Supporting Information for

Copper-Catalyzed Dehydrogenative Cross-Coupling of Benzothiazoles with Thiazoles and Polyfluoroarene

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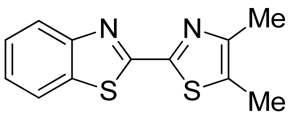
General information: ^{1}H NMR and ^{13}C NMR spectra were recorded on a Bruker AM300 and AM400 spectrometer. ^{19}F NMR was recorded on a Bruker AM300 spectrometer ($CFCl_3$ as outside standard and low field is positive). Chemical shifts (δ) are reported in ppm, and coupling constants (*J*) are in Hertz (Hz). The following abbreviations were used to explain the multiplicities: s = singlet, d = doublet, t = triplet, q = quartet, m = multiplet, br = broad. NMR yield was determined by ^{19}F NMR using fluorobenzene as an internal standard before working up the reaction.

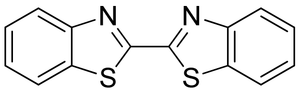
Materials: All reagents were used as received from commercial sources, unless specified otherwise, or prepared as described in the literature. All reagents were weighed and handled in air, and refilled with an inert atmosphere of N_2 at room temperature. DMF, DMSO and DCE were distilled under reduced pressure from CaH_2. 1,4-Dioxane was distilled from sodium and benzophenone immediately before use.

Screens for Copper-Catalyzed Dehydrogenative Cross-Coupling of Benzothiazoles with Thiazoles (Table 1). To a septum capped 25 mL of sealed tube were added Cu-catalyst (10 mol%), ligand (10 mol%), oxidant (2.0 equiv) and base (3.0 equiv) under N_2, followed by solvent (2.5 mL) with stirring. Benzothiazole **1a** (0.3 mmol, 1.0 equiv) and 4,5-dimethylthiazole **2a** (2.0 euqiv) were then added subsequently. The sealed tube was screw capped and heated to 80 ^{o}C (oil bath). After stirring for 10 h, the reaction mixture was cooled to room temperature, filtered and concentrated. The residue was purified with silica gel chromatography (Petroleum ether / Dichloromethane = 2:1) to give product.

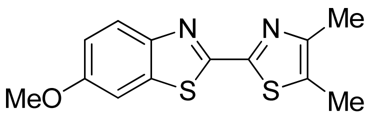
General Procedure for Copper-Catalyzed Dehydrogenative Cross-Coupling of Benzothiazoles with Thiazoles. To a septum capped 25 mL of sealed tube were added CuI (10 mol%), Ag_2CO_3 (2.0 equiv) and *t*BuOLi (3.0-4.0 equiv) under N_2, followed by solvent (2.5 mL) with stirring. Benzothiazole **1a** (0.3 mmol, 1.0 euqiv) and thiazole (2.0-3.0 equiv) were then added subsequently. The sealed tube was screw capped and heated to 80 ^{o}C (oil bath). After stirring for 10 h, the reaction mixture was cooled to room temperature, filtered and concentrated. The residue was purified with silica gel chromatography to provide pure product.



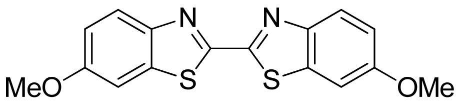
2-(4,5-Dimethylthiazol-2-yl)benzo[d]thiazole (3a). 3.0 equiv of thiazole was used. The product (52 mg, 71% yield) as a white solid was purified with silica gel chromatography (Petroleum ether / Dichloromethane = 2:1). This compound is known.[1] M.P. 194 ^{o}C; ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.06 (d, *J* = 8.7 Hz, 1H), 7.92 (d, *J* = 7.5 Hz, 1H), 7.50 (t, *J* = 7.2 Hz, 1H), 7.41 (t, *J* = 7.2 Hz, 1H), 2.46 (s, 3H), 2.44 (s, 3H).



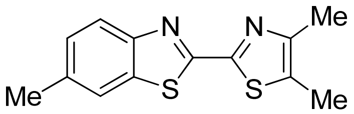
2,2'-Bibenzo[d]thiazole. Homocoupling compound of **1a** (6 mg, 14% yield) as a white solid was purified with silica gel chromatography (Petroleum ether / Dichloromethane = 2:1). ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.17 (d, *J* = 8.1 Hz, 2H), 8.00 (d, *J* = 8.1 Hz, 2H), 7.57 (t, *J* = 6.9 Hz, 2H), 7.50 (t, *J* = 6.9 Hz, 2H).



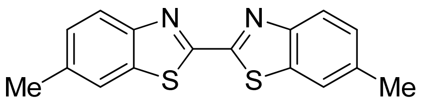
2-(4,5-Dimethylthiazol-2-yl)-6-methoxybenzo[d]thiazole (3b). 3.0 equiv of thiazole was used. The product (45 mg, 54% yield) as a white solid was purified with silica gel chromatography (Petroleum ether / Dichloromethane = 2:1). M.P. 167 ^{o}C; ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.93 (d, *J* = 9.0 Hz, 1H), 7.35 (d, *J* = 2.7 Hz, 1H), 7.09 (dd, *J* = 9.0 Hz, 2.7 Hz, 1H), 3.89 (s, 3H), 2.44 (s, 3H), 2.42 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 159.3, 158.3, 156.6, 150.3, 148.1, 136.6, 130.2, 123.9, 116.1, 103.9, 55.8, 14.8, 11.7. IR (thin film): ν_{max} 1603, 1465, 1266 cm^{-1}. MS (EI): *m/z* (%) 276 (M^+, 100), 261. HRMS: Calculated for $C_{13}H_{12}N_2OS_2$: 276.0391; Found: 276.0396.



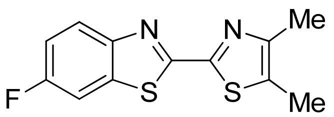
6,6'-Dimethoxy-2,2'-bibenzo[d]thiazole. Homocoupling compound of **1b** (9 mg, 20% yield) as a white solid was purified with silica gel chromatography (Petroleum ether / Dichloromethane = 2:1). ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.04 (d, *J* = 8.7 Hz, 2H), 7.43 (s, 2H), 7.16 (dd, *J* = 8.7 Hz, 2.4 Hz, 2H), 3.92 (s, 6H).



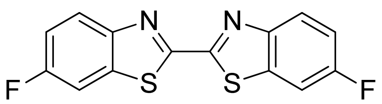
2-(4,5-Dimethylthiazol-2-yl)-6-methylbenzo[d]thiazole (3c). 3.0 equiv of thiazole was used. The product (52 mg, 67% yield) as a white solid was purified with silica gel chromatography (Petroleum ether / Dichloromethane = 2:1). M.P. 173 ^{o}C; ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.92 (d, *J* = 8.4 Hz, 1H), 7.68 (s, 1H), 7.28 (d, *J* = 8.4 Hz, 1H), 2.47 (s, 3H), 2.42 (s, 3H), 2.41 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 161.5, 157.3, 152.4, 151.1, 136.8, 136.0, 131.3, 128.8, 123.6, 122.3, 22.3, 15.6, 12.5. IR (thin film): ν_{max} 2916, 1557, 1449 cm^{-1}. MS (EI): *m/z* (%) 260 (M^+, 100), 86. HRMS: Calculated for $C_{13}H_{12}N_2S_2$: 260.0442; Found: 260.0448.



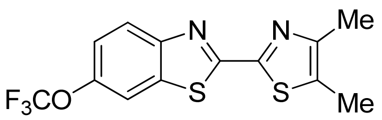
6,6'-Dimethyl-2,2'-bibenzo[d]thiazole. Homocoupling compound of **1c** (8 mg, 16% yield) as a white solid was purified with silica gel chromatography (Petroleum ether / Dichloromethane = 2:1). ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.05 (d, *J* = 8.7 Hz, 2H), 7.76 (s, 2H), 7.34 (d, *J* = 8.7 Hz, 2H), 2.52 (s, 6H).



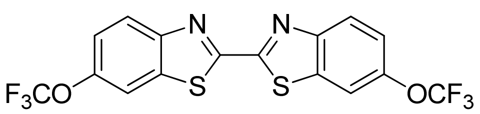
2-(4,5-Dimethylthiazol-2-yl)-6-fluorobenzo[d]thiazole (3d). 3.0 equiv of thiazole was used. The product (51 mg, 64% yield) as a white solid was purified with silica gel chromatography (Petroleum ether / Dichloromethane = 2:1). M.P. 194 ^{o}C; ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.98 (dd, *J* = 8.7 Hz, 4.8 Hz, 1H), 7.58 (dd, *J* = 8.4 Hz, 2.7 Hz, 1H), 7.22 (dd, *J* = 9.3 Hz, 2.7 Hz, 1H), 2.45 (s, 3H), 2.42 (s, 3H). ^{19}F NMR (282 MHz, $CDCl_3$) δ -115.1 (m, 1F). ^{13}C NMR (100 MHz, $CDCl_3$) δ 162.1, 161.6 (d, *J* = 3.0 Hz), 157.8 (d, *J* = 273.9 Hz), 150.7, 150.2, 136.3 (d, *J* = 11.1 Hz), 131.0, 124.4 (d, *J* = 9.7 Hz), 115.2 (d, *J* = 24.6 Hz), 108.0 (d, *J* = 26.8 Hz), 14.8, 11.8. IR (thin film): ν_{max} 2917, 1566, 1453 cm^{-1}. MS (EI): *m/z* (%) 264 (M^+, 100), 86, 71. HRMS: Calculated for $C_{12}H_9N_2FS_2$: 264.0191; Found: 264.0186.



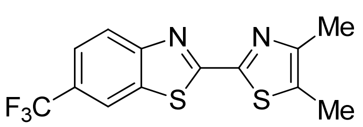
6,6'-Difluoro-2,2'-bibenzo[d]thiazole. Homocoupling compound of **1d** (5 mg, 12% yield) as a white solid was purified with silica gel chromatography (Petroleum ether / Dichloromethane = 2:1). ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.12 (dd, J = 9.0 Hz, 5.4 Hz, 2H), 7.64 (dd, J = 7.2 Hz, 2.4 Hz, 2H), 7.29 (td, J = 9.0 Hz, 2.7 Hz, 2H). ^{19}F NMR (282 MHz, $CDCl_3$) δ -116.3 (m, 2F).



2-(4,5-Dimethylthiazol-2-yl)-6-(trifluoromethoxy)benzo[d]thiazole (3e). 3.0 equiv of thiazole was used. The product (64 mg, 65% yield) as a white solid was purified with silica gel chromatography (Petroleum ether / Dichloromethane = 2:1). M.P. 172 ^{o}C; ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.03 (d, J = 9.0 Hz, 1H), 7.77 (s, 1H), 7.36 (d, J = 9.0 Hz, 1H), 2.46 (s, 3H), 2.43 (s, 3H). ^{19}F NMR (282 MHz, $CDCl_3$) δ -58.4 (s, 3F). ^{13}C NMR (100 MHz, $CDCl_3$) δ 163.0, 155.7, 152.0, 150.9, 146.9, 136.0, 131.5, 124.1, 120.5 (q, J = 256.8 Hz), 120.3, 114.3, 14.8, 11.8. IR (thin film): ν_{max} 1603, 1465, 1266 cm^{-1}. MS (EI): m/z (%) 330 (M^+, 100), 232, 71. HRMS: Calculated for $C_{13}H_9N_2OF_3S_2$: 330.0108; Found: 330.0107.

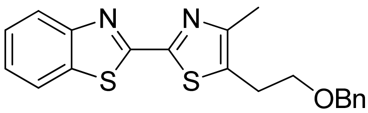


6,6'-Bis(trifluoromethoxy)-2,2'-bibenzo[d]thiazole. Homocoupling compound of **1e** (9 mg, 12% yield) as a white solid was purified with silica gel chromatography (Petroleum ether / Dichloromethane = 2:1). ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.15 (d, J = 9.0 Hz, 2H), 7.84 (d, J = 0.9 Hz, 2H), 7.28 (dd, J = 9.0 Hz, 0.9 Hz, 2H). ^{19}F NMR (282 MHz, $CDCl_3$) δ -58.5 (s, 6F).

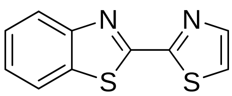


2-(4,5-Dimethylthiazol-2-yl)-6-(trifluoromethyl)benzo[d]thiazole (3f). 3.0 equiv of thiazole was used. The product (52 mg, 55% yield) as a white solid was purified with silica gel chromatography

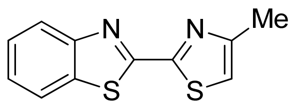
(Petroleum ether / Dichloromethane = 2:1). M.P. 181 °C; ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.21 (s, 1H), 8.12 (d, *J* = 7.8 Hz, 1H), 7.33 (d, *J* = 7.8 Hz, 1H), 2.47 (s, 3H), 2.44 (s, 3H). ^{19}F NMR (282 MHz, $CDCl_3$) δ -61.9 (s, 3F). ^{13}C NMR (100 MHz, $CDCl_3$) δ 164.8, 155.5, 151.2, 135.2, 132.1, 127.9, 127.6, 124.1 (q, *J* = 271.0 Hz), 123.6, 123.4 (q, *J* = 3.0 Hz), 119.5 (q, *J* = 3.7 Hz), 14.8, 11.8. IR (thin film): ν_{max} 1321, 1142, 1109 cm^{-1}. MS (EI): *m/z* (%) 314 (M^+), 232(100), 129. HRMS: Calculated for $C_{13}H_9N_2F_3S_2$: 314.0159; Found: 314.0160.



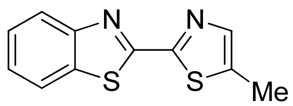
2-(5-(2-(Benzyloxy)ethyl)-4-methylthiazol-2-yl)benzo[d]thiazole (3g). 3.0 equiv of thiazole was used. The product (59 mg, 54% yield) as a white solid was purified with silica gel chromatography (Petroleum ether / Diethyl Ether = 15:1). M.P. 161 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.06 (d, *J* = 8.0 Hz, 1H), 7.90 (d, *J* = 8.0 Hz, 1H), 7.49 (t, *J* = 8.4 Hz, 1H), 7.40 (t, *J* = 8.4 Hz, 1H), 7.34-7.25 (m, 5H), 4.55 (s, 2H), 3.70 (t, *J* = 6.4 Hz, 2H), 3.09 (t, *J* = 6.0 Hz, 2H), 2.44 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 161.9, 157.5, 153.6, 150.9, 137.9, 135.2, 133.0, 128.4, 127.7, 127.6, 126.5, 125.8, 123.4, 121.8, 73.2, 69.8, 27.6, 15.2. IR (thin film): ν_{max} 2856, 1482, 1175 cm^{-1}. MS (EI): *m/z* (%) 366 (M^+), 245 (100), 91. HRMS: Calculated for $C_{20}H_{18}N_2OS_2$: 366.0861; Found: 366.0858. Homocoupling compound of **1a** (5 mg, 12% yield) as a white solid was purified with silica gel chromatography (Petroleum ether / Dichloromethane = 2:1).



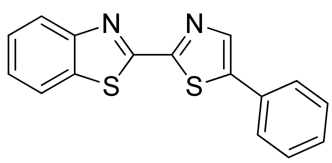
2-(Thiazol-2-yl)benzo[d]thiazole (3h). 3.0 equiv of thiazole was used. The product (34 mg, 52% yield) as a white solid was purified with silica gel chromatography (Petroleum ether / Dichloromethane = 2:1). This compound is known.[1] M.P. 138 °C; ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.11 (d, *J* = 8.1 Hz, 1H), 7.99 (d, *J* = 3.0 Hz, 1H), 7.96 (d, *J* = 7.8 Hz, 1H), 7.56 (d, *J* = 2.7 Hz, 1H), 7.54 (td, *J* = 7.8 Hz, 1.2 Hz, 1H), 7.46 (td, *J* = 7.5 Hz, 1.2 Hz, 1H). Homocoupling compound of **1a** (3 mg, 8% yield) as a white solid was purified with silica gel chromatography (Petroleum ether / Dichloromethane = 2:1).



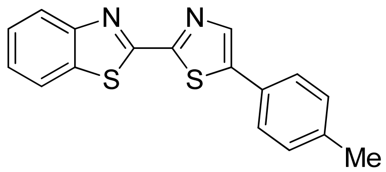
2-(4-Methylthiazol-2-yl)benzo[d]thiazole (3i). 3.0 equiv of thiazole was used. The product (51 mg, 73% yield) as a white solid was purified with silica gel chromatography (Petroleum ether / Dichloromethane = 2:1). This compound is known.[1] M.P. 136 °C; ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.08 (d, *J* = 8.1 Hz, 1H), 7.93 (d, *J* = 7.8 Hz, 1H), 7.52 (t, *J* = 7.8 Hz, 1H), 7.43 (t, *J* = 8.1 Hz, 1H), 7.10 (s, 1H), 2.55 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 161.5, 160.6, 154.8, 153.5, 126.6, 126.1, 123.6, 122.0, 121.9, 117.2, 17.2. IR (thin film): ν_{max} 1474, 1454, 1376 cm^{-1}. MS (EI): *m/z* (%) 232 (M^+, 100), 72. HRMS: Calculated for $C_{11}H_8N_2S_2$: 232.0129; Found: 232.0135. Homocoupling compound of **1a** (8 mg, 10% yield) as a white solid was purified with silica gel chromatography (Petroleum ether / Dichloromethane = 2:1).



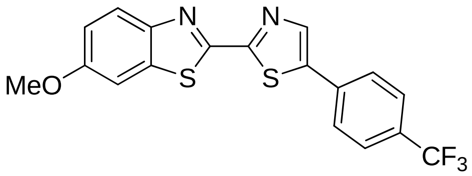
2-(5-Methylthiazol-2-yl)benzo[d]thiazole (3j). 3.0 equiv of thiazole was used. The product (49 mg, 70% yield) as a white solid was purified with silica gel chromatography (Petroleum ether / Dichloromethane = 2:1). M.P. 147 °C; ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.07 (d, *J* = 7.8 Hz, 1H), 7.93 (d, *J* = 7.8 Hz, 1H), 7.63 (s, 1H), 7.51 (t, *J* = 6.9 Hz, 1H), 7.40 (t, *J* = 6.9 Hz, 1H), 2.58 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 161.7, 159.8, 153.5, 142.3, 137.9, 135.2, 126.6, 126.0, 123.5, 121.9, 12.3. IR (thin film): ν_{max} 1455, 1415, 939 cm^{-1}. MS (EI): *m/z* (%) 232 (M^+, 100), 72. HRMS: Calculated for $C_{11}H_8N_2S_2$: 232.0129; Found: 232.0131. Homocoupling compound of **1a** (3 mg, 8% yield) as a white solid was purified with silica gel chromatography (Petroleum ether / Dichloromethane = 2:1).



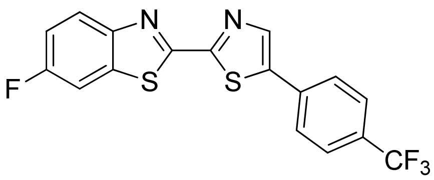
2-(5-Phenylthiazol-2-yl)benzo[d]thiazole (3k). 2.0 equiv of thiazole was used. The product (62 mg, 70% yield) as a yellow solid was purified with silica gel chromatography (Petroleum ether / Dichloromethane = 2:1). M.P. 177 °C; ^{1}H NMR (400 MHz, CD_2Cl_2) δ 8.21 (s, 1H), 8.04 (dd, *J* = 9.2 Hz, 4.8 Hz, 1H), 7.81-7.72 (m, 4H), 7.65 (dd, *J* = 8.4 Hz, 2.4 Hz, 1H), 7.30 (td, *J* = 9.2 Hz, 2.4 Hz, 1H). ^{19}F NMR (282 MHz, $CDCl_3$) δ -63.1 (s, 3F), -114.5 (m). ^{13}C NMR (100 MHz, $CDCl_3$) δ 161.4, 160.1, 153.5, 142.8, 139.8, 135.3, 130.7, 129.3, 129.1, 126.9, 126.7, 126.2, 123.6, 121.9. IR (thin film): ν_{max} 1606, 1455 cm^{-1}. MS (EI): *m/z* (%) 380 (M^+, 100), 202. HRMS: Calculated for $C_{17}H_8N_2F_4S_2$: 380.0069; Found: 380.0065. Homocoupling compound of **1a** (4 mg, 10% yield) as a white solid was purified with silica gel chromatography (Petroleum ether / Dichloromethane = 2:1).



2-(5-(*p*-Tolyl)thiazol-2-yl)benzo[d]thiazole (3l). 2.0 equiv of thiazole was used. The product (56 mg, 61% yield) as a yellow solid was purified with silica gel chromatography (Petroleum ether / Dichloromethane = 2:1). M.P. 150 °C; ^{1}H NMR (400 MHz, CD_2Cl_2) δ 8.21 (s, 1H), 8.04 (dd, *J* = 9.2 Hz, 4.8 Hz, 1H), 7.81-7.72 (m, 4H), 7.65 (dd, *J* = 8.4 Hz, 2.4 Hz, 1H), 7.30 (td, *J* = 9.2 Hz, 2.4 Hz, 1H). ^{19}F NMR (282 MHz, $CDCl_3$) δ -63.1 (s, 3F), -114.5 (m). ^{13}C NMR (100 MHz, $CDCl_3$) δ 161.4, 159.5, 153.5, 143.1, 139.3, 135.3, 130.0, 127.8, 126.8, 126.7, 126.1, 123.6, 121.9, 21.3. IR (thin film): ν_{max} 1606, 1455 cm^{-1}. MS (EI): *m/z* (%) 380 (M^+, 100), 202. HRMS: Calculated for $C_{17}H_8N_2F_4S_2$: 380.0069; Found: 380.0065. Homocoupling compound of **1a** (3 mg, 8% yield) as a white solid was purified with silica gel chromatography (Petroleum ether / Dichloromethane = 2:1).



6-methoxy-2-(5-(4-(trifluoromethyl)phenyl)thiazol-2-yl)benzo[d]thiazole (3m). 2.0 equiv of thiazole was used. The product (96 mg, 82% yield) as a yellow solid was purified with silica gel chromatography (Petroleum ether / Dichloromethane = 2:1). M.P. 160 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.14 (s, 1H), 7.98 (d, *J* = 8.8 Hz, 1H), 7.74-7.68 (m, 4H), 7.37 (d, *J* = 2.0 Hz, 1H), 7.14 (dd, *J* = 8.8 Hz, 2.0Hz, 1H), 3.91 (s, 3H). ^{19}F NMR (282 MHz, $CDCl_3$) δ -63.1 (s, 3F). ^{13}C NMR (100 MHz, $CDCl_3$) δ 161.5, 158.7, 158.3, 148.1, 140.6, 140.2, 137.1, 134.2, 130.6 (q, *J* = 33.2 Hz), 127.0, 126.3 (q, *J* = 3.7 Hz), 124.3, 123.8 (q, *J* = 270.7 Hz), 116.7, 103.9, 55.8. IR (thin film): ν_{max} 1615, 1464, 1326 cm^{-1}. MS (EI): *m/z* (%) 392 (M^+, 100), 377, 349. HRMS: Calculated for $C_{18}H_{11}N_2OF_3S_2$: 392.0262; Found: 392.0261. Homocoupling compound of **1b** (7 mg, 14% yield) as a white solid was purified with silica gel chromatography (Petroleum ether / Dichloromethane = 2:1).

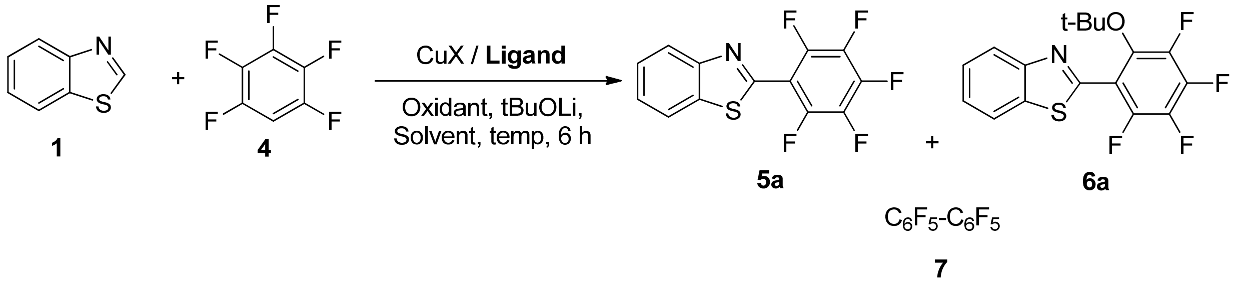


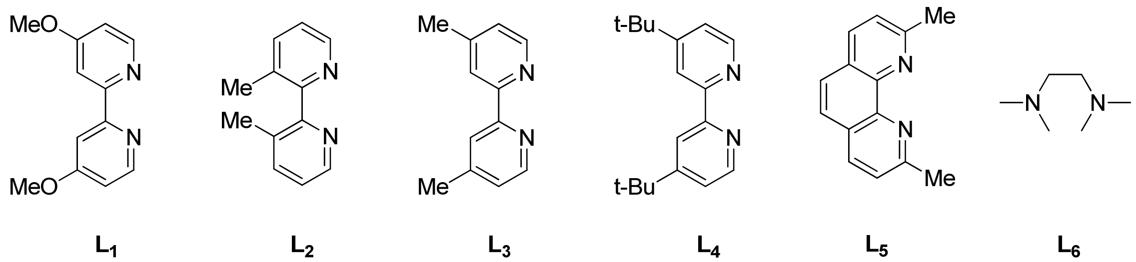
6-Fluoro-2-(5-(4-(trifluoromethyl)phenyl)thiazol-2-yl)benzo[d]thiazole (3n). 2.0 equiv of thiazole was used. The product (73 mg, 64% yield) as a yellow solid was purified with silica gel chromatography (Petroleum ether / Dichloromethane = 2:1). M.P. 168 ^{o}C; ^{1}H NMR (400 MHz, CD_2Cl_2) δ 8.21 (s, 1H), 8.04 (dd, *J* = 9.2 Hz, 4.8 Hz, 1H), 7.81-7.72 (m, 4H), 7.65 (dd, *J* = 8.4 Hz, 2.4 Hz, 1H), 7.30 (td, *J* = 9.2 Hz, 2.4 Hz, 1H). ^{19}F NMR (282 MHz, $CDCl_3$) δ -63.1 (s, 3F), -114.5 (m). ^{13}C NMR (100 MHz, $CDCl_3$) δ 161.1 (d, *J* = 246.0 Hz), 160.8, 150.3, 141.0, 140.8, 136.7, 134.2, 130.5 (q, *J* = 32.7 Hz), 127.1, 127.0, 126.2 (q, *J* = 3.5 Hz), 124.7 (d, *J* = 9.5 Hz), 123.9 (q, *J* = 270.9 Hz), 115.5 (q, *J* = 25.0Hz), 108.1 (q, *J* = 26.9 Hz). IR (thin film): ν_{max} 1606, 1455 cm^{-1}. MS (EI): *m/z* (%) 380 (M^+, 100), 202. HRMS: Calculated for $C_{17}H_8N_2F_4S_2$: 380.0069; Found: 380.0065. Homocoupling compound of **1d** (5 mg, 12% yield) as a white solid was purified with silica gel chromatography (Petroleum ether / Dichloromethane = 2:1).

Screens for Cu-Catalyzed Dehydrogenative Cross-Coupling of Benzothiazoles 1 with Pentafluorobenzene 4

In a glove box, to a 25 mL of dry sealed tube were added Cu-catalyst (10 mol%), ligand (10 mol%), oxidant (2.0 equiv), base (3.0 equiv), then remove the sealed tube out of glove box. Solvent (2.5 mL) benzothiazole **1** (2.0 euqiv) and pentafluorobenzene **4** (0.3 mmol, 1.0 equiv) were added subsequently under N_2. The sealed tube was screw capped and heated to 80 ^{o}C (oil bath). After stirring for 10 h, the reaction mixture was cooled to room temperature, filtered and concentrated. The residue was purified with silica gel chromatography (Petroleum ether / Dichloromethane = 2:1) to provide pure product.

Table S1. Screens for Cu-Catalyzed Dehydrogenative Cross-Coupling of Benzothiazoles 1 with Pentafluorobenzene 4[a]



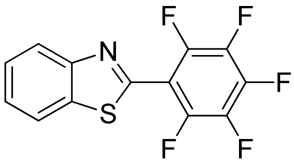


Entry	Cu (equiv)	ligand (equiv)	oxidant (equiv)	solvent	temp (^{o}C)	Yield[b] **5a/6a/7/1**
1	$Cu(OAc)_2$(0.3)	phen(0.3)	air	DCE (1.5mL)	60	nr
2	$Cu(OAc)_2$(0.3)	phen(0.3)	O_2	DCE (1.5mL)	60	nr
3	$Cu(OAc)_2$(0.3)	phen(0.3)	BPO(3.0)	DCE (1.5mL)	60	trace
4	$Cu(OAc)_2$(0.3)	phen(0.3)	tBuOOH(3.0)	DCE (1.5mL)	60	nr
5	$Cu(OAc)_2$(0.3)	phen(0.3)	tBuOOtBu(3.0)	DCE (1.5mL)	60	18/15/5/25
6	$Cu(OAc)_2$(0.3)	phen(0.3)	tBuOOtBu(3.0)	DMF (1.5mL)	60	nr
7	$Cu(OAc)_2$(0.3)	phen(0.3)	tBuOOtBu(3.0)	DMSO (1.5mL)	60	trace
8	$Cu(OAc)_2$(0.3)	phen(0.3)	tBuOOtBu(3.0)	Toluene (1.5mL)	60	trace
9	$Cu(OAc)_2$(0.3)	phen(0.3)	tBuOOtBu(3.0)	Dioxane (1.5mL)	60	trace
10	$Cu(OAc)_2$(0.3)	phen(0.3)	tBuOOtBu(3.0)	DME (1.5mL)	60	trace
11	$Cu(OAc)_2$(0.3)	phen(0.3)	tBuOOtBu(3.0)	Diglyme (1.5mL)	60	trace
12	$Cu(OAc)_2$(0.3)	phen(0.3)	tBuOOtBu(3.0)	DCE(2.5mL)	60	34/15/15/23
13	$Cu(OAc)_2$(0.3)	bpy(0.3)	tBuOOtBu(3.0)	DCE (2.5mL)	60	15/0/0/85
14	$Cu(OAc)_2$(0.3)	$\mathbf{L_1}$(0.3)	tBuOOtBu(3.0)	DCE(2.5mL)	60	55(42)/22/5/14
15	$Cu(OAc)_2$(0.3)	$\mathbf{L_2}$(0.3)	tBuOOtBu(3.0)	DCE(2.5mL)	60	41/15/17/10

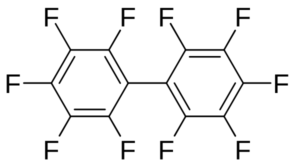
16	$Cu(OAc)_2$(0.3)	$\mathbf{L_3}$(0.3)	tBuOOtBu(3.0)	DCE(2.5mL)	60	54/10/5/27
17	$Cu(OAc)_2$(0.3)	$\mathbf{L_4}$(0.3)	tBuOOtBu(3.0)	DCE(2.5mL)	60	46/17/12/14
18	$Cu(OAc)_2$(0.3)	$\mathbf{L_5}$(0.3)	tBuOOtBu(3.0)	DCE(2.5mL)	60	0/0/0/100
19	$Cu(OAc)_2$(0.3)	$\mathbf{L_6}$(0.3)	tBuOOtBu(3.0)	DCE(2.5mL)	60	30/--/3/64
20	$Cu(acac)_2$(0.3)	$\mathbf{L_1}$(0.3)	tBuOOtBu(3.0)	DCE(2.5mL)	60	60/15/4/17
21	CuBr $_2$(0.3)	$\mathbf{L_1}$(0.3)	tBuOOtBu(3.0)	DCE(2.5mL)	60	37/6/5/48
22	CuCl (0.3)	$\mathbf{L_1}$(0.3)	tBuOOtBu(3.0)	DCE(2.5mL)	60	63/18/6/6
23	CuBr (0.3)	$\mathbf{L_1}$(0.3)	tBuOOtBu(3.0)	DCE(2.5mL)	60	48/10/4/33
24	CuI (0.3)	$\mathbf{L_1}$(0.3)	tBuOOtBu(3.0)	DCE(2.5mL)	60	0/0/0/93
25[c]	CuCl (0.2)	$\mathbf{L_1}$(0.2)	tBuOOtBu(3.0)	DCE(2.5mL)	60	63/0/3/31
26[c]	**CuCl (0.2)**	$\mathbf{L_1}$**(0.2)**	**tBuOOtBu(3.0)**	**DCE(2.5mL)**	**80**	**67(71)/6/7/15**
27[c]	CuCl (0.2)	$\mathbf{L_1}$(0.2)	tBuOOtBu(3.0)	DCE(2.5mL)	100	59/0/6/30
28[c]	CuCl (0.2)	$\mathbf{L_1}$(0.2)	tBuOOtBu(3.0)	DCE(2.5mL)	120	45/0/2/50
29[c]	----	$\mathbf{L_1}$(0.2)	tBuOOtBu(3.0)	DCE(2.5mL)	80	0/0/0/100
30[c]	CuCl (0.2)	----	tBuOOtBu(3.0)	DCE(2.5mL)	80	0/0/0/100
31[d]	CuCl (0.2)	$\mathbf{L_1}$(0.2)	tBuOOtBu(3.0)	DCE(2.5mL)	80	0/0/0/100

[a]Reaction conditions (unless otherwise specified): **1** (2.0 equiv), **4** (0.3 mmol, 1.0 equiv), tBuOLi (2.5 equiv), 6 h. [b]NMR yield determined by ^{19}F NMR using fluorobenzene as internal standard and number in parenthesis is isolated yield. [c]0.5 equiv of *t*BuOLi was used. [d]Reaction run in the absence of *t*BuOLi.

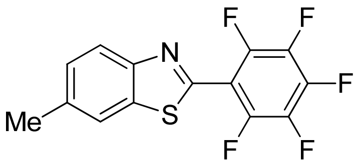
Typical Procedure for Copper-Catalyzed Dehydrogenative Cross-Coupling of Benzothiazoles with Pentafluorobenzene. In glove box, to a 25 mL of dry sealed tube were added CuCl (10 mol%), L_1 (10 mol%), tBuOOtBu (2.0 equiv), tBuOLi (3.0 equiv), then remove the sealed tube out of glove box. DCE (2.5 mL), benzothiazole **1** (2.0 euqiv) and pentafluorobenzene (0.3 mmol, 1.0 equiv) were added subsequently under N_2. The sealed tube was screw capped and heated to 80 ^{o}C (oil bath). After stirring for 10 h, the reaction mixture was cooled to room temperature, filtered and concentrated. The residue was purified with silica gel chromatography (Petroleum ether / Diethyl Ether = 250:1) to provide pure product (64 mg, 71% yield).



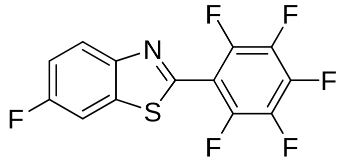
2-(Perfluorophenyl)benzo[d]thiazole (5a). 0.5 equiv of tBuOLi was used. The product (64 mg, 71% yield) as a white solid was purified with silica gel chromatography (Petroleum ether / Diethyl Ether = 250:1). This compound is known.[2] M.P. 125 ^{o}C; ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.20 (d, *J* = 7.8 Hz, 1H), 8.00 (d, *J* = 7.8 Hz, 1H), 7.59 (td, *J* = 8.1 Hz, 1.2 Hz, 1H), 7.51 (td, *J* = 8.4 Hz, 1.2 Hz, 1H). ^{19}F NMR (282 MHz, $CDCl_3$) δ -138.7 (m, 2F), -150.6 (t, *J* = 21.7 Hz, 1F), -161.0 (m, 2F).



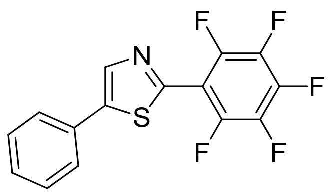
Perfluoro-1,1'-biphenyl. Homocoupling compound of **4** (9 mg, 18% yield) as a white solid was purified with silica gel chromatography (Petroleum ether / Diethyl Ether = 250:1). ^{19}F NMR (282 MHz, $CDCl_3$) δ -137.8 (dd, *J* = 21.7 Hz, 7.9 Hz, 4F), -150.1 (t, *J* = 19.7 Hz, 2F), -160.6 (m, 4F).



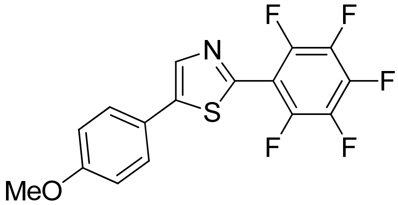
6-Methyl-2-(perfluorophenyl)benzo[d]thiazole (5b). 2.5 equiv of tBuOLi was used. The product (47 mg, 50% yield) as a white solid was purified with silica gel chromatography (Petroleum ether / Diethyl Ether = 250:1). M.P. 108 ^{o}C; ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.07 (d, *J* = 8.7 Hz, 1H), 7.77 (s, 1H), 7.39 (d, *J* = 8.7 Hz, 1H), 2.54 (s, 3H). ^{19}F NMR (282 MHz, $CDCl_3$) δ -138.3 (dm, *J* = 25.7 Hz, 2F), -150.9 (t, *J* = 21.7 Hz, 1F), -161.2 (m, 2F). ^{13}C NMR (100 MHz, $CDCl_3$) δ 151.0, 145.0 (dm, *J* = 258.1 Hz), 142.0 (dm, *J* = 257.1 Hz), 138.0 (dm, *J* = 244.9 Hz), 136.8, 135.8, 131.7, 128.4, 123.6, 121.0, 109.8 (m), 21.6. IR (thin film): ν_{max} 2923, 1652, 1554 cm^{-1}. MS (EI): *m/z* (%) 315 (M^+, 100), 121, 77. HRMS: Calculated for $C_{14}H_6NF_5S$: 315.0141; Found: 315.0143. Homocoupling compound of **4** (6 mg, 12% yield) as a white solid was purified with silica gel chromatography (Petroleum ether / Diethyl Ether = 250:1).



6-Fluoro-2-(perfluorophenyl)benzo[d]thiazole (5c). 0.5 equiv of tBuOLi was used. The product (52 mg, 55% yield) as a white solid was purified with silica gel chromatography (Petroleum ether / Diethyl Ether = 250:1). M.P. 82 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.14 (dd, *J* = 9.2 Hz, 5.2 Hz, 1H), 7.65 (dd, *J* = 7.6 Hz, 2.0 Hz, 1H), 7.32 (td, *J* = 9.2 Hz, 2.8 Hz, 1H). ^{19}F NMR (282 MHz, $CDCl_3$) δ -113.9 (m, 1F), -138.7 (dm, *J* = 17.8 Hz, 2F), -150.2 (t, *J* = 21.7 Hz, 1F), -160.8 (m, 2F). ^{13}C NMR (100 MHz, $CDCl_3$) δ 161.1 (d, *J* = 247.1 Hz), 152.3, 149.5, 144.9 (dm, *J* = 255.1 Hz), 142.2 (dm, *J* = 244.3 Hz), 138.0 (dm, *J* = 240.9 Hz), 136.5, 125.3 (d, *J* = 4.0 Hz), 115.7 (d, *J* = 24.9 Hz), 109.3 (m), 107.5 (d, *J* = 26.9 Hz). IR (thin film): ν_{max}1614, 1576, 1474 cm^{-1}. MS (EI): *m/z* (%) 319 (M^+, 100), 126, 69. HRMS: Calculated for $C_{13}H_3NF_6S$: 318.9891; Found: 318.9890. Homocoupling compound of **4** (8 mg, 16% yield) as a white solid was purified with silica gel chromatography (Petroleum ether / Diethyl Ether = 250:1).



2-(Perfluorophenyl)-5-phenylthiazole (5d). 1.5 equiv of tBuOLi was used. The product (54 mg, 55% yield) as a white solid was purified with silica gel chromatography (Petroleum ether / Diethyl Ether = 250:1). M.P. 140 °C; ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.19 (s, 1H), 7.62 (d, *J* = 7.2 Hz, 2H), 7.48-7.39 (m, 3H). ^{19}F NMR (282 MHz, $CDCl_3$) δ -139.4 (dm, *J* = 17.8 Hz, 2F), -152.2 (t, *J* = 21.7 Hz, 1F), -161.3 (m, 2F). ^{13}C NMR (100 MHz, $CDCl_3$) δ 151.0, 144.6 (dm, *J* = 254.0 Hz), 142.8, 141.5 (dm, *J* = 256.5 Hz), 139.2, 138.0 (dm, *J* = 252.9 Hz), 130.3, 129.3, 129.0, 127.0, 109.5 (m). IR (thin film): ν_{max} 2919, 1530, 1504 cm^{-1}. MS (EI): *m/z* (%) 327 (M^+), 134 (100), 90. HRMS: Calculated for $C_{15}H_6NF_5S$: 327.0141; Found: 327.0140. Homocoupling compound of **4** (7 mg, 14% yield) as a white solid was purified with silica gel chromatography (Petroleum ether / Diethyl Ether = 250:1).

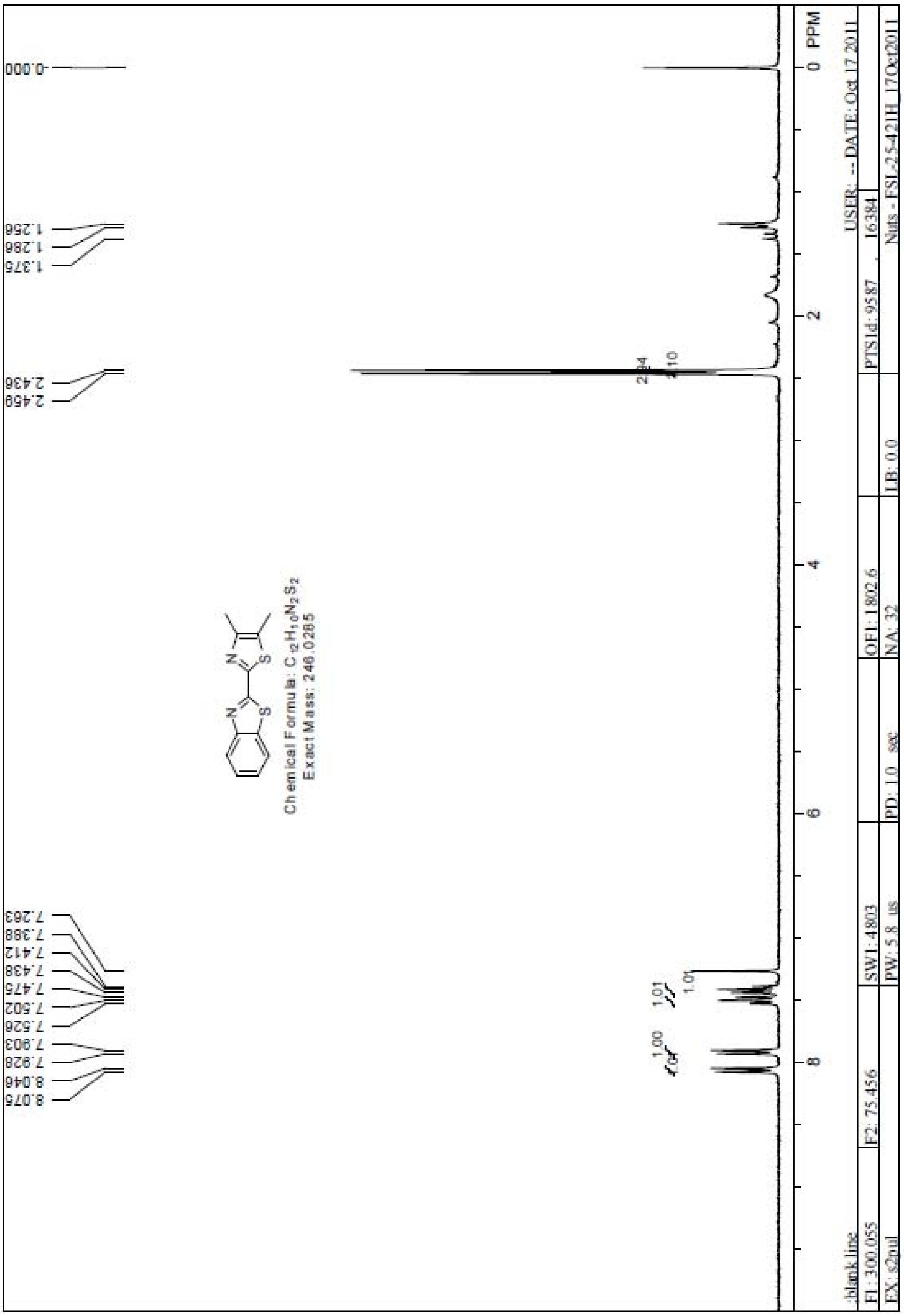


5-(4-Methoxyphenyl)-2-(perfluorophenyl)thiazole (5e). 1.5 equiv of tBuOLi was used. The product (43 mg, 41% yield) as a white solid was purified with silica gel chromatography (Petroleum ether / Diethyl Ether = 250:1). M.P. 145 ^{o}C; ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.09 (s, 1H), 7.55 (d, J = 9.0 Hz, 2H), 6.96 (d, J = 9.0 Hz, 2H), 3.86 (s, 3H). ^{19}F NMR (282 MHz, $CDCl_3$) δ -139.6 (d, J = 15.8 Hz, 2F), -152.5 (t, J = 21.7 Hz, 1F), -161.5 (m, 2F). ^{13}C NMR (100 MHz, $CDCl_3$) δ 160.3, 144.5 (dm, J = 257.0 Hz), 142.3, 141.4 (dm, J = 243.4 Hz), 138.2, 138.0 (dm, J = 252.7 Hz), 128.3, 122.8, 114.7, 109.6 (m), 55.4. IR (thin film): ν_{max} 2921, 1574, 1039 cm^{-1}. MS (EI): *m/z* (%) 357 (M^+), 149, 55 (100). HRMS: Calculated for $C_{16}H_8NOF_5S$: 357.0247; Found: 357.0244. Homocoupling compound of **4** (10 mg, 20% yield) as a white solid was purified with silica gel chromatography (Petroleum ether / Diethyl Ether = 250:1).

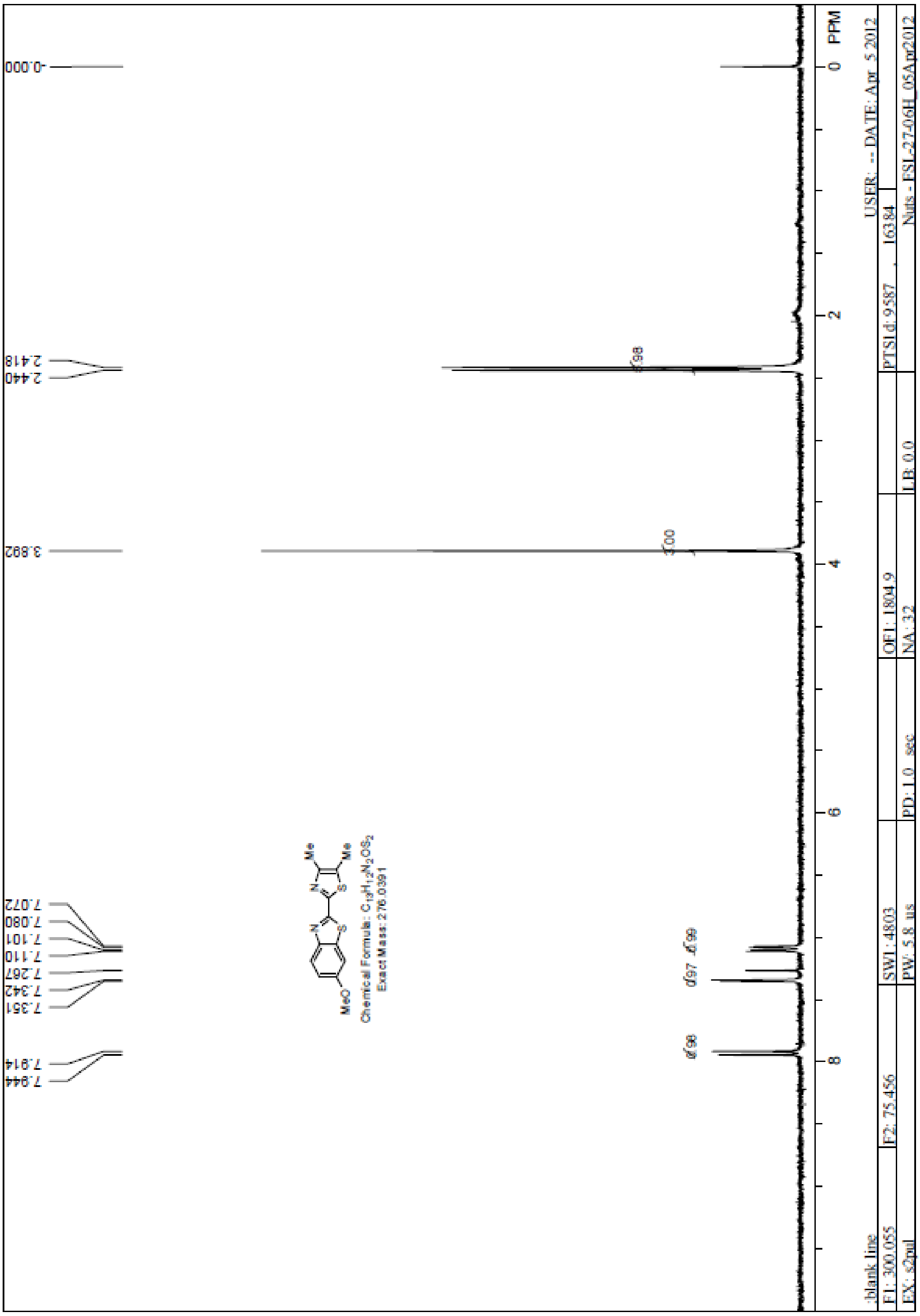
References:

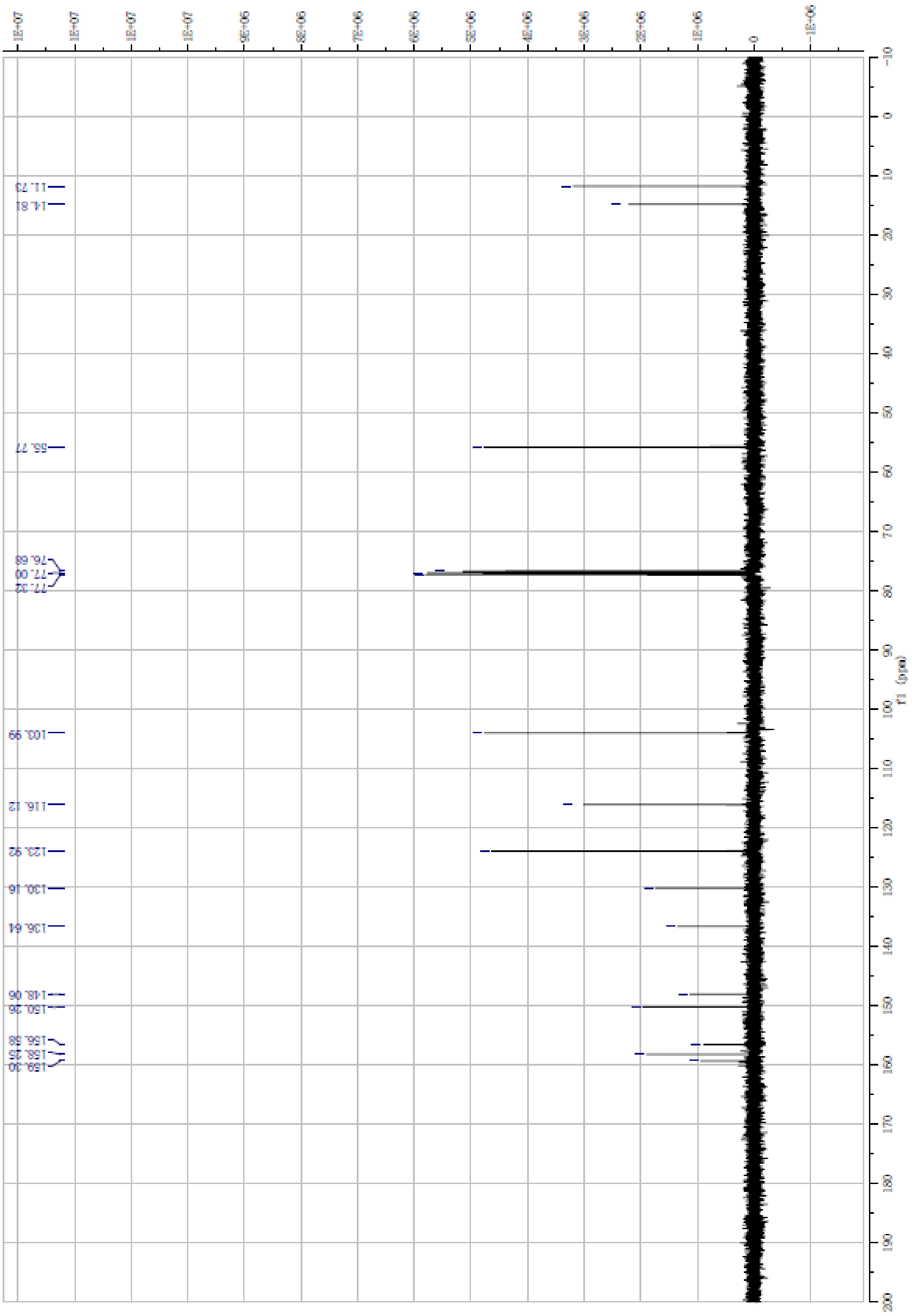
1) Han, W.; Mayer, P.; Ofial, A. R. *Angew. Chem. Int. Ed.* **2011**, *50*, 2178.
2) Xie, K.; Yang, Z.; Zhou, X.; Li, X.; Wang, S.; Tan, Z.; An, X.; Guo, C.-C. *Org. Lett.* **2010**, *12*, 1564.

2-(4,5-Dimethylthiazol-2-yl)benzo[d]thiazole (3a)



2-(4,5-Dimethylthiazol-2-yl)-6-methoxybenzo[d]thiazole (3b)

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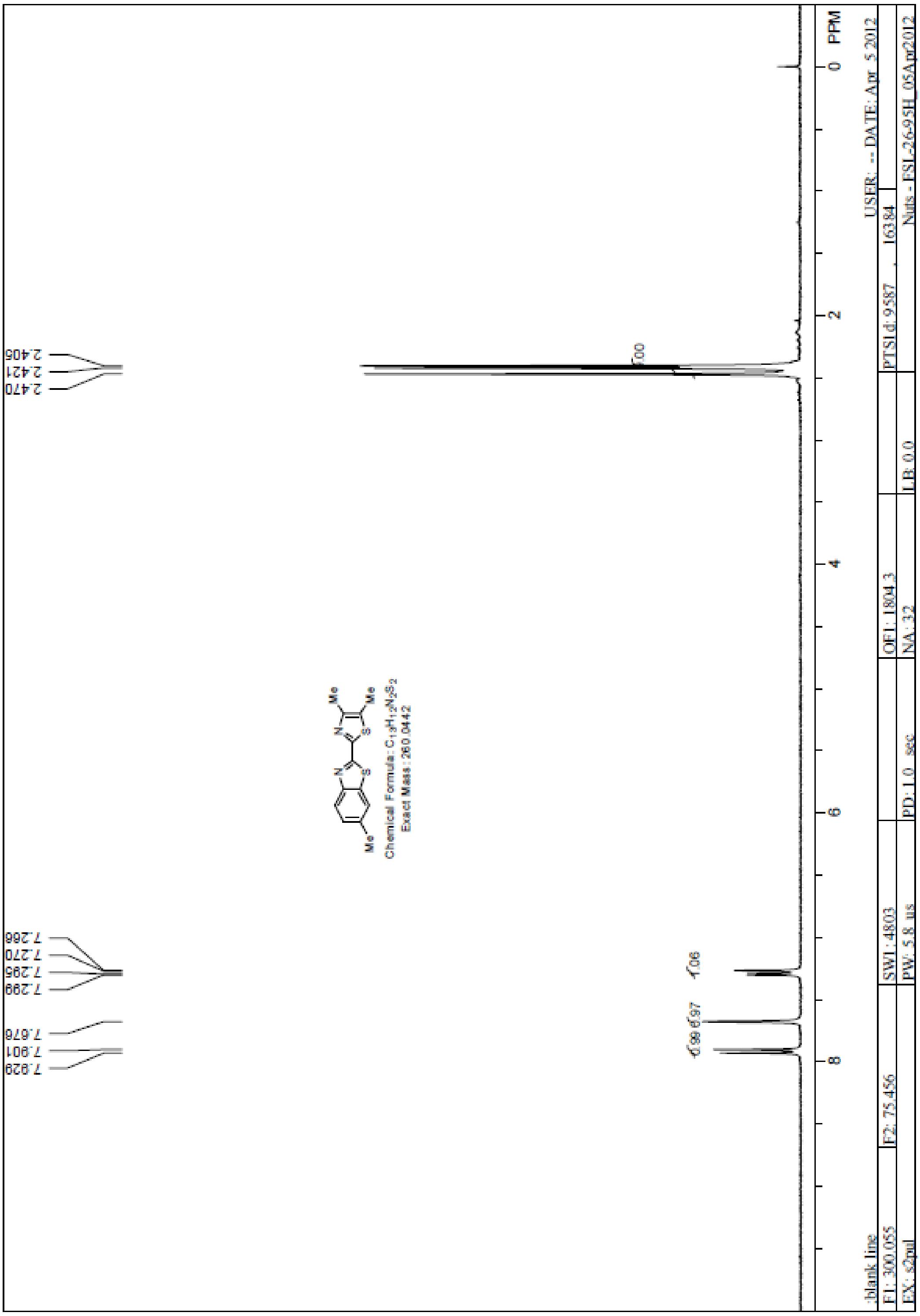
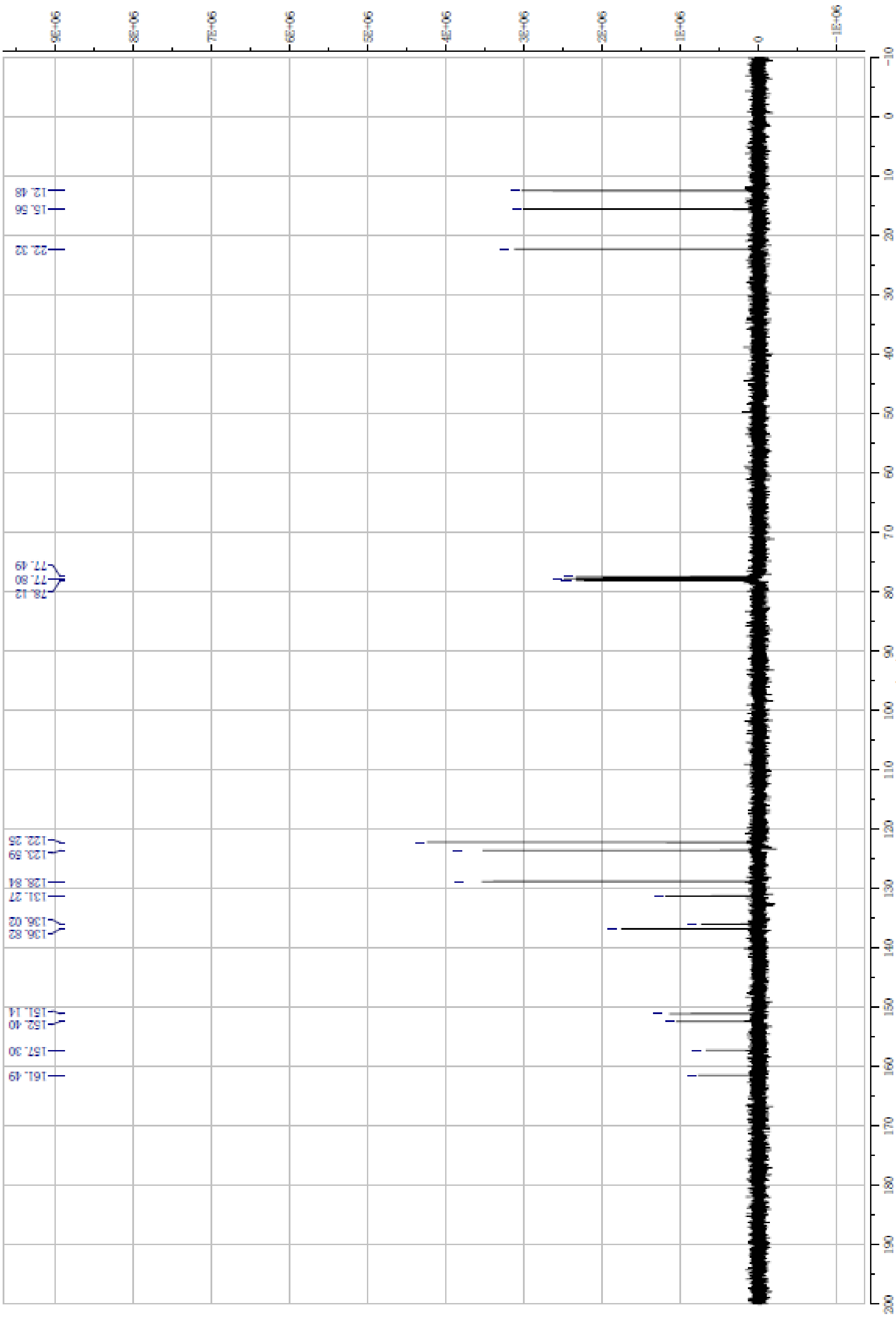
158.25
159.30
f1 (ppm)

2-(4,5-Dimethylthiazol-2-yl)-6-methylbenzo[d]thiazole (3c)





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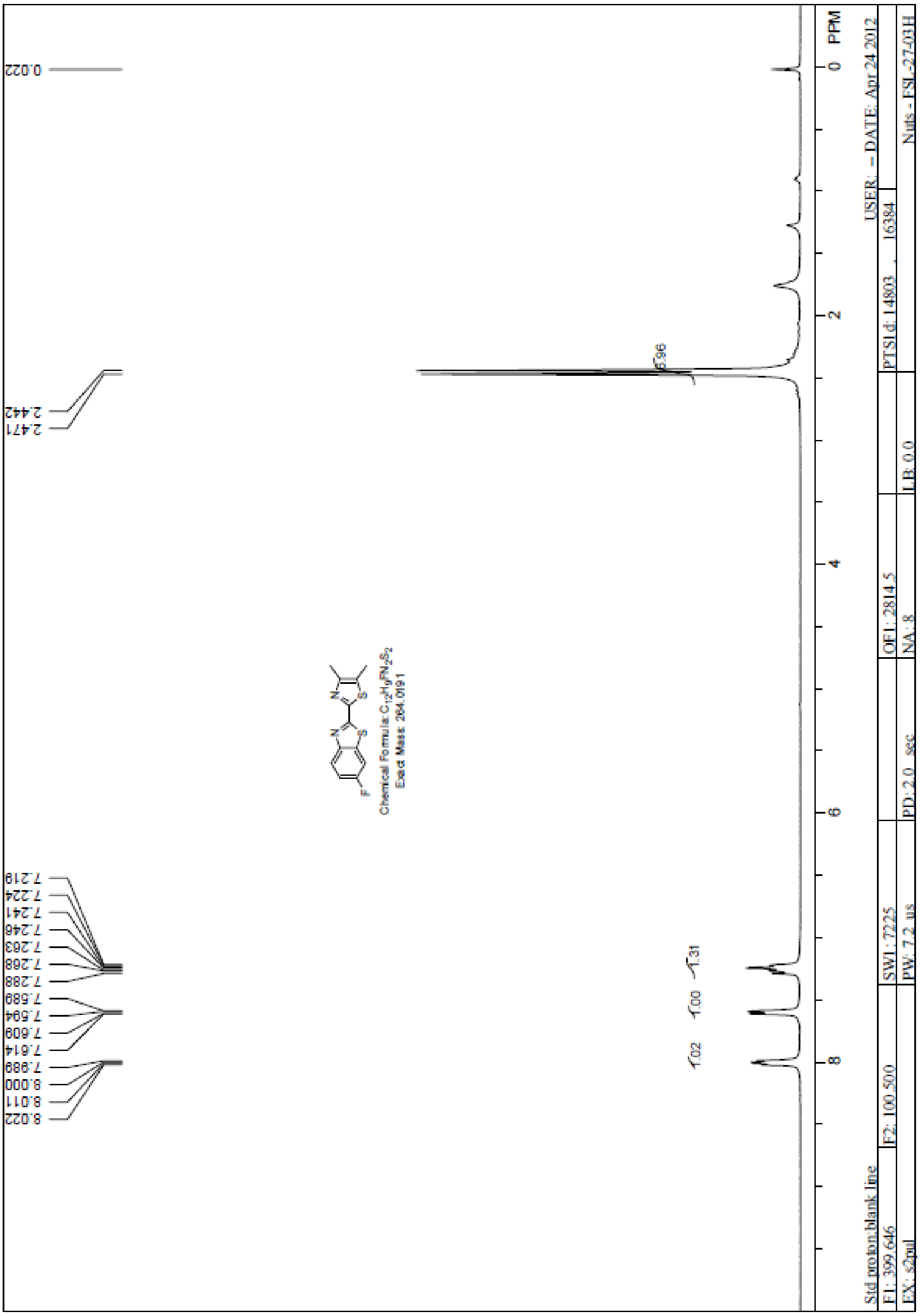
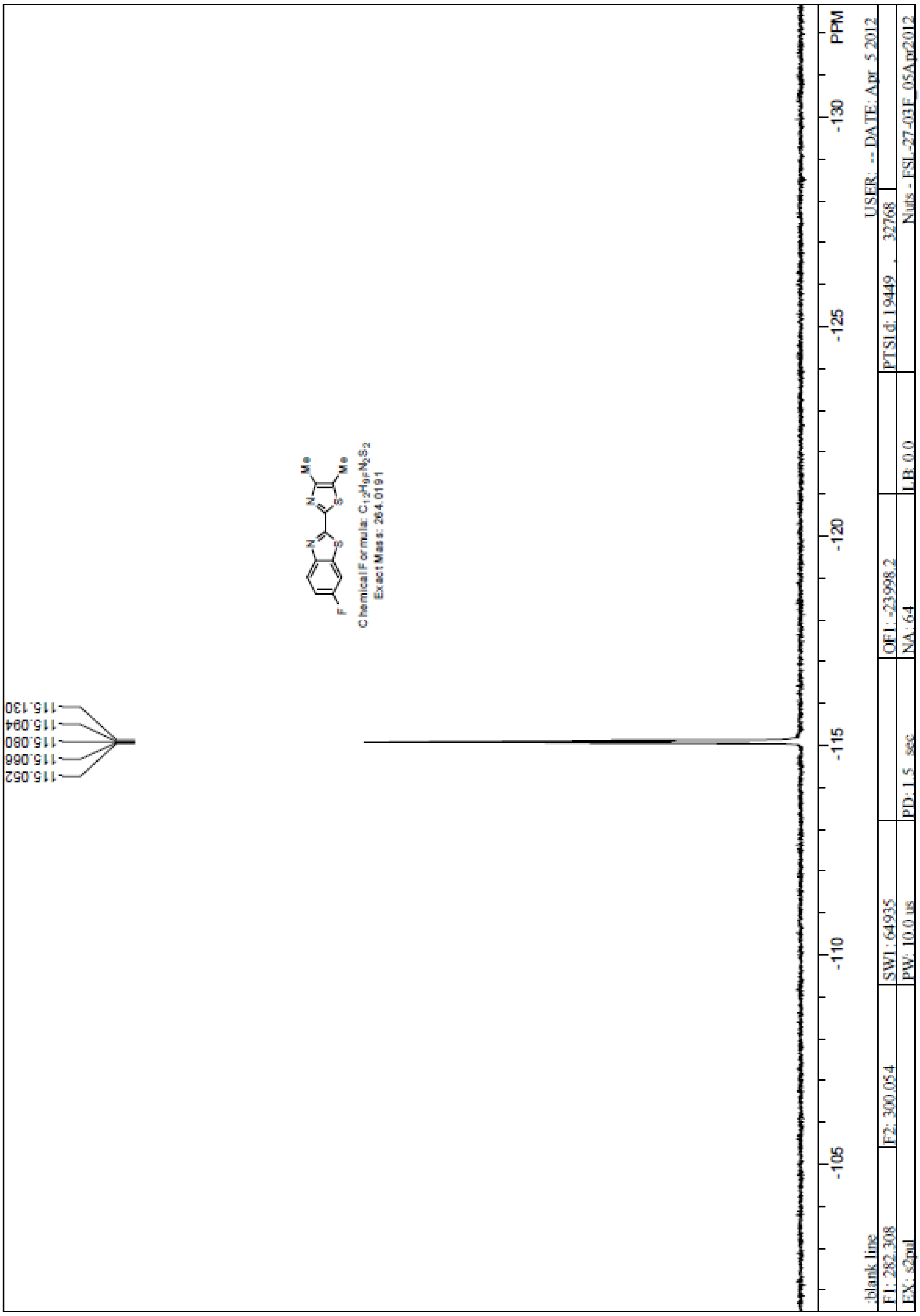
f1 (ppm)

2-(4,5-Dimethylthiazol-2-yl)-6-fluorobenzo[d]thiazole (3d)

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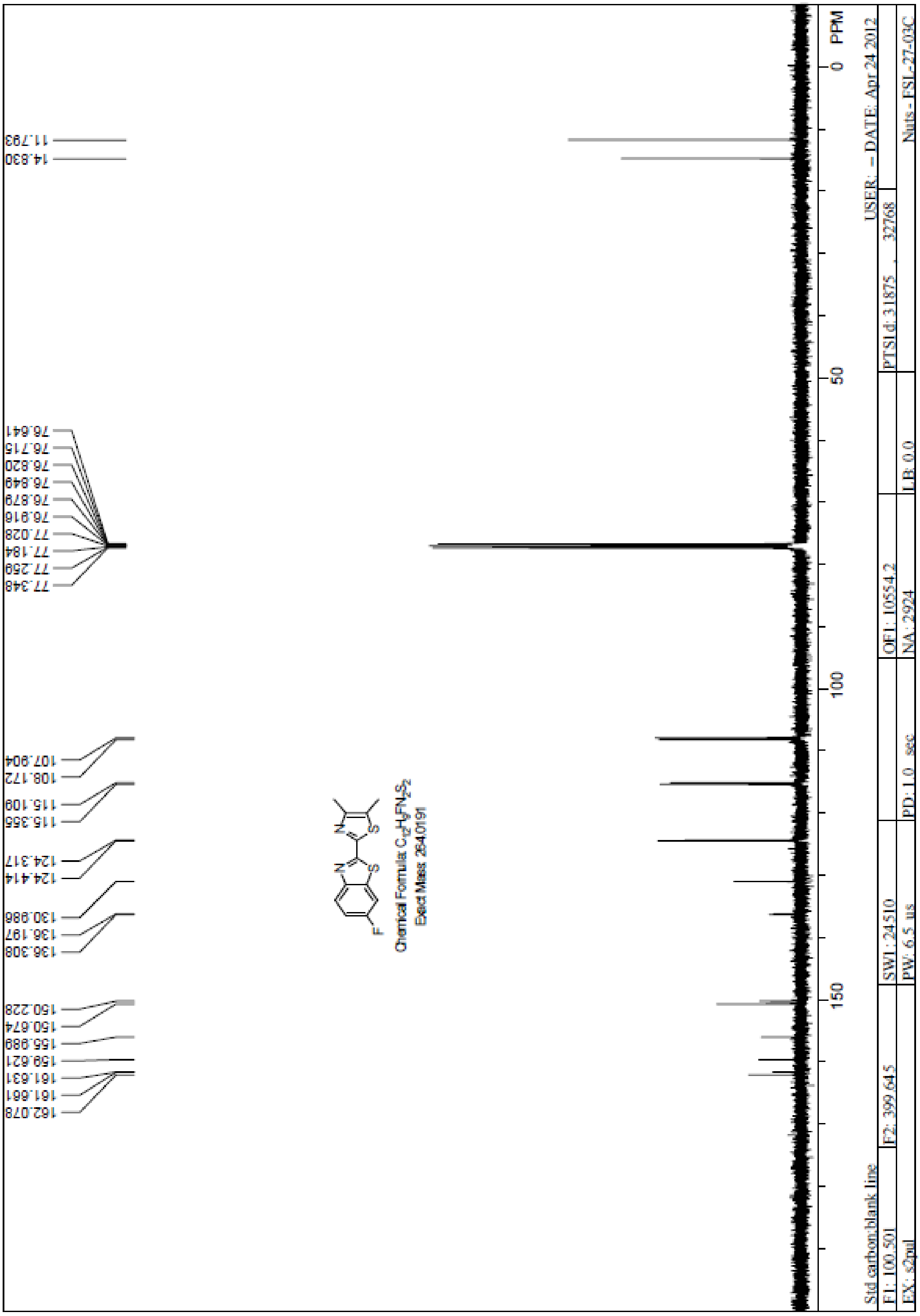
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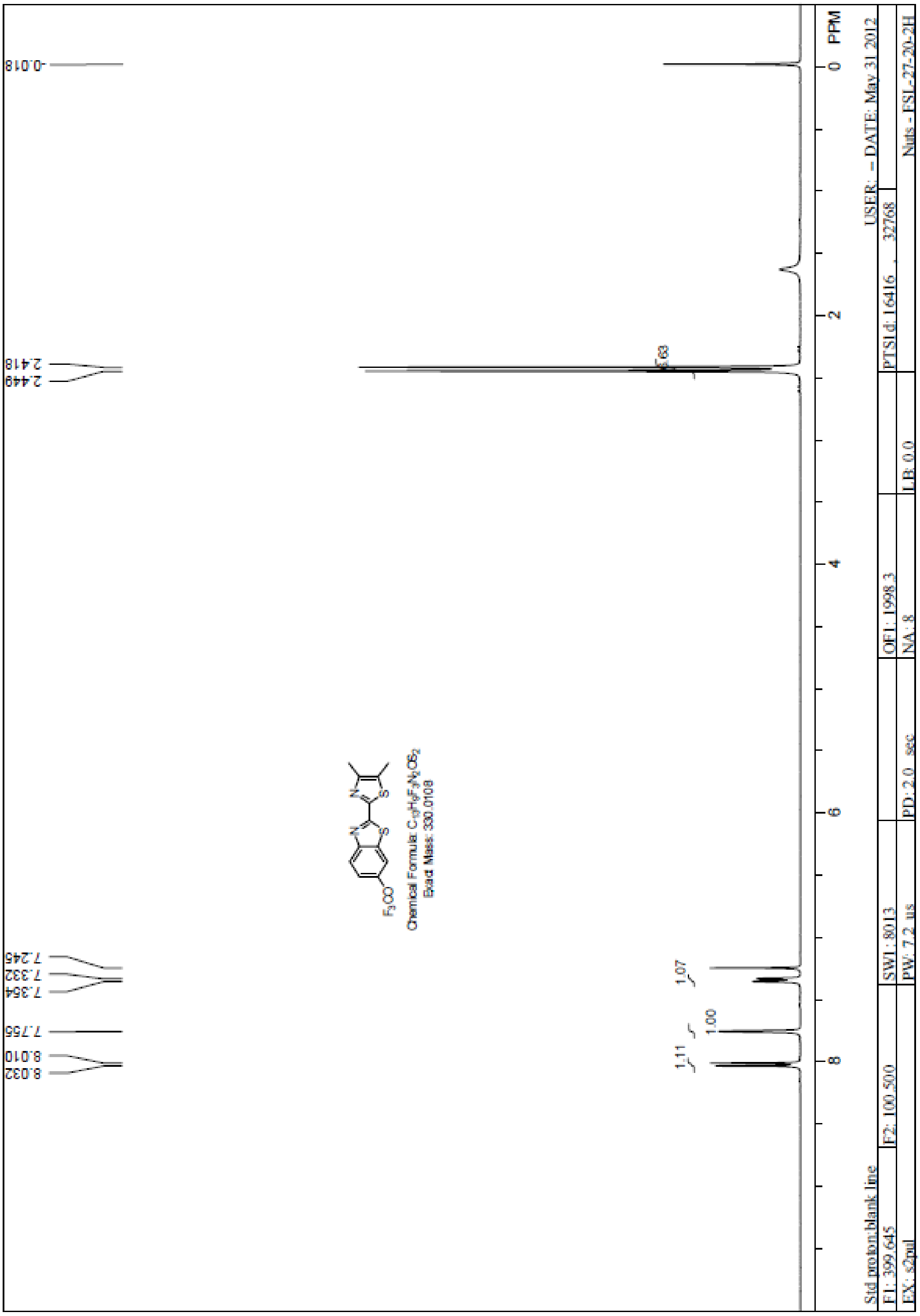
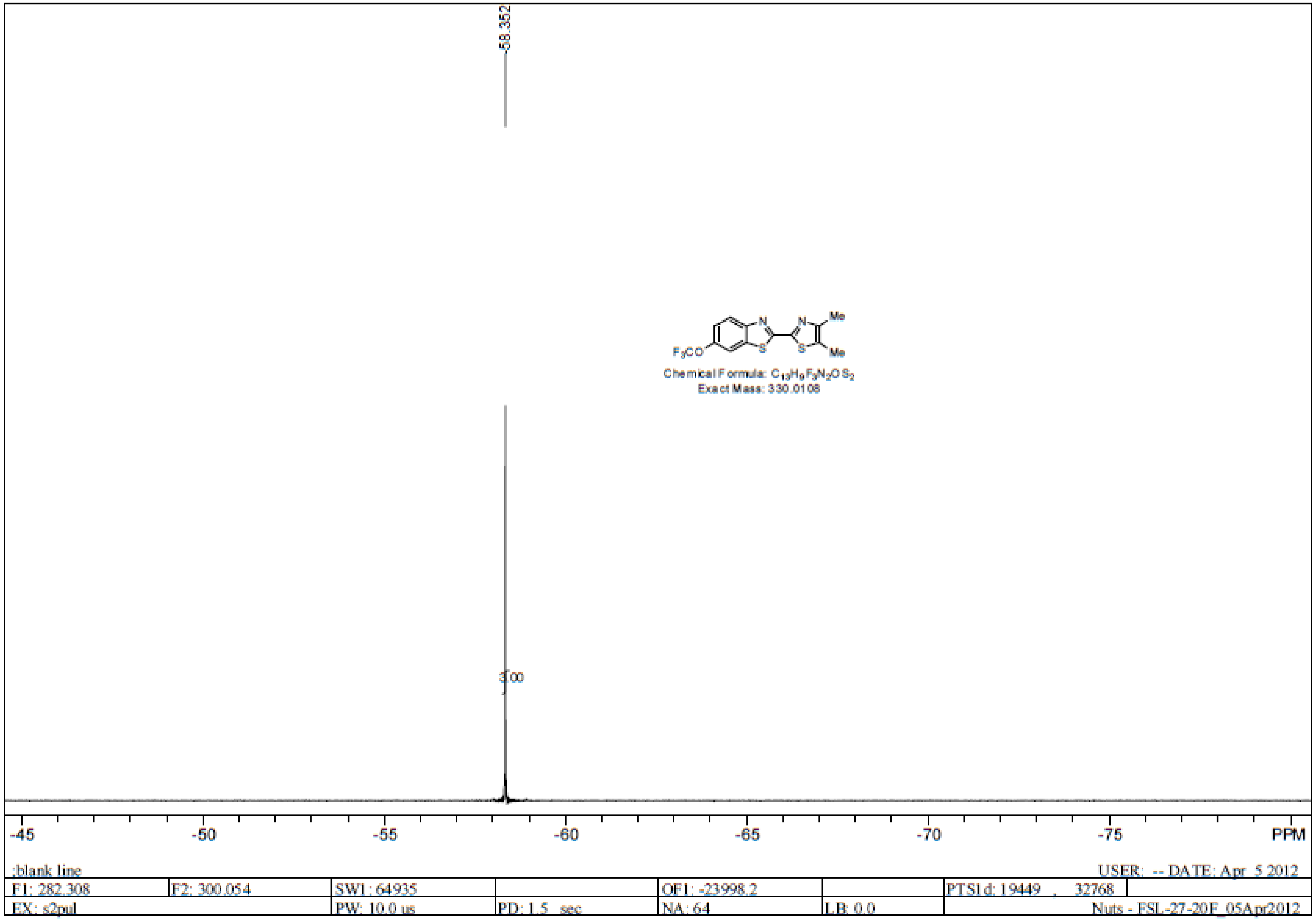
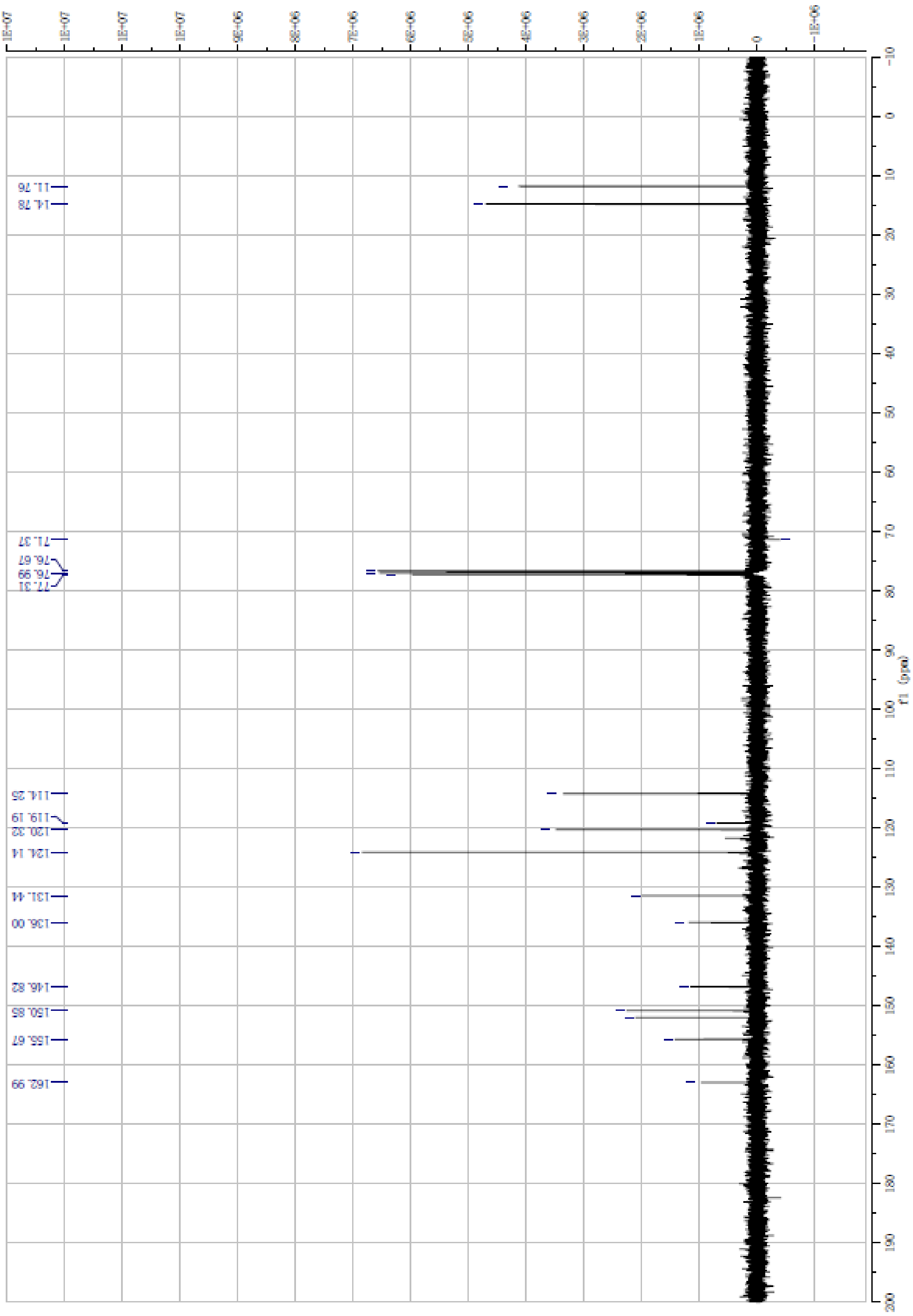
Nuts - FSI-27-03C

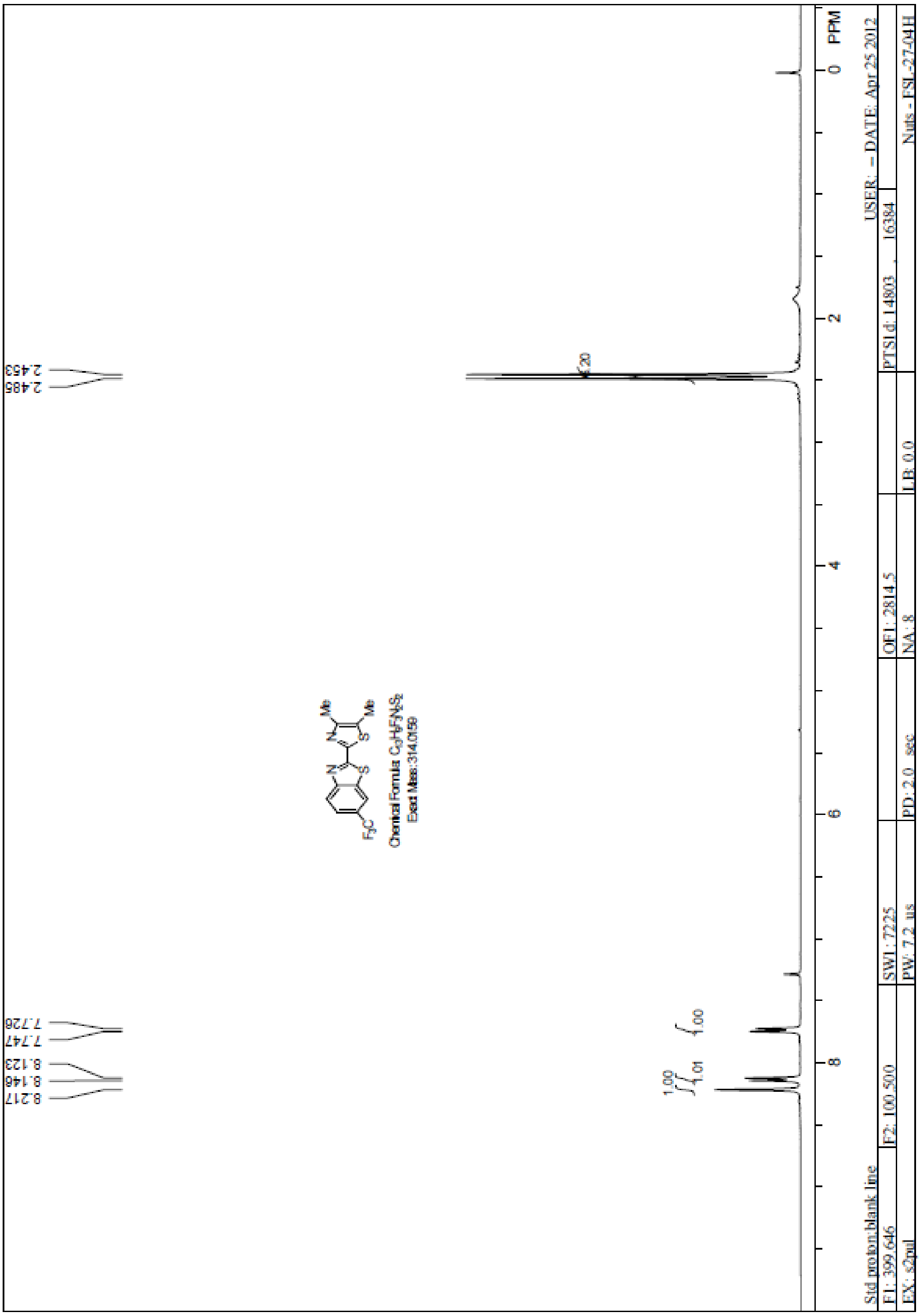
2-(4,5-Dimethylthiazol-2-yl)-6-(trifluoromethoxy)benzo[d]thiazole (3e)

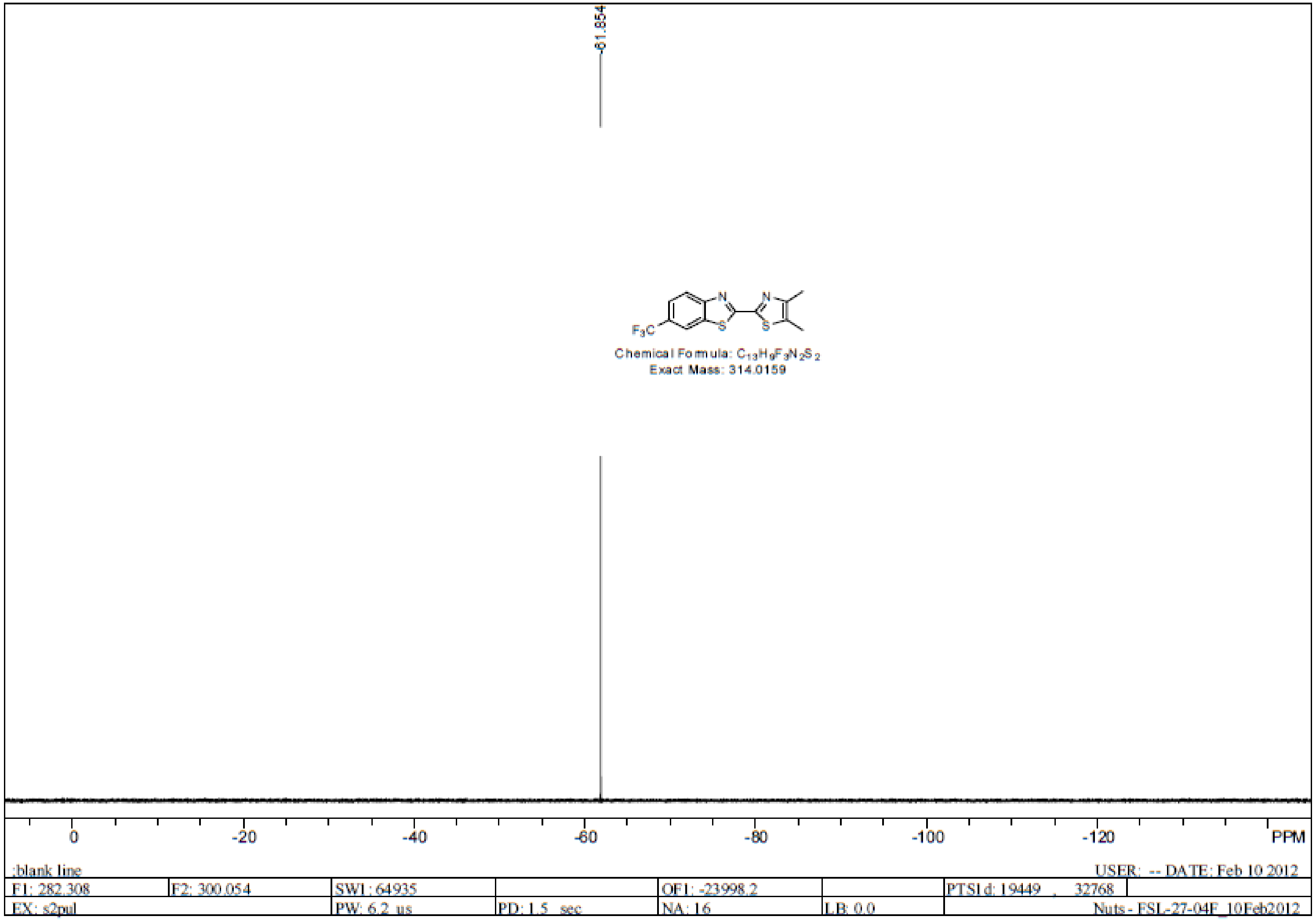



-58.352
3.00
F3CO
N
S
N
S
Me
Me
Chemical Formula: C13H9F3N2OS2
Exact Mass: 330.0108
-45
-50
-55
-60
-65
-70
-75
PPM
;blank line
USER: -- DATE: Apr 5 2012
F1: 282.308
F2: 300.054
SW1: 64935
OF1: -23998.2
PTS1d: 19449 , 32768
EX: s2pul
PW: 10.0 us
PD: 1.5 sec
NA: 64
LB: 0.0
Nuts - FSL-27-20F_05Apr2012

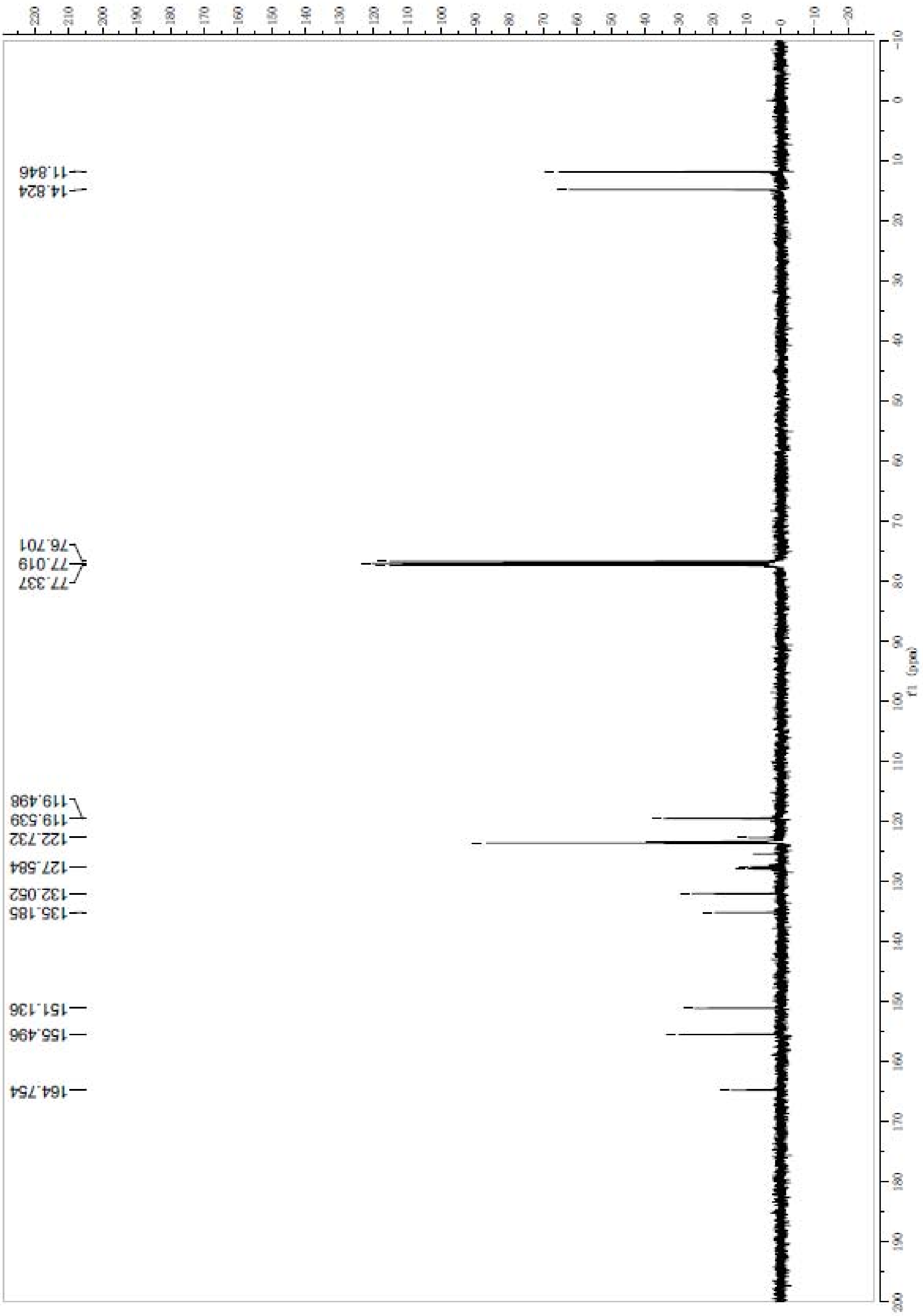

11.76
14.78
71.37
76.67
76.99
77.31
114.25
119.19
120.32
124.14
131.44
136.00
146.82
150.85
155.67
162.99
f1 (ppm)

2-(4,5-Dimethylthiazol-2-yl)-6-(trifluoromethyl)benzo[d]thiazole (3f)

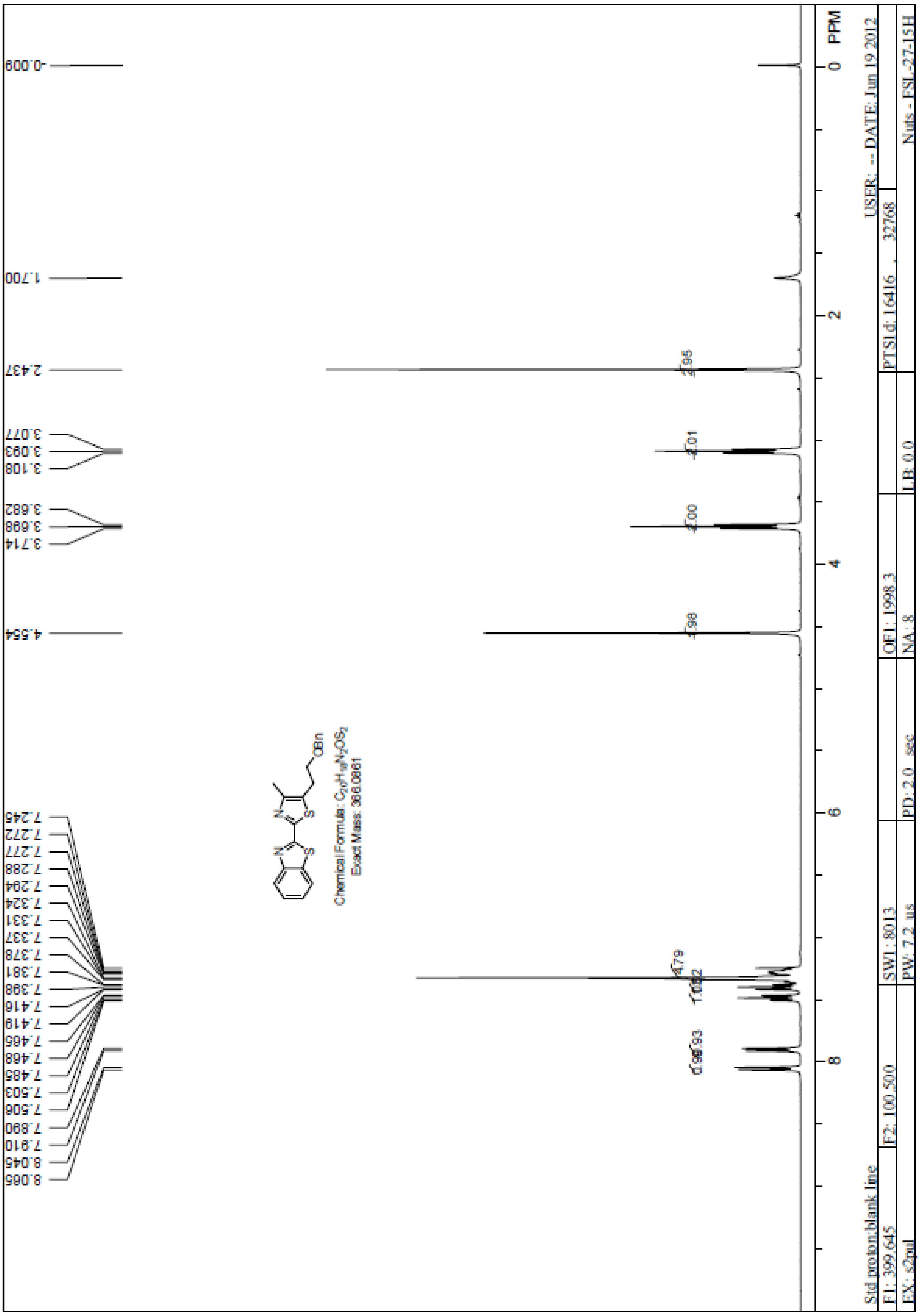


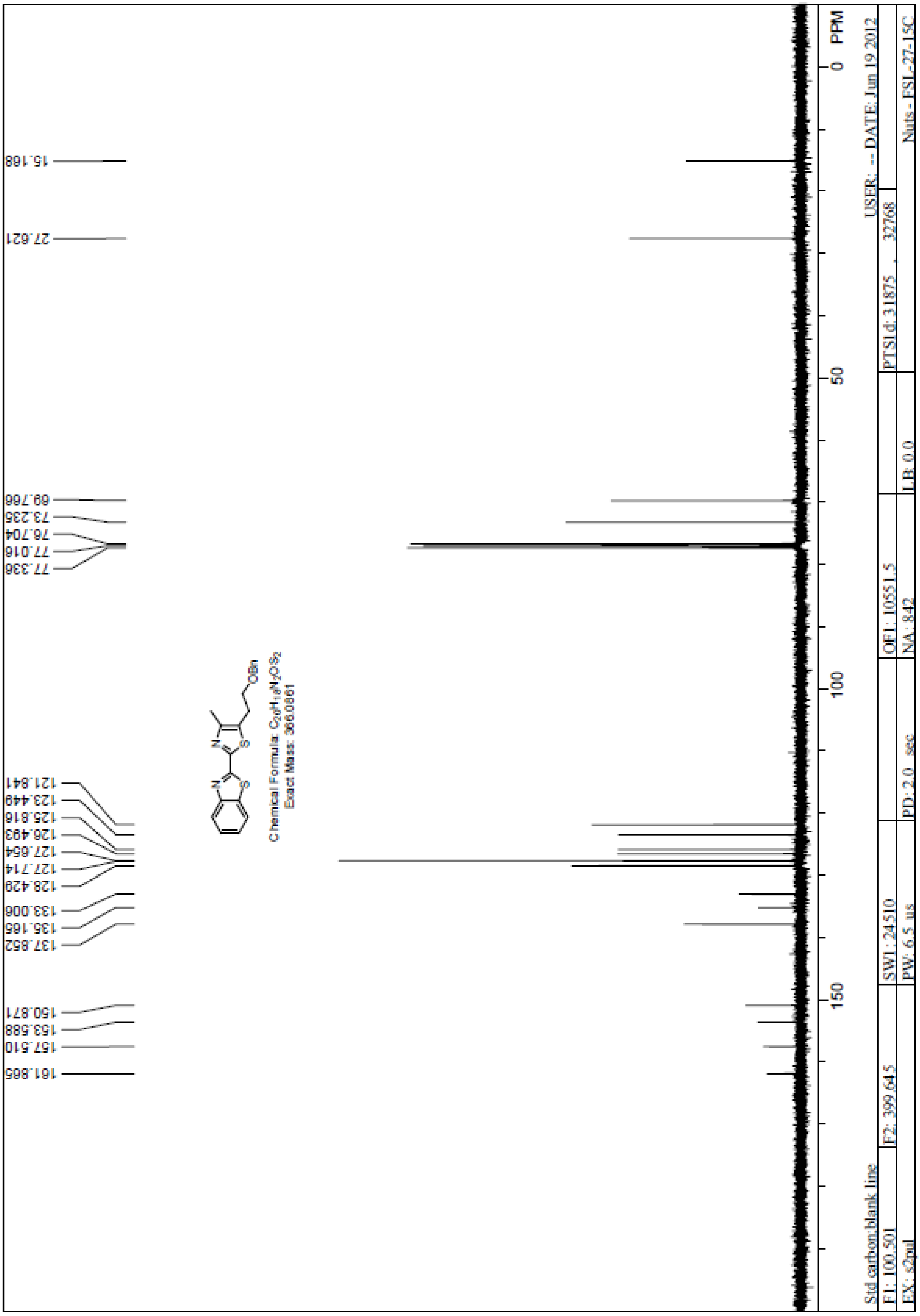


-61.854
F_3C
N
S
Chemical Formula: $C_{13}H_9F_3N_2S_2$
Exact Mass: 314.0159
0
-20
-40
-60
-80
-100
-120
PPM
;blank line
USER: -- DATE: Feb 10 2012
F1: 282.308
F2: 300.054
SW1: 64935
OF1: -23998.2
PTS1d: 19449 , 32768
EX: s2pul
PW: 6.2 us
PD: 1.5 sec
NA: 16
LB: 0.0
Nuts - FSL-27-04F_10Feb2012

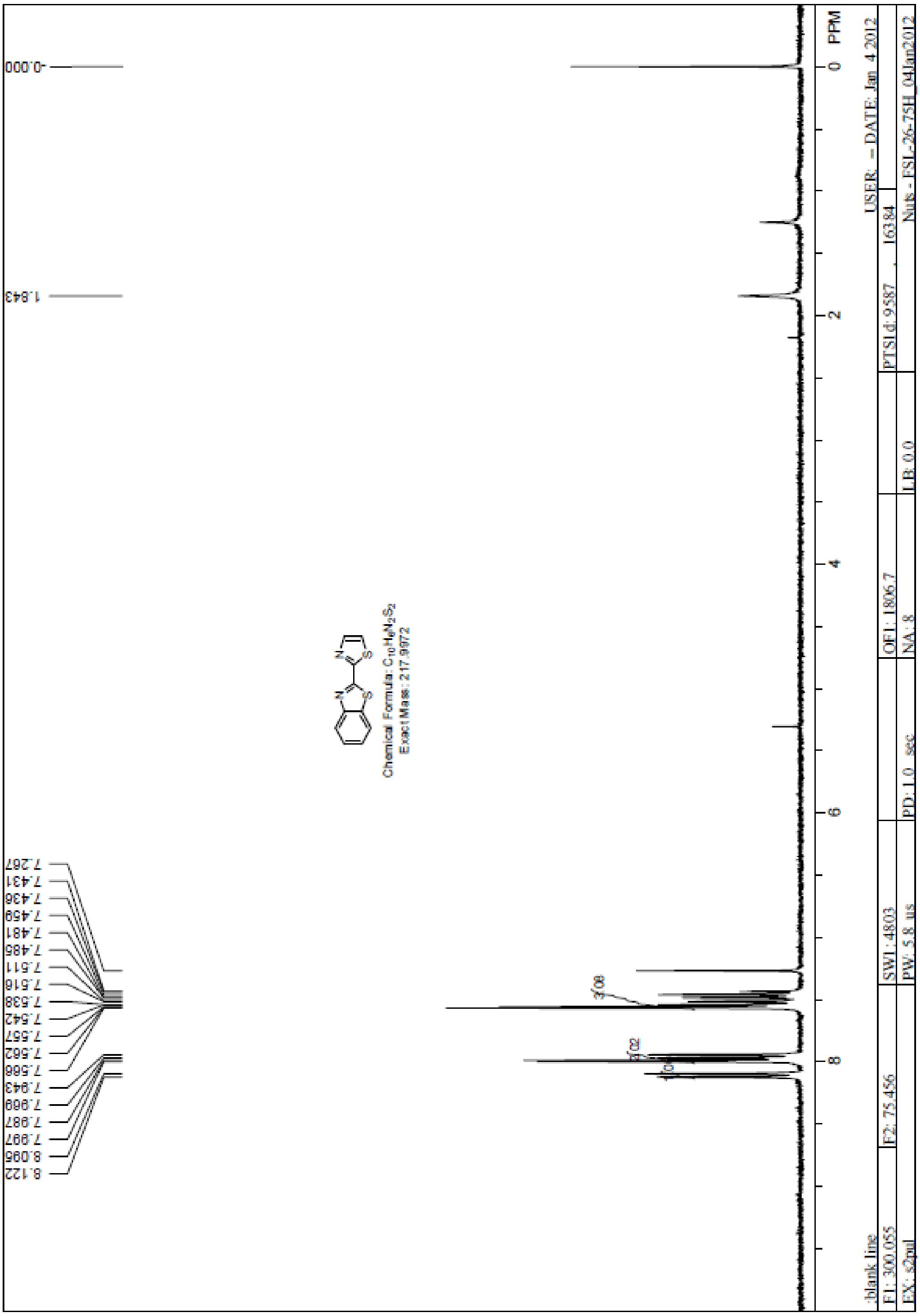

11.846
14.824
76.701
77.019
77.337
119.498
119.539
122.732
127.584
132.052
135.185
151.136
155.496
164.754
f1 (ppm)

2-(5-(2-(Benzyloxy)ethyl)-4-methylthiazol-2-yl)benzo[d]thiazole (3g)

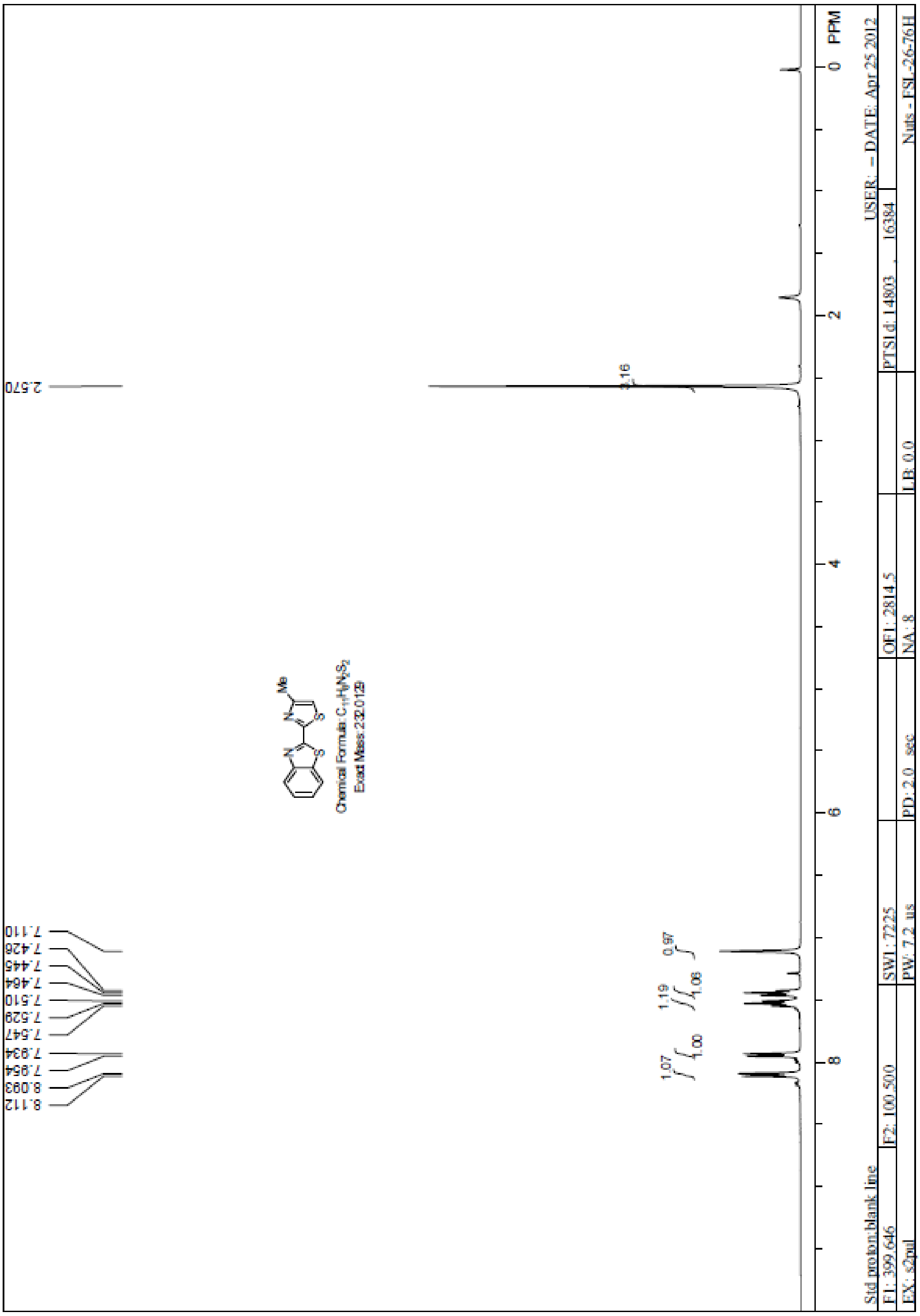


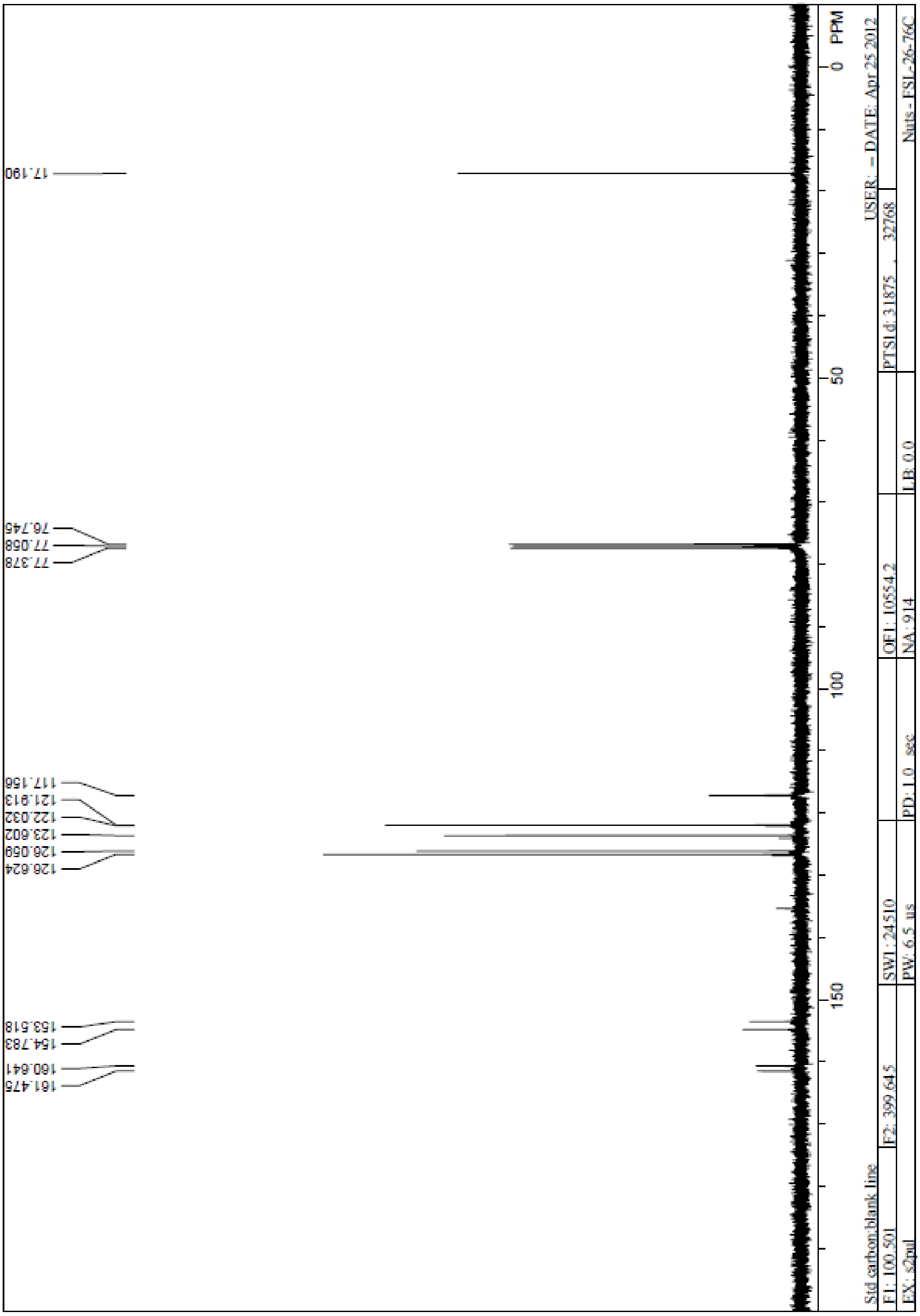

15.168
27.621
69.766
73.235
76.704
77.018
77.336
121.841
123.449
125.816
126.493
127.654
127.714
128.429
133.006
135.165
137.852
150.871
153.588
157.510
161.865
OBn
Chemical Formula: $C_{20}H_{18}N_2OS_2$
Exact Mass: 366.0861
0 PPM
50
100
150
Std carbon blank line
USER: -- DATE: Jun 19 2012
F1: 100.501
F2: 399.645
SW1: 24510
OF1: 10551.5
PTS1d: 31875 , 32768
EX: s2pul
PW: 6.5 us
PD: 2.0 sec
NA: 842
LB: 0.0
Nuts - FSL-27-15C

2-(Thiazol-2-yl)benzo[d]thiazole (3h)

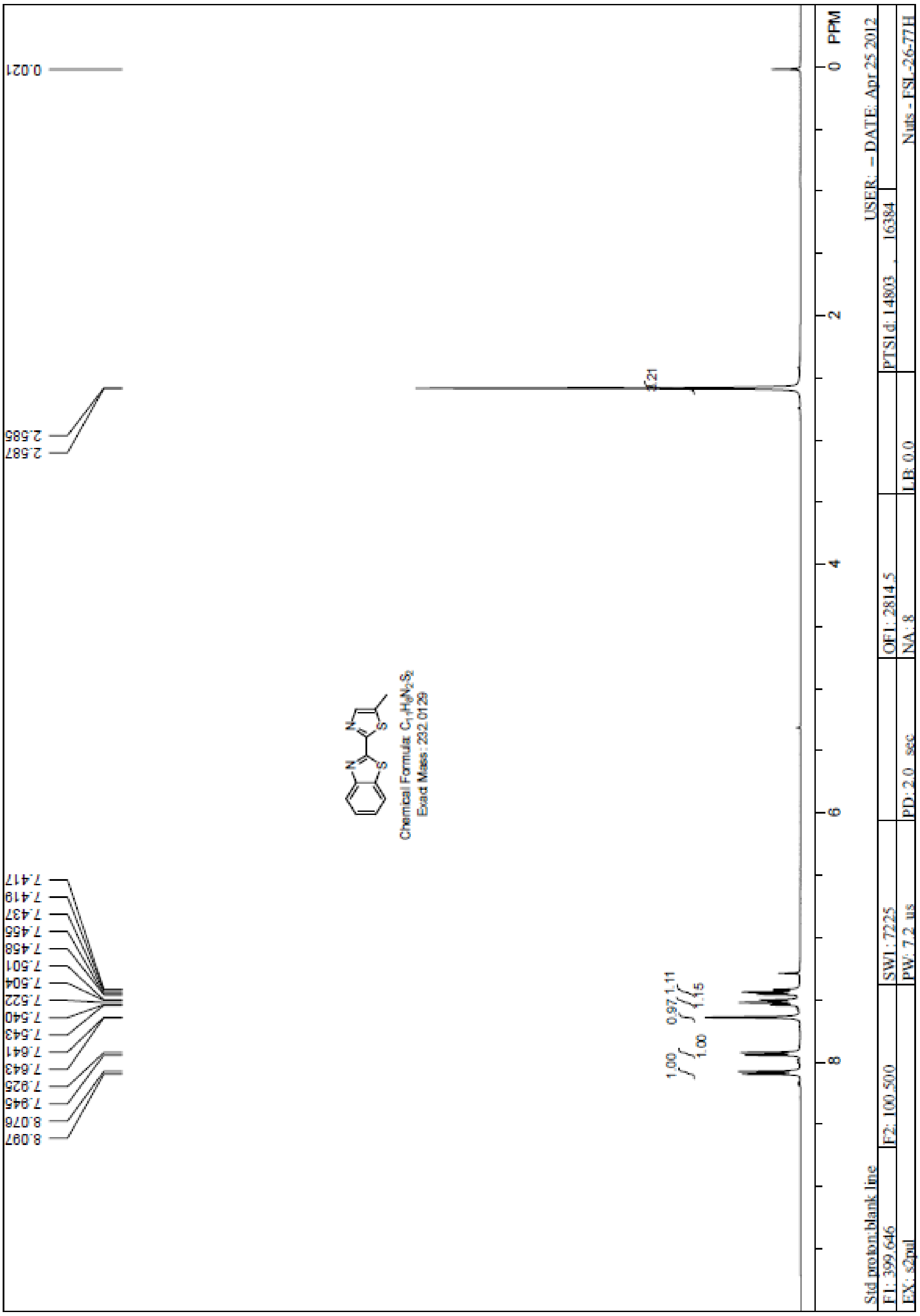


2-(4-Methylthiazol-2-yl)benzo[d]thiazole (3i)

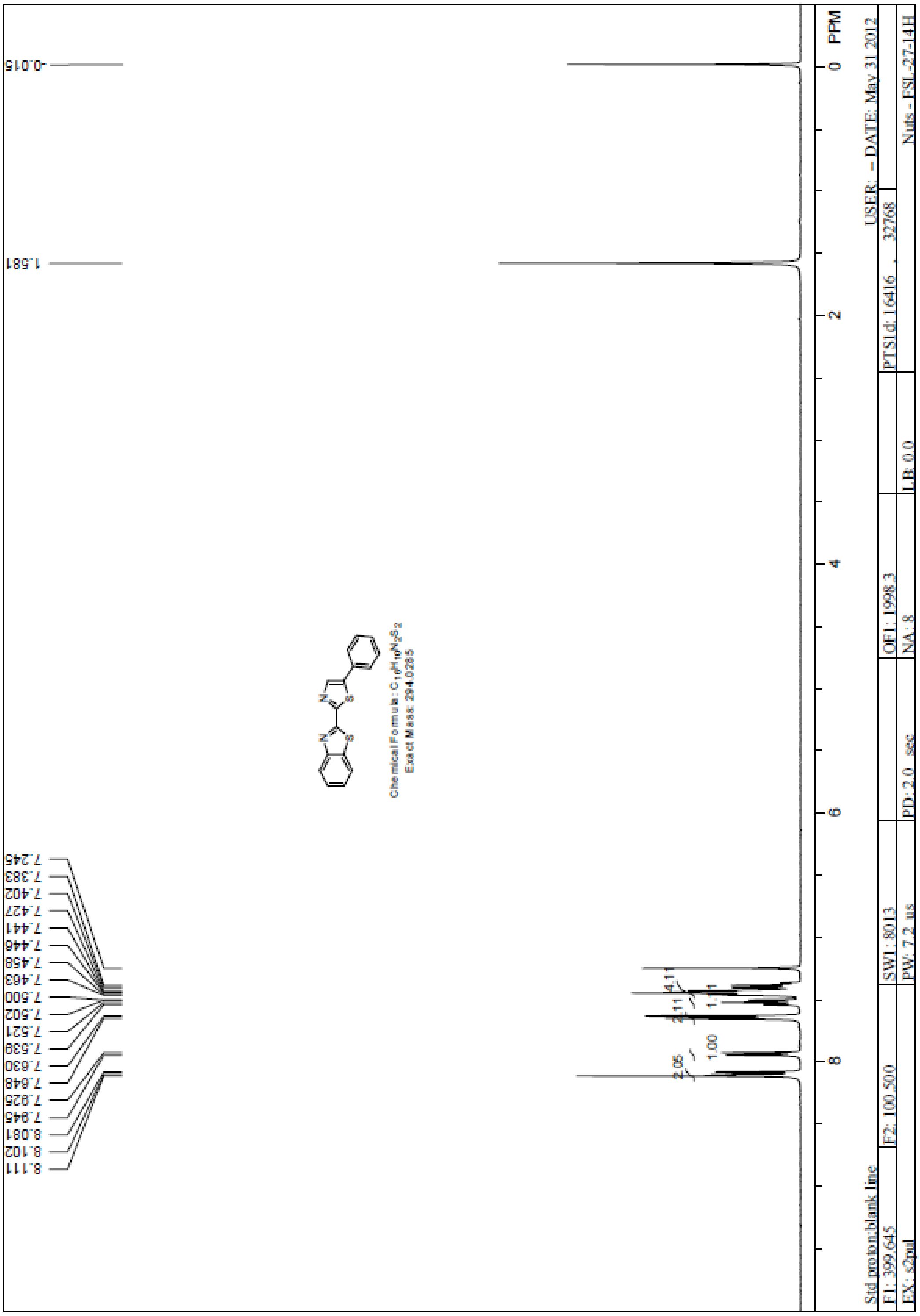


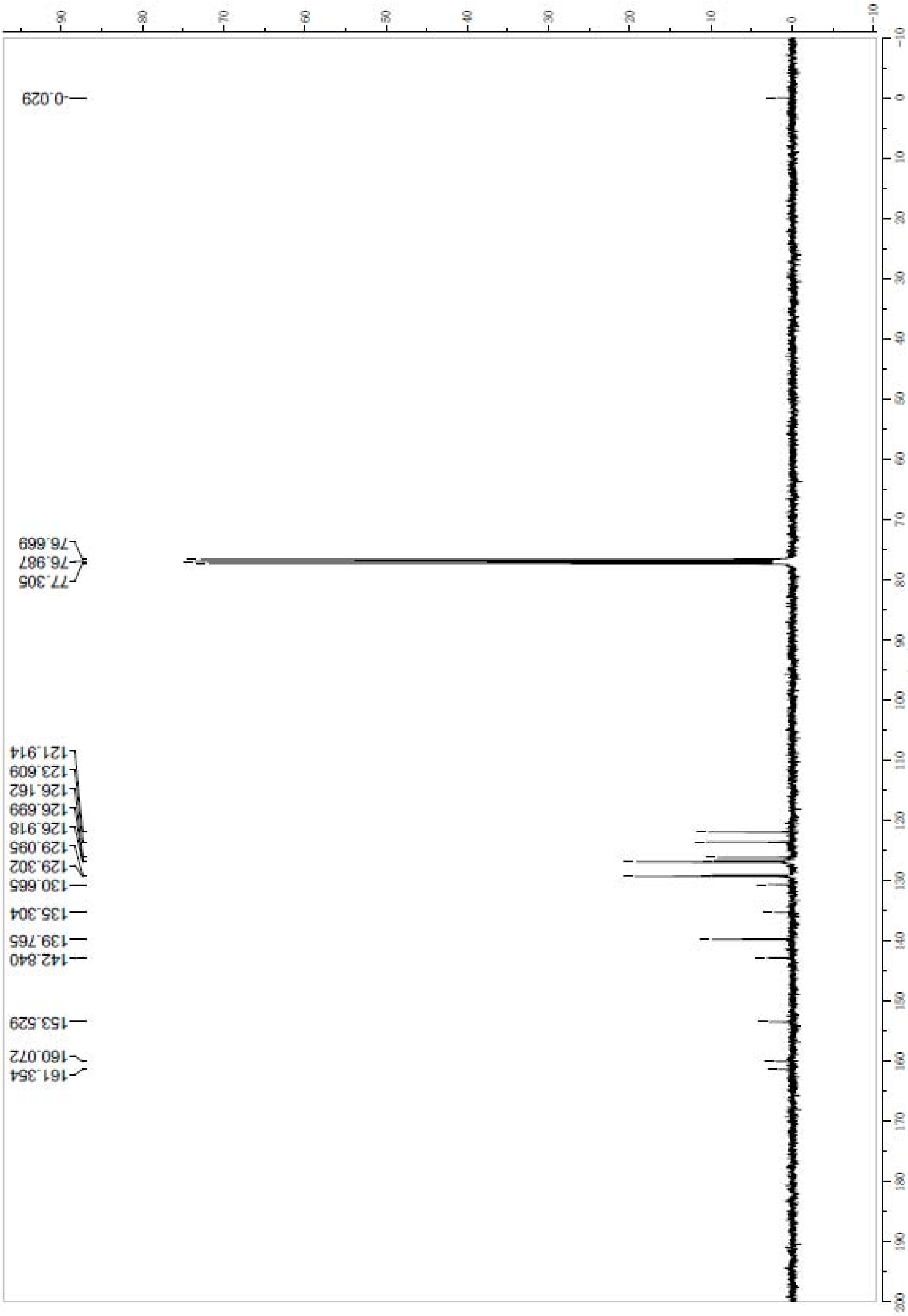

17.190
76.745
77.058
77.378
117.156
121.913
122.032
123.602
126.059
126.624
153.518
154.783
160.641
161.475
0 PPM
50
100
150
Std carbon;blank line
USER: -- DATE: Apr 25 2012
F1: 100.501
F2: 399.645
SW1: 24510
OF1: 10554.2
PTS1d: 31875 , 32768
EX: s2pul
PW: 6.5 us
PD: 1.0 sec
NA: 914
LB: 0.0
Nuts - FSI-26-76C

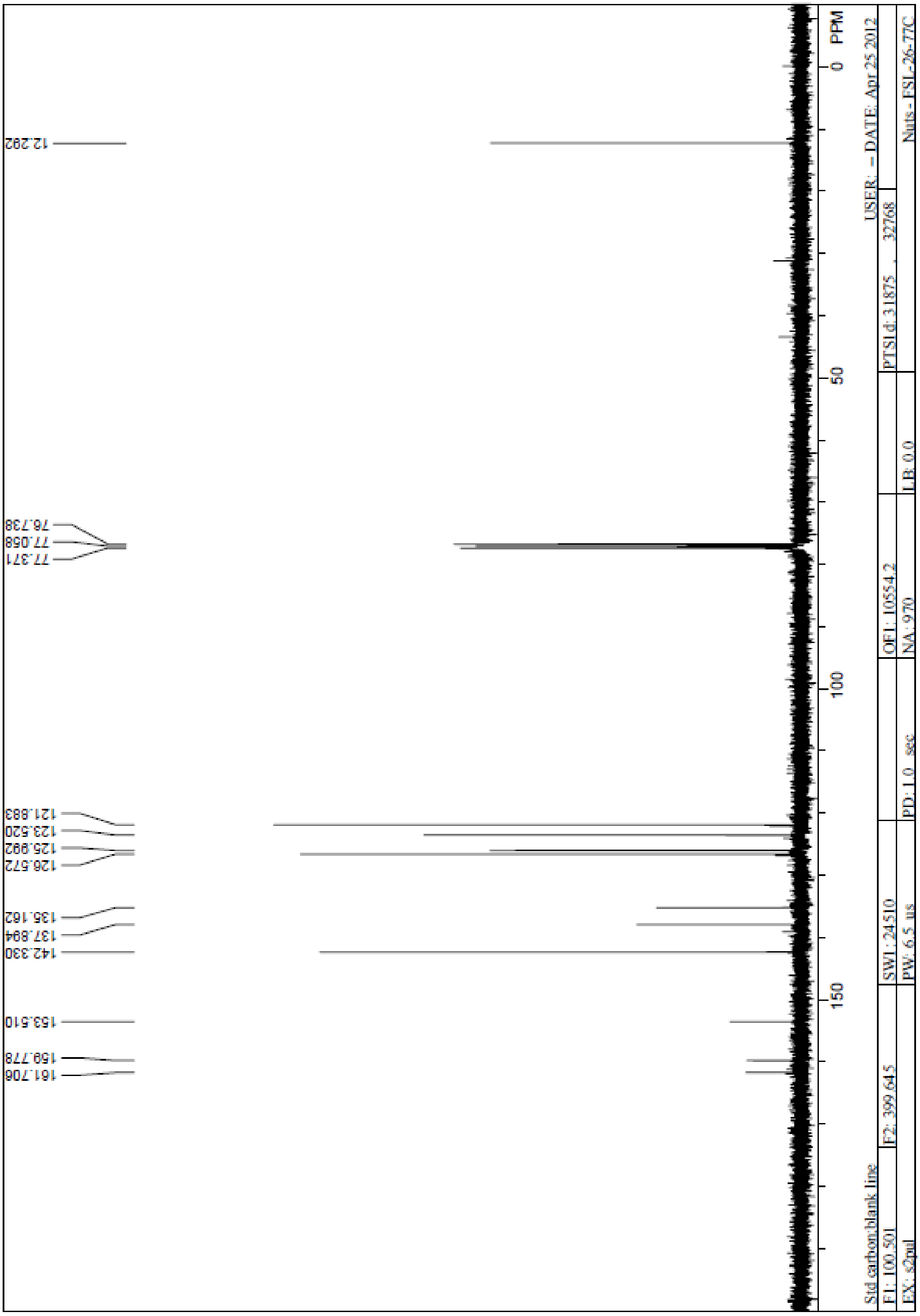
2-(5-Methylthiazol-2-yl)benzo[d]thiazole (3j)



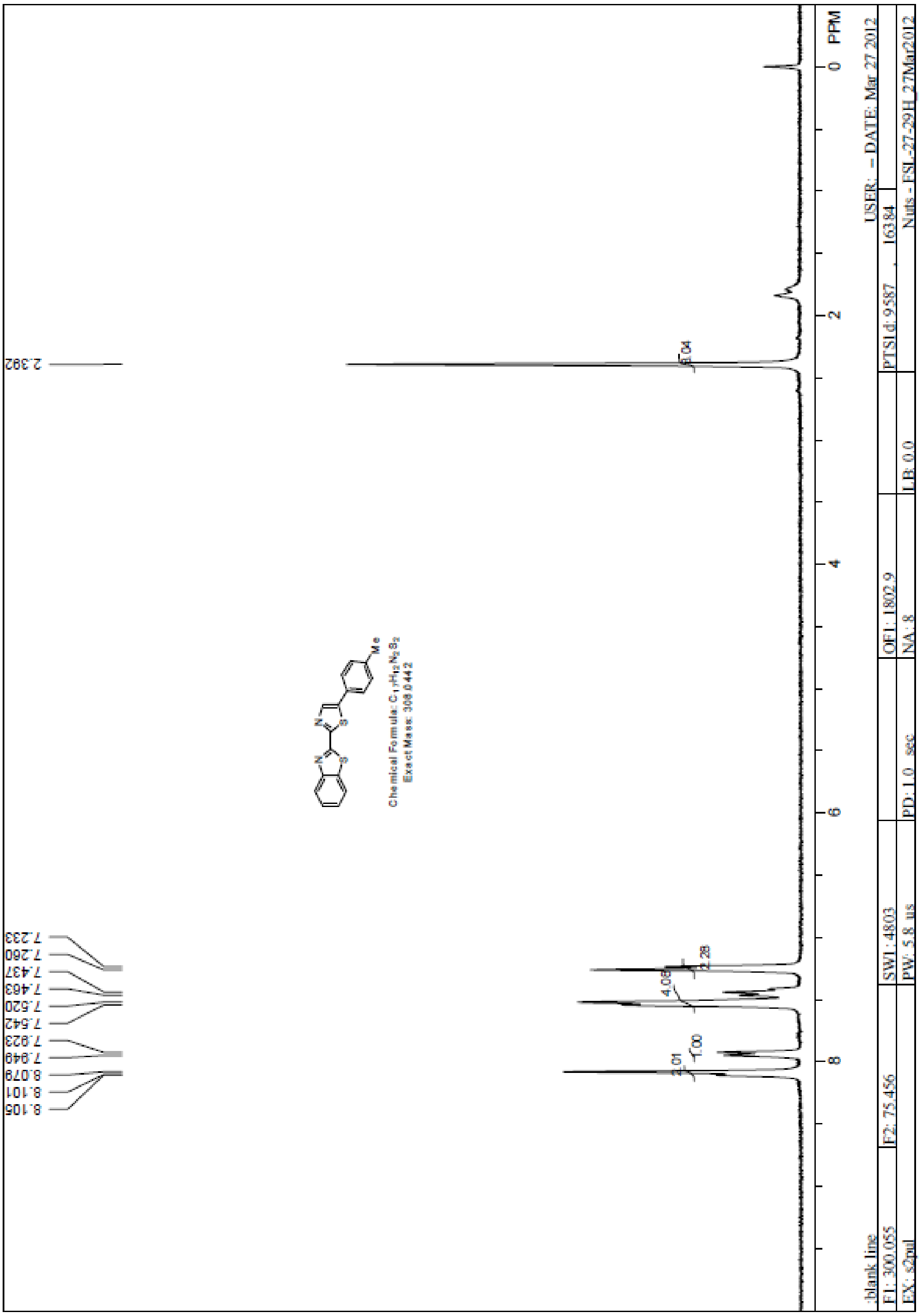
2-(5-Phenylthiazol-2-yl)benzo[d]thiazole (3k)

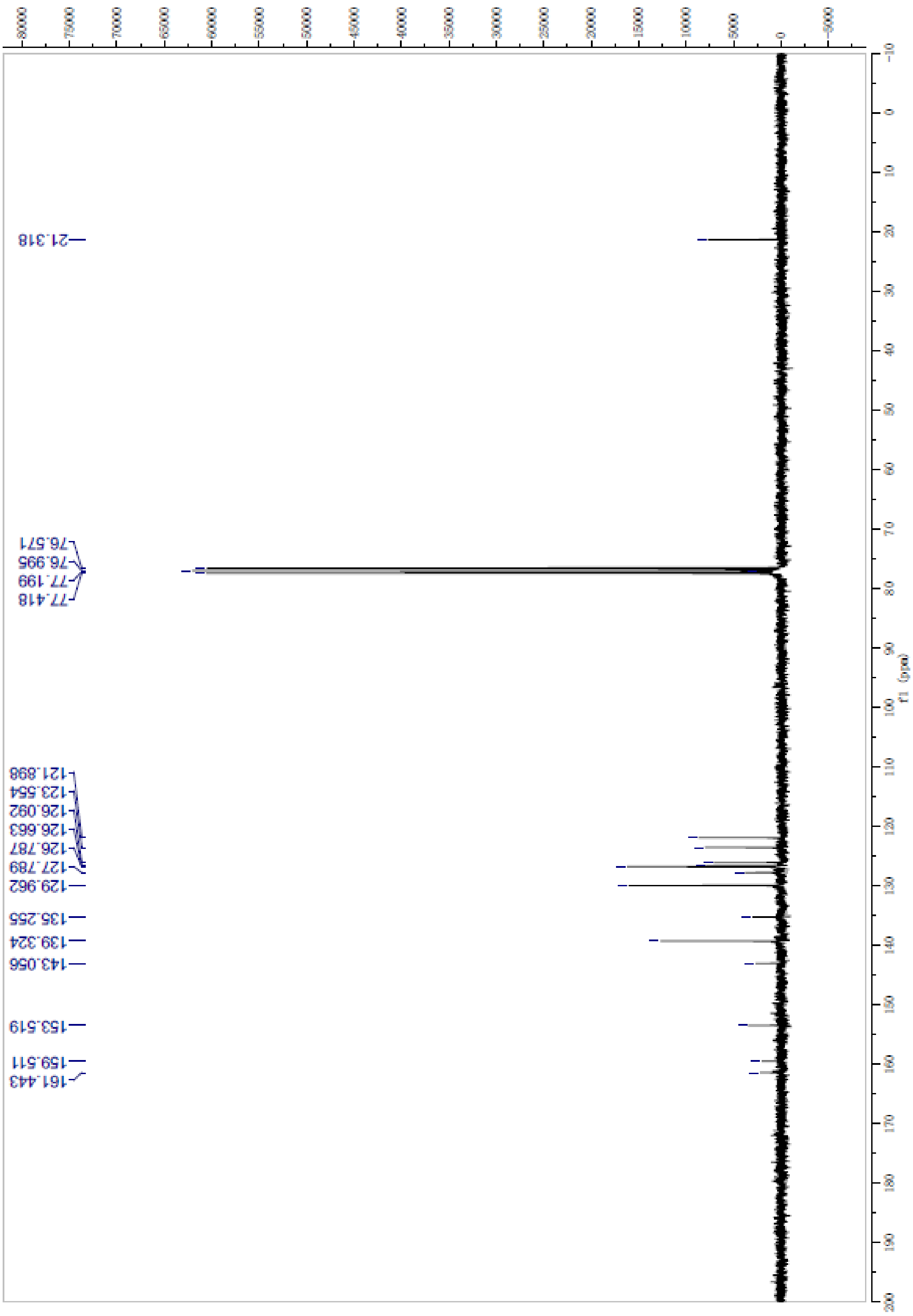



-0.029
76.669
76.987
77.305
121.914
123.609
126.162
126.699
126.918
129.095
129.302
130.665
135.304
139.765
142.840
153.529
160.072
161.354
f1 (ppm)


12.292
76.738
77.058
77.371
121.883
123.520
125.992
126.572
135.162
137.894
142.330
153.510
159.778
161.706
PPM
0
50
100
150
Std carbon;blank line
USER: -- DATE: Apr 25 2012
F1: 100.501
F2: 399.645
SW1: 24510
OF1: 10554.2
PTS1d: 31875 , 32768
EX: s2pul
PW: 6.5 us
PD: 1.0 sec
NA: 970
LB: 0.0
Nuts - FSI-26-77C

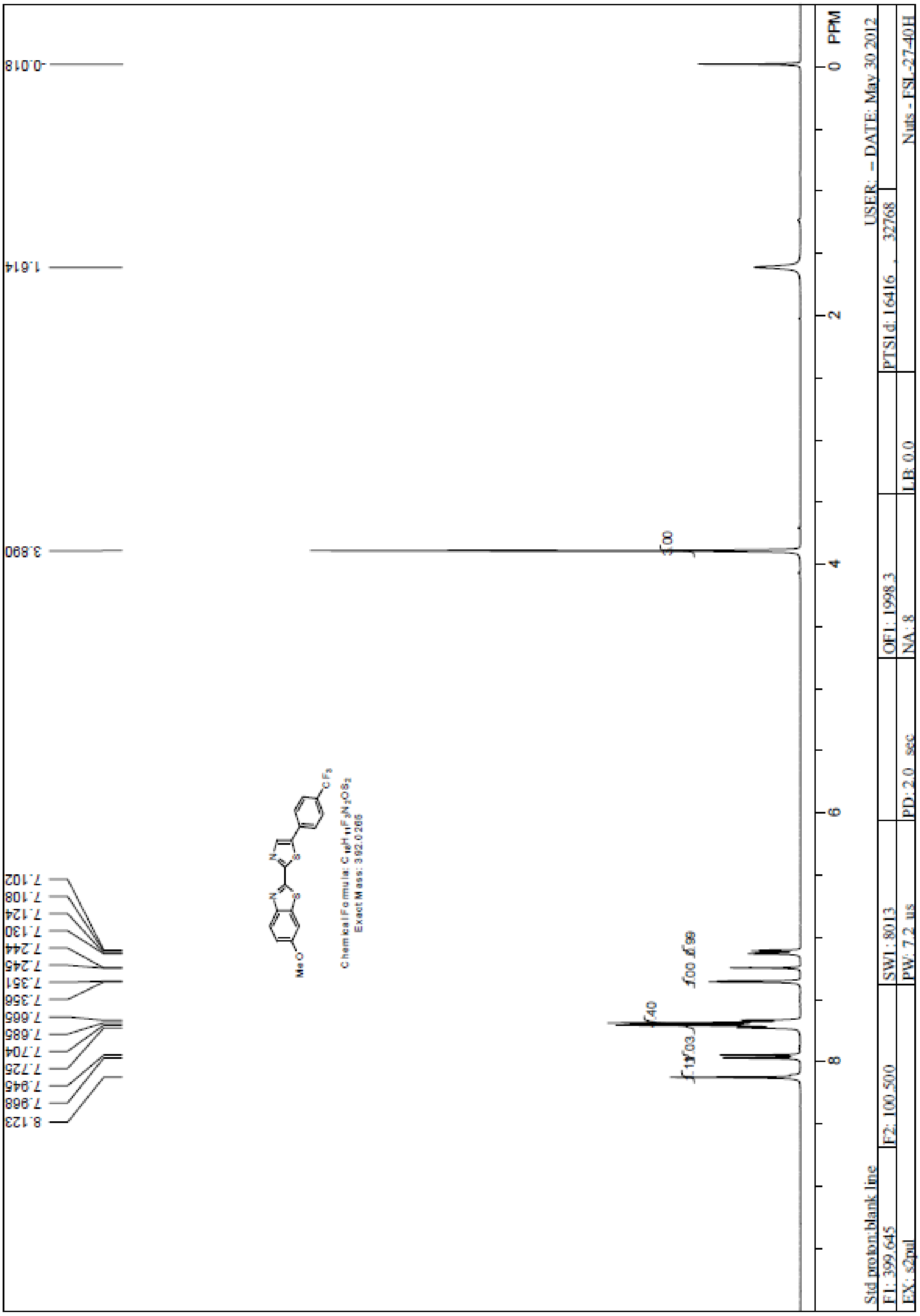
2-(5-(p-Tolyl)thiazol-2-yl)benzo[d]thiazole (3l)

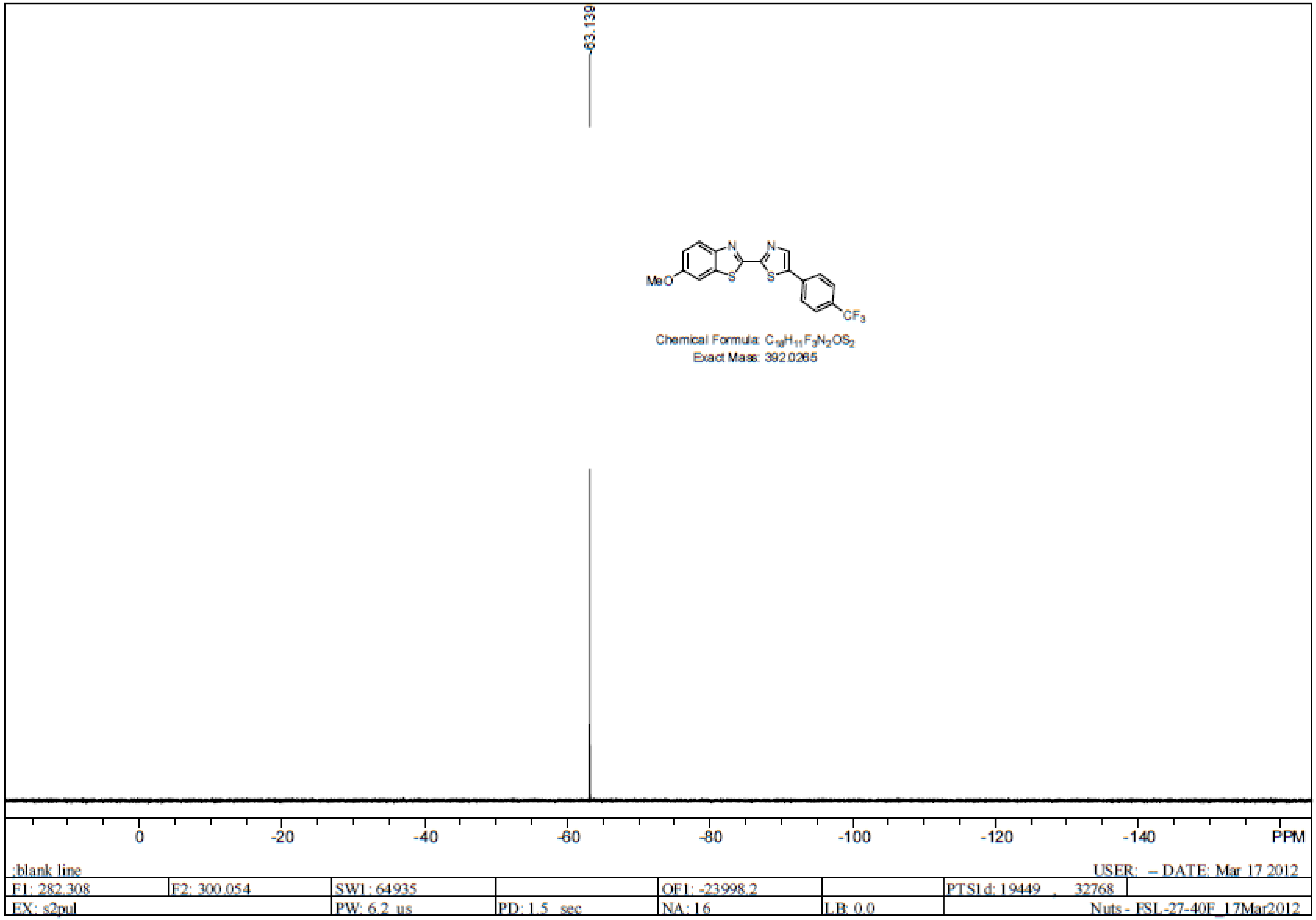




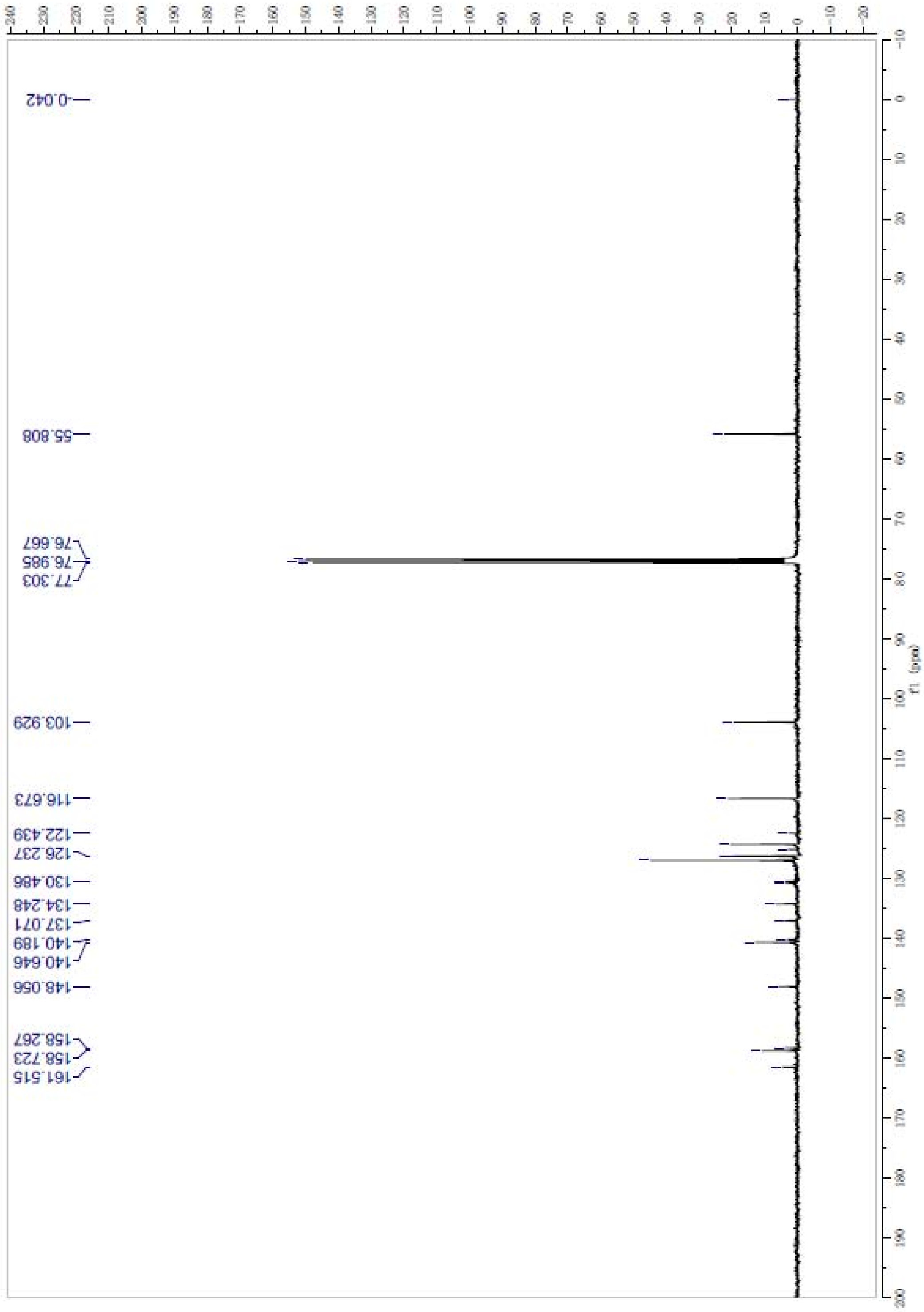
21.318
76.571
76.995
77.199
77.418
121.698
123.554
126.092
126.663
126.787
127.789
129.962
135.255
139.324
143.056
153.519
159.511
161.443
f1 (ppm)

6-Methyl-2-(5-(4-(trifluoromethyl)phenyl)thiazol-2-yl)benzo[d]thiazole (3m).

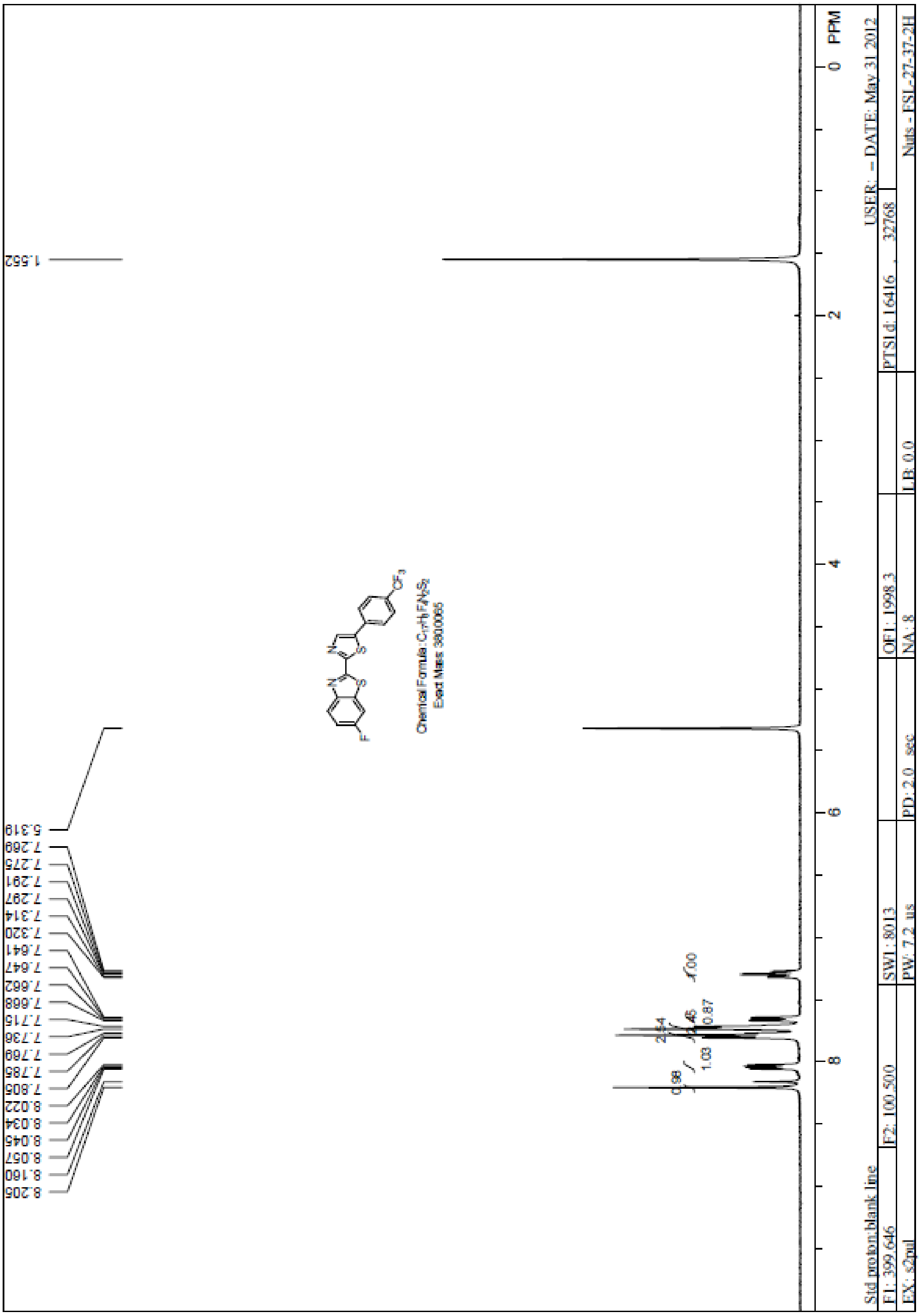


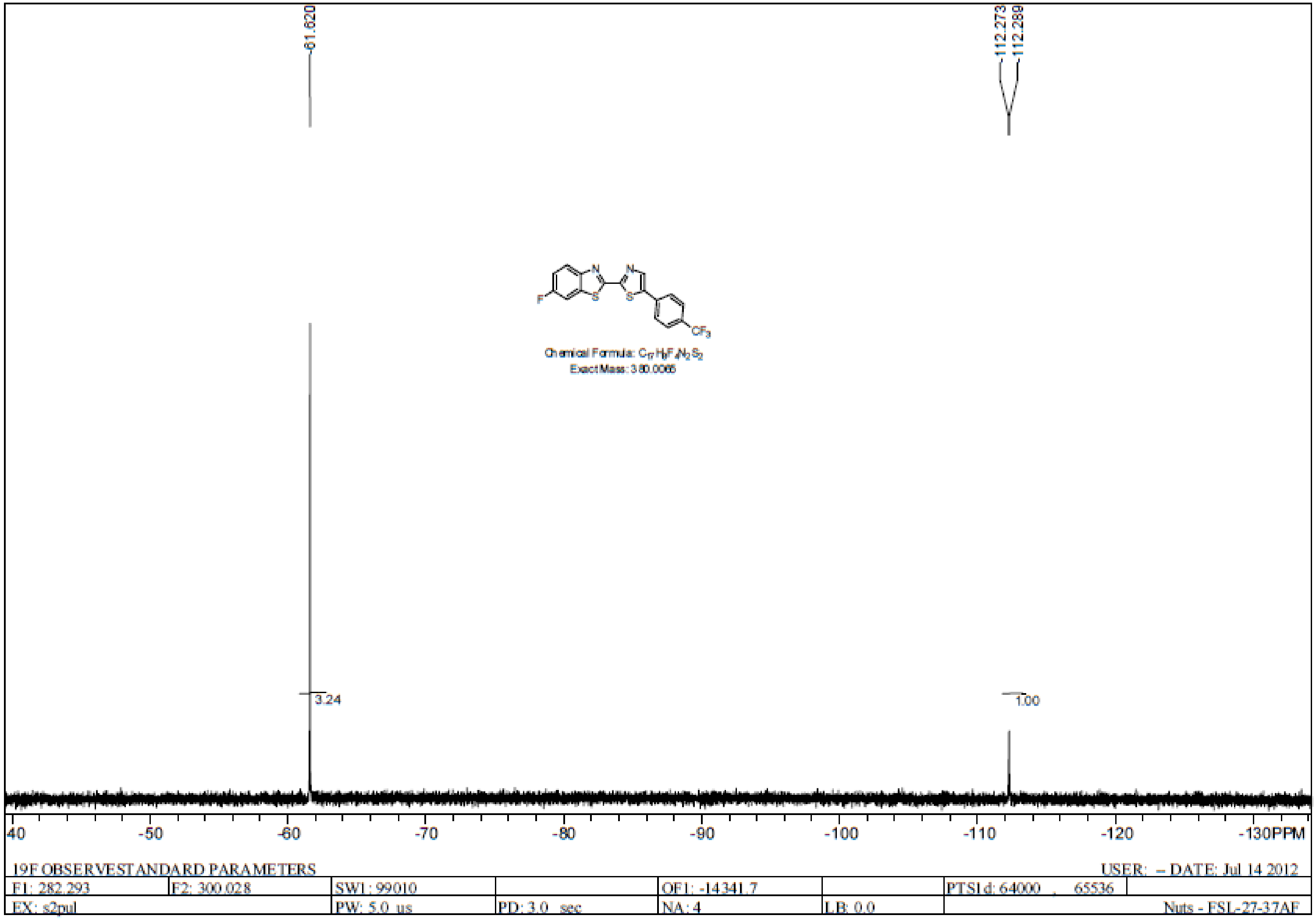


-63.139
MeO
N
S
N
S
CF3
Chemical Formula: C18H11F3N2OS2
Exact Mass: 392.0265
0
-20
-40
-60
-80
-100
-120
-140
PPM
;blank line
USER: -- DATE: Mar 17 2012
F1: 282.308
F2: 300.054
SW1: 64935
OF1: -23998.2
PTS1d: 19449 , 32768
EX: s2pul
PW: 6.2 us
PD: 1.5 sec
NA: 16
LB: 0.0
Nuts - FSL-27-40F_17Mar2012

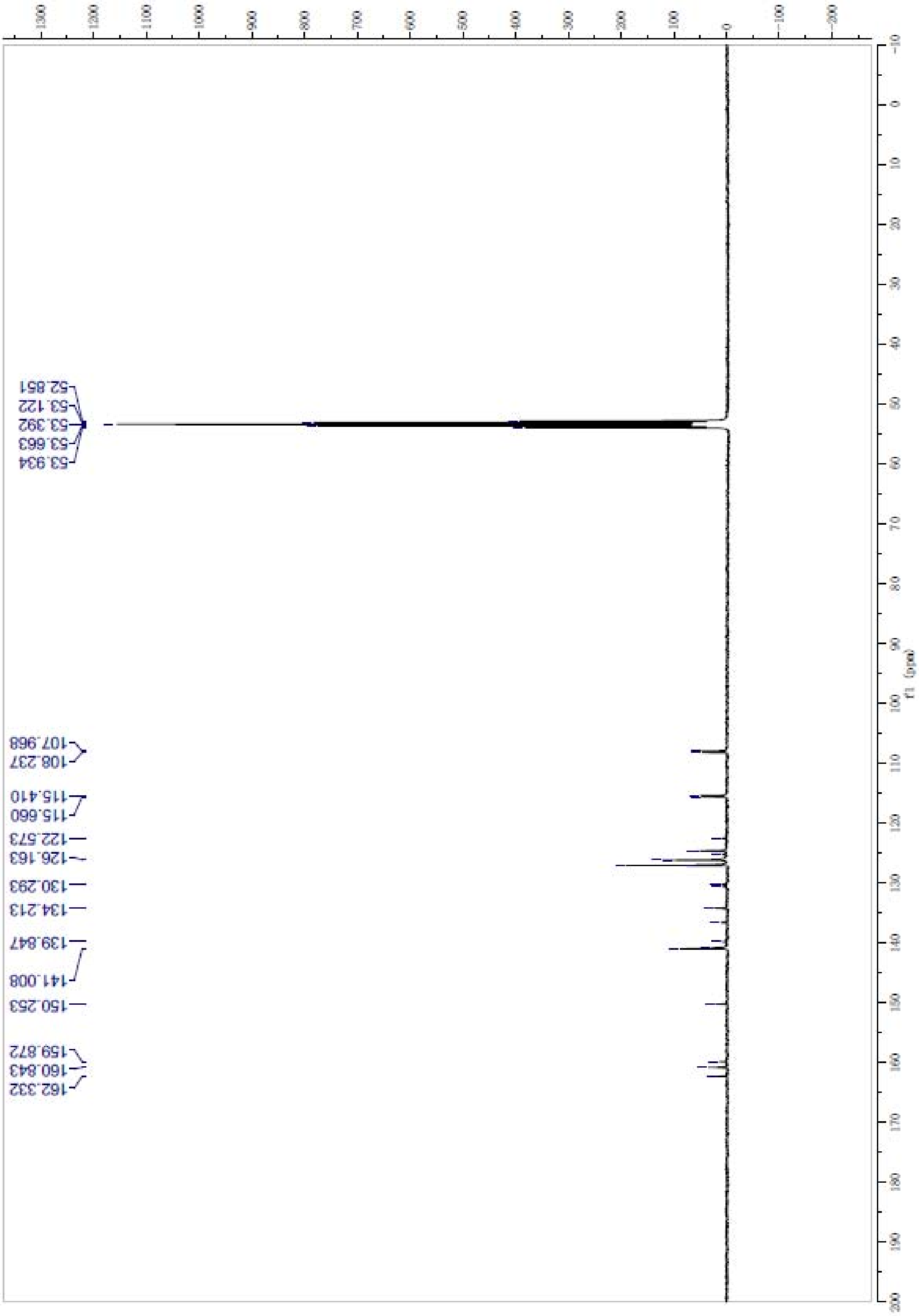

-0.042
55.808
76.667
76.985
77.303
103.929
116.673
122.439
126.237
130.486
134.248
137.071
140.189
140.646
148.056
158.267
158.723
161.515
f1 (ppm)

6-Fluoro-2-(5-(4-(trifluoromethyl)phenyl)thiazol-2-yl)benzo[d]thiazole (3n)



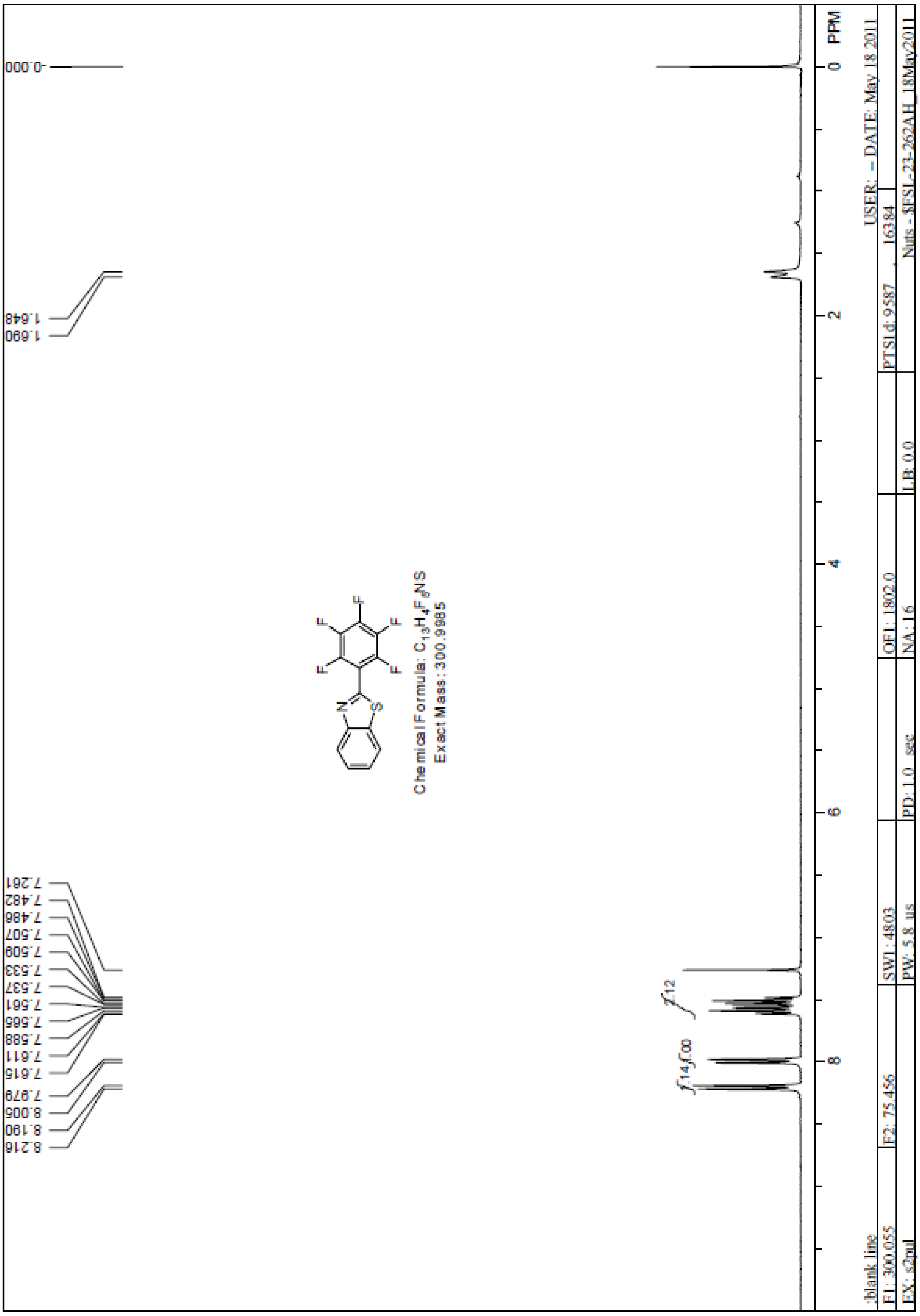


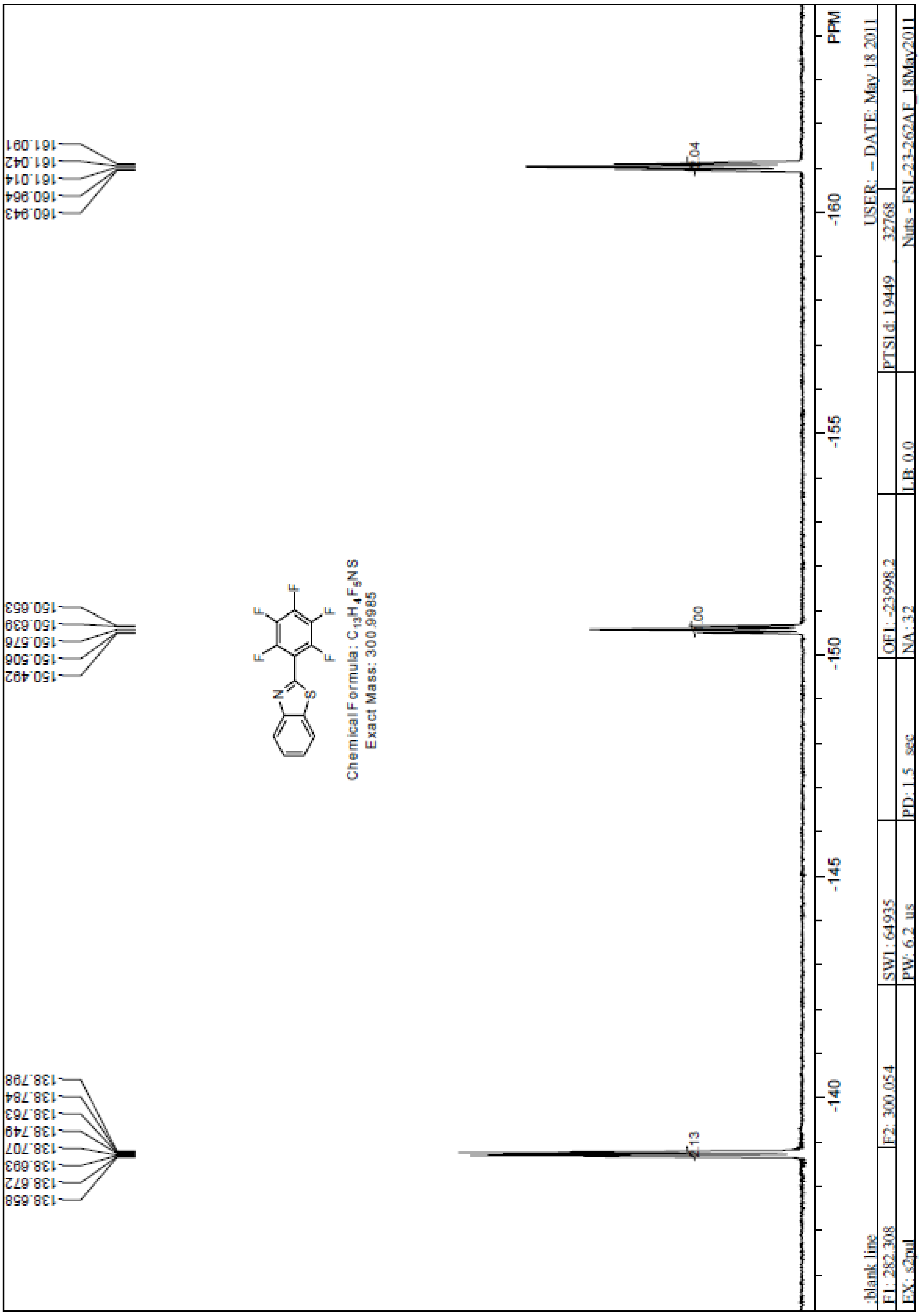
-61.620
-112.273
-112.289
3.24
1.00
Chemical Formula: C17H8F4N2S2
Exact Mass: 380.0065
40
-50
-60
-70
-80
-90
-100
-110
-120
-130PPM
19F OBSERVESTANDARD PARAMETERS
USER: -- DATE: Jul 14 2012
F1: 282.293
F2: 300.028
SW1: 99010
OF1: -14341.7
PTS1d: 64000 , 65536
EX: s2pul
PW: 5.0 us
PD: 3.0 sec
NA: 4
LB: 0.0
Nuts - FSL-27-37AF



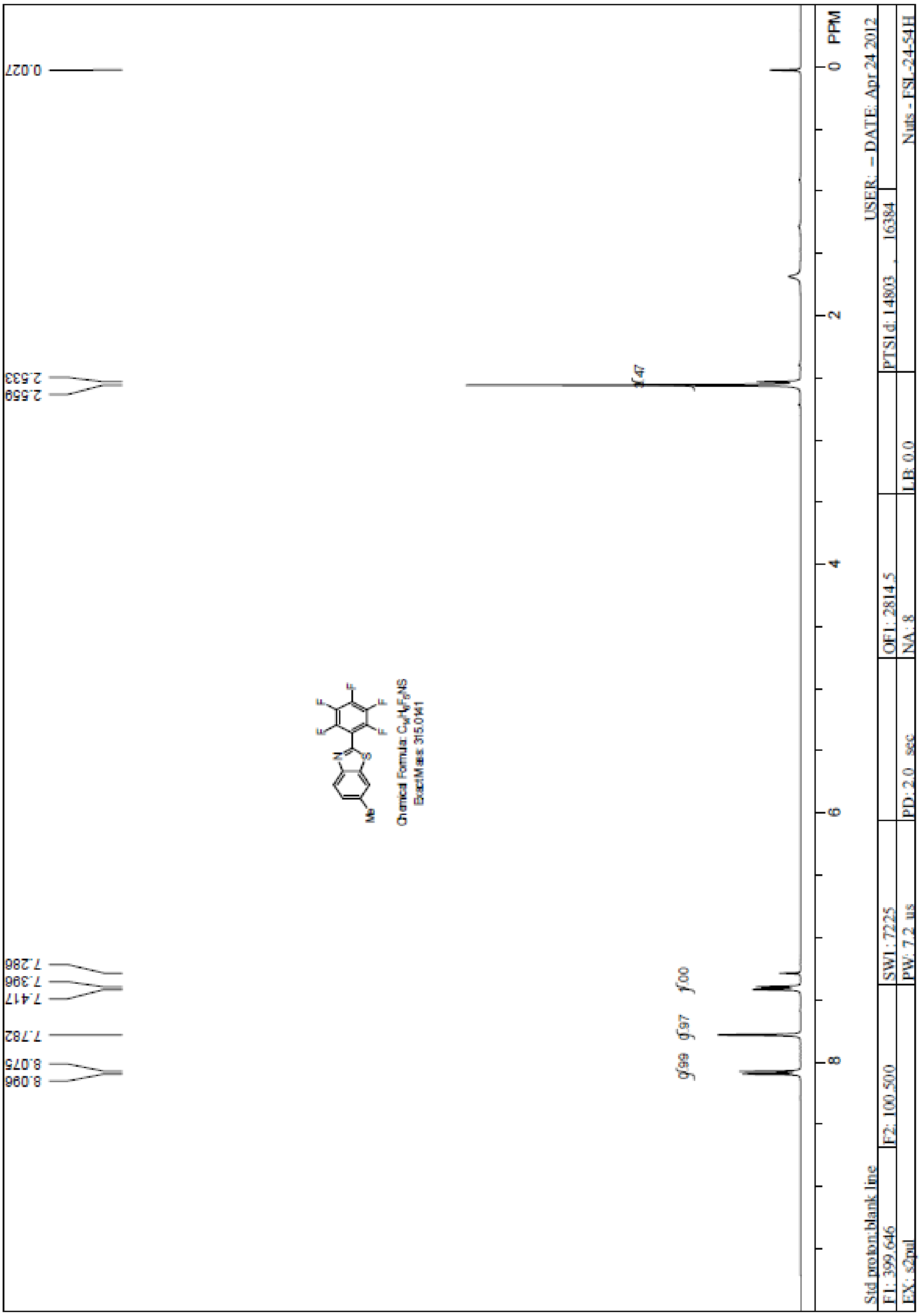
52.851
53.122
53.392
53.663
53.934
107.968
108.237
115.410
115.660
122.573
126.163
130.293
134.213
139.847
141.008
150.253
159.872
160.843
162.332
f1 (ppm)

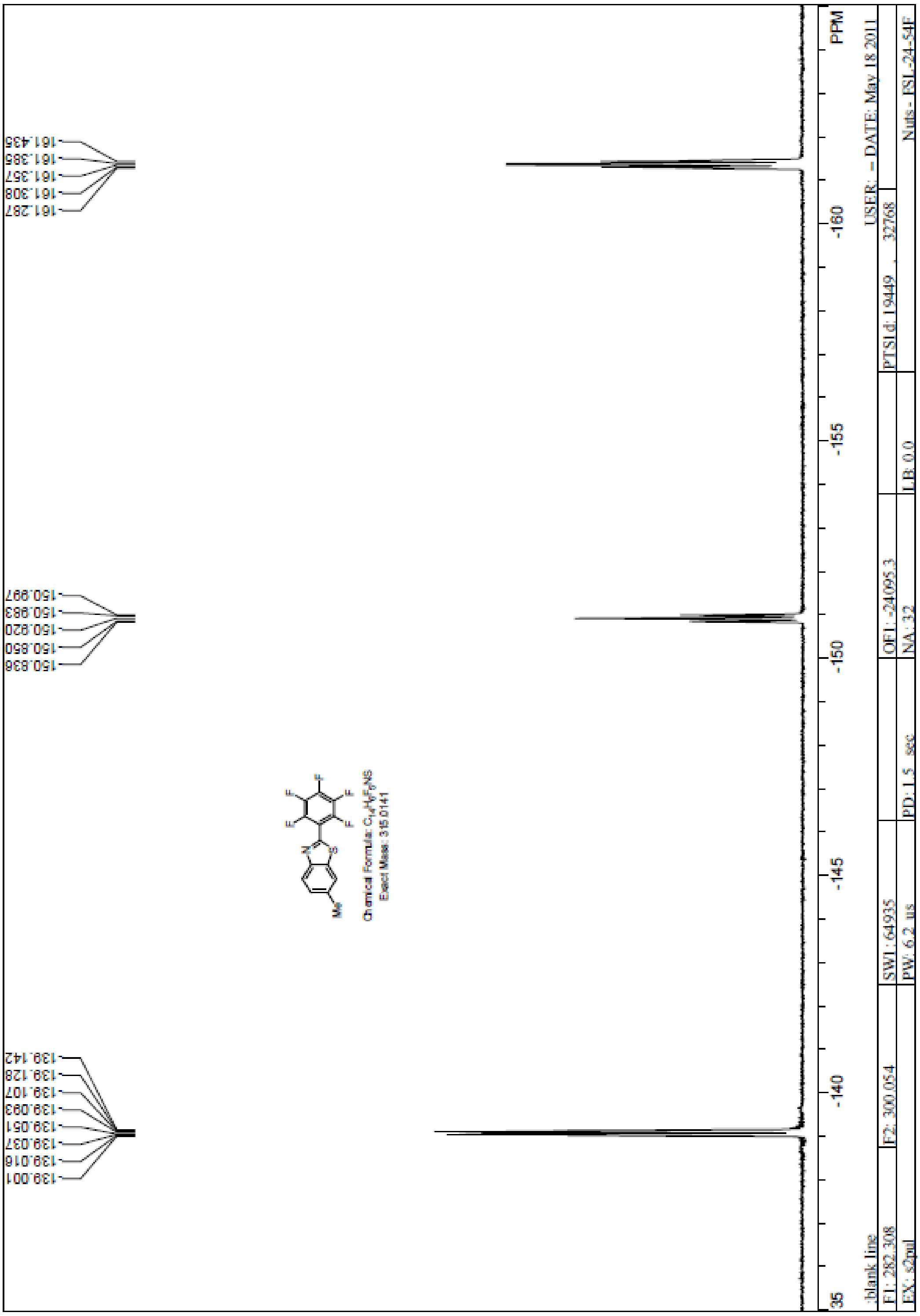
2-(Perfluorophenyl)benzo[d]thiazole (5a)

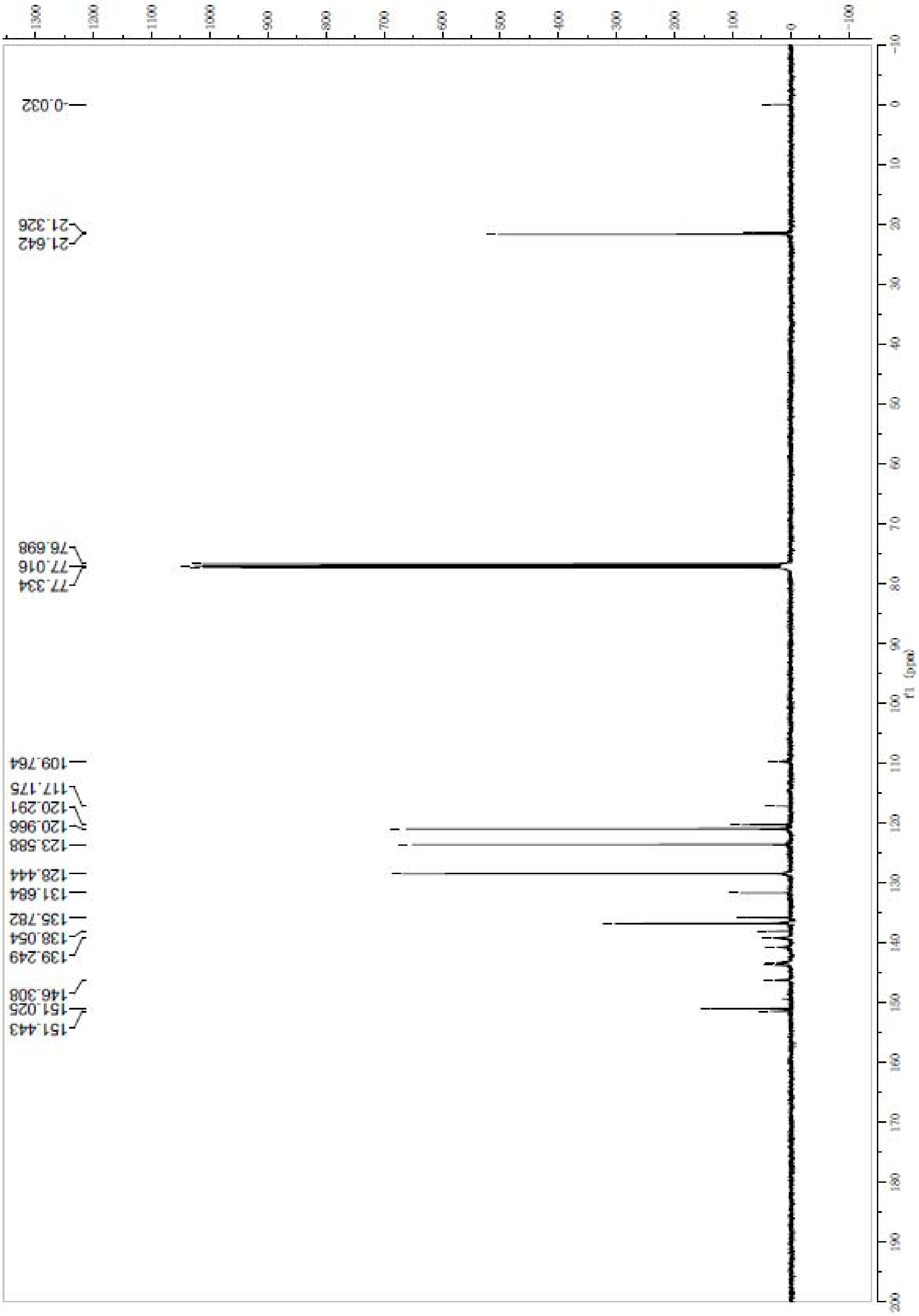



-161.091
-161.042
-161.014
-160.964
-160.943
-150.653
-150.639
-150.576
-150.506
-150.492
-138.798
-138.784
-138.763
-138.749
-138.707
-138.693
-138.672
-138.658
Chemical Formula: $C_{13}H_4F_5NS$
Exact Mass: 300.9985
2.13
1.00
2.04
-140
-145
-150
-155
-160
PPM
blank line
F1: 282.308
F2: 300.054
SW1: 64935
OF1: -23998.2
PTS1d: 19449
32768
USER: -- DATE: May 18 2011
EX: s2pul
PW: 6.2 us
PD: 1.5 sec
NA: 32
LB: 0.0
Nuts - FSI-23-262AF_18May2011

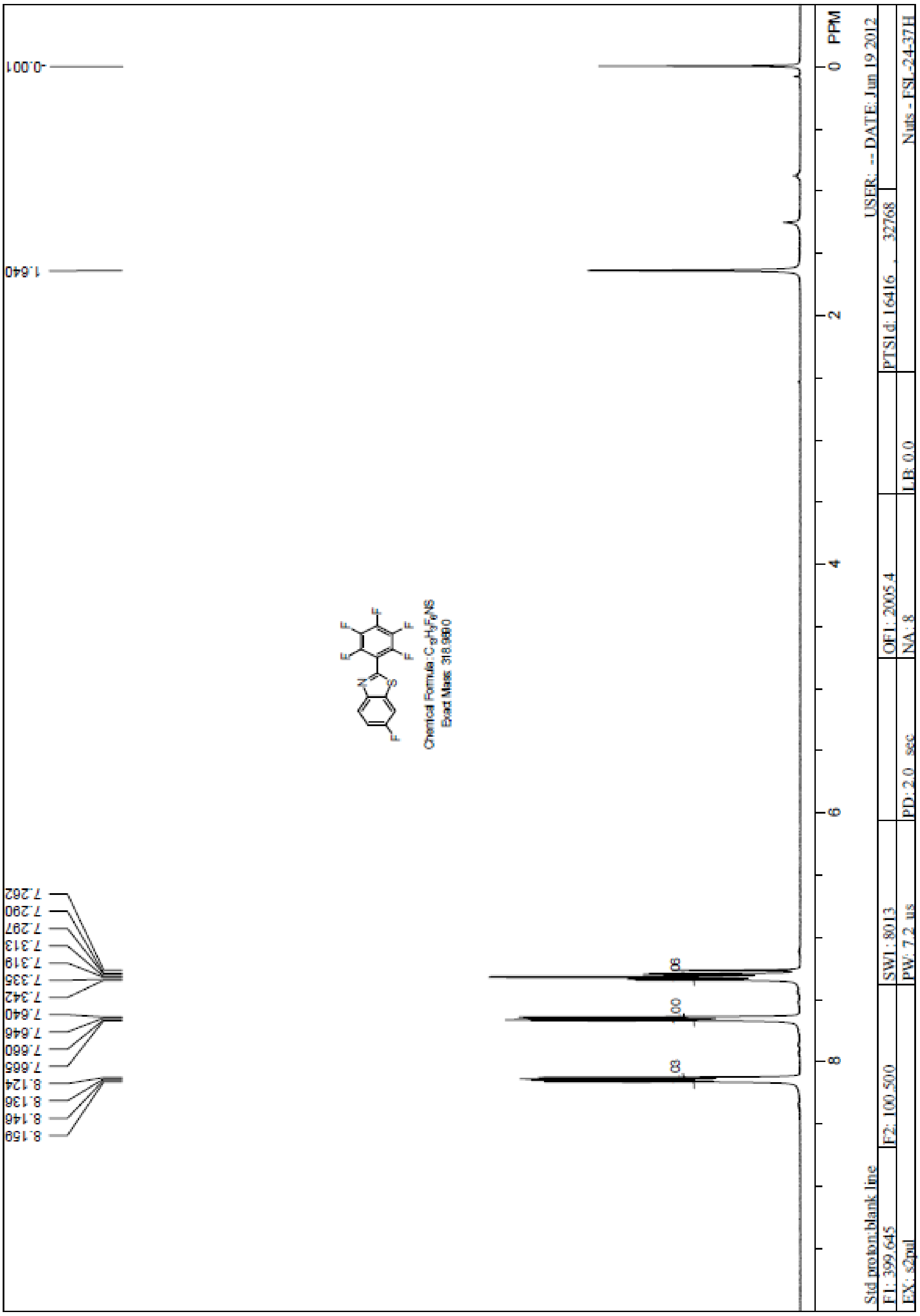
6-Methyl-2-(perfluorophenyl)benzo[d]thiazole (5b)

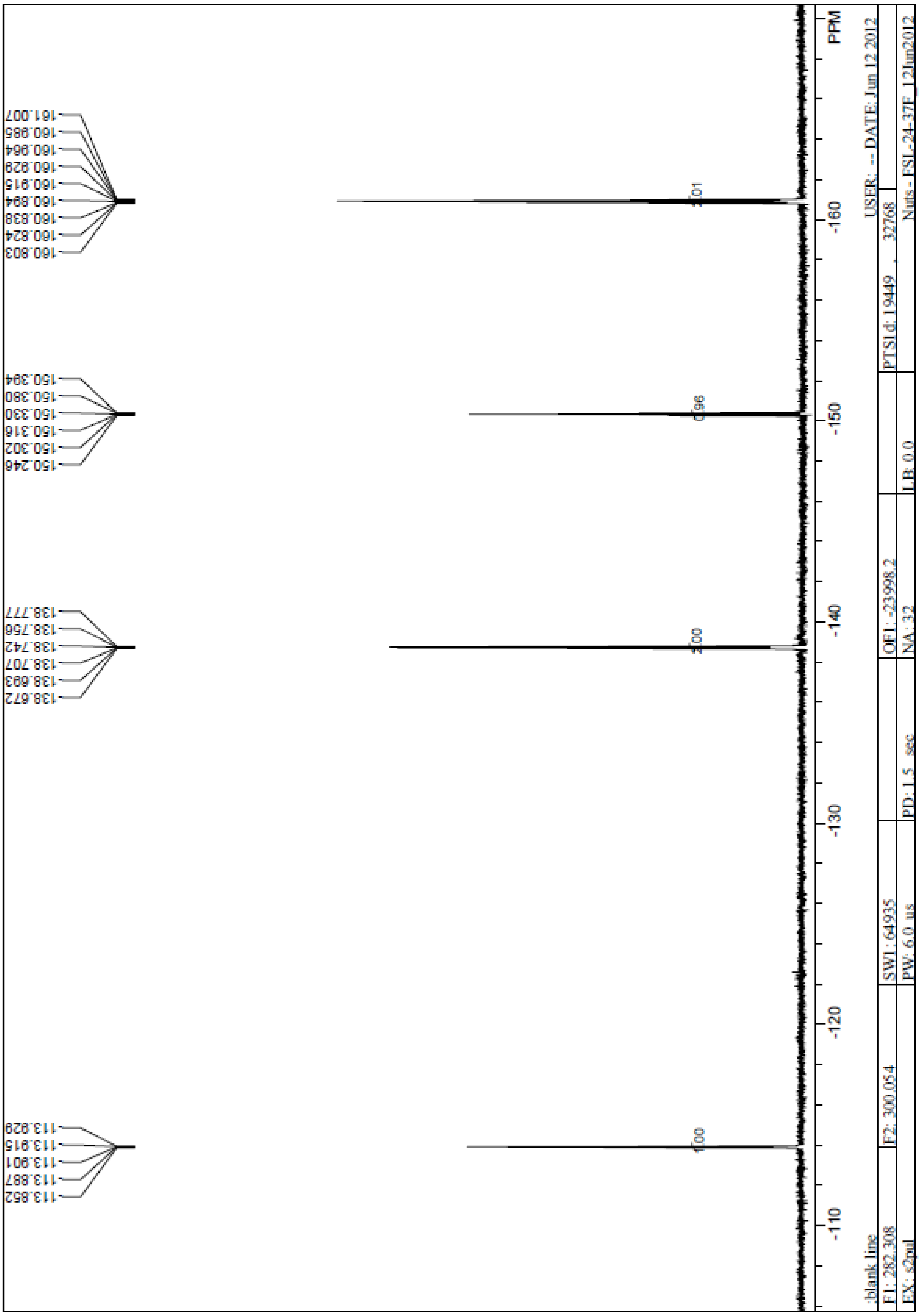


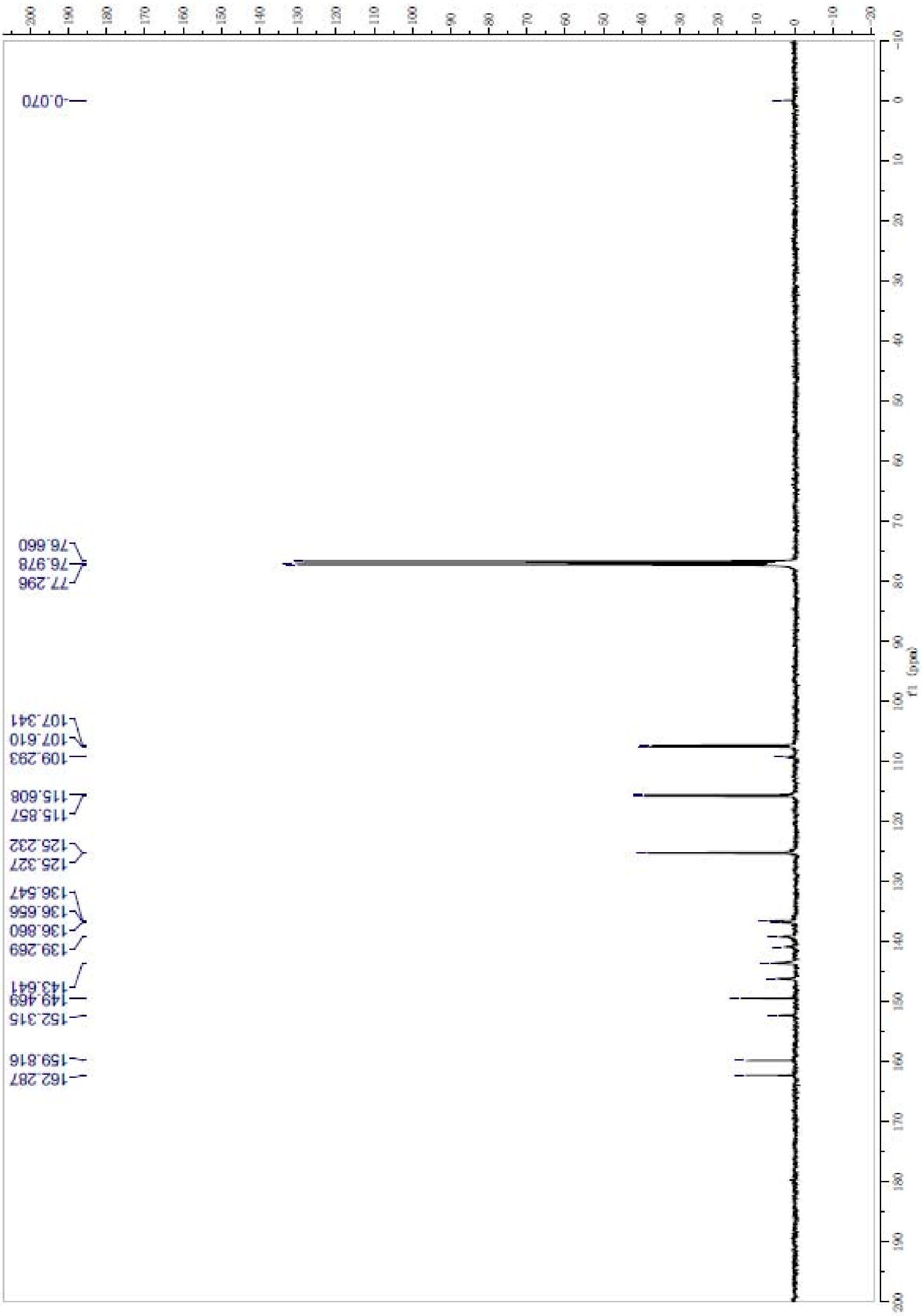

161.435
161.385
161.357
161.308
161.287
150.997
150.983
150.920
150.850
150.836
139.142
139.128
139.107
139.093
139.051
139.037
139.016
139.001
Chemical Formula: $C_{14}H_6F_5NS$
Exact Mass: 315.0141
PPM
-160
-155
-150
-145
-140
USER: -- DATE: May 18 2011
PTS1d: 19449 , 32768
OF1: -24095.3
SW1: 64935
F2: 300.054
F1: 282.308
:blank line
Nuts - FSL-24-54F
LB: 0.0
NA: 32
PD: 1.5 sec
PW: 6.2 us
EX: s2pul


0.032
21.326
21.642
76.698
77.016
77.334
109.764
117.175
120.291
120.966
123.588
128.444
131.684
135.782
138.054
139.249
146.308
151.025
151.443
f1 (ppm)

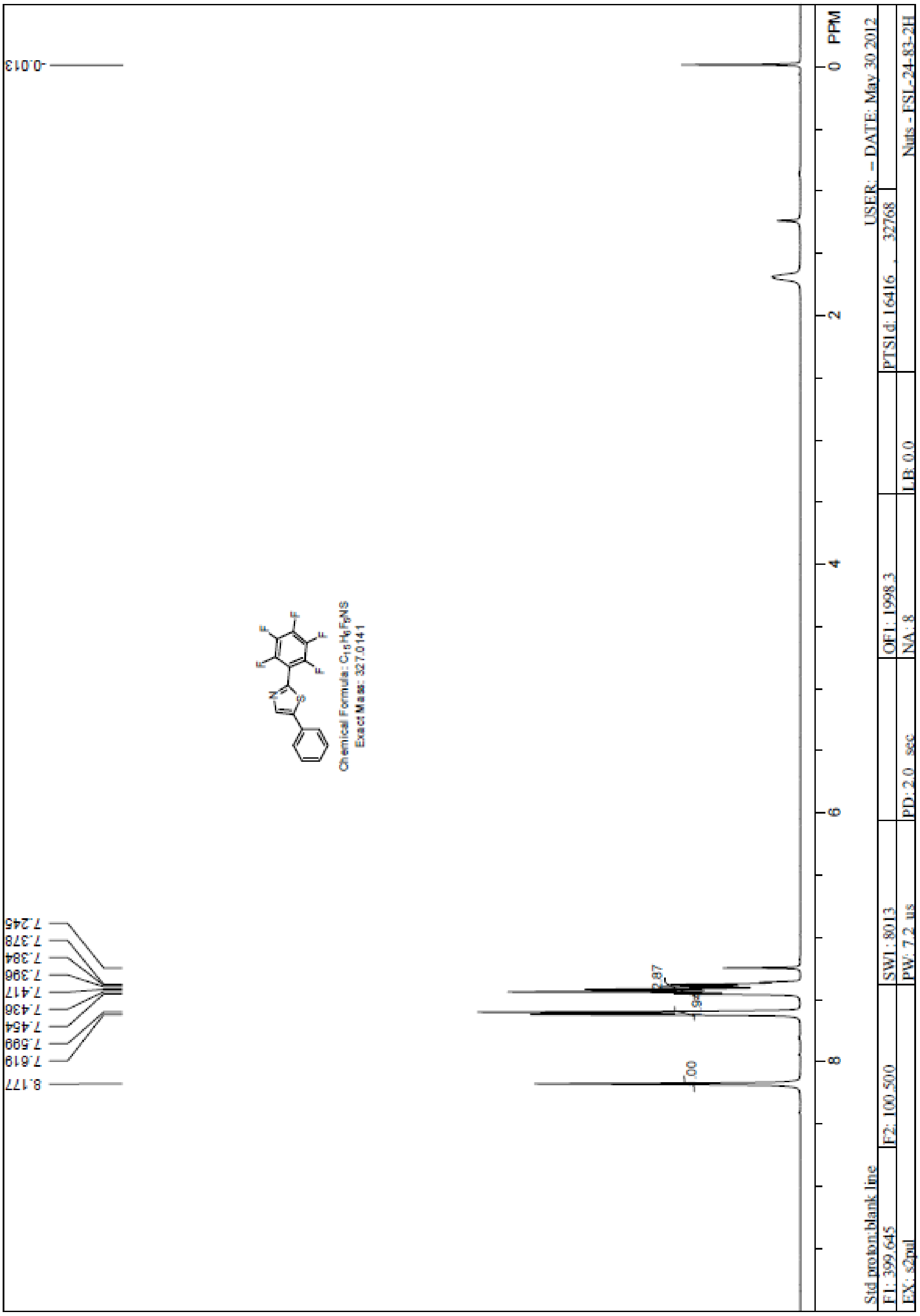
6-Fluoro-2-(perfluorophenyl)benzo[d]thiazole (5c)

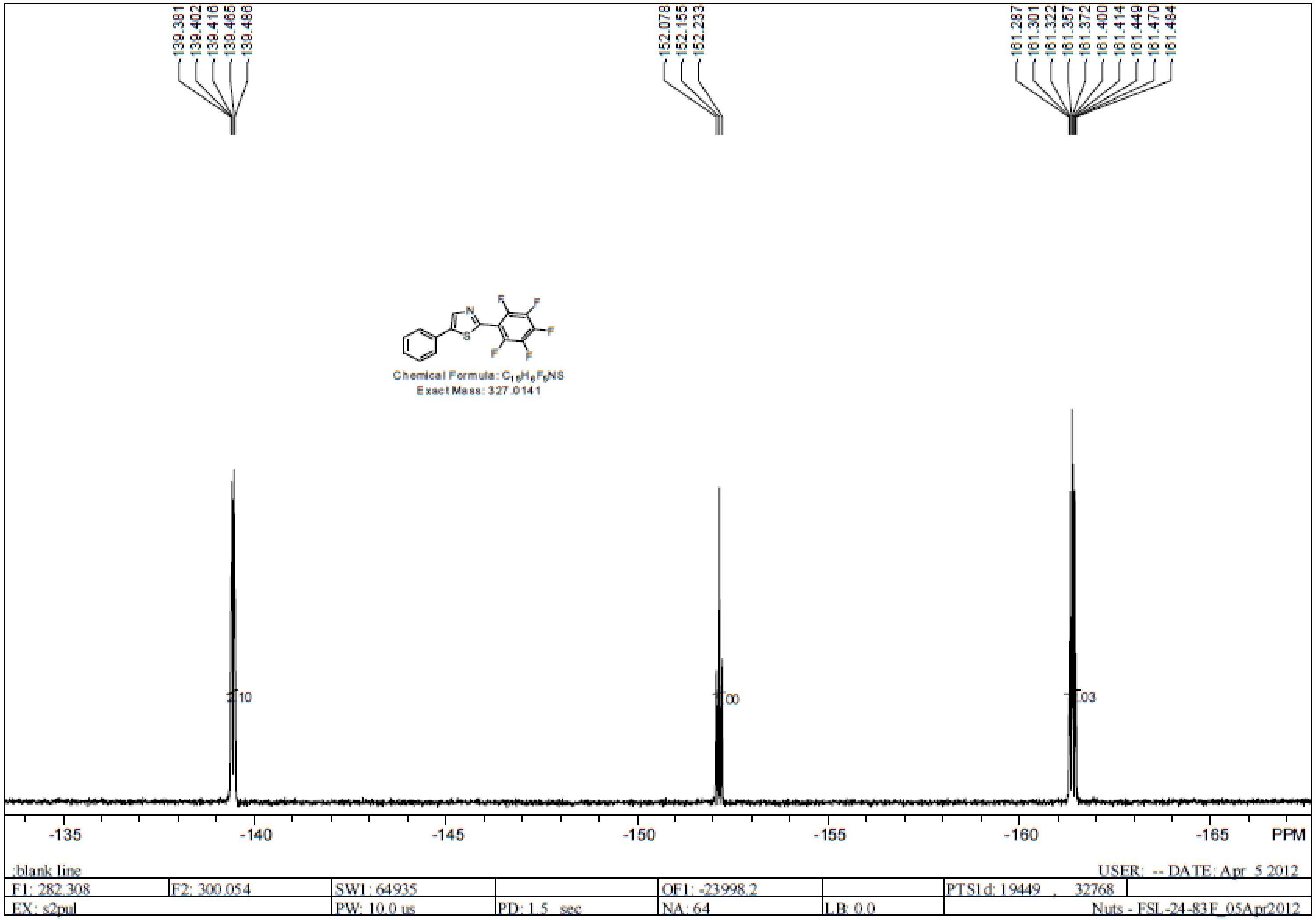



161.007
160.985
160.964
160.929
160.915
160.894
160.838
160.824
160.803
150.394
150.380
150.330
150.316
150.302
150.246
138.777
138.756
138.742
138.707
138.693
138.672
113.929
113.915
113.901
113.887
113.852
PPM
-160
-150
-140
-130
-120
-110
USER: -- DATE: Jun 12 2012
Nuts - FSL-24-37F_12Jun2012
PTS1d: 19449 , 32768
LB: 0.0
OF1: -23998.2
NA: 32
PD: 1.5 sec
SW1: 64935
PW: 6.0 us
F2: 300.054
blank line
F1: 282.308
EX: s2pul

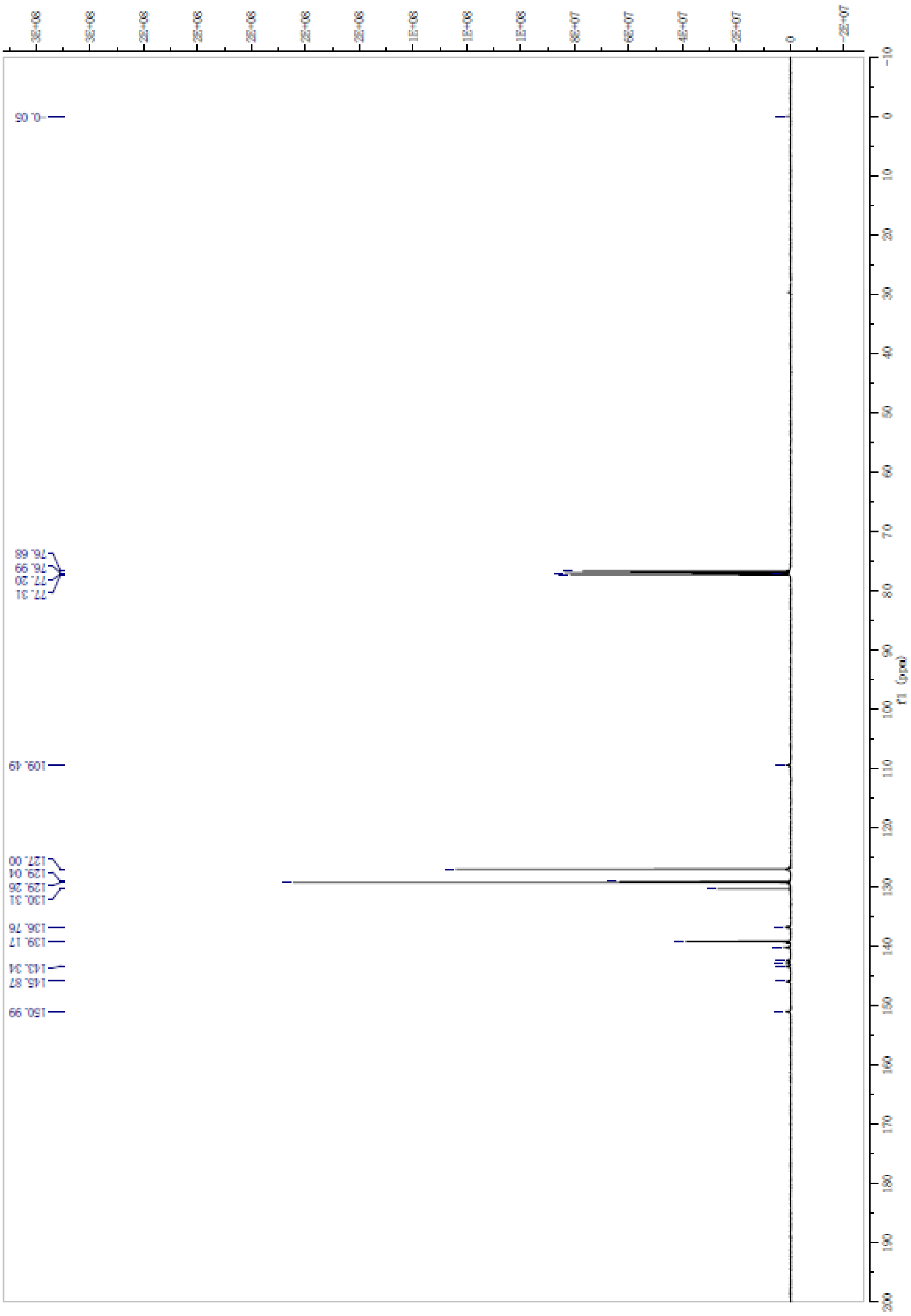

-0.070
76.660
76.978
77.296
107.341
107.610
109.293
115.608
115.857
125.232
125.327
136.547
136.656
136.860
139.269
143.641
149.469
152.315
159.816
162.287
f1 (ppm)

2-(Perfluorophenyl)-5-phenylthiazole (5d)

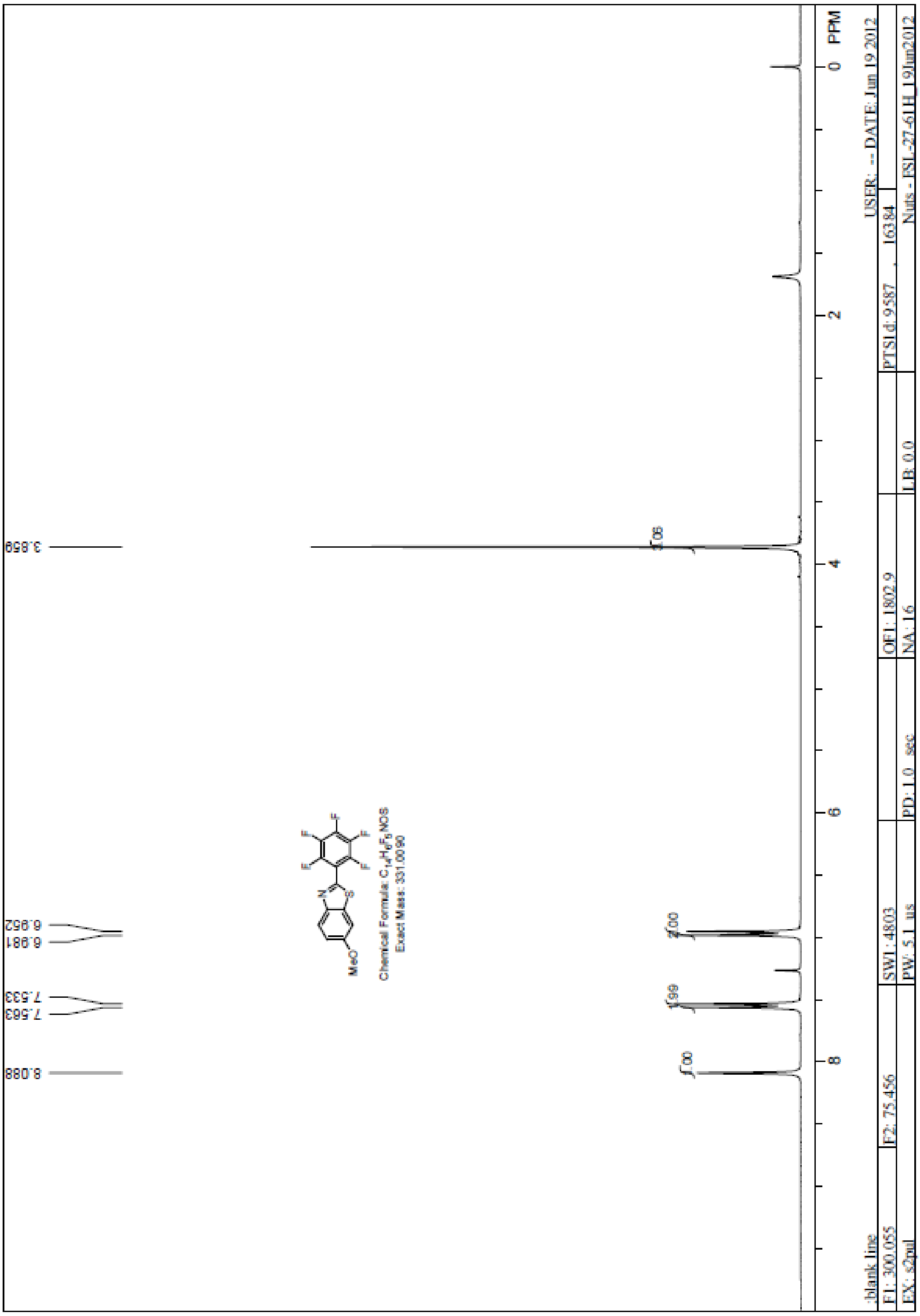


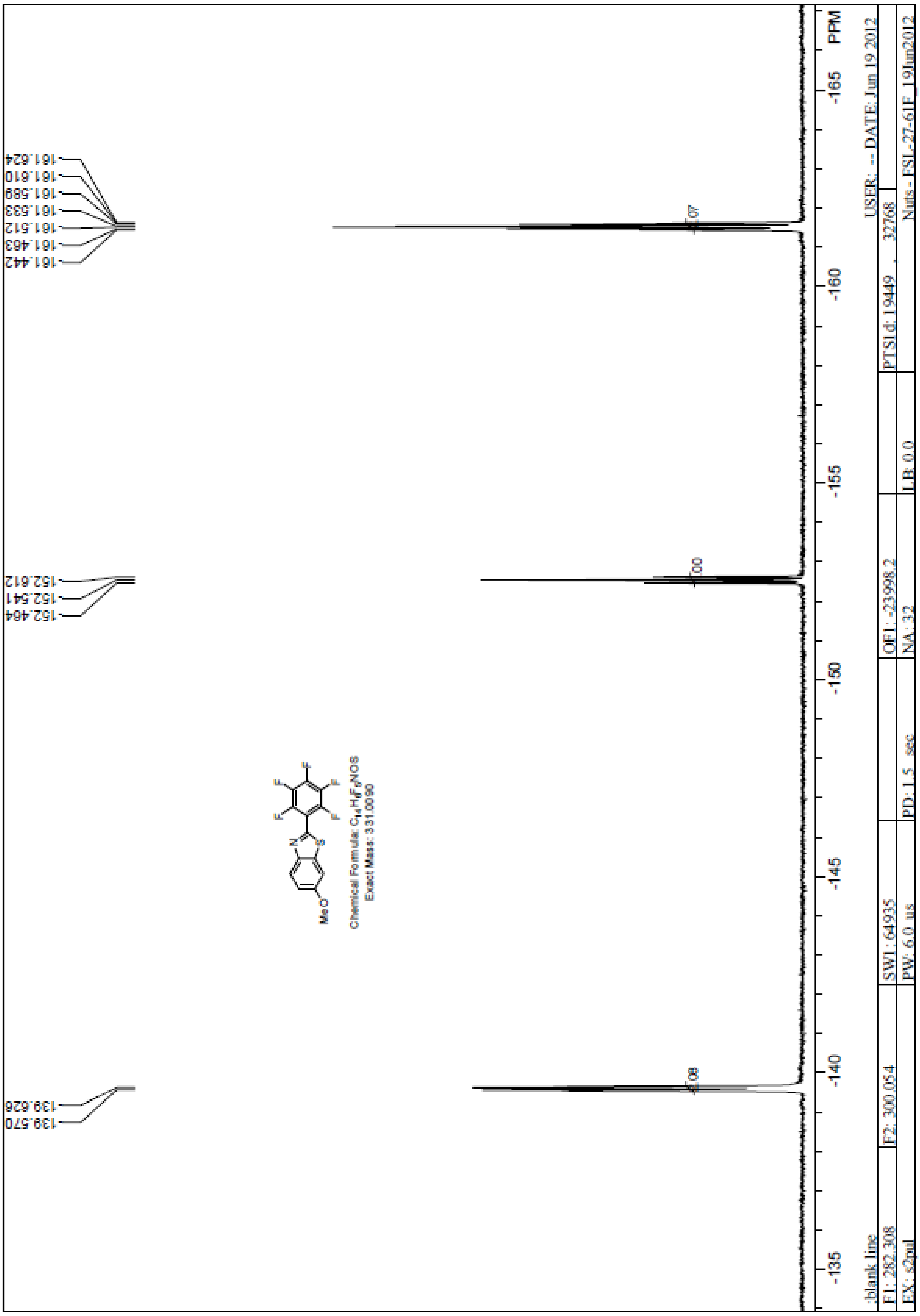


139.381
139.402
139.416
139.465
139.486
152.078
152.155
152.233
161.287
161.301
161.322
161.357
161.372
161.400
161.414
161.449
161.470
161.484
Chemical Formula: C15H6F5NS
Exact Mass: 327.0141
-135
-140
-145
-150
-155
-160
-165
PPM
;blank line
USER: -- DATE: Apr 5 2012
F1: 282.308
F2: 300.054
SW1: 64935
OF1: -23998.2
PTS1d: 19449 , 32768
EX: s2pul
PW: 10.0 us
PD: 1.5 sec
NA: 64
LB: 0.0
Nuts - FSL-24-83F_05Apr2012

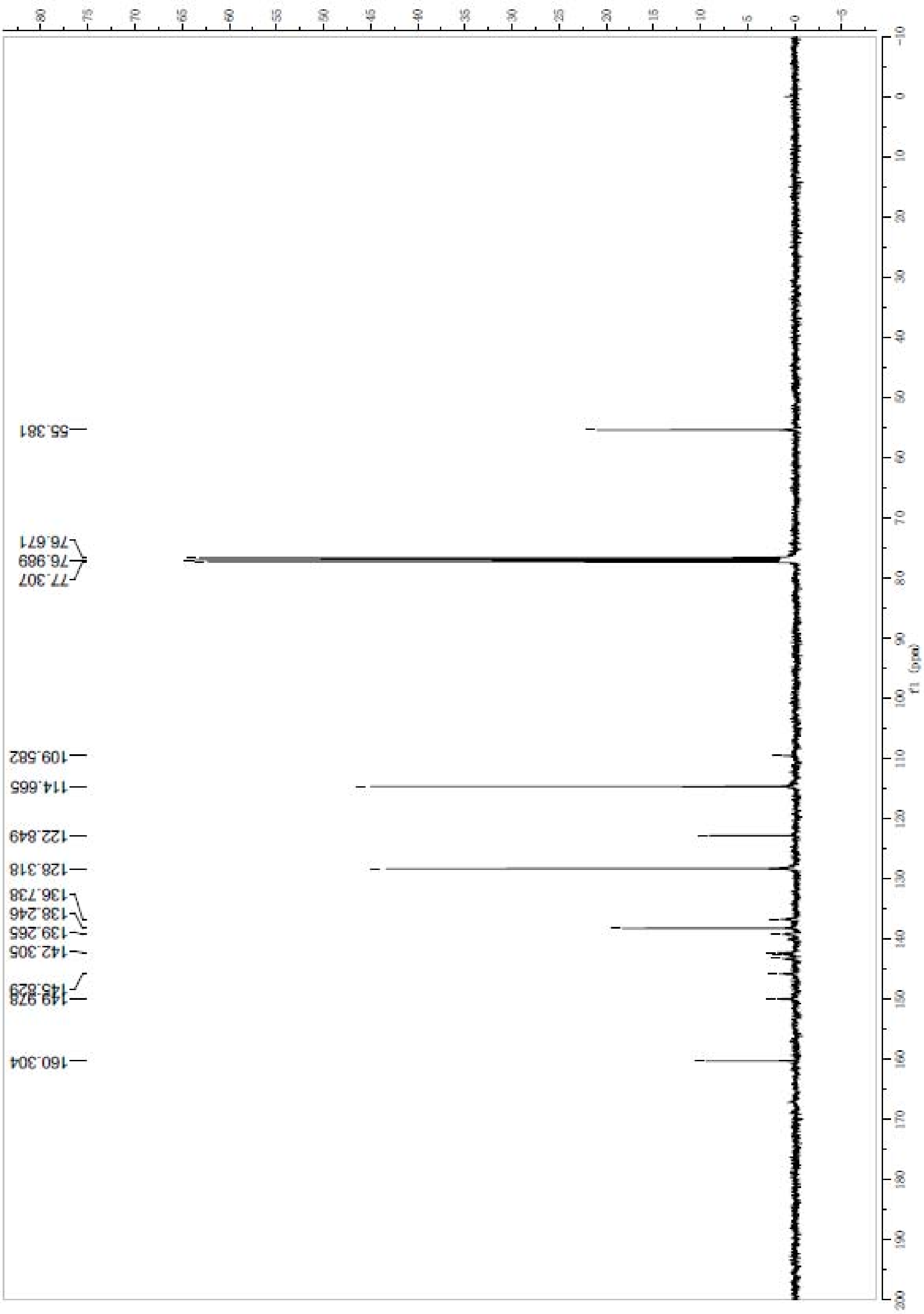

0.06
76.68
76.99
77.30
77.31
109.49
127.00
129.04
129.26
130.31
136.76
139.17
143.34
145.87
150.99
f1 (ppm)

5-(4-Methoxyphenyl)-2-(perfluorophenyl)thiazole (5e)





-139.570
-139.626
-152.464
-152.541
-152.612
-161.442
-161.463
-161.512
-161.533
-161.589
-161.610
-161.624
MeO
Chemical Formula: $C_{14}H_6F_5NOS$
Exact Mass: 331.0090
2.08
2.00
1.07
-135
-140
-145
-150
-155
-160
-165
PPM
:blank line
F1: 282.308
F2: 300.054
SW1: 64935
OF1: -23998.2
PTS1d: 19449 , 32768
USER: -- DATE: Jun 19 2012
EX: s2pul
PW: 6.0 us
PD: 1.5 sec
NA: 32
LB: 0.0
Nuts - FSL-27-61F_19Jun2012


55.381
76.671
76.969
77.307
109.582
114.665
122.849
128.318
136.738
138.246
139.265
142.305
160.304
f1 (ppm)