Supporting Informations

Tandem Regioselective Synthesis of Tetrazoles and Related Heterocycles Using Iodine

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General procedure for the preparation of phenyl-(1-phenyl-1*H*-tetrazol-5-yl)-amine (7a). Aniline **4a** (186 mg, 2 mmol) was added to phenyl isothiocyanate **1a** (270 mg, 2 mmol) in DMF (4 mL) and the reaction was stirred at room temperature for 20 min. During this time complete formation of 1,3-diphenylthiourea **5a** was observed. To this was added sequentially, NaN_3 (390 mg, 6 mmol), I_2 (559 mg, 2.2 mmol) and drop wise addition of triethylamine (835 μL, 6 mmol) over a period of 5 min. During the addition of triethylamine reaction was exothermic. After complete addition of triethylamine, the reaction mixture was stirred for an additional 4.5 h. Complete conversion of the in situ generated 1,3-diphenylthiourea **5a** to phenyl-(1-phenyl-*1H*-tetrazol-5-yl)-amine **7a** was observed by thin layer chromatography (TLC). The reaction mixture was treated with a 5% hypo solution (5 mL) and the product was extracted with ethyl acetate (3 x 10 mL). The combined ethyl acetate layer was washed with water (3 x 5 mL), dried over anhydrous Na_2SO_4 and concentrated under reduced pressure. The product was purified over a column of silica gel (saturated with 1% triethyl amine) and eluted with (8:2 hexane:ethylacetate) to give **7a** (356 mg, 75%). mp: 159 ^oC (Lit.[23d] 158–159 ^oC); ^1H NMR (400 MHz, $CDCl_3$): δ (ppm) 6.54 (brs, 1H), 7.03 (t, J = 7.2 Hz, 1H), 7.08 (t, J = 7.2 Hz, 1H), 7.14 (d, J = 8.0 Hz, 1H), 7.24 (t, J = 7.2 Hz, 1H), 7.34 (m, 1H), 7.52–7.71 (m, 5H); ^{13}C NMR (100 MHz, $CDCl_3$): δ (ppm) 118.4, 122.1, 123.6, 125.0, 129.5, 130.0, 132.8, 138.3, 151.8; IR (KBr): 3384, 3193, 3040, 2996, 2926, 1601, 1570, 1530, 1495, 1453, 1325, 1238, 1122, 1090, 764, 745 cm^{-1}; Elemental analysis: $C_{13}H_{11}N_5$ (237.26): calcd. C, 65.81; H, 4.67; N, 29.52; found C, 65.86; H, 4.71; N, 29.42.

General procedure for the preparation of (1-phenyl-1*H*-tetrazol-5-yl)-*p*-tolyl-amine / phenyl-(1-*p*-tolyl-1*H*-tetrazol-5-yl)-amine (9a+10a).

Similar to general procedure described above, except *p*-methyl aniline (214 mg, 2 mmol) **13** was used instead of aniline to give product **9a+10a** (377 mg, 75%). ^1H NMR (400 MHz, $CDCl_3$): δ (ppm) 2.30 (s, 3H), 2.46 (s, 3H), 6.58 (br s, 2H), 7.07 (t, J = 7.6 Hz, 1H), 7.12 (d, J = 8.4 Hz, 1H), 7.30–7.43 (m, 10H), 7.44–7.60 (m, 5H); ^{13}C NMR (100 MHz, $CDCl_3$): δ (ppm) 20.9, 21.5, 118.3, 118.7, 123.5, 124.9, 129.4, 129.9, 130.1, 130.5, 130.6, 131.2, 138.3, 141.1, 151.8; IR (KBr): 3239, 3193, 3056, 2924, 2853, 1607, 1569, 1560, 1531, 1514, 1498,

1457, 1401, 1230, 1178, 1121, 1078, 819, 745 cm^{-1}; Elemental analysis: $C_{14}H_{13}N_5$(251.29): calcd. C, 66.92; H, 5.21; N, 27.87. found: C, 65.85; H, 5.25; N, 27.75.

General procedure for the Preparation of Guanidine (13a).

To a solution of phenyl isothiocyanate **1a** (270 mg, 2 mmol.) in EtOH (2 mL) was added drop wise piperidine **k** (197 μL, 2 mmol), dissolved in EtOH (2 mL) at room temperature. Formation of thiourea **11a** was observed within 15 minutes as judged from thin layer chromatography (TLC). To this was then added I_2 (254 mg, 1 mmol.) pinch wise over a period of 10 minutes. The reaction was kept for stirring at room temperature and complete conversion to *anti*-Hugerschoff product was observed within 30 min as can be judged from TLC. After completion of the reaction, solvent was evaporated, and the reaction mixture was quenched with 5% hypo solution (5 mL) and admixed with ethyl acetate (15 mL). The ethyl acetate layer was washed with water (2 x 5 mL), dried over anhydrous Na_2SO_4 and concentrated under reduced pressure. The pure product was isolated by silica gel column (saturated with 1% triethyl amine) (2:8 ethyl acetate and hexane) to give **13a** (353 mg, 87%). mp: 186–188 ^oC (Lit.[28c] 186–188 ^oC); ^1H NMR (400 MHz, $CDCl_3$): δ(ppm) 0.84–1.67 (m, 12H), 2.63–3.82 (m, 8H), 6.90 (t, J = 7.6 Hz, 2H), 7.02–7.12 (m, 3H), 7.16 (t, J = 8.4 Hz, 2H), 7.26–7.40 (m, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ(ppm) 23.6, 24.5, 24.6, 24.9, 47.4, 51.4, 122.1, 122.3, 124.1, 128.4, 129.2, 143.7, 149.7, 150.0, 184.9; IR (KBr): 2936, 2854, 1632, 1588, 1481, 1454, 1416, 1295, 1261, 1240, 1207, 1028, 989, 903, 749 cm^{-1}; HRMS (ESI): 407.2269 (MH^+).

General Procedure for the Preparation of N^2, N^5-Diphenyl-1,3,4-thiadiazole-2,5-diamine (17a).

Hydrazine hydrate (50 mg, 1 mmol) was added to phenyl isothiocyanate **1a** (270 mg, 2 mmol) in EtOH (2 mL) and the reaction was stirred at room temperature for 20 minutes. During this time complete formation of *bis*-thiourea **15a** was observed. To this was added triethylamine (2 equiv) followed by I_2 (0.5 equiv) pinch wise over a period of 5 min. The complete conversion of *bis*-thiourea **15a** to N^2,N^5-diphenyl-1,3,4-thiadiazole-2,5-diamine **17a** was observed within 30 min. After completion, the reaction mixture was quenched with 5%

hypo solution (5 mL), and product was extracted with ethyl acetate (2 x 10mL), dried over on anhydrous Na_2SO_4 and concentrated under reduced pressure. The pure product was isolated by silica gel column (1:9 ethylacetate : hexane) to give product 1**7a** (217 mg, 81%). mp: 239–242 ^oC (Lit.[43] 239–241 ^oC); ^1H NMR (400 MHz, $CDCl_3$): δ (ppm) 6.94 (t, J = 7.6 Hz, 2H), 7.27 (t, J = 7.6 Hz, 4H), 7.54 (d, J = 7.6 Hz, 4H), 9.38 (br s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ (ppm) 116.8, 120.9, 128.5, 140.9, 156.3; IR (KBr) 3233, 3186, 2965, 2846, 1601, 1551, 1497, 1481, 1445, 1311, 1294, 1254, 1194, 1092, 896, 832, 746 cm^{-1}; Elemental analysis: $C_{14}H_{12}N_4S$ (268.34): calcd. C, 62.66; H, 4.51; N, 20.88; S, 11.95; found: C, 62.72; H, 4.55; N, 20.81; S, 11.90.

Characterization of known Compounds: Compounds **3a**[22a], **3b**[19a], **3e**, [22c] **3f**,[22b] **7a**,[23d] **7e**,[42a] **7f**,[42b] **9g**,[23c] **13a-13h**, **14a**, **14h**,[28c] **17a**,[43] **17c**,[44] **17d**.[45]

References and Notes:

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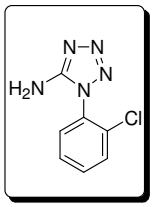
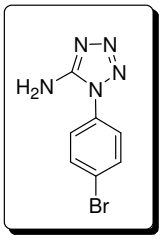
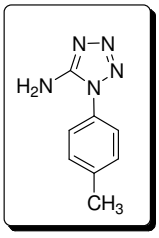
Spectral Data:



1-(2-Chloro-phenyl)-1*H*-tetrazol-5-ylamine (3b). mp: 183−185 °C (Lit.[19a] 187−189 °C); ^{1}H NMR (400 MHz, $CDCl_3$ + DMSO-d_6): δ (ppm) 6.35 (br s, 2H), 7.42−7.60 (m, 3H), 7.65 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$ + DMSO-d_6): δ (ppm) 128.1, 129.2, 130.5, 131.5, 131.8, 155.4; IR (KBr): 3329, 3158, 2983, 1659, 1594, 1578, 1498, 1460, 1317, 1141, 1130, 1093, 1081, 1040, 760 cm^{-1}; Elemental analysis: $C_7H_6ClN_5$ (195.61): calcd. C, 42.98; H, 3.09; N, 35.80; found: C, 43.03; H, 3.13; N, 35.69.

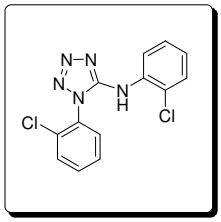


1-(4-Bromo-phenyl)-1*H*-tetrazol-5-ylamine (3e). mp: 240−242 °C (Lit.[22b] 239−240 °C); ^{1}H NMR (400 MHz, $CDCl_3$ + DMSO-d_6): δ 6.81 (br s, 2H), 7.53 (d, J = 8.8 Hz, 2H), 7.76 (d, J = 8.8 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$ + DMSO-d_6): δ (ppm) 121.3, 124.4, 131.3, 131.6, 153.5; IR (KBr): 3348, 3148, 2963, 2923, 1651, 1594, 1575, 1494, 1454, 1404, 1324, 1142, 1107, 1097, 1068, 1008, 836, 818 cm^{-1}; HRMS (ESI): 239.9885 (MH^+).

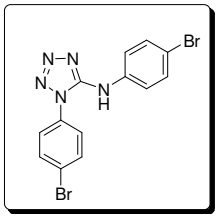


1-*p*-Tolyl-1*H*-tetrazol-5-ylamine (3f). mp: 188 °C (Lit.[22b] 178−179 °C); ^{1}H NMR (400 MHz, $CDCl_3$ + DMSO-d_6): δ (ppm) 2.46 (m, 3H), 6.46 (br s, 2H), 7.37 (d, J = 6.4 Hz, 2H), 7.43 (d, J = 6.4 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$ + DMSO-d_6): δ (ppm) 21.0, 123.5,

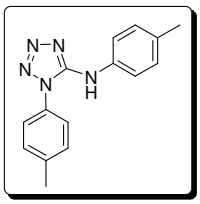
130.3, 130.6, 139.7, 154.4; IR (KBr): 3306, 3141, 2980, 1657, 1594, 1572, 1519, 1467, 1320, 1142, 1119, 1091, 1046, 1017, 839, 818, 765 cm^{-1}; HRMS (ESI): 176.0936 (MH^+).



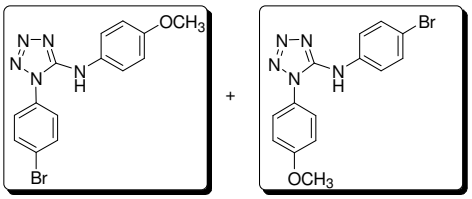
(2-Chloro-phenyl)-[1-(2-chloro-phenyl)-1*H*-tetrazol-5-yl]-amine (7b). mp: 106–108 °C; ^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) 6.86 (br s, 1H), 7.03 (t, J = 8.0 Hz, 1H), 7.40 (t, J = 8.0 Hz, 2H), 7.53–7.66 (m, 3H), 7.72 (d, J = 7.6 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ (ppm) 119.1, 121.7, 123.9, 128.2, 128.9, 129.1, 129.4, 129.6, 131.4, 130.0, 134.5, 151.8; IR (KBr): 3389, 1595, 1566, 1514, 1492, 1469, 1309, 1272, 1230, 1092, 1077, 1056, 1036, 766, 748 cm^{-1}; Elemental analysis: $C_{13}H_9Cl_2N_5$ (306.15): calcd. C, 51.00; H, 2.96; N, 22.88; found: C, 50.94; H, 3.01; N, 22.99.



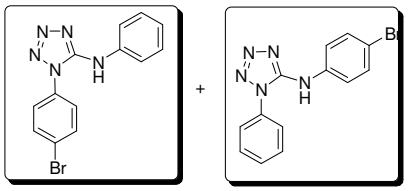
4-Bromo-phenyl)-[1-(4-bromo-phenyl)-1*H*-tetrazol-5-yl]-amine (7e). mp: 191–193 °C (Lit.[42a] 194–195 °C); ^{1}H NMR (400 MHz, $CDCl_3$ + DMSO-d_6): δ (ppm) 7.40 (d, J = 9.2 Hz, 2H), 7.52 (d, J = 8.8 Hz, 2H), 7.57 (d, J = 9.2 Hz, 2H), 7.76 (d, J = 8.8 Hz, 2H), 9.20 (br s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$ + DMSO-d_6): δ (ppm) 113.9, 119.6, 123.0, 126.3, 130.9, 131.5, 132.3, 138.0, 151.5; IR (KBr): 3259, 3191, 3096, 1741, 1606, 1563, 1526, 1488, 1403, 1235, 1091, 1070, 1010, 823, 804, 718 cm^{-1}; Elemental analysis: $C_{13}H_9Br_2N_5$ (395.05): calcd. C, 39.52; H, 2.30; N, 17.73; found: C, 39.47; H, 2.33; N, 17.80.



***p*-Tolyl-(1-*p*-tolyl-1*H*-tetrazol-5-yl)-amine (7f).** mp: 206–208 °C (Lit.[42b] 211 °C); ^{1}H NMR (400 MHz, $CDCl_3$ + DMSO-d_6): δ (ppm) 2.29 (s, 3H), 2.50 (s, 3H), 7.08 (d, J = 8.4 Hz, 2H), 7.40–7.49 (m, 6H), 8.82 (br s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$+ DMSO-d_6): δ (ppm) 20.5, 21.1, 118.6, 122.9, 124.9, 129.2, 130.3, 131.6, 136.9, 139.9, 152.5; IR (KBr): 3226, 3178, 3018, 2922, 1605, 1562, 1506, 1387, 1231, 1123, 1079, 824, 808, 788 cm^{-1}; Elemental analysis: $C_{15}H_{15}N_5$ (265.31): calcd. C, 67.90; H, 5.70; N, 26.40; found: C, 67.94; H, 5.65; N, 26.31.

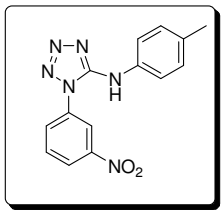


[1-(4-Bromo-phenyl)-1*H*-tetrazol-5-yl]-(4-methoxy-phenyl)-amine / (4-Bromo-phenyl)-[1-(4-methoxy-phenyl)-1*H*-tetrazol-5-yl]-amine (9c+10c). ^{1}H NMR (400 MHz, $CDCl_3$ + DMSO-d_6): δ (ppm) 3.78 (s, 3H), 3.88 (s, 3H), 6.83 (d, J = 8.0 Hz, 2H), 7.08 (m, 3H), 7.38 (d, J = 7.80 Hz, 2H), 7.45–7.50 (m, 5H), 7.57 (d, J = 7.80 Hz, 2H), 7.71 (d, J = 7.80 Hz, 2H), 8.64 (br s, 1H), 8.76 (br s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$ + DMSO-d_6): δ (ppm) 54.9, 55.9, 113.6, 114.2, 114.6, 119.7, 120.5, 123.0, 125.1, 126.3, 126.6, 131.2, 131.9, 132.5, 138.3, 151.9, 152.4, 155.1, 160.2; IR (KBr): 3253, 3190, 3090, 2960, 2927, 1613, 1573, 1537, 1514, 1489, 1462, 1441, 1313, 1301, 1256, 1180, 1170, 1121, 1099, 1072, 1030, 1007, 827 cm^{-1}; HRMS (ESI): 346.0303 (MH^+).

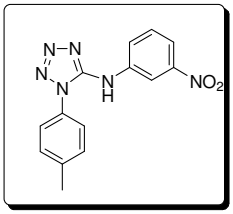


1-(4-Bromophenyl)-*N*-phenyl-1*H*-tetrazol-5-amine/*N*-(4-bromophenyl)-1-phenyl-1*H*-tetrazol-5-amine (9d+10d). ^{1}H NMR (400 MHz, $CDCl_3$ + DMSO-d_6): δ (ppm) 7.03 (t, J = 7.6 Hz, 2H), 7.30 (t, J = 7.6 Hz, 2H), 7.40 (d, J = 8.8 Hz, 2H), 7.52 (d, J = 8.4 Hz, 2H), 7.60 (m, 8H), 7.75 (d, J = 8.4 Hz, 2H), 8.97 (br s, 1H), 9.09 (br s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$ + DMSO-d_6): δ (ppm) 114.8, 119.0, 120.7, 122.9, 123.8, 125.5, 127.4, 129.2, 130.3, 131.9, 132.7, 133.3, 139.3, 139.9, 152.5, 152.8; IR (KBr): 3189, 3030, 1600, 1574, 1314,

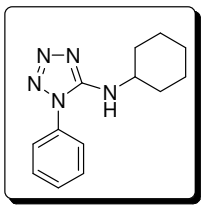
1238, 1179, 1126, 1095, 1069, 834, 823, 762, 747 cm^{-1}; Elemental analysis: $C_{13}H_{10}BrN_5$ (316.16): calcd. C, 49.39; H, 3.19; N, 22.15; found: C, 49.45; H, 3.14; N, 22.26.



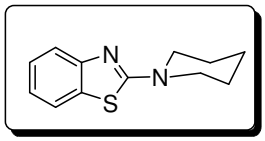
1-(3-Nitrophenyl)-*N*-*p*-tolyl-1*H*-tetrazol-5-amine (9e). mp: 203-205 ^oC; ^1H NMR (400 MHz, $CDCl_3$ + DMSO-d_6): δ (ppm) 2.50 (s, 3H), 7.40–7.55 (m, 3H), 7.83 (d, J = 8.0 Hz, 2H), 8.22 (d, J = 8.0 Hz, 2H), 8.53 (s, 1H), 9.34 (br s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$ + DMSO-d_6): δ (ppm) 20.5, 112.2, 115.8, 123.3, 124.6, 129.0, 129.7, 138.7, 140.3, 147.7, 151.2; IR (KBr): 3447, 2923, 2851, 1607, 1572, 1526, 1380, 1355, 1097, 1079, 834, 823, 733 cm^{-1}; Elemental analysis: $C_{14}H_{12}N_6O_2$ (296.28): calcd. C, 56.75; H, 4.08; N, 28.36; found: C, 56.71; H, 4.11; N, 28.46.



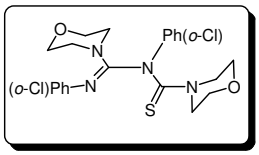
***N*-(3-Nitrophenyl)-1-*p*-tolyl-1*H*-tetrazol-5-amine (10e).** mp: 173-175 ^oC; ^1H NMR (400 MHz, $CDCl_3$ + DMSO-d_6): δ (ppm) 2.48 (s, 3H), 7.45–7.62 (m, 3H), 7.83 (d, J = 8.4 Hz, 2H), 8.13 (d, J = 8.4 Hz, 2H), 8.65 (s, 1H), 9.82 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$ + DMSO-d_6): δ (ppm) 20.7, 112.5, 116.0, 123.4, 124.8, 128.5, 129.2, 129.9, 139.9, 140.6, 147.9, 151.5; IR (KBr): 3432, 2923, 2846, 1608, 1574, 1525, 1344, 1110, 1089, 823, 733 cm^{-1}; HRMS (ESI): 297.1100 (MH^+).



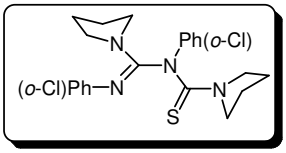
Cyclohexyl-(1-phenyl-1*H*-tetrazol-5-yl)-amine (9g). mp: 128−130 °C (Lit.[23c] 121−122 °C); ^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) 1.11−1.50 (m, 5H), 1.62−1.80 (m, 4H), 2.14 (d, J = 9.2 Hz, 1H), 3.77 (m, 1H), 4.17 (d, J = 7.2 Hz, 1H), 7.43−7.53 (m, 2H), 7.54 (m, 1H), 7.60 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$): δ (ppm) 24.9, 25.6, 33.5, 53.7, 124.2, 129.9, 130.5, 133.5, 154.1; IR (KBr): 3230, 2927, 2853, 1595, 1514, 1498, 1449, 1372, 1137, 1095, 1071, 1018, 765, 693 cm^{-1}; Elemental analysis: $C_{13}H_{17}N_5$ (243.31): calcd. C, 64.17; H, 7.04; N, 28.78; found: C, 64.22; H, 6.99; N, 28.71.



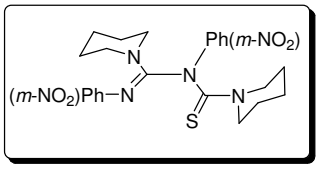
2-(Piperidin-1-yl)benzo[*d*]thiazole (14a). mp: 93 °C (Lit.[28c] 93 °C); ^{1}H NMR (400 MHz, $CDCl_3$): δ(ppm) 1.67 (s, 6H), 3.58 (s, 4H), 7.03 (t, J = 7.6 Hz,1H), 7.26 (t, J = 8.0 Hz,1H), 7.55 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$): δ(ppm) 24.4, 25.5, 49.8, 118.9, 120.7, 121.2, 126.0, 130.8, 153.1, 169.0; IR (KBr): 2961, 2858, 1608, 1562, 1542, 1473, 1443, 1356, 1305, 1270, 1220, 1058, 1038, 868, 838 cm^{-1}; Elemental analysis: $C_{12}H_{14}N_2S$ (218.32): calcd. C, 66.02; H, 6.46; N, 12.83; S, 14.69; found: C, 66.08; H, 6.88; N, 12.76; S, 14.74.



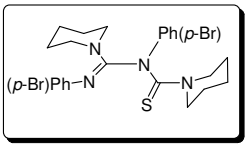
***N*-((*E*)-(2-Chlorophenylimino)(morpholino)methyl)-*N*-(2-chlorophenyl)morpholine-4-carbothioamide (13c).** mp: 157 °C (Lit.[28c].157 °C); ^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) 2.50–4.60 (m, 16H), 6.39–7.16 (m, 5H), 7.22–7.68 (m, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ (ppm) 47.1, 47.5, 50.9, 66.1, 122.8, 123.9, 126.5, 127.3, 128.0, 129.1, 131.0, 139.7, 145.7, 148.6, 187.2; IR (KBr): 2950, 2894, 2849, 1632, 1580, 1470, 1427, 1401, 1363, 1303, 1272, 1237, 1219, 1206, 1159, 1150, 1119, 1109, 1051, 1031, 999, 953, 876, 757, 750 cm^{-1}; Elemental analysis: $C_{22}H_{24}Cl_2N_4O_2S$ (479.42): calcd. C, 55.12; H, 5.05; N, 11.69; S, 6.69; found: C, 55.18; H, 5.09; N, 11.82; S 6.75.



***N*-((*E*)-(2-Chlorophenylimino)(pyrrolidin-1-yl)methyl)-*N*-(2-chlorophenyl)pyrrolidine-1-carbothioamide (13d).** mp: 154 °C (Lit.[28c] 154 °C); ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 1.70–2.21 (m, 10H), 3.14–4.02 (m, 6H), 6.43–6.86 (m, 3H), 6.90–7.06 (m, 2H), 7.12–7.53 (m, 2H), 7.77 (br s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ (ppm) 24.5, 25.1, 26.1, 26.7, 46.9, 48.1, 51.6, 54.5, 122.3, 123.3, 123.8, 125.3, 126.3, 127.2, 127.5, 128.2, 128.9, 130.9, 138.6, 146.6, 183.2; IR (KBr): 2968, 2949, 2862, 1623, 1580, 1440, 1413, 1330, 1283, 1261, 1205, 1177, 1051, 947, 874, 756 cm^{-1}; Elemental analysis: $C_{22}H_{24}Cl_2N_4S$ (447.42): calcd. C, 59.06; H, 5.41; N, 12.52; S, 7.17; found: C, 59.12; H, 5.46; N, 12.48; S 7.21.

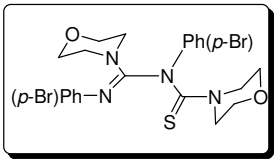


***N*-((*E*)-(3-Nitrophenylimino)(piperidin-1-yl)methyl)-*N*-(3-nitrophenyl)piperidine-1-carbothioamide (13e).** mp: 186 °C (Lit.[28c] 186 °C); ^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) 0.91–1.92 (m, 12H), 3.35 (m, 8H), 7.14–7.41 (m, 3H), 7.50 (t, J = 7.6 Hz, 1H), 7.63–7.86 (m, 3H), 7.93 (d, J = 7.6 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ (ppm) 23.7, 24.3, 25.0, 47.9, 52.1, 116.8, 117.1, 119.3, 127.4, 129.3, 130.4, 144.4, 148.7, 148.9, 150.5, 184.1; IR (KBr): 2942, 2925, 2851, 1637, 1606, 1522, 1479, 1444, 1417, 1352, 1299, 1280, 1244, 1206, 1182, 1027, 901, 739 cm^{-1}; Elemental analysis: $C_{24}H_{28}N_6O_4S$ (496.58): calcd. C, 58.05; H, 5.68; N, 16.92; S, 6.46; found: C, 57.99; H, 5.72; N, 16.88; S, 6.38.

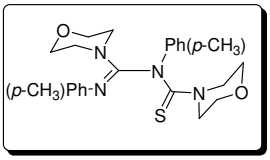


***N*-((*E*)-(4-Bromophenylimino)(piperidin-1-yl)methyl)-*N*-(4-bromophenyl)piperidine-1-carbothioamide (13f).** mp:177–179 °C (Lit.[28c] 177–179 °C); ^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) 1.01–1.85 (m, 13H), 2.81–3.82 (m, 7H), 6.77 (m, 2H), 6.88 (d, J = 8.4 Hz, 2H), 7.26 (d, J = 8.4 Hz, 2H), 7.43 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$): δ (ppm) 23.8, 24.5, 24.9, 25.1, 47.7, 51.9, 115.2, 117.4, 123.1, 124.2, 131.5, 132.5, 142.8, 148.8, 150.1, 184.7; IR (KBr): 2936, 2917, 2851, 1630, 1578, 1483, 1423, 1362, 1297, 1270, 1240, 1205, 1185,

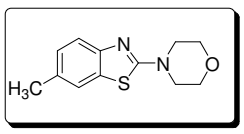
1066, 1051, 1026, 1005, 987, 891, 851, 822, 776 cm^{-1}; Elemental analysis: $C_{24}H_{28}Br_2N_4S$ (564.38): calcd. C, 51.08; H, 5.00; N, 9.93; S, 5.68; found: C, 51.14; H, 5.03; N, 9.87; S, 5.66.



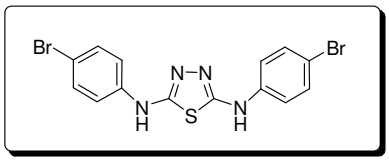
***N*-((*E*)-(4-Bromophenylimino)(morpholino)methyl)-*N*-(4-bromophenyl)morpholine-4-carbothioamide (13g).** mp: 173–175 °C (Lit.[28c] 173–175 °C); ^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) 2.60–3.81 (m, 16H), 6.61–7.12 (m, 4H), 7.31 (d, J = 8.4 Hz, 2H), 7.49 (br s, 2H); ^{13}C NMR (100 MHz, $CDCl_3$): δ (ppm) 46.9, 50.9, 65.5, 66.3, 115.8, 118.0, 121.9, 123.9, 131.8, 132.9, 141.7, 148.7, 148.3, 149.3, 184.8; IR (KBr): 2964, 2921, 2853, 1633, 1578, 1485, 1417, 1359, 1296, 1274, 1235, 1156, 1113, 1067, 999, 854, 831, 785 cm^{-1}; Elemental analysis: $C_{22}H_{24}Br_2N_4O_2S$ (568.32): calcd. C, 46.49; H, 4.26; N, 9.86; S, 5.64; found: C, 46.43; H, 4.30; N, 9.81; S, 5.68.



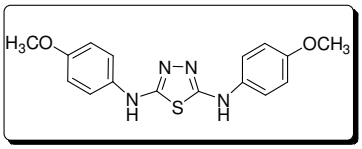
***N*-((*E*)-(*p*-Tolylimino)(morpholino)methyl)-*N*-*p*-tolylmorpholine-4-carbothioamide (13h).**[28c] Gummy; ^{1}H NMR (400 MHz, $CDCl_3$): δ(ppm) 2.25 (s, 3H), 2.33 (s, 3H), 2.74–3.75 (m, 16H), 6.80 (br s, 1H), 6.85 (d, J = 8.0 Hz, 2H), 7.05 (d, J = 8.0 Hz, 2H), 7.08–7.27 (m, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ (ppm) 20.8, 20.9, 46.7, 50.6, 65.4, 66.2, 121.2, 121.9, 129.2, 130.2, 131.8, 134.4, 140.2, 146.7, 149.5, 185.2; IR (KBr): 2963, 2919, 2857, 1632, 1607, 1506, 1472, 1422, 1360, 1296, 1279, 1236, 1160, 1115, 1066, 1034, 1018, 999, 940, 911, 855, 829, 818, 732 cm^{-1}; Elemental analysis: $C_{24}H_{30}N_4O_2S$ (438.58): calcd. C, 65.72; H, 6.89; N, 12.77; S, 7.31; found: C, 65.68; H, 6.84; N, 12.81; S 7.26.



6-Methyl-2-morpholinobenzo[*d*]thiazole (14h). mp: 133 °C (Lit.[28c] 133 °C); ^{1}H NMR (400 MHz, $CDCl_3$) δ(ppm) 2.40 (s, 3H), 3.60 (t, J = 5.2 Hz, 4H), 3.83 (t, J = 5.2 Hz, 4H), 7.12 (d, J = 8.0 Hz, 1H), 7.42 (s, 1H), 7.46 (d, J = 8.0 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 21.4, 48.6, 66.4, 119.1, 121.0, 127.4, 130.8, 131.6, 150.4, 168.7; IR (KBr): 2964, 2911, 2857, 1604, 1577, 1466, 1439, 1379, 1352, 1282, 1271, 1237, 1113, 1070, 1027, 945, 914, 840, 812 cm^{-1}; Elemental analysis: $C_{12}H_{14}N_2OS$ (234.38): calcd. C, 61.51; H, 6.02; N, 11.96; S, 13.68; found: C, 61.55; H, 5.97; N, 11.89; S, 13.61.



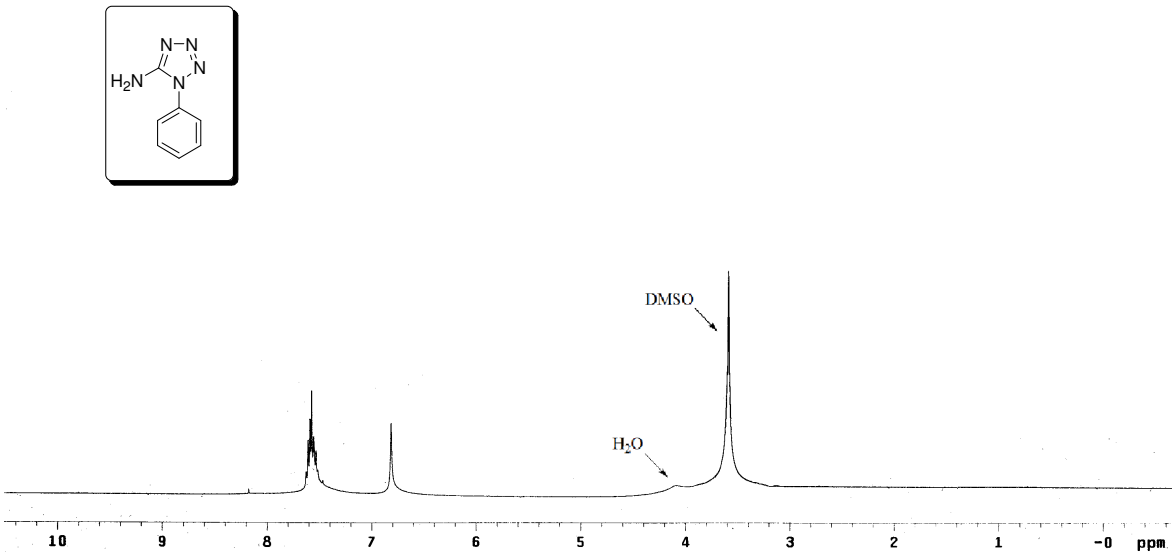
***N*^{2}, *N*^{5}-Bis(4-bromophenyl)-1,3,4-thiadiazole-2,5-diamine (17c).** mp: 244–246 °C (Lit.[44] 247–248 °C); ^{1}H NMR (400 MHz, $CDCl_3$ + DMSO-d_6): δ(ppm) 7.35 (d, J = 8.8 Hz, 4H), 7.54 (d, J = 8.8 Hz, 4H), 9.76 (br s, 2H); ^{13}C NMR (100 MHz, $CDCl_3$ + DMSO-d_6): δ(ppm) 112.0, 118.1, 130.6, 139.5, 155.4; IR (KBr): 3387, 2923, 1624, 1588, 1574, 1531, 1487, 1440, 1393, 1336, 1311, 1218, 1116, 1075, 1017, 827, 803 cm^{-1}; HRMS (ESI): 424.9071 (MH^+).



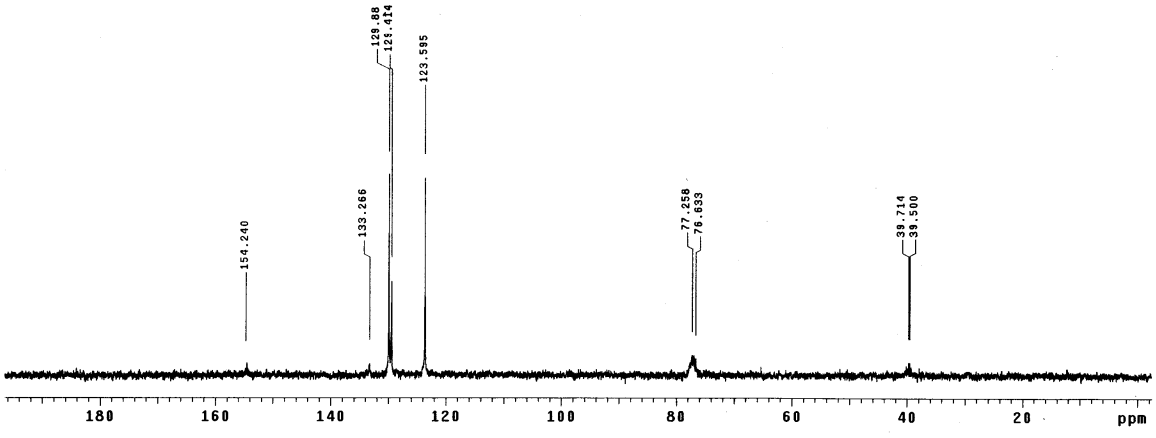
***N*^{2}, *N*^{5}-Bis(4-methoxyphenyl)-1,3,4-thiadiazole-2,5-diamine (17d).** mp: 235–237 °C (Lit.[45] 232 °C); ^{1}H NMR (400 MHz, $CDCl_3$+ DMSO-d_6): δ(ppm) 3.80 (s, 6H), 6.82 (d, J = 9.2 Hz, 4H), 7.45 (d, J = 9.2 Hz, 4H), 9.07 (br s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$+ DMSO-d_6): δ(ppm) 54.9, 113.6, 118.7, 134.5, 153.9, 156.6; IR (KBr): 3393, 3293, 3186, 3126, 3005, 2923, 2857, 1599, 1531, 1509, 1434, 1298, 1243, 1229, 1177, 1111, 1083, 1026, 819, 770 cm^{-1}; HRMS (ESI): 329.1072 (MH^+).

Spectra:

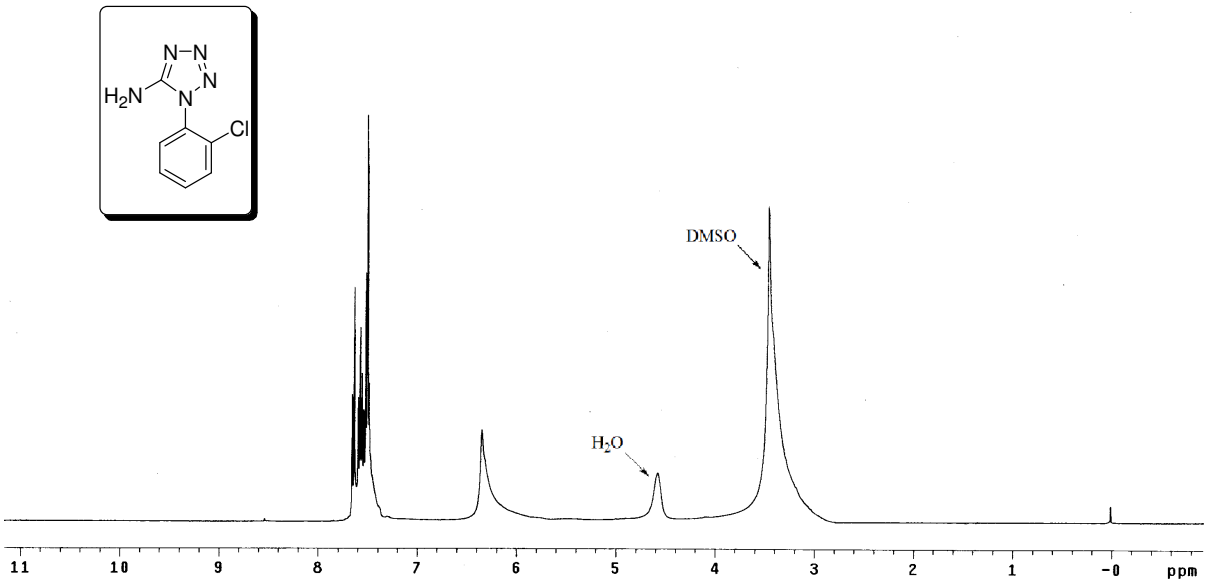
1-Phenyl-1*H*-tetrazol-5-ylamine (3a): ^{1}H NMR (400 MHz, $CDCl_3$ + DMSO-d_6):



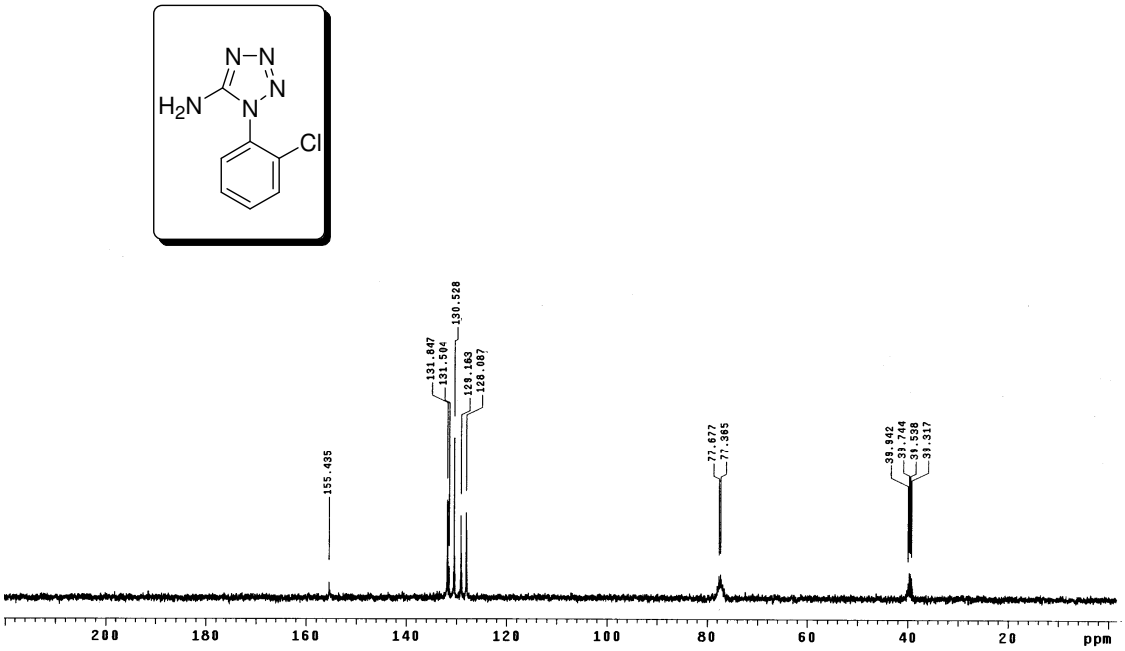
1-Phenyl-1*H*-tetrazol-5-ylamine (3a): ^{13}C NMR (100 MHz, $CDCl_3$ + DMSO-d_6):



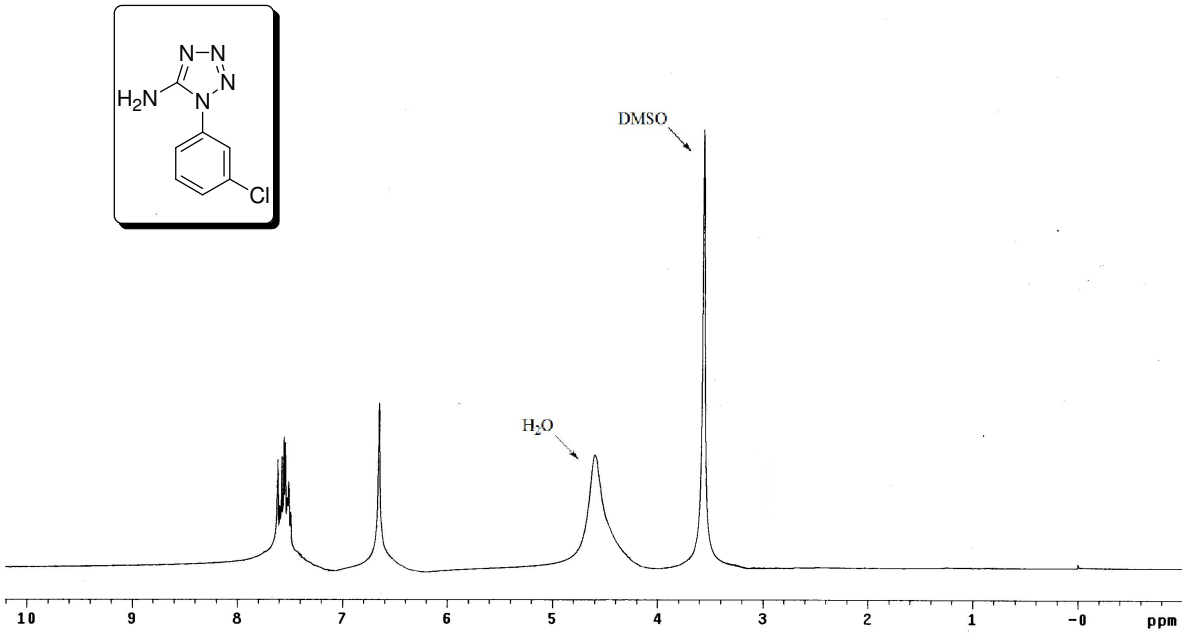
1-(2-Chloro-phenyl)-1*H*-tetrazol-5-ylamine (3b). ^{1}H NMR (400 MHz, $CDCl_3$ + DMSO-d_6):



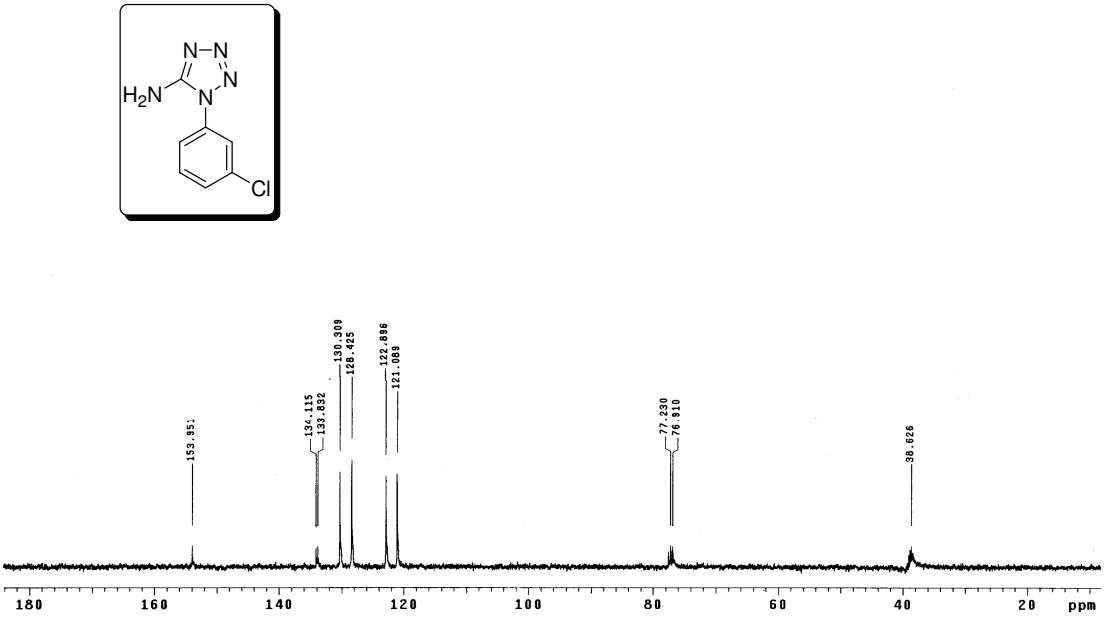
1-(2-Chloro-phenyl)-1*H*-tetrazol-5-ylamine (3b): ^{13}C NMR (100 MHz, $CDCl_3$+ DMSO-d_6):



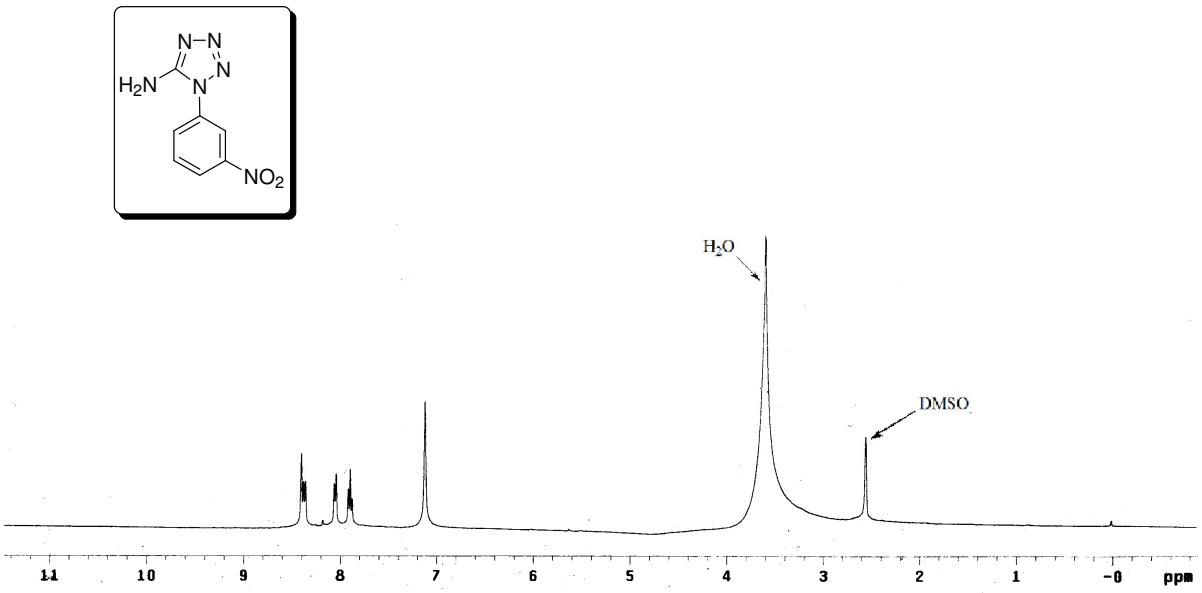
1-(3-Chloro-phenyl)-1*H*-tetrazol-5-ylamine (3c): ^{1}H NMR (400 MHz, $CDCl_3$ + DMSO-d_6):



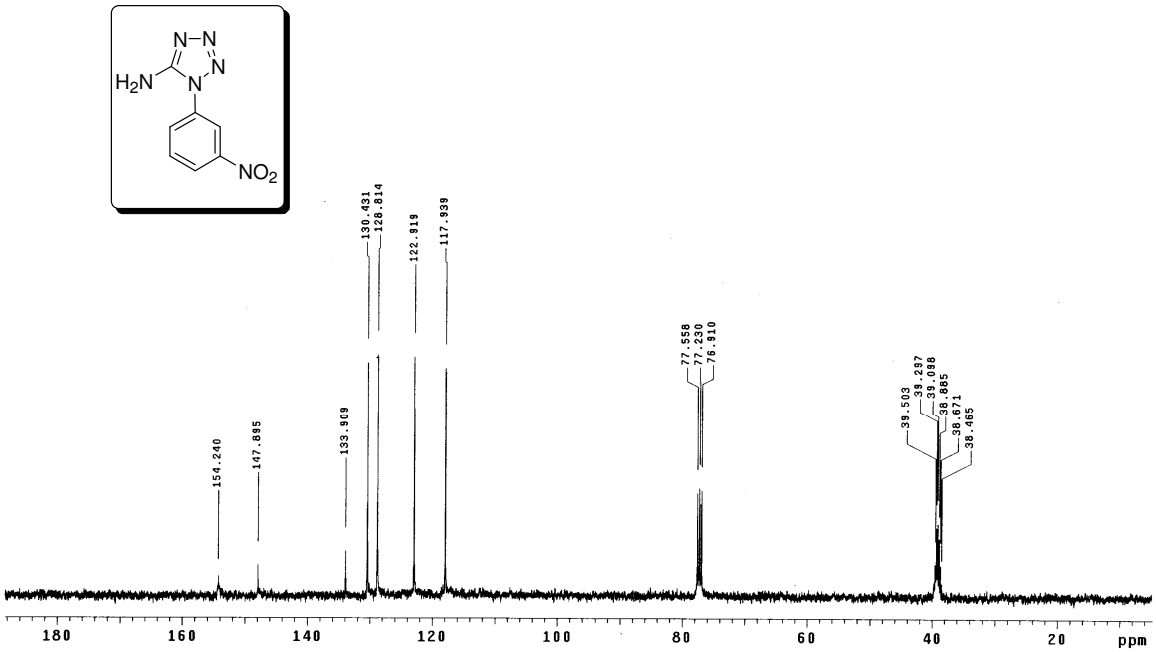
1-(3-Chloro-phenyl)-1*H*-tetrazol-5-ylamine (3c): ^{13}C NMR (100 MHz, $CDCl_3$ + DMSO-d_6):



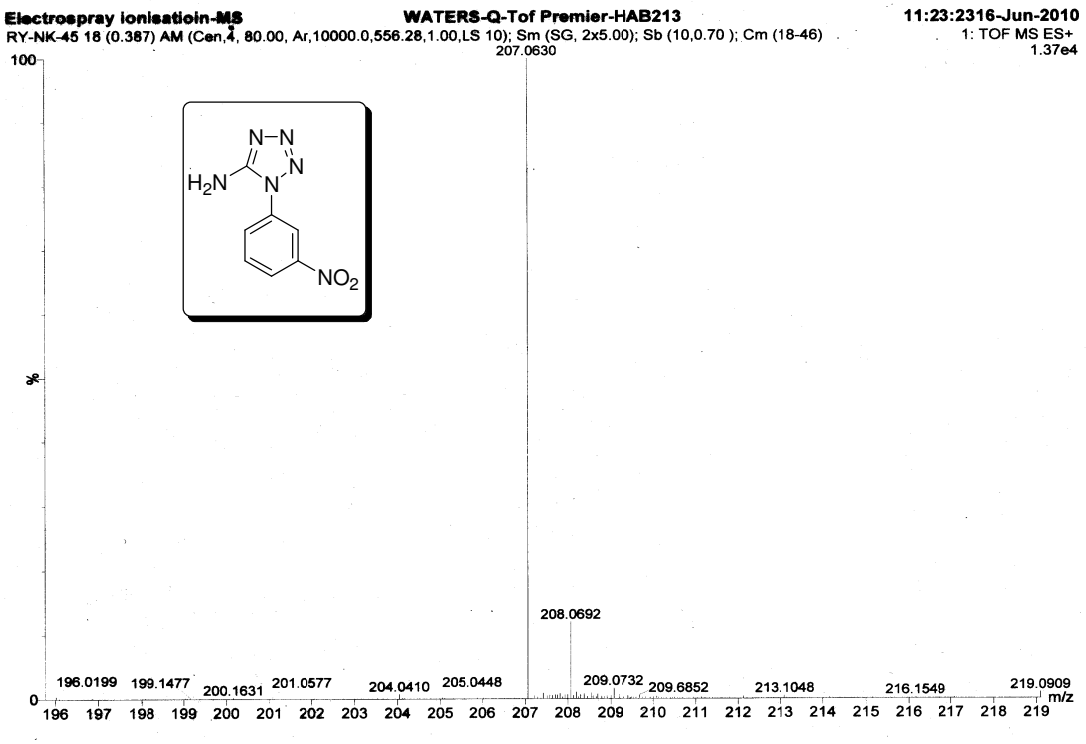
1-(3-Nitro-phenyl)-1*H*-tetrazol-5-ylamine (3d): ^{1}H NMR (400 MHz, $CDCl_3$ + DMSO-d_6):



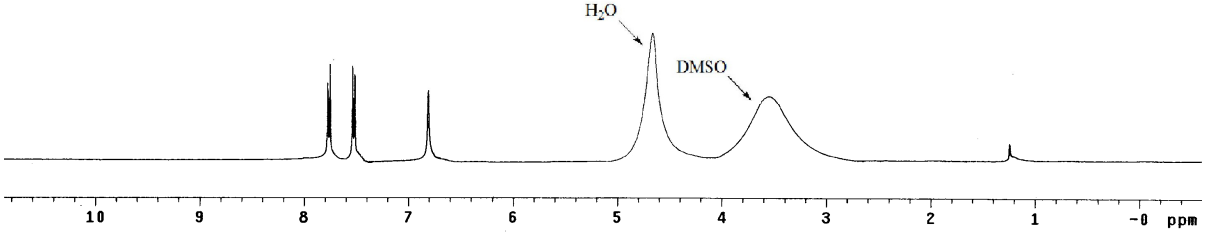
1-(3-Nitro-phenyl)-1*H*-tetrazol-5-ylamine (3d): ^{13}C NMR (100 MHz, $CDCl_3$ + DMSO-d_6):



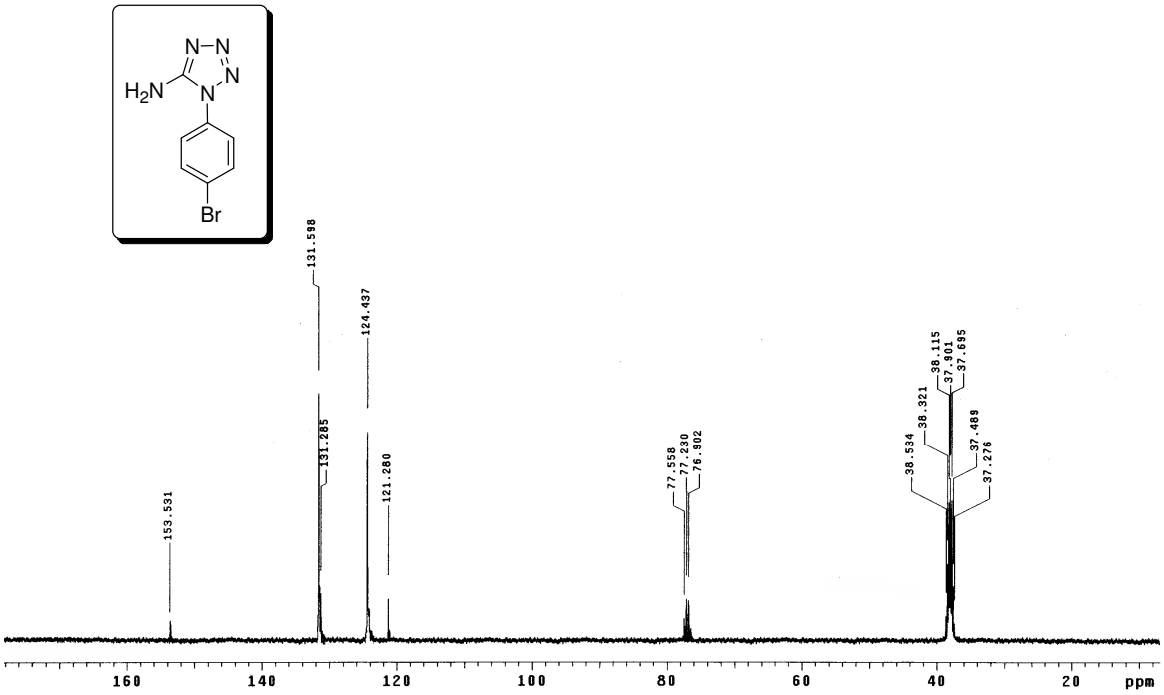
1-(3-Nitro-phenyl)-1*H*-tetrazol-5-ylamine (3d): MASS SPECTRA



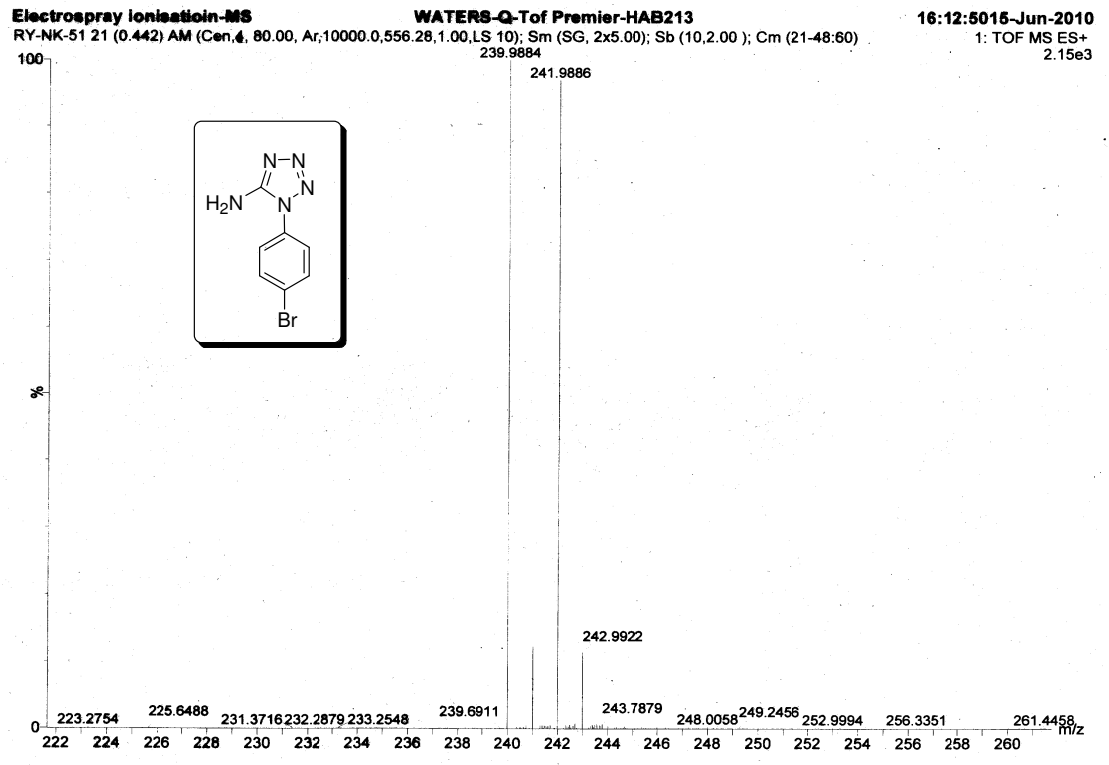
1-(4-Bromo-phenyl)-1*H*-tetrazol-5-ylamine (3e): ^{1}H NMR (400 MHz, $CDCl_3$ + DMSO-d_6):



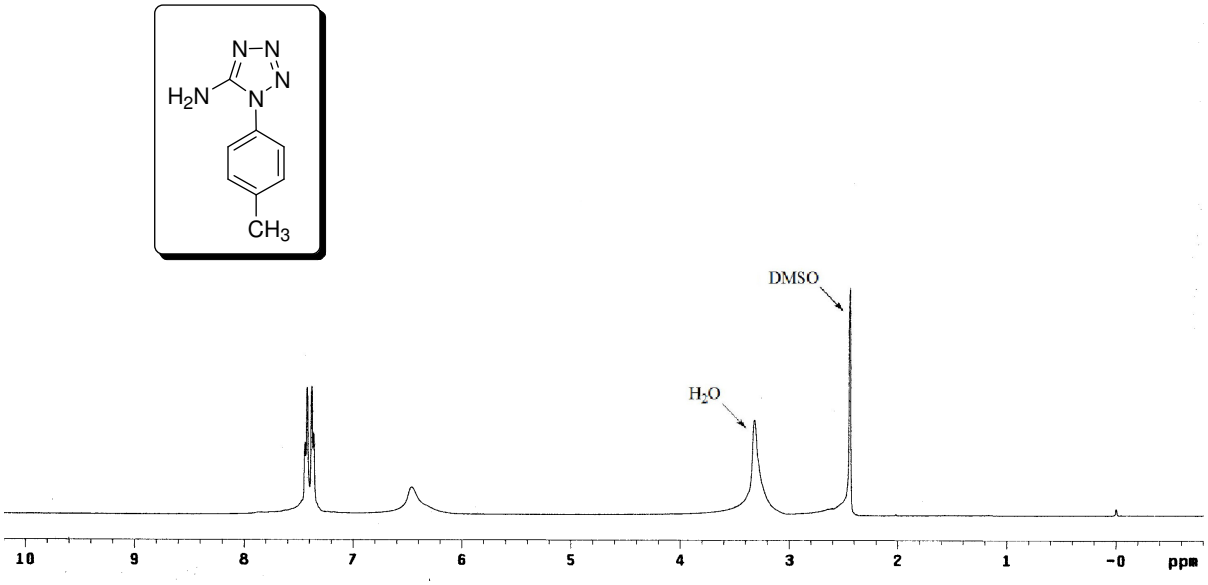
1-(4-Bromo-phenyl)-1*H*-tetrazol-5-ylamine (3e): ^{13}C NMR (100 MHz, $CDCl_3$ + DMSO-d_6):



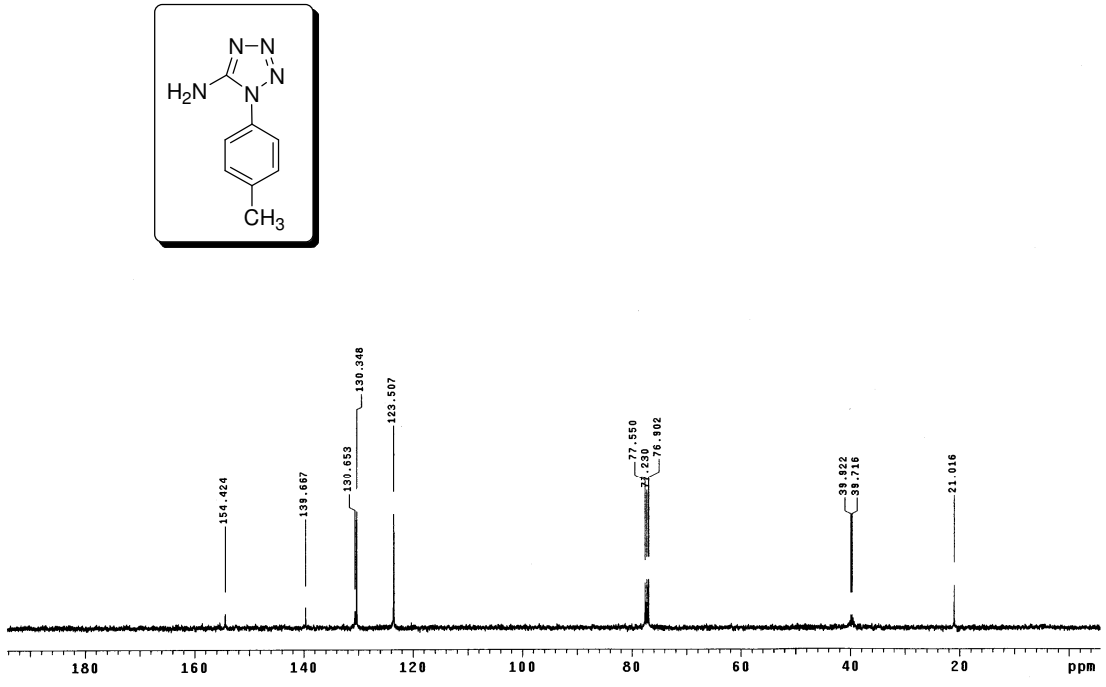
1-(4-Bromo-phenyl)-1*H*-tetrazol-5-ylamine (3e): MASS SPECTRA



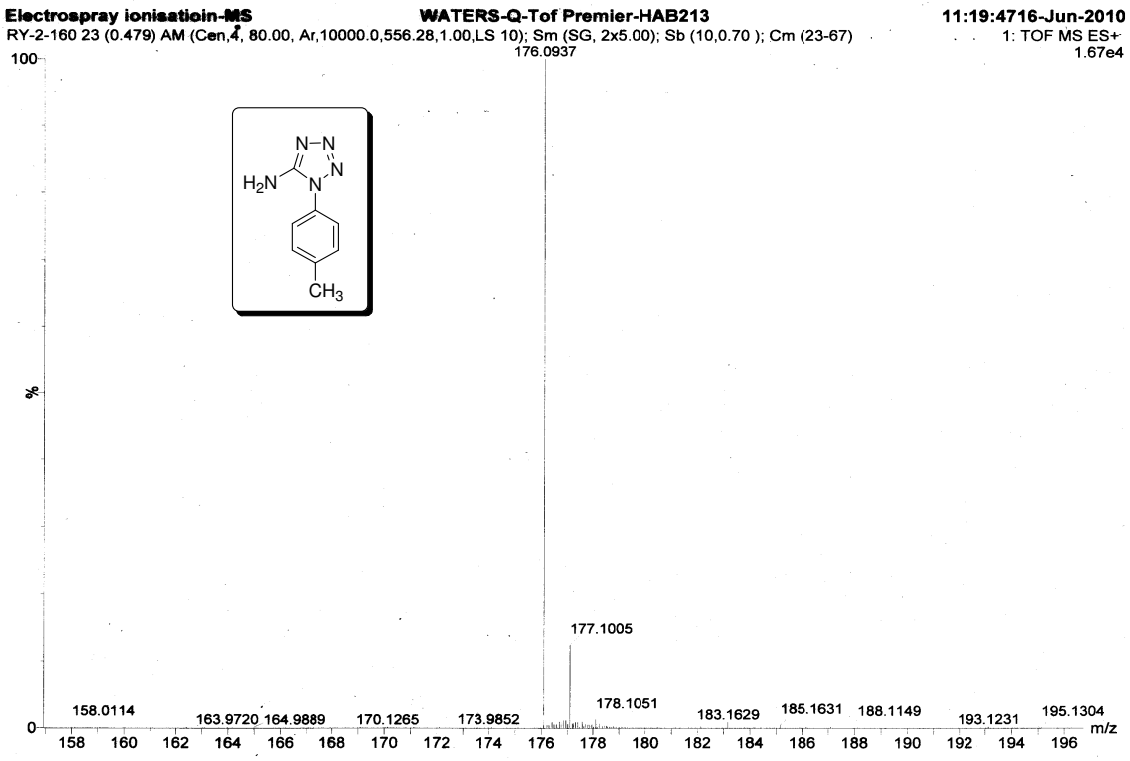
1-*p*-Tolyl-1*H*-tetrazol-5-ylamine (3f): ^{1}H NMR (400 MHz, $CDCl_3$ + DMSO-d_6):



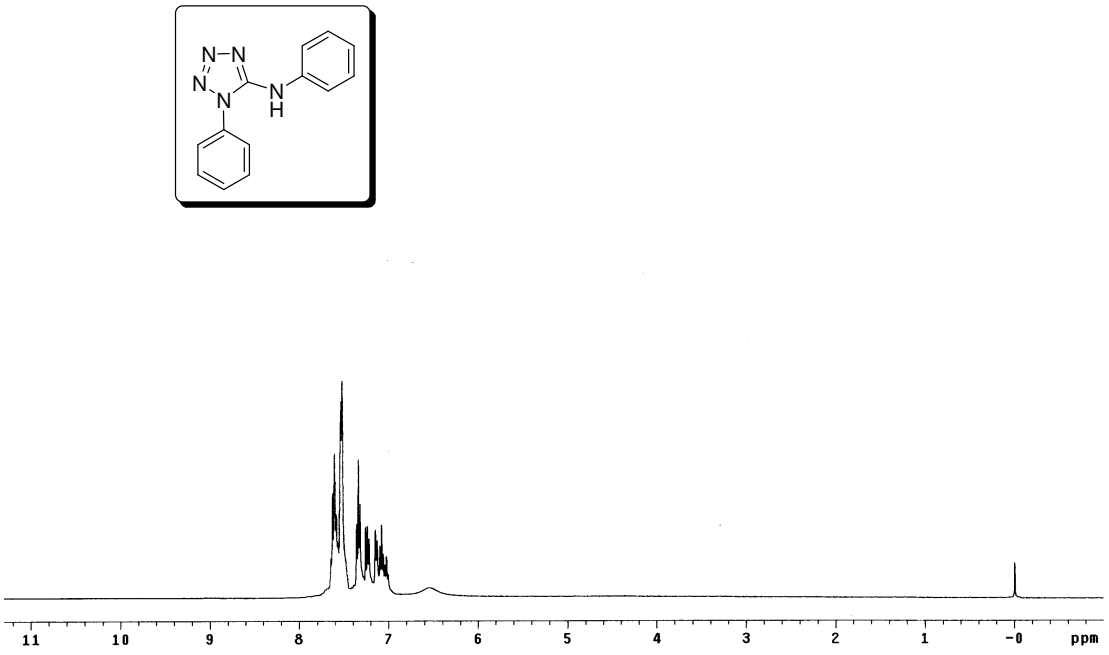
1-*p*-Tolyl-1*H*-tetrazol-5-ylamine (3f): ^{13}C NMR (100 MHz, $CDCl_3$ + DMSO-d_6):



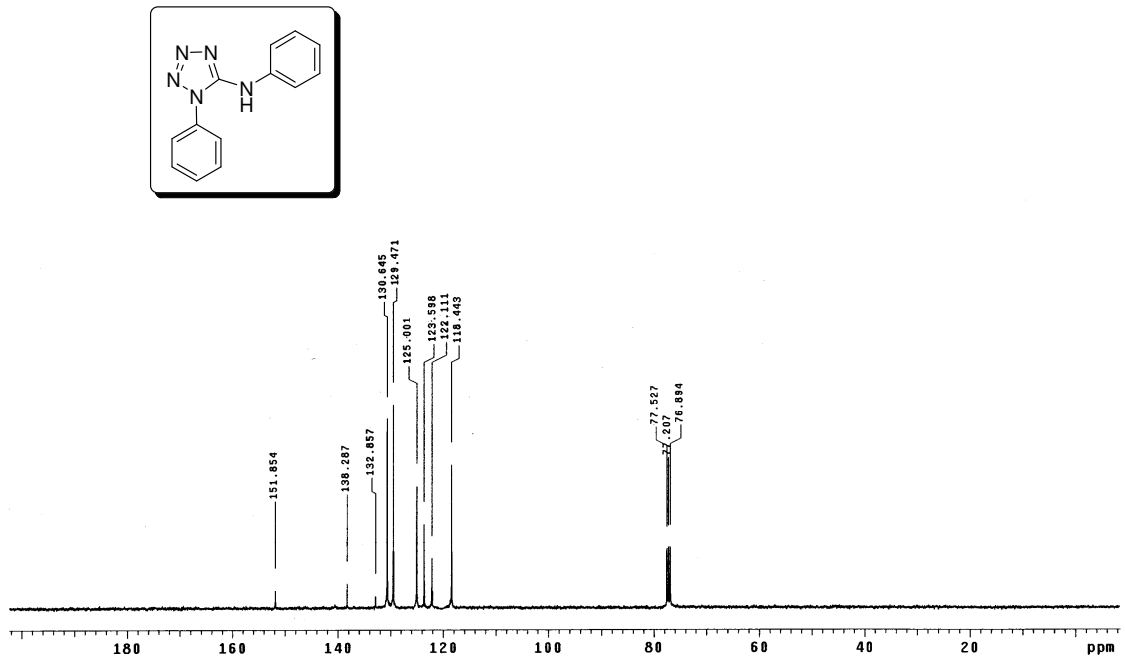
1-*p*-Tolyl-1*H*-tetrazol-5-ylamine (3f): MASS SPECTRA



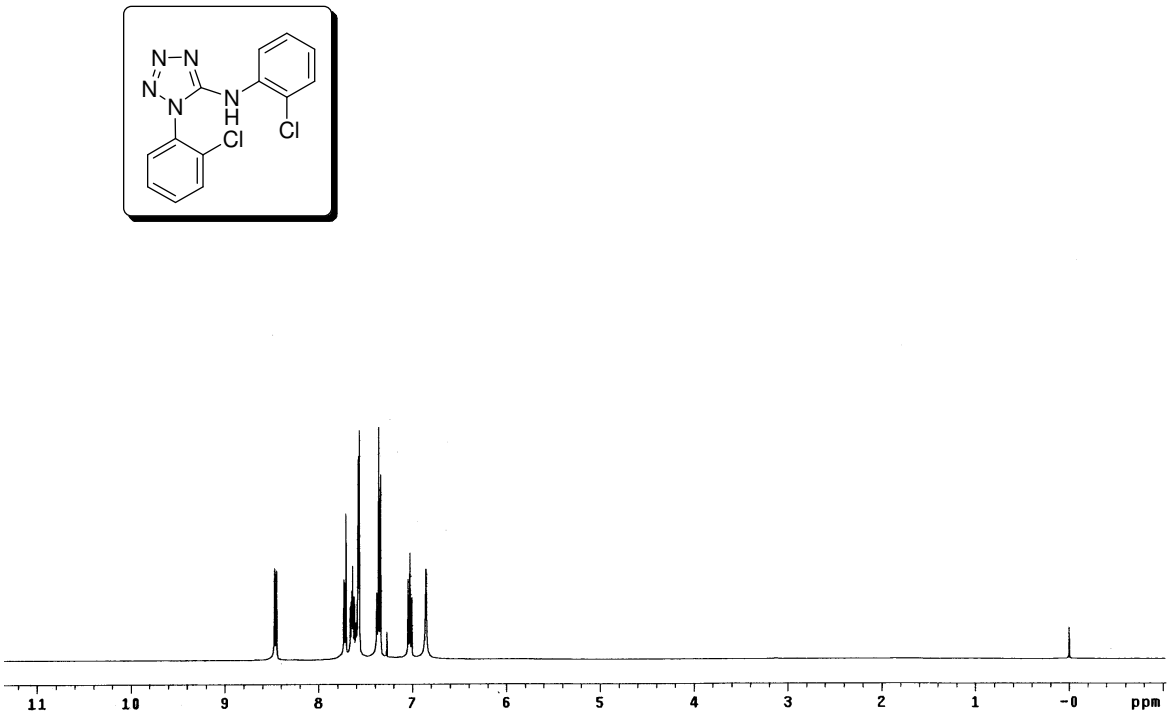
Phenyl-(1-phenyl-1*H*-tetrazol-5-yl)-amine (7a): ^{1}H NMR (400 MHz, $CDCl_3$):



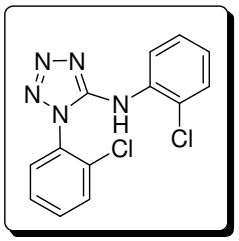
Phenyl-(1-phenyl-1*H*-tetrazol-5-yl)-amine (7a): ^{13}C NMR (100 MHz, $CDCl_3$):

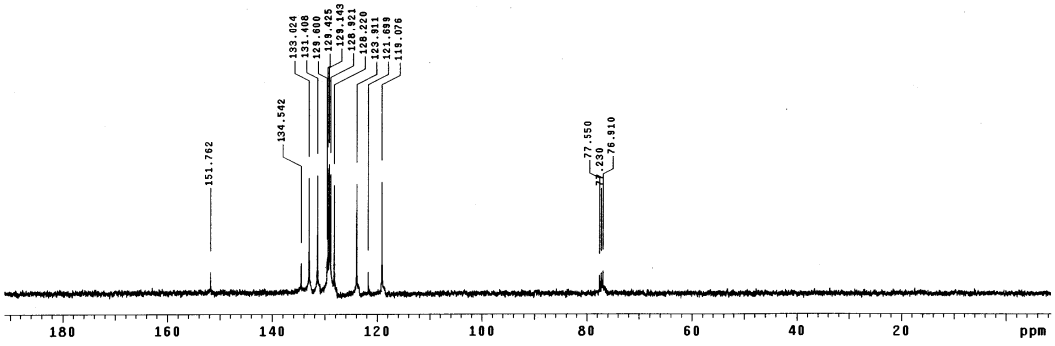


(2-Chloro-phenyl)-[1-(2-chloro-phenyl)-1*H*-tetrazol-5-yl]-amine (7b): ^{1}H NMR (400 MHz, $CDCl_3$):

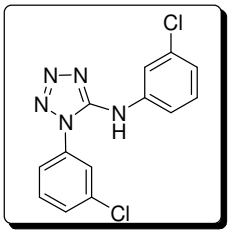


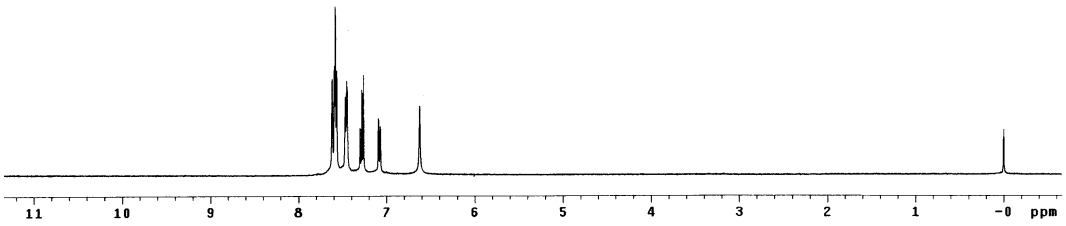
(2-Chloro-phenyl)-[1-(2-chloro-phenyl)-1*H*-tetrazol-5-yl]-amine (7b): ^{13}C NMR (100 MHz, $CDCl_3$):



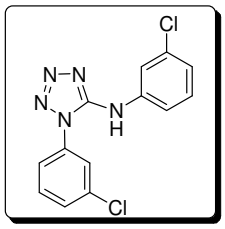


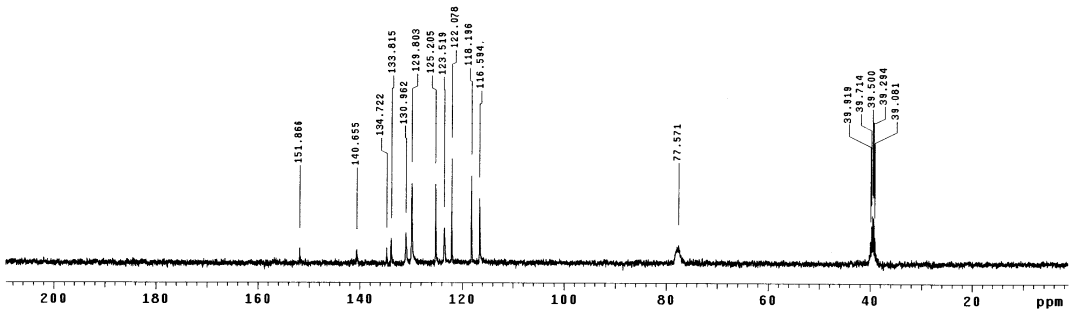
(3-Chloro-phenyl)-[1-(3-chloro-phenyl)-1*H*-tetrazol-5-yl]-amine (7c): ^{1}H NMR (400 MHz, $CDCl_3$):



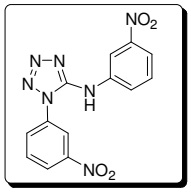


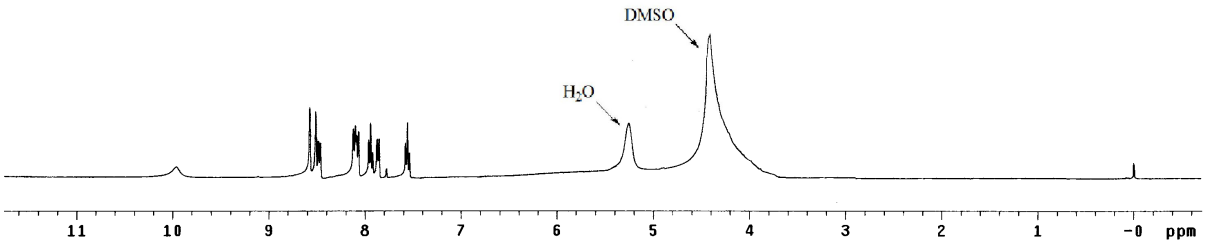
(3-Chloro-phenyl)-[1-(3-chloro-phenyl)-1*H*-tetrazol-5-yl]-amine (7c): ^{13}C NMR (100 MHz, $CDCl_3$-d_6):



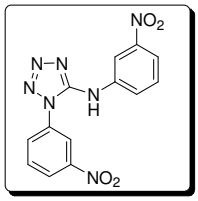


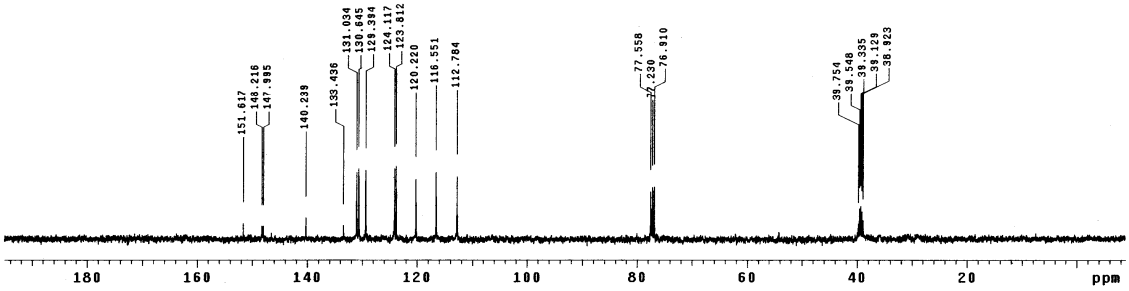
(3-Nitro-phenyl)-[1-(3-nitro-phenyl)-1*H*-tetrazol-5-yl]-amine (7d): ^{1}H NMR (400 MHz, $CDCl_3$ + DMSO-d_6):



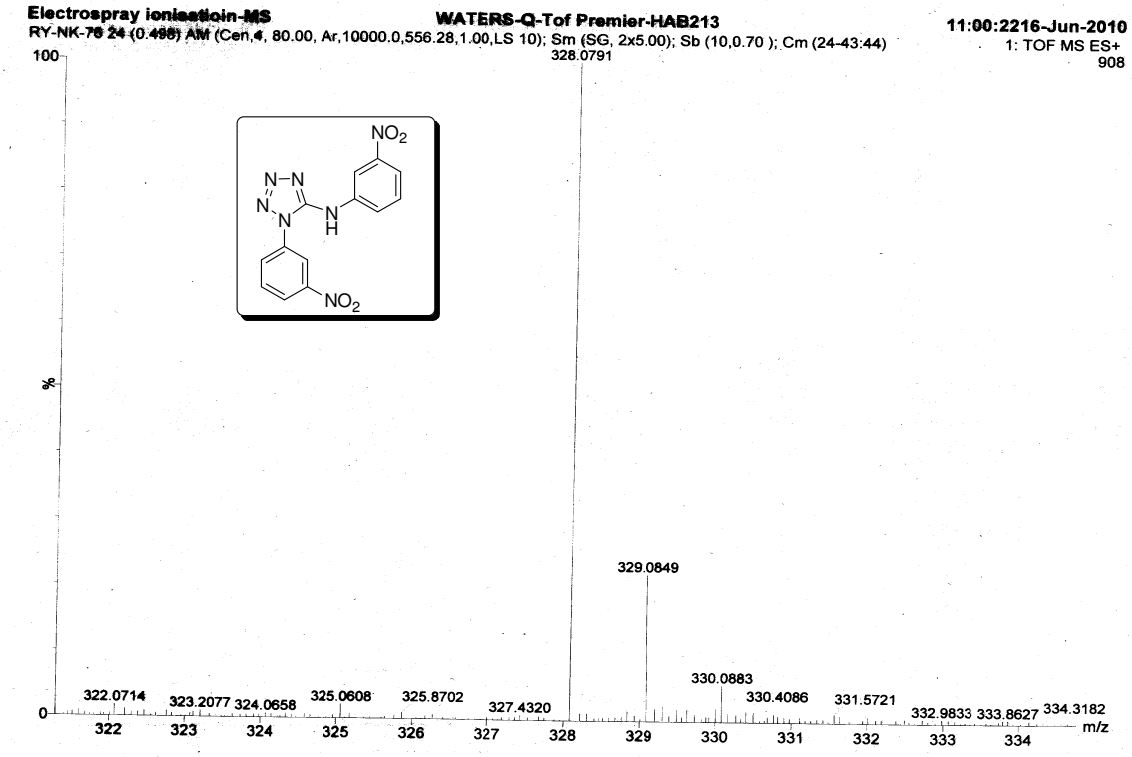


(3-Nitro-phenyl)-[1-(3-nitro-phenyl)-1*H*-tetrazol-5-yl]-amine (7d): ^{13}C NMR (100 MHz, $CDCl_3$ + DMSO-d_6):

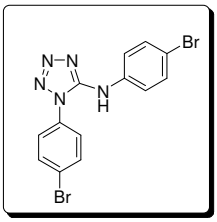


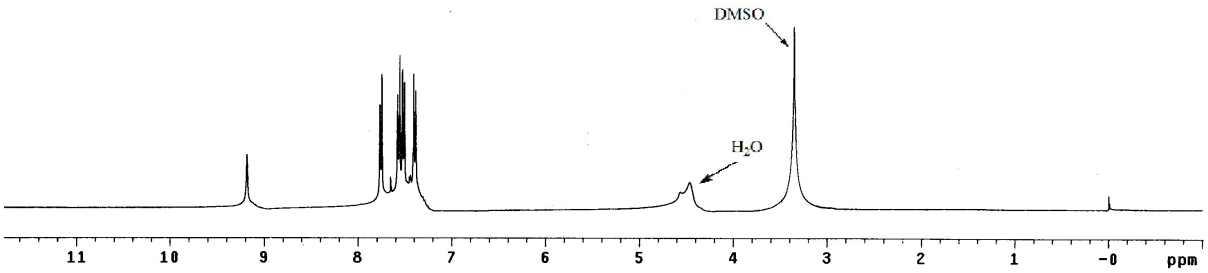


(3-Nitro-phenyl)-[1-(3-nitro-phenyl)-1*H*-tetrazol-5-yl]-amine (7d): MASS SPECTRA

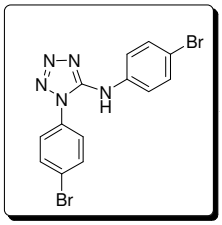


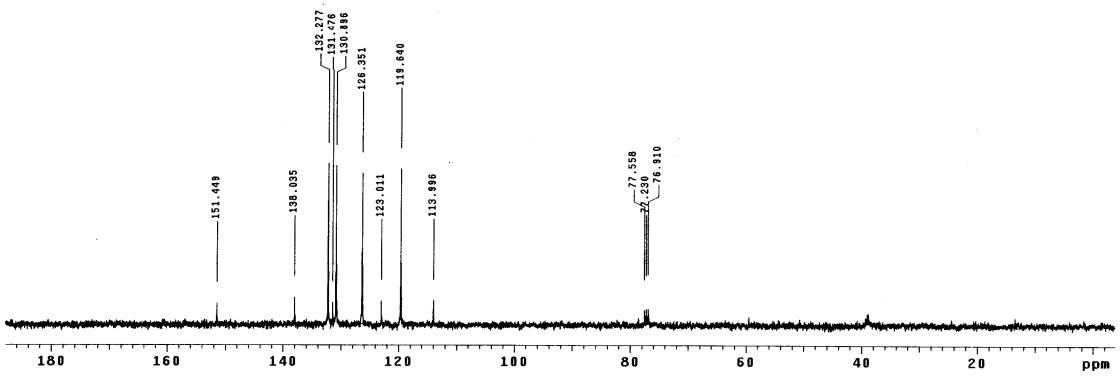
4-Bromo-phenyl)-[1-(4-bromo-phenyl)-1*H*-tetrazol-5-yl]-amine (7e): ^{1}H NMR (400 MHz, $CDCl_3$ + DMSO-d_6):



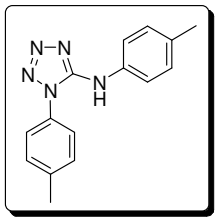


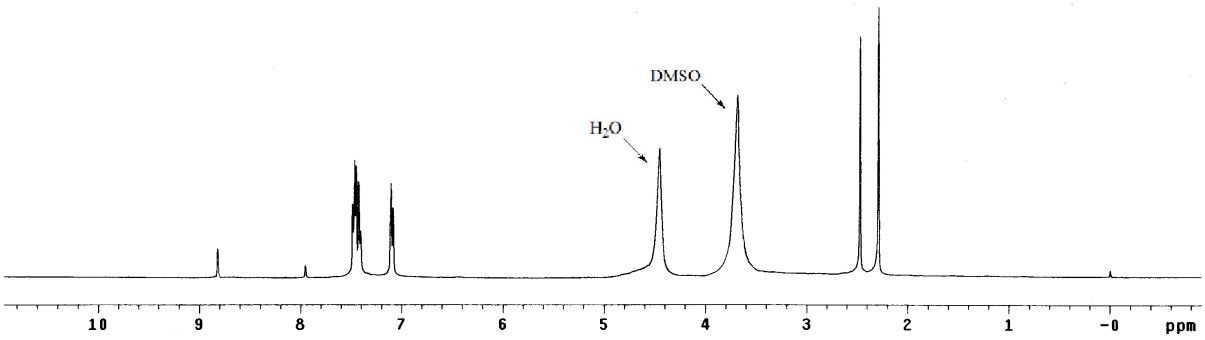
4-Bromo-phenyl)-[1-(4-bromo-phenyl)-1*H*-tetrazol-5-yl]-amine (7e): ^{13}C NMR (100 MHz, $CDCl_3$ + DMSO-d_6):



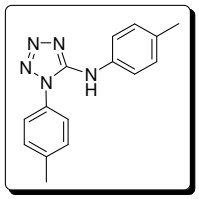


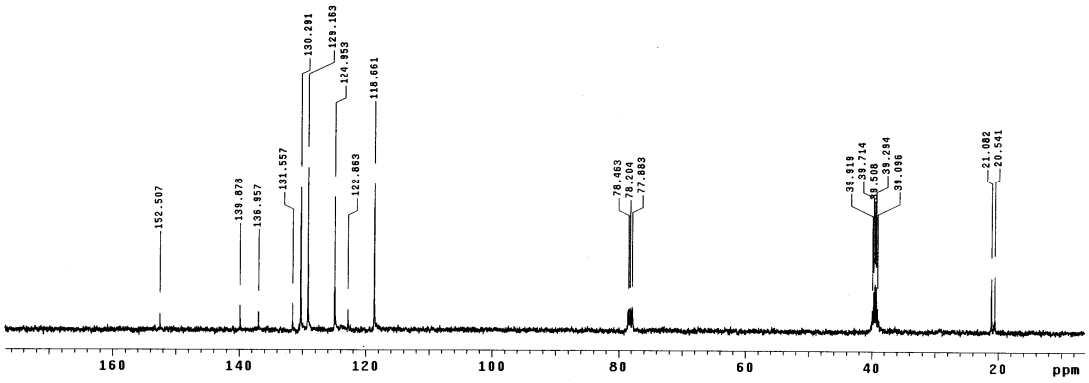
***p*-Tolyl-(1-*p*-tolyl-1*H*-tetrazol-5-yl)-amine (7f): ^{1}H NMR (400 MHz, $CDCl_3$ + DMSO-d_6):**



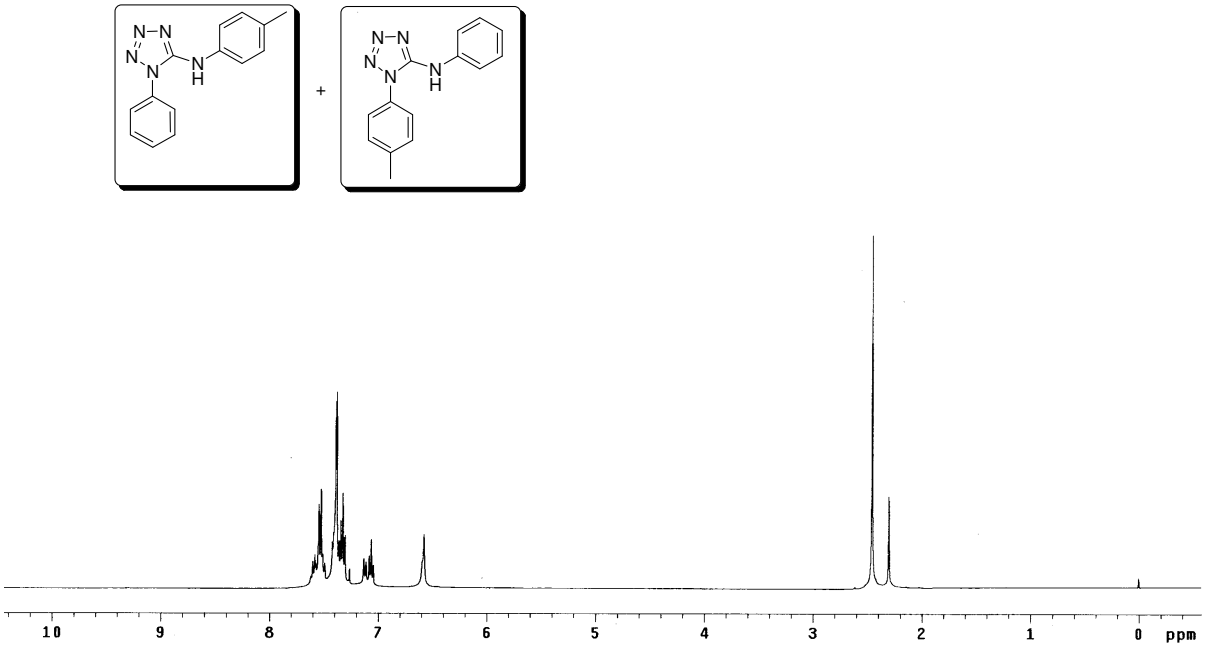


***p*-Tolyl-(1-*p*-tolyl-1*H*-tetrazol-5-yl)-amine (7f): ^{13}C NMR (100 MHz, $CDCl_3$ + DMSO-d_6):**

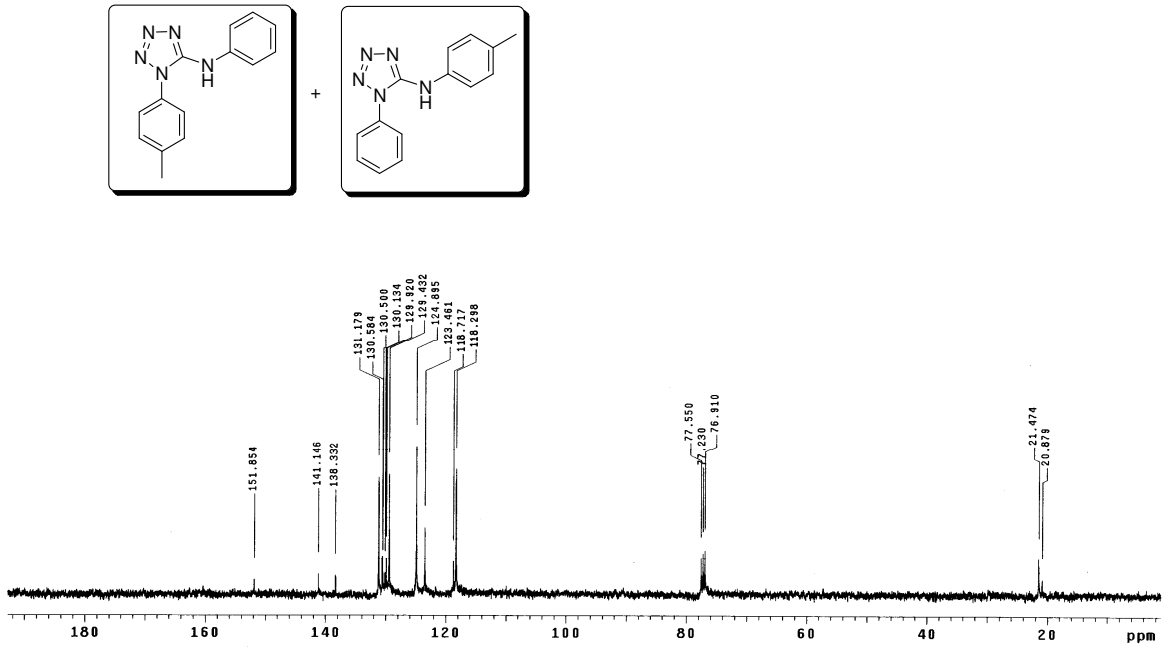




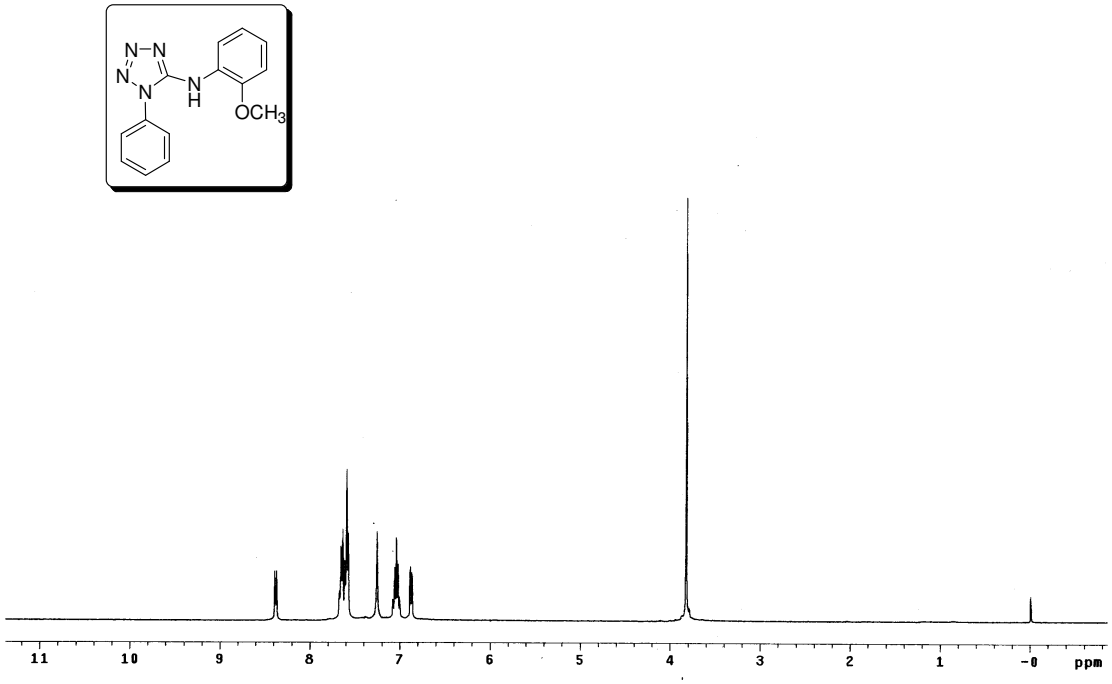
(1-Phenyl-1*H*-tetrazol-5-yl)-*p*-tolyl-amine / Phenyl-(1-*p*-tolyl-1*H*-tetrazol-5-yl)-amine (9a + 10a): ^{1}H NMR (400 MHz, $CDCl_3$):



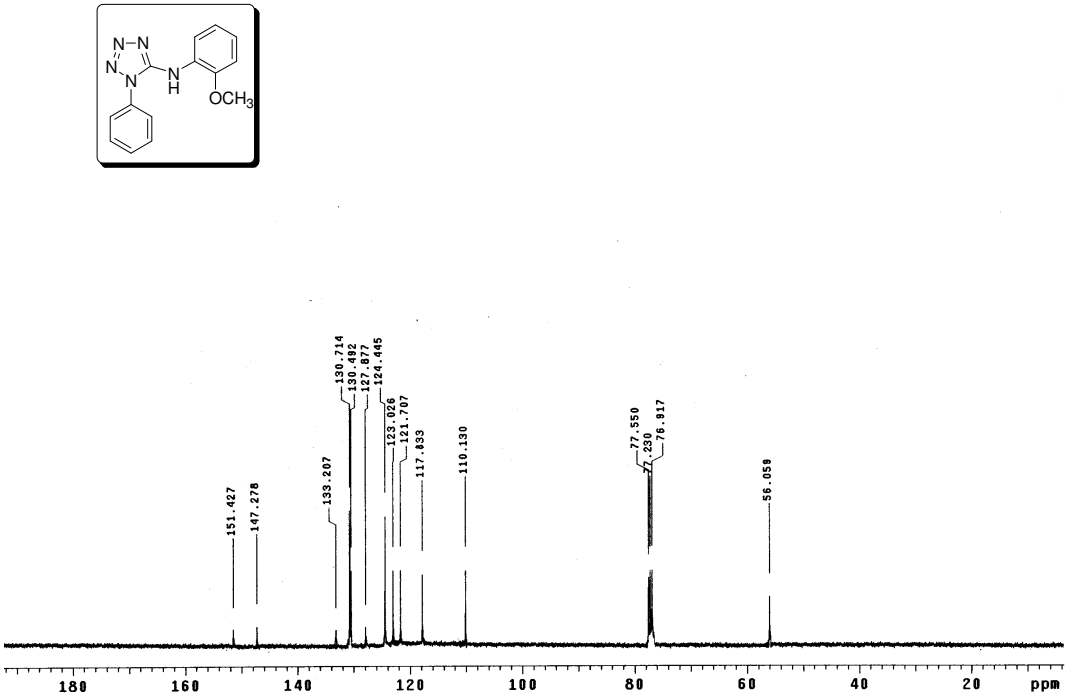
(1-Phenyl-1*H*-tetrazol-5-yl)-*p*-tolyl-amine / Phenyl-(1-*p*-tolyl-1*H*-tetrazol-5-yl)-amine (9a + 10a):^{13}C NMR (100 MHz, $CDCl_3$):



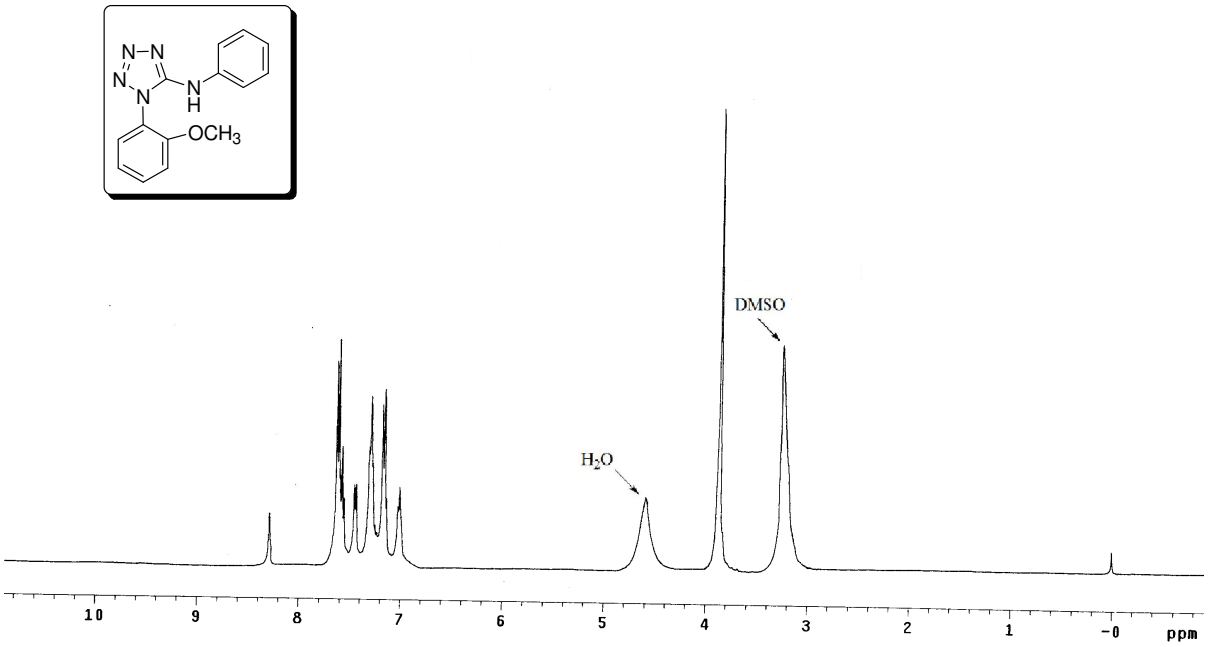
(2-Methoxy-phenyl)-(1-phenyl-1*H*-tetrazol-5-yl)-amine (9b): ^{1}H NMR (400 MHz, $CDCl_3$):



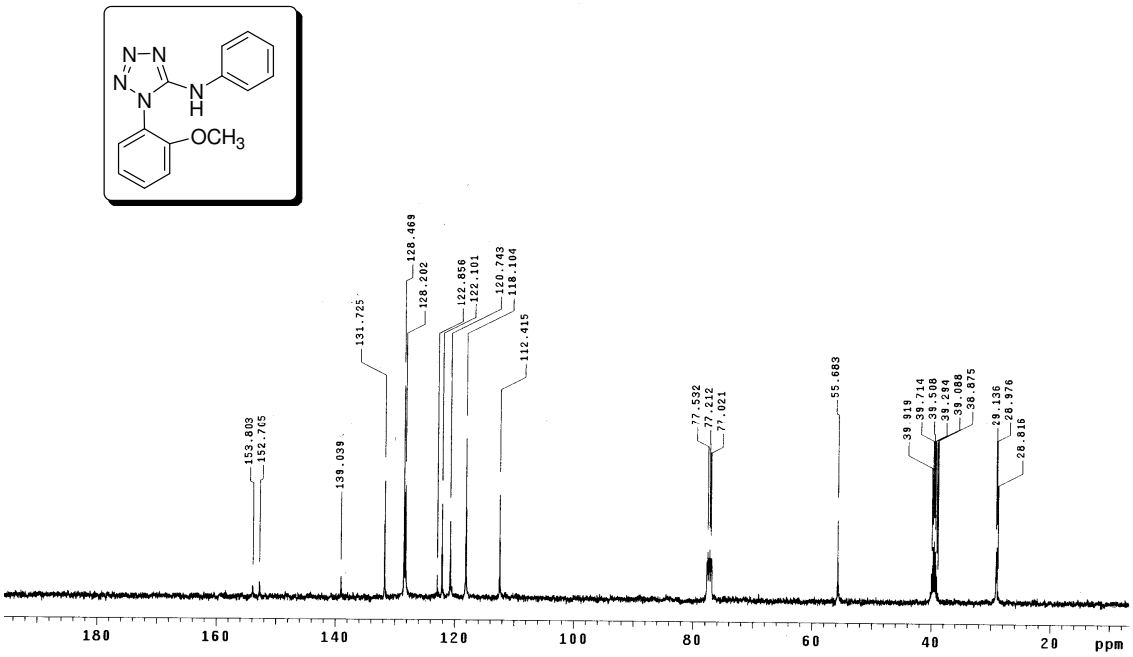
(2-Methoxy-phenyl)-(1-phenyl-1*H*-tetrazol-5-yl)-amine (9b): ^{13}C NMR (100 MHz, $CDCl_3$):



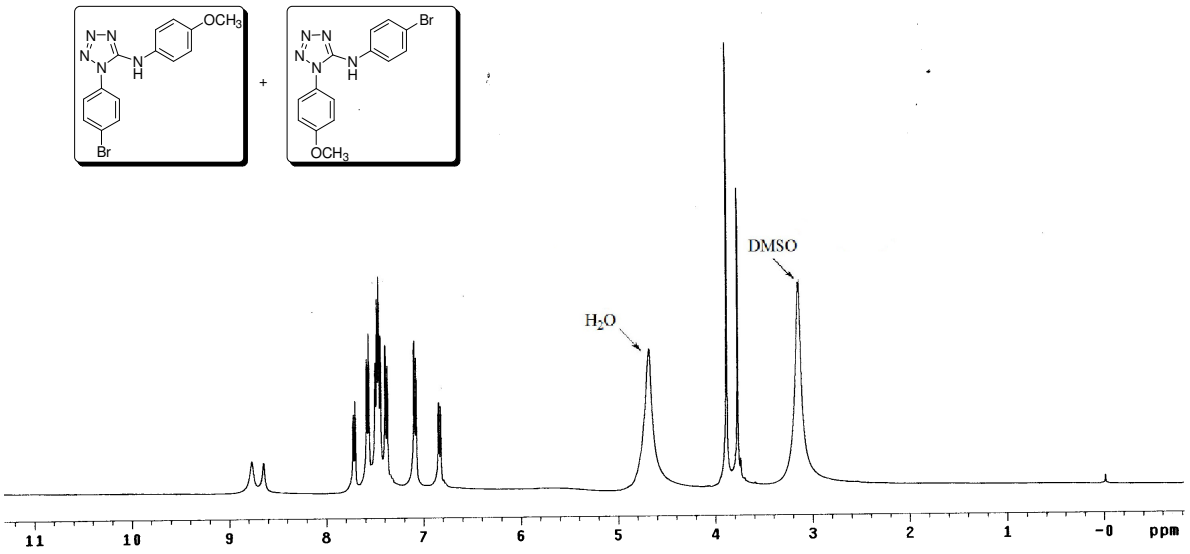
[1-(2-Methoxy-phenyl)-1*H*-tetrazol-5-yl]-phenyl-amine (10b): ^{1}H NMR (400 MHz, $CDCl_3$ + DMSO-d_6):



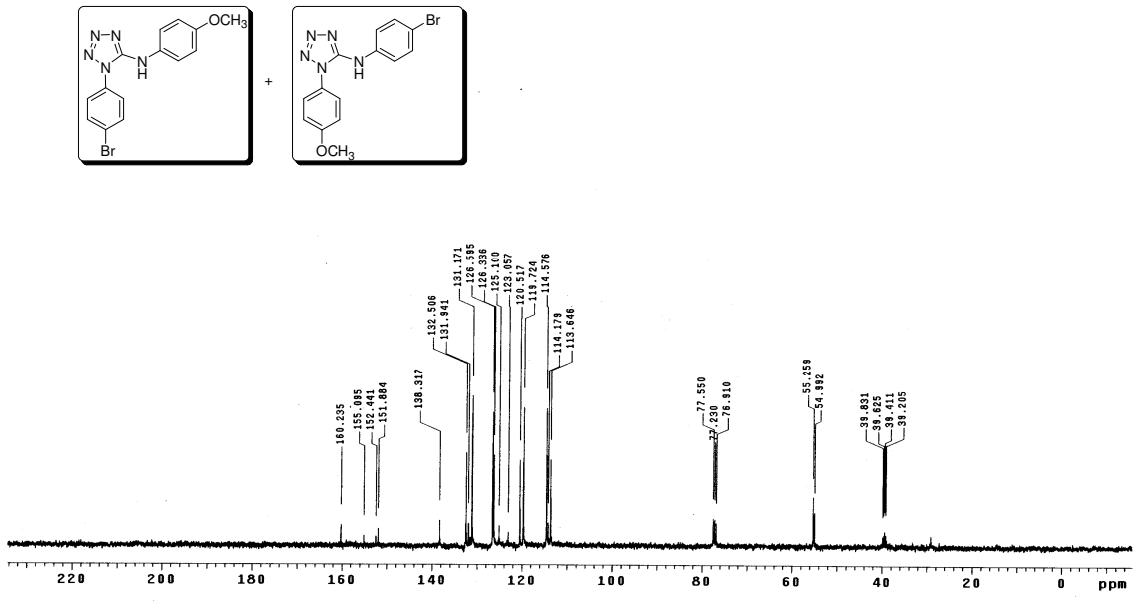
[1-(2-Methoxy-phenyl)-1*H*-tetrazol-5-yl]-phenyl-amine (10b): ^{13}C NMR (100 MHz, $CDCl_3$ + DMSO-d_6):



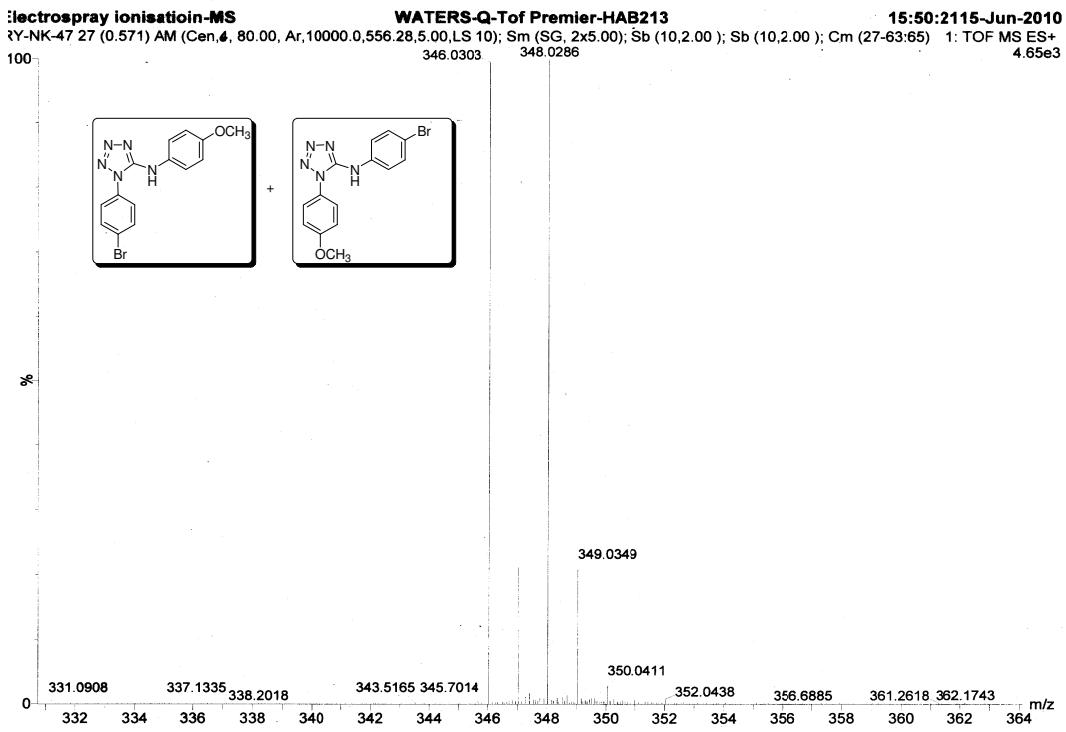
[1-(4-Bromo-phenyl)-1*H*-tetrazol-5-yl]-(4-methoxy-phenyl)-amine / (4-Bromo-phenyl)-[1-(4-methoxy-phenyl)-1*H*-tetrazol-5-yl]-amine (9c+10c): ^{1}H NMR (400 MHz, $CDCl_3$ + DMSO-d_6):



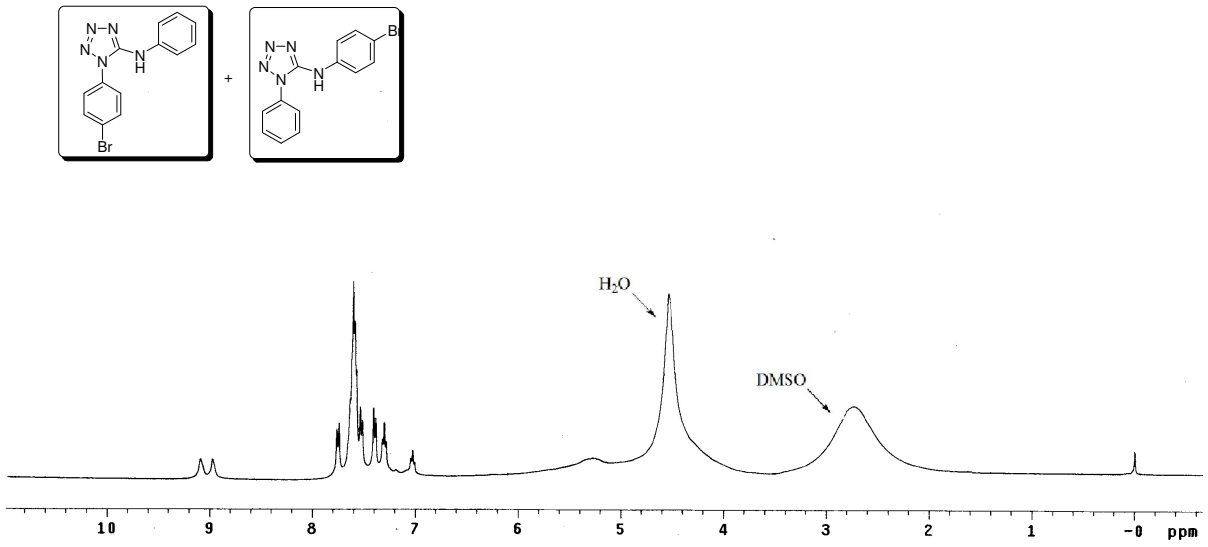
[1-(4-Bromo-phenyl)-1*H*-tetrazol-5-yl]-(4-methoxy-phenyl)-amine / (4-Bromo-phenyl)-[1-(4-methoxy-phenyl)-1*H*-tetrazol-5-yl]-amine (9c+10c): ^{13}C NMR (100 MHz, $CDCl_3$ + DMSO-d_6):



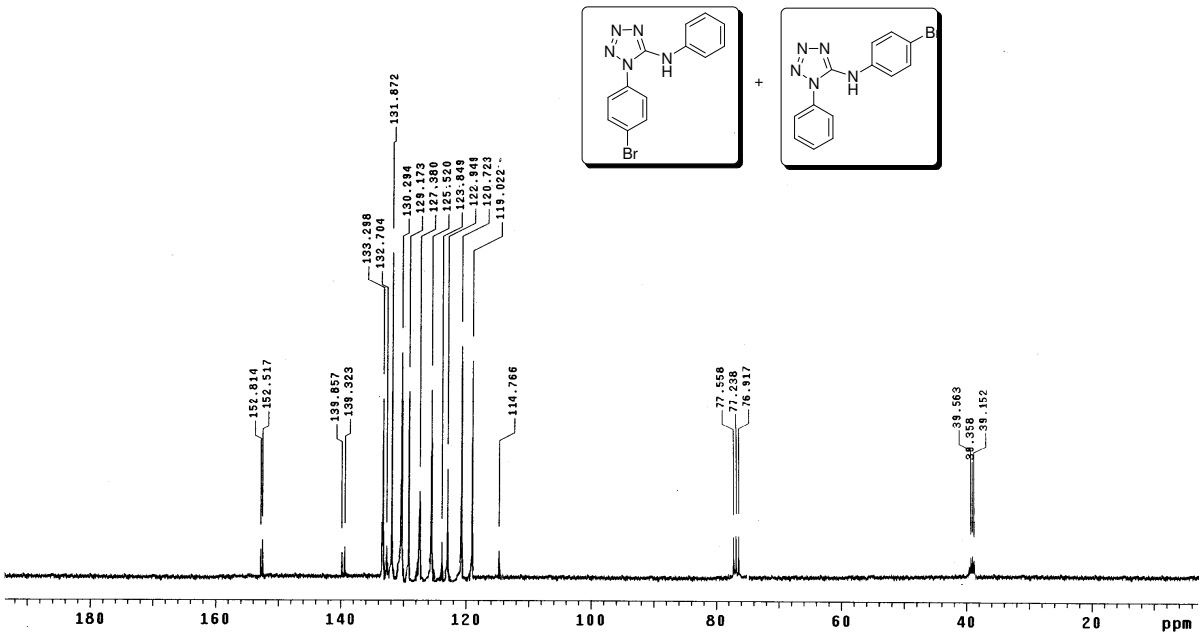
[1-(4-Bromo-phenyl)-1*H*-tetrazol-5-yl]-(4-methoxy-phenyl)-amine / (4-Bromo-phenyl)-[1-(4-methoxy-phenyl)-1*H*-tetrazol-5-yl]-amine (9c+10c): Mass Spectra



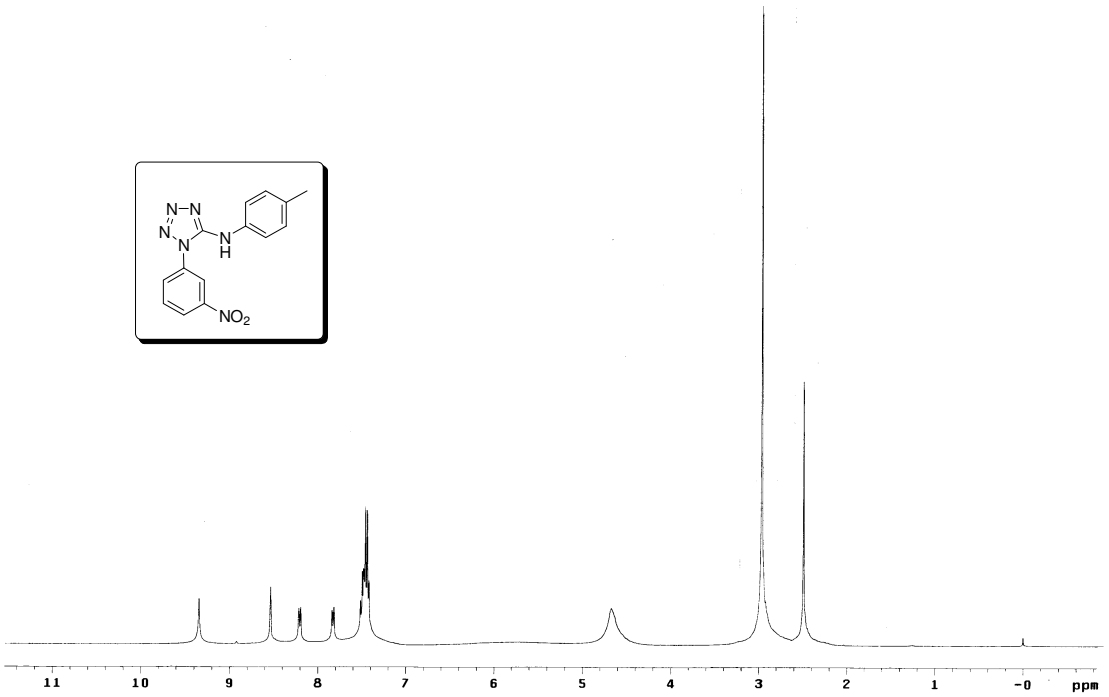
1-(4-Bromophenyl)-*N*-phenyl-1*H*-tetrazol-5-amine / *N*-(4-bromophenyl)-1-phenyl-1*H*-tetrazol-5-amine (9d+10d): ^{1}H NMR (400 MHz, $CDCl_3$ + DMSO-d_6):



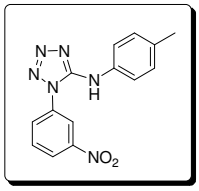
1-(4-Bromophenyl)-N-phenyl-1*H*-tetrazol-5-amine / N-(4-bromophenyl)-1-phenyl-1*H*-tetrazol-5-amine (9d+10d): ^{13}C NMR (100 MHz, $CDCl_3$ + DMSO-d_6):

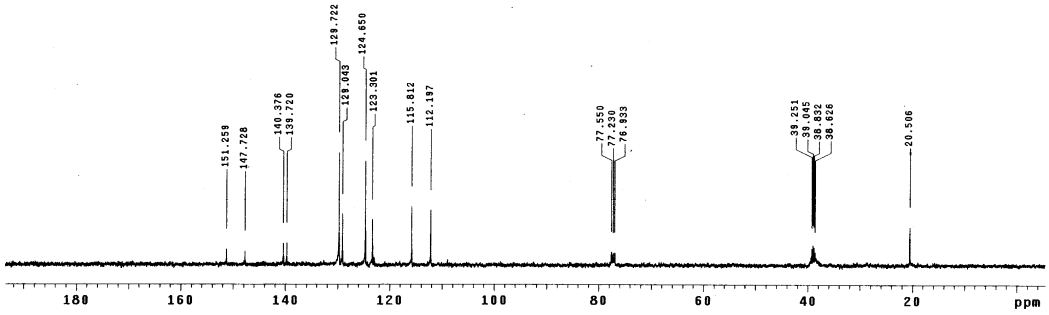


1-(3-nitrophenyl)-*N*-p-tolyl-1H-tetrazol-5-amine (9e): ^{1}H NMR (400 MHz, $CDCl_3$ + DMSO-d_6):

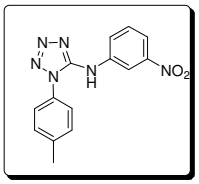


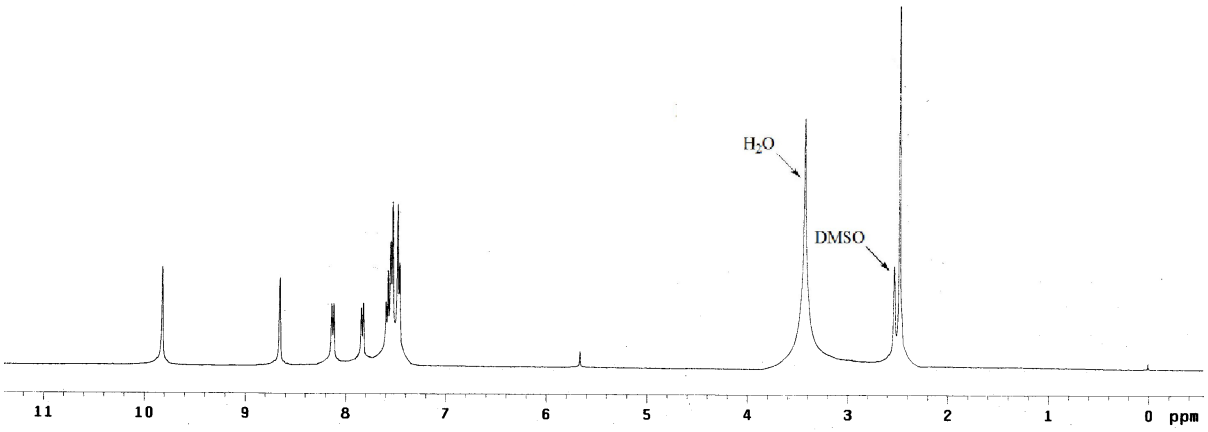
1-(3-nitrophenyl)-N-p-tolyl-1H-tetrazol-5-amine (9e): ^{13}C NMR (100 MHz, $CDCl_3$ + DMSO-d_6):



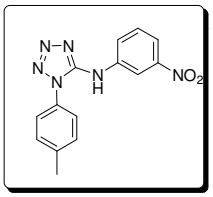


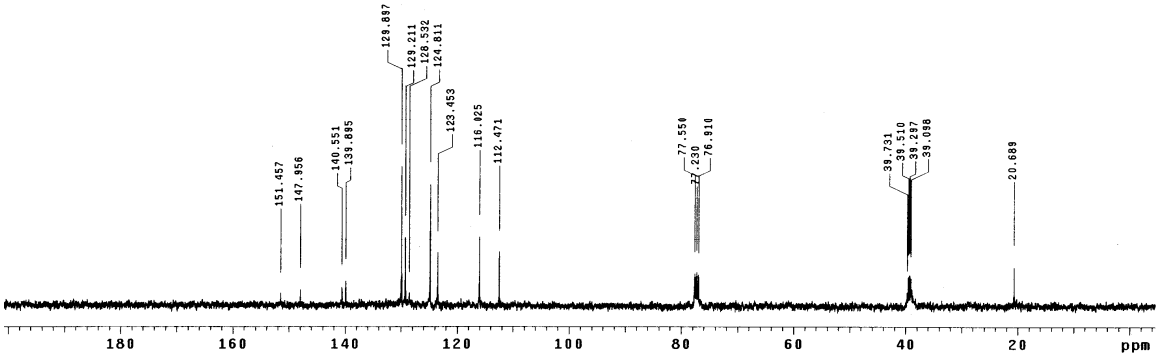
***N*-(3-Nitrophenyl)-1-*p*-tolyl-1*H*-tetrazol-5-amine (10e): ^{1}H NMR (400 MHz, $CDCl_3$ + DMSO-d_6):**



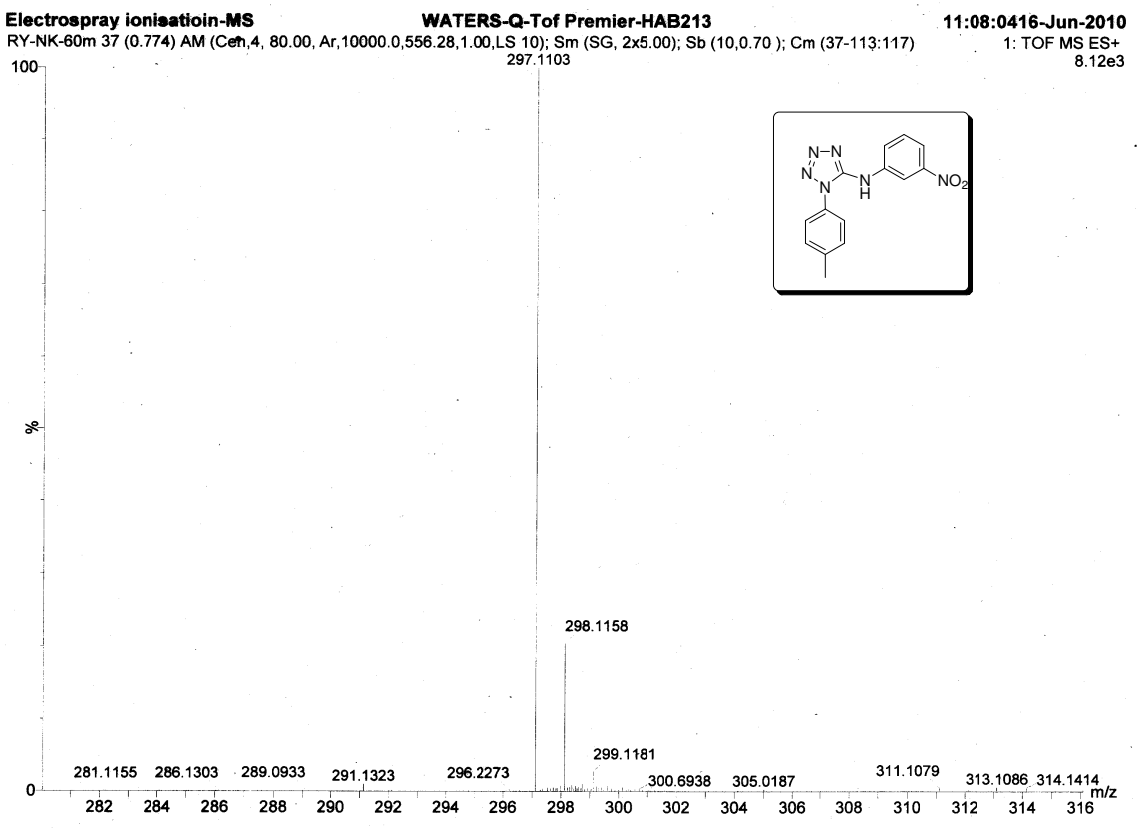


_N_-(3-Nitrophenyl)-1-_p_-tolyl-1_H_-tetrazol-5-amine (10e): ^{13}C NMR (100 MHz, $CDCl_3$ + DMSO-d_6):

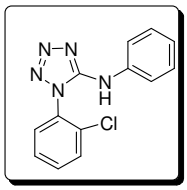


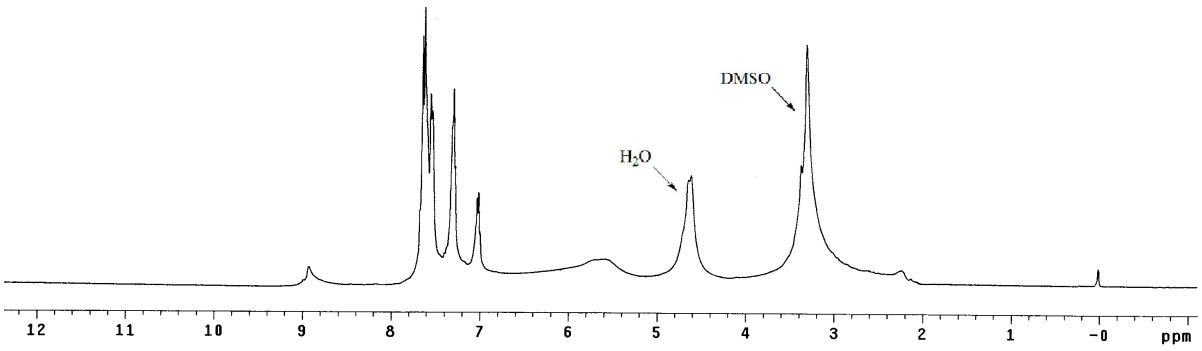


_N_-(3-Nitrophenyl)-1-_p_-tolyl-1_H_-tetrazol-5-amine (10e): MASS SPECTRA

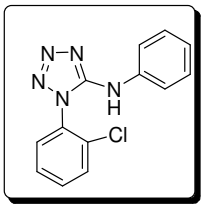


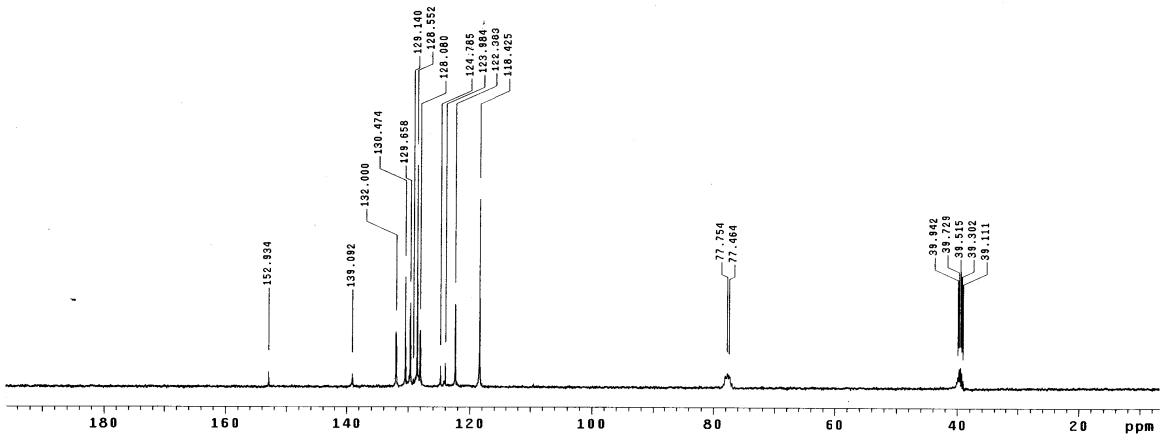
[1-(2-Chloro-phenyl)-1*H*-tetrazol-5-yl]-phenyl-amine (9f): ^{1}H NMR (400 MHz, $CDCl_3$+ DMSO-d_6):



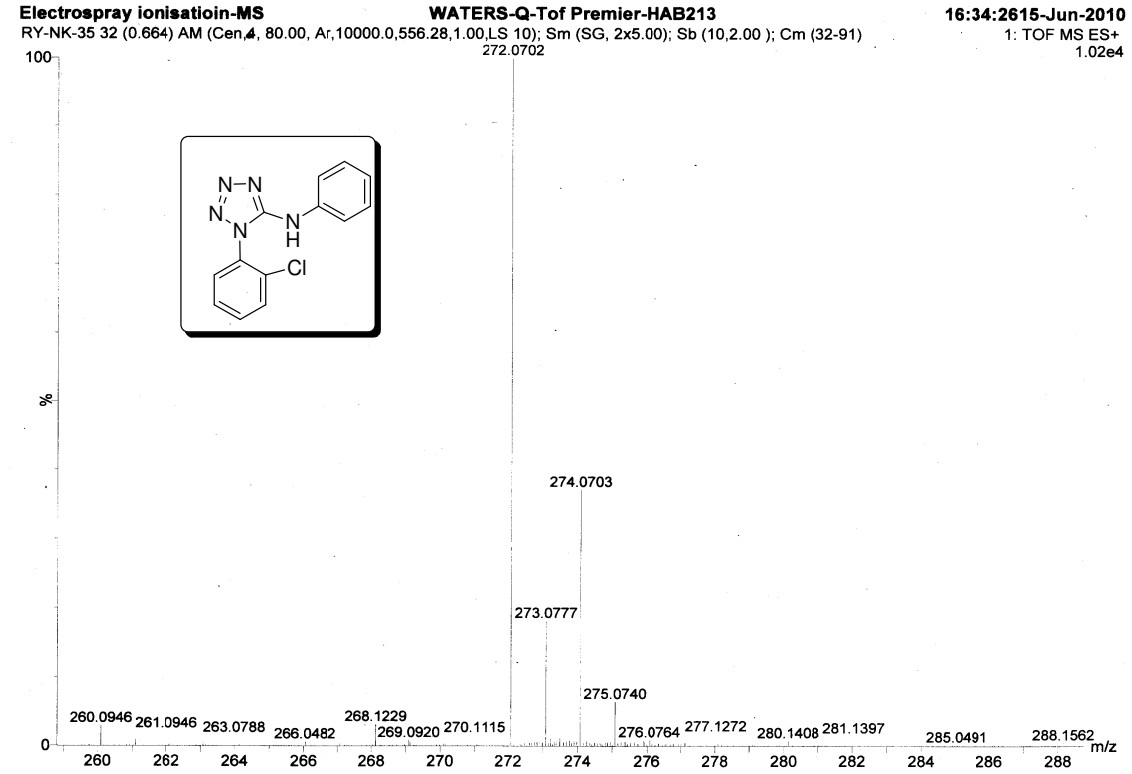


[1-(2-Chloro-phenyl)-1*H*-tetrazol-5-yl]-phenyl-amine (9f): ^{13}C NMR (100 MHz, $CDCl_3$ + DMSO-d_6):

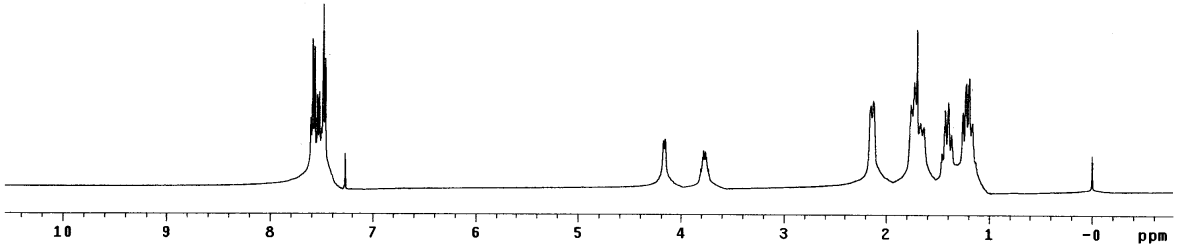




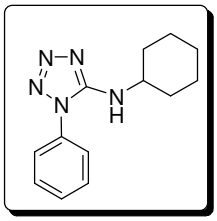
[1-(2-Chloro-phenyl)-1*H*-tetrazol-5-yl]-phenyl-amine (9f): Mass Spectra

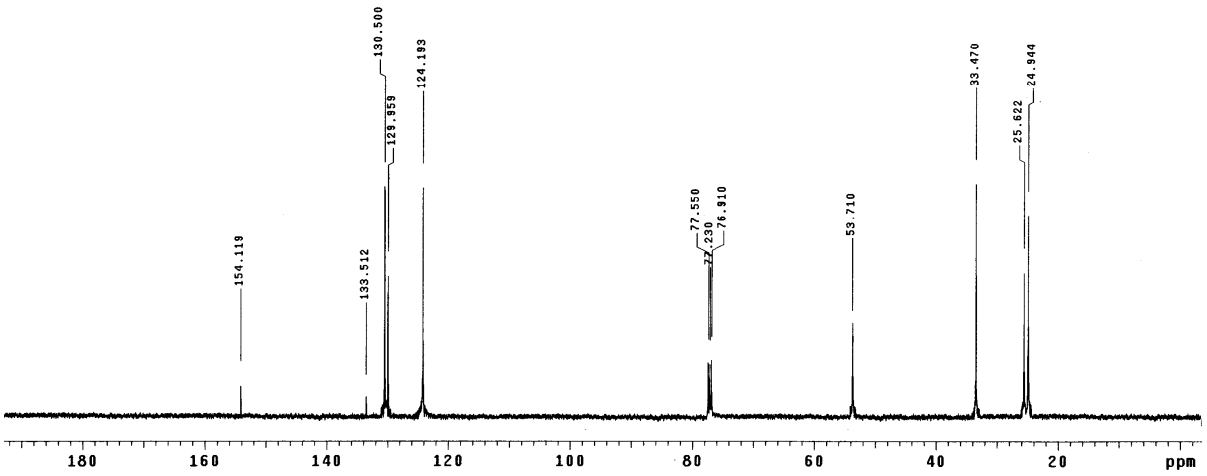


Cyclohexyl-(1-phenyl-1*H*-tetrazol-5-yl)-amine (9g): ^{1}H NMR (400 MHz, $CDCl_3$):

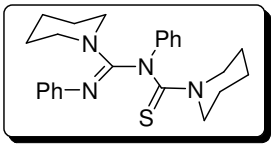


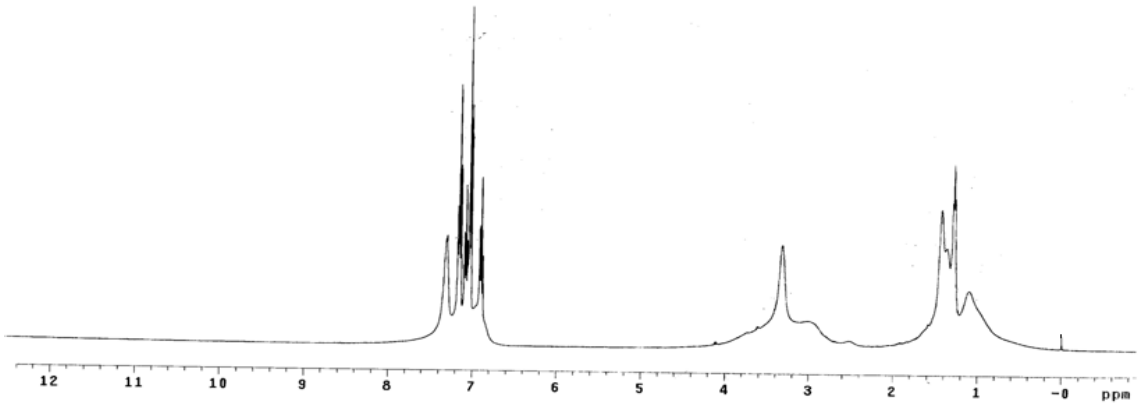
Cyclohexyl-(1-phenyl-1*H*-tetrazol-5-yl)-amine (9g). ^{13}C NMR (100 MHz, $CDCl_3$):





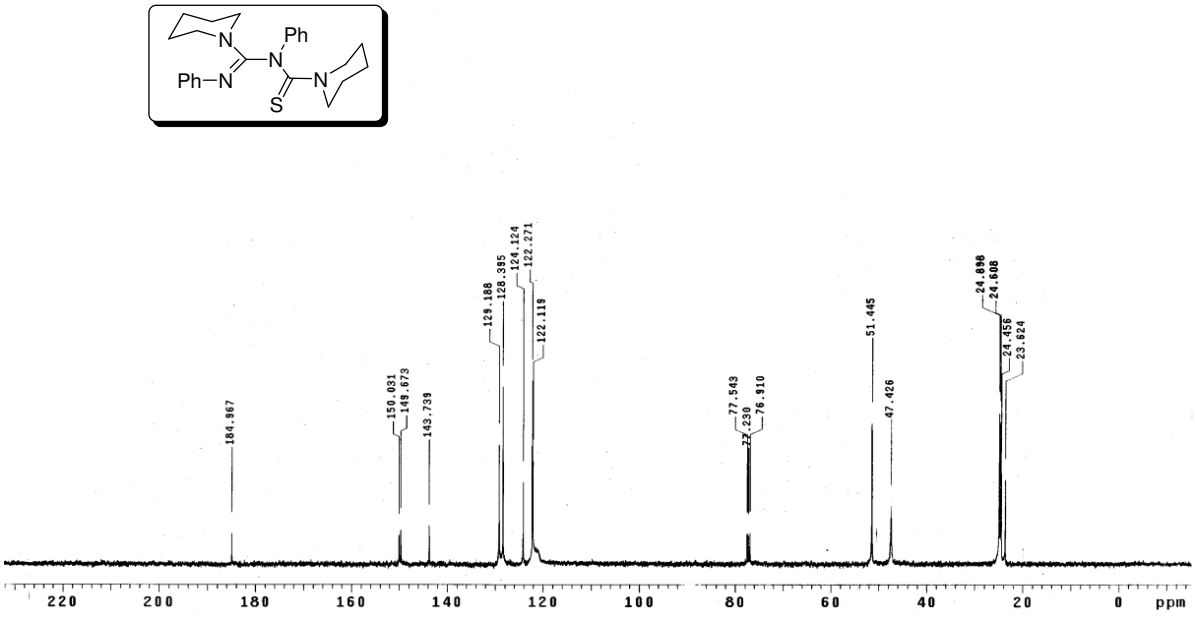
***N*-Phenyl-*N*-((*E*)-(phenylimino)(piperidin-1-yl)methyl)piperidine-1-carbothioamide (13a). ^{1}H NMR (400 MHz, $CDCl_3$):**





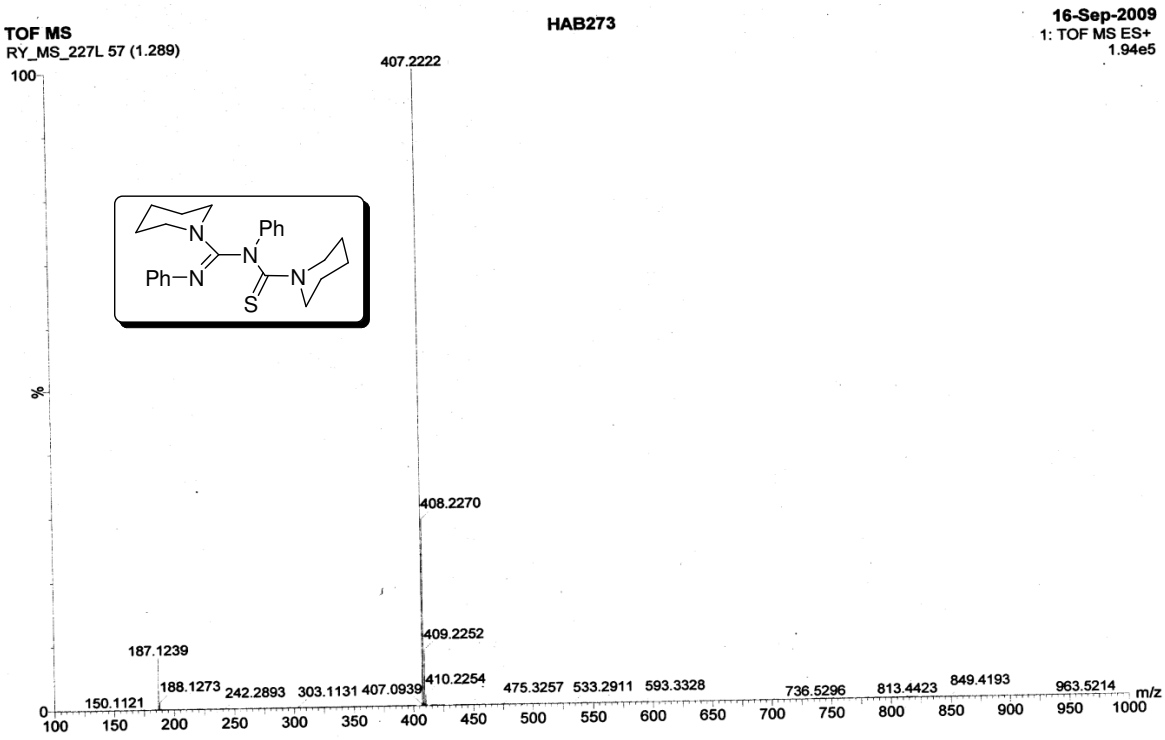
***N*-Phenyl-*N*-((*E*)-(phenylimino)(piperidin-1-yl)methyl)piperidine-1-carbothioamide (13a).**

^{13}C NMR (100 MHz, $CDCl_3$):

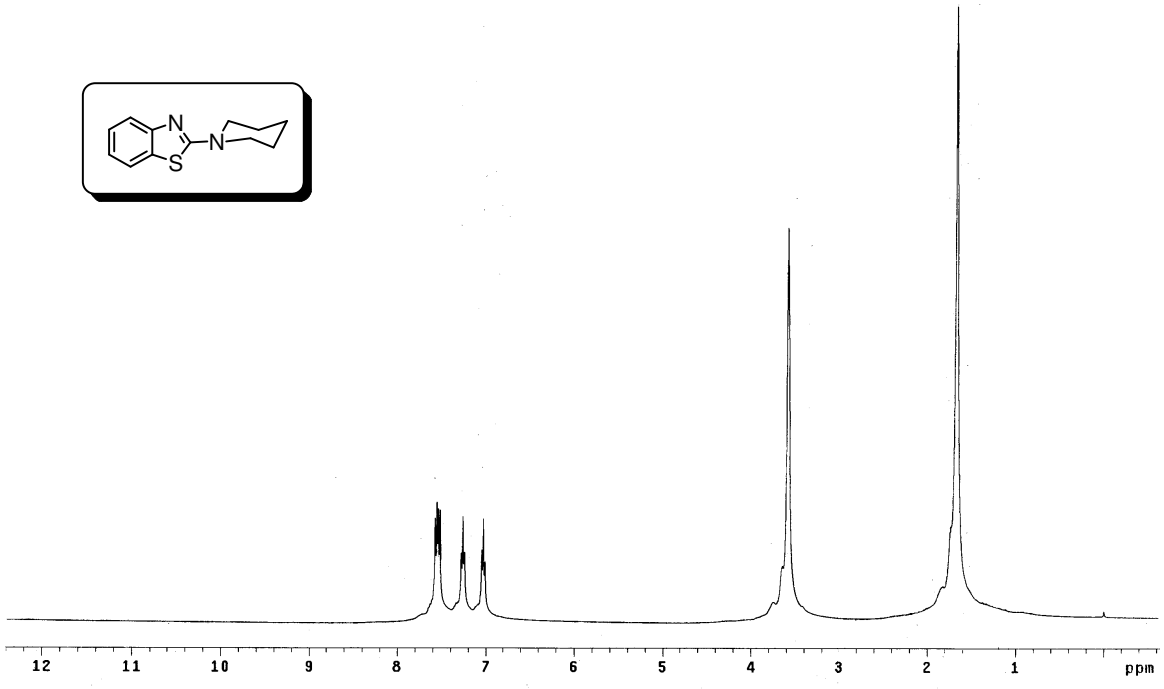


***N*-Phenyl-*N*-((*E*)-(phenylimino)(piperidin-1-yl)methyl)piperidine-1-carbothioamide (13a).**

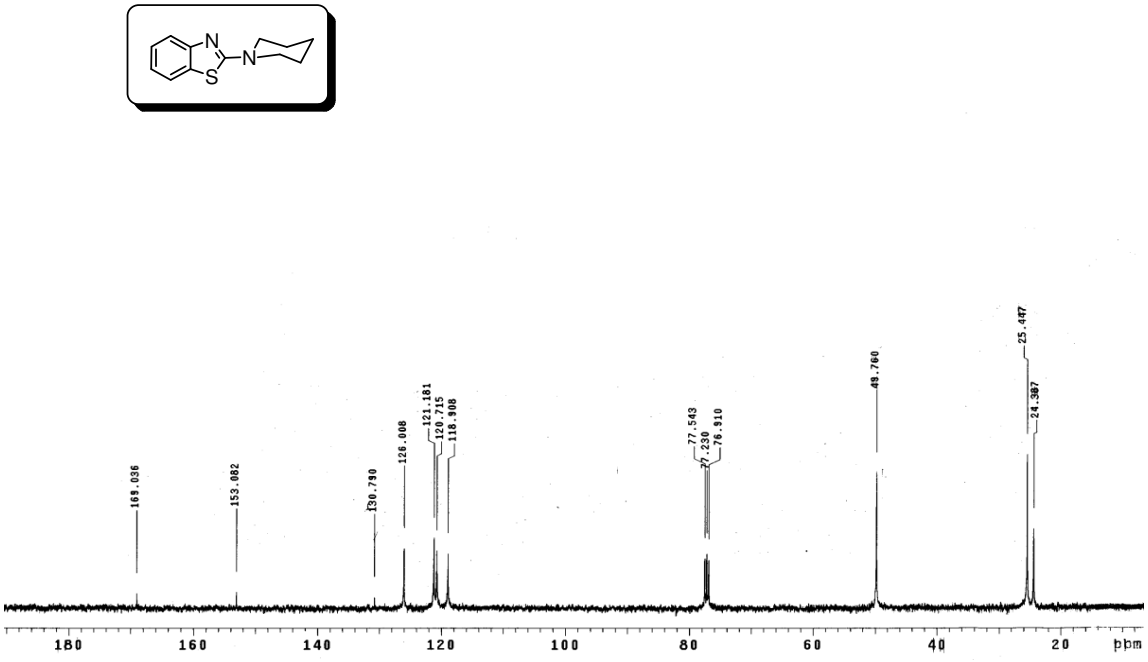
Mass Spectra:



2-(Piperidin-1-yl)benzo[*d*]thiazole (14a). ^{1}H NMR (400 MHz, $CDCl_3$):

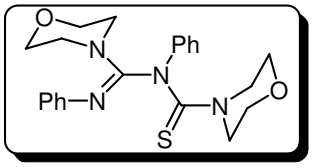


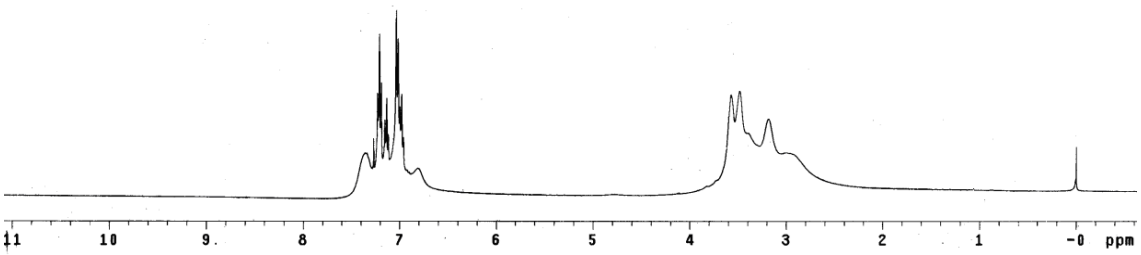
2-(Piperidin-1-yl)benzo[*d*]thiazole (14a). ^{13}C NMR (100 MHz, $CDCl_3$):



***N*-((*E*)-Morpholino(phenylimino)methyl)-*N*-phenylmorpholine-4-carbothioamide (13b).**

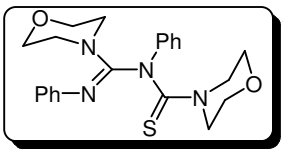
^{1}H NMR (400 MHz, $CDCl_3$):

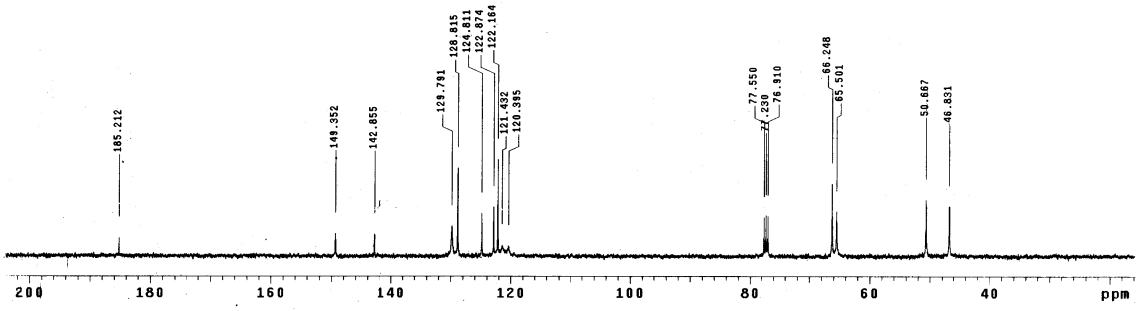




***N*-((*E*)-Morpholino(phenylimino)methyl)-*N*-phenylmorpholine-4-carbothioamide (13b).**

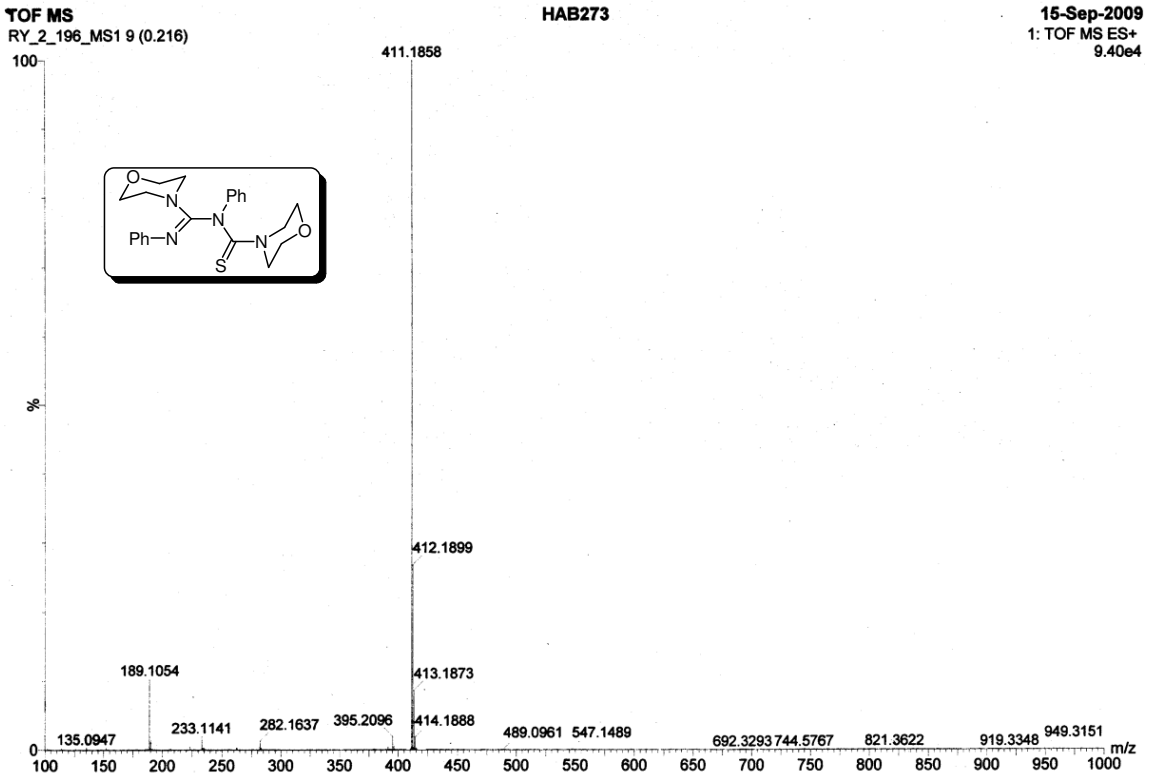
^{13}C NMR (100 MHz, $CDCl_3$):



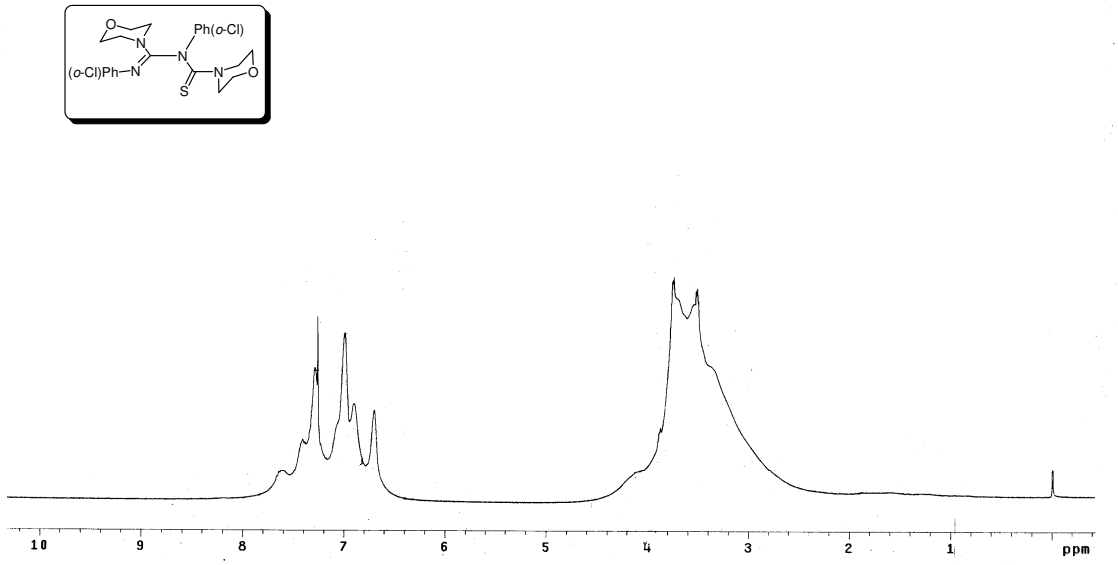


***N*-((*E*)-Morpholino(phenylimino)methyl)-*N*-phenylmorpholine-4-carbothioamide (13b).**

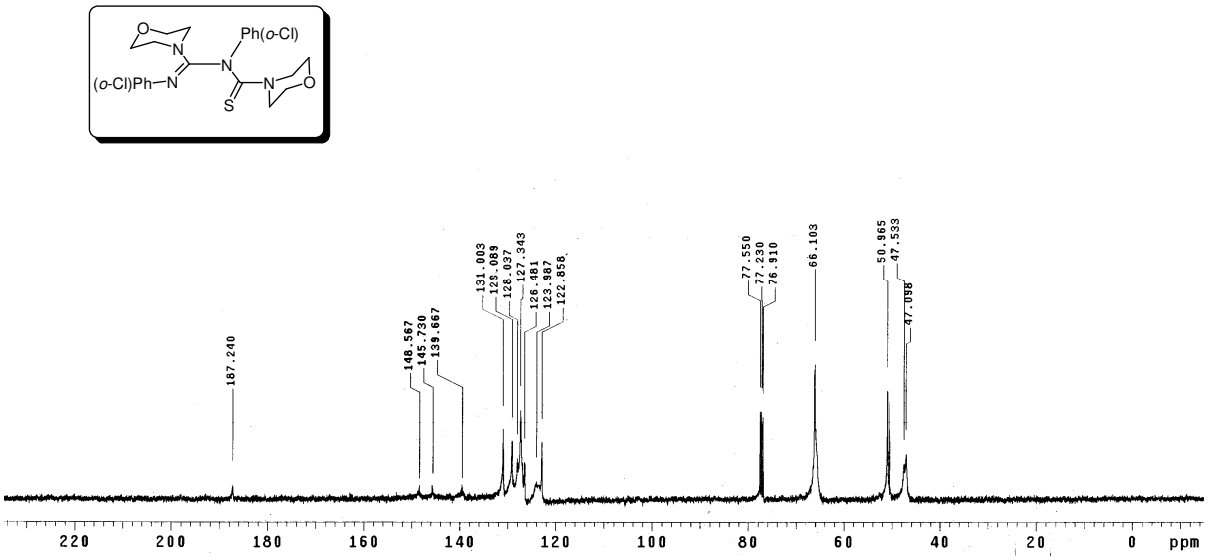
MASS SPECTRA:



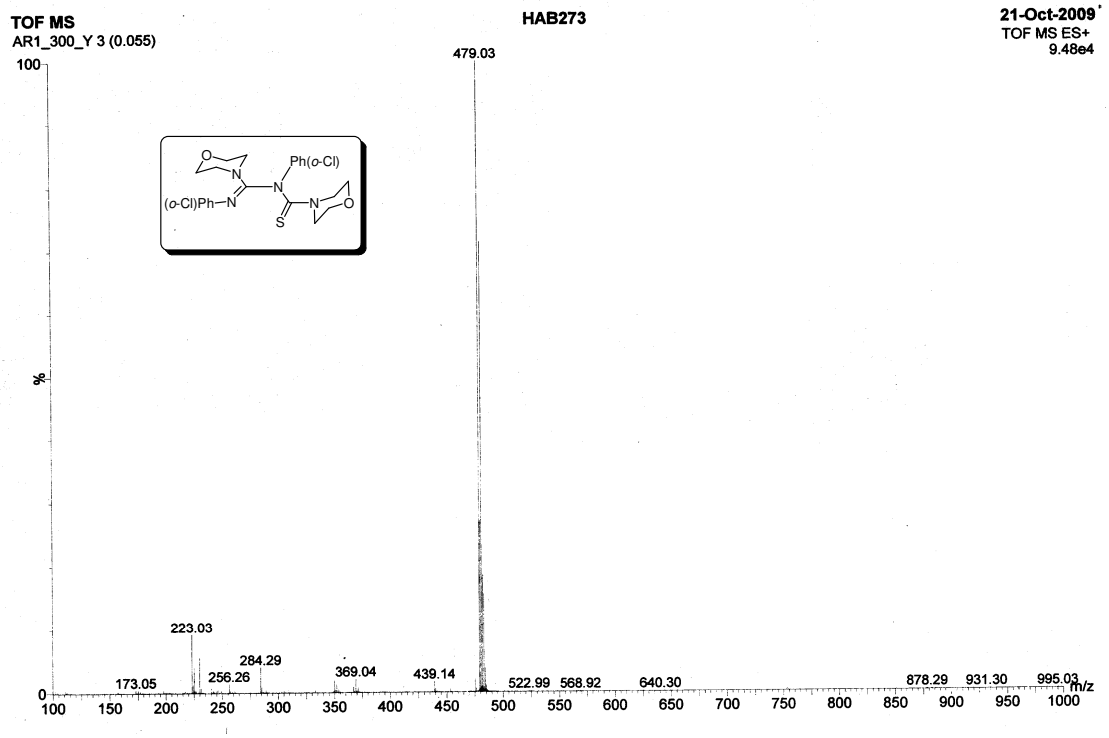
***N*-((*E*)-(2-Chlorophenylimino)(morpholino)methyl)-*N*-(2-chlorophenyl)morpholine-4-carbothioamide (13c). ^{1}H NMR (400 MHz, $CDCl_3$):**



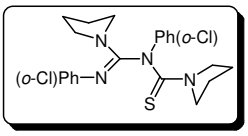
_N_-((_E_)-(2-Chlorophenylimino)(morpholino)methyl)-_N_-(2-chlorophenyl)morpholine-4-carbothioamide (13c). ^{13}C NMR (100 MHz, $CDCl_3$):

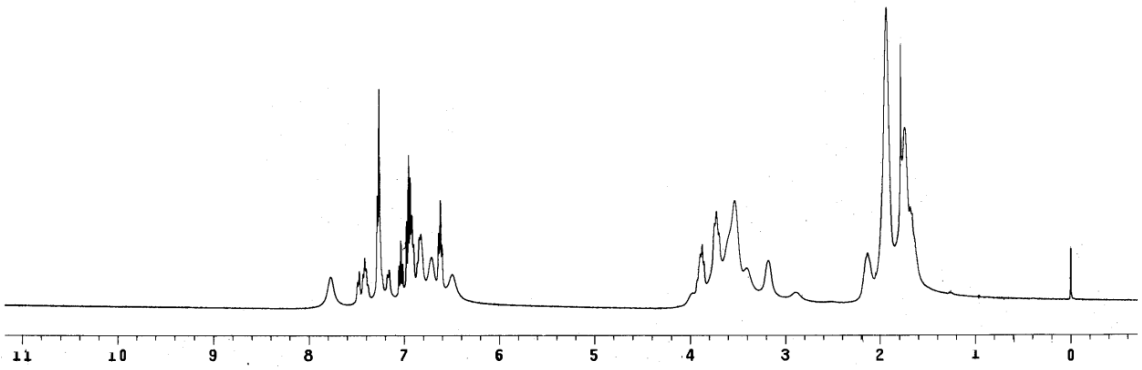


_N_-((_E_)-(2-Chlorophenylimino)(morpholino)methyl)-_N_-(2-chlorophenyl)morpholine-4-carbothioamide (13c): Mass Spectra

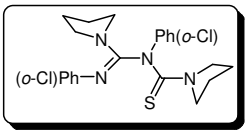


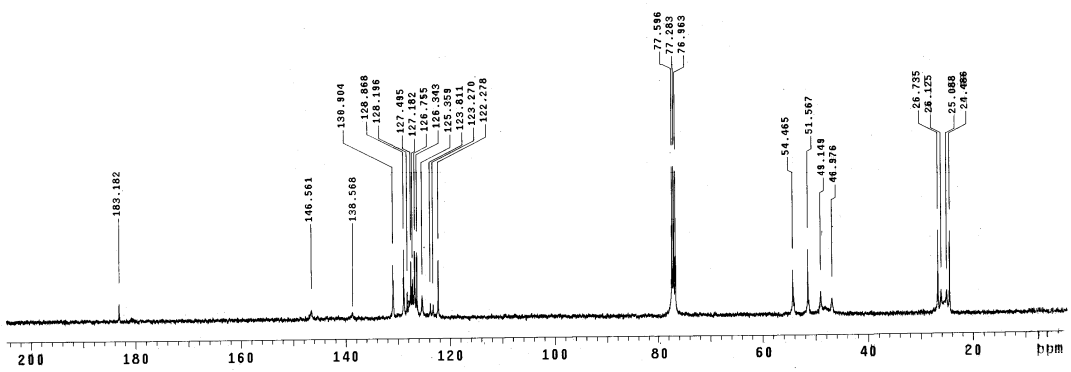
_N_-((_E_)-(2-Chlorophenylimino)(pyrrolidin-1-yl)methyl)-_N_-(2-chlorophenyl)pyrrolidine-1-carbothioamide (13d).^{1}H NMR (400 MHz, $CDCl_3$):



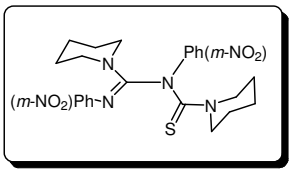


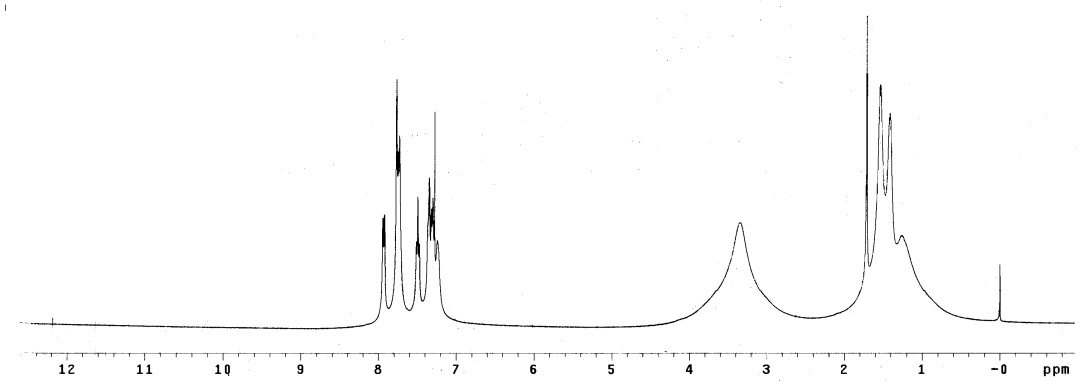
_N_-((_E_)-(2-Chlorophenylimino)(pyrrolidin-1-yl)methyl)-_N_-(2-chlorophenyl)pyrrolidine-1-carbothioamide (13d).^{13}C NMR (100 MHz, $CDCl_3$):



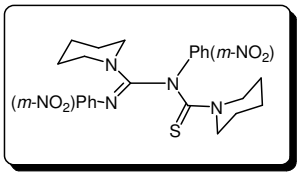


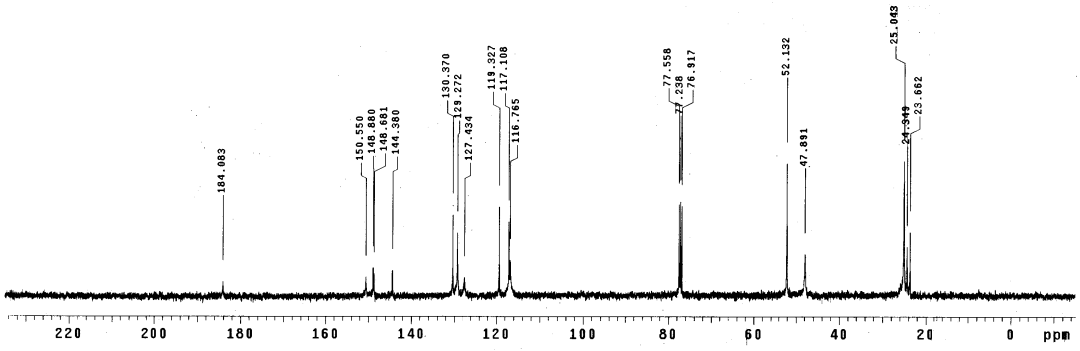
_N_-((_E_)-(3-Nitrophenylimino)(piperidin-1-yl)methyl)-_N_-(3-nitrophenyl)piperidine-1-carbothioamide (13e).^{1}H NMR (400 MHz, $CDCl_3$):



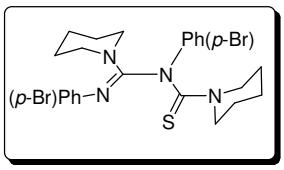


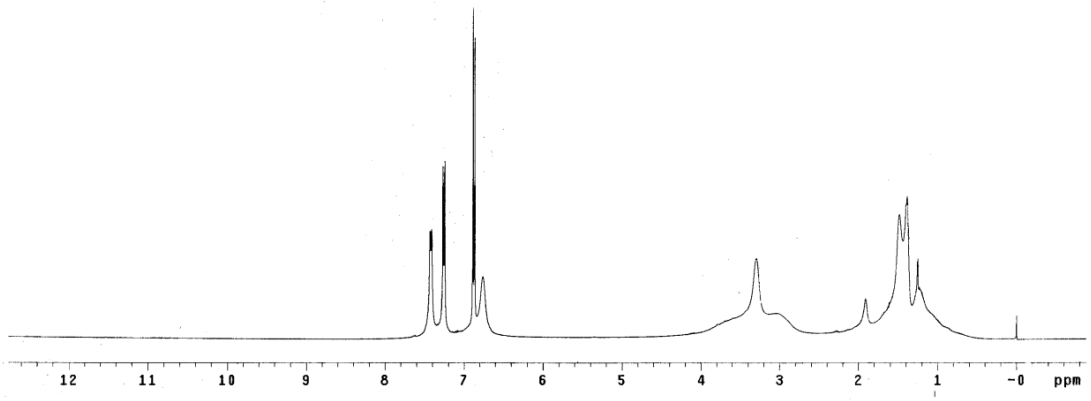
_N_-((_E_)-(3-Nitrophenylimino)(piperidin-1-yl)methyl)-_N_-(3-nitrophenyl)piperidine-1-carbothioamide (13e).^{13}C NMR (100 MHz, $CDCl_3$):



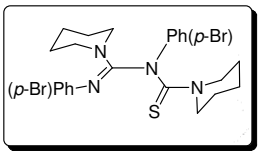


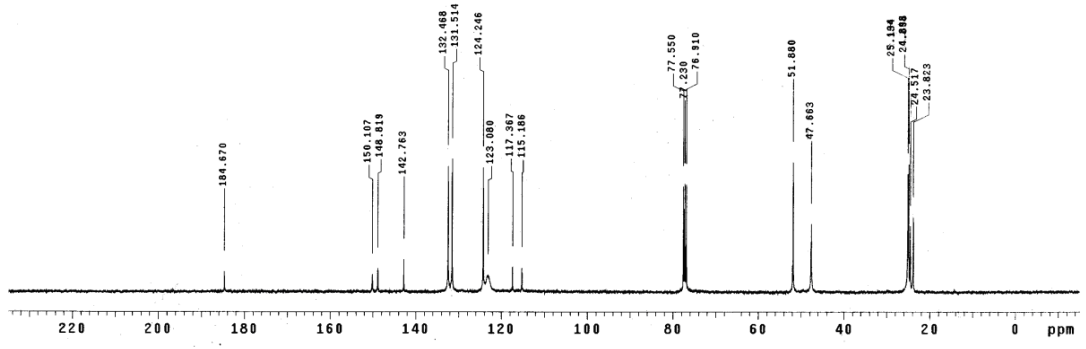
_N_-((_E_)-(4-Bromophenylimino)(piperidin-1-yl)methyl)-_N_-(4-bromophenyl)piperidine-1-carbothioamide (13f). ^{1}H NMR (400 MHz, $CDCl_3$):



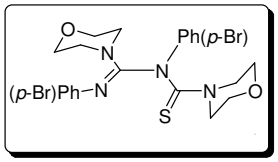


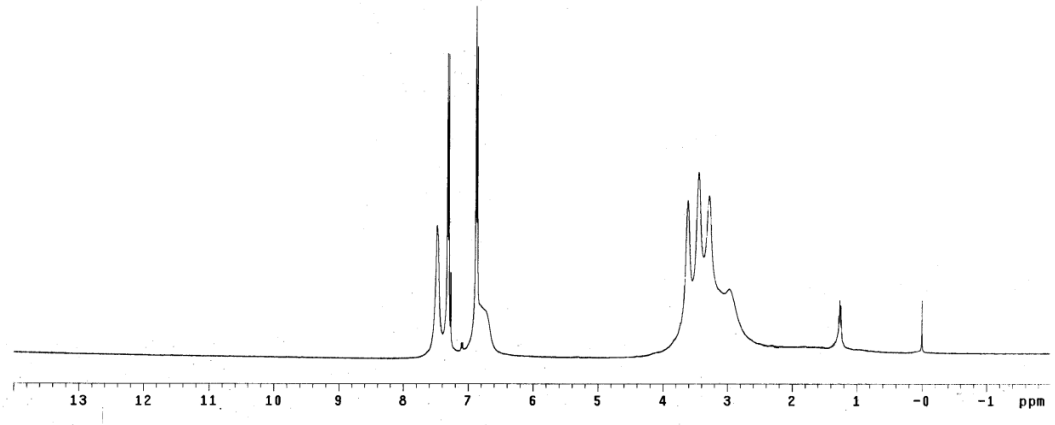
_N_-((_E_)-(4-Bromophenylimino)(piperidin-1-yl)methyl)-_N_-(4-bromophenyl)piperidine-1-carbothioamide (13f). ^{13}C NMR (100 MHz, $CDCl_3$):



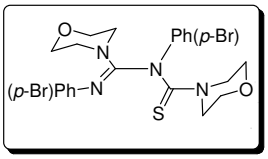


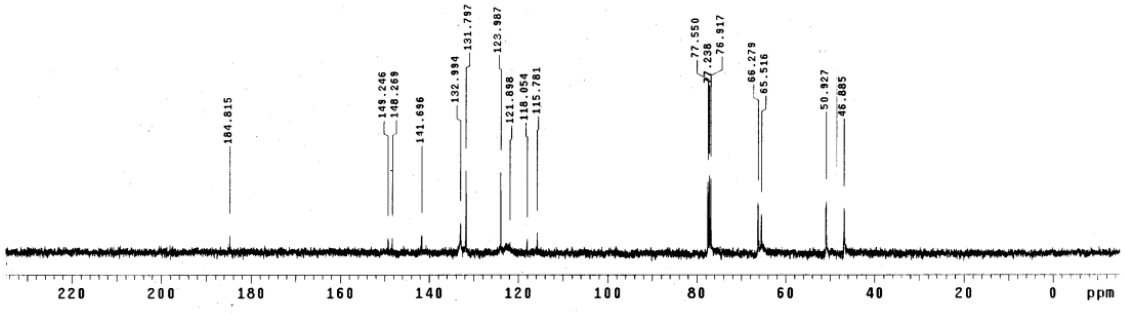
_N_-((_E_)-(4-Bromophenylimino)(morpholino)methyl)-_N_-(4-bromophenyl)morpholine-4-carbothioamide (13g). ^{1}H NMR (400 MHz, $CDCl_3$):



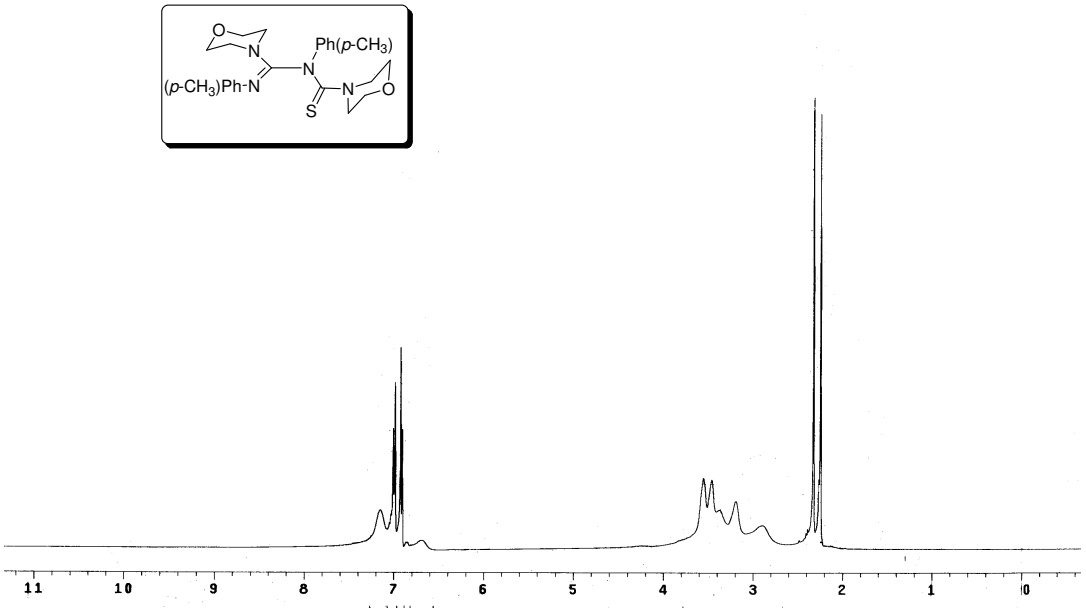


_N_-((_E_)-(4-Bromophenylimino)(morpholino)methyl)-_N_-(4-bromophenyl)morpholine-4-carbothioamide (13g).^{13}C NMR (100 MHz, $CDCl_3$):

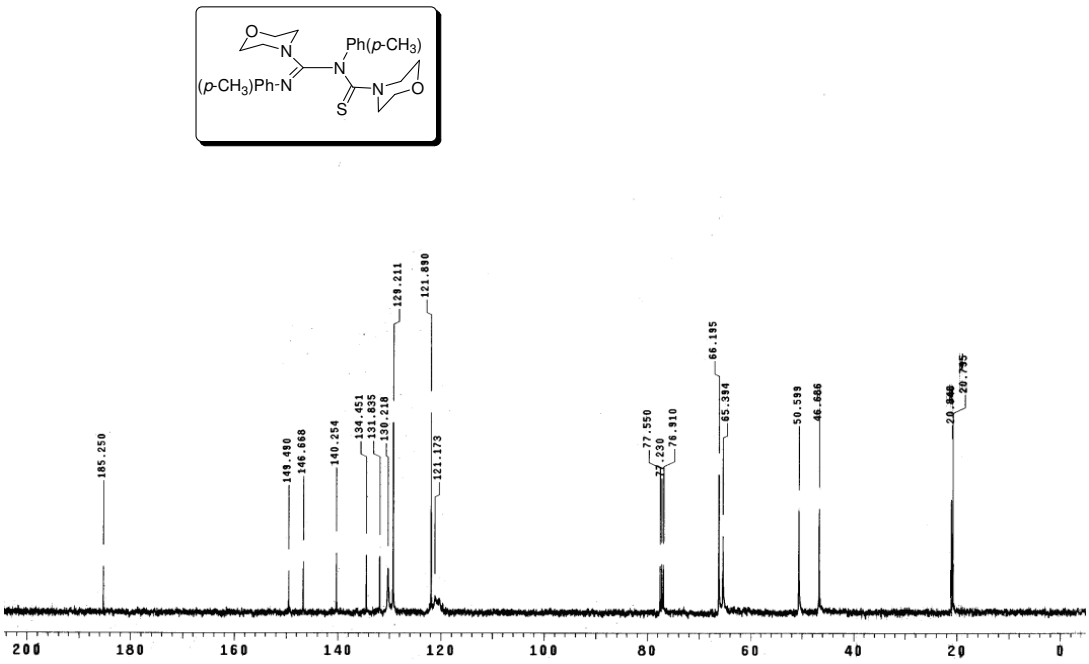




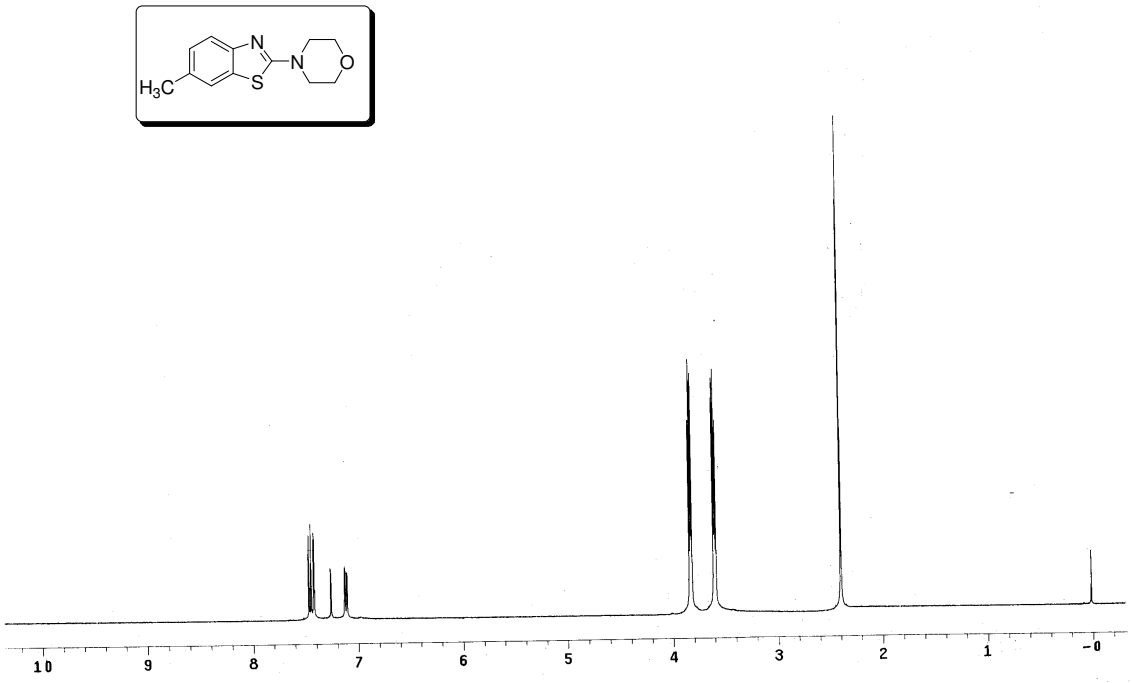
***N*-((*E*)-(*p*-Tolylimino)(morpholino)methyl)-*N*-*p*-tolylmorpholine-4-carbothioamide (13h). ^{1}H NMR (400 MHz, $CDCl_3$):**



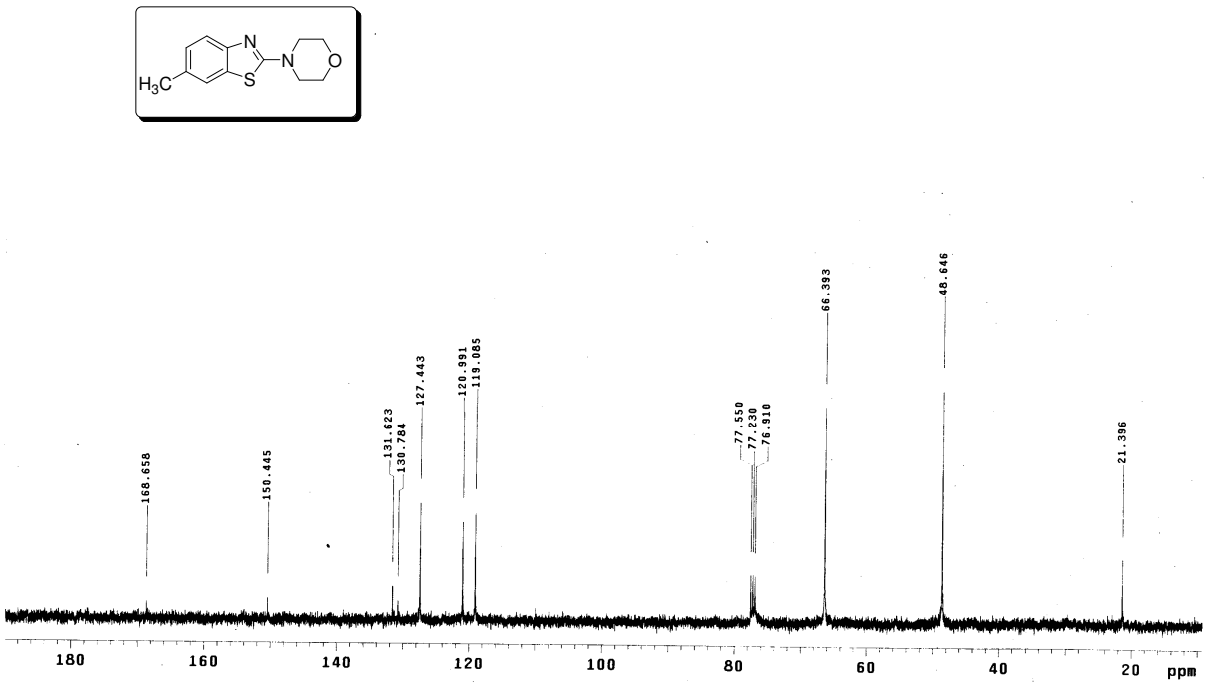
***N*-((*E*)-(*p*-Tolylimino)(morpholino)methyl)-*N*-*p*-tolylmorpholine-4-carbothioamide (13h). ^{13}C NMR (100 MHz, $CDCl_3$):**



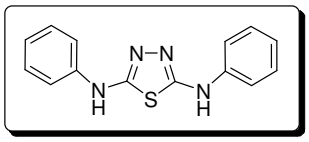
6-Methyl-2-morpholinobenzo[*d*]thiazole (14h). ^{1}H NMR (400 MHz, $CDCl_3$):

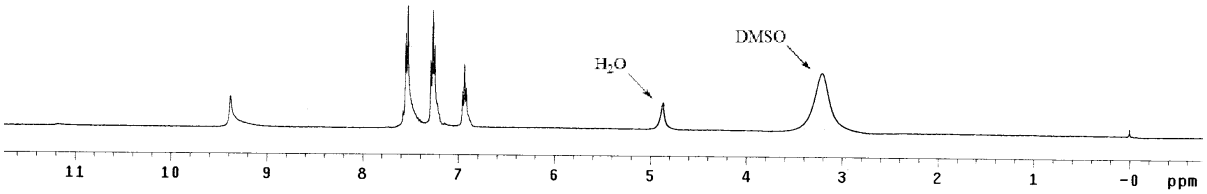


6-Methyl-2-morpholinobenzo[*d*]thiazole (14h). ^{13}C NMR (100 MHz, $CDCl_3$):

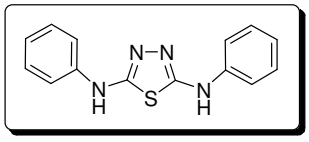


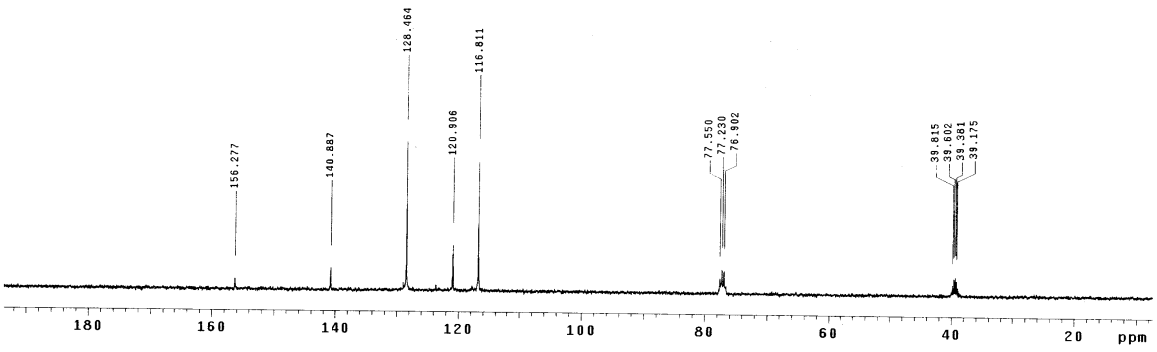
N^2, N^5-diphenyl-1,3,4-thiadiazole-2,5-diamine (17a). ^{1}H NMR (400 MHz, $CDCl_3$ + DMSO-d_6):



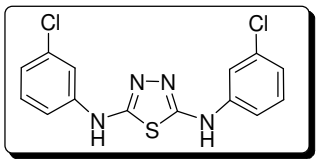


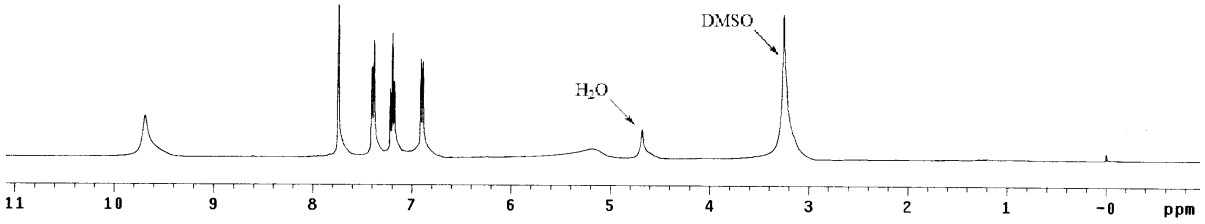
N^2, N^5-diphenyl-1,3,4-thiadiazole-2,5-diamine (17a). ^{13}C NMR (100 MHz, $CDCl_3$ + DMSO-d_6):



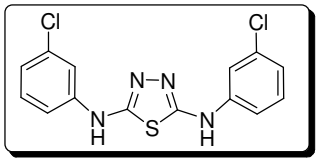


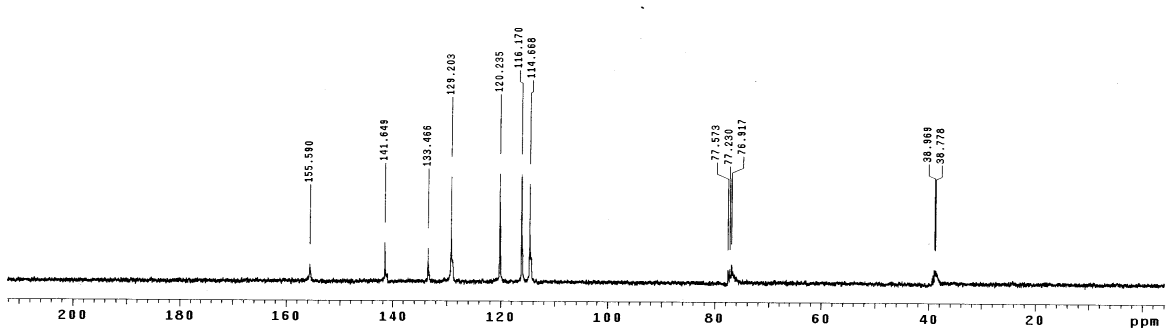
N^2, N^5-bis(3-chlorophenyl)-1,3,4-thiadiazole-2,5-diamine (17b). ^{1}H NMR (400 MHz, $CDCl_3$ + DMSO-d_6):



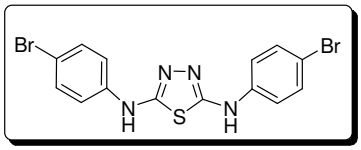


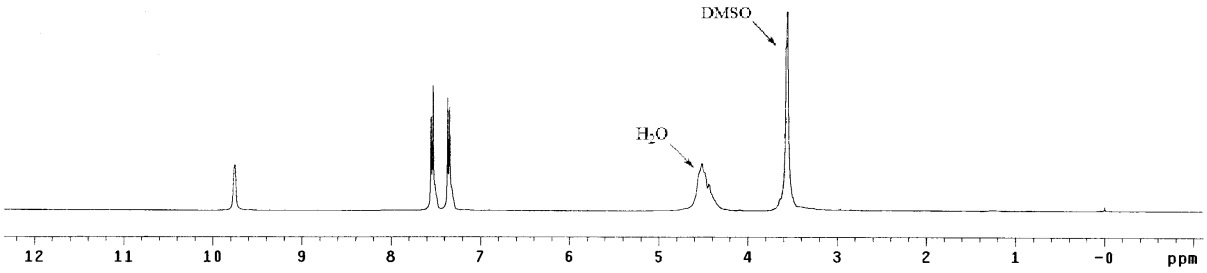
N^2, N^5-bis(3-chlorophenyl)-1,3,4-thiadiazole-2,5-diamine (17b). ^{13}C NMR (100 MHz, $CDCl_3$ + DMSO-d_6):



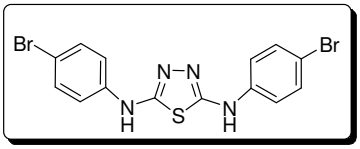


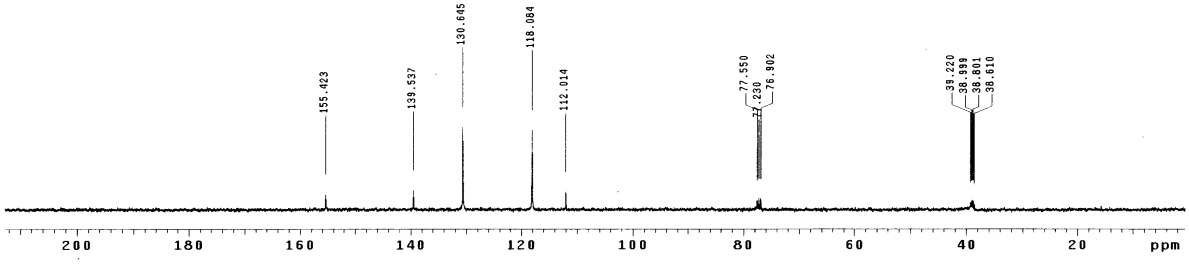
N^2, N^5-bis(4-bromophenyl)-1,3,4-thiadiazole-2,5-diamine (17c). ^{1}H NMR (400 MHz, $CDCl_3$ + DMSO-d_6):



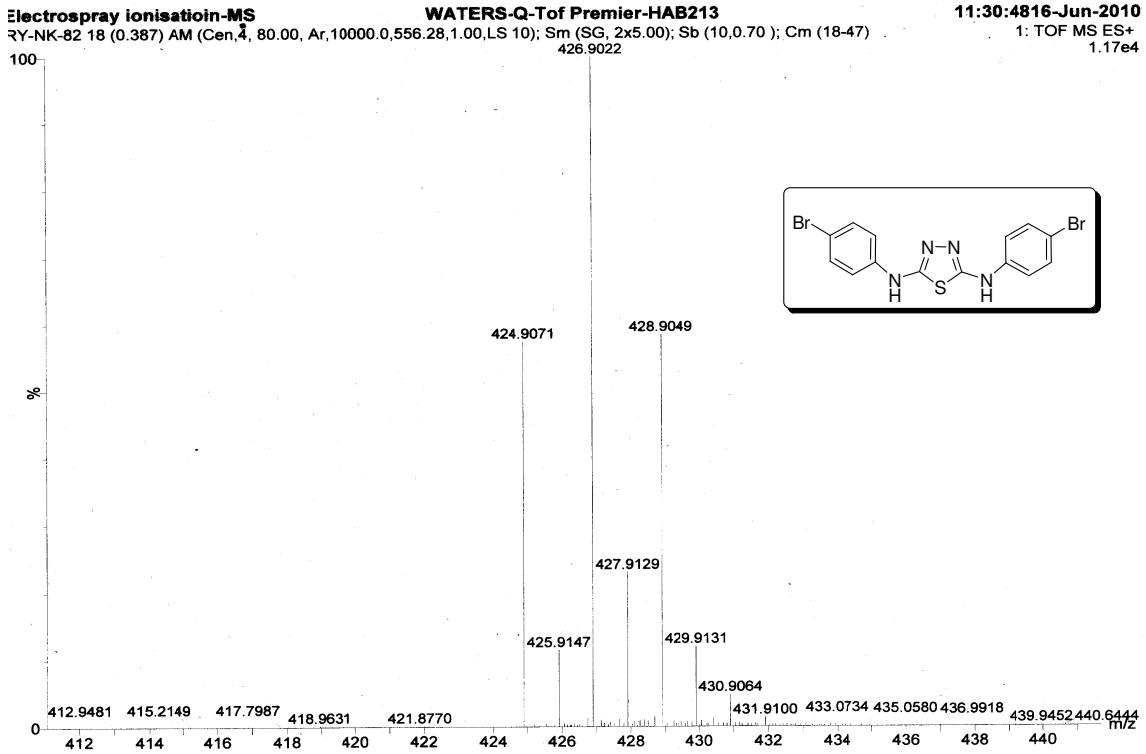


N^2, N^5-bis(4-bromophenyl)-1,3,4-thiadiazole-2,5-diamine (17c). ^{13}C NMR (100 MHz, $CDCl_3$ + DMSO-d_6):

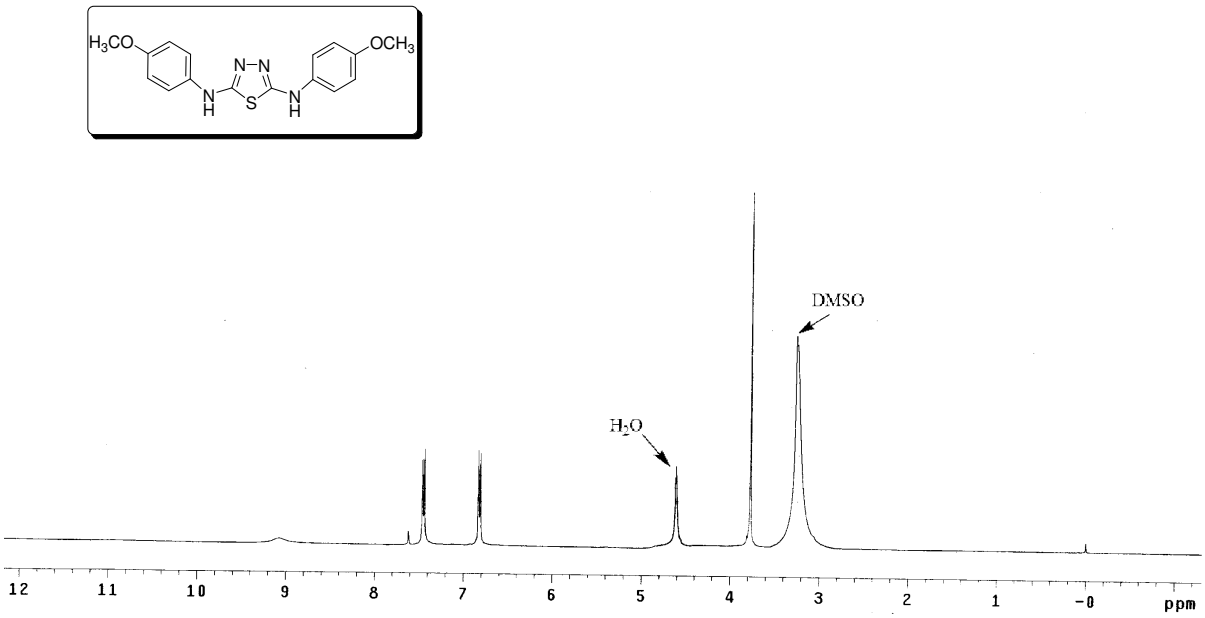




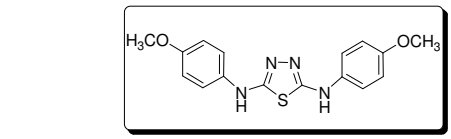
N^2, N^5-bis(4-bromophenyl)-1,3,4-thiadiazole-2,5-diamine (17c). MASS SPECTRA

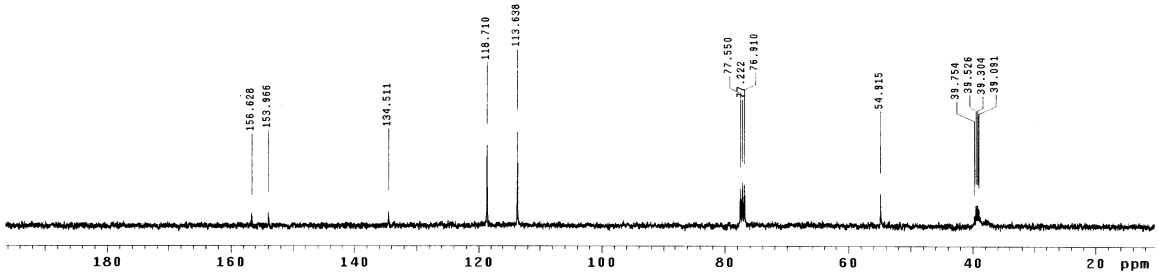


N^2, N^5-bis(4-methoxyphenyl)-1,3,4-thiadiazole-2,5-diamine (17d). ^{1}H NMR (400 MHz, $CDCl_3$+ DMSO-d_6):



N^2, N^5-bis(4-methoxyphenyl)-1,3,4-thiadiazole-2,5-diamine (17d). ^{13}C NMR (100 MHz, $CDCl_3$ + DMSO-d_6):





N^2, N^5-bis(4-methoxyphenyl)-1,3,4-thiadiazole-2,5-diamine (17d). Mass Spectra