

# A one pot synthesis of [1,3,4]-oxadiazoles mediated by molecular iodine

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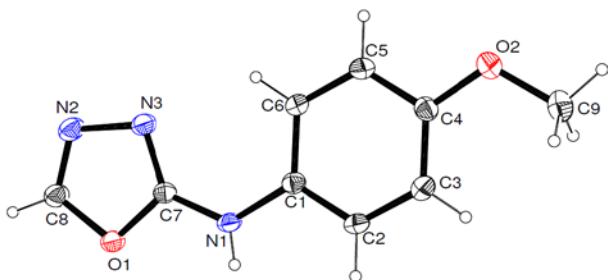
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## Experimental:

### General remarks

Unless otherwise stated, all reagents were purchased from commercial sources and used without further purification. Reaction progress was monitored by TLC using Merck silica gel 60 F254 (0.25mm) with detection by UV or iodine. Chromatography was performed using Merck silica gel (60-120) mesh size with freshly distilled solvents. Columns were typically packed as slurry and equilibrated with the appropriate solvent system prior to use. <sup>1</sup>H NMR (400 MHz) and <sup>13</sup>C NMR (100 MHz) spectra were recorded on a Varian FT-400 MHz instrument using TMS as an internal standard. Data are presented as follows: chemical shift (ppm), multiplicity (s = singlet, d = doublet, t = triplet, m = multiplet, b = broad, brs = broad singlet, brm= broad multiplet, coupling constant *J* (Hz). Elemental analyses were carried out on a Perkin–Elmer 2400 automatic carbon, hydrogen, nitrogen and sulfur analyser. 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. Mass data were obtained with a WATERS MS system, Q-tof premier and data analyzed using Mass Lynx4.1.

**Crystallographic Analysis:** Crystal data were collected with Bruker Smart Apex-II CCD diffractometer using graphite by using graphite-monochromated Mo- $K_{\alpha}$  radiation ( $\lambda = 0.71073 \text{ \AA}$ ) at 298 K. Cell parameters were retrieved using SMART <sup>1</sup>USA, 1995 software and refined with SAINT<sup>1</sup> for all observed reflections. Data reduction was performed with the SAINT software and corrected for Lorentzian and polarization effects. Absorption corrections were applied with the SADABS program.<sup>2</sup> The structures were solved by direct methods implemented in the SHELX-97<sup>3</sup> program and refined by full-matrix least-squares methods on  $F^2$ . All non-hydrogen atom positions were located in difference Fourier maps and refined anisotropically. The hydrogen atoms were placed in their geometrically generated positions. The crystals were isolated in rectangular shape from ethyl acetate and hexane mixture at room temperature.



**Fig. 2** ORTEP view of *N*-(4-Methoxyphenyl)-1,3,4-oxadiazol-2-amine (**4a**).

**Crystallographic description of *N*-(4-Methoxyphenyl)-1,3,4-oxadiazol-2-amine (**4a**):**

$C_9H_9N_3O_2$ , crystal dimensions  $0.38 \times 0.32 \times 0.28$  mm,  $M_r = 191.19$ , triclinic, space group P-1,  $a = 8.2269(8)$ ,  $b = 10.1265(11)$ ,  $c = 11.1995(11)$  Å,  $\alpha = 84.312(6)^\circ$ ,  $\beta = 86.837(6)^\circ$ ,  $\gamma = 76.573(7)^\circ$ ,  $V = 902.56(16)$  Å<sup>3</sup>,  $Z = 4$ ,  $\rho_{\text{calcd}} = 1.407$  mg/m<sup>3</sup>,  $\mu = 0.103$  mm<sup>-1</sup>,  $F(000) = 400.0$ , reflection collected / unique = 4510 / 2747, refinement method = full-matrix least-squares on  $F^2$ , final  $R$  indices [ $I > 2\sigma(I)$ ]:  $R_1 = 0.0782$ ,  $wR_2 = 0.2253$ ,  $R$  indices (all data):  $R_1 = 0.1067$ ,  $wR_2 = 0.2489$ , goodness of fit = 1.093. CCDC-824583 for *N*-(4-Methoxyphenyl)-1,3,4-oxadiazol-2-amine (**4a**) 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

**N-Phenyl-1,3,4-oxadiazol-2-amine (1a):** Pinkish solid; M.p. 149-150 °C (Lit. M.p. 153-154 °C).<sup>4</sup> <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>): δ = 7.01 (t, 1H, J = 7.6 Hz), 7.31 (t, 2H, J = 7.6 Hz), 7.52 (d, 2H, J = 8.0 Hz), 8.44 (s, 1H) ppm. <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>): δ = 118.9, 123.9, 130.3, 139.9, 149.4, 162.1 ppm. IR (KBr): 3255, 3155, 3092, 3044, 2316, 1614, 1591, 1211, 1098, 1012, 755 cm<sup>-1</sup>. C<sub>8</sub>H<sub>7</sub>N<sub>3</sub>O (161.08): calcd. C 59.65, H 4.38, N 26.09; found C 59.61, H 4.32, N 26.13.

**N-p-Tolyl-1,3,4-oxadiazol-2-amine (2a):** White solid; M.p. 129-132 °C. <sup>1</sup>H NMR (400 MHz, CD<sub>3</sub>OD): δ = 2.29 (s, 3H), 7.14 (d, 2H, J = 8.4 Hz), 7.38 (d, 2H, J = 8.4 Hz), 8.43 (s, 1H) ppm. <sup>13</sup>C NMR (100 MHz, CD<sub>3</sub>OD): δ = 20.9, 119.0, 130.8, 133.6, 137.4, 149.3, 162.3 ppm. IR (KBr): 3159, 2956, 2923, 2854, 1626, 1614, 1596, 1514, 1217, 1095, 1015, 819 cm<sup>-1</sup>. C<sub>9</sub>H<sub>9</sub>N<sub>3</sub>O (175.19): calcd. C 61.70, H 5.18, N 23.99; found C 61.66, H 5.23, N 23.96.

**N-(2-Methoxyphenyl)-1,3,4-oxadiazol-2-amine (3a):** White solid; M.p. 103-105 °C. <sup>1</sup>H NMR (400 MHz, CD<sub>3</sub>OD): δ = 3.91 (s, 3H), 6.94-7.07 (m, 3H), 7.95 (d, 1H, J = 8 Hz), 8.46 (s, 1H) ppm. <sup>13</sup>C NMR (100 MHz, CD<sub>3</sub>OD): δ = 56.4, 111.9, 119.7, 121.9, 124.7, 128.7, 149.5, 150.2, 162.3 ppm. IR (KBr): 3367, 3147, 3087, 2940, 2840, 1623, 1590, 1548, 1464, 1252, 1097, 1023, 773, 758 cm<sup>-1</sup>. C<sub>9</sub>H<sub>9</sub>N<sub>3</sub>O<sub>2</sub> (191.19): calcd. C 56.54, H 4.74, N 21.98; found C 56.51, H 4.72, N 21.91.

**N-(4-Methoxyphenyl)-1,3,4-oxadiazol-2-amine (4a):** Pink solid; M.p. 164-166 °C. <sup>1</sup>H NMR (400 MHz, CD<sub>3</sub>OD): δ = 3.76 (s, 3H), 6.90 (d, 2H, J = 9.2 Hz), 7.40 (d, 2H, J = 9.2), 8.40 (s, 1H) ppm. <sup>13</sup>C NMR (100 MHz, CD<sub>3</sub>OD): δ = 56.1, 115.6, 120.9, 133.1, 149.3, 157.3, 162.6 ppm. IR (KBr): 3234, 3142, 3046, 2341, 1614, 1511, 1237, 1097, 1032, 829 cm<sup>-1</sup>. C<sub>9</sub>H<sub>9</sub>N<sub>3</sub>O<sub>2</sub> (191.19): calcd. C 56.54, H 4.74, N 21.98; found C 56.59, H 4.69, N 21.97.

**N-(3,4-Dimethylphenyl)-1,3,4-oxadiazol-2-amine (5a):** White solid; M.p. 133-135 °C. <sup>1</sup>H NMR (400 MHz, CD<sub>3</sub>OD): δ = 2.17 (s, 3H), 2.21 (s, 3H), 7.03 (d, 1H, J = 8.4 Hz), 7.19 (d, 1H, J = 8.4 Hz), 7.25 (s, 1H), 8.40 (s, 1H) ppm. <sup>13</sup>C NMR (100 MHz, CD<sub>3</sub>OD): δ = 19.3, 20.2, 116.5, 120.2, 131.2, 132.1, 137.5, 138.6, 149.2, 162.2 ppm. IR (KBr): 3444, 3228,

2923, 2854, 2288, 1626, 1503, 1328, 1096, 871, 817, 723  $\text{cm}^{-1}$ .  $\text{C}_{10}\text{H}_{11}\text{N}_3\text{O}$  (189.22): calcd. C 63.48, H 5.86, N 22.21; found C 63.44, H 5.89, N 22.19.

**N-(2-Chlorophenyl)-1,3,4-oxadiazol-2-amine (6a):** White solid; M.p. 57-60 °C.  $^1\text{H}$  NMR (400 MHz,  $\text{CD}_3\text{OD}$ ):  $\delta$  = 7.07 (dt, 1H,  $J_1$  = 8.0 Hz,  $J_2$  = 1.6 Hz), 7.31 (dt, 1H,  $J_1$  = 8.0 Hz,  $J_2$  = 1.6 Hz), 7.41 (dd, 1H,  $J_1$  = 8.0 Hz,  $J_2$  = 1.2 Hz), 8.02 (dd, 1H,  $J_1$  = 7.6 Hz,  $J_2$  = 1.6 Hz), 8.51 (s, 1H) ppm.  $^{13}\text{C}$  NMR (100 MHz,  $\text{CD}_3\text{OD}$ ):  $\delta$  = 122.6, 125.9, 129.0, 131.0, 136.5, 143.4, 150.1, 162.3 ppm. IR (KBr): 3428, 3230, 2357, 1614, 1444, 1321, 1120, 1039, 737  $\text{cm}^{-1}$ .  $\text{C}_8\text{H}_6\text{ClN}_3\text{O}$  (195.61): calcd. C 49.12, H 3.09, N 21.48; found C 49.16, H 3.05, N 21.41.

**N-(3-Chlorophenyl)-1,3,4-oxadiazol-2-amine (7a):** White solid; M.p. 119-122 °C.  $^1\text{H}$  NMR (400 MHz,  $\text{CD}_3\text{OD}$ ):  $\delta$  = 6.96 (d, 1H,  $J$  = 8.0 Hz), 7.24 (t, 1H,  $J$  = 8.4 Hz), 7.36 (d, 1H,  $J$  = 8.4 Hz), 7.63 (s, 1H), 8.47 (s, 1H) ppm.  $^{13}\text{C}$  NMR (100 MHz,  $\text{CD}_3\text{OD}$ ):  $\delta$  = 116.8, 118.4, 123.5, 131.5, 135.9, 141.2, 149.6, 161.6 ppm. IR (KBr): 3435, 3153, 2924, 2853, 1687, 1599, 1502, 1484, 1217, 1065, 1025, 904, 852, 755  $\text{cm}^{-1}$ . HRMS (ESI): calcd. for  $\text{C}_8\text{H}_6\text{ClN}_3\text{O}$  ( $\text{MH}^+$ ) 196.0272; found 196.0278.

**N-(4-Bromophenyl)-1,3,4-oxadiazol-2-amine (8a):** Pink solid; M.p. 167-169 °C.  $^1\text{H}$  NMR (400 MHz,  $\text{CD}_3\text{OD}$ ):  $\delta$  = 7.38-7.44 (m, 4 H), 8.45 (s, 1H) ppm.  $^{13}\text{C}$  NMR (100 MHz,  $\text{CD}_3\text{OD}$ ):  $\delta$  = 115.9, 120.4, 133.2, 139.2, 149.5, 161.7 ppm. IR (KBr): 3277, 3092, 2925, 2854, 2399, 1609, 1405, 1093, 1008, 825, 777  $\text{cm}^{-1}$ .  $\text{C}_8\text{H}_6\text{BrN}_3\text{O}$  (240.06): calcd. C 40.03, H 2.52, N 17.50; found C 40.07, H 2.46, N 17.48.

**N-(3-Nitrophenyl)-1,3,4-oxadiazol-2-amine (9a):** Yellowish white solid; M.p. 189-191 °C.  $^1\text{H}$  NMR (400 MHz,  $\text{CD}_3\text{OD}$ ):  $\delta$  = 7.53 (t, 1H,  $J$  = 8.4 Hz), 7.83 (m, 2H), 8.52 (m, 3H) ppm.  $^{13}\text{C}$  NMR (100 MHz,  $\text{CD}_3\text{OD}$ ):  $\delta$  = 113.0, 118.0, 124.2, 131.4, 141.4, 149.9, 150.4, 161.5 ppm. IR (KBr): 3437, 3329, 3153, 2856, 1685, 1520, 1352, 1226, 1078, 1025, 934, 834, 735  $\text{cm}^{-1}$ .  $\text{C}_8\text{H}_6\text{N}_4\text{O}_3$  (206.16): calcd. C 46.61, H 2.93, N 27.18; found C 46.57, H 2.98, N 27.11. HRMS (ESI): calcd. for  $\text{C}_8\text{H}_6\text{N}_4\text{O}_3$  ( $\text{MH}^+$ ) 207.0513; found 207.0523.

**N-(4-(Trifluoromethyl)phenyl)-1,3,4-oxadiazol-2-amine (10a):** White solid; M.p. 166-169 °C.  $^1\text{H}$  NMR (400 MHz,  $\text{CD}_3\text{OD}$ ):  $\delta$  = 7.59 (d, 2H,  $J$  = 8.4 Hz), 7.69 (d, 2H,  $J$  = 8.4 Hz), 8.51 (s, 1H) ppm.  $^{13}\text{C}$  NMR (100 MHz,  $\text{CD}_3\text{OD}$ ):  $\delta$  = 118.4, 124.7, 125.1, 125.4, 127.5, 127.6,

143.4, 149.9, 161.6 ppm. IR (KBr): 3444, 3268, 2924, 1614, 1422, 1332, 1164, 1113, 1070, 1015, 838, 787 cm<sup>-1</sup>. C<sub>9</sub>H<sub>6</sub>F<sub>3</sub>N<sub>3</sub>O (229.16): calcd. C 47.17, H 2.64, F 24.87, N 18.34; found C 47.23, H 2.61, F 24.84, N 18.37. HRMS (ESI): calcd. for C<sub>9</sub>H<sub>6</sub>F<sub>3</sub>N<sub>3</sub>O (MH<sup>+</sup>) 230.0536; found 230.0539.

**N-(Naphthalen-1-yl)-1,3,4-oxadiazol-2-amine (11a):** Black solid; M.p. 136-139 °C. <sup>1</sup>H NMR (400 MHz, CD<sub>3</sub>OD): δ = 7.47-7.57 (m, 3H), 7.70 (d, 1H, J = 8 Hz), 7.86-7.91 (m, 2H), 8.12 (m, 1H), 8.48 (s, 1H) ppm. <sup>13</sup>C NMR (100 MHz, CD<sub>3</sub>OD): δ = 119.4, 122.8, 126.2, 126.8, 127.36, 127.42, 128.4, 129.6, 135.0, 135.9, 149.8, 163.6. ppm. IR (KBr): 3175, 2961, 2845, 1574, 1400, 1217, 1088, 1006, 780, 724 cm<sup>-1</sup>. C<sub>12</sub>H<sub>9</sub>N<sub>3</sub>O (211.22): calcd. C 68.24, H 4.29, N 19.89; found C 68.29, H 4.26, N 19.83. HRMS (ESI): calcd for C<sub>12</sub>H<sub>9</sub>N<sub>3</sub>O (MH<sup>+</sup>) 212.0818; found 212.0824.

**N,5-Diphenyl-1,3,4-oxadiazol-2-amine (12a):** White solid; M.p. 218-220 °C.(Lit. M.p. 214.9-215.9 °C).<sup>5</sup> <sup>1</sup>H NMR (400 MHz, CD<sub>3</sub>OD): δ = 7.06 (t, 1H, J = 7.6 Hz), 7.36 (t, 2H, J = 6.8 Hz), 7.55 (m, 5H), 7.96 (m, 2H) ppm. <sup>13</sup>C NMR (100 MHz, CD<sub>3</sub>OD + DMSO-d<sub>6</sub>): δ = 118.9, 123.9, 125.4, 127.2, 130.5, 130.6, 132.6, 140.0, 160.2, 162.0 ppm. IR (KBr): 3446, 3264, 3053, 2923, 1620, 1580, 1500, 1444, 1242, 1050, 1021, 745, 722, 685 cm<sup>-1</sup>. C<sub>14</sub>H<sub>11</sub>N<sub>3</sub>O (237.26): calcd. C 70.87, H 4.67, N 17.71; found C 70.81; H 4.69, N 17.75. HRMS (ESI): calcd. for C<sub>14</sub>H<sub>11</sub>N<sub>3</sub>O (MH<sup>+</sup>) 238.0975; found 238.0981.

**5-Phenyl-N-p-tolyl-1,3,4-oxadiazol-2-amine (13a):** White solid; M.p. 214-217 °C (Lit. M.p. 214-216 °C).<sup>6</sup> <sup>1</sup>H NMR (400 MHz, CD<sub>3</sub>OD): δ = 2.31 (s, 3H), 7.17 (d, 2H, J = 8.4 Hz), 7.43 (d, 2H, J = 8.4 Hz), 7.54 (m, 3H), 7.95 (m, 2H) ppm. <sup>13</sup>C NMR (100 MHz, CD<sub>3</sub>OD + DMSO-d<sub>6</sub>): δ = 21.2, 119.0, 125.5, 127.1, 129.0, 130.6, 131.0, 132.5, 137.6, 159.9, 162.0 ppm. IR (KBr): 3435, 3298, 3044, 2917, 1613, 1581, 1518, 1286, 1244, 1232, 1050, 818, 719, 682 cm<sup>-1</sup>. C<sub>15</sub>H<sub>13</sub>N<sub>3</sub>O (251.29): calcd. C 71.70, H 5.21, N 16.72; found C 71.74, H 5.17, N 16.66.

**N-(2-Fluorophenyl)-5-phenyl-1,3,4-oxadiazol-2-amine (14a):** White solid; M.p. 120-122 °C. <sup>1</sup>H NMR (400 MHz, CD<sub>3</sub>OD): δ = 7.05 (m, 1H), 7.13-7.20 (m, 2H), 7.49 (m, 3H), 7.93 (m, 2H), 8.09 (t, 1H, 8.0 Hz) ppm. <sup>13</sup>C NMR (100 MHz, CD<sub>3</sub>OD): δ = 116.4, 116.6, 121.8, 125.0, 125.1, 125.2, 125.8, 125.9, 127.2, 127.8, 127.9, 130.4, 132.5, 153.1, 155.5, 160.7, 162.0 ppm. IR (KBr): 3391, 3063, 1620, 1581, 1557, 1488, 1461, 1252, 1051, 749, 719, 688

$\text{cm}^{-1}$ .  $\text{C}_{14}\text{H}_{10}\text{FN}_3\text{O}$  (255.24): calcd. C 65.88, H 3.95, N 16.46; found C 65.83, H 3.99, N 16.41. HRMS (ESI): calcd. for  $\text{C}_{14}\text{H}_{10}\text{FN}_3\text{O} (\text{MH}^+)$  256.0881; found 256.0883.

**N-Cyclohexyl-5-phenyl-1,3,4-oxadiazol-2-amine (15a):** White solid; M.p. 146-148 °C (Lit. M.p. 152.8-152.9 °C).<sup>7</sup>  $^1\text{H}$  NMR (400 MHz,  $\text{CD}_3\text{OD}$ ):  $\delta$  = 1.22-1.48 (m, 5H), 1.66 (m, 1H), 1.81 (m, 2H), 2.07 (m, 2H), 3.49 (m, 1H), 7.49 (m, 3H), 7.87 (m, 2H) ppm  $^{13}\text{C}$  NMR (100 MHz,  $\text{CD}_3\text{OD}$ ):  $\delta$  = 26.1, 26.8, 34.0, 53.77, 125.6, 126.8, 130.3, 132.1, 159.9, 164.8 ppm. IR (KBr): 3264, 3022, 2919, 2852, 1621, 1586, 1452, 1379, 1346, 1048, 770, 736, 693  $\text{cm}^{-1}$ .  $\text{C}_{14}\text{H}_{17}\text{N}_3\text{O}$  (243.31): calcd. C 69.11, H 7.04, N 17.27; found C 69.15, H 7.06, N 17.20.

**(R)-5-Phenyl-N-(1-phenylethyl)-1,3,4-oxadiazol-2-amine (16a).** White solid; M.p. 179-180 °C (Lit. M.p. 181-183 °C).<sup>7</sup>  $^1\text{H}$  NMR (400 MHz,  $\text{CD}_3\text{OD}$ ):  $\delta$  = 1.58 (d, 3H,  $J$  = 6.8 Hz), 4.94 (m, 1H), 7.25 (m, 1H), 7.35 (t, 2H,  $J$  = 8.0 Hz), 7.42 (m, 2H), 7.49 (m, 3H), 7.85 (m, 2H) ppm.  $^{13}\text{C}$  NMR (100 MHz,  $\text{CD}_3\text{OD}$ ):  $\delta$  = 23.6, 54.6, 125.5, 126.9, 127.2, 128.6, 129.8, 130.3, 132.2, 142.7, 145.2, 164.7 ppm. IR (KBr): 3231, 3036, 2976, 2936, 1614, 1494, 1256, 1127, 1048, 700, 691  $\text{cm}^{-1}$ .  $\text{C}_{16}\text{H}_{15}\text{N}_3\text{O}$  (265.31): calcd. C 72.43, H 5.70, N 15.84; found C 72.39, H 5.73, N 15.77. HRMS (ESI): calcd. for  $\text{C}_{16}\text{H}_{15}\text{N}_3\text{O} (\text{MH}^+)$  266.1288; found 266.1293.

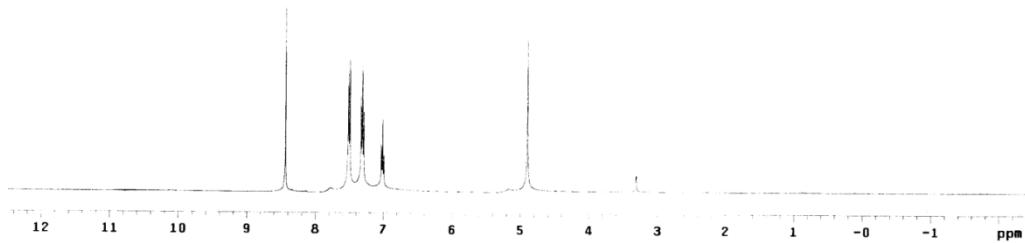
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## SPECTRA

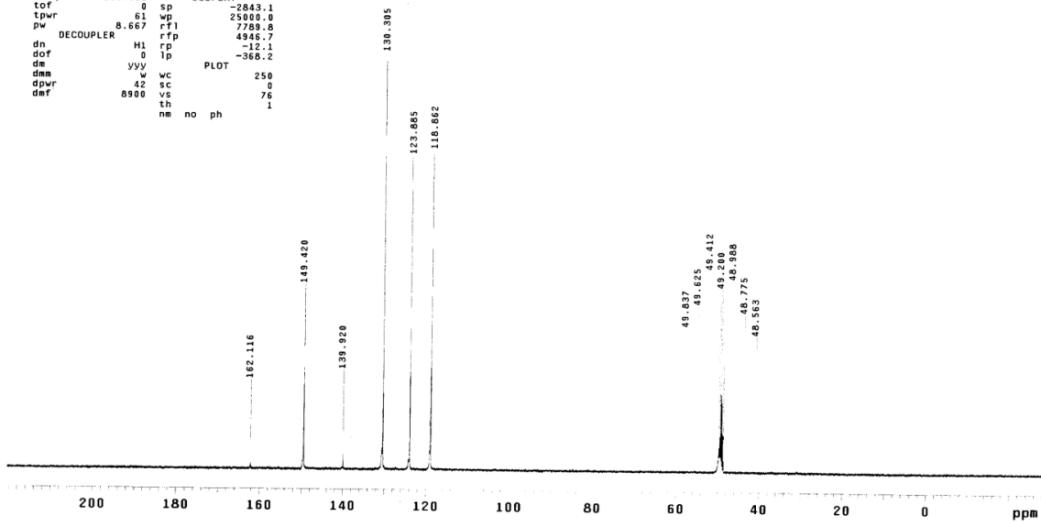
**N-Phenyl-1,3,4-oxadiazol-2-amine (1a):  $^1\text{H}$  NMR ( $\text{CD}_3\text{OD}$ , 400 MHz)**

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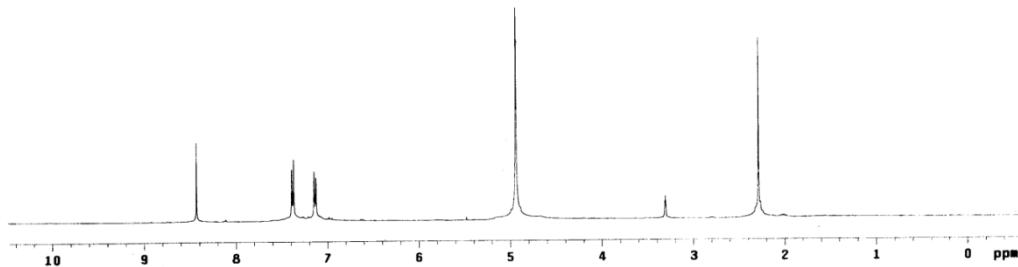
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*N-p-Tolyl-1,3,4-oxadiazol-2-amine (2a): <sup>1</sup>H NMR (CD<sub>3</sub>OD, 400 MHz)*

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solvent CD3OD   gain    not used
file   exp      spin    not used
      ACQUISITION hst      0.000
      sw      6389.8 pw99    19.700
      at      1.398 alfa   20.000
      np      256   flags
      rb      not used 11   n
      bs      4   in
      d1      1.000   y
      nt      32   hs
      ct      32   PROCESSING nn
      TRANSMITTER hb
      tn      H1 fn    65536
      sfrq   399.855 DISPLAY
      tof     367.5 sp    239.3
      tpwv   57   wp    4432.3
      pw     9.850 rfp   2116.8
      DECOUPLER C13 rfp   132.0
      dn      C13 rp    -108.0
      dof     0   lp    -88.2
      de     nnn   PLOT
      dse     c   wc    258
      dpwr   50   sc    0
      daf     15980 vs    53
      th     nm cdc ph  20

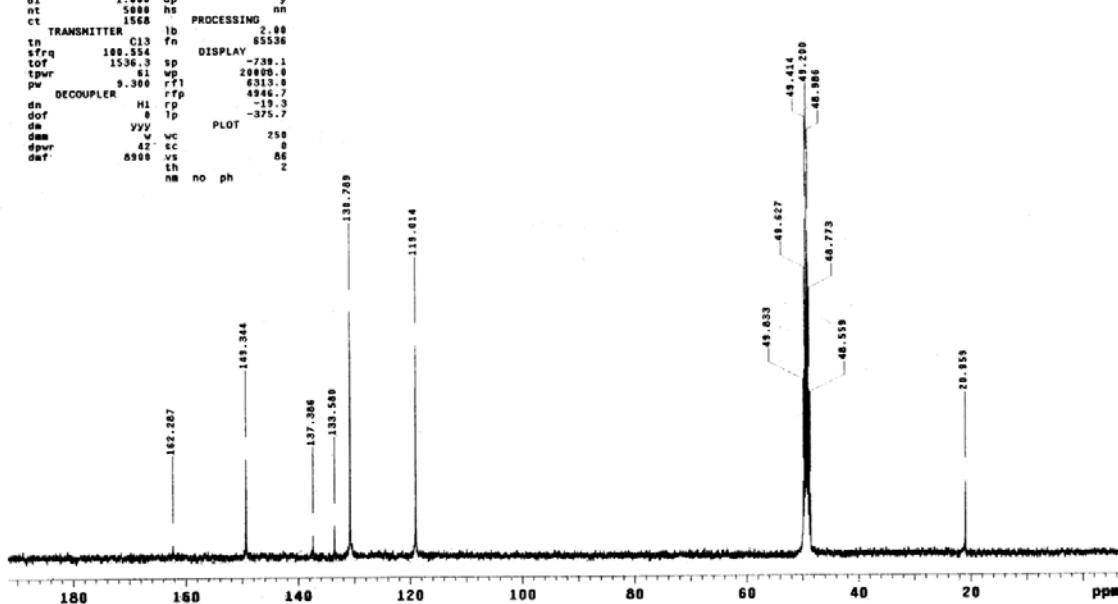
```



*N-p-Tolyl-1,3,4-oxadiazol-2-amine (2a): <sup>13</sup>C NMR (CD<sub>3</sub>OD, 100 MHz)*

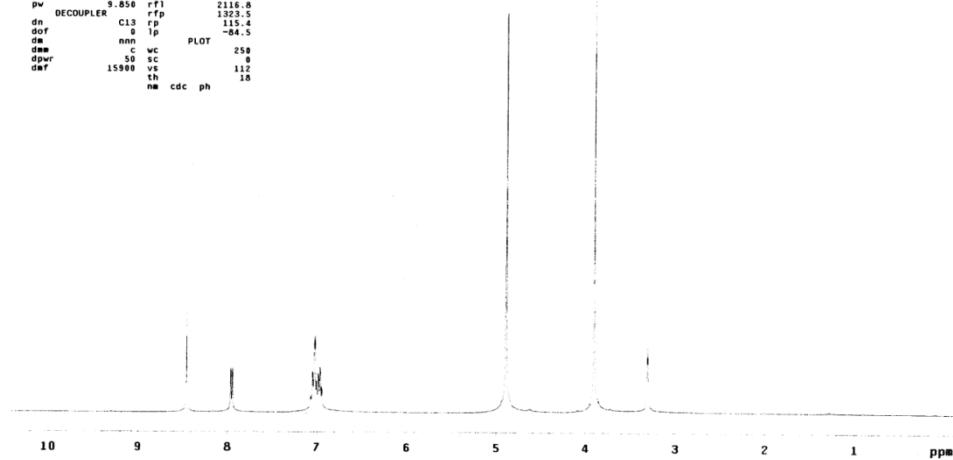
```
expt s2pul
SAMPLE          SPECIAL
date Jan 19 2011 temp    not used
solvent CD3OD   gain    not used
file   exp      spin    not used
      ACQUISITION hst      0.000
      sw      25125.6 pw99    10.000
      at      1.398 alfa   20.000
      np      256   flags
      rb      13888 11   n
      bs      32   in
      d1      1.000   y
      nt      5000 hs
      ct      1568 PROCESSING 2.00
      TRANSMITTER hb
      tn      C13 fn    65536
      sfrq   100.554 DISPLAY -739.1
      tof     1536.3 sp    28800.0
      tpwv   61   wp    28800.0
      pw     5.300 rfp   4946.7
      DECOUPLER C13 rfp   4946.7
      dn      H1 rp    -19.3
      dof     0   lp    -375.7
      de     yyv   PLOT
      dse     v   wc    258
      dpwr   47   sc    0
      daf     8988 vs    86
      th     nm no ph

```



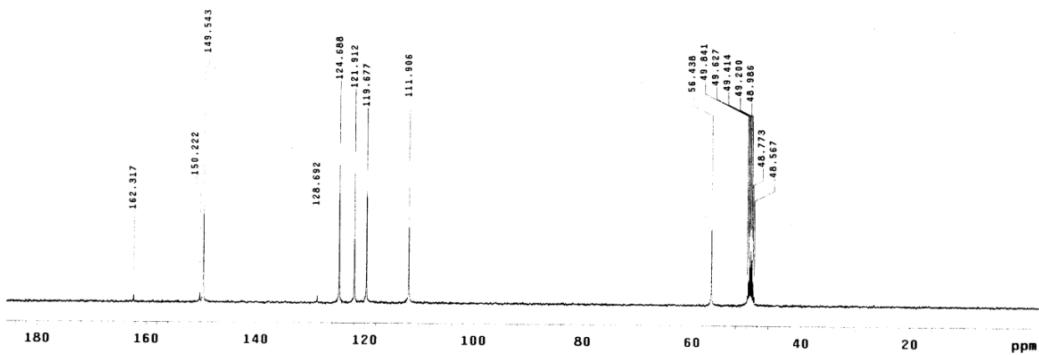
*N*-(2-Methoxyphenyl)-1,3,4-oxadiazol-2-amine (3a):  $^1\text{H}$  NMR (CD<sub>3</sub>OD, 400 MHz)

```
expt s2pul
SAMPLE SPECIAL
date May 17 2011 temp not used
solvent CD3OD gain not used
file exp spin not used
ACQUISITION hst 0.008
sw 6389.8 pw0 1.798
at 1.998 alfa 20.000
tp not used t1 1.000
fb not used d1 in n
dt 1.000 dp y
nt 32 hs nn
ct 32 PROCESSING
TRANSMITTER lb 0.10
tn H1 fn 65536
sfrq 393.455 DISPLAY
tof 365.7 sp -42.8
tpwr 57 wp 4231.8
pw 9.858 r1 2316.8
DECOUPLER C13 rfp 1322.5
dn C13 rfp 115.4
dof 0 ip -84.5
de mnm PLOT
dme c wc 250
dpwr 56 sc 0
dft 15889 vs 112
th th 18
nm cdc ph
```



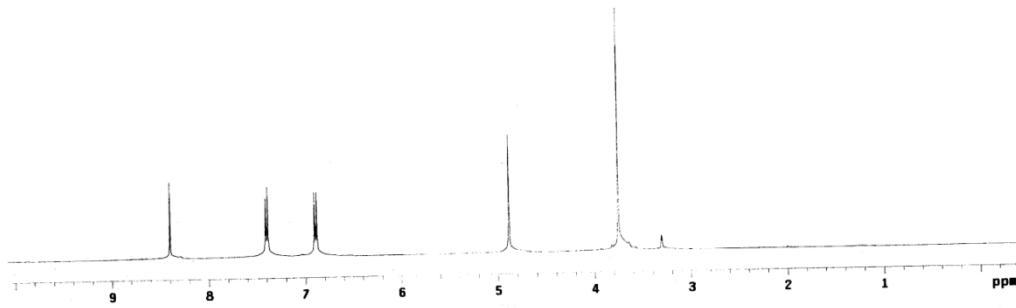
*N*-(2-Methoxyphenyl)-1,3,4-oxadiazol-2-amine (3a):  $^{13}\text{C}$  NMR (CD<sub>3</sub>OD, 100 MHz)

```
expt s2pul
SAMPLE SPECIAL
date May 17 2011 temp not used
solvent CD3OD gain not used
file exp spin not used
ACQUISITION hst 0.008
sw 25125.6 pw0 18.500
at 1.199 pw1fa 29.000
np 60270 FLAGS
fb 1380 t1 in n
bs 32 in n
di 1.800 dp y
nt 5000 hs nn
ct 416 PROCESSING
TRANSMITTER lb 2.00
tn H1 fn 65536
sfrq 100.554 DISPLAY
tof 1536.3 sp -415.5
tpwr 61 wp 19083.3
pw 9.300 r1 6300.0
DECOUPLER C13 rfp 4946.7
dn H1 rfp -15.6
dof 0 ip -350.3
de yyv PLOT
dme v wc 250
dpwr 42 sc 0
dft 8900 vs 33
th th 2
nm no ph
```



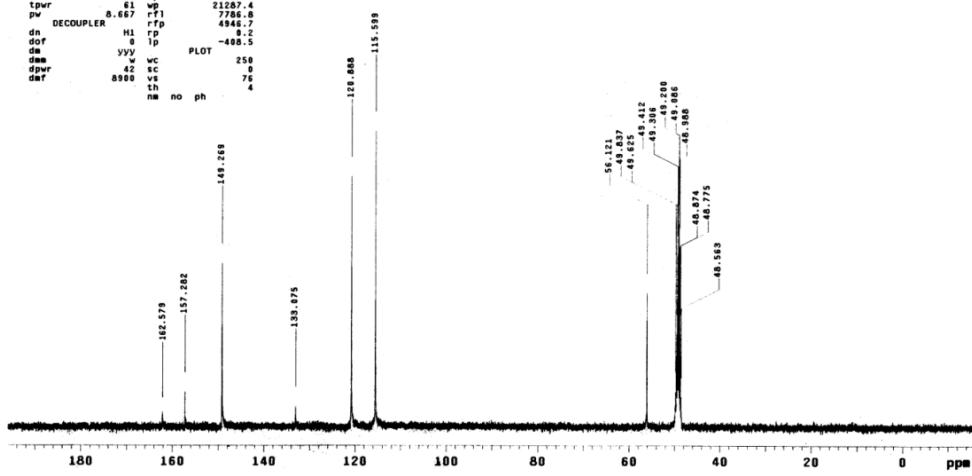
*N*-(4-Methoxyphenyl)-1,3,4-oxadiazol-2-amine (4a):  $^1\text{H}$  NMR ( $\text{CD}_3\text{OD}$ , 400 MHz)

```
exp1 std1h
SAMPLE          SPECIAL
date Dec 21 2010 temp not used
solvent CD3OD   gain  not used
file   exp    spin  not used
      ACQUISITION hst   fwhm  6.750
      sw    8000.0   t90   16.750
      at    1.995   aita  20.000
      np    23994   flags
      rb    not used 11   n
      bs    4       in   n
      di    1.000   dp   y
      nt    32      hs   nn
      ct    32      PROCESSING
      TRANSMITTER fm   not used
      HI   DISPLAY
      sfrq  399.855 sp   -166.7
      tof   0       w1   4189.7
      tpwr  61      r1   2282.2
      pw   7.000   rfp  1323.5
      DECOUPLER C13  rp   193.8
      d1    C13   ip   -59.2
      dof   0       PLOT
      de   nnn wc   250
      dm   c sc   9
      dppr 51 ts   60
      dprf  15900 th   20
      dmt   nm cdc ph
```



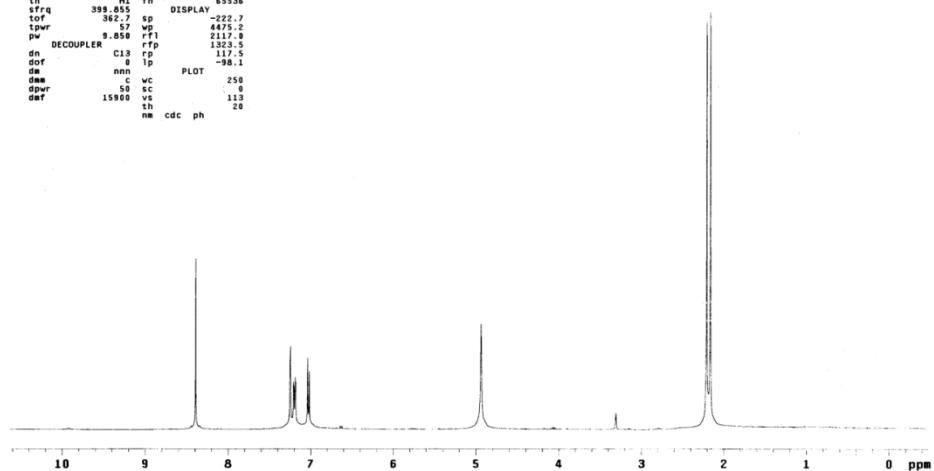
*N*-(4-Methoxyphenyl)-1,3,4-oxadiazol-2-amine (4a):  $^{13}\text{C}$  NMR ( $\text{CD}_3\text{OD}$ , 100 MHz)

```
exp1 std13c
SAMPLE          SPECIAL
date Dec 21 2010 temp not used
solvent CD3OD   gain  not used
file   exp    spin  not used
      ACQUISITION hst   fwhm  8.000
      sw    25000.0   t90   16.600
      at    1.995   aita  20.000
      np    34992   flags
      rb    13880   11   n
      bs    32      in   n
      di    0       dp   y
      nt    5000   hs   nn
      ct    2144   PROCESSING
      TRANSMITTER C13  fm   1.00
      HI   DISPLAY
      sfrq  100.000 sp   -1591.9
      tof   0       w1   21287.4
      tpwr  61      r1   22771.4
      pw   8.667   rfp  4946.7
      DECOUPLER C13  rp   193.8
      d1    H1   rp   -9.2
      dof   0       ip   -488.5
      de   vyy wc   250
      dm   c sc   9
      dppr 42 ts   76
      dprf  8500 th   4
      dmt   nm no ph
```



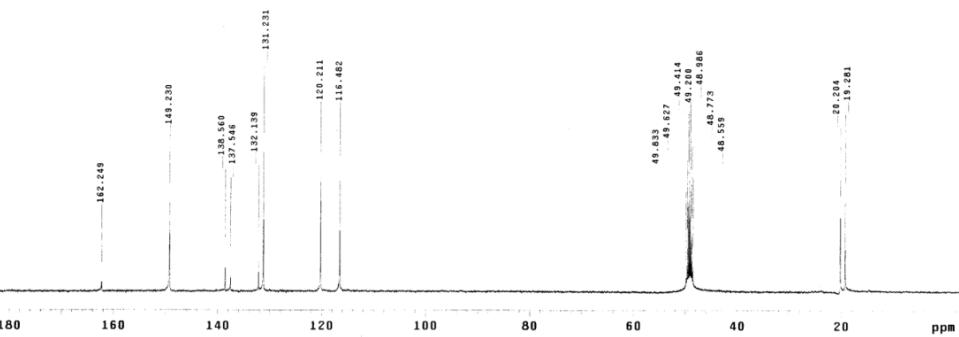
**N-(3,4-Dimethylphenyl)-1,3,4-oxadiazol-2-amine (5a):  $^1\text{H}$  NMR (CD<sub>3</sub>OD, 400 MHz)**

```
exp1 s2pu1
SAMPLE SPECIAL
date Jan 18 2011 temp not used
solvent CD3OD gain not used
file exp spin not used
ACQUISITION hst 0.008
sw 139.5 139.5 139.5
at 1.998 alfa 20.000
nu 2500000
fb not used il n
bs 32 4 in n
d1 1.000 sp y
nt 32 hs nn
ct 32 PROCESSING
TRANSMITTER C13 lb 9.18
tn H1 fm 65536
sfrq 393.7 sp DISPLAY -222.7
tot 362.7
tpwr 57 wp 4475.2
pw 9.859 r1 1323.5
DECOUPLER rfp 1323.5
dn C13 rp 117.5
dof 8 lp 50.1
dss nnn PLOT
dme 250
dpw 50 tc 250
def 15900 vs 113
drt 15900 th 20
nm cdc ph
```

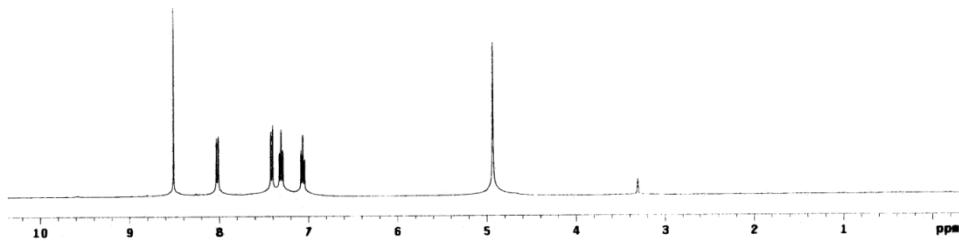


**N-(3,4-Dimethylphenyl)-1,3,4-oxadiazol-2-amine (5a):  $^{13}\text{C}$  NMR (CD<sub>3</sub>OD, 100 MHz)**

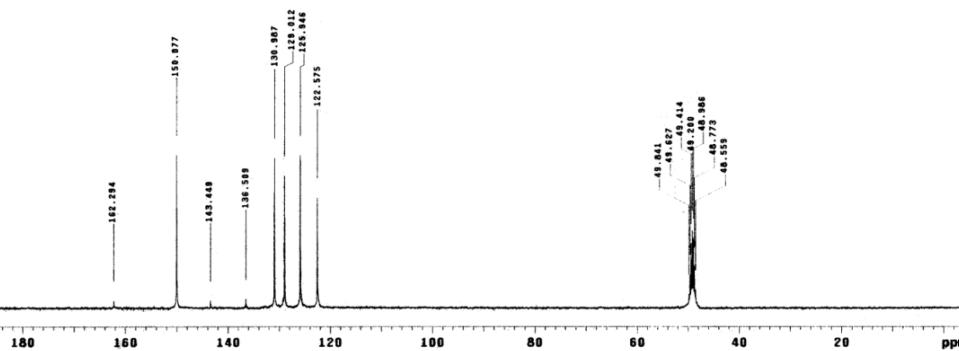
```
exp1 s2pu1
SAMPLE SPECIAL
date Jan 18 2011 temp not used
solvent CD3OD gain not used
file exp spin not used
ACQUISITION hst 0.008
sw 25125.6 25125.6 25125.6
at 1.199 alfa 20.000
nu 68000
fb 138000 il n
bs 32 in n
d1 1.000 sp y
nt 5000 hs nn
ct 1088 PROCESSING
TRANSMITTER C13 lb 2.00
tn H1 fm 65536
sfrq 100.554 DISPLAY
tot 153.0 sp -281.3
tpwr 61 wp 18853.9
pw 9.300 r1 6316.9
DECOUPLER rfp 4446.5
dn C13 rp -62.5
dof 8 lp -271.4
dss yyy PLOT
dme 250
dpw 42 tc 50
def 8900 vs 35
drt 8900 th z
nm no ph
```



**N-(2-Chlorophenyl)-1,3,4-oxadiazol-2-amine (6a):**  $^1\text{H}$  NMR ( $\text{CD}_3\text{OD}$ , 400 MHz)



**N-(2-Chlorophenyl)-1,3,4-oxadiazol-2-amine (6a):**  $^{13}\text{C}$  NMR ( $\text{CD}_3\text{OD}$ , 100 MHz)

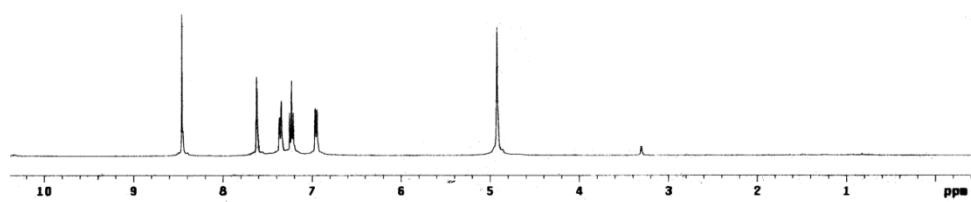


**N-(3-Chlorophenyl)-1,3,4-oxadiazol-2-amine (7a):**  $^1\text{H}$  NMR ( $\text{CD}_3\text{OD}$ , 400 MHz)

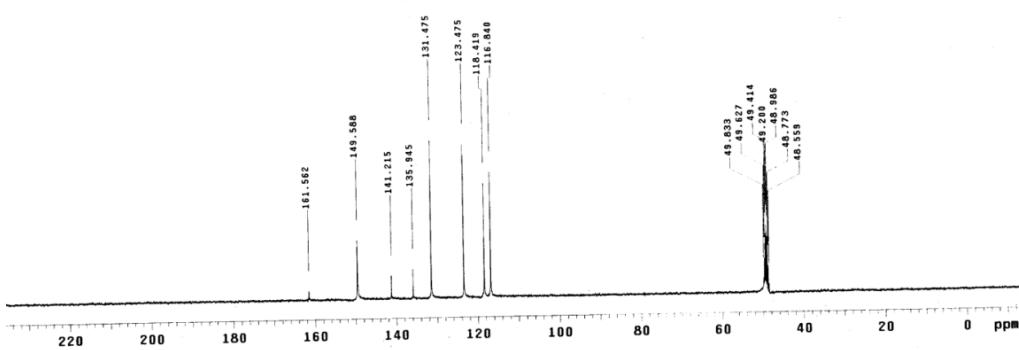
```

exp1 s2pul          SAMPLE           SPECIAL
date Jan 7 2011      tame    not used
solvent CD300       gain    not used
file exp            spin   not used
sw ACQUISITION      6386.8     pw08   15.788
at 1.0000           1.0000    alfa   28.000
sp 1000              1000     flags   000
dt not used        11      in      n
dt             1.0000    dp      m
dt             32      ns      v
ct             32      nc      p
                                         PROCESSING 0.10
tn TRANSMITTER      H1      HI      65536
tqf 388.81          388.81    DISPLAY -163.0
tqf 387.62          387.62    3d      4315.7
tpwr 5.57            5.57      w      1323.5
tpwr 9.88            9.88      r      1323.5
decoupler        C13     rfp      1323.5
dn               nm      rp      1323.5
de               nm      ip      1323.5
de               nm      c      PLOT 250
de               nm      c      37
de               nm      vs      37
de               nm      vr      37
de               nm      ph      cdc
de               nm      ph      ph

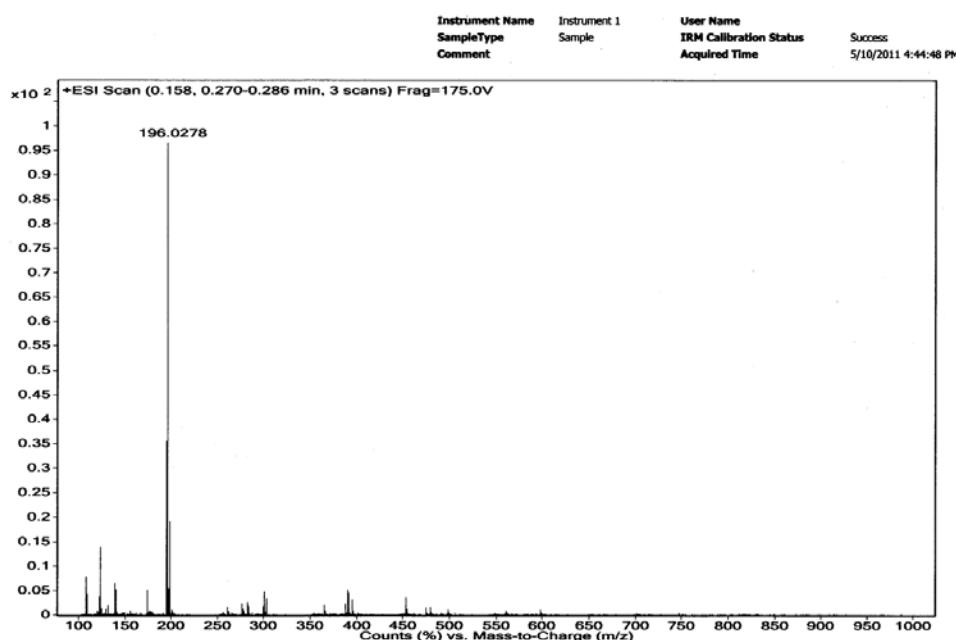
```



**N-(3-Chlorophenyl)-1,3,4-oxadiazol-2-amine (7a):**  $^{13}\text{C}$  NMR ( $\text{CD}_3\text{OD}$ , 100 MHz)

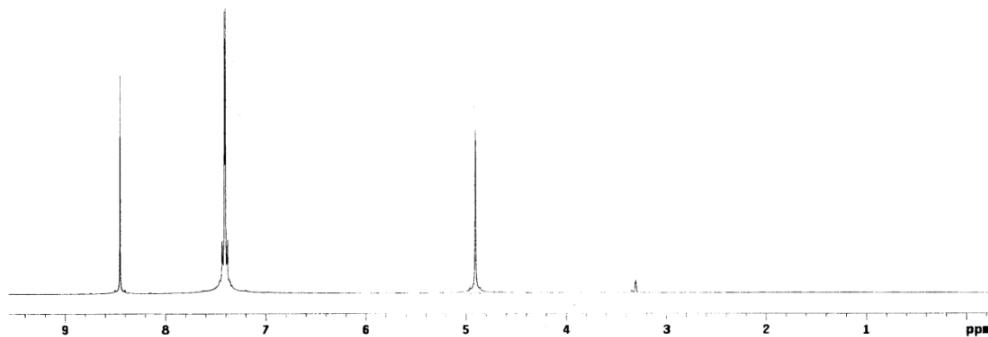


**N-(3-Chlorophenyl)-1,3,4-oxadiazol-2-amine (7a): (Mass Spectra)**

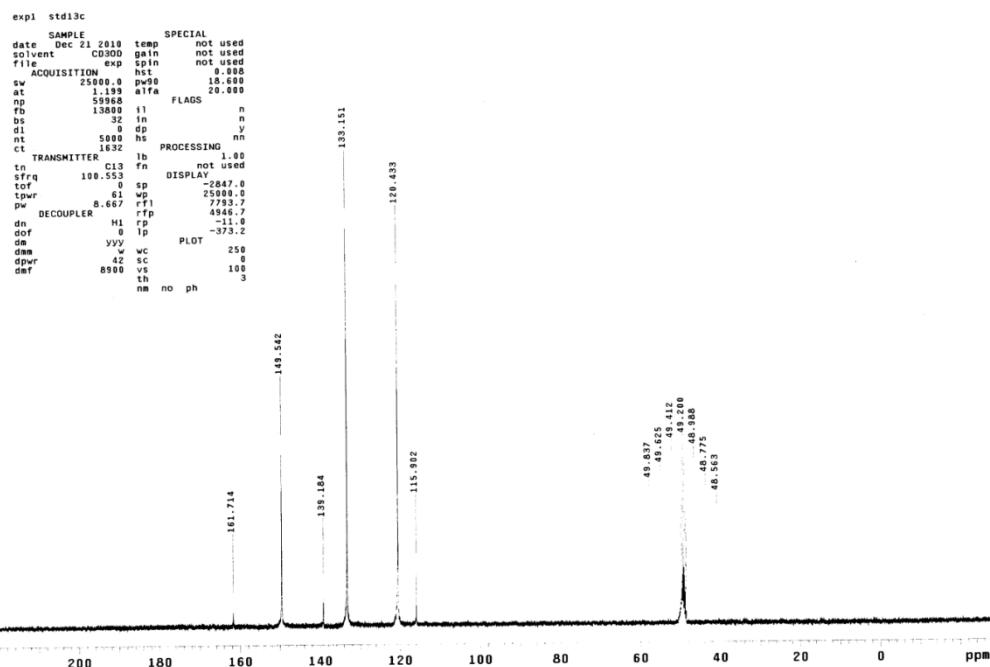


**N-(4-Bromophenyl)-1,3,4-oxadiazol-2-amine (8a):  $^1\text{H}$  NMR ( $\text{CD}_3\text{OD}$ , 400 MHz)**

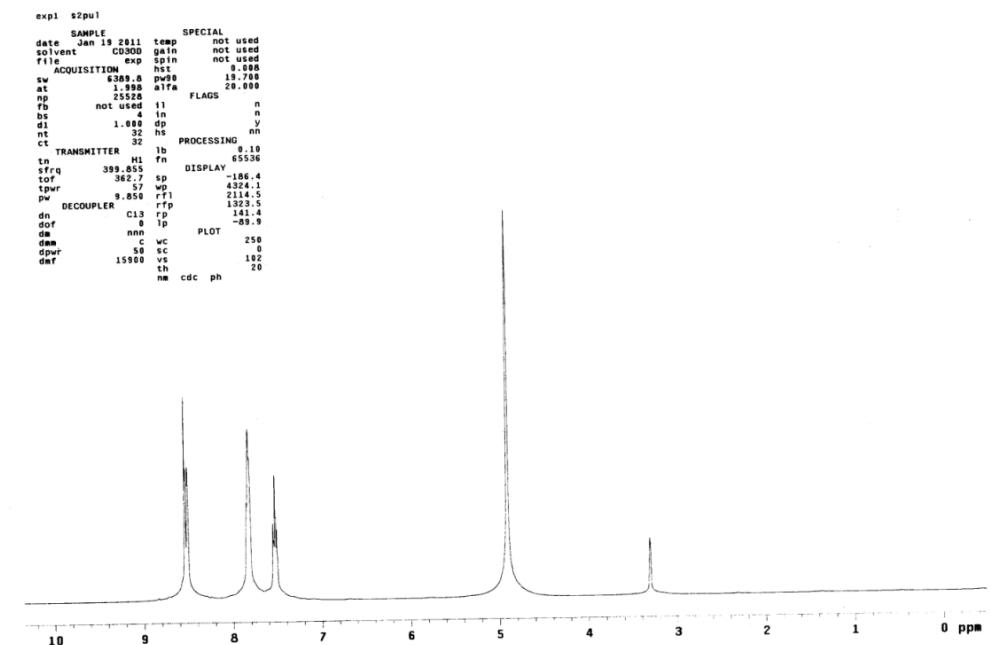
```
expt stdih
SAMPLE          SPECIAL
date Dec 21 2010 temp not used
solvent   CD3OD  gain not used
file      exp  spin not used
ACQUISITION exp  int 1000
sw       6006.0 pw90 19.700
at       1.995 alfa 28.000
np       2048   16
dp       256    128   FLAGS
fb       not used 11   n
bs       4      in   n
dt       1.000   g   y
nt       32    hs  nn
ct       32    PROCESSING nn
TRANSMITTER H1 fn not used
tn        H1 DISPLAY
sfrq     399.855 sp -112.1
tr       1.000   1
tppr     57    rF1  2287.6
pw       7.000 rFp 1323.5
pwr      1000   rf 112.0
dec      64    c64 -81.2
d1       C13 1p PLOT
dof      0      256
dm      nnn wc  256
dme      c  sc   8
dpwpr    50    vs  73
dmtf    15900 th  26
dmf      nm cdc ph
```



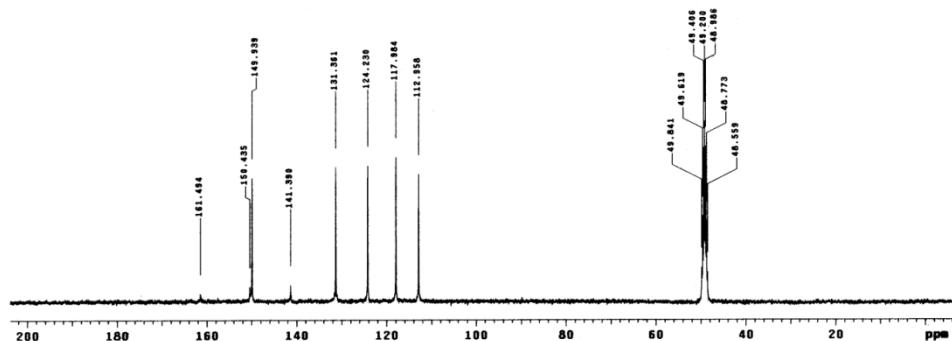
**N-(4-Bromophenyl)-1,3,4-oxadiazol-2-amine (8a):  $^{13}\text{C}$  NMR ( $\text{CD}_3\text{OD}$ , 100 MHz)**



**N-(3-Nitrophenyl)-1,3,4-oxadiazol-2-amine (9a):  $^1\text{H}$  NMR ( $\text{CD}_3\text{OD}$ , 400 MHz)**

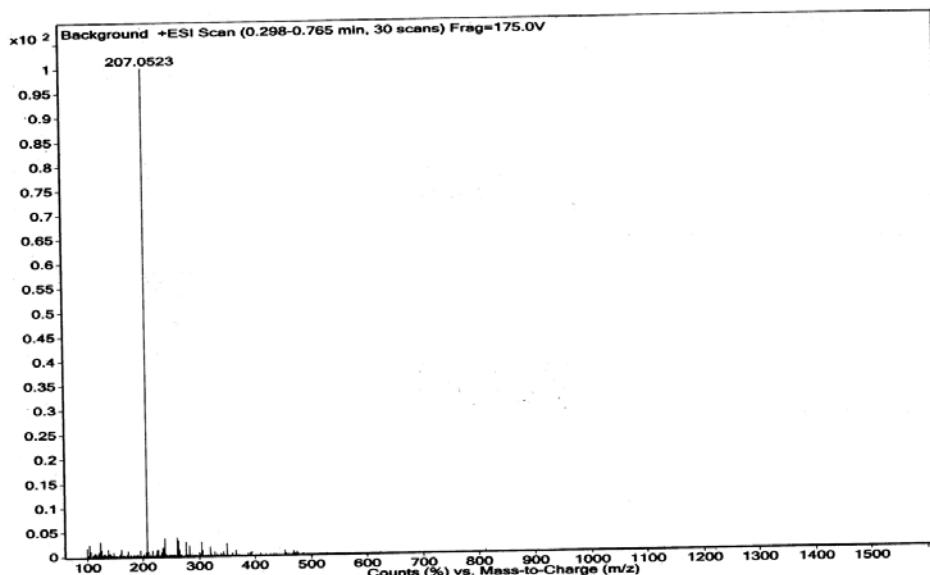


**N-(3-Nitrophenyl)-1,3,4-oxadiazol-2-amine (9a):**  $^{13}\text{C}$  NMR ( $\text{CD}_3\text{OD}$ , 100 MHz)



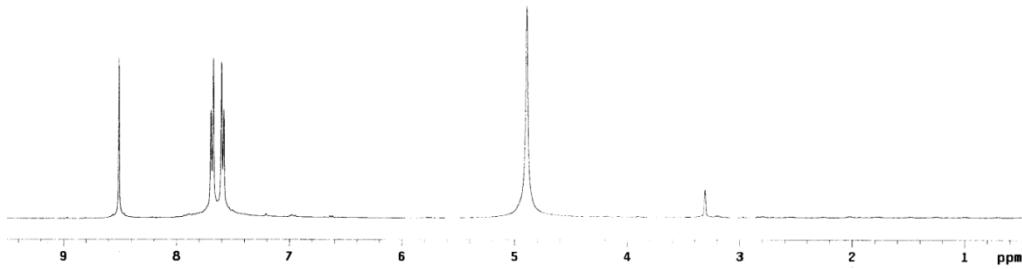
### ***N*-(3-Nitrophenyl)-1,3,4-oxadiazol-2-amine (9a): (Mass Spectra)**

Instrument Name	Instrument 1	User Name	
SampleType	Sample	IRM Calibration Status	Success
Comment		Acquired Time	5/9/2011 8:14:47 PM



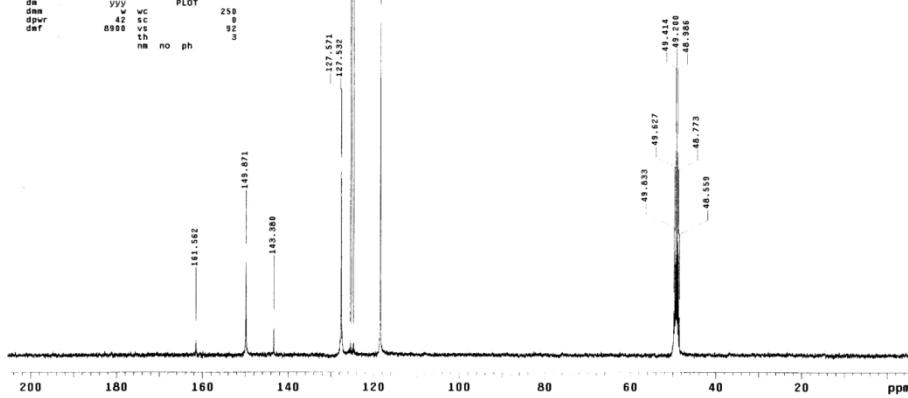
*N*-(4-(Trifluoromethyl)phenyl)-1,3,4-oxadiazol-2-amine (10a):  $^1\text{H}$  NMR (CD<sub>3</sub>OD, 400 MHz)

```
exp1 s2pul
SAMPLE          SPECIAL
date Dec 21 2010 temp not used
solvent CD3OD gain not used
file   exp spin not used
ACQUISITION hst    0.088
sw    6389.8   16.00
at    1.998 alfa  20.000
np    25528   flags
fb    not used  11   n
bs    4       in   n
di    1.000 dp   y
nt    32      hs   nn
ct    32      PROCESSING
TRANSMITTER 1b   0.10
tr    H1 fn   65536
sfrq  399.855 DISPLAY
t0f   362.7 sp   179.8
tpwr  5    w1   3644.1
pw    9.650 r1   111.6
p     1.000 rfp  1323.5
DECOUPLER C13  rfp  121.9
dof   nnn   lp   -98.4
dm   nnn   wc   250
dmm   c   sc   0
dpwr  15900 vs   52
def   15900 th   20
nm   cdc ph
```



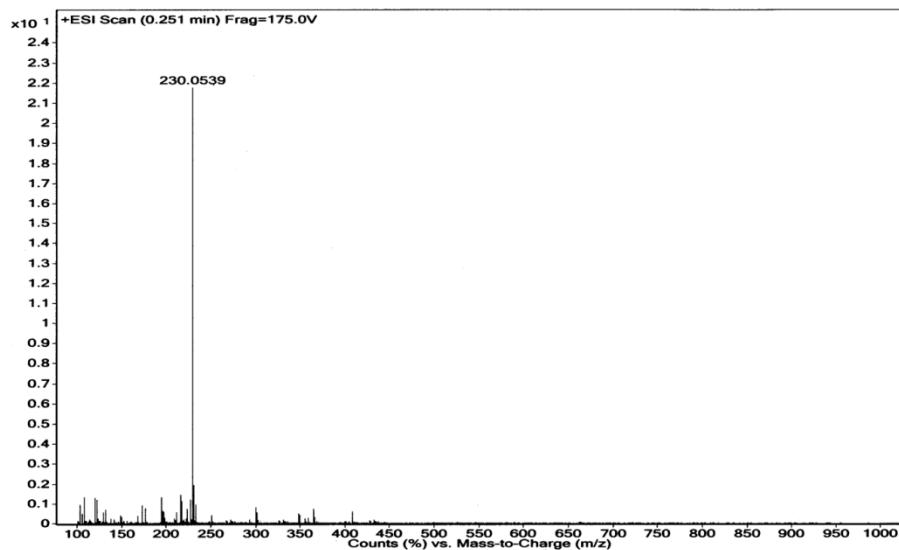
*N*-(4-(Trifluoromethyl)phenyl)-1,3,4-oxadiazol-2-amine (10a):  $^{13}\text{C}$  NMR (CD<sub>3</sub>OD, 100 MHz)

```
exp1 s2pul
SAMPLE          SPECIAL
date Dec 21 2010 temp not used
solvent CD3OD gain not used
file   exp spin not used
ACQUISITION hst    0.088
sw    25125.6   16.00
at    1.998 alfa  20.000
np    4096   flags
fb    138000  11   n
bs    32      in   n
di    1.000 dp   y
nt    50000 hs   nn
ct    1024    PROCESSING
TRANSMITTER 1b   2.00
tr    C13 fn   65536
sfrq  100.000 DISPLAY
t0f   1536.3 sp   -440.2
tpwr  5    w1   6513.5
pw    9.385 r1   4946.7
p     1.000 rfp  121.1
DECOUPLER H1   rfp  -371.9
dn   yyy   wc   250
dmm   42   sc   0
dpwr  8900 vs   92
def   8900 th   5
nm   no ph
```

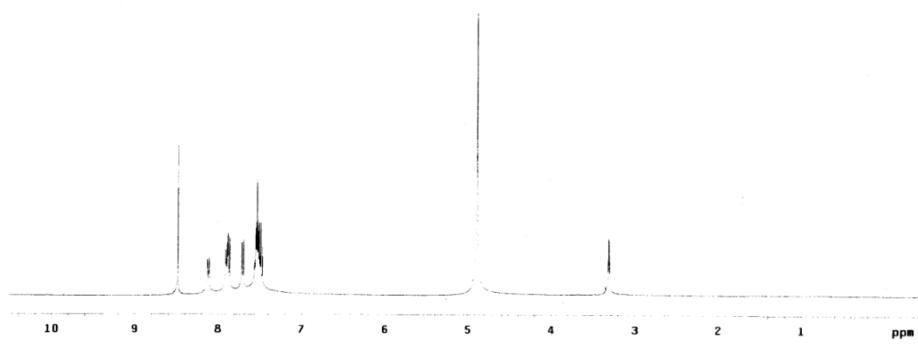


### **N-(4-(Trifluoromethyl)phenyl)-1,3,4-oxadiazol-2-amine (10a): (Mass Spectra)**

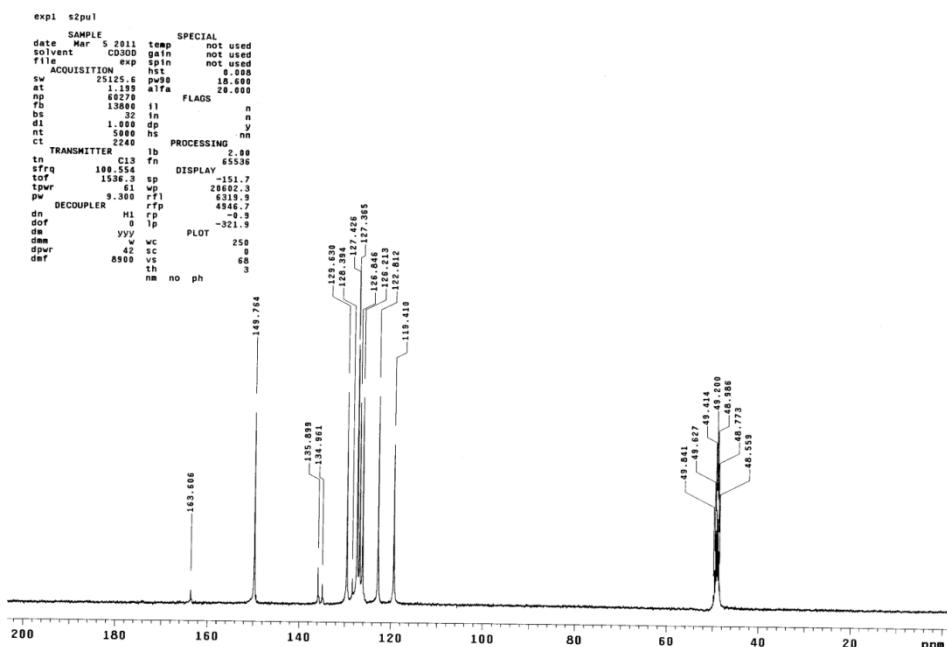
Instrument Name	Instrument 1	User Name	
SampleType	Sample	IRM Calibration Status	Success
Comment		Acquired Time	5/10/2011 5:21:08 PM



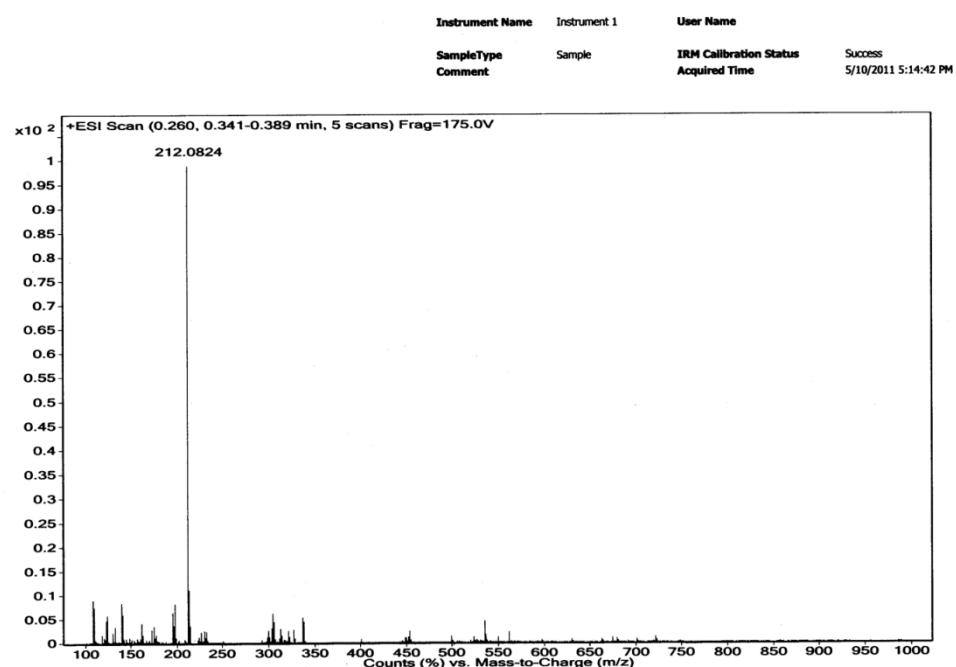
**N-(Naphthalen-1-yl)-1,3,4-oxadiazol-2-amine (11a):**  $^1\text{H}$  NMR ( $\text{CD}_3\text{OD}$ , 400 MHz)



**N-(Naphthalen-1-yl)-1,3,4-oxadiazol-2-amine (11a):  $^{13}\text{C}$  NMR ( $\text{CD}_3\text{OD}$ , 100 MHz)**

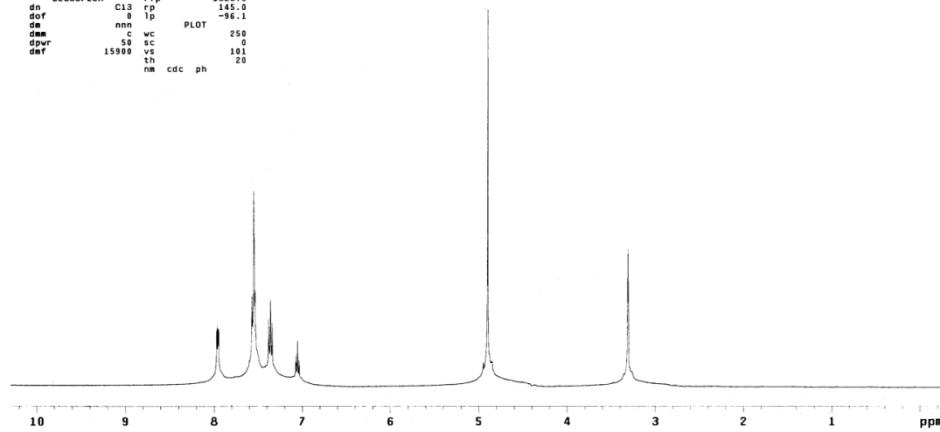


**N-(Naphthalen-1-yl)-1,3,4-oxadiazol-2-amine (11a): (Mass Spectra)**



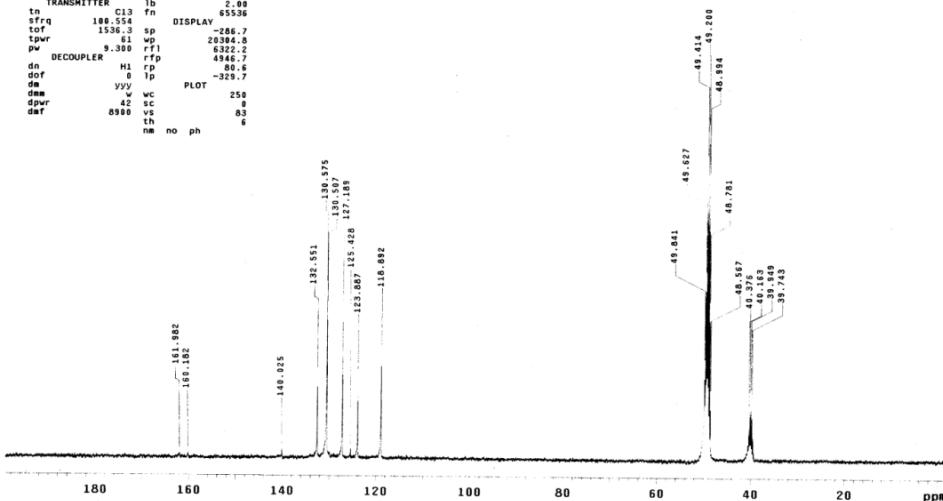
**N,5-Diphenyl-1,3,4-oxadiazol-2-amine (12a):  $^1\text{H}$  NMR ( $\text{CD}_3\text{OD}$ , 400 MHz)**

```
exp1 s2pul
SAMPLE      SPECIAL
date Feb 54 2011 temp    not used
solvent CD3OD gain     not used
file        exp spin    not used
ACQUISITION t1       1.000   pw98   19.700
            t2       0.000   alfa   20.000
at         1.100   alpha  25528   FLAGs
np         25528   flags
fb         not used 11   n
bs         4        in    n
di         1.000   dp     y
nt         32      hs    nn
ct         32      PROCESSING
TRANSMITTER lb      0.10
tn         H1      fn    65536
sfreq     399.855  DISPLAY
t0f        362.7   sp    -121.7
tpwr      61       wp    20.2
pw        9.850   rfp   2116.8
DECOUPLER C13     rfp   132.5
dn         C13     rfp   145.0
dof        0        lp    -96.1
de         n       PLOT
dm         c       wc    250
dpw       50      sc    0
dpwr     19980   th    181
def       8980   th    83
nm       cdc   ph
```

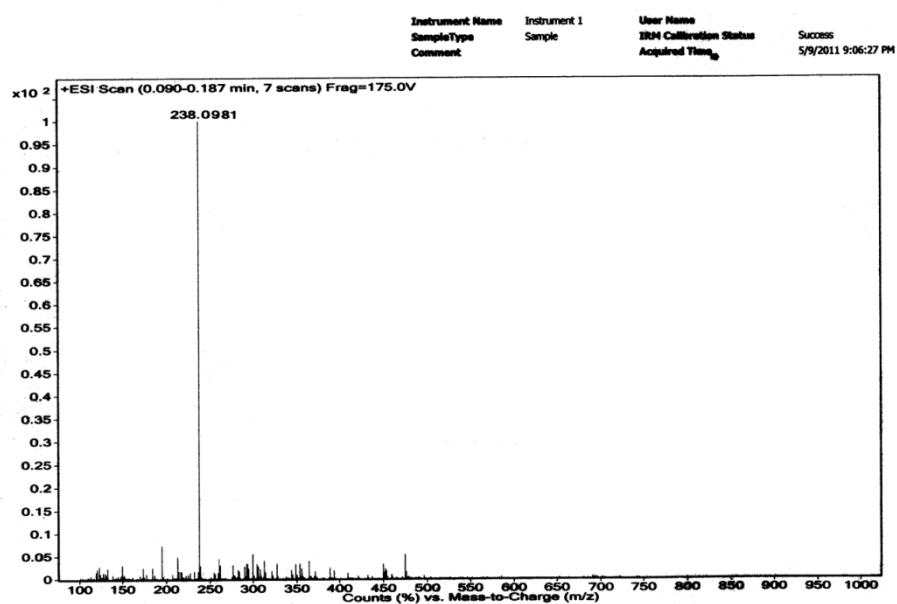


**N,5-Diphenyl-1,3,4-oxadiazol-2-amine (12a):  $^{13}\text{C}$  NMR ( $\text{CD}_3\text{OD} + \text{DMSO}-d_6$ , 100 MHz)**

```
exp1 s2pul
SAMPLE      SPECIAL
date May 2 2011 temp    not used
solvent CD3OD gain     not used
file        exp spin    not used
ACQUISITION t1       1.000   pw98   19.600
            t2       0.000   alfa   20.000
at         1.100   alpha  25125.6   FLAGs
np         25125.6   flags
fb         138000  11   n
bs         1.000   dp     y
nt         16000   hs    nn
ct         16000   PROCESSING
TRANSMITTER lb      2.00
tn         C13     fn    65536
sfreq     100.000  DISPLAY
t0f        1536.3   sp    -266.7
tpwr      61       wp    20384.8
pw        9.300   rfp   4946.7
DECOUPLER H1     rfp   80.6
dn         H1     rfp   -329.7
dof        0        lp    6
de         vvy   PLOT
dm         vvy   wc    250
dpw       42      sc    8
dpwr     8980   th    83
nm       no   ph
```

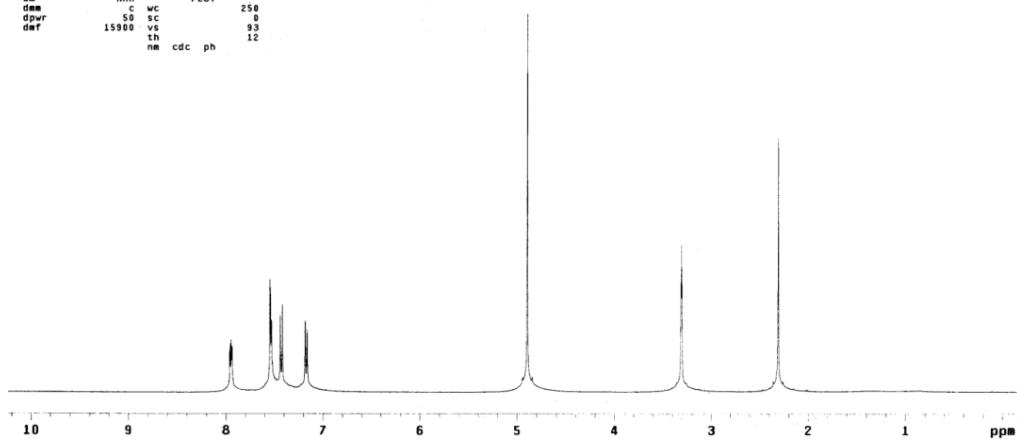


**N,5-Diphenyl-1,3,4-oxadiazol-2-amine (12a): (Mass Spectra)**

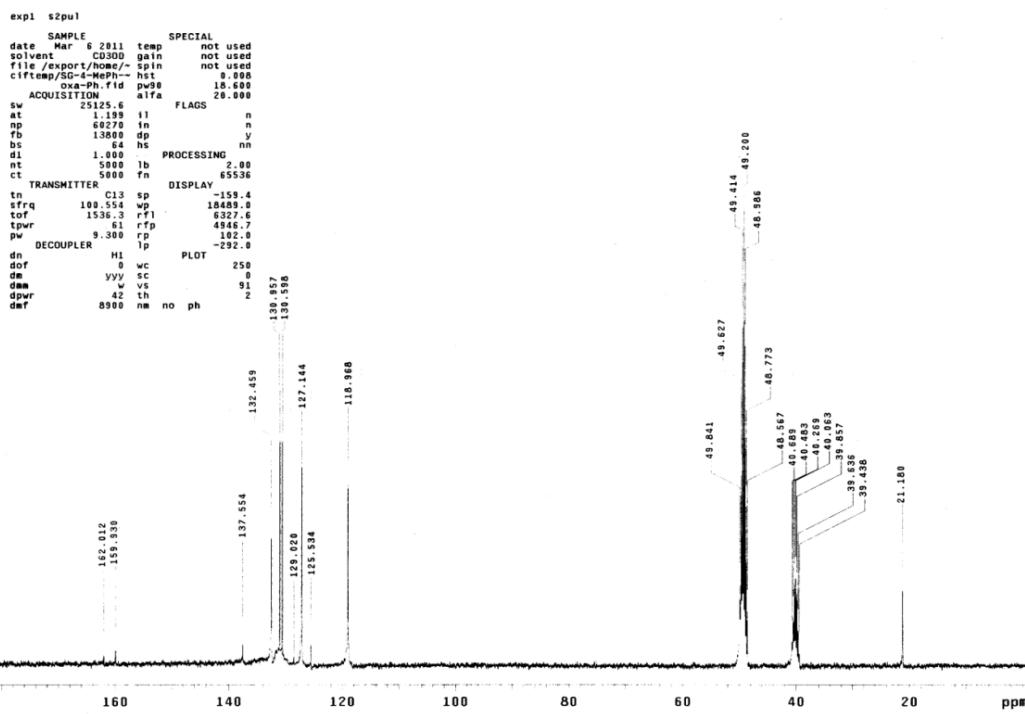


**5-Phenyl-N-p-tolyl-1,3,4-oxadiazol-2-amine (13a):  $^1\text{H}$  NMR (CD<sub>3</sub>OD, 400 MHz)**

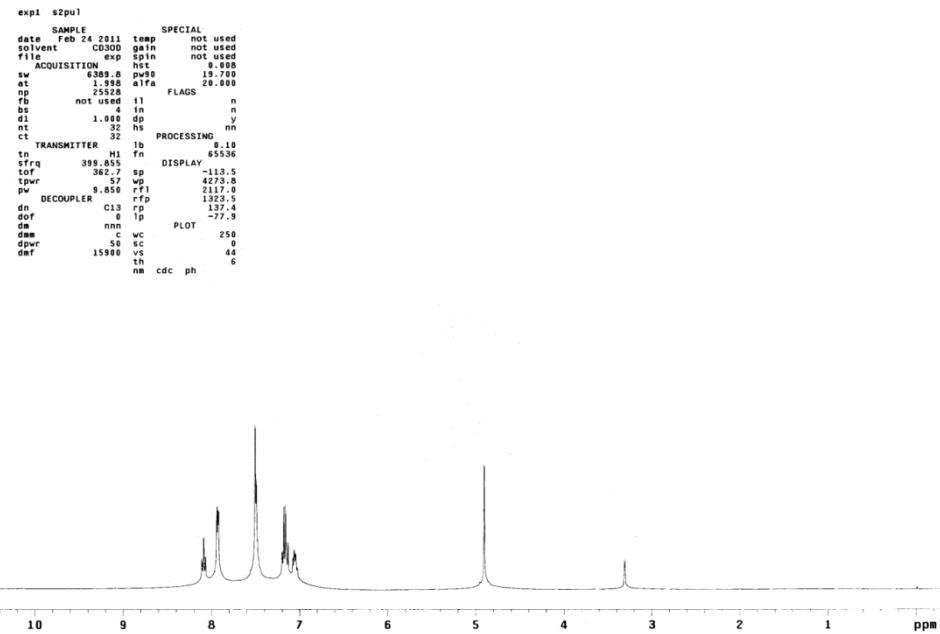
```
exp1 s2pul
SAMPLE          SPECIAL.
date  Feb 24 2011 temp  not used
solvent   CD3OD  gain  not used
rf1off    0.000  not used
ACQUISITION disp  hstn   0.008
sw      6380.00  pw90  15.700
et      1.358  a17a  28.000
np      25528  FLAGS
fb      not used  f1    n
bs      1.000  dp    y
d1      1.000  dp    nn
nt      32      hc    nn
ct      32      PROCESSING
TRANSMITTER 1b    0.10
tn      H1  fn   65536
tffq    399.80  DISPLAY -70.8
tof     362.7  sp    4189.7
tpwr    57      wp    211.2
pw     9.850  rfp   1323.5
DECOUPLER   C13  rfp   147.6
dn      8      tp    -99.1
dof     nm      PLOT
dmm    c      wc    250
dpwr   15900  sc    9.3
def     nm      th    12
nm      cdc  ph
```



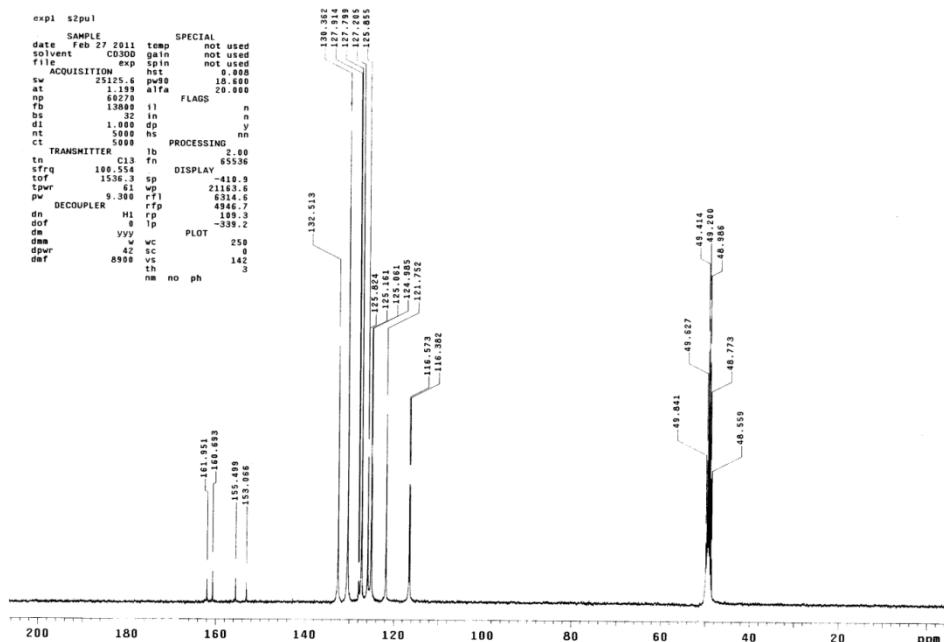
**5-Phenyl-N-p-tolyl-1,3,4-oxadiazol-2-amine (13a):  $^{13}\text{C}$  NMR ( $\text{CD}_3\text{OD} + \text{DMSO}-d_6$ , 100 MHz)**



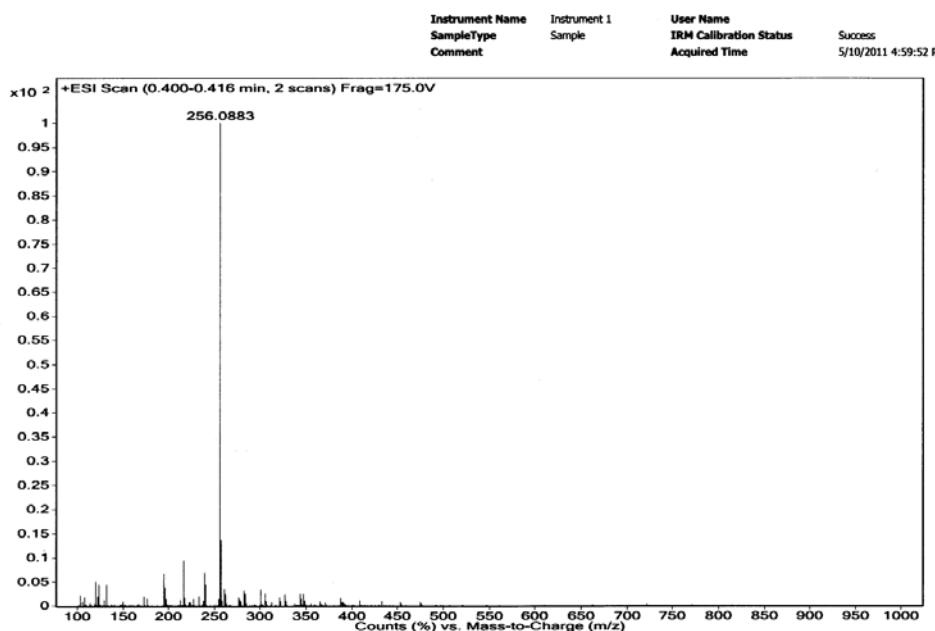
**N-(2-Fluorophenyl)-5-phenyl-1,3,4-oxadiazol-2-amine (14a):  $^1\text{H}$  NMR ( $\text{CD}_3\text{OD}$ , 400 MHz)**



*N*-(2-Fluorophenyl)-5-phenyl-1,3,4-oxadiazol-2-amine (14a):  $^{13}\text{C}$  NMR ( $\text{CD}_3\text{OD}$ , 100 MHz)

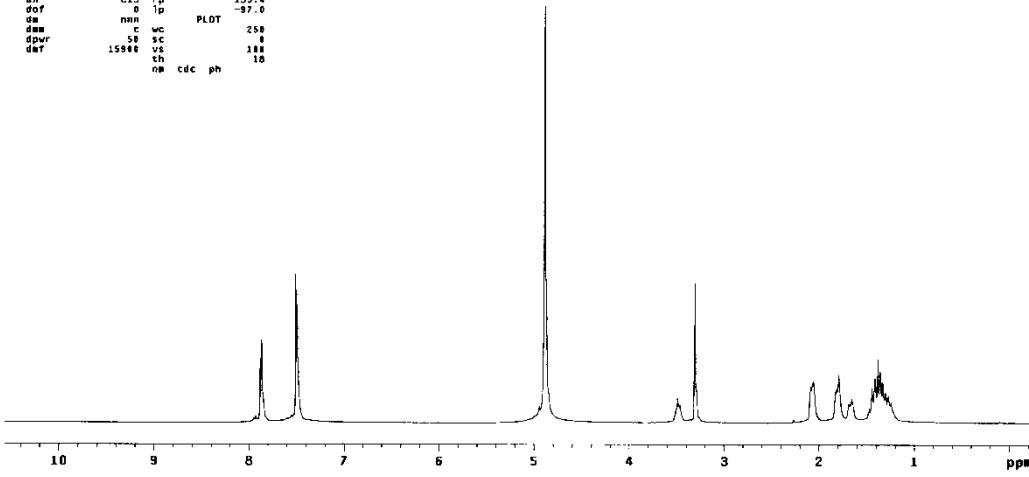


### **N-(2-Fluorophenyl)-5-phenyl-1,3,4-oxadiazol-2-amine (14a): (Mass Spectra)**



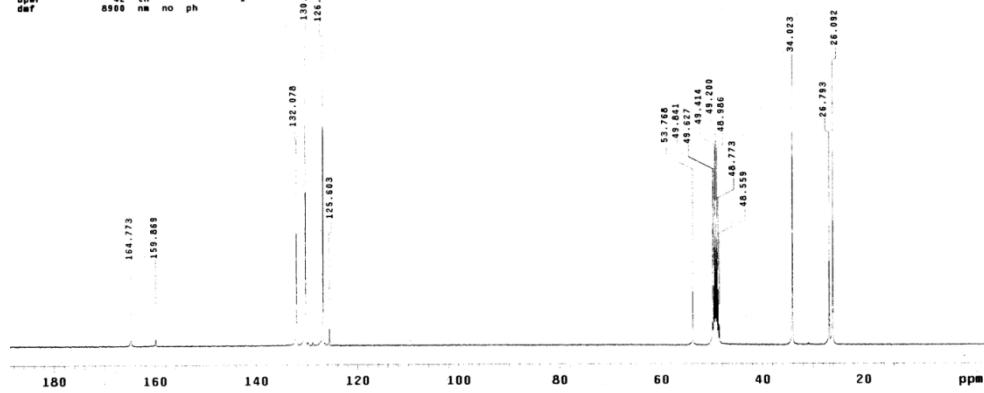
*N*-Cyclohexyl-5-phenyl-1,3,4-oxadiazol-2-amine (15a):  $^1\text{H}$  NMR (CD<sub>3</sub>OD, 400 MHz)

```
expt s2pul
SAMPLE      SPECIAL
date May 13 2011 temp not used
solvent CD3OD gain not used
file      exp spin not used
ACQUISITION 1.000 sec 1.000
sw       6388.6 pw180 19.788
at        1.998 alfa 29.000
zt        25328 flags
tb      not used 11 n
bs         4 in n
di        1.000 dp y
nt        32 hs nn
ct        32 PROCESSING
ct      TRANSMITTER 1b 0.10
tn      H1 fn 65536
sfreq  399.855 DISPLAY
t0f    362.7 sp -113.1
tpwr   65 r1 2116.6
pw     9.659 rfp 1323.5
DECOUPLER C13 rfp 135.4
dof      0 ip -97.0
dm      nnn PLOT
dme      c wc 258
dpwr   58 sc 1
dfr    15998 vs 100
dft    15998 th 10
dop    no cdc ph
```



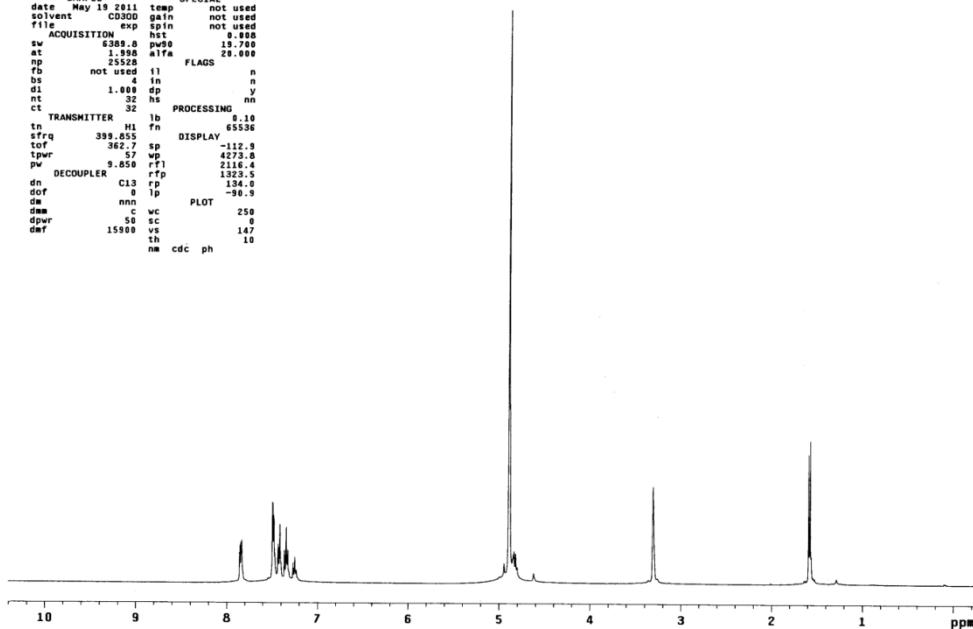
*N*-Cyclohexyl-5-phenyl-1,3,4-oxadiazol-2-amine (15a):  $^{13}\text{C}$  NMR (CD<sub>3</sub>OD, 100 MHz)

```
expt s2pul
SAMPLE      SPECIAL
date May 14 2011 temp not used
solvent CD3OD gain not used
ciftemp/SG=cyclohex- h1s 8.088
file      exp spin not used
ACQUISITION 1.000 sec 2.000
sw       25125.6 pw180 29.000
at        1.998 alfa 65536
zt        25328 flags
tb      not used 11 n
bs         68270 in n
fb        13808 dp y
di        1.000 hs nn
dt        1.000 PROCESSING
nt        10000 lb 2.00
zf        10000 fn 65536
ct      TRANSMITTER DISPLAY
tn      C13 sp -443.1
sfreq  104.773 pw180 100.000
t0f    1536.3 rfp 6313.8
tpwr   61 rfp 4946.7
pw     9.398 ip 22.5
d0f    10000 PLOT
dme      v wc 258
dme      v vs 56
dpwr   42 th 1
dfr    8500 nm no ph
```



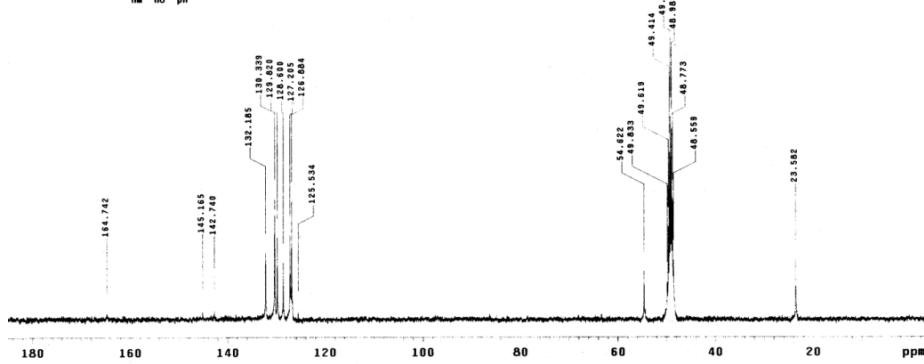
(R)-5-Phenyl-N-(1-phenylethyl)-1,3,4-oxadiazol-2-amine (16a):  $^1\text{H}$  NMR (CD<sub>3</sub>OD, 400 MHz)

```
expt s2pul
SAMPLE      SPECIAL
date May 19 2011 temp not used
solvent CD3OD  gain not used
file      exp  gain not used
ACQUISITION hst  0.008
sw       2500.0  sp  100.0
at       1.000  a1fa 20.000
np      25528  flags
tr       0.000  t1  n
bs       4  in  n
d1      1.000  dp  y
rt      0.000  hs  nm
ct      32  PROCESSING 0.10
tn  TRANSMITTER 1b  PROCESSING 0.10
fn      H1  fn  65536
sfrq    399.855  DISPLAY
t0f     362.7  sp  -112.8
t0r     359.5  sp  44.0
pw      9.850  rfp  2116.4
DECOUPLER C13  rfp  1323.5
dn      C13  1p  1323.5
dof     0  1p  -98.5
de      nnn  PLOT
dm      c  wc  250
dpwv   50  sc  0
dmf    15900  vs  147
dt      0  th  10
nm  cdc ph
```



(R)-5-Phenyl-N-(1-phenylethyl)-1,3,4-oxadiazol-2-amine (16a):  $^{13}\text{C}$  NMR (CD<sub>3</sub>OD, 100 MHz)

```
SPECIAL
date May 14 2011 temp not used
solvent CD3OD  gain not used
file      exp  gain not used
ACQUISITION hst  0.008
sw       25125.6  pw90  18.400
t0f     6027.0  sp  374.5
t0r     5994.0  sp  19148.2
pw      9.300  rfp  6311.5
DECOUPLER C13  rfp  448.5
dn      H1  1p  49.5
dof     0  1p  -319.0
de      v  wc  250
dm      v  tc  54.0
dpwv   42  sc  0
dmf    8500  vs  147
dt      0  th  2
nm  no ph
```



**(R)-5-Phenyl-N-(1-phenylethyl)-1,3,4-oxadiazol-2-amine (16a): (Mass Spectra)**

Instrument Name	Instrument 1	User Name
SampleType	Sample	IRM Calibration Status
Comment	Acquired Time	Success

