

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

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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. ¹H NMR (400 MHz) and ¹³C 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*_α radiation ($\lambda = 0.71073 \text{ \AA}$) at 298 K. Cell parameters were retrieved using SMART ¹USA, 1995 software and refined with SAINT¹ 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.² The structures were solved by direct methods implemented in the SHELX-97³ 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.

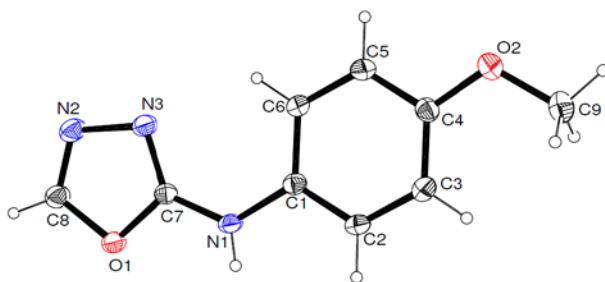


Fig. 2 ORTEP view of *N*-(4-Methoxyphenyl)-1,3,4-oxadiazol-2-amine (**4a**).

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

$C_9H_9N_3O_2$, crystal dimensions 0.38 x 0.32 x 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, $\alpha = 84.312(6)^\circ$, $\beta = 86.837(6)^\circ$, $\gamma = 76.573(7)^\circ$, $V = 902.56(16)$ Å³, $Z = 4$, $\rho_{\text{calcd}} = 1.407$ mg/m³, $\mu = 0.103$ mm⁻¹, $F(000) = 400.0$, 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.

Spectral Data

***N*-Phenyl-1,3,4-oxadiazol-2-amine (1a):** Pinkish solid; M.p. 149-150 °C (Lit. M.p. 153-154 °C).⁴ ¹H NMR (400 MHz, CDCl₃): 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. ¹³C NMR (100 MHz, CDCl₃): 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⁻¹. C₈H₇N₃O (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. ¹H NMR (400 MHz, CD₃OD): 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. ¹³C NMR (100 MHz, CD₃OD): 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⁻¹. C₉H₉N₃O (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. ¹H NMR (400 MHz, CD₃OD): δ = 3.91 (s, 3H), 6.94-7.07 (m, 3H), 7.95 (d, 1H, *J* = 8 Hz), 8.46 (s, 1H) ppm. ¹³C NMR (100 MHz, CD₃OD): 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⁻¹. C₉H₉N₃O₂ (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. ¹H NMR (400 MHz, CD₃OD): 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. ¹³C NMR (100 MHz, CD₃OD): 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⁻¹. C₉H₉N₃O₂ (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. ¹H NMR (400 MHz, CD₃OD): 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. ¹³C NMR (100 MHz, CD₃OD): 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 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. ^1H NMR (400MHz, CD_3OD): δ = 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}C NMR (100 MHz, CD_3OD): δ = 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 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. ^1H NMR (400 MHz, CD_3OD): δ = 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}C NMR (100 MHz, CD_3OD): δ = 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 cm^{-1} . HRMS (ESI): calcd. for $\text{C}_8\text{H}_6\text{ClN}_3\text{O}$ (MH^+) 196.0272; found 196.0278.

***N*-(4-Bromophenyl)-1,3,4-oxadiazol-2-amine (8a)**: Pink solid; M.p. 167-169 °C. ^1H NMR (400 MHz, CD_3OD): δ = 7.38-7.44 (m, 4 H), 8.45 (s, 1H) ppm. ^{13}C NMR (100 MHz, CD_3OD): δ = 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 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. ^1H NMR (400 MHz, CD_3OD): δ = 7.53 (t, 1H, J = 8.4 Hz), 7.83 (m, 2H), 8.52 (m, 3H) ppm. ^{13}C NMR (100 MHz, CD_3OD): δ = 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 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 $\text{C}_8\text{H}_6\text{N}_4\text{O}_3$ (MH^+) 207.0513; found 207.0523.

***N*-(4-(Trifluoromethyl)phenyl)-1,3,4-oxadiazol-2-amine (10a)**: White solid; M.p. 166-169 °C. ^1H NMR (400 MHz, CD_3OD): δ = 7.59 (d, 2H, J = 8.4 Hz), 7.69 (d, 2H, J = 8.4 Hz), 8.51 (s, 1H) ppm. ^{13}C NMR (100 MHz, CD_3OD): δ = 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^{-1} . $\text{C}_9\text{H}_6\text{F}_3\text{N}_3\text{O}$ (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 $\text{C}_9\text{H}_6\text{F}_3\text{N}_3\text{O}$ (MH^+) 230.0536; found 230.0539.

***N*-(Naphthalen-1-yl)-1,3,4-oxadiazol-2-amine (11a)**: Black solid; M.p. 136-139 °C. ^1H NMR (400 MHz, CD_3OD): 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. ^{13}C NMR (100 MHz, CD_3OD): 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^{-1} . $\text{C}_{12}\text{H}_9\text{N}_3\text{O}$ (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 $\text{C}_{12}\text{H}_9\text{N}_3\text{O}$ (MH^+) 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). ^5H NMR (400 MHz, CD_3OD): 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. ^{13}C NMR (100 MHz, CD_3OD + $\text{DMSO-}d_6$): 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^{-1} . $\text{C}_{14}\text{H}_{11}\text{N}_3\text{O}$ (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 $\text{C}_{14}\text{H}_{11}\text{N}_3\text{O}$ (MH^+) 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). ^6H NMR (400 MHz, CD_3OD): 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. ^{13}C NMR (100 MHz, CD_3OD + $\text{DMSO-}d_6$): 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^{-1} . $\text{C}_{15}\text{H}_{13}\text{N}_3\text{O}$ (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. ^1H NMR (400 MHz, CD_3OD): 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. ^{13}C NMR (100 MHz, CD_3OD): 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

cm⁻¹. C₁₄H₁₀FN₃O (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 C₁₄H₁₀FN₃O (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).⁷ ¹H NMR (400 MHz, CD₃OD): δ = 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 ¹³C NMR (100 MHz, CD₃OD): δ = 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 cm⁻¹. C₁₄H₁₇N₃O (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).⁷ ¹H NMR (400 MHz, CD₃OD): δ = 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. ¹³C NMR (100 MHz, CD₃OD): δ = 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 cm⁻¹. C₁₆H₁₅N₃O (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 C₁₆H₁₅N₃O (MH⁺) 266.1288; found 266.1293.

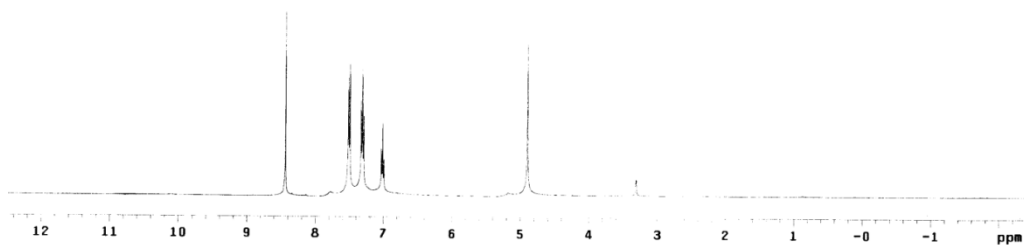
References:

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SPECTRA

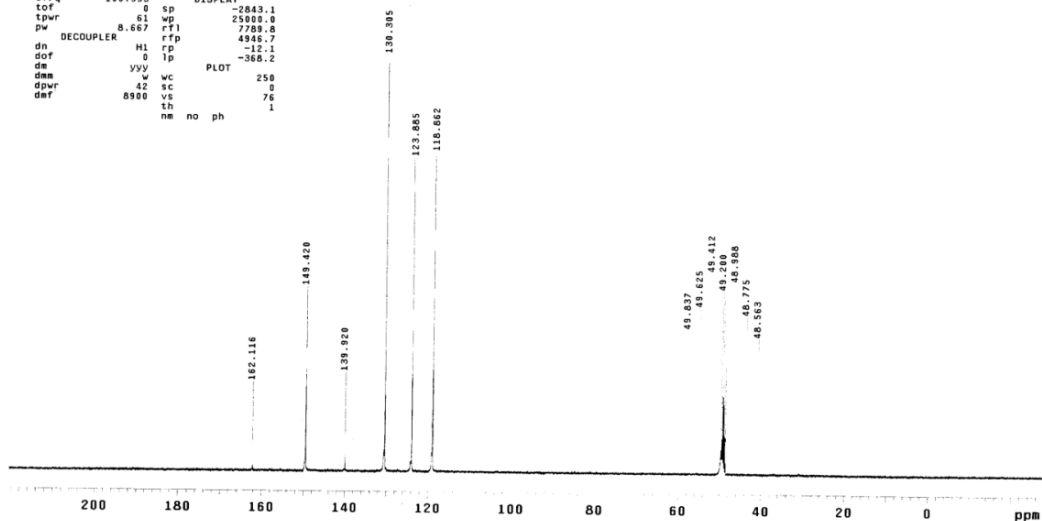
N-Phenyl-1,3,4-oxadiazol-2-amine (1a): ^1H NMR (CD_3OD , 400 MHz)

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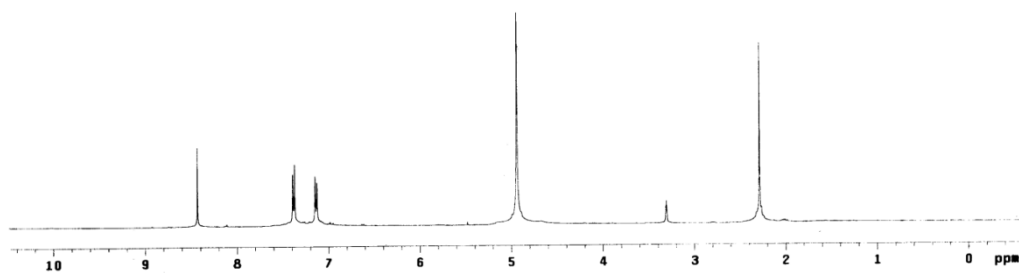
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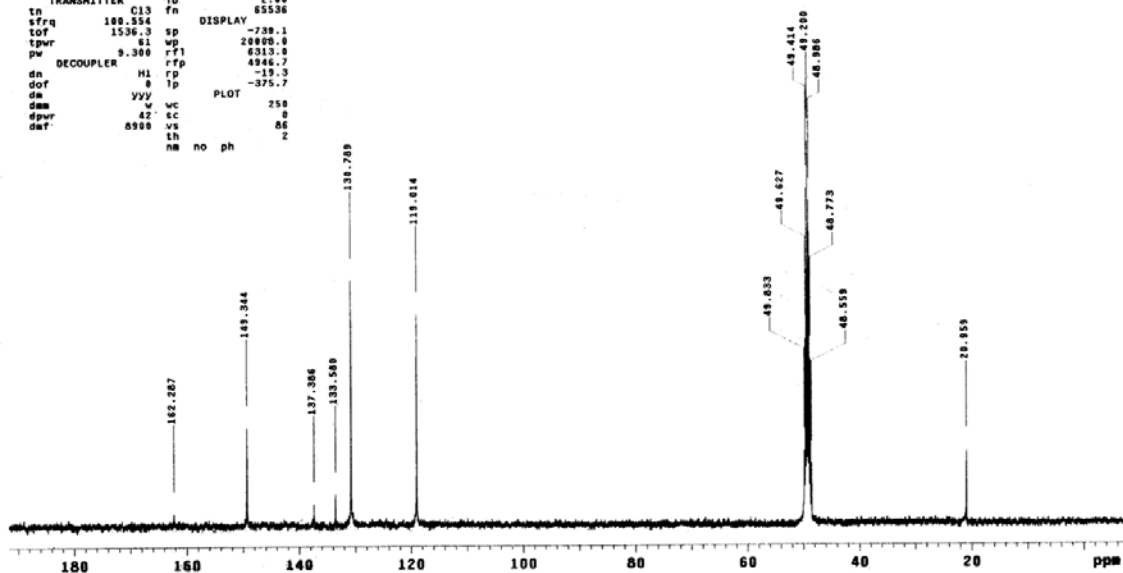
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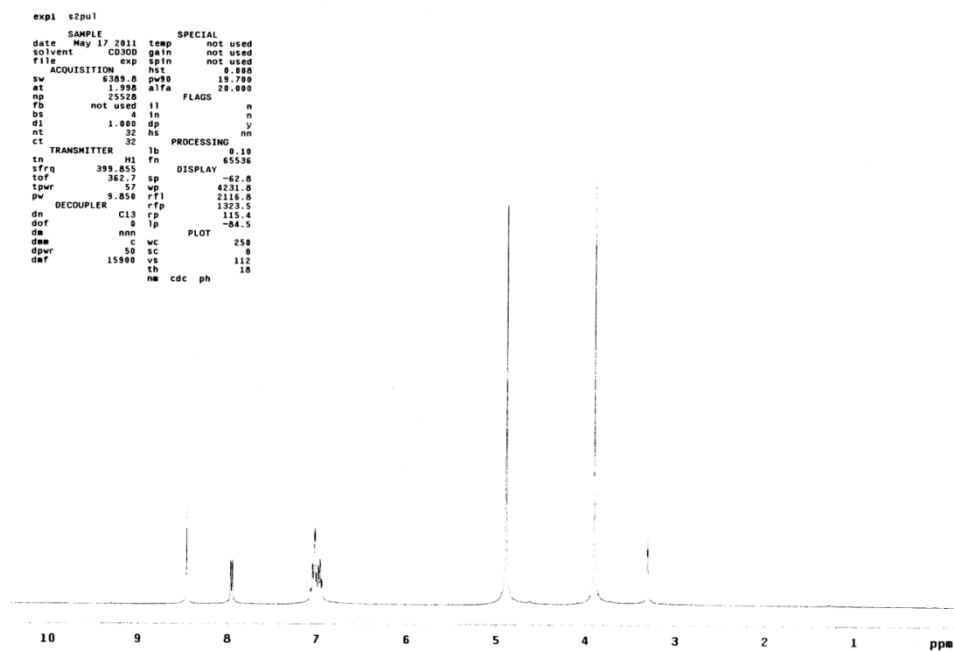


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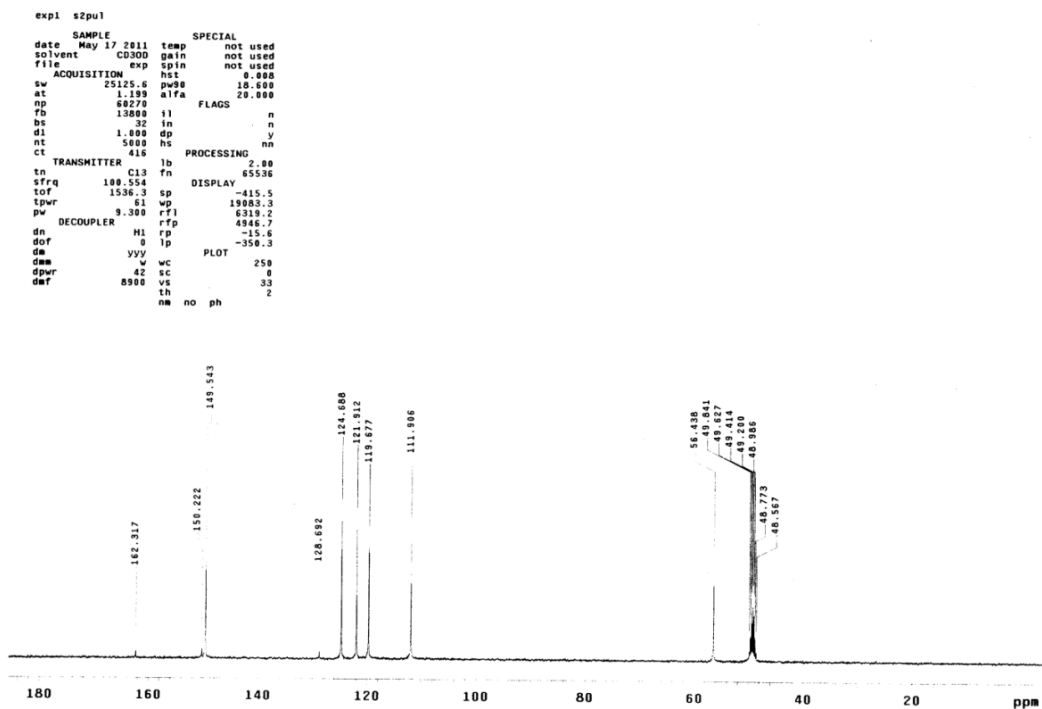
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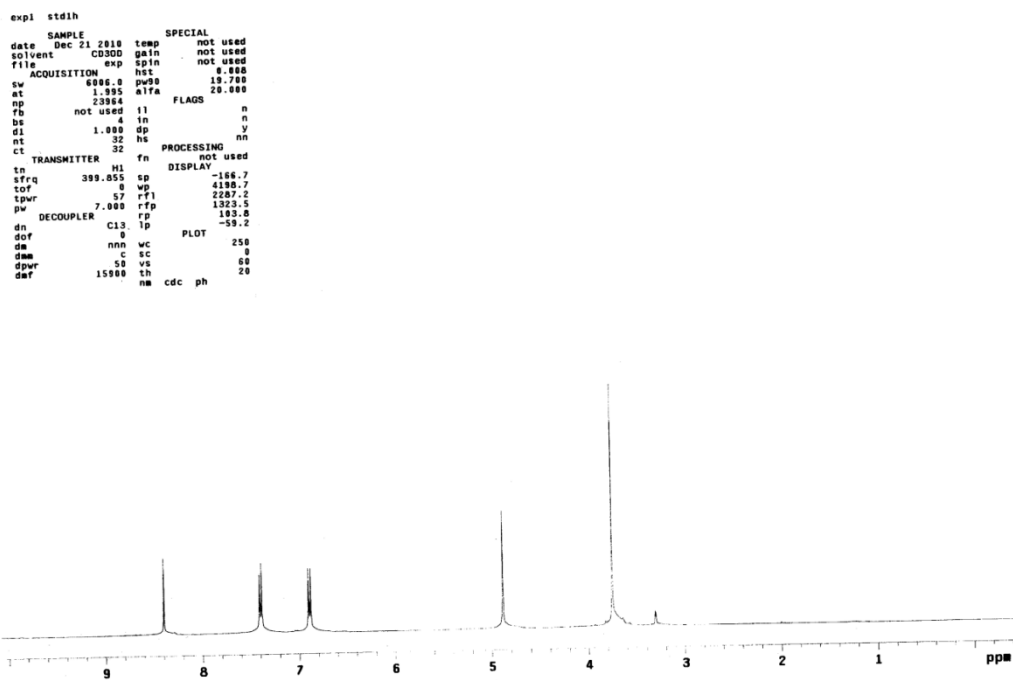
N-(2-Methoxyphenyl)-1,3,4-oxadiazol-2-amine (3a): ^1H NMR (CD_3OD , 400 MHz)



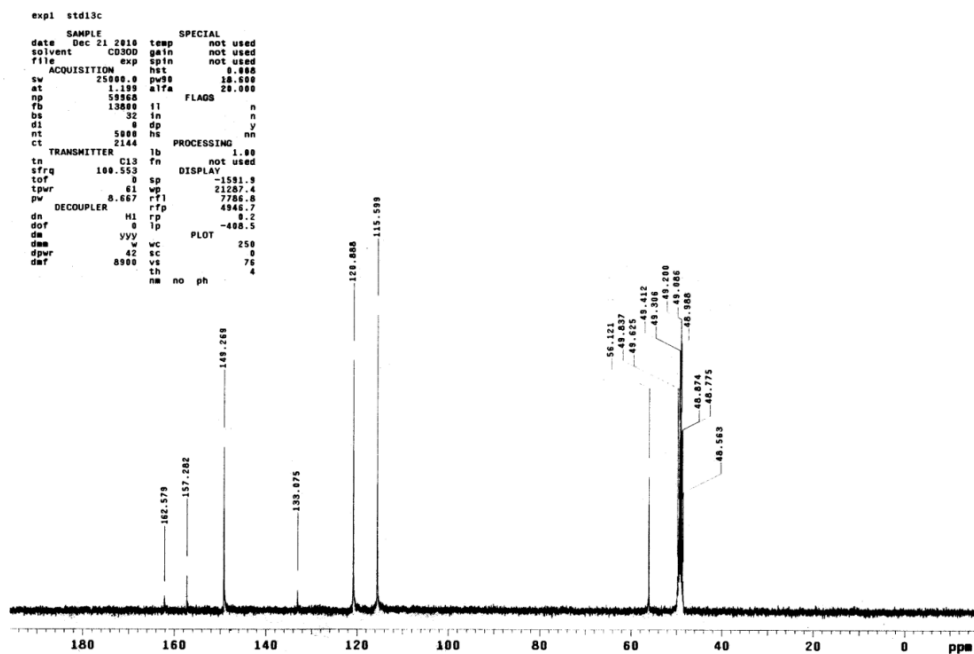
N-(2-Methoxyphenyl)-1,3,4-oxadiazol-2-amine (3a): ^{13}C NMR (CD_3OD , 100 MHz)



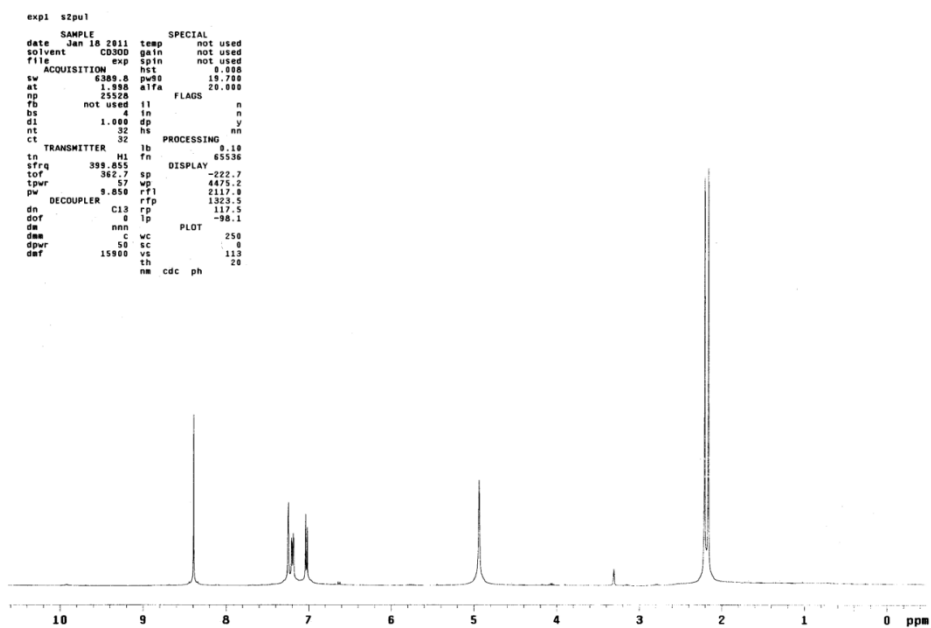
N-(4-Methoxyphenyl)-1,3,4-oxadiazol-2-amine (4a): ^1H NMR (CD_3OD , 400 MHz)



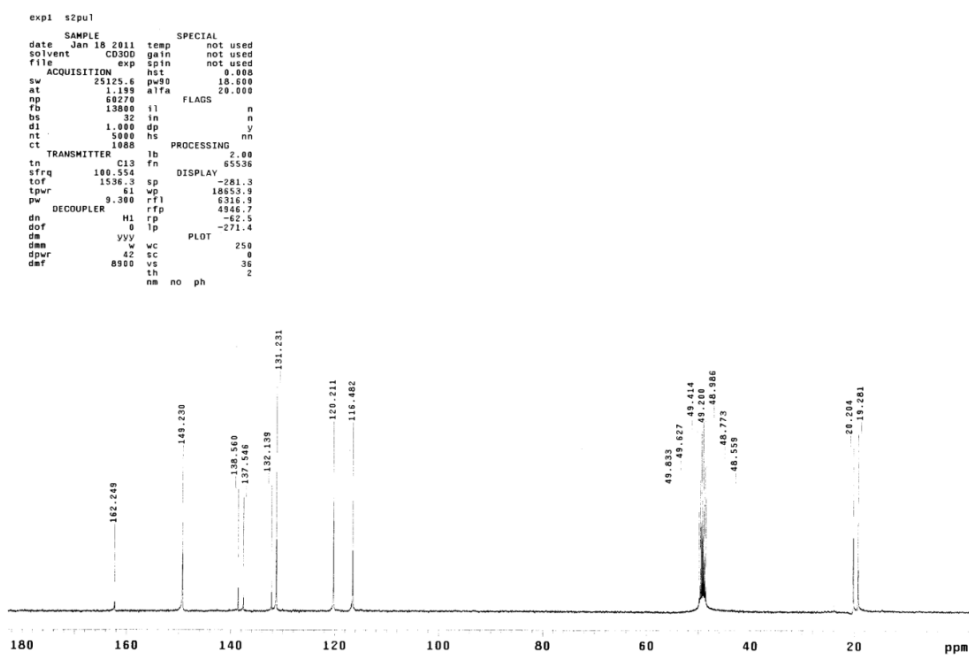
N-(4-Methoxyphenyl)-1,3,4-oxadiazol-2-amine (4a): ^{13}C NMR (CD_3OD , 100 MHz)



***N*-(3,4-Dimethylphenyl)-1,3,4-oxadiazol-2-amine (5a): ¹H NMR (CD₃OD, 400 MHz)**

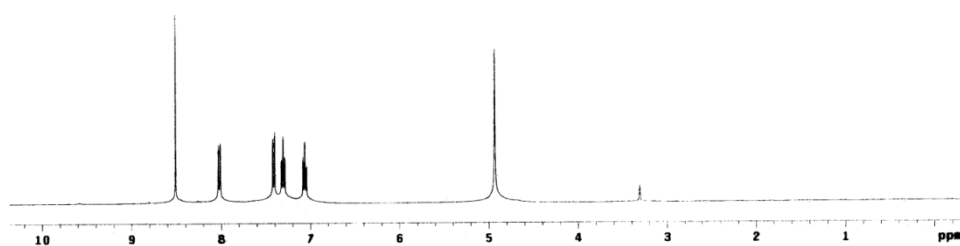


***N*-(3,4-Dimethylphenyl)-1,3,4-oxadiazol-2-amine (5a): ¹³C NMR (CD₃OD, 100 MHz)**



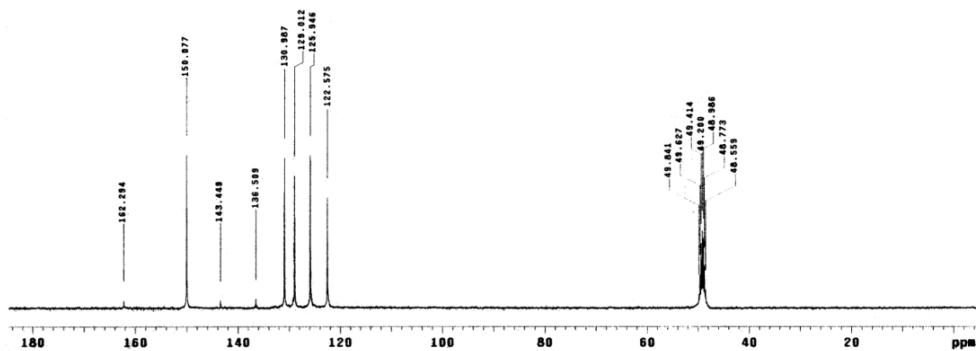
N-(2-Chlorophenyl)-1,3,4-oxadiazol-2-amine (6a): ^1H NMR (CD_3OD , 400 MHz)

```
exp1 szpu1
SAMPLE
date Jan 19 2011 temp not used
solvent CD3OD gain not used
file ACQUISITION exp spin not used
sw 6389.8 pu98 19.700
at 1.950 a1fa 28.488
np 25528 FLAGS n
fb not used i1 n
bs not used i1 n
d1 1.000 dp y
nt 32 hs nn
ct TRANSMITTER 32 PROCESSING 8.10
tn H1 fn 65536
sfrq 399.855 DISPLAY -137.9
tof 362.7 sp 4282.1
tpwr 9.850 rF1 2116.2
pw DECOUPLER C13 rfp 1323.5
dn H1 rp 123.7
dof 0 lp -88.5
dm nnn PLOT 250
dms c wc 0
dpr 15800 vs 0
drt nm th 20
nm cdc ph
```



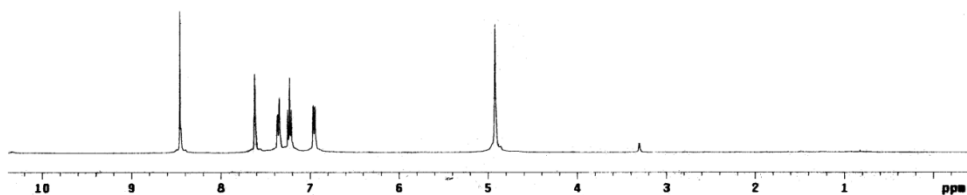
N-(2-Chlorophenyl)-1,3,4-oxadiazol-2-amine (6a): ^{13}C NMR (CD_3OD , 100 MHz)

```
exp1 szpu1
SAMPLE
date Jan 19 2011 temp not used
solvent CD3OD gain not used
file ACQUISITION exp spin not used
sw 25123.6 pu98 18.800
at 1.159 a1fa 28.488
np 68270 FLAGS n
fb 13000 i1 n
bs 32 i1 n
d1 1.000 dp y
nt 5000 hs nn
ct TRANSMITTER 1668 PROCESSING 2.00
tn C13 fn 65536
sfrq 100.624 DISPLAY -512.9
tof 1536.3 sp 19883.3
tpwr 9.300 rF1 6317.6
pw DECOUPLER H1 rfp 4946.7
dn H1 rp 36.5
dof 0 lp -375.3
dm vvv PLOT 250
dms c wc 0
dpr 8900 vs 33
drt nm th 2
nm no ph
```



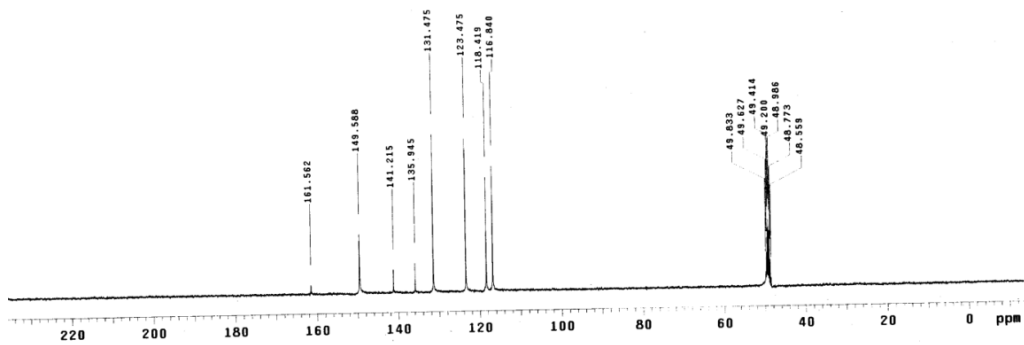
N-(3-Chlorophenyl)-1,3,4-oxadiazol-2-amine (7a): ¹H NMR (CD₃OD, 400 MHz)

```
exp1 s2pul
SAMPLE
date Jan 7 2011 temp SPECIAL
solvent CD300 gain not used
file exp spin not used
ACQUISITION hst 0.000
sw 6360.0 pw90 13.700
at 1.990 a1Fa 20.000
np 25520 FLAGS n
fb not used i1 n
bs 32 in n
d1 1.000 dp y
nt 32 hs nm
ct
TRANSMITTER 32 PROCESSING 0.10
tn H1 fn 65536
sfrq 300.855 DISPLAY 65536
tof 362.7 sp -163.0
tpwr 57 wp 6315.7
pw 9.050 rF1 2116.2
DECOUPLER rFp 1323.5
dn C13 rFp 130.0
dof 0 lp -100.0
dm nnn PLOT
dwm c wc 250
dpr 50 sc 0
daf 15000 vs 37
nm cdc ph 20
```

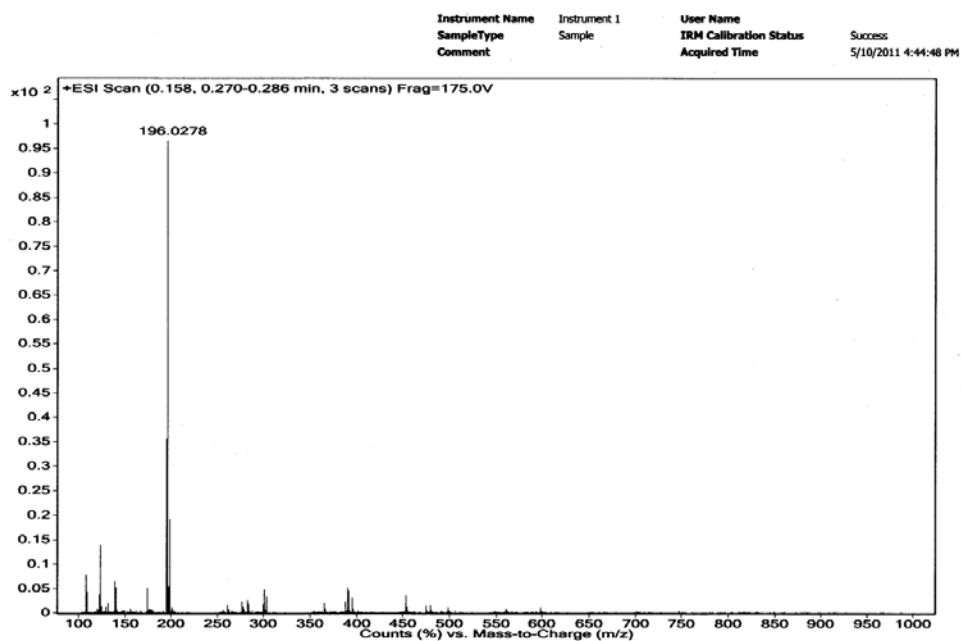


N-(3-Chlorophenyl)-1,3,4-oxadiazol-2-amine (7a): ¹³C NMR (CD₃OD, 100 MHz)

```
exp1 s2pul
SAMPLE
date Jan 7 2011 temp SPECIAL
solvent CD300 gain not used
file exp spin not used
ACQUISITION hst 0.000
sw 25125.6 pw90 10.000
at 1.190 a1Fa 20.000
np 60270 FLAGS n
fb 13000 i1 n
bs 32 in n
d1 1.000 dp y
nt 5000 hs nm
ct
TRANSMITTER 544 PROCESSING 2.00
tn C13 fn 65536
sfrq 100.554 DISPLAY 65536
tof 1536.3 sp -1374.0
tpwr 61 wp 25125.6
pw 9.300 rF1 6320.7
DECOUPLER rFp 4946.7
dn H1 rFp 17.4
dof 0 lp -420.3
dm yyy PLOT
dwm c wc 250
dpr 42 sc 0
daf 8900 vs 30
nm no ph 2
```

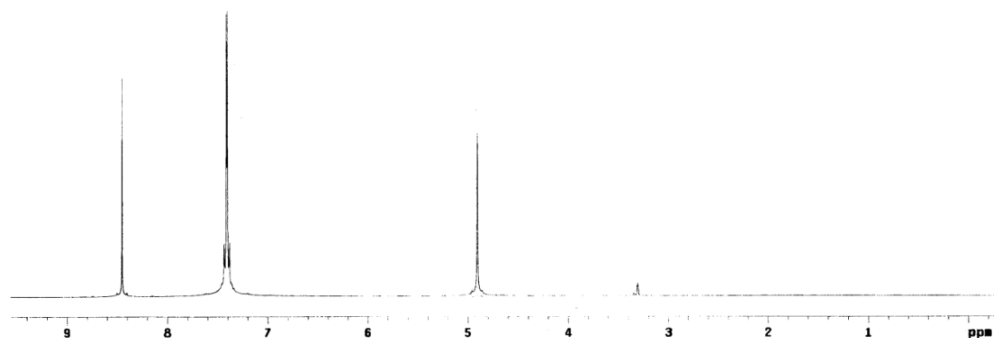


N-(3-Chlorophenyl)-1,3,4-oxadiazol-2-amine (7a): (Mass Spectra)

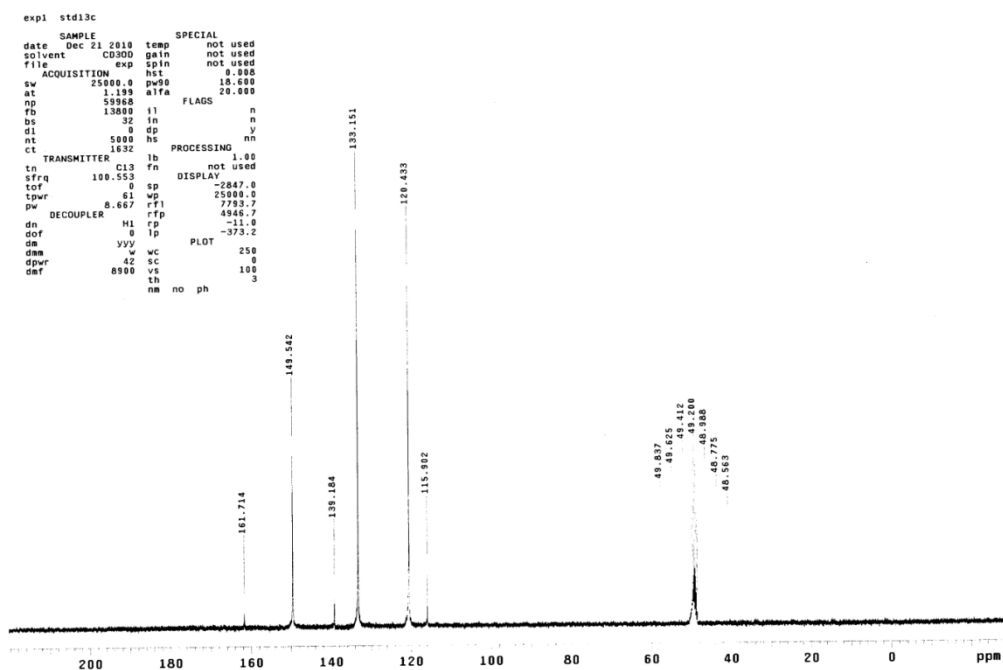


N-(4-Bromophenyl)-1,3,4-oxadiazol-2-amine (8a): ¹H NMR (CD₃OD, 400 MHz)

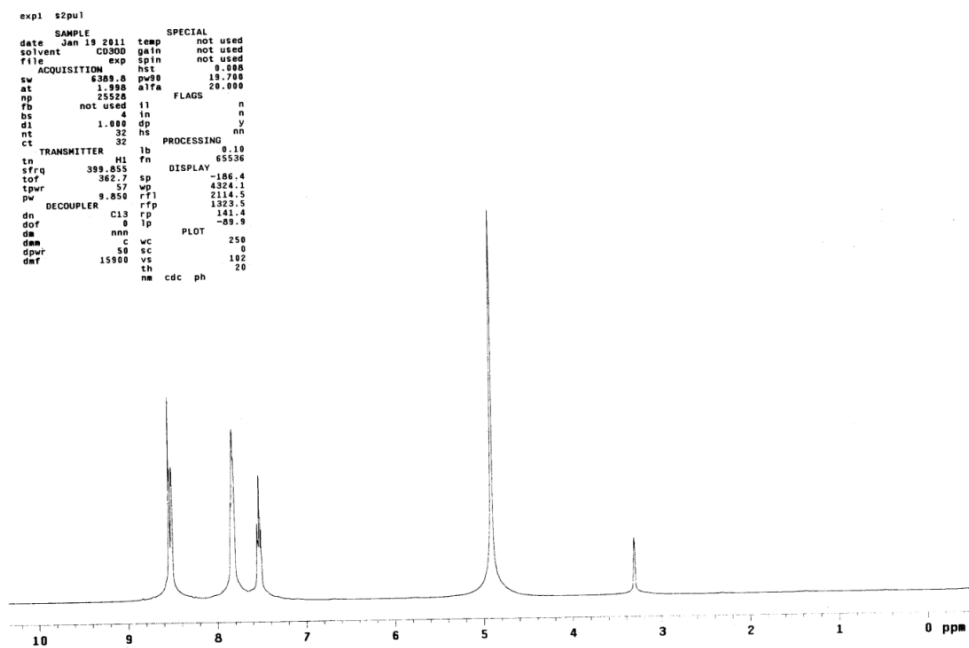
```
expl stdih
SAMPLE
date Dec 21 2010 temp SPECIAL not used
solvent CD300 gain not used
file exp spin not used
ACQUISITION hst 0.000
sw 6000.0 pw90 13.700
at 1.995 altfa 20.000
np 23964 FLAGS n
fb not used i1 n
bs 4 in n
d1 1.000 dp y
nt 32 hs nn
ct 32 fn PROCESSING nn
TRANSMITTER H1 not used
tn 399.855 sp DISPLAY -112.1
tof 0 wp 3930.0
tpwr 57 rfl 2287.0
pw 7.000 rfp 1323.5
DECOUPLER C13 rp 112.0
dn 0 lp -81.2
dof 0 nnn wc PLOT 250
dm c sc 0
dpr 50 vs 73
dprf 15900 tn 20
dpr nm cdc ph
```



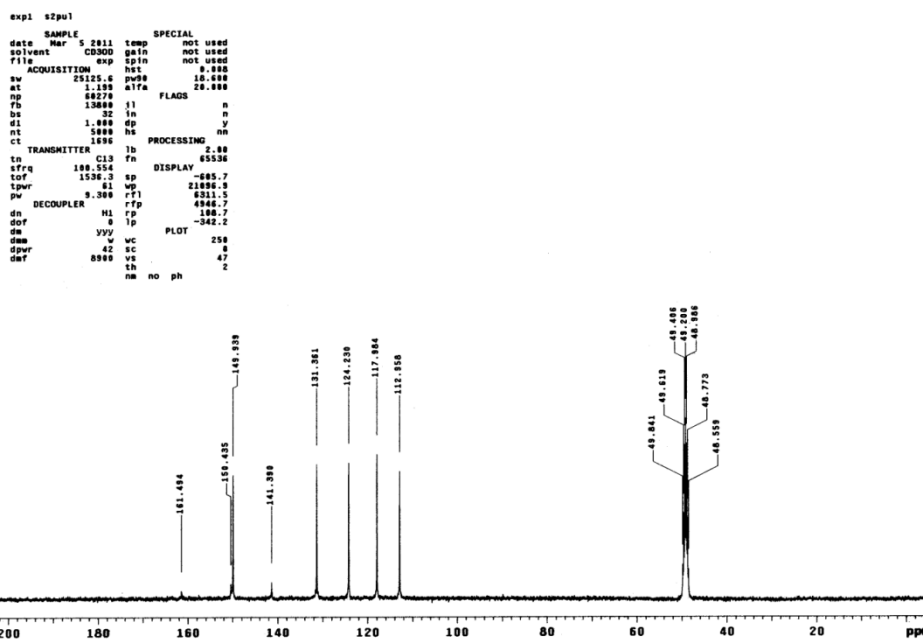
***N*-(4-Bromophenyl)-1,3,4-oxadiazol-2-amine (8a): ¹³C NMR (CD₃OD, 100 MHz)**



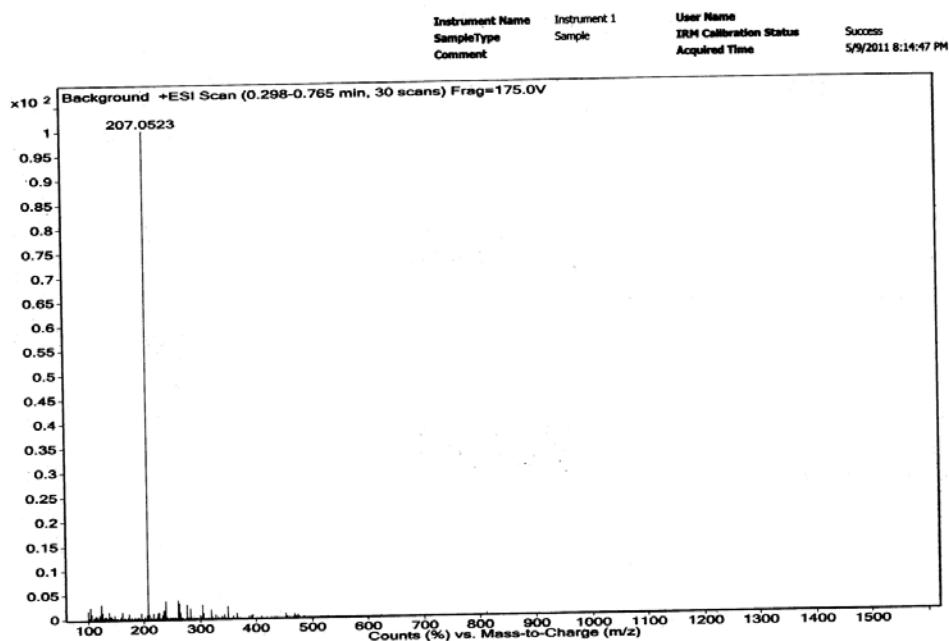
***N*-(3-Nitrophenyl)-1,3,4-oxadiazol-2-amine (9a): ¹H NMR (CD₃OD, 400 MHz)**



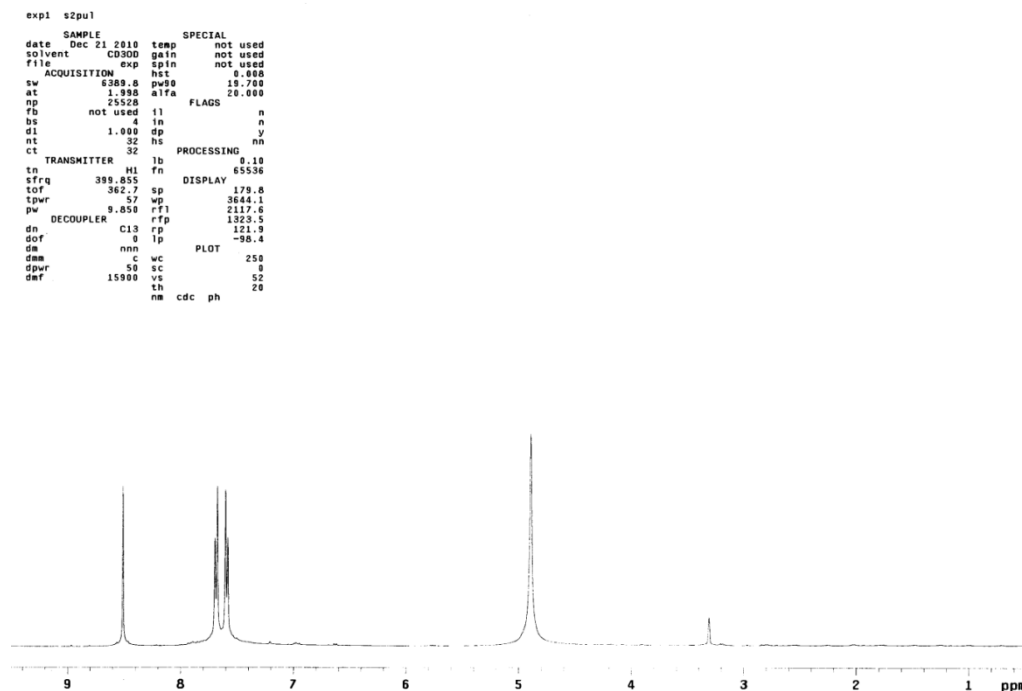
N-(3-Nitrophenyl)-1,3,4-oxadiazol-2-amine (9a): ^{13}C NMR (CD_3OD , 100 MHz)



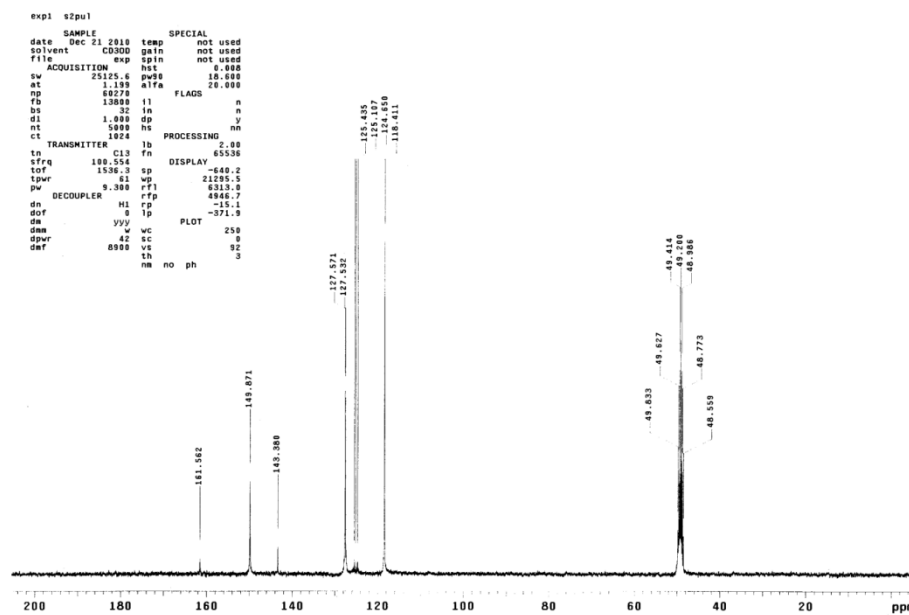
N-(3-Nitrophenyl)-1,3,4-oxadiazol-2-amine (9a): (Mass Spectra)



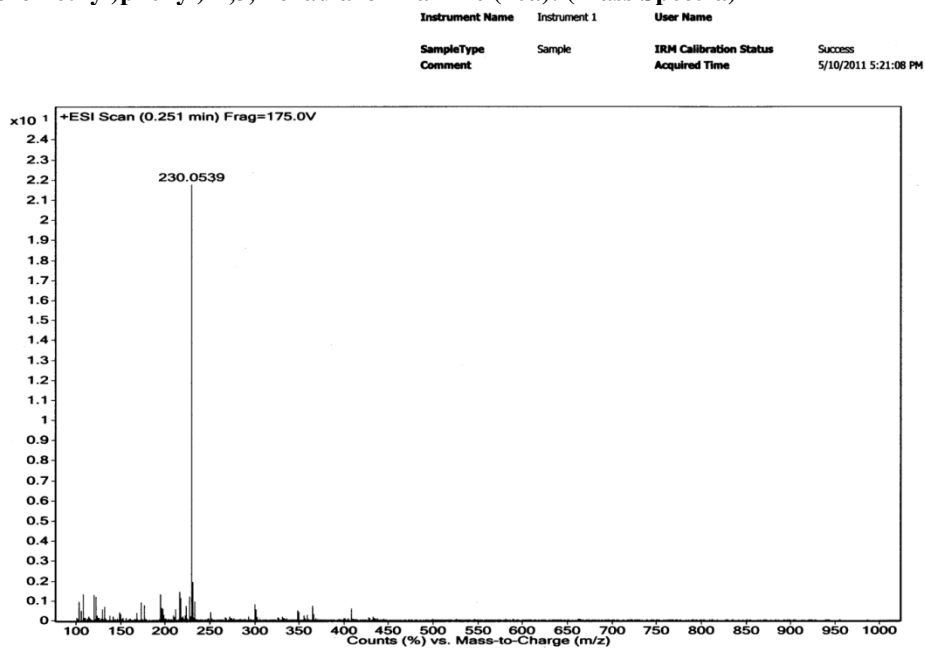
N-(4-(Trifluoromethyl)phenyl)-1,3,4-oxadiazol-2-amine (10a): ¹H NMR (CD₃OD, 400 MHz)



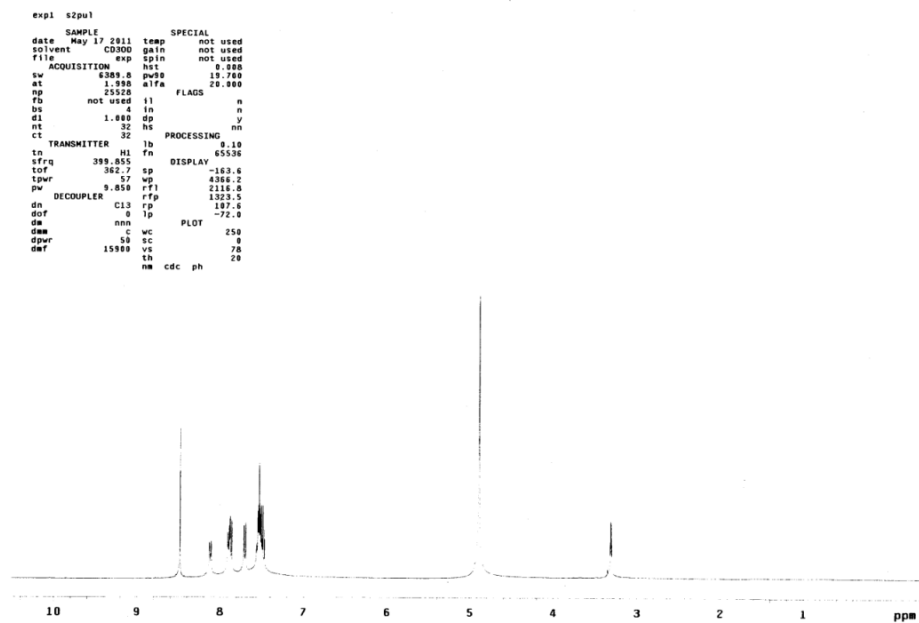
N-(4-(Trifluoromethyl)phenyl)-1,3,4-oxadiazol-2-amine (10a): ¹³C NMR (CD₃OD, 100 MHz)



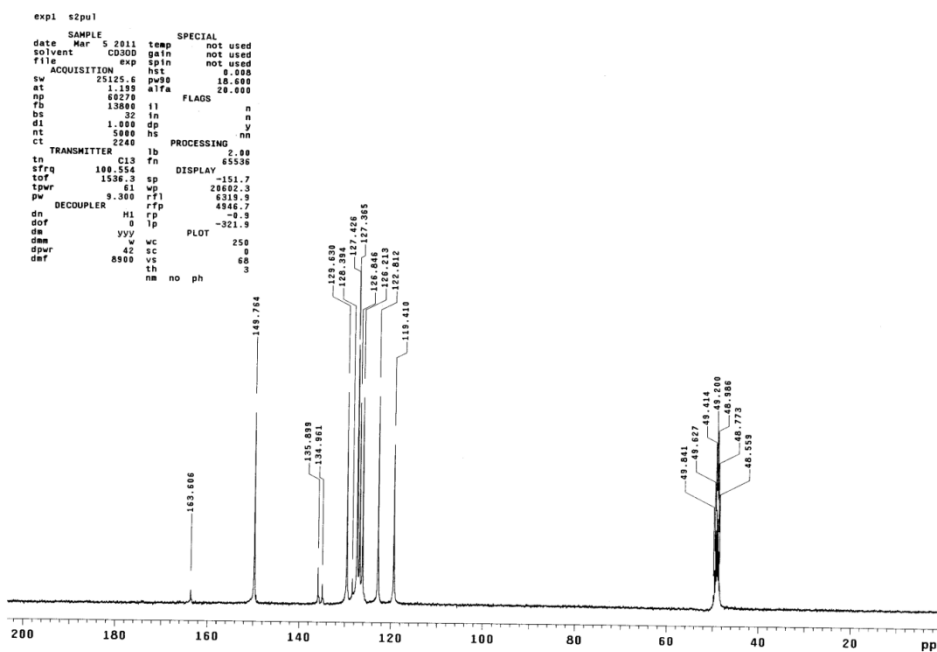
N-(4-(Trifluoromethyl)phenyl)-1,3,4-oxadiazol-2-amine (10a): (Mass Spectra)



N-(Naphthalen-1-yl)-1,3,4-oxadiazol-2-amine (11a): ¹H NMR (CD₃OD, 400 MHz)



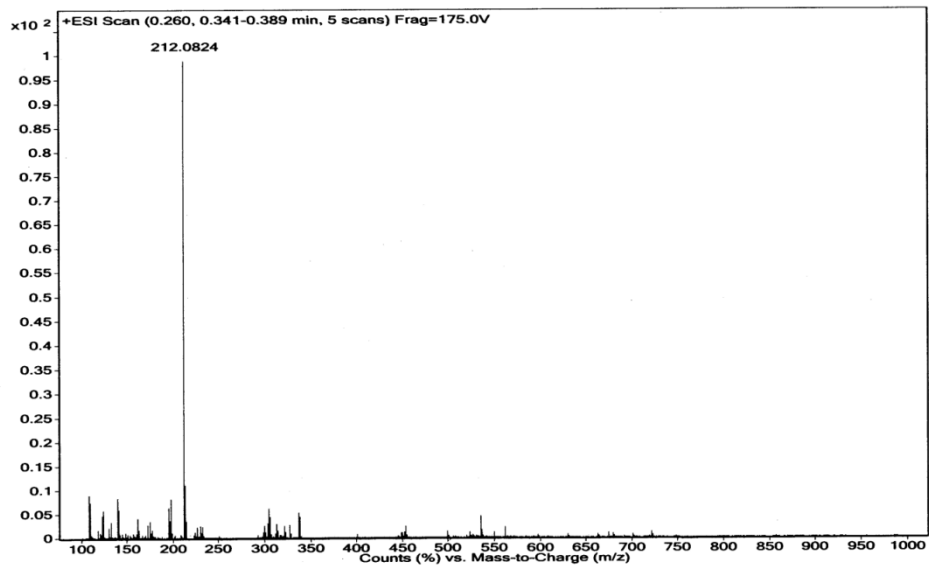
N-(Naphthalen-1-yl)-1,3,4-oxadiazol-2-amine (11a): ^{13}C NMR (CD_3OD , 100 MHz)



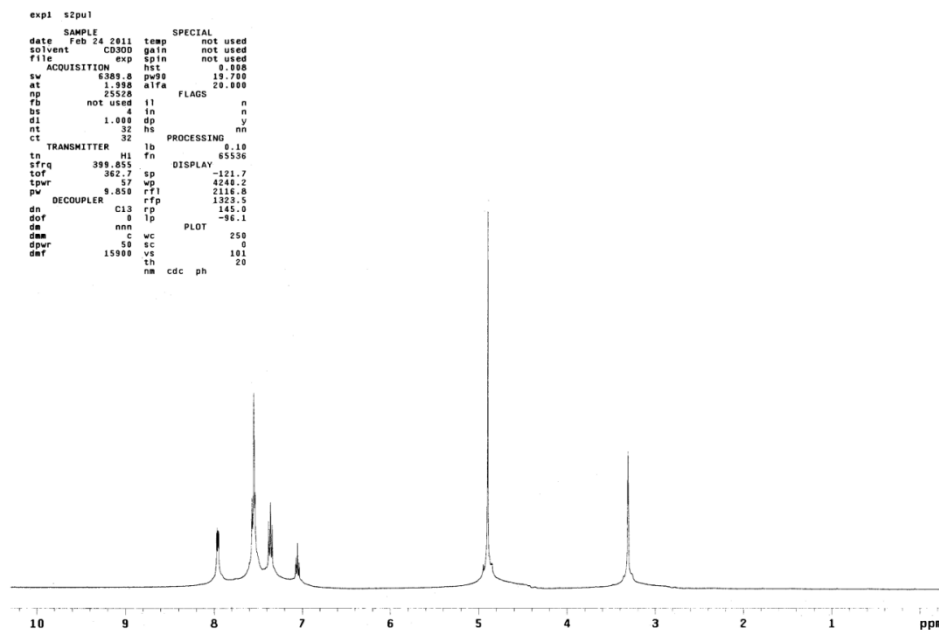
N-(Naphthalen-1-yl)-1,3,4-oxadiazol-2-amine (11a): (Mass Spectra)

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

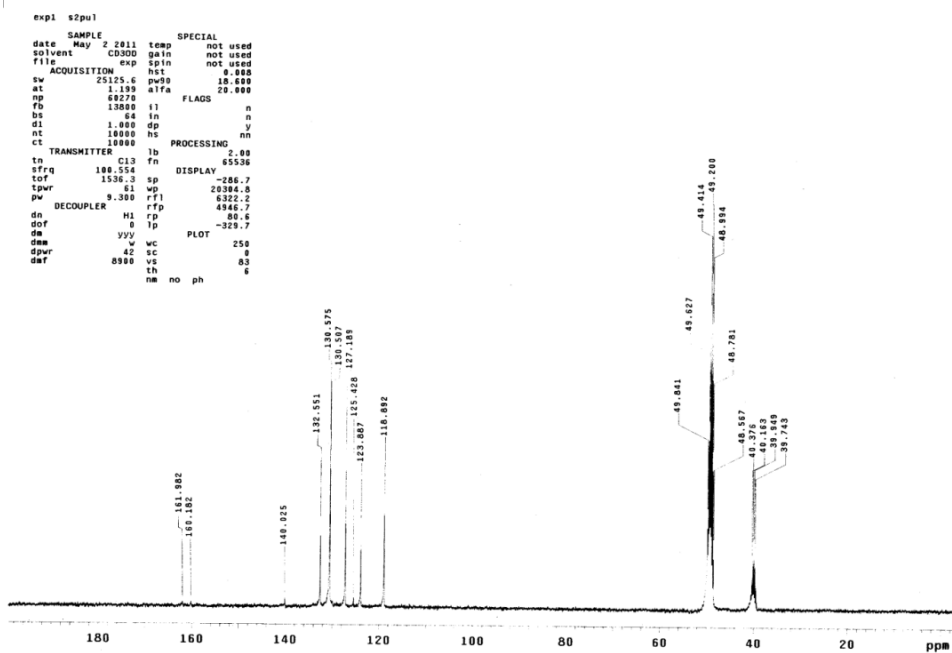
Success
5/10/2011 5:14:42 PM



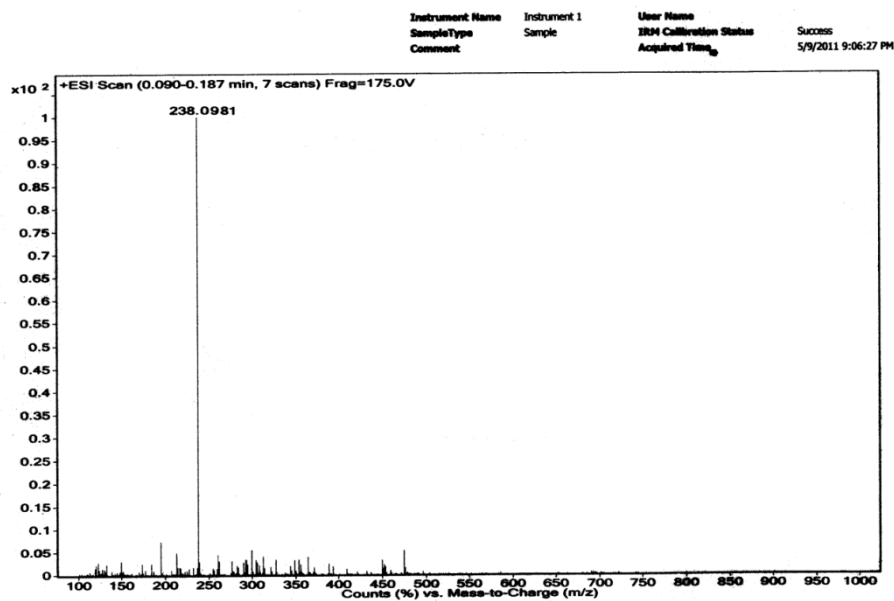
***N*,5-Diphenyl-1,3,4-oxadiazol-2-amine (12a): ¹H NMR (CD₃OD, 400 MHz)**



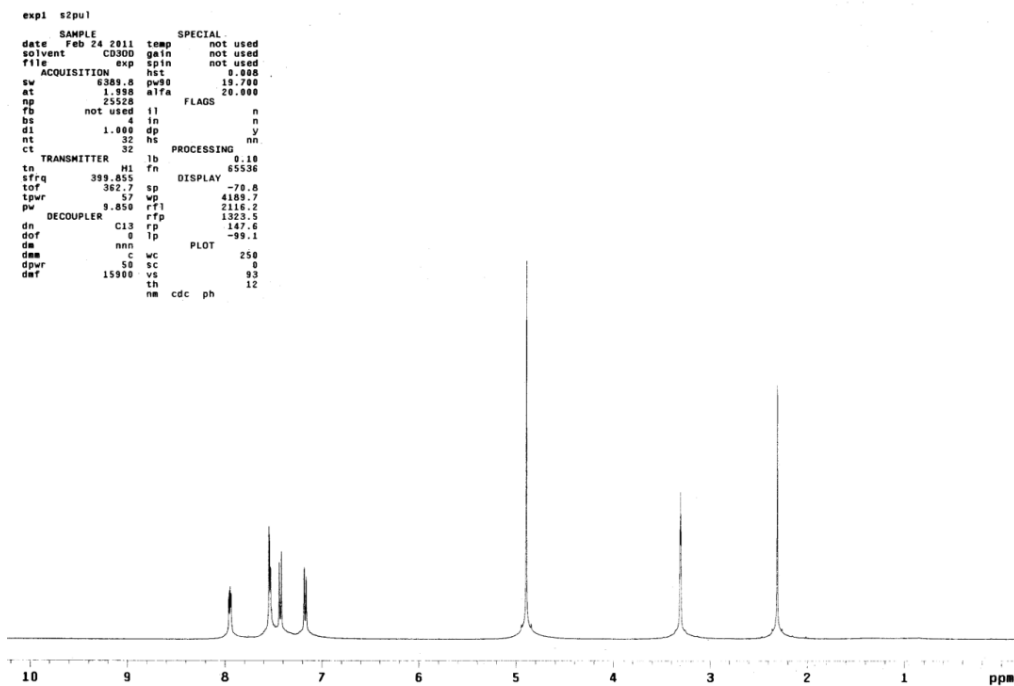
***N*,5-Diphenyl-1,3,4-oxadiazol-2-amine (12a): ¹³C NMR (CD₃OD + DMSO-*d*₆, 100 MHz)**



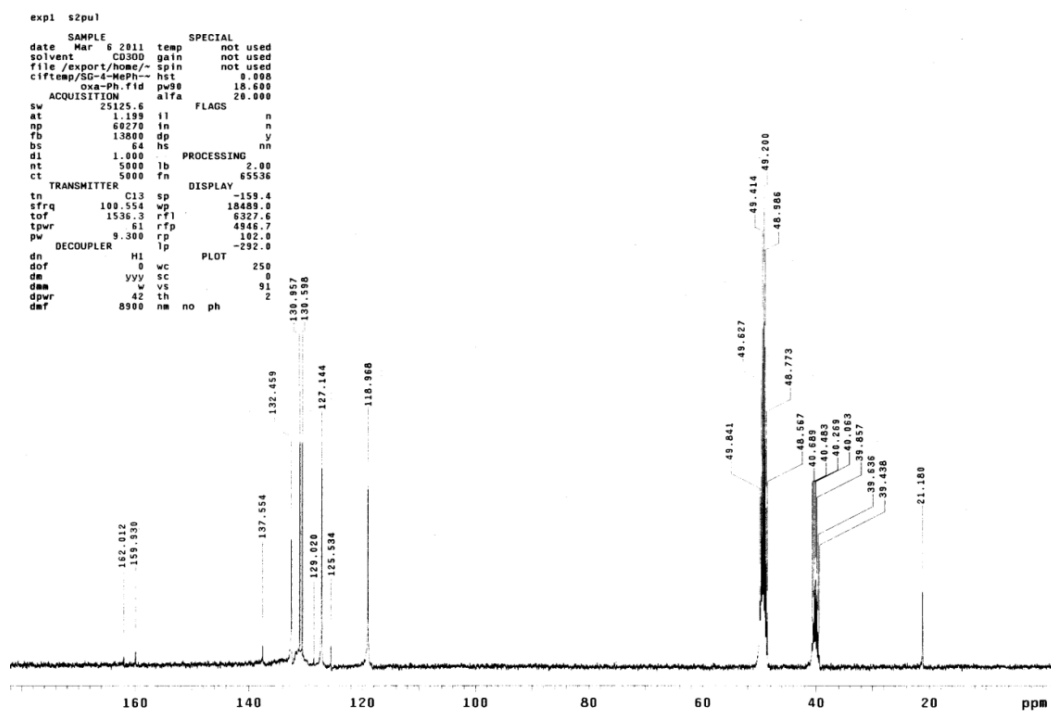
N,5-Diphenyl-1,3,4-oxadiazol-2-amine (12a): (Mass Spectra)



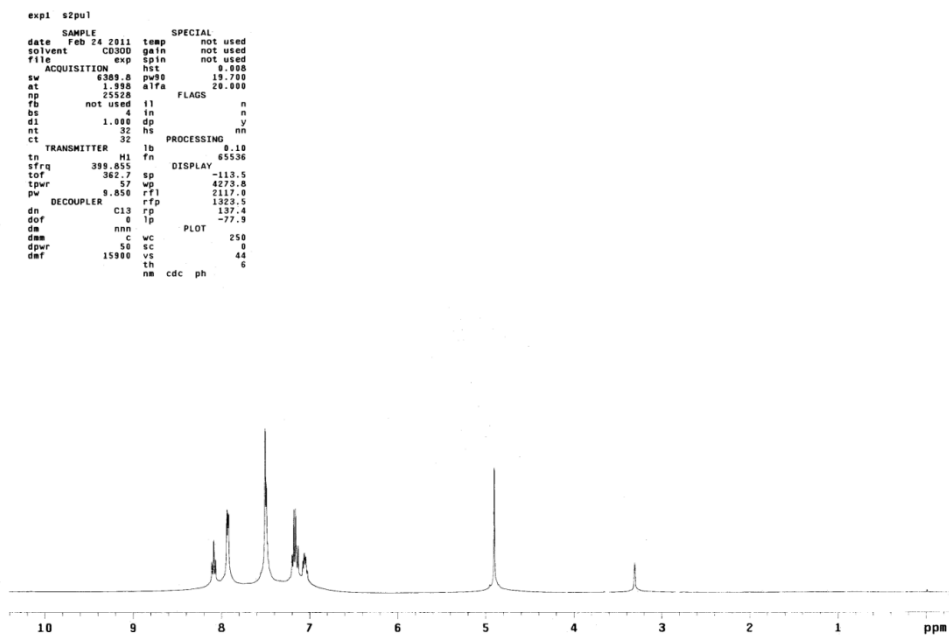
5-Phenyl-N-p-tolyl-1,3,4-oxadiazol-2-amine (13a): ¹H NMR (CD₃OD, 400 MHz)



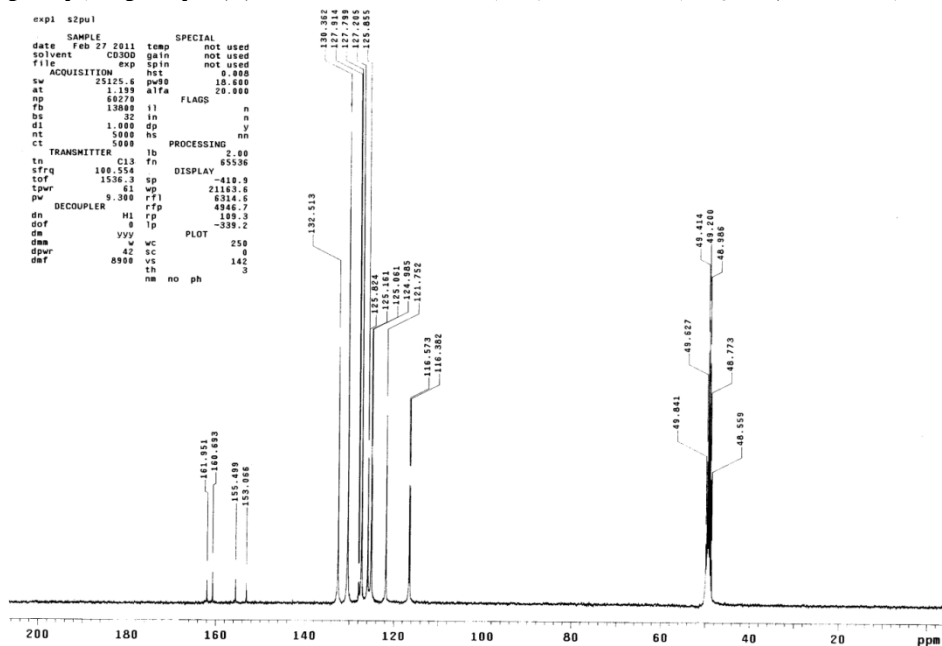
5-Phenyl-*N-p*-tolyl-1,3,4-oxadiazol-2-amine (13a): ^{13}C NMR ($\text{CD}_3\text{OD} + \text{DMSO-}d_6$, 100 MHz)



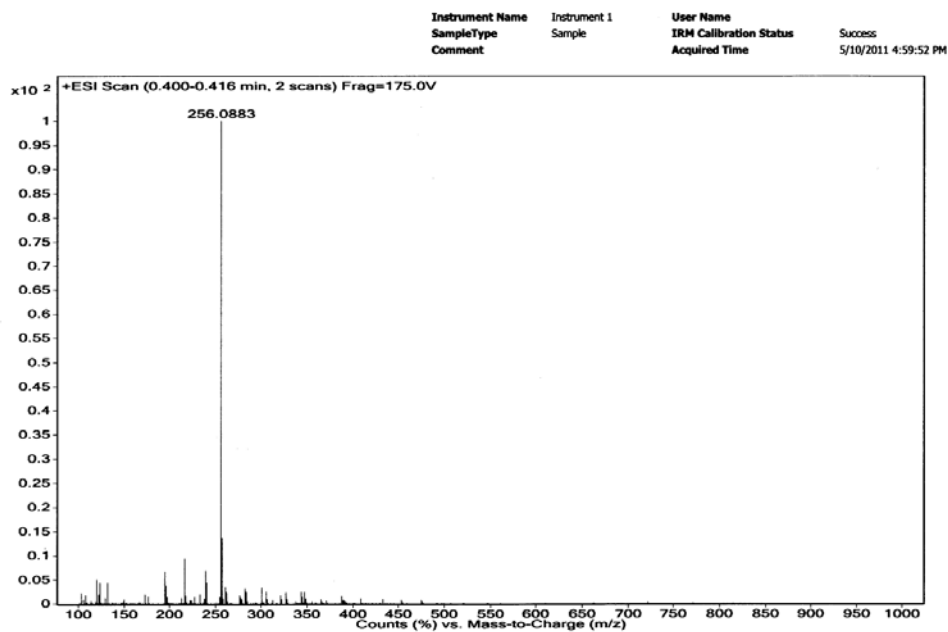
N-(2-Fluorophenyl)-5-phenyl-1,3,4-oxadiazol-2-amine (14a): ^1H NMR (CD_3OD , 400 MHz)



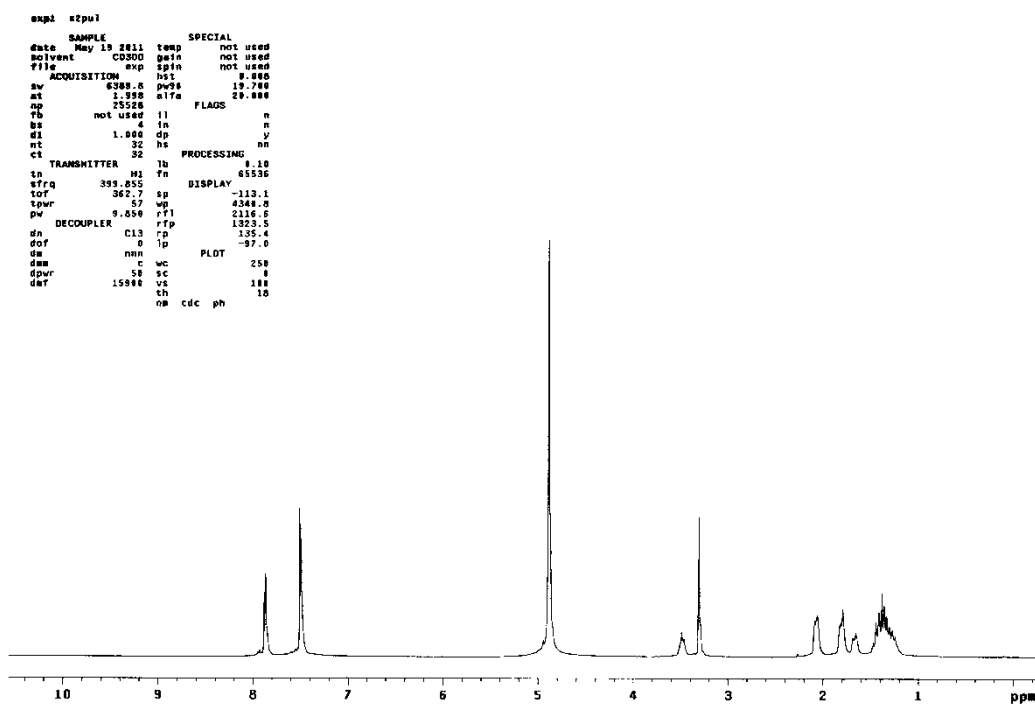
***N*-(2-Fluorophenyl)-5-phenyl-1,3,4-oxadiazol-2-amine (14a): ^{13}C NMR (CD_3OD , 100 MHz)**



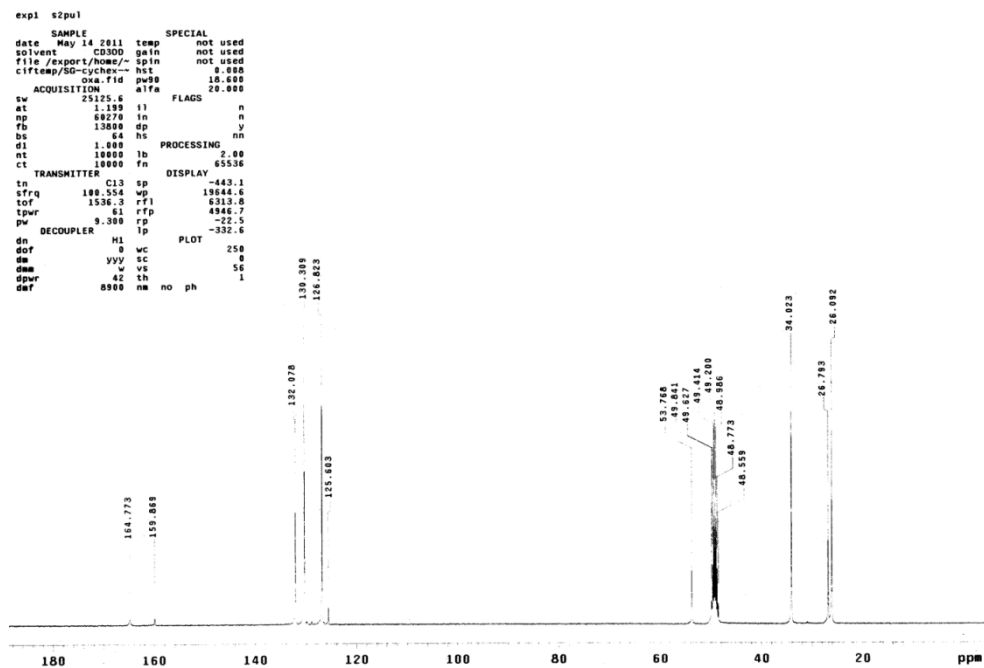
***N*-(2-Fluorophenyl)-5-phenyl-1,3,4-oxadiazol-2-amine (14a): (Mass Spectra)**



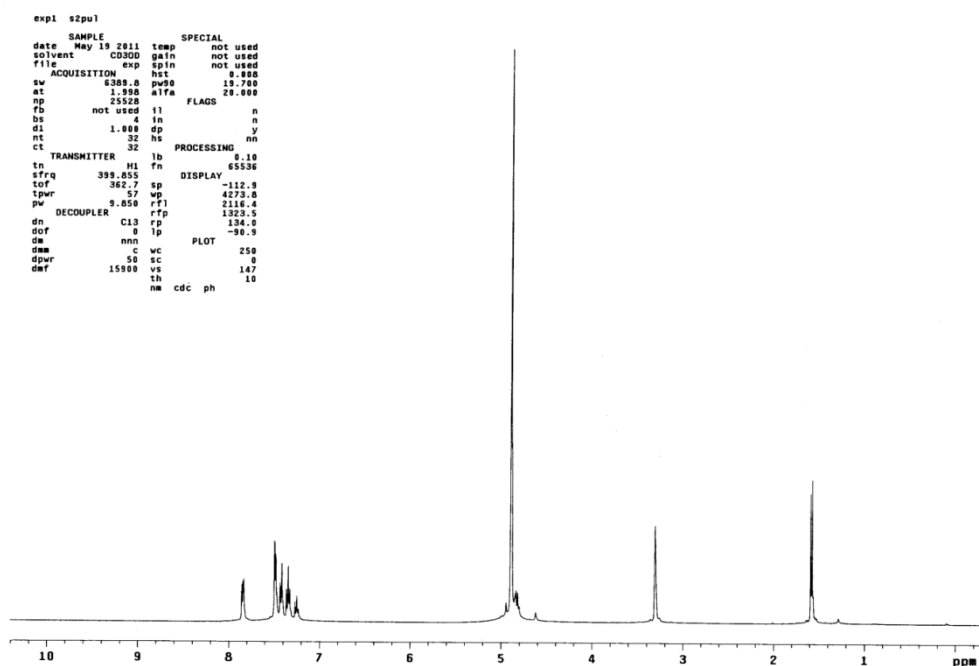
N-Cyclohexyl-5-phenyl-1,3,4-oxadiazol-2-amine (15a): ¹H NMR (CD₃OD, 400 MHz)



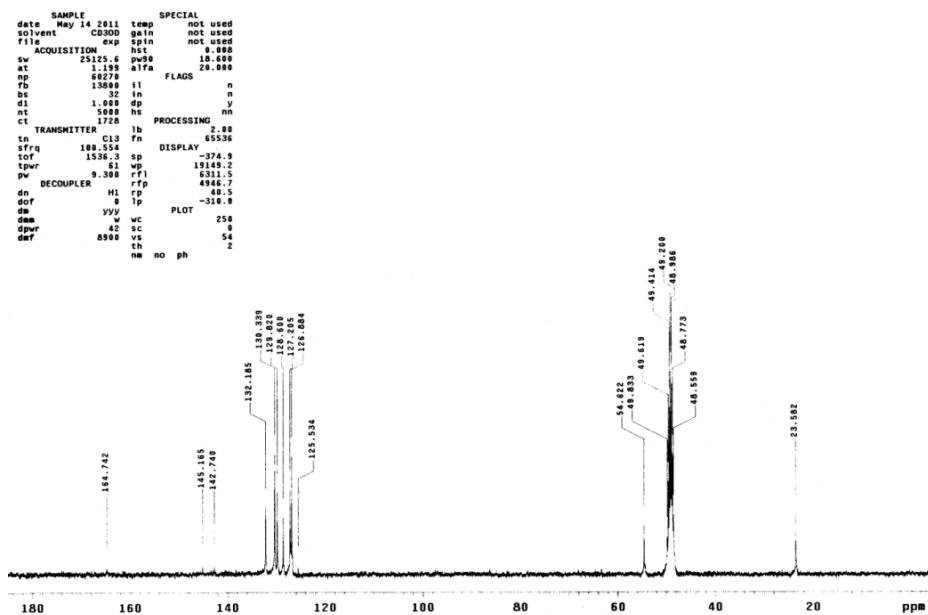
N-Cyclohexyl-5-phenyl-1,3,4-oxadiazol-2-amine (15a): ¹³C NMR (CD₃OD, 100 MHz)



(*R*)-5-Phenyl-*N*-(1-phenylethyl)-1,3,4-oxadiazol-2-amine (16a): ^1H NMR (CD_3OD , 400 MHz)



(*R*)-5-Phenyl-*N*-(1-phenylethyl)-1,3,4-oxadiazol-2-amine (16a): ^{13}C NMR (CD_3OD , 100 MHz)



(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	Success
Comment		Acquired Time	5/10/2011 5:05:33 PM

