -----
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 0.00 dB
PL12 15.00 dB
PL13 15.50 dB
SFO2 500.1330005 MHz

F2 - Processing parameters
SI 32768
SF 125.7577395 MHz
WDW CM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

1D NMR plot parameters
CX 20.00 cm
CY 12.50 cm
F1P 211.744 ppm
F1 26628.44 Hz
F2P -2.915 ppm
F2 -365.95 Hz
PPMCM 10.73269 ppm/cm
HZCM 1345.71524 Hz/cm



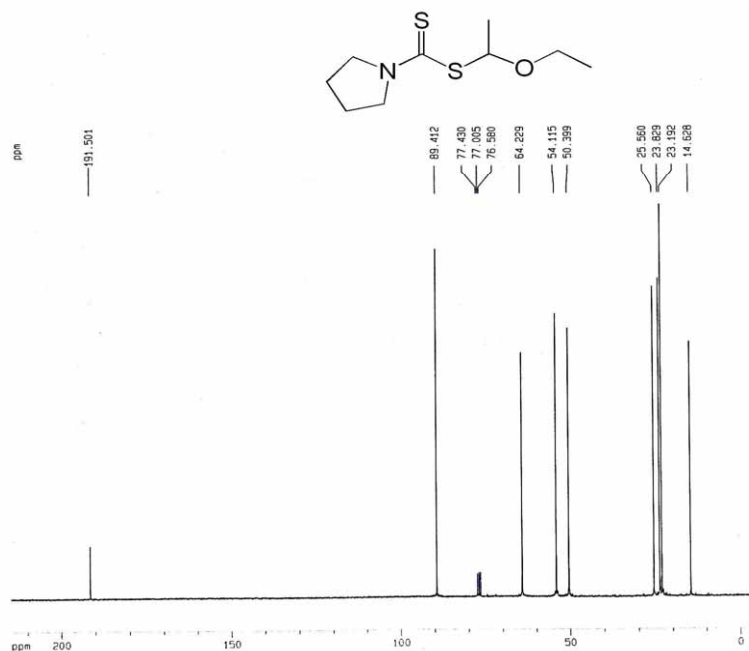
Current Data Parameters
NAME Zi111
EXPNO 87
PROCNO 1

F2 - Acquisition Parameters
Date_ 20090512
Time 8.44
INSTRUM spect
PROBHD 5 mm Multinuc1
PULPROG zg
TD 16384
SOLVENT CDCl3
NS 16
DS 2
SWH 6172.839 Hz
FIDRES 0.376760 Hz
AQ 1.3271540 sec
RG 16
DN 81.000 usec
DE 6.00 usec
TE 300.0 K
D1 6.00000000 sec

***** CHANNEL f1 *****
NUC1 1H
P1 10.00 usec
PL1 0.00 dB
SF01 300.1315007 MHz

F2 - Processing parameters
SI 32768
SF 300.130036 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

1D NMR plot parameters
CX 20.00 cm
CY 12.50 cm
F1P 10.500 ppm
F1 3151.36 Hz
F2P -0.300 ppm
F2 -0.04 Hz
PRCH 0.54000 ppm/cm
ZDCH 162.07021 Hz/cm



Current Data Parameters
NAME Zi111
EXPNO 88
PROCNO 1

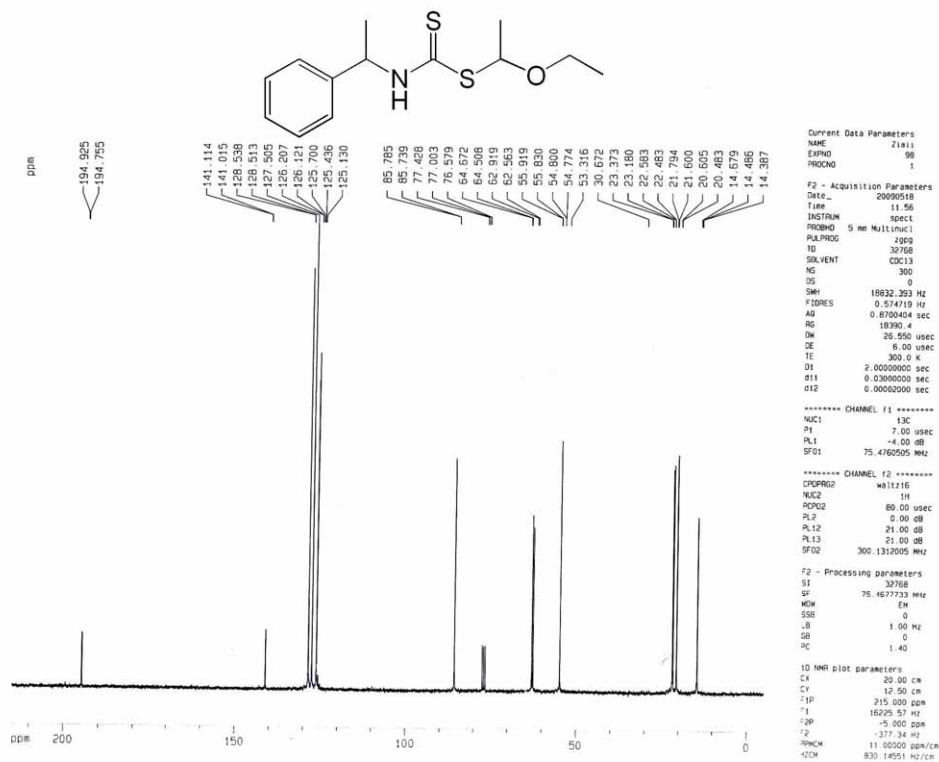
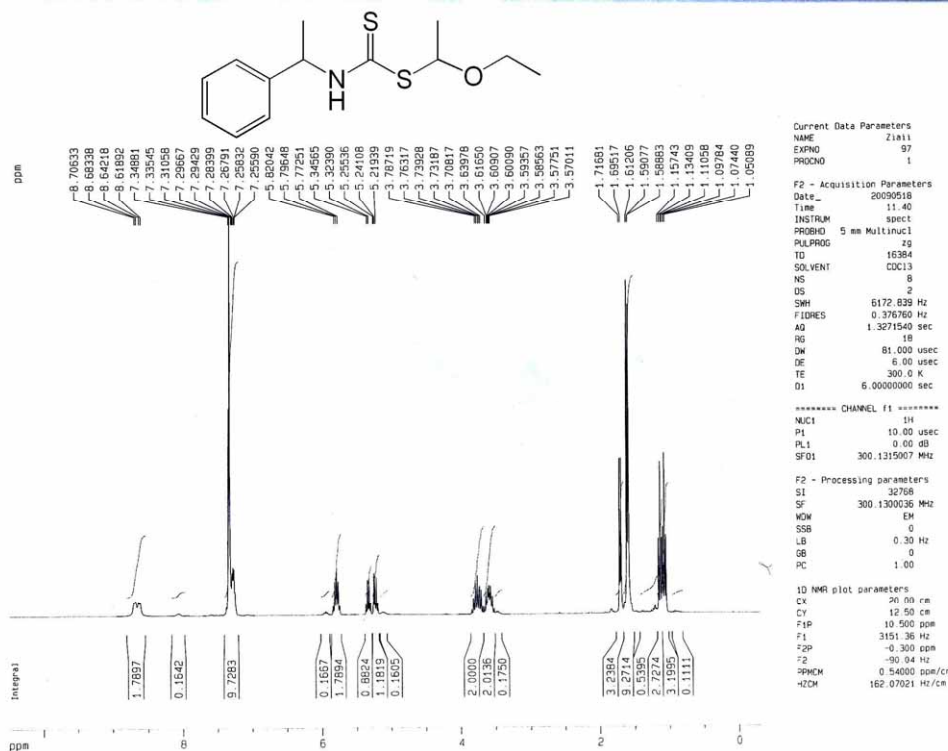
F2 - Acquisition Parameters
Date_ 20090512
Time 9.05
INSTRUM spect
PROBHD 5 mm Multinuc1
PULPROG zgpg
TD 32768
SOLVENT CDCl3
NS 624
DS 0
SWH 18832.393 Hz
FIDRES 0.574719 Hz
AQ 0.8700404 sec
RG 1836.4
DN 26.550 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
d11 0.03000000 sec
d12 0.00002000 sec

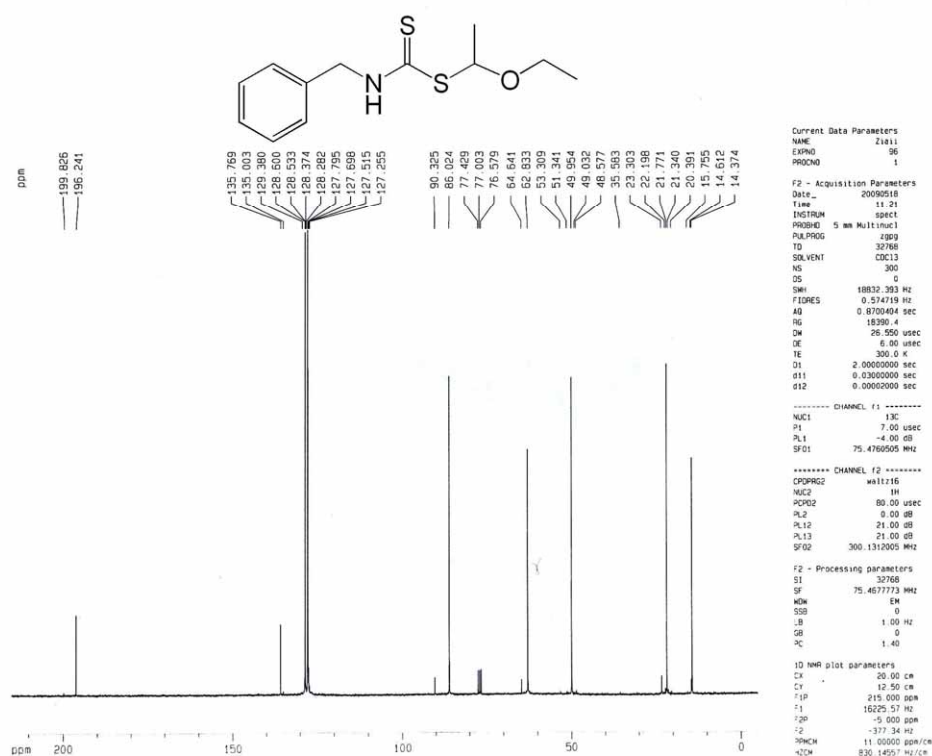
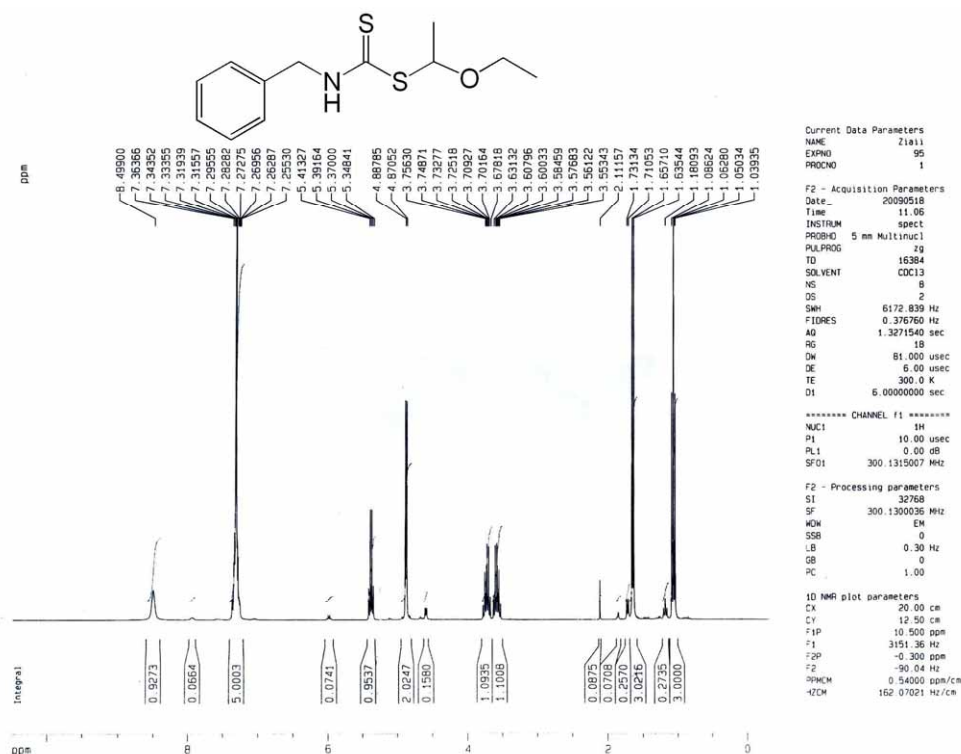
***** CHANNEL f1 *****
NUC1 13C
P1 7.00 usec
PL1 -4.00 dB
SF01 75.4760565 MHz

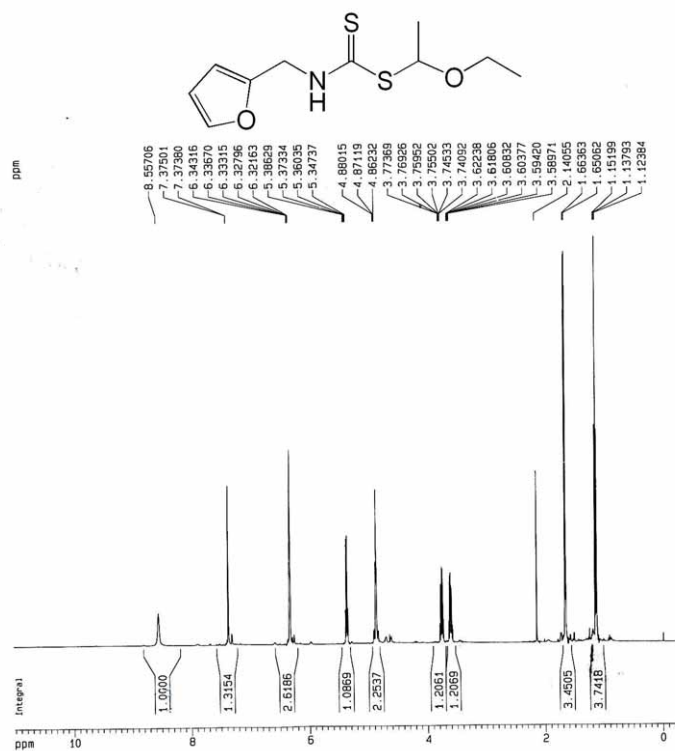
***** CHANNEL f2 *****
CPDPRG2 waltz16
NUC2 1H
P2P2 80.00 usec
PL2 0.00 dB
PL12 21.00 dB
PL13 21.00 dB
SF02 300.1312005 MHz

F2 - Processing parameters
SI 32768
SF 75.4677739 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

1D NMR plot parameters
CX 20.00 cm
CY 12.50 cm
F1P 215.000 ppm
F1 16235.57 Hz
F2P -5.000 ppm
F2 -37.134 Hz
PRCH 11.00000 ppm/cm
ZDCH 830.14551 Hz/cm







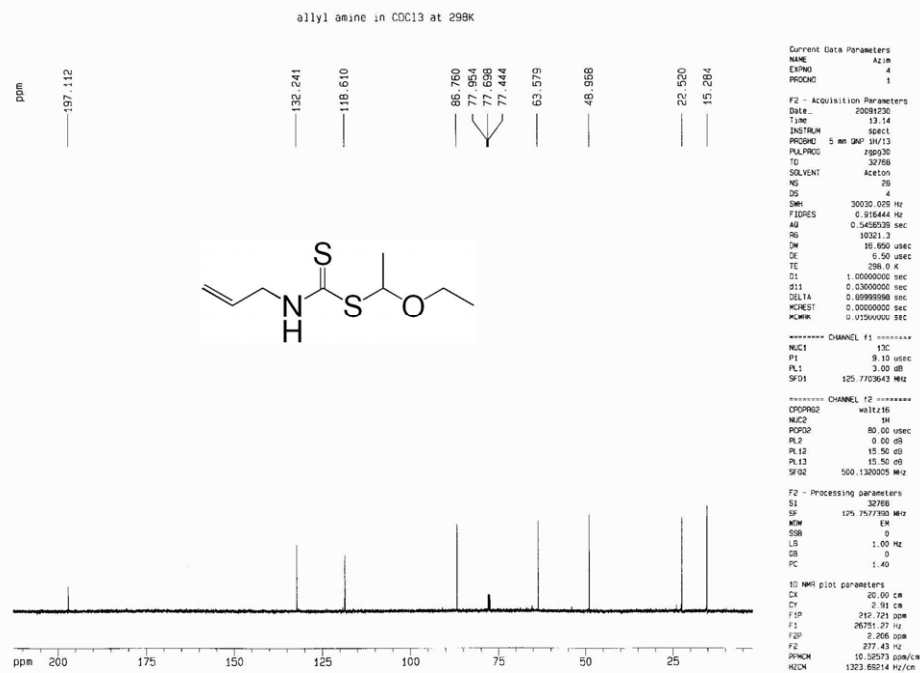
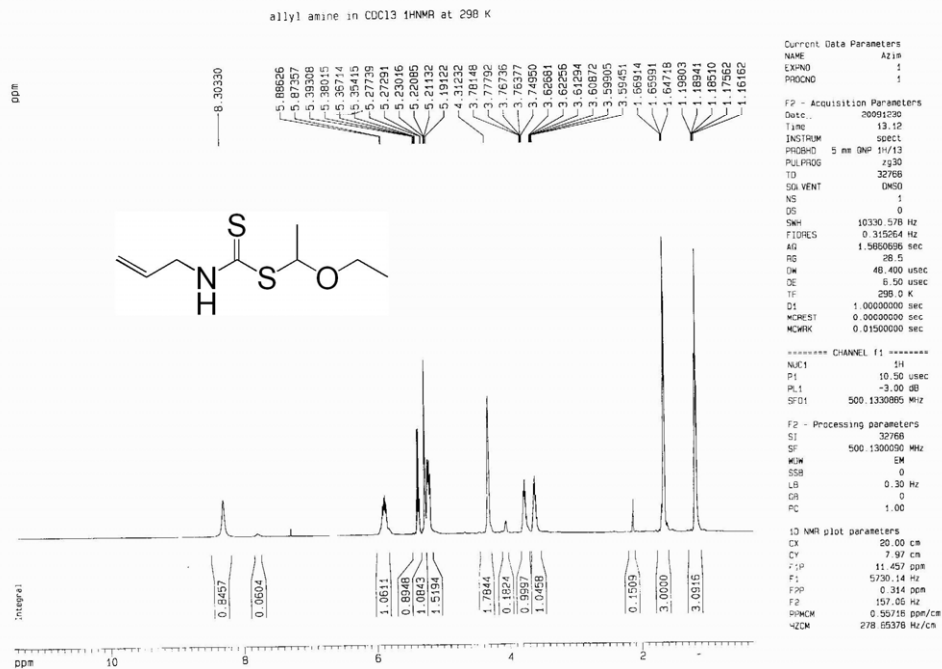
Current Date Parameters
NAME Azim
EXPNO 1
PROCNO 1

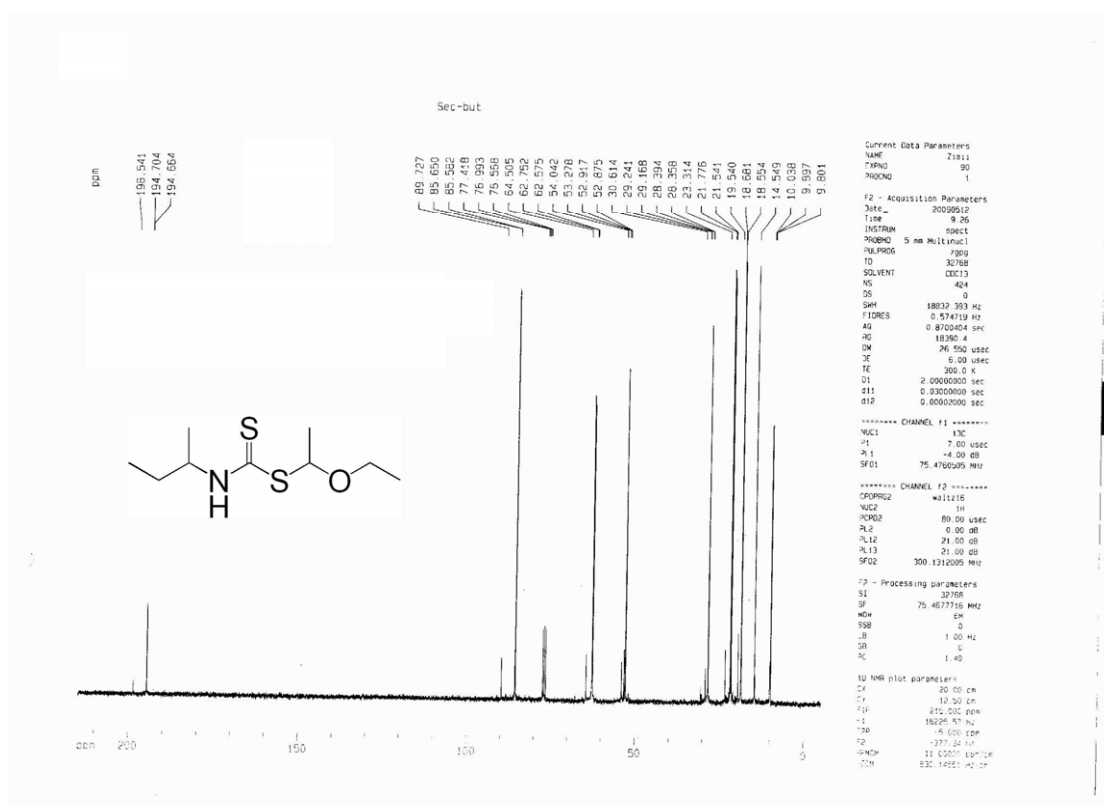
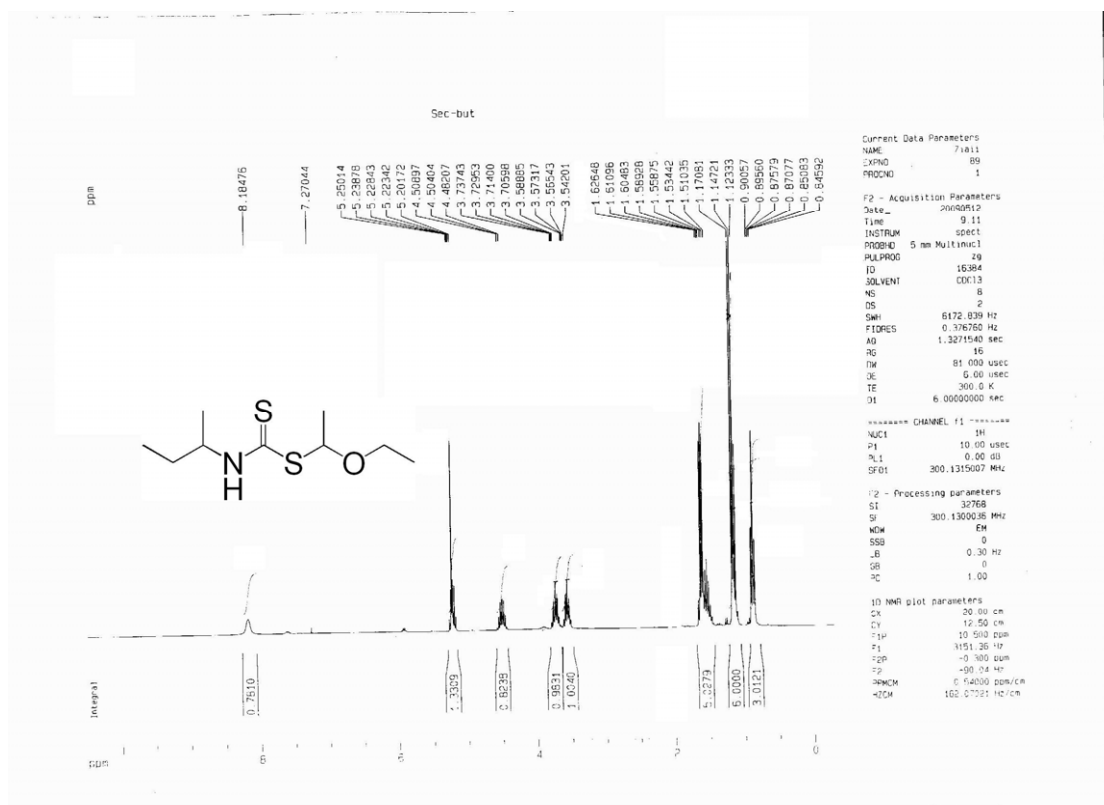
F2 - Acquisition Parameters
Date_ 20090904
Time 12.53
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 1
DS 0
SWH 10330.578 Hz
FIDRES 0.315264 Hz
AQ 1.5862096 sec
RG 35.9
DM 48.400 usec
DE 6.50 usec
TE 298.0 K
D1 1.00000000 sec
MCHES1 0.00000000 sec
MCHES2 0.01500000 sec

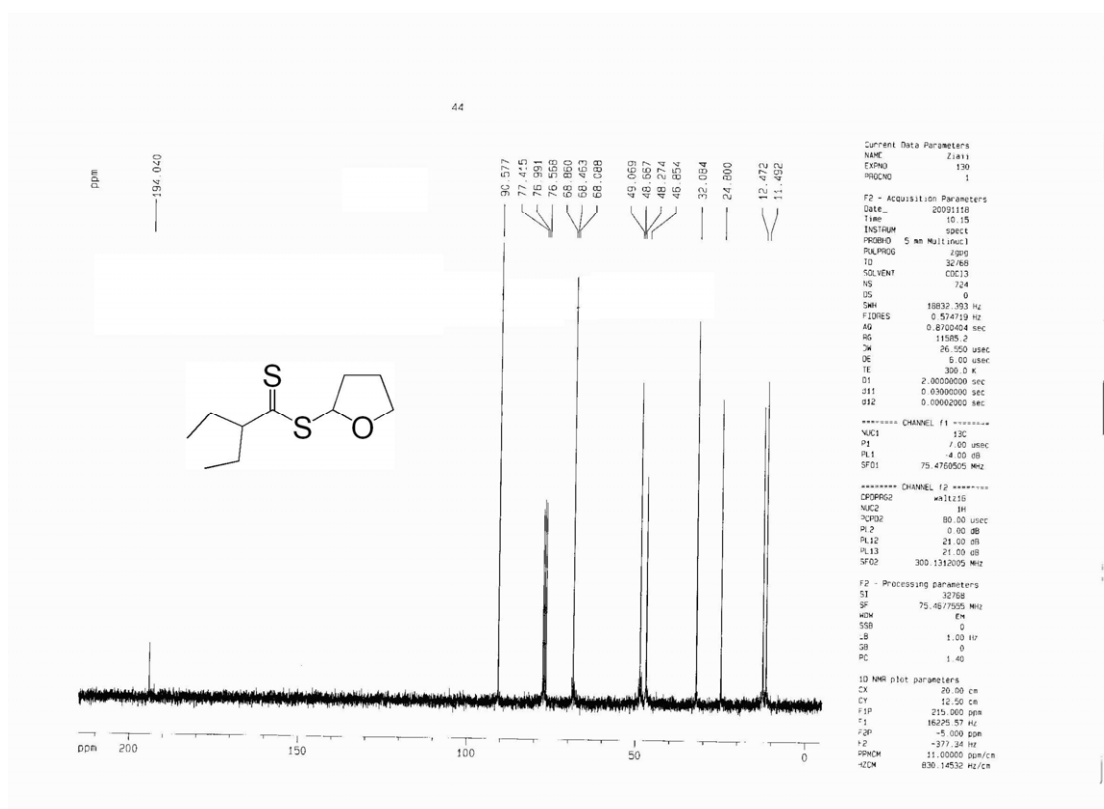
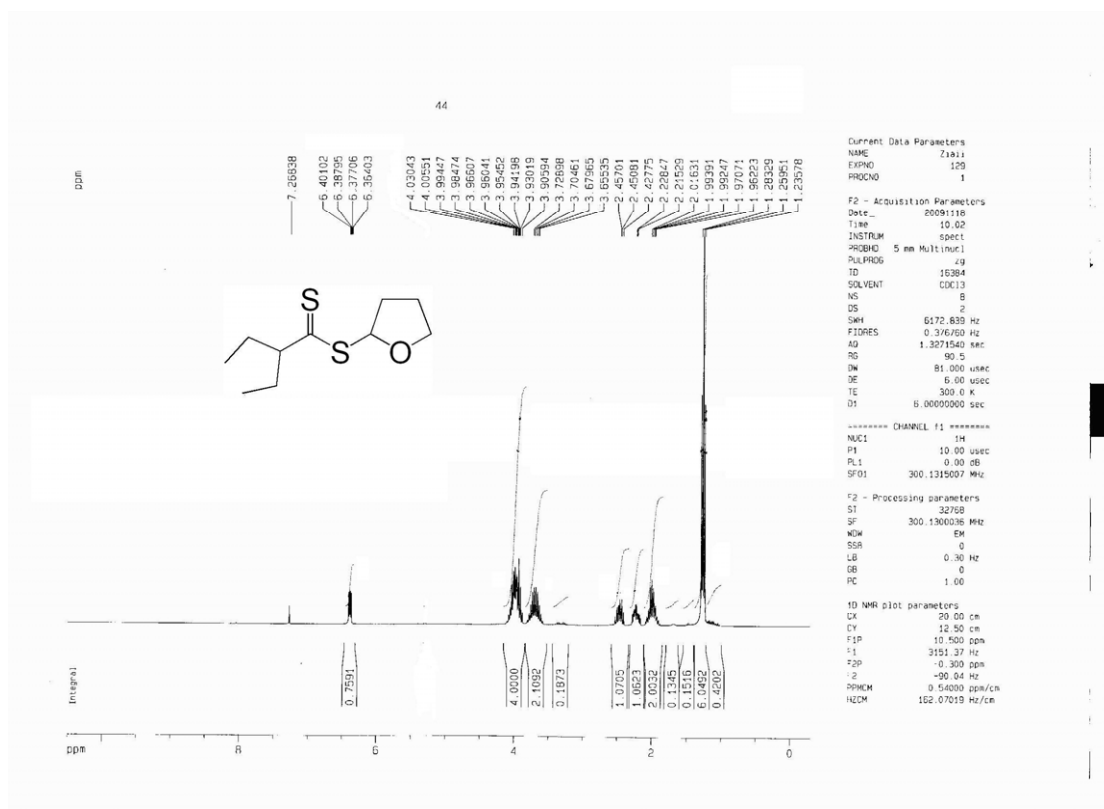
----- CHANNEL f1 -----
NUC1 1H
P1 10.50 usec
PL1 -3.00 dB
SFO1 500.1330685 MHz

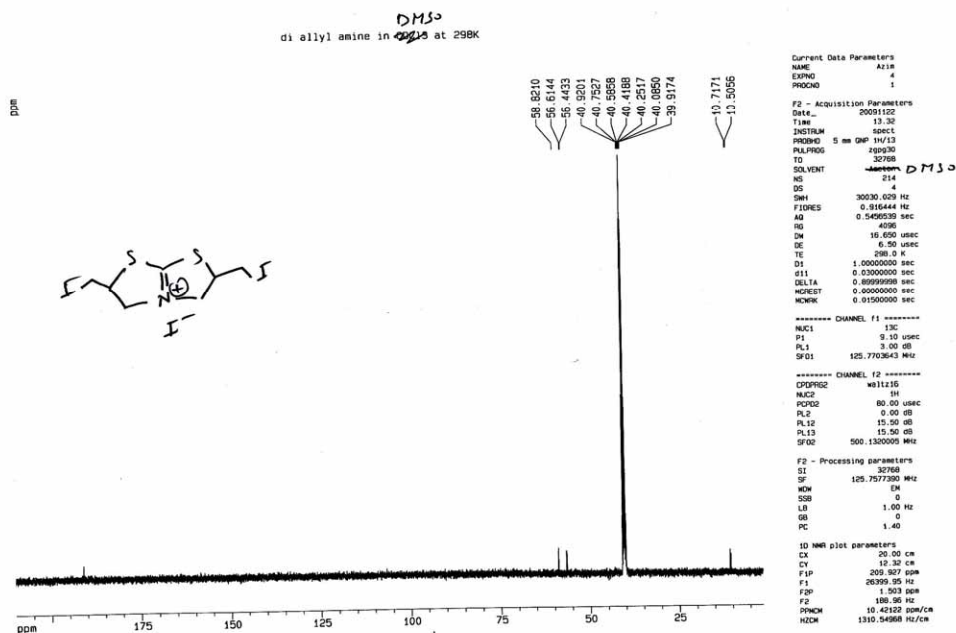
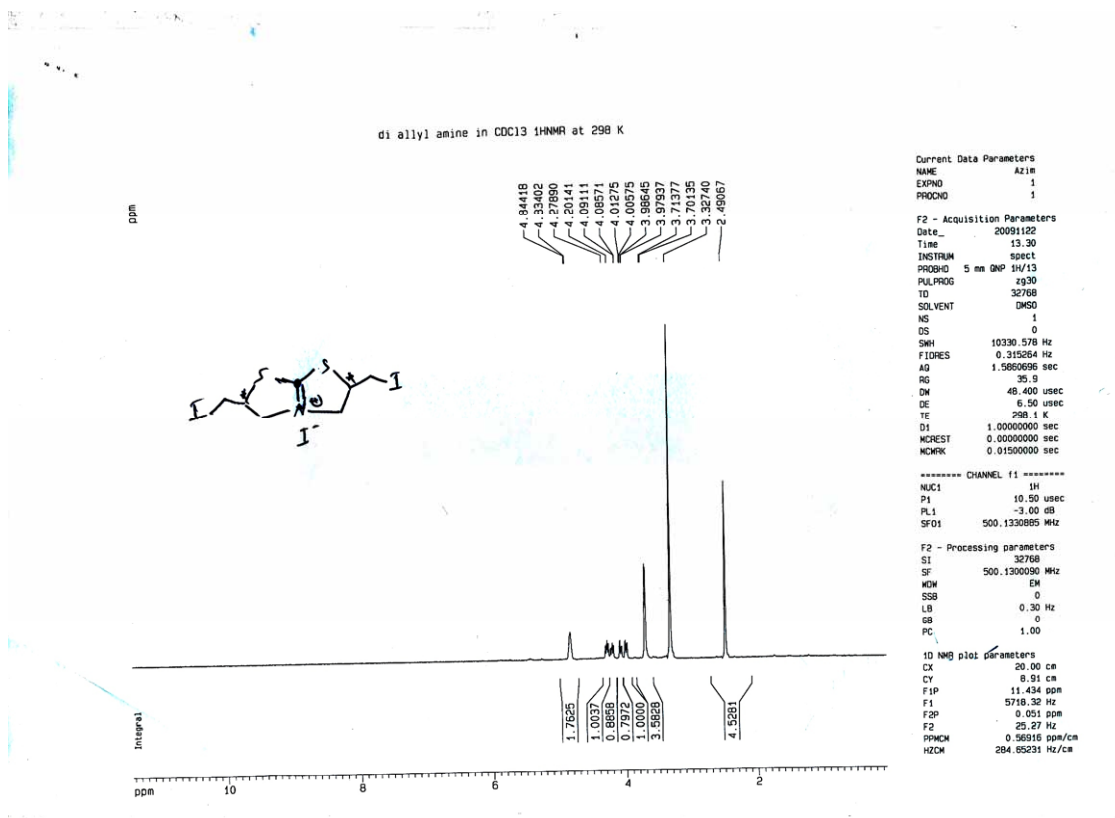
F2 - Processing parameters
SI 32768
SF 500.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

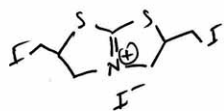
10 NMR plot parameters
CX 18.00 cm
CY 11.00 cm
F1P 11.025 ppm
F1 5513.55 Hz
F2P -0.313 ppm
F2 -155.64 Hz
PCHW 0.62990 ppm/cm
HZCM 315.03275 Hz/cm



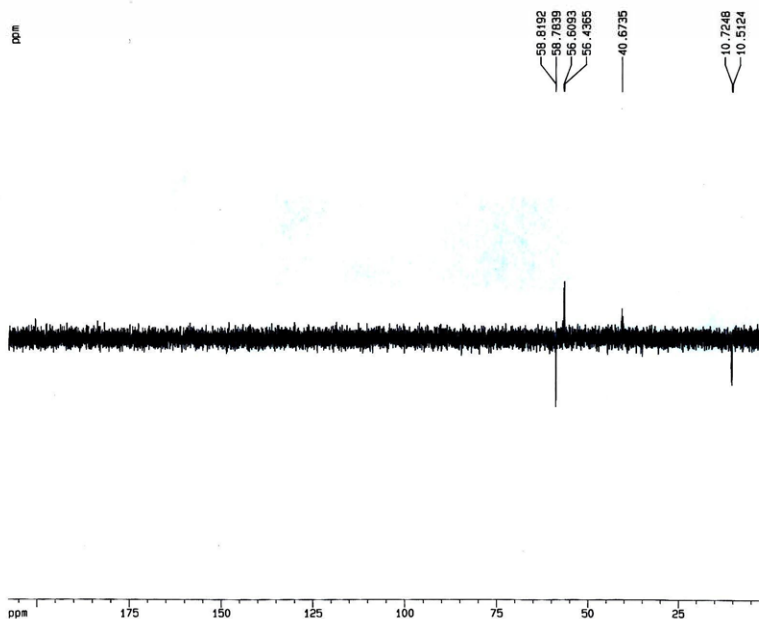








DEPT135 in DMSO at 298 K 88/9/1



Current Data Parameters
NAME Atis
EXPNO 30
PROCNO 1

F2 - Acquisition Parameters
Date_ 20091122
Time 13.39
INSTRUM spect
PROBHD 5 mm DNP 1H/13
PULPROG dept135
TD 65536
SOLVENT DMSO
NS 52
DS 4
SWH 30030.029 Hz
FIDRES 0.458022 Hz
AQ 1.0912410 sec
RG 7298.2
DM 16.650 usec
DE 6.50 usec
TE 298.0 K
CHST2 145.0000000
D1 2.00000000 sec
G2 0.00344020 sec
r12 0.00000000 sec
DELTA 0.00001159 sec
MORPH 0.00000000 sec
MORPH 0.01500000 sec

***** CHANNEL f1 *****
NUC1 13C
P1 9.10 usec
P2 18.20 usec
PL1 3.00 dB
SFO1 125.770543 MHz

***** CHANNEL f2 *****
CHPROG zgpg30
NUC2 1H
P3 13.00 usec
P4 26.00 usec
PCPD2 80.00 usec
PL3 0.00 dB
PL12 15.50 dB
SFO2 500.132005 MHz

F2 - Processing parameters
SI 32768
SF 125.7577390 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

1D NMR plot parameters
CX 20.00 cm
CY 1.50 cm
FSP 207.851 ppm
F1 20138.82 Hz
F2 201.60 Hz
FREQ 10.30442 ppm/c
HZCN 1099.86198 Hz/cm