

## An “on-water” exploration of CuO nano particle catalysed synthesis of 2-aminobenzothiazoles

Saroj Kumar Rout, Srimanta Guin, Jayashree Nath and Bhisma K. Patel\*

Department of Chemistry, Indian Institute of Technology Guwahati

Email: patel@iitg.ernet.in

### List of Contents

1. General information and procedure	S1
2. Crystallographic description	S2 – S4
3. Spectral data of all compounds	S5 – S17
4. Spectra ( $^1\text{H}$ NMR, $^{13}\text{C}$ NMR, HRMS)	S18 – S48

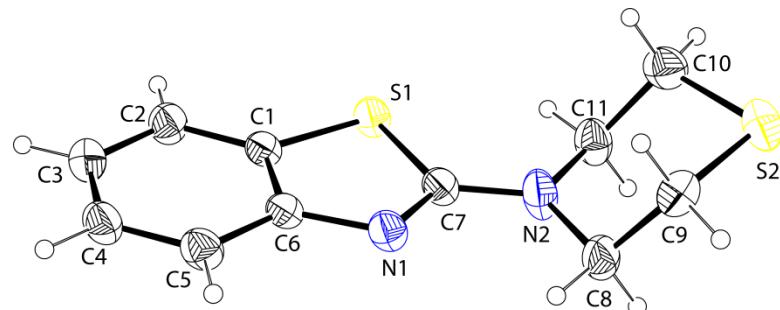
### General information:

All the reagents were commercial grade and purified according to the established procedures. Organic extracts were dried over anhydrous sodium sulphate. Solvents were removed in a rotary evaporator under reduced pressure. Silica gel (60–120 mesh size) was used for the column chromatography. Reactions were monitored by TLC on silica gel 60 F<sub>254</sub> (0.25mm). NMR spectra were recorded in CDCl<sub>3</sub> and DMSO-d<sub>6</sub> with tetramethylsilane as the internal standard for  $^1\text{H}$  NMR (400 MHz) CDCl<sub>3</sub> and DMSO-d<sub>6</sub> solvent as the internal standard for  $^{13}\text{C}$  NMR (100 MHz). Mass spectra were recorded using WATERS MS system, Q-tof premier and data analyzed using Mass Lynx 4.1. Specific rotations were recorded on Perkin Elmer instruments model 343 polarimeter. Elemental analysis was performed with a Perkin Elmer 2400 elemental analyzer. Melting points were recorded on Buchi B-545 melting point apparatus and are uncorrected. IR spectra were recorded in KBr or neat on a Nicolet Impact 410 spectrophotometer.

### Crystallographic Description:

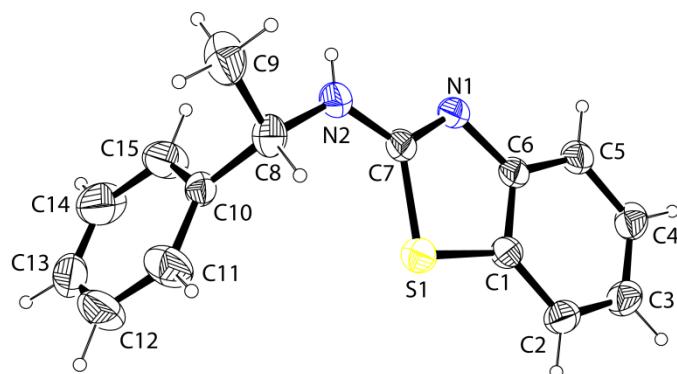
Crystal data were collected with Bruker Smart Apex-II CCD diffractometer using graphite monochromated MoK $\alpha$  radiation ( $\lambda = 0.71073 \text{ \AA}$ ) at 298 K. Cell parameters were retrieved using SMART<sup>[a]</sup> software and refined with SAINT<sup>[a]</sup> on all observed reflections. Data reduction was performed with the SAINT software and corrected for Lorentz and polarization effects. Absorption corrections were applied with the program SADABS<sup>[b]</sup>. The structure was solved by direct methods implemented in SHELX-97<sup>[c]</sup> program and refined by full-matrix least-squares methods on F2. All non-hydrogen atomic positions were located in difference Fourier maps and refined anisotropically. The hydrogen atoms were placed in their geometrically generated positions. colorless crystals were isolated in rectangular shape from acetonitrile at room temperature.

- a. SMART V 4.043 Software for the CCD Detector System; Siemens Analytical Instruments Division: Madison, WI, 1995.
- b. SAINT V 4.035 Software for the CCD Detector System; Siemens Analytical Instruments Division: Madison, WI, 1995.
- c. Sheldrick, G. M. SHELXL-97, Program for the Refinement of Crystal Structures; University of Göttingen: Göttingen (Germany), **1997**



**Fig. 3** ORTEP view of **2-Thiomorpholinobenzo[d]thiazole (1b)**

**Crystallographic description of 2-Thiomorpholinobenzo[*d*]thiazole (**1b**):** C<sub>11</sub>H<sub>12</sub>N<sub>2</sub>S<sub>2</sub>, crystal dimensions 0.42 x 0.35 x 0.28 mm,  $M_r = 236.37$ , monoclinic, space group P 21/c,  $a = 10.130(2)$ ,  $b = 8.1511(15)$ ,  $c = 13.600(2)$  Å,  $\alpha = 90^\circ$ ,  $\beta = 93.902(10)^\circ$ ,  $\gamma = 90^\circ$ ,  $V = 1120.4(3)$  Å<sup>3</sup>,  $Z = 4$ ,  $\rho_{\text{calcd}} = 1.401$  mg/m<sup>3</sup>,  $\mu = 0.442$  mm<sup>-1</sup>,  $F(000) = 496.0$ , reflection collected / unique = 2761 / 2255, refinement method = full-matrix least-squares on  $F^2$ , final  $R$  indices [ $I > 2\sigma(I)$ ]:  $R_1 = 0.0379$ ,  $wR_2 = 0.1007$ ,  $R$  indices (all data):  $R_1 = 0.0469$ ,  $wR_2 = 0.1069$ , goodness of fit = 1.070. CCDC-876212 for **2-Thiomorpholinobenzo[*d*]thiazole (**1b**)** contains the supplementary crystallographic data for this paper. These data can be obtained free of charge from The Cambridge Crystallographic Data Centre via [www.ccdc.cam.ac.uk/data\\_request/cif](http://www.ccdc.cam.ac.uk/data_request/cif).



**Fig. 3** ORTEP view of *N*-((*R*)-1-phenylethyl)benzo[*d*]thiazol-2-amine (**10q**)

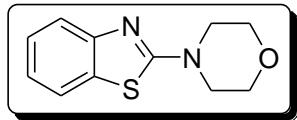
**Crystallographic description of *N*-((*R*)-1-phenylethyl)benzo[*d*]thiazol-2-amine (**10q**):** C<sub>15</sub>H<sub>13</sub>N<sub>2</sub>S, crystal dimensions 0.45 x 0.34 x 0.25 mm,  $M_r = 253.34$ , tetragonal, space group I 41,  $a = 14.9330(16)$ ,  $b = 14.9330(16)$ ,  $c = 12.2771(16)$  Å,  $\alpha = 90^\circ$ ,  $\beta = 90^\circ$ ,  $\gamma = 90^\circ$ ,  $V = 2737.7(5)$  Å<sup>3</sup>,  $Z = 8$ ,  $\rho_{\text{calcd}} = 1.229$  mg/m<sup>3</sup>,  $\mu = 0.220$  mm<sup>-1</sup>,  $F(000) = 1064.0$ , reflection collected / unique = 2726 / 2243, refinement method = full-matrix least-squares on  $F^2$ , final  $R$  indices [ $I > 2\sigma(I)$ ]:  $R_1$

= 0.0553,  $wR_2$  = 0.1214,  $R$  indices (all data):  $R_1$  = 0.0641,  $wR_2$  = 0.1302, goodness of fit = 1.019.

CCDC-829313 for ***N-((R)-1-phenylethyl)benzo[d]thiazol-2-amine (10q)*** contains the supplementary crystallographic data for this paper. These data can be obtained free of charge from The Cambridge Crystallographic Data Centre via [www.ccdc.cam.ac.uk/data\\_request/cif](http://www.ccdc.cam.ac.uk/data_request/cif).

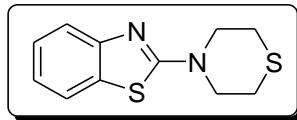
## Spectral Data

### 2-Morpholinobenzo[d]thiazole (1a):



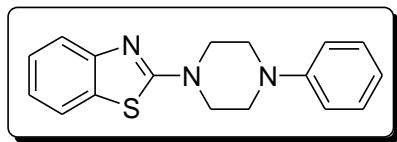
White solid; M.p. 120–122 °C;  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  (ppm) 3.59 (t, 4H,  $J = 4.4$  Hz), 3.80 (t, 4H,  $J = 4.4$  Hz), 7.07 (t, 1H,  $J = 7.6$  Hz), 7.28 (t, 1H,  $J = 8.0$  Hz), 7.57 (dd, 2H,  $J_1 = 6.4$  Hz,  $J_2 = 4.0$  Hz);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ ):  $\delta$  (ppm) 48.6, 66.3, 119.4, 120.9, 121.8, 126.2, 130.7, 152.6, 169.1; IR (KBr): 2918, 2854, 1591, 1537, 1441, 1377, 1289, 1229, 1113, 1067, 1032, 945, 859, 756  $\text{cm}^{-1}$ ; HRMS (ESI) calcd for  $\text{C}_{11}\text{H}_{12}\text{N}_2\text{OS}$  ( $\text{M}+\text{H}$ ) $^+$  221.0743; found 221.0749.

### 2-Thiomorpholinobenzo[d]thiazole (1b):



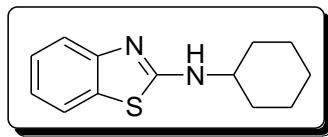
Yellow solid; M.p. 98-99 °C;  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  (ppm) 2.71 (t, 4H,  $J = 5.2$  Hz), 3.93 (t, 4H,  $J = 4.8$  Hz), 7.06 (t, 1H,  $J = 7.2$  Hz), 7.28 (t, 1H,  $J = 8.0$  Hz), 7.52 (d, 1H,  $J = 8.0$  Hz), 7.57 (d, 1H,  $J = 7.6$  Hz);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ ):  $\delta$  (ppm) 26.7, 51.4, 119.3, 120.9, 121.7, 126.2, 130.8, 152.8, 168.2; IR (KBr): 3059, 2936, 2858, 1599, 1531, 1444, 1385, 1359, 1313, 1218, 1054, 1020, 899, 750  $\text{cm}^{-1}$ ; Anal. calcd for  $\text{C}_{11}\text{H}_{12}\text{N}_2\text{S}_2$ : C 55.90, H 5.12, N 11.85; found C 55.88, H 5.17, N 11.79.

**2-(4-Phenylpiperazine-1-yl)benzo[d]thiazole (1c):**



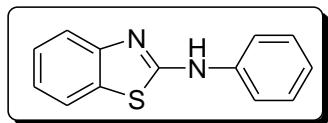
White solid; M.p. 165–167 °C;  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  (ppm) 3.32 (t, 4H,  $J$  = 5.2 Hz), 3.80 (t, 4H,  $J$  = 5.2 Hz), 6.92 (t, 1H,  $J$  = 7.2 Hz), 6.97 (d, 2H,  $J$  = 8.4 Hz), 7.10 (t, 1H,  $J$  = 7.2 Hz), 7.28–7.33 (m, 3H), 7.57–7.63 (m, 2H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ ):  $\delta$  (ppm) 48.4, 49.2, 117.0, 119.4, 120.8, 120.9, 121.7, 126.2, 129.4, 131.0, 151.1, 152.9, 168.8; IR (KBr): 3054, 2838, 1594, 1539, 1504, 1444, 1230, 1158, 1024, 935, 754, 724  $\text{cm}^{-1}$ ; Anal. calcd for  $\text{C}_{17}\text{H}_{17}\text{N}_3\text{S}$ : C 69.12, H 5.80, N 14.22; found C 69.07, H 5.86, N 14.16.

**Benzothiazol-2-yl-cyclohexyl-amine (1d):**



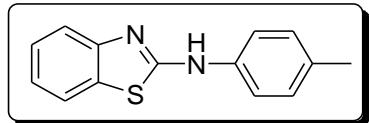
White solid; M.p. 107–108 °C;  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  (ppm) 1.17–1.46 (m, 5H), 1.61–1.65 (m, 1H), 1.73–1.79 (m, 2H), 2.10 (m, 2H), 3.53 (s, 1H), 5.70 (brs, 1H), 7.05 (t, 1H,  $J$  = 8.0 Hz), 7.25–7.29 (m, 1H), 7.51 (d, 1H,  $J$  = 8.0 Hz), 7.56 (d, 1H,  $J$  = 8.0 Hz);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  (ppm) 24.9, 25.6, 33.4, 54.8, 118.8, 119.8, 120.9, 121.4, 123.4, 126.0, 129.2, 167.1; IR (KBr) 3202, 3017, 2927, 2852, 1590, 1538, 1445, 1365, 1345, 1248, 1209, 1076, 885, 804, 746, 720  $\text{cm}^{-1}$ ; Anal. calcd for  $\text{C}_{13}\text{H}_{16}\text{N}_2\text{S}$ : C 67.20, H 6.94, N 12.06; found C 67.16, H 6.98, N 11.99.

**N-Phenylbenzo[d]thiazol-2-amine (1e):**



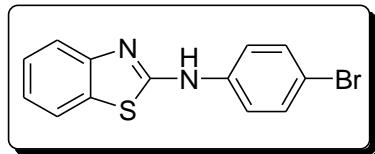
Grey solid; M.p. 156–158 °C;  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  (ppm) 7.11–7.19 (m, 2H), 7.31 (t, 1H,  $J$  = 8 Hz), 7.40 (t, 2H,  $J$  = 8 Hz), 7.50 (d, 2H,  $J$  = 8.8 Hz), 7.54 (d, 1H,  $J$  = 8 Hz), 7.61 (d, 1H,  $J$  = 8 Hz);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ ):  $\delta$  (ppm) 119.4, 120.7, 121.1, 122.5, 124.7, 126.3, 129.8, 130.0, 140.2, 151.5, 165.4; IR (KBr) 3234, 3187, 3128, 3053, 2996, 2935, 1625, 1602, 1571, 1558, 1466, 1429, 1248, 1224, 921, 744, 720, 688, 592  $\text{cm}^{-1}$ ; Anal. calcd for  $\text{C}_{13}\text{H}_{10}\text{N}_2\text{S}$ : C 69.00, H 4.45, N 12.38; found C 69.05, H 4.51, N 12.32.

**Benzothiazol-2-yl-p-tolyl-amine (1f):**



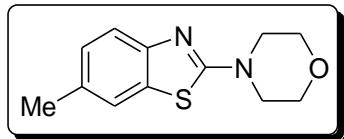
White solid; M.p. 177–178 °C;  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  (ppm) 2.37 (s, 3H), 7.12 (t, 1H,  $J$  = 8.0 Hz), 7.21 (d, 2H,  $J$  = 8.0 Hz), 7.29 (t, 1H,  $J$  = 8.0 Hz), 7.35–7.40 (m, 2H), 7.50 (d, 1H,  $J$  = 8.0 Hz), 7.60 (d, 1H,  $J$  = 7.2 Hz);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  (ppm) 21.1, 119.2, 121.0, 121.5, 122.4, 126.3, 129.7, 130.3, 134.9, 137.5, 151.5, 166.3; IR (KBr) 3183, 3029, 2914, 1624, 1572, 1514, 1447, 1404, 1330, 1271, 1247, 919  $\text{cm}^{-1}$ ; Anal. calcd for  $\text{C}_{14}\text{H}_{12}\text{N}_2\text{S}$ : C 69.97, H 5.03, N 11.66; found C 69.92, H 5.07, N 11.63.

**Benzothiazol-2-yl-(4-bromo-phenyl)-amine (1g):**



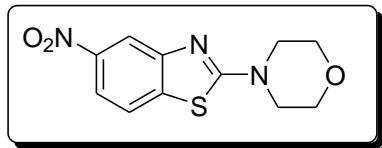
White solid; M.p. 217–218 °C;  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3 + \text{DMSO}-d_6$ )  $\delta$  (ppm) 7.15 (t, 1H,  $J = 7.6$  Hz), 7.32 (t, 1H,  $J = 7.2$  Hz), 7.43 (d, 2H,  $J = 8.8$  Hz), 7.61 (d, 1H,  $J = 8.0$  Hz), 7.66 (d, 1H,  $J = 8.0$  Hz), 7.76 (d, 2H,  $J = 8.8$  Hz), 10.34 (brs, 1H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3 + \text{DMSO}-d_6$ )  $\delta$  (ppm) 114.1, 119.9, 120.2, 120.9, 122.8, 126.1, 130.6, 131.8, 140.4, 152.5, 161.9; IR (KBr) 3174, 3069, 2956, 2899, 1619, 1584, 1562, 1454, 1448, 1445, 1311, 1298, 1270, 1246, 1226, 1076  $\text{cm}^{-1}$ ; Anal. calcd for  $\text{C}_{13}\text{H}_9\text{BrN}_2\text{S}$ : C 51.16, H 2.97, N 9.18; found C 51.12, H 2.94, N 9.25.

**6-Methyl-2-morpholinobenzo[d]thiazole (2a):**



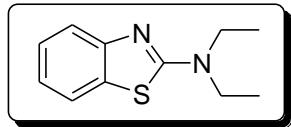
Pale white; Mp 134–136 °C;  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  (ppm) 2.37 (s, 3H), 3.56 (t, 4H,  $J = 4.8$  Hz), 3.79 (t, 4H,  $J = 4.8$  Hz), 7.09 (d, 1H,  $J = 8.0$  Hz), 7.39 (s, 1H), 7.44 (d, 1H,  $J = 8.0$  Hz);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ ):  $\delta$  (ppm) 21.4, 48.6, 66.4, 119.1, 120.9, 127.4, 130.8, 131.6, 150.4, 168.6; IR (KBr): 2963, 2912, 2856, 1599, 1575, 1544, 1464, 1434, 1352, 1281, 1235, 1113, 1026, 943, 811  $\text{cm}^{-1}$ ; HRMS (ESI) calcd for  $\text{C}_{12}\text{H}_{14}\text{N}_2\text{OS} (\text{M}+\text{H})^+$  235.1035; found 235.1035.

**2-Morpholino-5-nitrobenzo[d]thiazole (3a):**



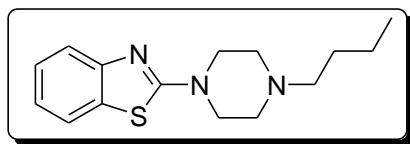
Yellow solid; M.p. 172–174 °C;  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  (ppm) 3.68 (t, 4H,  $J$  = 5.2 Hz), 3.86 (t, 4H,  $J$  = 5.2 Hz), 7.70 (d, 1H,  $J$  = 8.8 Hz), 7.97 (dd, 1H,  $J_1$  = 8.8 Hz,  $J_2$  = 2.4 Hz), 8.35 (ds, 1H,  $J$  = 2.4 Hz);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ ):  $\delta$  (ppm) 48.6, 66.2, 114.0, 116.3, 120.9, 138.0, 147.1, 153.0, 170.4; IR (KBr) 3095, 3064, 3019, 2979, 2913, 2866, 1602, 1539, 1531, 1508, 1343, 1228, 1119, 815, 738, 723  $\text{cm}^{-1}$ ; Anal. calcd for  $\text{C}_{11}\text{H}_{11}\text{N}_3\text{O}_3\text{S}$ : C 49.80, H 4.18, N 15.84; found C 49.83, H 4.14, N 15.78.

***N,N*-Diethylbenzo[d]thiazol-2-amine (4h):**



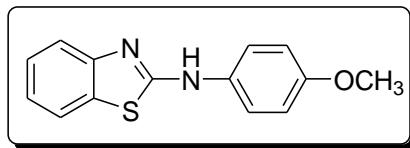
Pale yellow solid; M.p. 113-114 °C;  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  (ppm) 1.26 (m, 6H), 3.55 (m, 4H), 7.03 (t, 1H,  $J$  = 8.0 Hz), 7.27 (t, 1H,  $J$  = 8.0 Hz), 7.57 (m, 2H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ ):  $\delta$  (ppm) 12.9, 45.4, 118.6, 120.6, 120.7, 125.8, 130.7, 153.3, 167.4; IR (KBr): 3056, 2972, 2931, 2862, 1596, 1561, 1542, 1444, 1360, 1315, 1260, 1135, 1079, 1013, 750  $\text{cm}^{-1}$ ; HRMS (ESI) calcd for  $\text{C}_{11}\text{H}_{14}\text{N}_2\text{S} (\text{M}+\text{H})^+$  207.0687; found 207.0687.

**2-(4-Butylpiperazin-1-yl)benzo[d]thiazole (4i):**



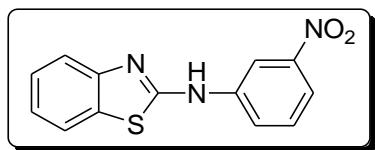
White solid; M.p. 92–93 °C;  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  (ppm) 0.94 (t, 3H,  $J$  = 7.2 Hz), 1.35 (sextet, 2H,  $J$  = 7.6 Hz), 1.51 (quin, 2H,  $J$  = 7.2 Hz), 2.40 (t, 2H,  $J$  = 7.6 Hz), 2.57 (t, 4H,  $J$  = 5.2 Hz), 3.66 (t, 4H,  $J$  = 5.2 Hz), 7.07 (t, 1H,  $J$  = 7.6 Hz), 7.29 (t, 1H,  $J$  = 7.6 Hz), 7.55 (d, 1H,  $J$  = 8.0 Hz), 7.60 (d, 1H,  $J$  = 8.4 Hz);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ ):  $\delta$  (ppm) 14.2, 20.9, 29.1, 48.5, 52.7, 58.6, 119.2, 120.9, 121.5, 126.2, 130.9, 152.9, 168.9; IR (KBr): 3047, 2955, 2935, 2860, 2814, 1601, 1544, 1445, 1347, 1291, 1245, 1235, 1127, 749, 722  $\text{cm}^{-1}$ ; Anal. Calcd for  $\text{C}_{15}\text{H}_{21}\text{N}_3\text{S}$ : C 65.41, H 7.69, N 15.26; found C 65.35, H 7.63, N 15.19.

**Benzothiazol-2-yl-(4-methoxy-phenyl)-amine (4j):**



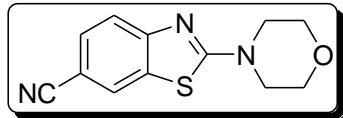
Grey solid; M.p. 160–161 °C;  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  (ppm) 3.84 (s, 3H), 6.95 (d, 2H,  $J$  = 8.8 Hz), 7.12 (t, 1H,  $J$  = 7.2 Hz), 7.31 (t, 1H,  $J$  = 7.2 Hz), 7.40 (d, 2H,  $J$  = 8.8 Hz), 7.54 (d, 1H,  $J$  = 8.0 Hz), 7.59 (d, 1H,  $J$  = 8.0 Hz);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ ):  $\delta$  (ppm) 55.8, 115.0, 119.3, 121.0, 122.3, 124.1, 126.3, 130.3, 133.1, 152.0, 157.6, 166.8; IR (KBr): 3181, 2835, 1619, 1572, 1511, 1444, 1414, 1241, 1037, 918  $\text{cm}^{-1}$ ; Anal. calcd for  $\text{C}_{14}\text{H}_{12}\text{N}_2\text{OS}$ : C 65.60, H 4.72, N 10.93; found C 65.64, H 4.69, N 10.99.

**N-(3-Nitrophenyl)benzo[d]thiazol-2-amine (4k):**



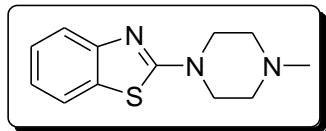
Yellow solid; M.p. 189–190 °C;  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3 + \text{DMSO-d}_6$ ):  $\delta$  (ppm) 7.23–7.26 (m, 1H), 7.41 (t, 1H,  $J = 8.0$  Hz), 7.54 (t, 1H,  $J = 8.0$  Hz), 7.70 (d, 1H,  $J = 8.0$  Hz), 7.74 (d, 1H,  $J = 8.0$  Hz), 7.96 (t, 2H,  $J = 7$  Hz), 8.56 (s, 1H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3 + \text{DMSO-d}_6$ ):  $\delta$  (ppm) 111.7, 115.5, 119.3, 120.0, 122.1, 123.0, 125.2, 129.0, 129.7, 141.3, 147.9, 151.3, 160.6; IR (KBr): 3226, 3181, 3073, 2947, 1619, 1567, 1532, 1460, 1445, 1351, 1243, 885, 745, 718  $\text{cm}^{-1}$ ; HRMS (ESI) calcd for  $\text{C}_{13}\text{H}_9\text{N}_3\text{O}_2\text{S}$  ( $\text{M}+\text{H}$ ) $^+$  272.0488; found 272.0472.

**2-Morpholinobenzo[d]thiazole-6-carbonitrile (6a):**



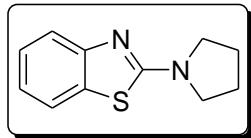
White solid; M.p. 173–175 °C;  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  (ppm) 3.57 (t, 4H,  $J = 4.8$  Hz), 3.74 (t, 4H,  $J = 4.4$  Hz), 7.42 (s, 2H), 7.75 (s, 1H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ ):  $\delta$  (ppm) 48.5, 66.0, 103.9, 119.3, 124.9, 130.0, 131.1, 155.9, 162.5, 171.0; IR (KBr): 2906, 2861, 2224, 1526, 1554, 1434, 1325, 1286, 1226, 1194, 1118, 1067, 1028, 949, 838  $\text{cm}^{-1}$ . HRMS (ESI) calcd for  $\text{C}_{12}\text{H}_{11}\text{N}_3\text{OS}$  ( $\text{M}+\text{H}$ ) $^+$  246.0702; found 246.0649.

**2-(4-Methylpiperazin-1-yl)benzo[d]thiazole (7l):**



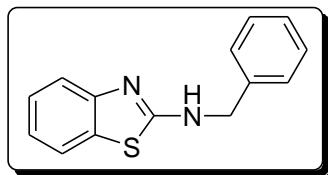
White solid; M.p. 94–95 °C;  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  (ppm) 2.36 (s, 3H), 2.55 (t, 4H,  $J$  = 5.2 Hz), 3.67 (t, 4H,  $J$  = 5.2 Hz), 7.08 (t, 1H,  $J$  = 8.0 Hz), 7.30 (t, 1H,  $J$  = 7.2 Hz), 7.55–7.61 (m, 2H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ ):  $\delta$  (ppm) 46.2, 48.2, 54.2, 119.1, 120.7, 121.4, 126.0, 130.8, 152.7, 168.7; IR (KBr): 3052, 2938, 2884, 2844, 2807, 1593, 1530, 1445, 1375, 1334, 1293, 1214, 1140, 1002, 748, 726  $\text{cm}^{-1}$ ; Anal. Calcd for  $\text{C}_{12}\text{H}_{15}\text{N}_3\text{S}$ : C 61.77, H 6.48, N 18.01; found C 61.74, H 6.45, N 18.07.

**2-(Pyrrolidin-1-yl)benzo[d]thiazole (7m):**



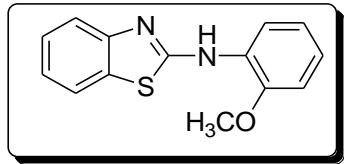
White solid; M.p. 101–103 °C;  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  (ppm) 2.04 (m, 4H), 3.57 (s, 4H), 7.02 (t, 1H,  $J$  = 7.6 Hz), 7.26 (t, 1H,  $J$  = 8.0 Hz), 7.57 (t, 2H,  $J$  = 8.0 Hz);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ ):  $\delta$  (ppm) 25.8, 49.8, 118.9, 120.9, 121.2, 126.2, 130.6, 153.2, 165.6; IR (KBr): 2924, 2851, 16, 1544, 1442, 1363, 1314, 1278, 1166, 1119, 853  $\text{cm}^{-1}$ . Anal. Calcd for  $\text{C}_{11}\text{H}_{12}\text{N}_2\text{S}$ : C 64.67, H 5.92, N 13.71; found C 64.61, H 5.96, N 13.76.

**N-Benzylbenzo[d]thiazol-2-amine (7n):**



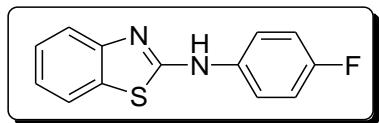
White solid; M.p. 163–165 °C;  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  (ppm) 4.63 (s, 2H), 6.36 (brs, 1H), 7.08 (t, 1H,  $J$  = 7.2 Hz), 7.25–7.47 (brm, 7H), 7.57 (d, 1H,  $J$  = 8.0 Hz);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ ):  $\delta$  (ppm) 49.6, 119.1, 121.0, 121.8, 126.2, 127.9, 128.1, 129.0, 130.6, 137.7, 152.5, 167.9; IR (KBr) 3183, 3085, 2980, 2897, 2853, 1620, 1574, 1447, 1355, 1268, 972, 743, 724, 698, 673  $\text{cm}^{-1}$ ; Anal. calcd for  $\text{C}_{14}\text{H}_{12}\text{N}_2\text{S}$ : C 69.97, H 5.03, N 11.66; found C 69.93, H 5.06, N 11.59.

**N-(2-Methoxyphenyl)benzo[d]thiazol-2-amine (7o):**



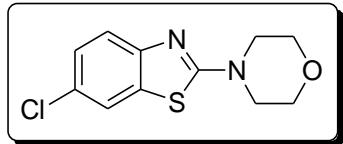
Grey solid; M.p. 146–148 °C;  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  (ppm) 3.86 (s, 3H), 6.88–6.90 (m, 1H), 7.01–7.04 (m, 2H), 7.15 (t, 1H,  $J$  = 8 Hz), 7.34 (t, 1H,  $J$  = 8 Hz), 7.63 (d, 1H,  $J$  = 8 Hz), 7.68 (d, 1H,  $J$  = 8 Hz), 8.26–8.28 (m, 1H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ ):  $\delta$  (ppm) 55.9, 110.4, 118.1, 120.1, 120.9, 121.3, 122.7, 123.1, 126.2, 129.6, 130.5, 148.1, 152.2, 162.5; IR (KBr) 3469, 3177, 3074, 2934, 1612, 1566, 1443, 1433, 1255, 1114, 1018, 755  $\text{cm}^{-1}$ ; Anal. calcd for  $\text{C}_{14}\text{H}_{12}\text{N}_2\text{OS}$ : C 65.60, H 4.72, N 10.93; found C 65.54, H 4.77, N 10.86.

**N-(4-Fluorophenyl)benzo[d]thiazol-2-amine (7p):**



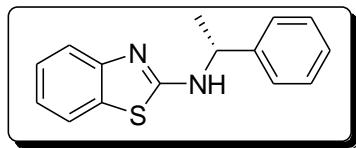
White solid; M.p. 196–197 °C;  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3 + \text{DMSO}-d_6$ ):  $\delta$  (ppm) 7.03 (t, 2H,  $J = 8.4$  Hz), 7.13 (t, 1H,  $J = 7.6$  Hz), 7.31 (t, 1H,  $J = 8$  Hz), 7.62 (d, 2H,  $J = 8$  Hz), 7.71–7.75 (m, 2H), 9.65 (brs, 1H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3 + \text{DMSO}-d_6$ ):  $\delta$  (ppm) 115.2, 115.4, 119.3, 120.0, 120.1, 120.4, 122.0, 125.6, 130.2, 136.8, 152.2, 162.5; IR (KBr) 3443, 3194, 3136, 3054, 2910, 1626, 1574, 1511, 1455, 1445, 1216, 921, 834, 745, 722  $\text{cm}^{-1}$ ; Anal. calcd for  $\text{C}_{13}\text{H}_9\text{FN}_2\text{S}$ : C 63.92, H 3.71, N 11.47; found C 63.98, H 3.76, N 11.42.

**6-Chloro-2-morpholinobenzo[d]thiazole (9a):**



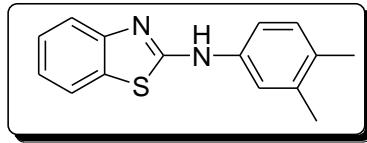
White solid; M.p. 122–124 °C  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  (ppm) 3.56 (t, 4H,  $J = 4.8$  Hz), 3.81 (t, 4H,  $J = 4.8$  Hz), 7.18 (dd, 1H,  $J_1 = 8.4$  Hz,  $J_2 = 2.0$  Hz), 7.43 (d, 1H,  $J = 8.4$  Hz), 7.69 (d, 1H,  $J = 2.0$  Hz);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ ):  $\delta$  (ppm) 48.6, 66.3, 119.4, 121.5, 121.9, 129.0, 132.1, 153.8, 170.1; IR (KBr): 3051, 2978, 2902, 2855, 1737, 1587, 1530, 147, 1375, 1325, 1279, 1234, 1142, 1116, 1070, 1035, 885, 872, 808, 678  $\text{cm}^{-1}$ ; HRMS (ESI) calcd for  $\text{C}_{11}\text{H}_{11}\text{N}_2\text{OSCl}(\text{M}+\text{H})^+$  255.0446; found 255.0448.

**N-((R)-1-Phenylethyl)benzo[d]thiazol-2-amine (10q):**



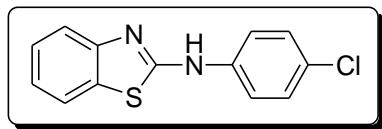
Yellow solid; M.p. 160-161 °C;  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  (ppm) 1.61 (d, 3H,  $J$  = 6.8 Hz), 4.75 (q, 1H,  $J$  = 6.8 Hz), 7.02 (t, 1H,  $J$  = 7.6 Hz), 7.21–7.27 (m, 2H), 7.31 (t, 2H,  $J$  = 7.6 Hz), 7.38, (d, 2H,  $J$  = 7.6 Hz), 7.47-7.52 (m, 2H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ ):  $\delta$  (ppm) 24.0, 55.8, 118.9, 121.0, 121.5, 126.0, 126.3, 127.7, 128.9, 130.7, 143.2, 152.1, 167.8; IR (KBr) 3444, 3178, 3077, 2965, 1605, 1569, 1556, 1445, 1309, 1271, 1207, 1141, 1122, 751, 700  $\text{cm}^{-1}$ ; Anal. calcd for  $\text{C}_{15}\text{H}_{14}\text{N}_2\text{S}$ : C 70.83, H 5.55, N 11.01; found C 70.78, H 5.49, N 10.98.

**N-(3,4-Dimethylphenyl)benzo[d]thiazol-2-amine (10r):**



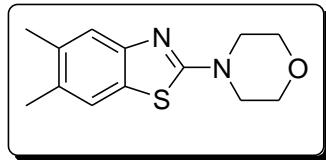
White solid; M.p. 140-142 °C;  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  (ppm) 2.27 (s, 3H), 2.28 (s, 3H), 7.10-7.17 (m, 2H), 7.22 (brs, 2H), 7.30 (t, 1H,  $J$  = 7.6 Hz), 7.53 (d, 1H,  $J$  = 8.4 Hz), 7.60 (d, 1H,  $J$  = 8 Hz);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ ):  $\delta$  (ppm) 19.4, 20.1, 118.9, 119.1, 121.0, 122.1, 123.0, 126.2, 129.9, 130.8, 133.5, 137.9, 138.2, 151.6, 166.7; IR (KBr) 3436, 3227, 3183, 1623, 1569, 1467, 1272, 1249, 887, 737, 717  $\text{cm}^{-1}$ ; Anal. calcd for  $\text{C}_{15}\text{H}_{14}\text{N}_2\text{S}$ : C 70.83, H 5.55, N 11.01; found C 70.78, H 5.58, N 10.95.

**N-(4-Chlorophenyl)benzo[d]thiazol-2-amine (10s):**



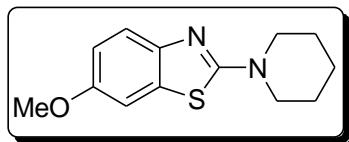
White solid; M.p. 114–116 °C;  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3 + \text{DMSO}-d_6$ ):  $\delta$  (ppm) 7.19 (t, 1H,  $J = 8$  Hz), 7.34–7.38 (m, 3H), 7.50 (d, 2H,  $J = 8.8$  Hz), 7.64 (t, 2H,  $J = 7.6$  Hz);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3 + \text{DMSO}-d_6$ ):  $\delta$  (ppm) 119.2, 119.3, 120.2, 122.0, 125.5, 126.3, 128.4, 130.0, 139.2, 151.9, 161.6; IR (KBr) 3444, 3054, 1567, 1474, 1434, 1315, 1250, 1089, 1012, 964, 828, 756, 731, 692  $\text{cm}^{-1}$ ; Anal. calcd for  $\text{C}_{13}\text{H}_9\text{ClN}_2\text{S}$ : C 59.88, H 3.48, N 10.74; found C 59.96, H 3.45, N 10.69.

**6,6-Dimethyl-2-morpholinobenzo[d]thiazole (11a):**



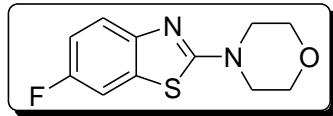
Brown solid; M.p. 156–158 °C;  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  (ppm) 2.30 (s, 3H), 2.31 (s, 3H), 3.59 (t, 4H,  $J = 5.2$  Hz), 3.83 (t, 4H,  $J = 4.8$  Hz), 7.37 (s, 2H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ ):  $\delta$  (ppm) 20.0, 20.3, 48.7, 66.4, 120.3, 121.2, 128.0, 130.7, 135.1, 151.1, 168.9; IR (KBr) 2966, 2892, 2857, 1530, 1443, 1375, 1283, 1227, 1114, 1020, 899, 857  $\text{cm}^{-1}$ ; HRMS (ESI) calcd for  $\text{C}_{13}\text{H}_{16}\text{N}_2\text{OS} (\text{M}+\text{H})^+$  249.1161; found 249.1164.

**6-Methoxy-2-(piperdin-1-yl)benzo[d]thiazole (12t):**



White solid; M.p. 96–97 °C;  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  (ppm) 1.63 (brs, 6H), 3.51 (brs, 4H), 3.76 (s, 3H), 6.87 (dd, 1H,  $J$  = 8.4, 2.4 Hz), 7.11 (s, 1H), 7.44 (d, 1H,  $J$  = 8.8 Hz);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ ):  $\delta$  (ppm) 24.2, 25.3, 49.6, 55.8, 105.2, 113.4, 119.2, 131.6, 147.8, 154.8, 167.6; IR (KBr): 2934, 2922, 2849, 1588, 1534, 1440, 1382, 1332, 1257, 1234, 1209, 1120, 1018, 749  $\text{cm}^{-1}$ ; Anal. Calcd for  $\text{C}_{13}\text{H}_{16}\text{N}_2\text{OS}$ : C 62.87, H 6.49, N 11.28; found C 62.81, H 6.56, N 11.21.

**6-Fluoro-2-morpholinobenzo[d]thiazole (13a):**

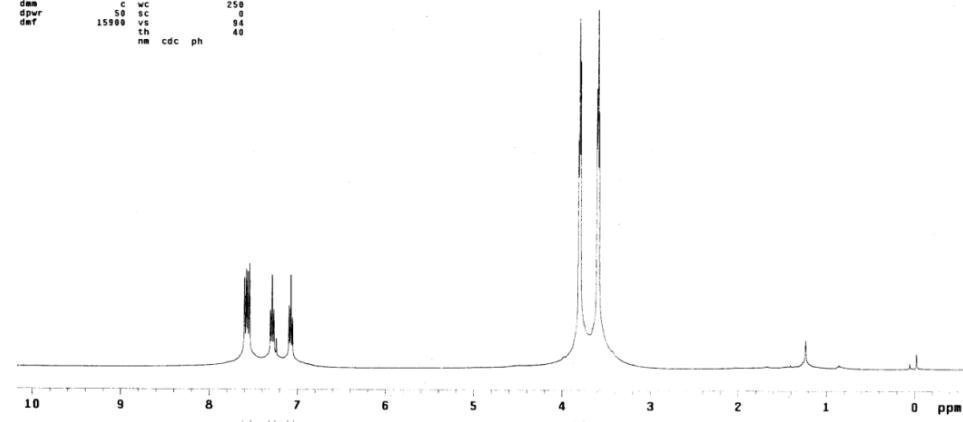


White solid; M.p. 157–158 °C;  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  (ppm) 3.51 (t, 4H,  $J$  = 4.8 Hz), 3.75 (t, 1H,  $J$  = 4.4 Hz), 6.97 (m, 1H), 7.25 (m, 1H), 7.44 (m, 1H);  $^{13}\text{CNMR}$  (100 MHz,  $\text{CDCl}_3$ ):  $\delta$  (ppm) 48.4, 66.2, 107.4, 107.7, 113.7, 113.9, 119.7, 119.8, 131.3, 131.4, 148.9, 157.0, 159.4, 168.6; IR (KBr): 2982, 2901, 2863, 1673, 1597, 1538, 1459, 1376, 1343, 1287, 1234, 1181, 1111, 1073, 1029, 948, 920, 844  $\text{cm}^{-1}$ ; HRMS (ESI) calcd for  $\text{C}_{11}\text{H}_{11}\text{N}_2\text{OSF}$  ( $\text{M}+\text{H}$ ) $^+$  239.0655; found 239.0651.

## Spectra

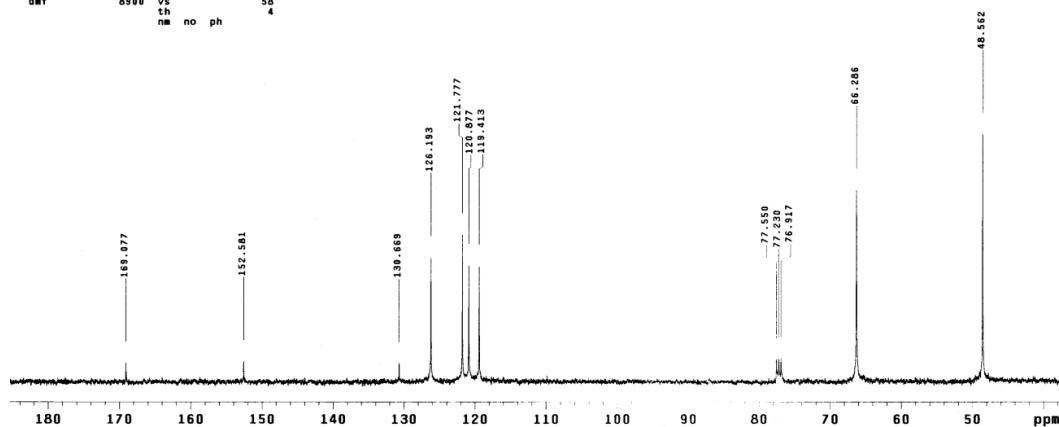
### 2-Morpholinobenzo[*d*]thiazole (1a): $^1\text{H}$ NMR (400 MHz, $\text{CDCl}_3$ ):

```
exp1 s2pul
SAMPLE          SPECIAL
date   Oct 7 2010 temp    not used
solvent        CDCl3 gain    not used
file      exp  spin    not used
ACQUISITION   hst    0.000
sw       6300.0  sp    15.000
at       1.000  a1fa   20.000
np      25528   FLAGs
fb       not used  t1    n
bs        4      in    n
d1      1.000  dp    y
dt       32     hs    nn
ct       32     PROCESSING nn
TRANSMITTER  1b    1.00
tn      H1    fn    6536
sfrq    399.853  DISPLAY
tot     362.0  sp    -252.4
tpwr    57     wpt   4943.8
pw      9.859  rfp   3698.1
DECOUPLER   rfp   2894.9
dn      C13   12    0
dof      0     1p   -74.2
dm      mm    PLOT
da      c     wc   250
dpwr    15900  sc    0
dmtf    15900  th   94
nm    cdc  ph   40
```

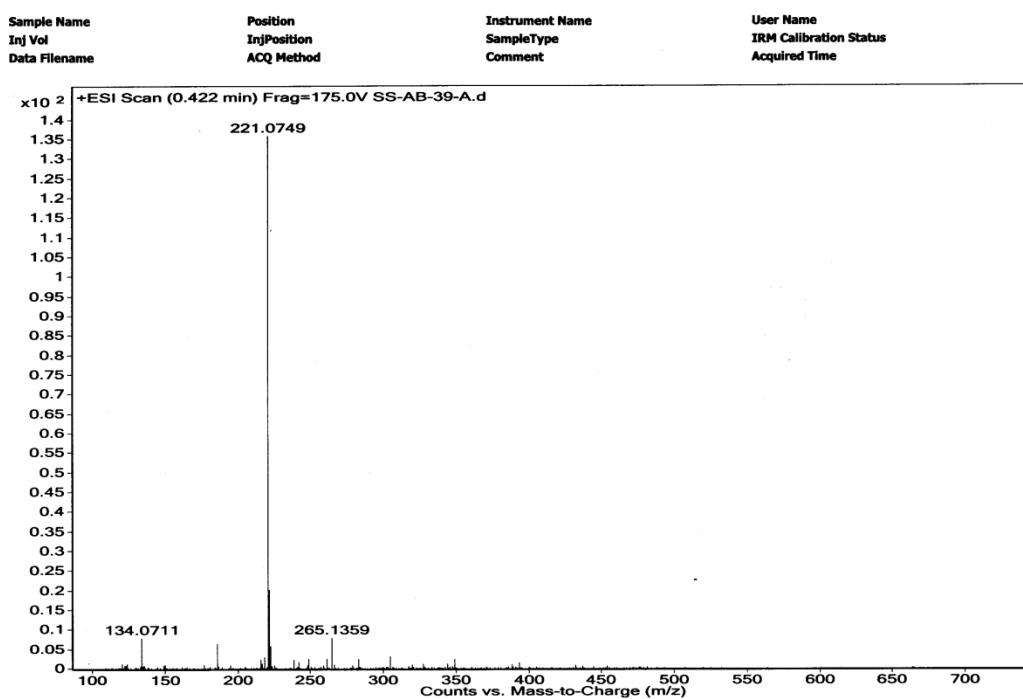


### 2-Morpholinobenzo[*d*]thiazole (1a): $^{13}\text{C}$ NMR (100 MHz, $\text{CDCl}_3$ ):

```
exp1 s2pul
SAMPLE          SPECIAL
date   Oct 11 2010 temp    not used
solvent        CDCl3 gain    not used
file      exp  spin    not used
ACQUISITION   hst    0.000
sw       25125.6  sp    18.000
at       1.199  a1fa   20.000
np      60270   FLAGs
fb       1380.0  t1    n
bs        16     in    n
d1      1.000  dp    y
nt      5000  hs    nn
ct       512     PROCESSING nn
TRANSMITTER  1b    2.00
tn      C13   fn    6536
sfrq    100.654  DISPLAY
tot     1536.3  sp    3727.7
tpwr    61     wpt   14549.5
pw      9.300  rfp   7764.9
DECOUPLER   rfp   -44.7
dn      H1    rfp   -345.1
dof      0     1p   -345.1
dm      yy    PLOT
da      w     wc   250
dpwr    8900   sc    0
dmtf    8900   th   55
nm    no   ph   4
```

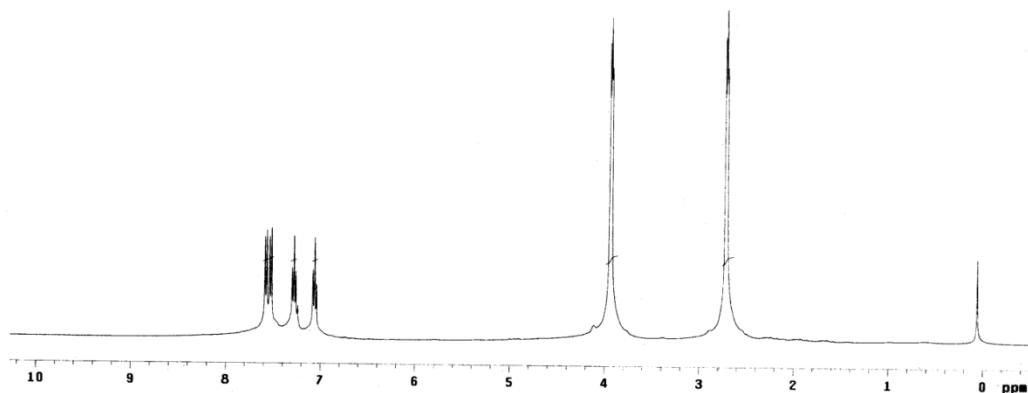


**2-Morpholinobenzo[*d*]thiazole (1a): MASS SPECTRA:**

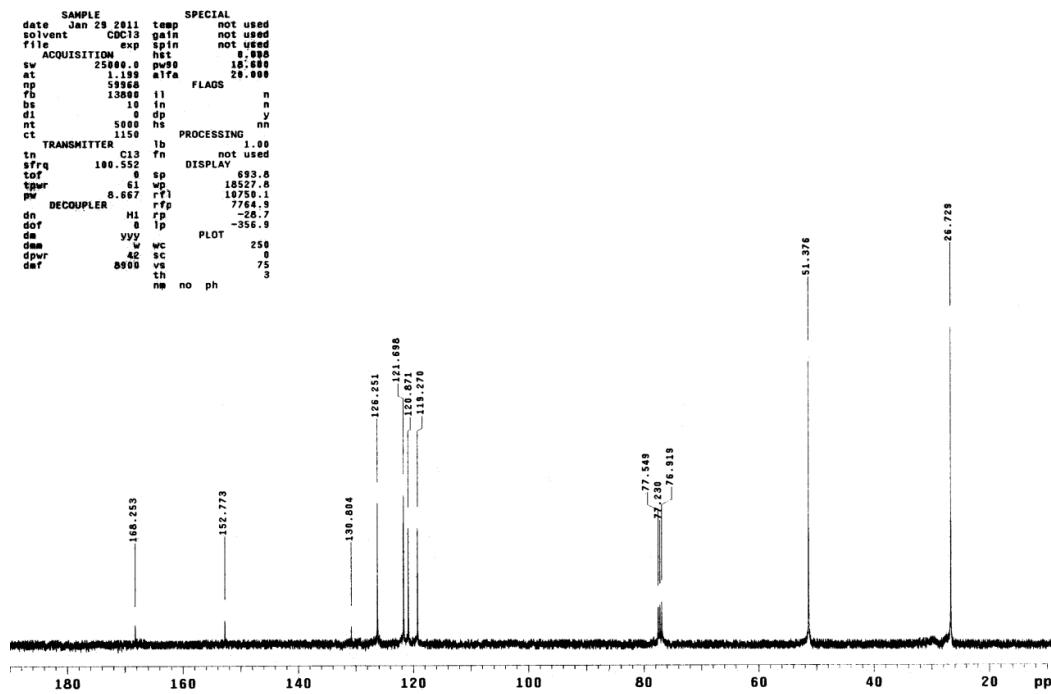


**2-Thiomorpholinobenzo[*d*]thiazole (1b):  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):**

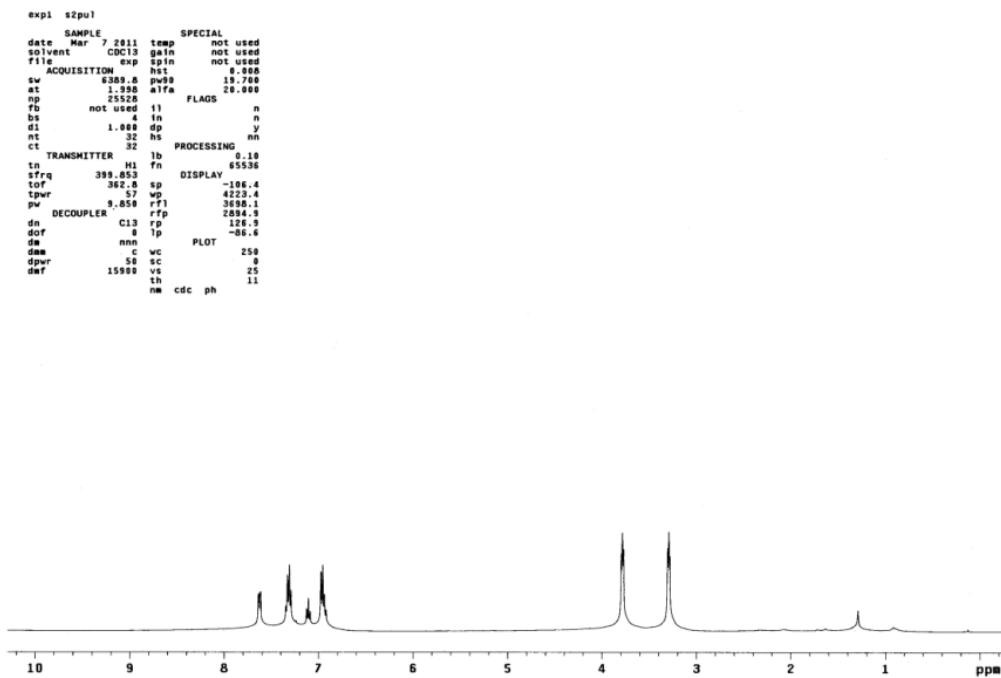
```
exp1 stdih
      SAMPLE      SPECIAL
date Jan 29 2011 temp    not used
solvent   CDCl3  gain    not used
file     exp    fn      not used
        ACQUISITION hst    8.988
        sw      6000.0 pw90  19.700
        at      1.000 a1fa  29.000
        np      23984  FLAGS
        tb      not used  t1      n
        ba      not used  tn      n
        di      1.000  dp      y
        nt      32    hs      nn
        ct      32    PROCESSING nn
        TRANSMITTER fn    not used
        tn      H1    DISPLAY
        stfQ    399.653 sp      -288.6
        tcf    100.000  fp      288.6
        tPwR    57    rrf1  3885.6
        Pw      7.000  rfp   2811.3
        DECOUPLER C13  1p      131.2
        dn      C13  1p      -71.8
        dof      0    PLOT
        dso      nm   wc      259
        das      c    sc      8
        dPwr    50    vs      83
        dAr     15980 th      20
                    nm cdc ph
```



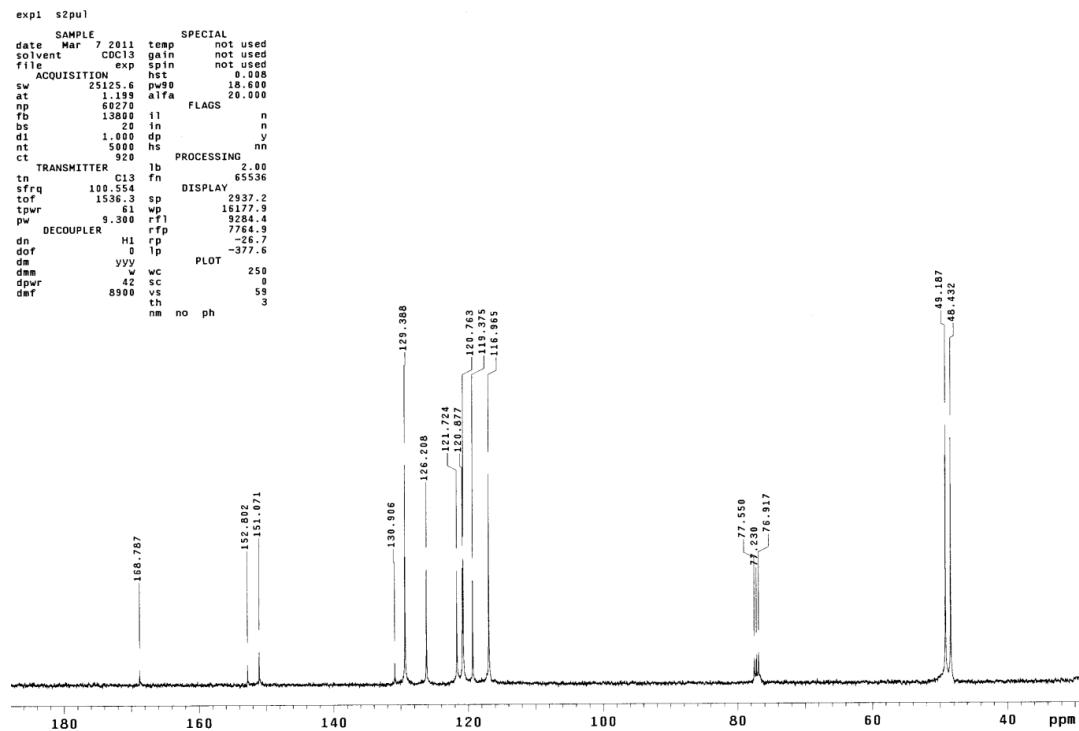
**2-Thiomorpholinobenzo[d]thiazole (1b):  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ ):**



**2-(4-Phenylpiperazine-1-yl)benzo[d]thiazole (1c):  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):**



**2-(4-Phenylpiperazine-1-yl)benzo[d]thiazole (1c):  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ ):**

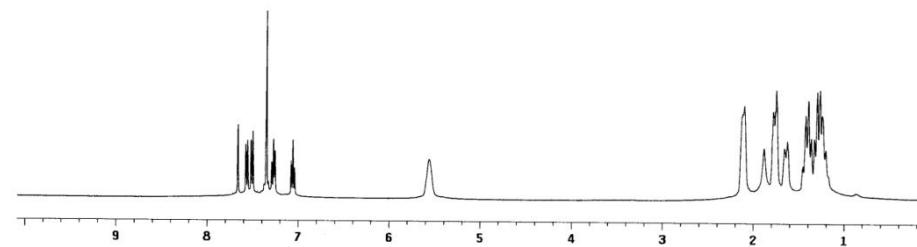


**Benzothiazol-2-yl-cyclohexyl-amine (1d):  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):**

```

exp1 s2pu1
SAMPLE SPECIAL
date May 28 2011 temp not used
solvent CDCl3 gain not used
file exp1 exp not used
ACQUISITION hst 0.005
sw 6389.8 pw90 15.700
at 25.28 alfa 26.000
np 25528 FLAGS
rb not used 11 n
bs 1.000 in n
d1 1.000 dp y
nt 32 hs nn
ct 32 PROCESSING
TRANSMITTER H1 fn 0.10
tn H1 fn 65536
sfrq 399.553 DISPLAY
tof 362.8 sp -416.7
tpwr 57 wp 4459.0
pw 9.856 rfi 794.5
DECOUPLER C13 rfp 0
dn C13 rfp 110.4
dof 0 1p -81.1
ds nno PLOT
dss c wc 250
dpwr 50 sc 0
dmf 15900 vs 65
th th 20
nm cdc ph

```

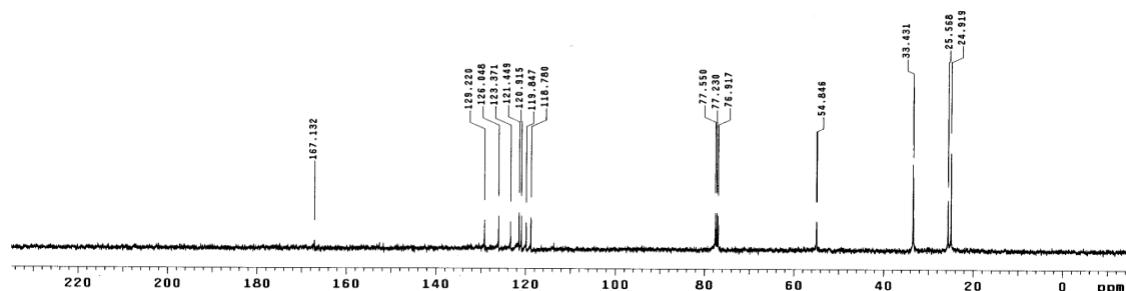


**Benzothiazol-2-yl-cyclohexyl-amine (1d):  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ ):**

```

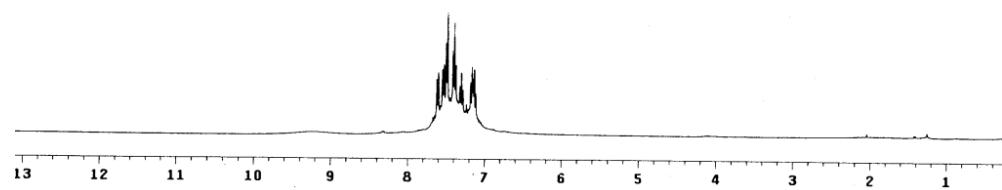
exp1 s2pu1
SAMPLE SPECIAL
date May 29 2011 temp not used
solvent CDCl3 gain not used
file exp1 exp not used
ACQUISITION hst 0.005
sw 2512.5 pw90 15.800
at 25.199 pw10 29.000
np 66270 FLAGS
rb 13800 il n
bs 13800 in n
d1 1.000 dp y
nt 32 hs nn
ct 672 PROCESSING
TRANSMITTER C13 lb 2.00
tn C13 lb 65536
sfrq 100.554 DISPLAY
tof 1536.3 sp -1509.5
tpwr 50 wp 2630.5
pw 9.300 rfi 3274.4
DECOUPLER C13 rfp 7764.9
dn H1 rfp 0 25 -235.3
dof 0 1p
ds vvy PLOT
dss c wc 250
dpwr 42 sc 0
dmf 8900 vs 25
th th 2
nm no ph

```



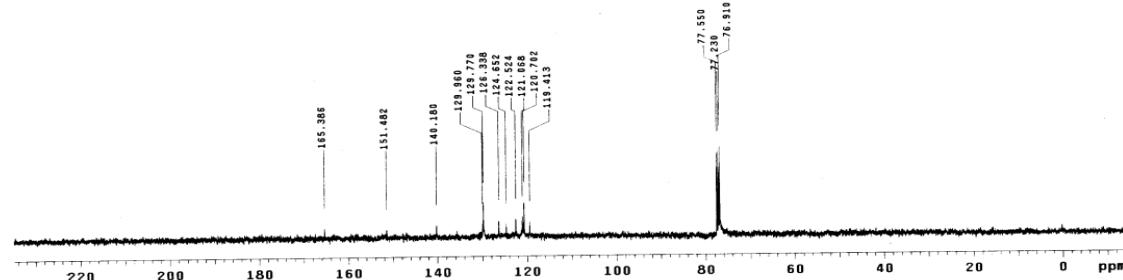
**N-Phenylbenzo[d]thiazol-2-amine (1e):  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):**

```
expt s2pul
SAMPLE SPECIAL
date Jun 18 2011 temp not used
solvent CDCl3 gain not used
file ACQUISITION exp spin not used
ACQUISITION hst 0.008
sw 639.8 pw90 15.000
at 1.998 alfa 20.000
np 25528 FLAGS
t0 not used t1 n
bs 4 in n
d1 1.000 dp y
nt 32 hs nn
ct 32 PROCESSING
TRANSMITTER lb 0.10
tn H1 fn 65536
sfrq 399.853 DISPLAY
tof 362.8 sp -527.1
tpwr 5 rp 5835.5
pw 9.850 rfp 604.0
DECOUPLER rfp 0
dn C13 rp 117.0 f
dof 1P -90.1
dm nnn PLOT
dme c wc 250
dpwr 50 sc 0
dmr 15900 vs 66
dtm th 20
nm cdc ph
```

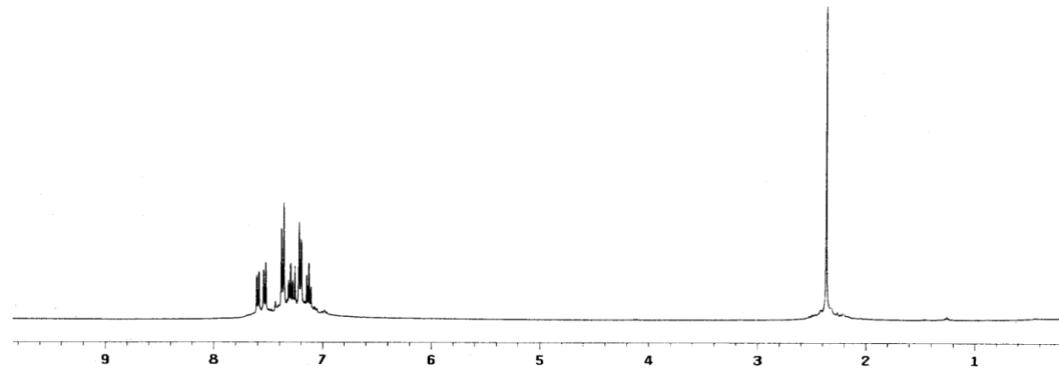


**N-Phenylbenzo[d]thiazol-2-amine (1e):  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ ):**

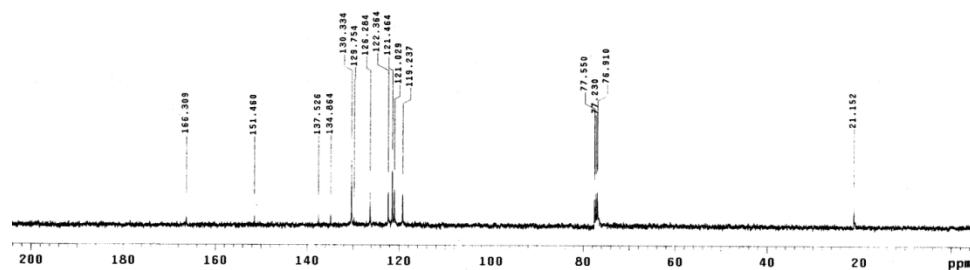
```
expt s2pul
SAMPLE SPECIAL
date Jun 18 2011 temp not used
solvent CDCl3 gain not used
file ACQUISITION exp spin not used
ACQUISITION hst 0.008
sw 25125.8 pw90 15.000
at 1.998 alfa 20.000
np 60270 FLAGS
t0 1360.0 t1 n
bs 32 in n
d1 1.000 dp y
nt 500 hs nn
ct 672 PROCESSING
TRANSMITTER lb 2.00
tn C13 fn 65536
sfrq 100.554 DISPLAY
tof 1536.3 sp -1508.0
tpwr 63 wp 2214.6
pw 9.000 rfp 9272.9
DECOUPLER rfp 7764.9
dn H1 rp -90.1
dof 0 p -271.4
dm vyy PLOT
dme v wc 250
dpwr 42 sc 0
dmr 8900 vs 22
dtm th 20
nm no ph
```



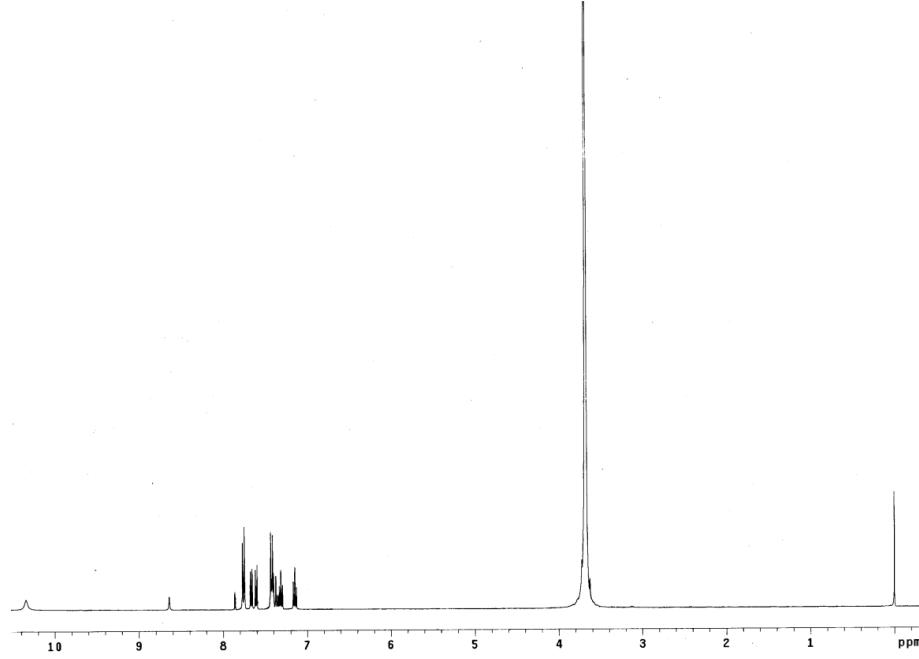
**Benzothiazol-2-yl-p-tolyl-amine (1f):  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):**



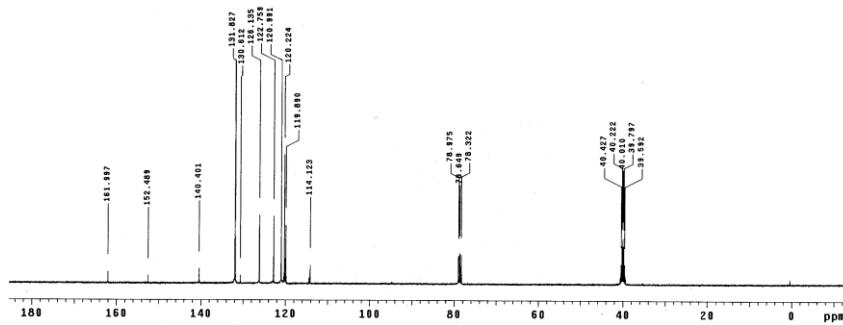
**Benzothiazol-2-yl-*p*-tolyl-amine (1f):**  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ ):



**Benzothiazol-2-yl-(4-bromo-phenyl)-amine (1g):**  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3 + \text{DMSO}-d_6$ )

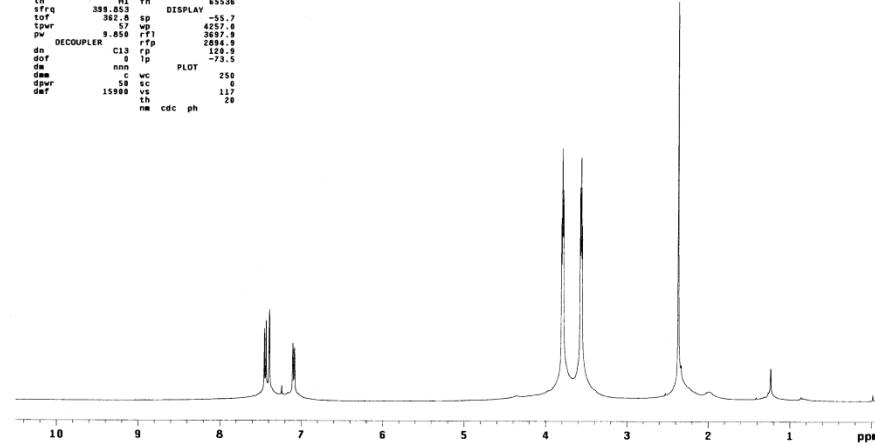


Benzothiazol-2-yl-(4-bromo-phenyl)-amine (1g): <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub> + DMSO-d<sub>6</sub>)



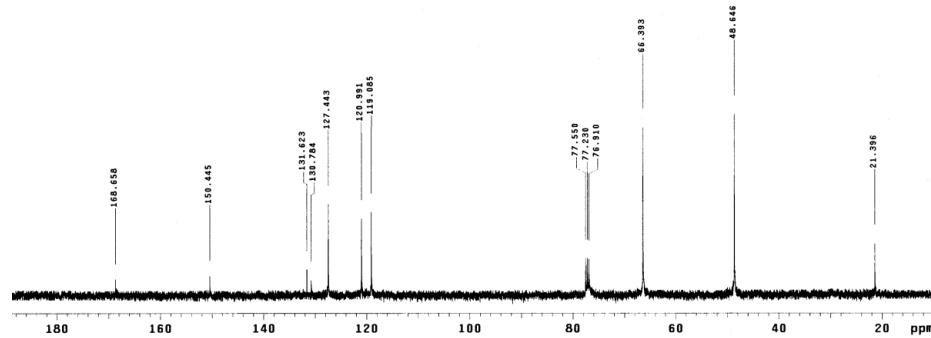
6-Methyl-2-morpholinobenzo[d]thiazole (2a): <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>):

```
exp1 s2pul
SAMPLE          SPECIAL
date Sep 30 2010 temp not used
solvent   CDCl3 gain not used
file      ex1 spin not used
ACQUISITION hst    0.005
sw       6389.5   hz
at        25228   alfa  20.000
np        25228   flags
rb       not used  t1
ds        32      in
dt       1.000   dp
n1        32      hs
nt        32      nn
ct        32      PROCESSING
TRANSMITTER H1   rp
tn       139.53   fm
sfrq    399.653  sp   DISPLAY 55.7
t0f      360.000  sp
t0r      57      wp
tpw     9.650   r1
pw       9.650   r1
DECOUPLER   C13   rp
dp       200.000
dn       C13   rp
d1       128.9   ip
dd       nnn   PLOT
de       vvv   250
dm       50    ec
dprw   15990   vs
def      15990   th
nm cdc ph
```

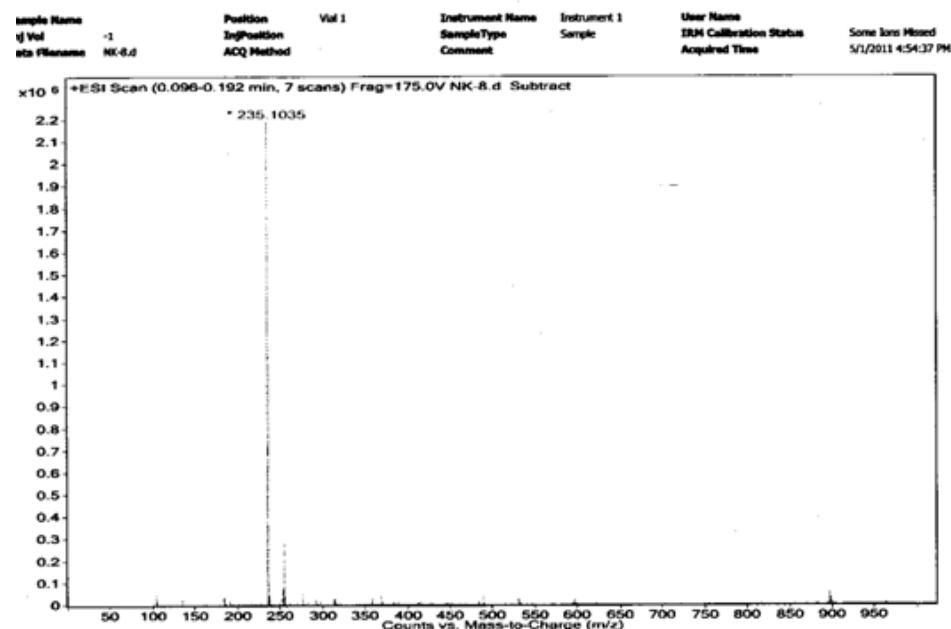


**6-Methyl-2-morpholinobenzo[*d*]thiazole (2a):  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ ):**

```
exp1 s2pul
SAMPLE          SPECIAL
date Sep 30 2010 temp not used
solvent   CDCl3 gain not used
file      ex1 spin not used
ACQUISITION hst    0.005
sw       25125.5   hz
at        139.53   alfa  10.000
np        66270   flags
rb       139.53   t1
ds        16      in
dt       1.000   dp
n1        16      hs
nt        560   nn
ct        560   PROCESSING
TRANSMITTER H1   rp
tn       139.53   fm
sfrq    100.554  sp   DISPLAY 65536
t0f      153.000  sp
t0r      61      wp
tpw     9.300   r1
pw       9.300   r1
DECOUPLER   C13   rp
dp       200.000
dn       H1   rp
d1       -33.0   ip
de       vvv   250
dm       50    ec
dprw   8590   vs
def      8590   th
nm no ph
```

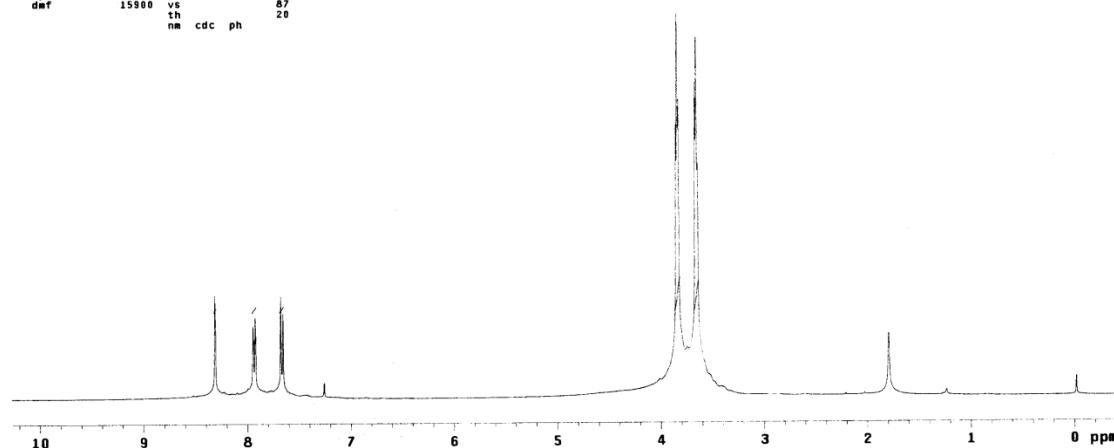


**6-Methyl-2-morpholinobenzo[*d*]thiazole (2a): MASS SPECTRA:**

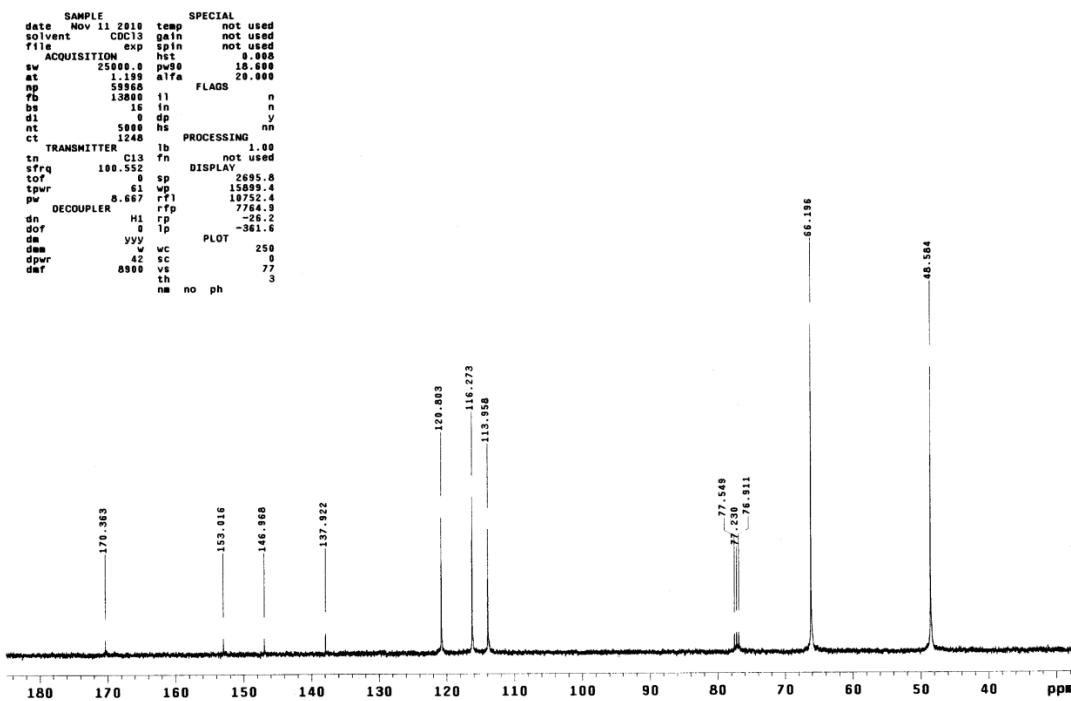


**2-Morpholino-5-nitrobenzo[d]thiazole (3a):  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):**

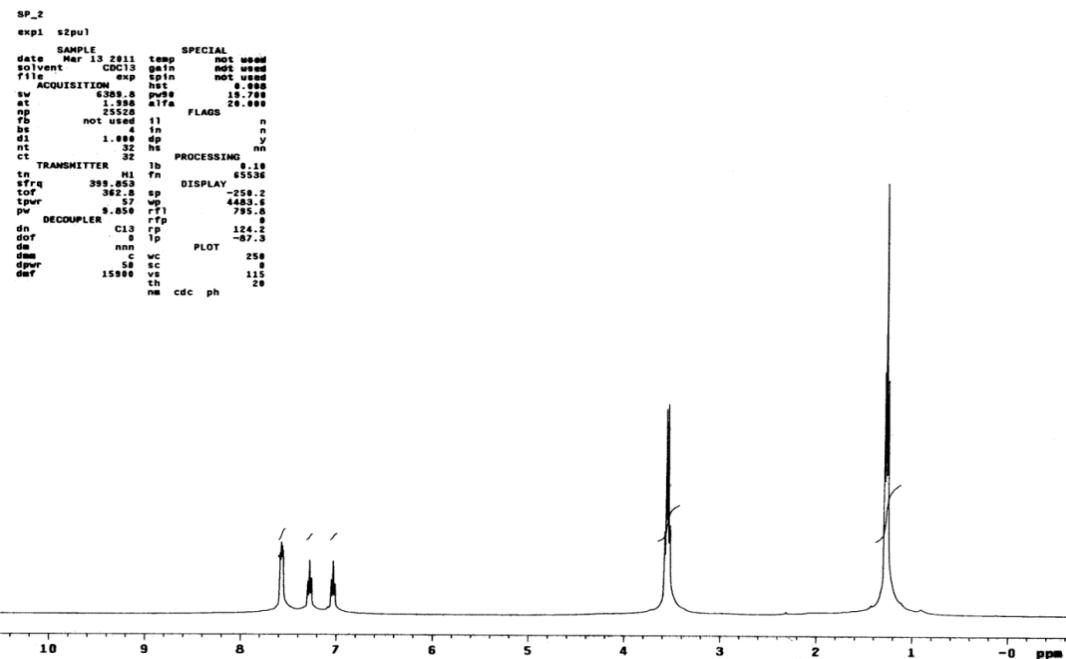
```
exp1 s2pu1
SAMPLE          SPECIAL
date Nov 11 2010 temp    not used
solvent   CDCl3  gain    not used
rfif     1000   exp  spin  not used
        hst      0.008
ACQUISITION      pw90    15.700
        6389.8   15.700
        25528   28.000
        25528   FLAGS
        not used 11      n
        1.000   0n      y
        32      hs      y
        32      nn      n
TRANSMITTER      1b      0.10
        H1      65536
        399.853  DISPLAY
        362.8   sp      -182.9
        57      w1      4298.5
        9.850   r1      795.6
DECOUPLER        rfp
        C13    rfp     121.1
        0      1p      -83.0
        nm      PLOT
dss      c      wc     250
dpvr    50      sc      0
dmf    15900   vs      87
        th      20
        nm      cdc ph
```



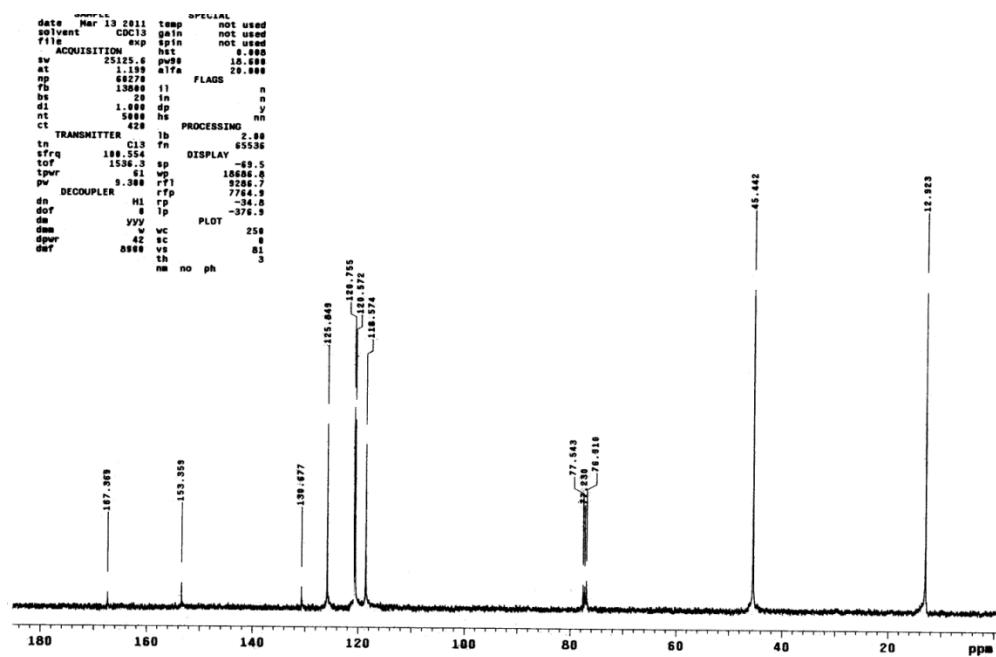
**2-Morpholino-5-nitrobenzo[d]thiazole (3a):  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ ):**



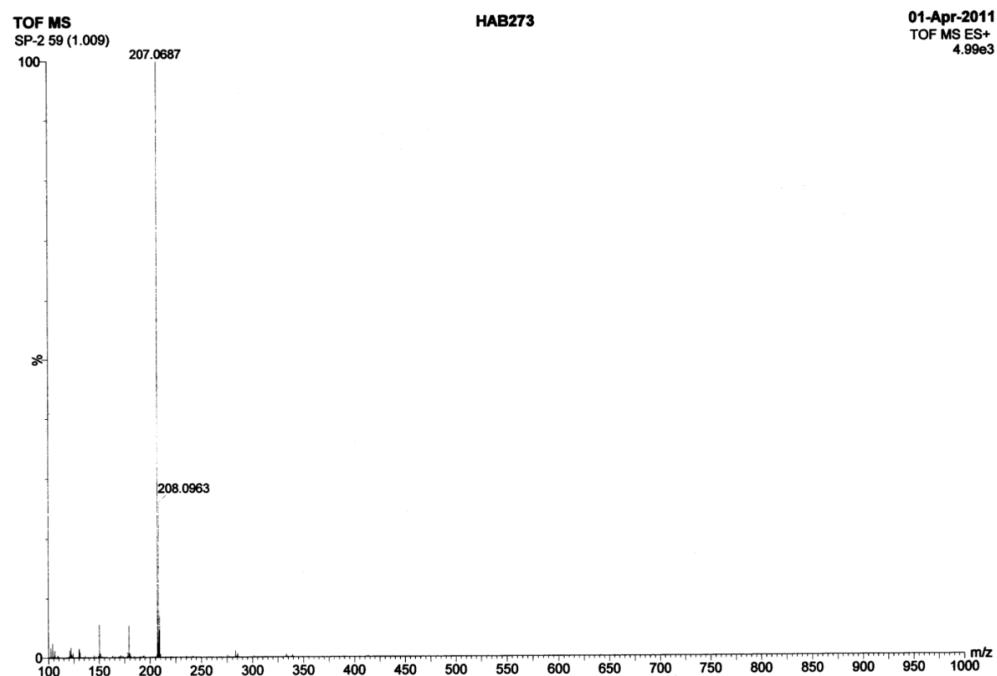
**N,N-Diethylbenzo[d]thiazol-2-amine (4h): <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>):**



**N,N-Diethylbenzo[d]thiazol-2-amine (4h): <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>):**



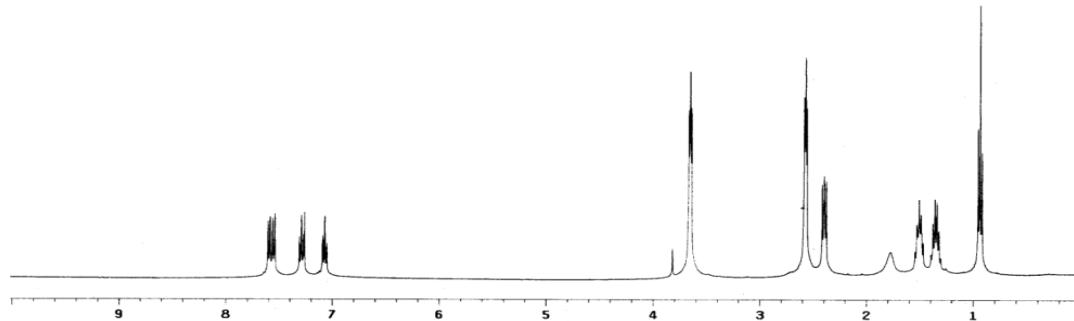
#### **N,N-Diethylbenzo[d]thiazol-2-amine (4h): MASS SPECTRA:**



**2-(4-Butylpiperazin-1-yl)benzo[d]thiazole (4i):**  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):

```

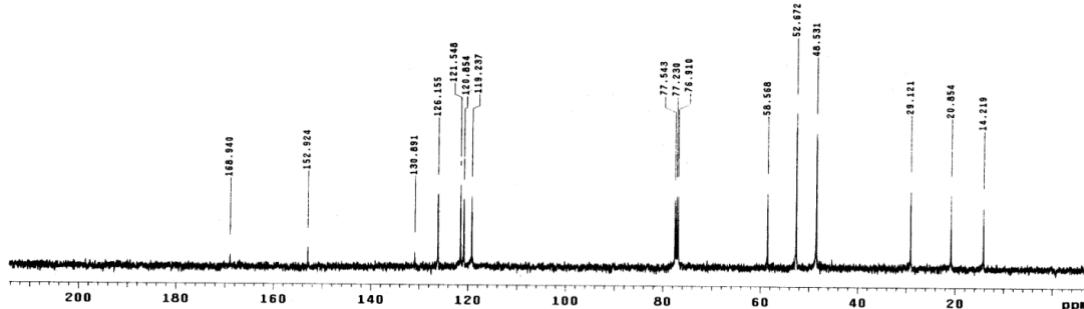
expt s2pul
SAMPLE      SPECIAL
date Mar 24 2011 temp not used
solvent CDCl3 gain not used
file exp spin not used
ACQUISITION exp width 8.000
sw 6389.5 bwpp 19.700
at 2.998 alfa 20.000
np 256 flags
fb not used 11 n
bs 1.000 tdp n
di 1.000 dp v
nt 32 ns nn
ct 32 PROCESSING
TRANSMITTER 32 lb 0.10
tn H1 fn 65536
sfrq 399.850 DISPLAY -358.2
tot 362.8 sp 4374.5
tpwr 57 vp 792.0
pw 9.633 rfp 0
DECOUPLER
dn C13 rp 111.2
dof 6 ip -98.9
dmf nnn p 0
dme c vc 250
dpwr 50 vs 0
dpr 15900 ts 778
dmt 0 th 6
nm cdc ph
    
```



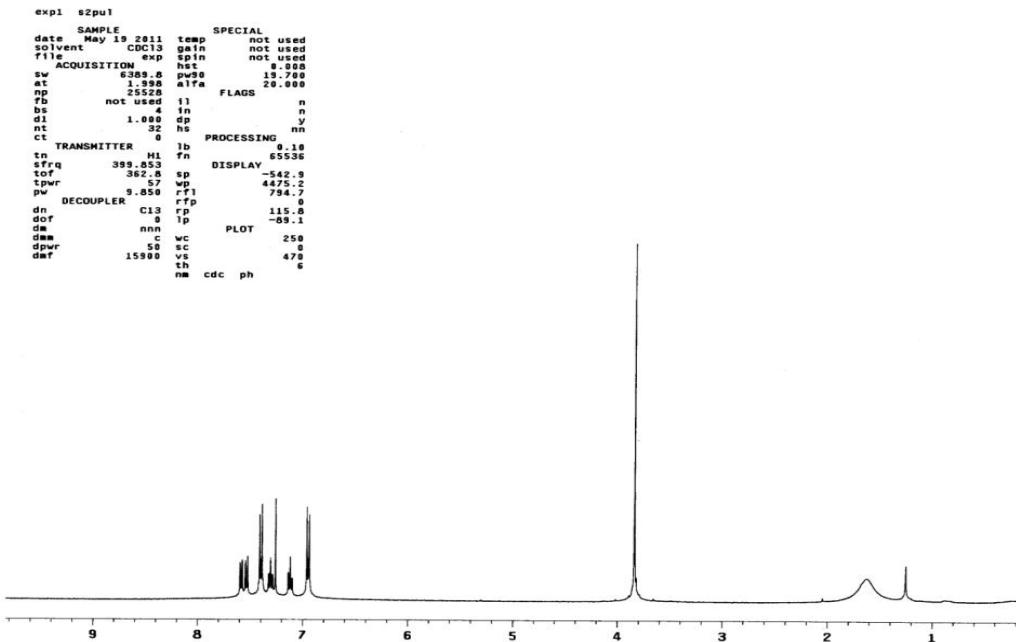
**2-(4-Butylpiperazin-1-yl)benzo[d]thiazole (4i):  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ ):**

```

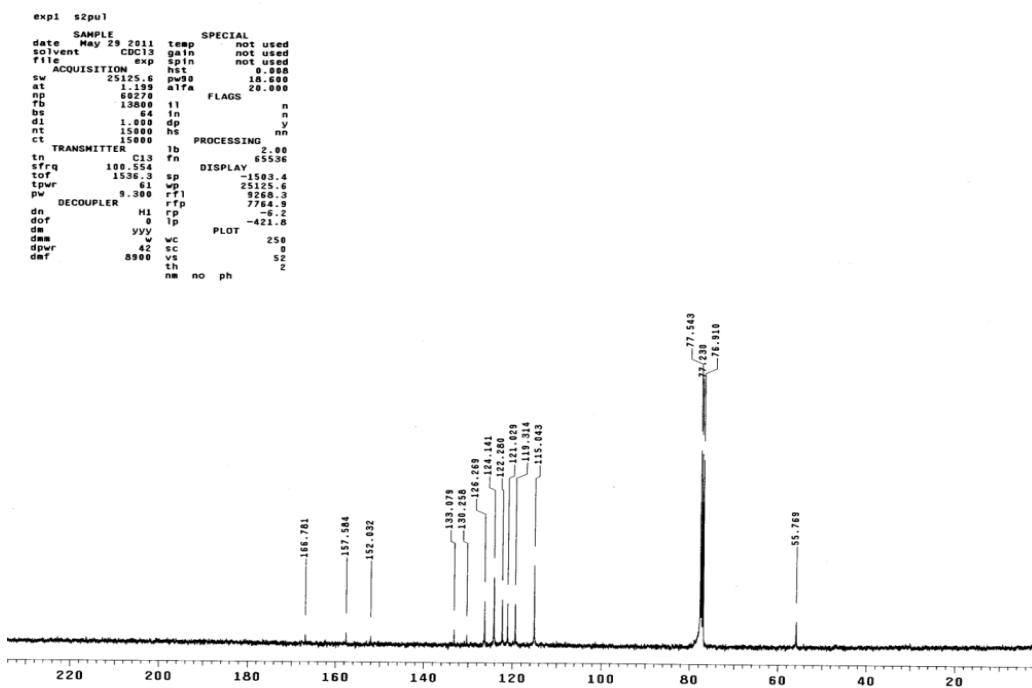
expt s2pul
SAMPLE      SPECIAL
date Mar 30 2011 temp not used
solvent CDCl3 gain not used
file exp spin not used
ACQUISITION exp het 8.000
sw 25125.6 bwpp 20.000
at 1.199 alfa 20.000
np 12800 flags
fb 12800 11 n
bs 1.000 tdp n
di 1.000 dp v
nt 5000 ns nm
ct 1010 PROCESSING 2.00
TRANSMITTER 1b 65536
tn H1 fn 65536
sfrq 100.550 DISPLAY -847.0
tot 1533.3 sp 22385.1
tpwr 61 vp 9272.9
pw 9.390 rfp 777.8
DECOUPLER
dn C13 rp -42.4
dof 6 ip -366.1
dmf vvy p 0
dme c vc 250
dpwr 42 vs 0
dpr 8900 ts 41
dmt 0 no ph 3
    
```



**Benzothiazol-2-yl-(4-methoxy-phenyl)-amine (4j):  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):**



Benzothiazol-2-yl-(4-methoxy-phenyl)-amine (4j): <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>):

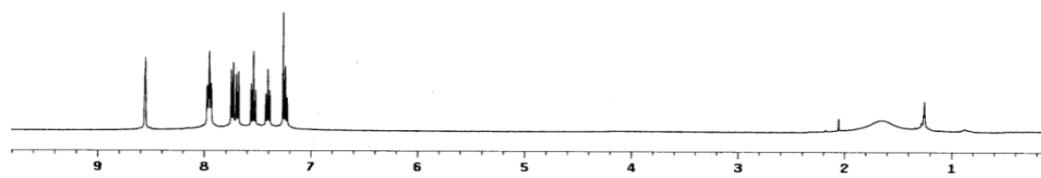


N-(3-Nitrophenyl)benzo[d]thiazol-2-amine (4k): <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub> + DMSO-d<sub>6</sub>):

```

expt s2pu1
SAMPLE          SPECIAL
date  May 19 2011 temp  not used
solvent   CDCl3 gain  not used
file    exp gain  not used
ACQUISITION hst      0.008
        18.500
sw       6389.8  flags
at       1.995  18.780
np      256.000
        28.980
fb      not used  11   n
bs        4   in
di       1.000  dp
nt       32   hs
ct       32   PROCESSING
        1b
TRANSMITTER H1  fn  655.36
tn      C13  fp  117.7
        2.19
        -88.4
dof      0
de      nme
dme      c  wc  250
dpwr     50  sc  0
dmt     15900  vs  459
        th  20
        nm  cdc ph

```

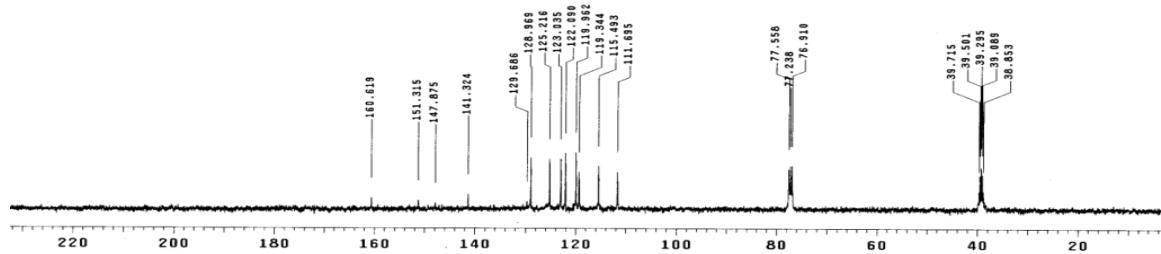


**N-(3-Nitrophenyl)benzo[d]thiazol-2-amine (4k):  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3 + \text{DMSO}-d_6$ ):**

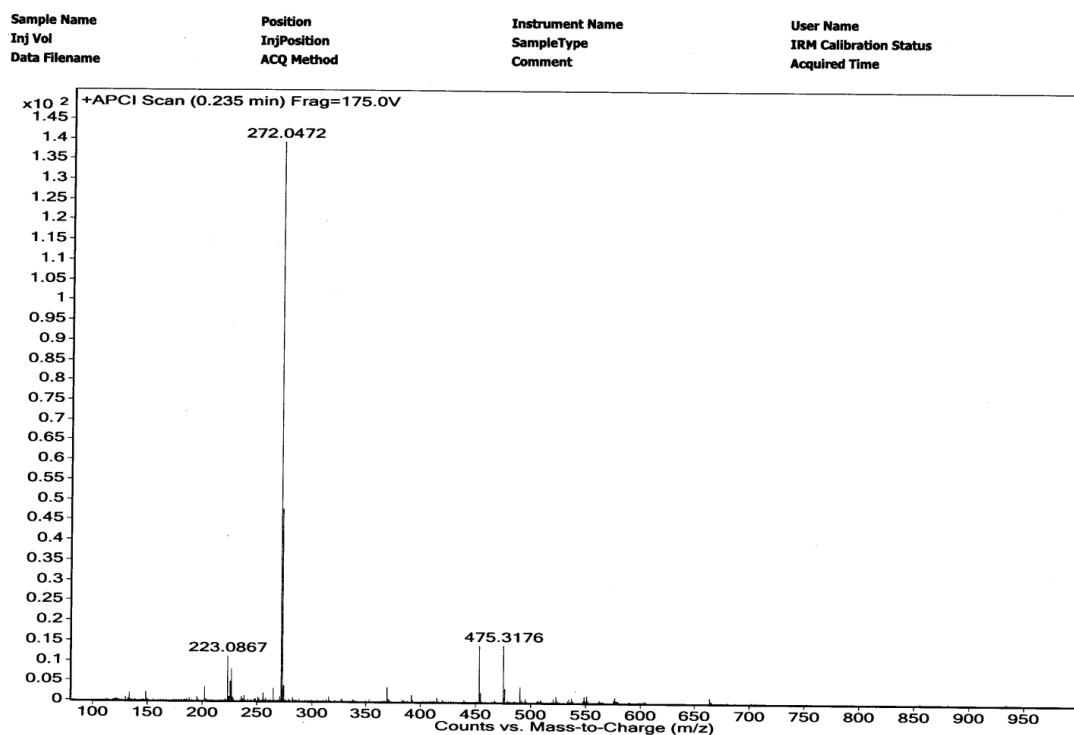
```

expt s2pu1
SAMPLE          SPECIAL
date  May 23 2011 temp  not used
solvent   CDCl3 gain  not used
file    exp gain  not used
ACQUISITION hst      0.008
        18.500
sw       6225.6  flags
at       1.199  18.500
        26.000
np      60270
        26.000
fb      13800  11   n
bs        16   in
di       1.000  dp
nt       5000  hs
ct       2250  PROCESSING
        1b
TRANSMITTER H1  fn  2.08
tn      C13  fp  655.36
        2.08
        -1570.8
        251.6
        9335.8
DECOUPLER   rfp
        7764.9
dn      H1
dof      0
de      vvy
dme      v  wc  250
dpwr     42  sc  0
dmt     8900  vs  14
        th  2
        nm  no ph

```

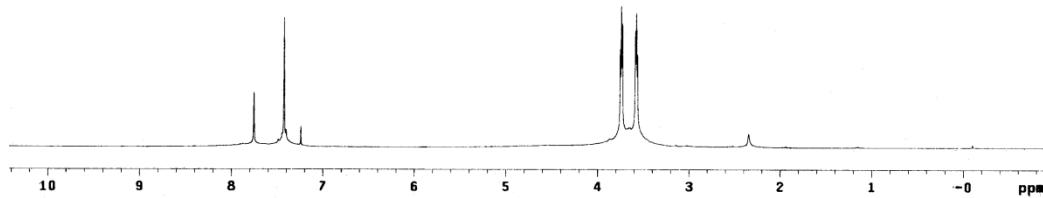


**N-(3-Nitrophenyl)benzo[d]thiazol-2-amine (4k): MASS SPECTRA**



**2-Morpholinobenzo[d]thiazole-6-carbonitrile (6a):  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):**

```
SAMPLE          SPECIAL
date Nov 15 2010 temp    not used
solvent   CDCl3 gain     not used
file      exp spin    not used
ACQUISITION freq    400.0
           width   10.0
           sw      6388.8 pw0s   15.750
           at      1.998 alfa   28.000
           25528   FLAGS
           not used t1      n
           bs      4      in      n
           di      1.000 dp      y
           nt      32     hs      nn
           ct      32     PROCESSING
           TRANSMITTER 1b      0.10
           tn      H1      Tn      65536
           sfrq   399.853 DISPLAY
           tor      362.8 sp      -374.6
           tpwr   57      pp      3657.5
           pw      9.859 r1      2894.9
           DECOUPLER C13 rfp      132.0
           dof      8      t1      -86.8
           dm      nnn      PLOT
           dmm      c      wc      250
           cpwr   15900   tc      34
           dat      th      nm      cdc ph
```

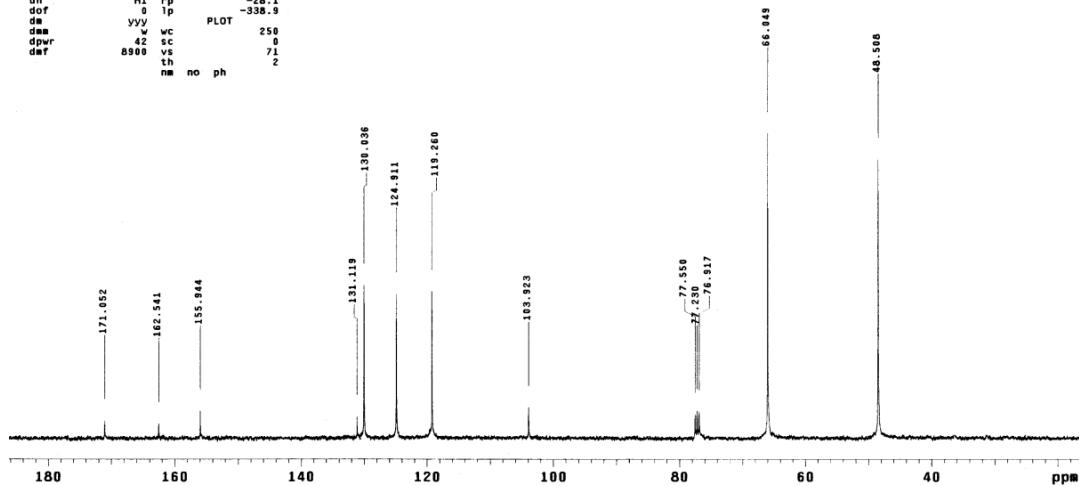


**2-Morpholinobenzo[d]thiazole-6-carbonitrile (6a):  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ ):**

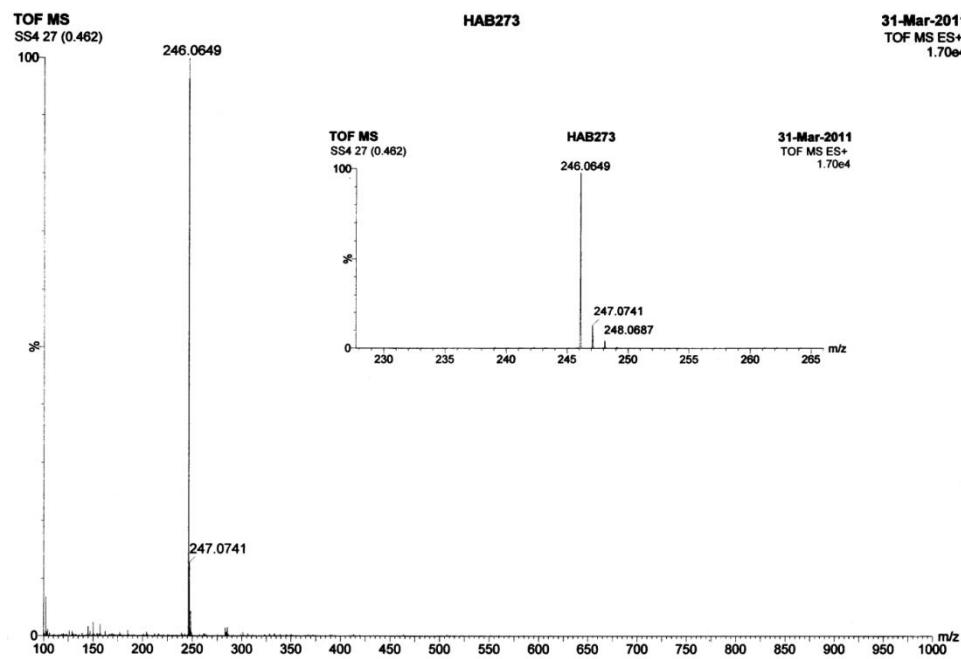
```

expl s2pu1           SAMPLE          SPECIAL
date Nov 15 2010      temp    not used
Solvent   CDCl3        gain    not used
file      exp        spin    not used
ACQUISITION   hst      pres    18.000
             25125.6    pres    18.000
at       1.199          n
np      66270          FLAGS
tr       15000          f1
bs       16             in
d1      1.000          dp
nt      5000           hs
             116          hs
TRANSMITTER   lb      PROCESSING
             C13      2.00
frq      100.0          fn      65536
tof      1536.3          DISPLAY
tpwr     61             sp      1611.4
             3.00          wp      17135.6
             8.300         rf      952.0
DECOUPLER    H1      PLOT
dn      rfp            -26.1
dof      0              ip      -338.9
dme     VVY            PLOT
dppr     Wc             250
dprw    42             sc             0
dav     8900           vs             71
             116          ph             2

```

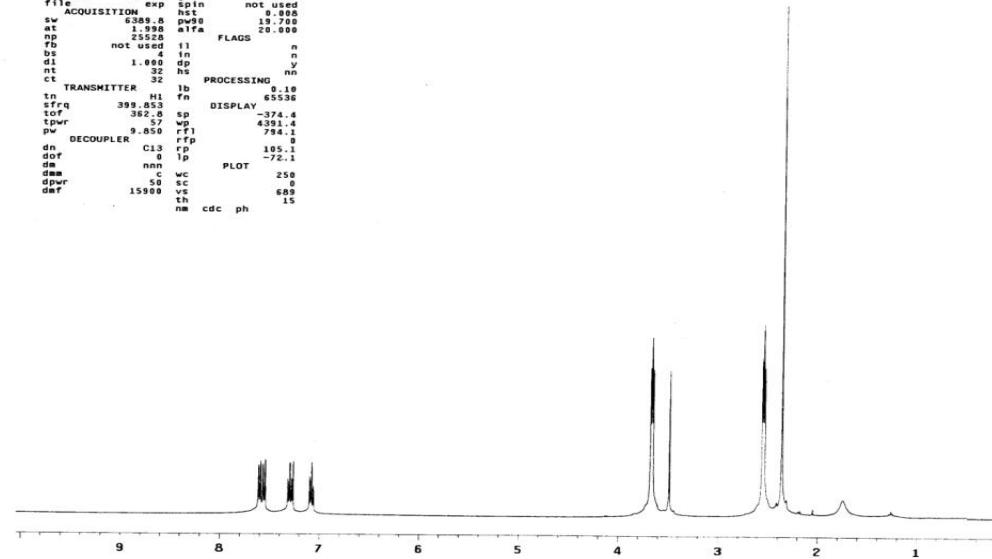


## 2-Morpholinobenzo[d]thiazole-6-carbonitrile (6a): MASS SPECTRA



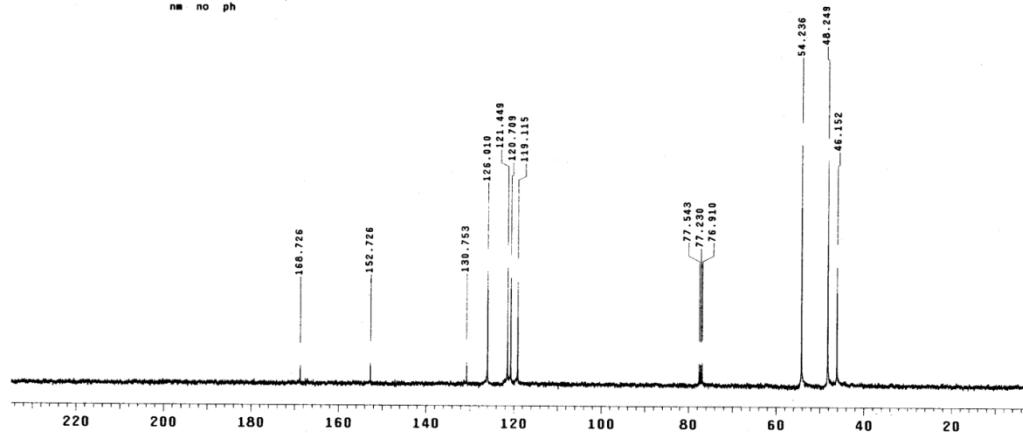
**2-(4-Methylpiperazin-1-yl)benzo[d]thiazole (7l):**  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):

```
expt s2pu1
SAMPLE          SPECIAL
date Mar 24 2011 temp not used
solvent   CDCl3 gain not used
file      exp spin not used
ACQUISITION    hst    0.008
sw        1369.8   17700  20.000
at        1.998   a1fa
np        2500      flags
rb        not used  11   n
ds        4         in   n
di        1.000   dp   y
nt        32        hs   nn
ct        32        PROCESSING 0.10
TRANSMITTER   C13  1b
tn        H1  fn   65536
sfrq     399.454   DISPLAY -374.4
t0f      382.6   sp
tpwr     9.850   rfp  794.1
pw        9.850   rfp
DECOUPLER    rfp
dn        C13  1p   105.1
dof       0        -72.1
dm        nnn      PLOT
dss       c        wc   250
dpwr     50       sc   0
dfr      15900    th   600
nm        cdc   ph   15
```



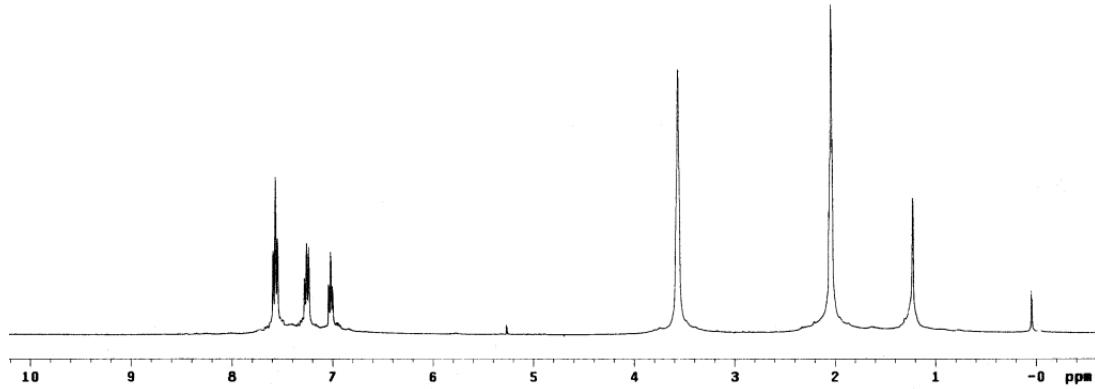
2-(4-Methylpiperazin-1-yl)benzo[d]thiazole (7l):  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ ):

```
expt s2pu1
SAMPLE          SPECIAL
date Mar 29 2011 temp not used
solvent   CDCl3 gain not used
file      exp spin not used
ACQUISITION    hst    0.008
sw        25125.6   10000  20.000
at        1.195   a1fa
np        60270      flags
t0       1369.8   11   n
ds        18       in   n
di        1.000   dp   y
nt        5000    hs   nn
ct        260    PROCESSING 2.00
TRANSMITTER   C13  1b
tn        H1  fn   65536
sfrq     100.554   DISPLAY -1524.1
t0f      1530.0   sp
tpwr     61       rfp  25125.6
pw        9.300   rfp  9289.0
DECOUPLER    rfp
dn        H1  1p   -483.1
dof       0        -289.7
dm        vvy      PLOT
dss       c        wc   250
dpwr     42       sc   0
dfr      8500    th   54
nm        no   ph
```



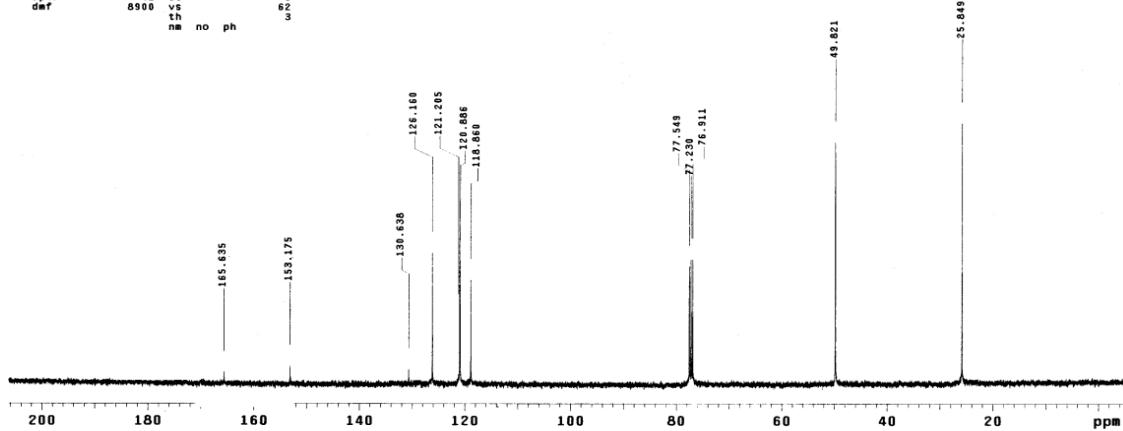
2-(Pyrrolidin-1-yl)benzo[d]thiazole (7m):  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):

```
date Nov 23 2010 sample
solvent CDCl3 temp not used
file exp spin not used
ACQUISITION hst 8.000
sw 686.0 pw90 19.780
at 23564 alfa 28.000
np 23564 FLAGS
fb not used 11 n
bs 4 in n
di 1.000 dp y
nt 32 hs nn
ct 32 PROCESSING
TRANSMITTER H1 fn not used
tn H1 sp DISPLAY
sfrq 399.853 0 -249.6
tof 0 wp 4372.1
tpwr 57 r1 3885.1
pw 7.000 rfp 2034.9
DECOUPLER C13 rp 106.4
dn C13 1p -92.0
dof nnn wc 250
dmm c sc 0
dpwr 50 vs 76
dmt 15900 th 7
dmf nm cdc ph
```



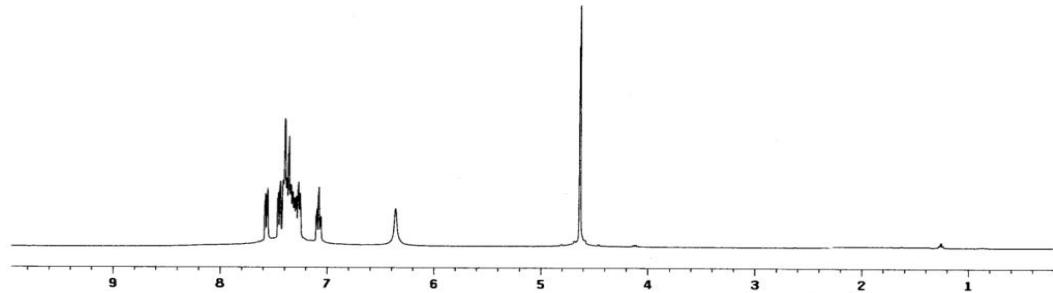
2-(Pyrrolidin-1-yl)benzo[*d*]thiazole (7m):  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ ):

```
exp1 std13c
SAMPLE SPECIAL
date Nov 23 2010 temp not used
solvent CDCl3 gain not used
file exp spin not used
ACQUISITION hst 8.000
sw 25000.0 pw90 10.000
at 1.199 alfa 20.000
np 59968 FLAGS
fb 13000 il n
bs 64 in n
di 0 dp y
nt 12000 hs nn
ct 12000 PROCESSING
TRANSMITTER C13 1p 1.00
tn C13 1p not used
sfrq 100.552 0 DISPLAY
tof 0 sp -514.8
tpwr 61 wp 21254.6
pw 8.667 r1 1000.0
DECOUPLER H1 rfp 7764.9
dn H1 rp -46.5
dof 0 1p -346.9
dmm vvv wc 250
dpwr 42 c 8
dmt 8900 vs 62
dmf nm no ph 3
```



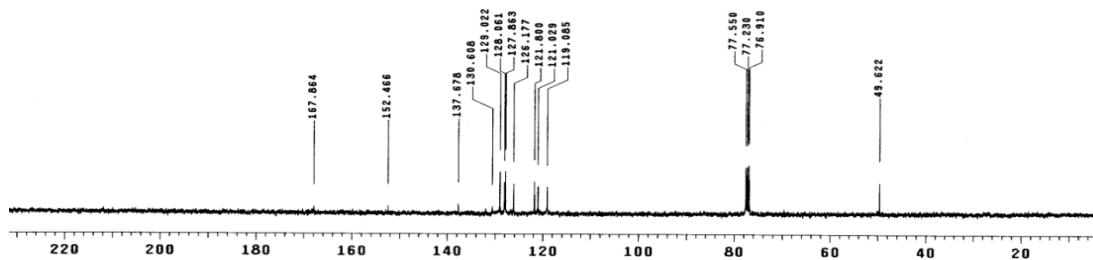
*N*-Benzylbenzo[*d*]thiazol-2-amine (7n):  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):

```
exp1 s2pul
SAMPLE SPECIAL
date May 28 2011 temp not used
solvent CDCl3 spin not used
file exp spin not used
ACQUISITION hst 0.005
sw 6389.0 pw90 18.600
at 1.898 a1f4 20.000
np 25528 FLAGS
fb not used 11 n
bs 32 in n
di 1.000 dp y
nt 32 ns mn
ct 32 PROCESSING
tn TRANSMITTER lb 0.10
HI fn 65536
sfrq 399.853 DISPLAY
t0f 362.8 sp -420.6
tpwr 7.0 rfp 438.7
pw 9.850 rfp 798.4
DECOUPLER rfp 0
dn C13 rf 129.3
dof 0 1p -94.9
dm vnm vc PLOT
dss 0 250
dpwr 50 xc 0
dmf 15900 vs 61
th 31
nm cdc ph
```



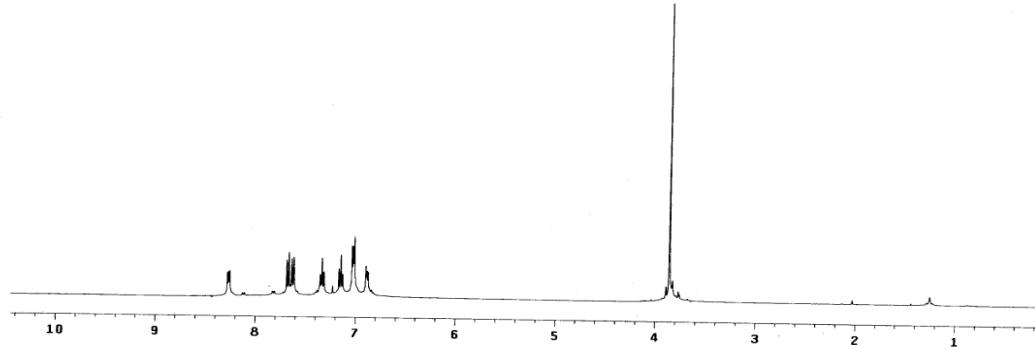
**N-Benzylbenzo[d]thiazol-2-amine (7n):  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ ):**

```
exp1 s2pul
SAMPLE SPECIAL
date May 29 2011 temp not used
solvent CDCl3 spin not used
file exp spin not used
ACQUISITION hst 0.005
sw 25125.6 pw90 18.600
at 6.0270 a1f4 20.000
np 60270 FLAGS
fb 13800 11 n
bs 32 in n
di 1.000 dp y
nt 5000 ns nn
ct 1152 PROCESSING 2.00
tn TRANSMITTER lb 0.00
C13 rf 65536
sfrq 100.554 DISPLAY
t0f 1536.8 sp -1505.7
tpwr 61 wp 25125.6
pw 9.300 rfp 9270.6
DECOUPLER rfp 7764.9
dn HI rf -4
dof 0 1p -351.1
dm vvv vc PLOT
dss 0 250
dpwr 42 xc 0
dmf 6900 vs 11
th 2
nm no ph
```



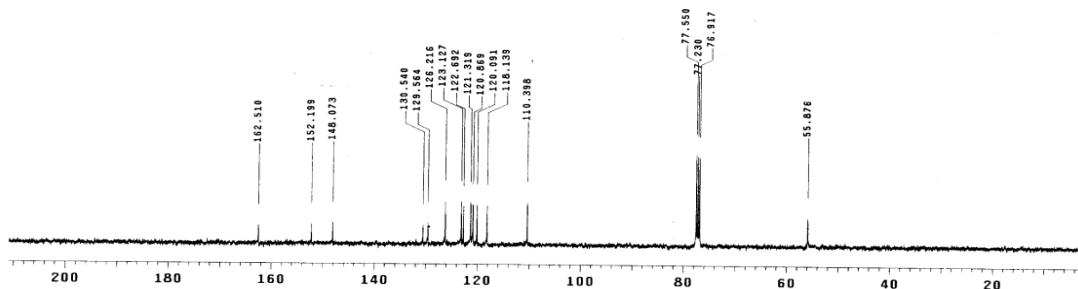
**N-(2-Methoxyphenyl)benzo[d]thiazol-2-amine (7o):  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):**

```
exp1_s2pul
SAMPLE          SPECIAL
date Sep 2 2011 temp not used
solvent   CDCl3 gain  not used
file    exp spin  not used
ACQUISITION      hst 0.005
sw       6383.8 pws 18.600
at        1.998 alfa 20.000
np       256      flags
rb       not used 11 n
bs        4 in n
dt       1.000 dp y
nt       32 hs nn
ct        32 PROCESSING nm
TRANSMITTER    C13 rp 0.18
tn      H1 fn 65536
sfrq    399.853 DISPLAY
tof      362.5 sp 135.9
tpwr    9.850 rfp 4314.1
pw       9.850 rfi 805.6
DECOPPLER      C13 rp 0
dof      0 ip 0
dn      C13 rp 126.2
dof      0 ip -87.8
dm      nc wc 250
dms     sc 0
dpwr    50 th 77
dfr     15900 ts 20
nm      cdc ph 20
```



**N-(2-Methoxyphenyl)benzo[d]thiazol-2-amine (7o):  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ ):**

```
exp1_s2pul
SAMPLE          SPECIAL
date Sep 24 2011 temp not used
solvent   CDCl3 gain  not used
file    exp spin  not used
ACQUISITION      hst 0.005
sw       2025.6 pws 18.600
at        1.199 alfa 20.000
np       60270 flags
ft      13800 11 n
bs        32 in n
dt       1.000 dp y
nt       500 hs nn
ct        512 PROCESSING 2.00
TRANSMITTER    C13 rp 65536
tn      C13 fn 65536
sfrq    100.554 DISPLAY
tof      1536.3 sp -622.3
tpwr    9.300 rfp 21823.8
Dw      9.300 rfi 527.2
DECOPPLER      H1 rp 7764.9
dn      H1 ip -59.4
dof      0 ip -271.4
dm      VVY wc 250
dms     SC 0
dpwr    42 ts 23
dfr     8900 vs 3
nm      no ph 3
```

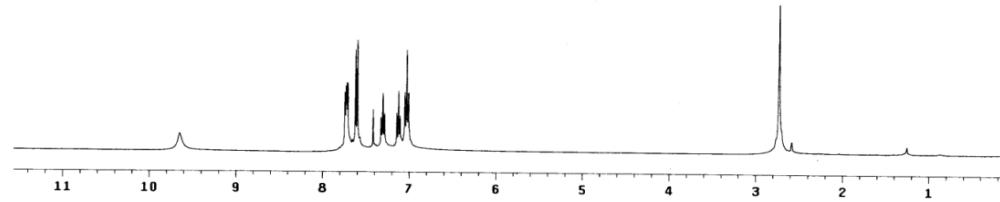


**N-(4-Fluorophenyl)benzo[d]thiazol-2-amine (7p):  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3 + \text{DMSO}-d_6$ ):**

```

exp1 s2pul
      SAMPLE          SPECIAL
date Sep 27 2011 temp   not used
solvent CDCl3 gain   not used
file   exp  spin   not used
      ACQUISITION   not used
      sw       6389.8 pw90  18.700
      at      1.998 alfa  20.000
      np      64   0.02   FLAGS
      fb      not used i1 n
      bs      4 in   n
      di      1.000 dp   y
      nt      32 hs   nn
      ct      32 PROCESSING
      TRANSMITTER   C13  1b   0.10
      tn      H1  fn   65536
      sfrq   399.853 DISPLAY
      t0f    362.8 sp   -294.8
      tpwr   61   wp   492.2
      pw     9.859 rfp   731.5
      DECOUPLER
      dn      C13  1p   125.8
      dof     0 ip   -102.4
      dmm   nnnn PLOT
      dsw   yy  wc   250
      dpwr   59   sc   0
      def    15900 vs   36
      nm cdc ph   20

```

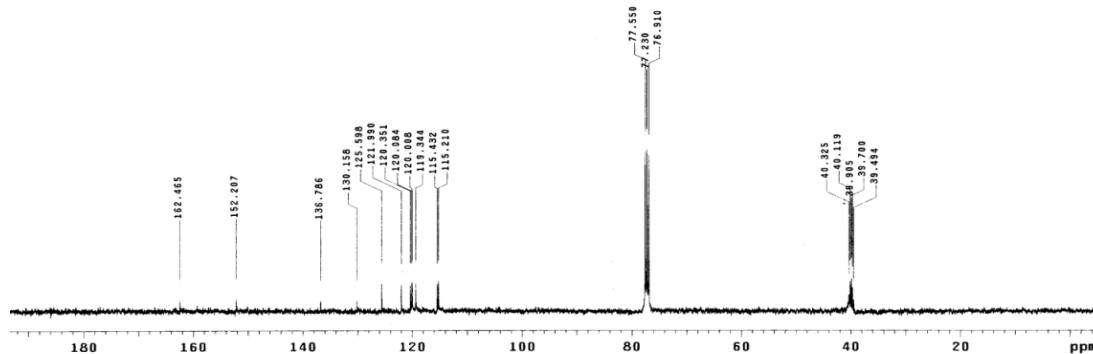


**N-(4-Fluorophenyl)benzo[d]thiazol-2-amine (7p):  $^{13}\text{C}$  NMR (400 MHz,  $\text{CDCl}_3 + \text{DMSO}-d_6$ ):**

```

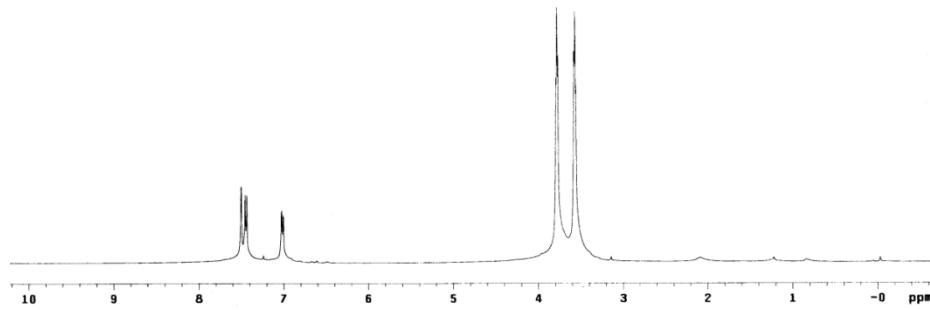
exp1 s2pul
      SAMPLE          SPECIAL
date Sep 27 2011 temp   not used
solvent CDCl3 gain   not used
file   exp  spin   not used
      ACQUISITION   not used
      sw       25125.6 pw90  18.600
      at      1.178 alfa  20.000
      np      64   0.02   FLAGS
      fb      13800 i1 n
      bs      32 in   n
      di      1.000 dp   y
      nt      5000 hs   nn
      ct      1120 lb   PROCESSING
      TRANSMITTER   C13  1b   2.00
      tn      H1  fn   65536
      sfrq   100.554 DISPLAY
      t0f    158.1 sp   -576.3
      tpwr   61   wp   29041.0
      pw     9.300 rfp   9285.2
      DECOUPLER
      dn      H1  rfp   40.1
      dof     0 ip   -479.2
      dmm   yy  wc   250
      dpwr   42   sc   0
      def    8500 vs   40
      nm no ph   2

```

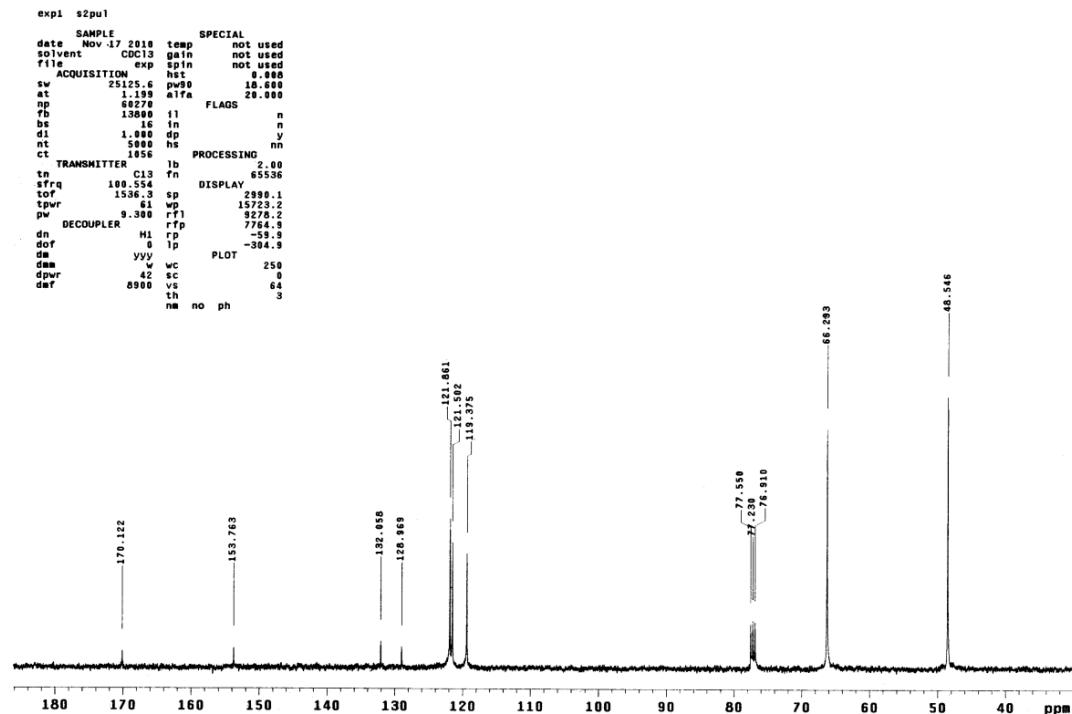


**6-Chloro-2-morpholinobenzo[d]thiazole (9a):  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):**

```
exp1 s2pu1
      SAMPLE          SPECIAL
date Nov 17 2010 temp    not used
start   0.000000 spin    not used
file   exp  spin    not used
      ACQUISITION hst    9.168
ss     8.000.0      10.000
at     1.898 alfa   29.000
nt     25528      FLAGS
fb    not used   11      n
bs     4        in      n
dl     1.000    np      y
nt     32        ns      nn
ct     32        PROCESSING 0.19
tn     H1 fn    65136
sfrq  399.853      DISPLAY -273.3
tfrq  399.853      sp
tpwr  57      wp    4400.1
pw     0.058      rfp   2894.9
      DECOUPLER C13 rfp   2894.9
dn     C13 rp    110.1
dof    mnn 1P    -61.3
dme   mnn c     PLOT
dme   mnn c     250
dppr  15900 vs    69
ddef   nm      h    20
      nm cdc ph
```

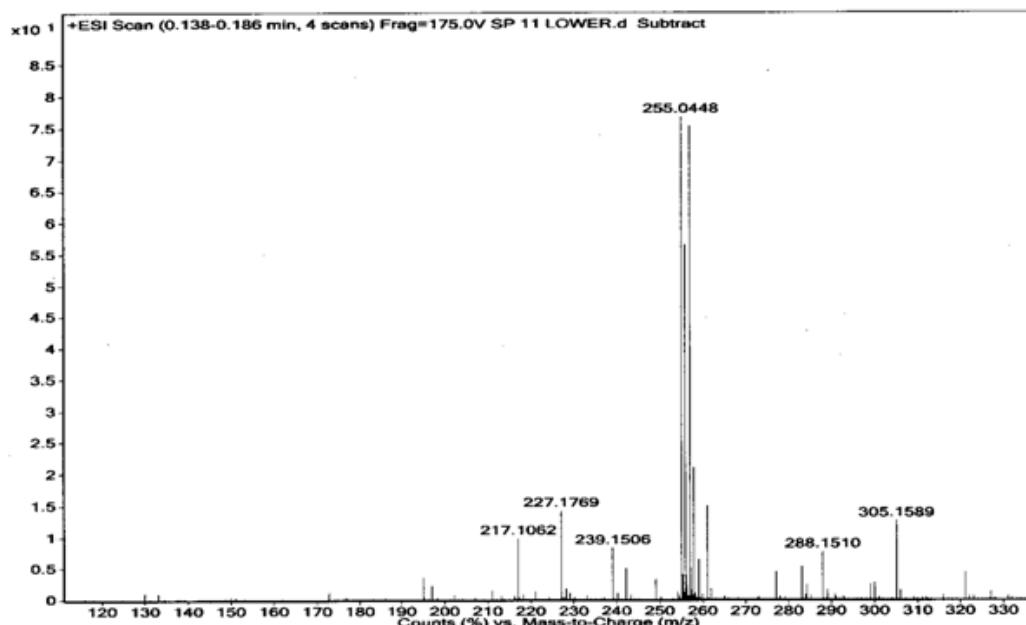


**6-Chloro-2-morpholinobenzo[*d*]thiazole (9a):  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ ):**



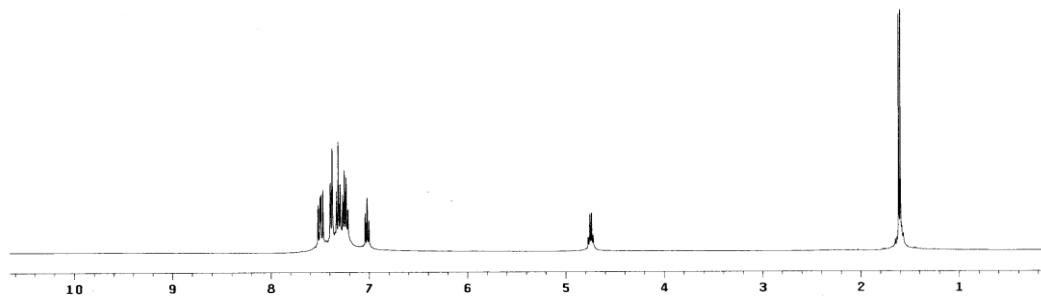
**6-Chloro-2-morpholinobenzo[*d*]thiazole (9a): MASS SPECTRA:**

Sample Name	SP11 LOWER	Position	Vial 1	Instrument Name	Instrument 1	User Name
Inj Vol	-1	Inj/Position		SampleType	Sample	IRM Calibration Status
Data Filename	SP 11 LOWER.d	ACQ Method		Comment		Acquired Time



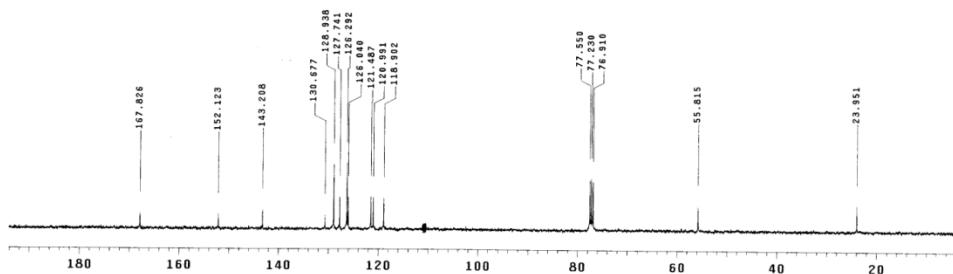
**N-((R)-1-Phenylethyl)benzo[d]thiazol-2-amine (10q):  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):**

```
exp1 s2pul
SAMPLE          SPECIAL
date  Sep 27 2011 temp  not used
solvent   CDCl3  gain  not used
file    exp1      exp  not used
ACQUISITION hst    npt  0.008
sw     6385.8   pw90  19.760
at     1350      r1fa  20.000
np     25528    FLAGs
fb     not used  l1  n
bs     4       in  n
dl     1.000   dp  y
nt     32      hs  nn
ct     32      PROCESSING
TRANSMITTER lb   0.10
tn     H1      fn  65536
trfq  399.853  DISPLAY
tof   362.8   sp  -188.0
tpwr  57      wp  4459.0
pw    9.850   rf1  889.3
DECOUPLER rfp
dn     C13    rp  118.0
dof    0      lp  -85.1
da     rnm    PLOT
dmm   wc   250
dpwr  56      sc  0
ddef  15900   vs  61
th     nm   cdc  ph
20
```

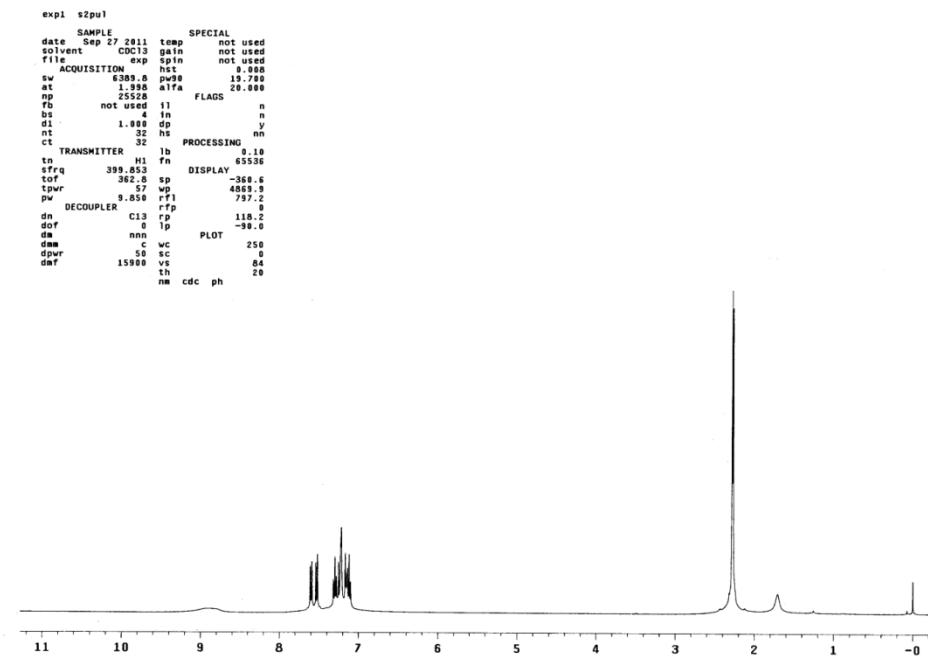


**N-((R)-1-Phenylethyl)benzo[d]thiazol-2-amine (10q):  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ ):**

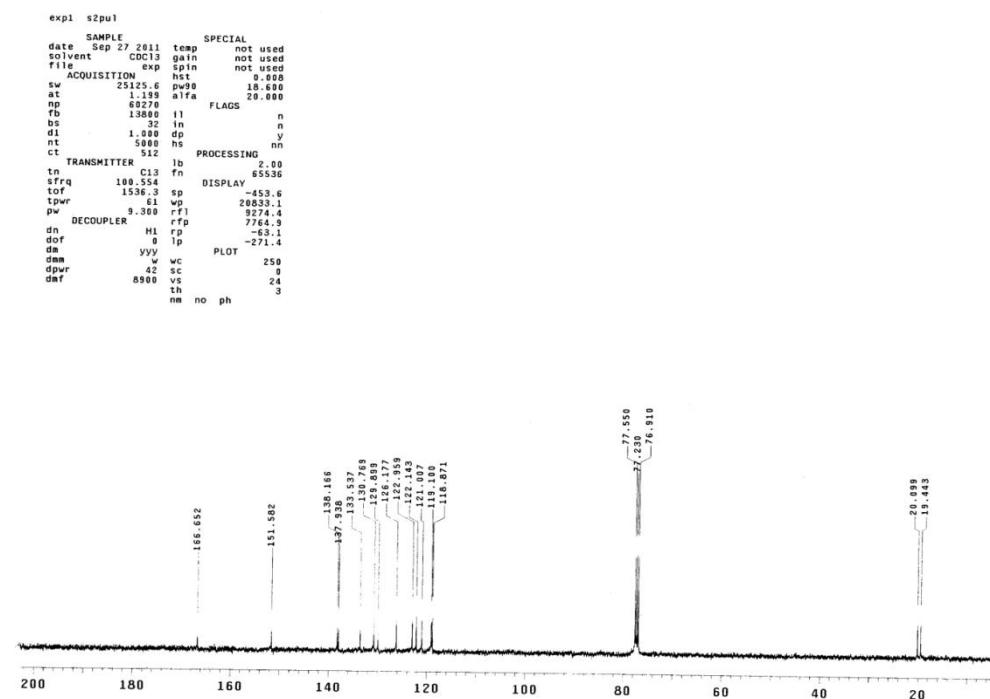
```
exp1 s2pul
SAMPLE          SPECIAL
date  Sep 27 2011 temp  not used
solvent   CDCl3  gain  not used
file    exp1      exp  not used
ACQUISITION hst    npt  0.008
sw     2512.6   pw90  18.600
at     1350      alfa  20.000
np     60270    FLAGs
fb     13800   l1  n
bs     1.000   dp  y
nt     5000   hs  nn
ct     512      PROCESSING
TRANSMITTER lb   2.00
tn     C13    fn  65536
trfq  100.000  DISPLAY
tof   1336.3   sp  -884.6
tpwr  61      wp  20403.7
pw    9.300   rf1  9276.7
DECOUPLER rfp
dn     H1    rp  -53.9
dof    0      lp  -305.1
da     v99    PLOT
dmm   w   wc  250
dpwr  42      sc  0
ddef  8890   vs  16
th     nm   no  ph
3
```



**N-(3,4-Dimethylphenyl)benzo[d]thiazol-2-amine (10r):  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):**

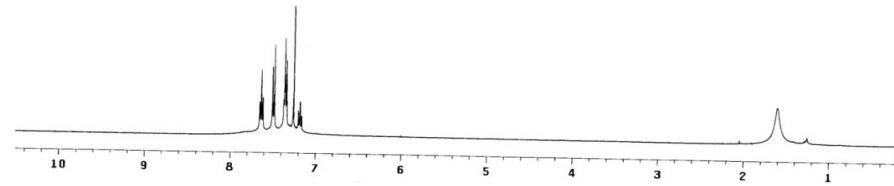


**N-(3,4-Dimethylphenyl)benzo[d]thiazol-2-amine (10r):  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ ):**



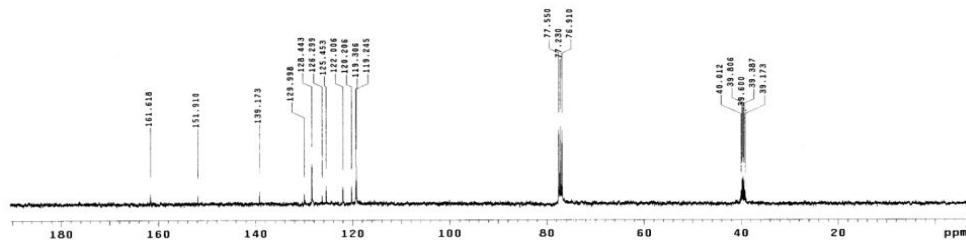
**N-(4-Chlorophenyl)benzo[d]thiazol-2-amine (10s):  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):**

```
expt s2pul
SAMPLE          SPECIAL
date Sep 17 2011 temp not used
solvent   CDCl3 gain  not used
file      exp gain  not used
ACQUISITION    hst    0.000
sw        6300.0 pws8  19.700
at        1.390.0 20.000
np        25528   FLAGs
fb       not used 11  n
bs        4  in  n
d1      1.000.0 dp  y
nt       32  sc  nn
ct        32  th  nn
TRANSMITTER   1b  PROCESSING
tn        H1  fn  65536
trfq     399.853  DISPLAY
tot       360.000  SP
tpwr     57  wp  4466.0
pw       9.850  rfp  754.8
DECOUPLER
d1f      C13  rp  111.1
dof      8  tp  0
d1n     nnn  tp  -65.6
dme      c  wc  250
dppr     50  sc  0
def      15900  vs  38
            th  no  cdc ph  19
```



**N-(4-Chlorophenyl)benzo[d]thiazol-2-amine (10s):  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3+\text{DMSO}-d_6$ ):**

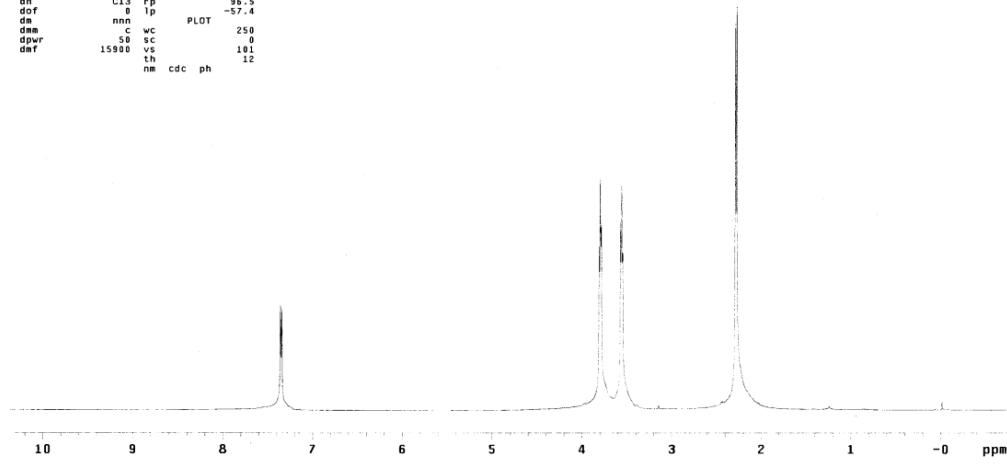
```
expt s2pul
SAMPLE          SPECIAL
date Sep 24 2011 temp not used
solvent   CDCl3 gain  not used
file      exp gain  not used
ACQUISITION    hst    0.000
sw        25125.6 pws8  19.400
at        1.195  altp  20.000
np        13868   FLAGs
fb       not used 11  n
bs        4  in  n
d1      1.998.0 dp  y
nt       544  sc  nn
ct        544  th  nn
TRANSMITTER   13  PROCESSING
tn        C13  fn  65536
trfq     100.514  DISPLAY
tot       13868.0 sp  -7531.4
tpwr     3.301  rfp  19980.3
pw       9.300  rfp  3.300
DECOUPLER
d1f      H1  rp  25.0
dof      8  tp  -360.6
dme      vvv  PLOT
dppr     42  sc  250
def      8398  vs  0
            th  no  ph  2
```



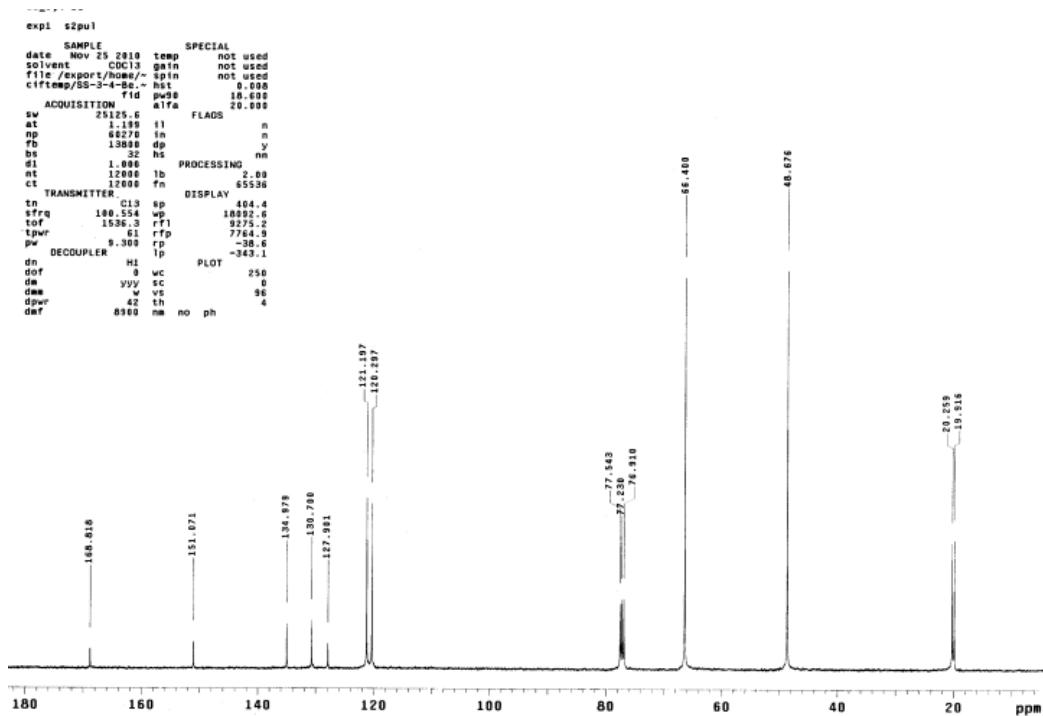
**6,6-Dimethyl-2-morpholinobenzo[d]thiazole (11a):  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):**

```
exptl s2pu1
SAMPLE
date Nov 25 2010 temp not used
solvent CDCl3 gain not used
file not used ph not used
ACQUISITION hst 0.008
sw 6389.8 pw90 15.700
at 1.258 tfa 28.000
np 25528 FLAGS
fb not used i n
bs 4 in n
d1 1.000 dp y
nt 32 hs PROCESSING nn
ct 32 ph

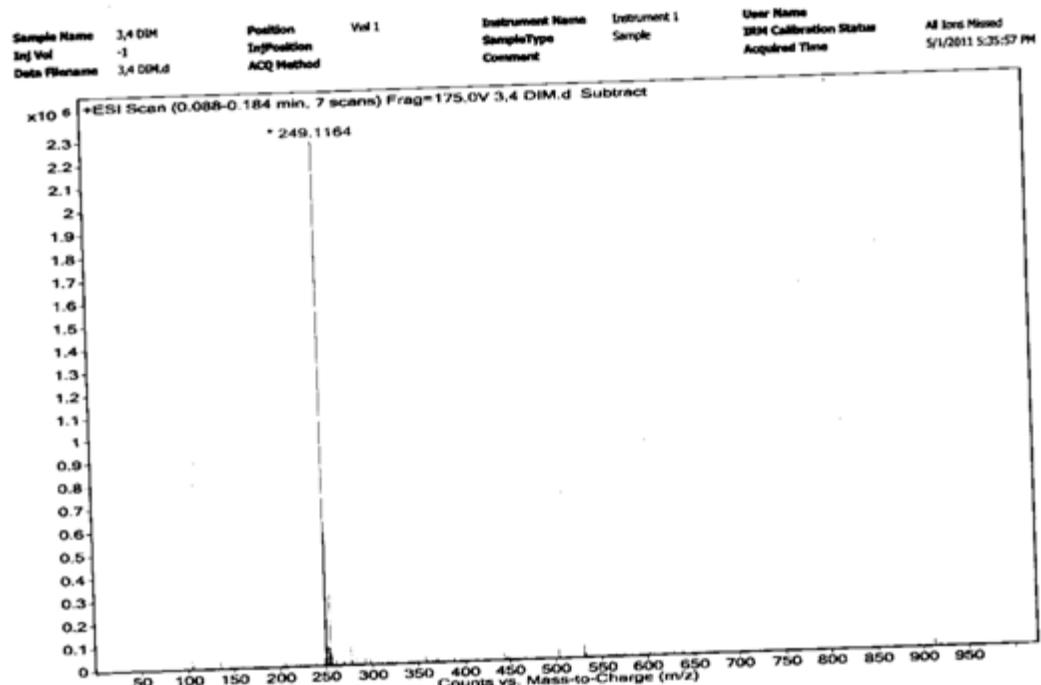
TRANSMITTER H1 f1 0.10
tn H1 fn 65536
sfrq 399.811 DISPLAY 65536
t0rf 362.8 sp -316.1
tpwr 57 vp 4508.9
pw 9.850 r1 383.1
DECOUPLER C13 rfp 2894.9
dn C13 rp 96.5
dof nnn lp -57.4
dmn c wc PLOT 250
dpwr 15900 vs 181
dmf 15900 th 12
nm cdc ph
```



**6,6-Dimethyl-2-morpholinobenzo[d]thiazole (11a):  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ ):**

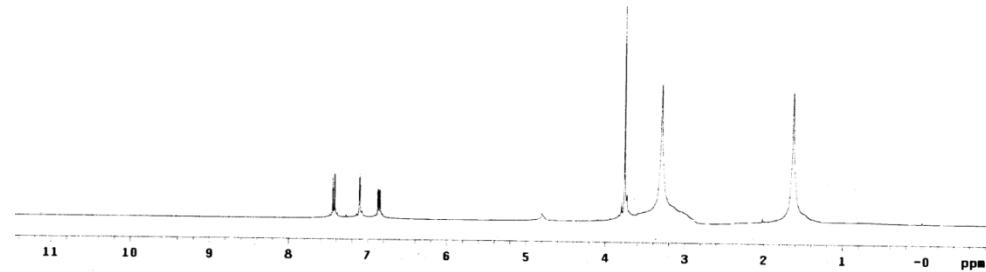


### 6,6-Dimethyl-2-morpholinobenzo[d]thiazole (11a) MASS SPECTRA:



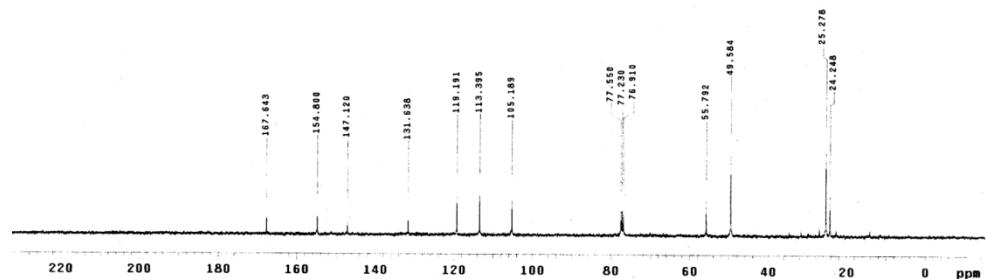
### 6-Methoxy-2-(piperdin-1-yl)benzo[d]thiazole (12t): $^1\text{H}$ NMR (400 MHz, $\text{CDCl}_3$ ):

```
exp1 s2pul
SAMPLE SPECIAL
date Jul 28 2011 temp not used
solvent CDCl3 gain not used
file exp exp ph not used
ACQUISITION hst 0.008
sw 6383.5 pw98 15.789
at 25915 p90 28.000
nt 25528
np 1
tr 25536
td 16384
rf 1.000
dt 32
ct 32 hs nn
rt 0
TRANSMITTER lb 0.10
t1 399.853 fn DISPLAY 65536
sfreq 399.853
tof 362.8 sp -343.4
tpwr 100 rf 4978.7
pw 9.853 rfp 708.4
DECOUPLER rfp 0
dn C13 rp 126.9
dof 0 lp -76.4
dm nnn PLOT
dme v 250
dpwr 50 wc 0
dmt 15900 vs 75
th 20
nm cdc ph
```



**6-Methoxy-2-(piperdin-1-yl)benzo[*d*]thiazole (12t):  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ ):**

```
exp1 s2pul
SAMPLE SPECIAL
date Jul 28 2011 temp not used
solvent CDCl3 gain not used
file exp exp ph not used
ACQUISITION hst 0.008
sw 25125.6 pw98 18.699
at 25915 p90 26.999
nt 60270
np 1
tr 13800
td 16384
rf 1.000
dt 32
ct 3000 hs nn
rt 0
TRANSMITTER lb 2.00
t1 188.554 fn DISPLAY 65536
sfreq 188.554
tof 1536.3 sp -1523.3
tpwr 100 rf 25125.6
pw 9.300 rfp 500.2
DECOUPLER rfp 7764.9
dn H1 rp -39.9
dof 0 lp -312.0
dm vvv PLOT
dme v 250
dpwr 42 wc 22
dmt 6500 vs 22
th 3
nm no ph
```



**6-Methoxy-2-(piperdin-1-yl)benzo[*d*]thiazole (12t): MASS SPECTRA:**

Sample Name: [REDACTED]  
 Inj Vol: [REDACTED]  
 Data File Name: [REDACTED]

Position: [REDACTED]  
 Inj Position: [REDACTED]  
 ACQ Method: [REDACTED]

Instrument Name: [REDACTED]  
 Sample Type: [REDACTED]  
 Comment: [REDACTED]

User Name: [REDACTED]  
 IRM Calibration Status: [REDACTED]  
 Acquired Time: [REDACTED]

+ESI Scan (0.435 min) Frag=175.0V

249.1053

134.0709

x10<sup>-2</sup>

1.2  
1.15  
1.1  
1.05  
1.0  
0.95  
0.9  
0.85  
0.8  
0.75  
0.7  
0.65  
0.6  
0.55  
0.5  
0.45  
0.4  
0.35  
0.3  
0.25  
0.2  
0.15  
0.1  
0.05  
0

100 125 150 175 200 225 250 275 300 325 350 375 400 425 450 475 500 525 550 575 600 625 650 675 700

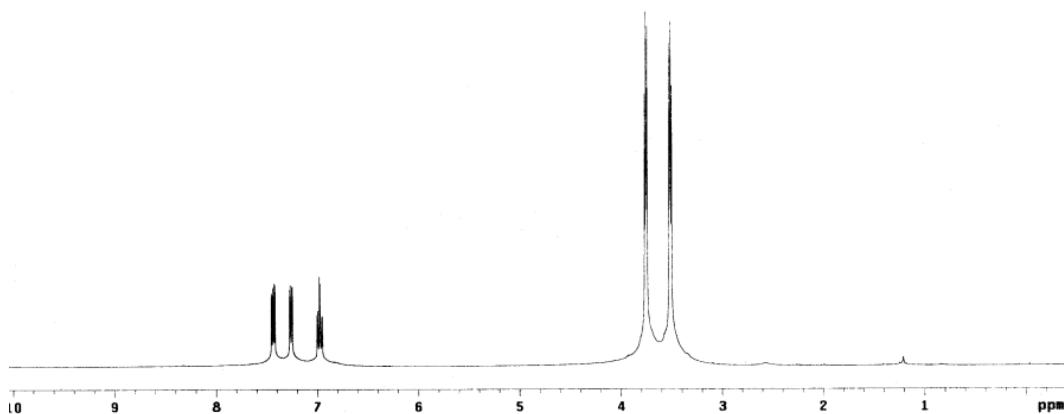
Counts vs. Mass-to-Charge (m/z)

**6-Fluoro-2-morpholinobenzo[*d*]thiazole (13a):**  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):

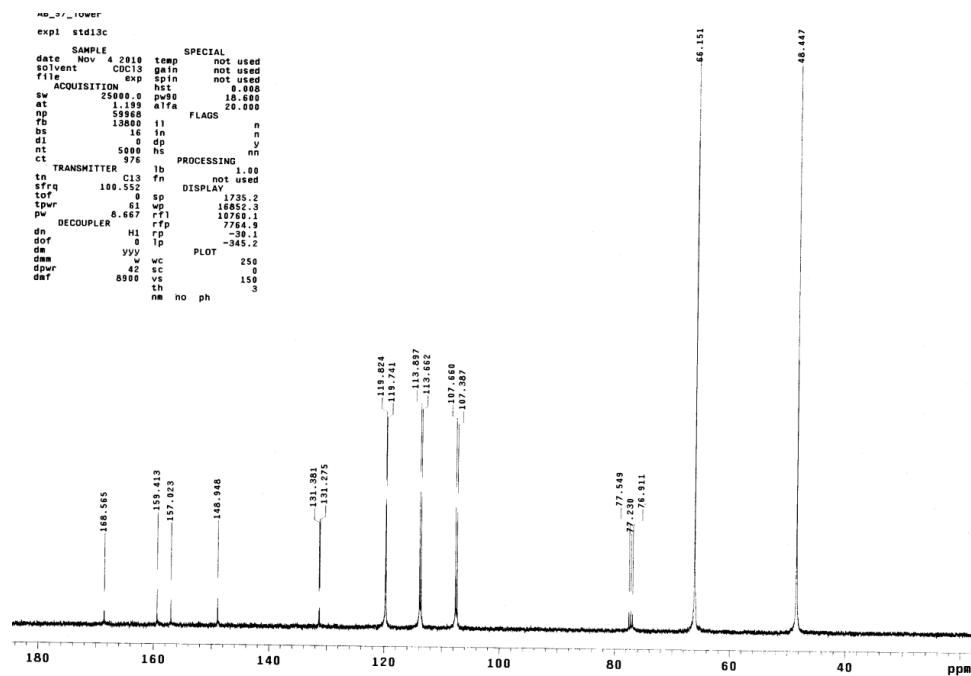
```

exp1 stdih
      SAMPLE          SPECIAL
date Nov 4 2010 temp  not used
solvent CDCl3 gain  not used
file   spin  not used
ACQUISITION    hz    8.000
sw     600.0 pw00 19.700
t1     1.995 alfa  20.000
238.0
fb    not used 11   n
bs     4 in    n
di     1.00 dp    y
rt     32.00 hs   n
      TRANSMITTER    DISPLAY
in      HI          not used
sfreq  395.035 sp   not used
tof    0 wp    4253.7
tpwrf rfp1  956.6
tpw    7.000 rfp2  128.7
      DECOUPLER      PLOT
dn      C13 1p    48.0
dof    0          not used
ns     nc    250
dm    c sc   0
dpwrf 50 vs   83.0
dav    15000 th   48.0
      Cdc ph

```



**6-Fluoro-2-morpholinobenzo[*d*]thiazole (13a):**  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ ):



### 6-Fluoro-2-morpholinobenzothiazole (13a): MASS SPECTRA:

