Supporting Information

Iodine–catalysed oxidative cyclisation of acylhydrazones to 2,5-substituted 1,3,4-oxadiazoles

Ganesh Majji, Saroj Kumar Rout, Srimanta Guin, Anupal Gogoi and Bhisma K. Patel

Department of Chemistry, Indian Institute of Technology Guwahati

Email: patel@iitg.ernet.in

Contents

Instrumentation and Chemicals:

All the reagents were commercial grade and used without purification. Organic extracts were dried over anhydrous sodium sulphate. Solvents were removed in a rotary evaporator under reduced pressure. Silica gel (60-120 mesh size) was used for the column chromatography. Reactions were monitored by TLC on silica gel 60 F_{254} (0.25mm). NMR spectra were recorded in $CDCl_3$ with tetramethylsilane as the internal standard for ^1H NMR (400 MHz), $CDCl_3$ solvent as the internal standard for ^{13}C NMR (100 MHz). HRMS spectra were recorded using ESI mode. IR spectra were recorded in KBr or neat. The arylidenearoylhydrazides, alkylidenearoylhydrazides were prepared by the condensation of one equivalent of corresponding hydrazides and aldehydes in ethanolic medium under reflux condition for 2-6 h.

Crystallographic Description:

Crystal data were collected with Bruker Smart Apex-II CCD diffractometer using graphite monochromated MoKα radiation (λ = 0.71073 Å) at 298 K. Cell parameters were retrieved using SMART[a] software and refined with SAINT[a] on all observed reflections. Data reduction was performed with the SAINT software and corrected for Lorentz and polarization effects. Absorption corrections were applied with the program SADABS[b]. The

structure was solved by direct methods implemented in SHELX-97[c] program and refined by full-matrix least-squares methods on F2. All non-hydrogen atomic positions were located in difference Fourier maps and refined anisotropically. The hydrogen atoms were placed in their geometrically generated positions. colourless crystals were isolated in rectangular shape from acetonitrile at room temperature.

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

CCDC number for compound 9a: CCDC 953478. This data can be obtained free of charge from the Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/datarequest/cif.

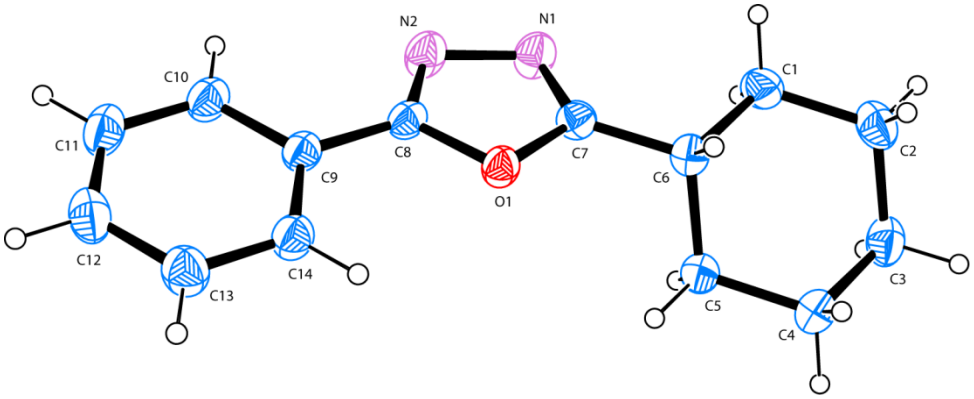
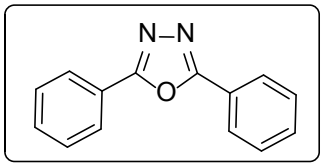


Figure S1: ORTEP view of **9a**

Crystallographic description of 9a: Crystal dimension (mm): 0.42 x 0.35 x 0.26. $C_{14}H_{16}N_2O$, Mr = 228.29 Triclinic, space group P -1; a = 5.7158 (2) Å, b = 9.9633 (4) Å, c = 11.1928 (4) Å; α = 108.896 (2)°, β = 92.553 (2) °, γ = 90.149 (2)°, V = 602.36 (4) Å^3; Z = 2; ρ_{cal} = 1.259 mg/m^3; μ (mm^{-1}) = 0.081; *F (000)* = 244.0; Reflection collected / unique = 3353 / 2055; Refinement method = Full-matrix least-squares on F^2; Final R indices [I>2σ_I] R1 = 0.0384, wR2 = 0.1139, R indices (all data) R1 = 0.0483, wR2 = 0.1213; goodness of fit = 1.062.

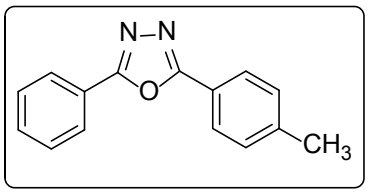
Spectral Data

2,5-Diphenyl-1,3,4-oxadiazole (1a):



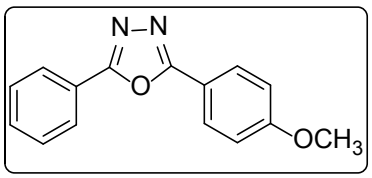
White Solid; M.p. 136-138 ^{o}C (Lit.[1] 138 ^{o}C); ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.53-7.55 (m, 6H), 8.13-8.15 (m, 4H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 124.1, 127.1, 129.3, 131.9, 164.8.; IR (KBr): 3058, 2919, 1547, 1484, 1445, 1268, 1155, 1068, 1019, 964, 922, 782, 710, 686 cm^{-1}. HRMS (*m/z*) (M+1) calcd for $C_{14}H_{10}N_2O$: 223.0866, found 223.0863.

2-Phenyl-5-p-tolyl-1,3,4-oxadiazole (2a):



White solid; M.p. 121-122 ^{o}C (Lit.[2] 121-122 ^{o}C); ^{1}H NMR (400 MHz, $CDCl_3$): δ 2.45 (s, 3H), 7.34 (d, 2H, *J* = 8.0 Hz), 7.53-7.56 (m, 3H), 8.04 (d, 2H, *J* = 8.0 Hz), 8.13-8.16 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 21.8, 121.3, 124.2, 127.0, 129.2, 129.9, 131.8, 142.5, 164.5, 164.9.; IR (KBr): 3060, 2919, 2852, 1610, 1581, 1550, 1496, 1486, 1445, 1271, 1173, 1076, 822, 728, 702, 687 cm^{-1}. HRMS (*m/z*) (M+1) calcd for $C_{15}H_{12}N_2O$: 237.1022, found 237.1020.

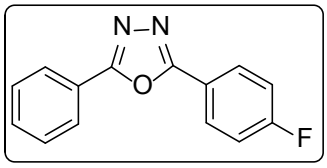
2-(4-Methoxy-phenyl)-5-phenyl-1,3,4-oxadiazole (3a):



White solid; M.p. 149-150 ^{o}C (Lit.[1] 148-150 ^{o}C); ^{1}H NMR (400 MHz, $CDCl_3$): δ 3.88 (s, 3H), 7.02 (d, 2H, *J* = 8.4 Hz), 7.52-7.53 (m, 3H), 8.07 (d, 2H, *J* = 8.4 Hz), 8.11-8.12 (m, 2H); ^{13}C NMR (100

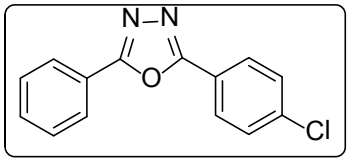
MHz, $CDCl_3$): δ 55.6, 114.7, 116.6, 124.2, 127.0, 128.9, 129.2, 131.7, 162.5, 164.3, 164.7.; IR (KBr): 2956, 2923, 2848, 1616, 1503, 1262, 1066, 1017, 831, 737, 706, 684 cm^{-1}. HRMS (*m/z*) (M+1) calcd for $C_{15}H_{12}N_2O_2$: 253.0972, found 253.0970.

2-(4-Fluorophenyl)-5-phenyl-1,3,4-oxadiazole (4a):



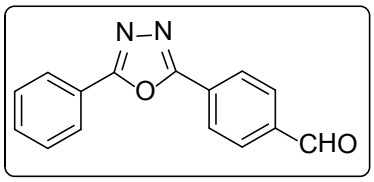
White solid; M.p. 151-152 °C (Lit.[3] 151-152 °C); ^1H NMR (400 MHz, $CDCl_3$): δ 7.22-7.27 (m. 2H), 7.54-7.57 (m, 3H), 8.13-8.18 (m, 4H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 116.5, 116.7, 120.5, 124.0, 127.1, 129.28, 129.33, 129.4, 132.0, 163.7, 164.0, 164.8, 166.2.; IR (KBr): 3061, 2921, 1606, 1549, 1496, 1221, 1149, 1069, 841, 733, 703, 687 cm^{-1}. HRMS (*m/z*) (M+1) calcd for $C_{14}H_9N_2OF$: 241.0772, found 241.0770.

2-(4-Chlorophenyl)-5-phenyl-1,3,4-oxadiazole (5a):



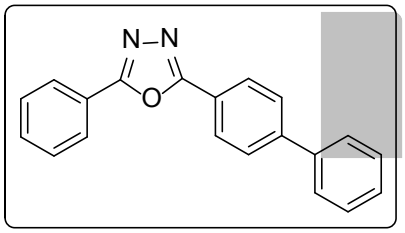
White solid; M.p. 161-162 °C (Lit.[4] 162-163 °C); ^1H NMR (400 MHz, $CDCl_3$): δ 7.49-7.53 (m, 5H), 8.06 (d, 2H, *J* = 8.0 Hz), 8.11 (d, 2H, *J* = 6.6 Hz); ^{13}C NMR (100 MHz, $CDCl_3$): δ 122.6, 123.9, 127.2, 128.4, 129.3, 129.7, 132.1, 138.2, 164.0, 164.9.; IR (KBr): 3061, 2920, 1605, 1550, 1478, 1406, 1086, 1074, 839, 730, 702, 687 cm^{-1}. HRMS (*m/z*) (M+1) calcd for $C_{14}H_9N_2OCl$: 257.0476, found: 257.0471.

4-(5-Phenyl-1,3,4-oxadiazol-2-yl)-benzaldehyde (6a):



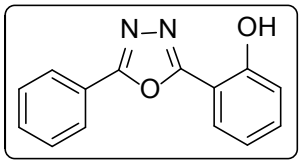
White solid; M.p. 168-169 ^{o}C (lit.[5] 162.7 ^{o}C); ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.53-7.59 (m, 3H), 8.05 (d, 2H, *J* = 8.4 Hz), 8.15 (d, 2H, *J* = 8 Hz), 8.31 (d, 2H, *J* = 8 Hz), 10.10 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 123.6, 127.3, 127.6, 129.0, 129.4, 130.4, 132.3, 138.3, 163.8, 165.4, 191.5.; IR (KBr): 3060, 2925, 2853, 1703, 1547, 1446, 1271, 1204, 1075, 833, 729, 704, 685 cm^{-1}. HRMS (*m/z*) (M+1) calcd for $C_{15}H_{10}N_2O_2$: 251.0815, found: 251.0815.

2-Biphenyl-4-yl-5-phenyl-1,3,4-oxadiazole (7a):



White solid; M.p. 164-166 ^{o}C (Lit.[6] 166-167 ^{o}C); ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.42 (d, 2H, *J* = 7.6 Hz), 7.49 (t, 2H, *J* = 16 Hz), 7.55-7.56 (m, 2H), 7.66 (d, 2H, *J* = 7.6 Hz), 7.77 (d, 2H, *J* = 8.4 Hz), 8.16-8.17 (m, 2H) 8.22 (d, 2H, *J* = 8 Hz); ^{13}C NMR (100 MHz, $CDCl_3$): δ 122.6, 123.9, 127.1, 127.4, 127.7, 128.2, 129.0, 129.1, 131.8, 139.7, 144.4, 164.5, 164.6.; IR (KBr): 3032, 2917, 1609, 1571, 1546, 1481, 1447, 1409, 1270, 1066, 854, 731, 710, 695cm^{-1}. HRMS (m/z) (M+1) calcd for $C_{20}H_{14}N_2O$: 299.1179, found: 299.1182.

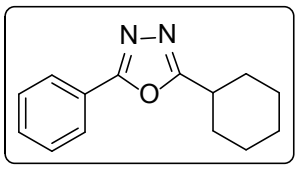
2-(5-Phenyl-1,3,4-oxadiazol-2-yl)-phenol (8a):



White solid; M.p. 185-187 ^{o}C (Lit.[7] 183-185 ^{o}C); ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.55-7.69 (m, 4H), 8.10-8.18 (m, 5H), 11.08 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 120.1, 123.1, 127.3, 129.4, 132.5,

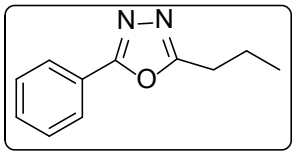
134.7, 134.8, 142.2, 150.2, 157.5, 163.0, 163.7.; IR (KBr): 3152, 2917, 1535, 1487, 1447, 1377, 1248, 1232, 1066, 823, 749, 707, 683cm^{-1}. Anal calcd for $C_{14}H_{10}N_2O_2$ (238.07): C 70.58, H 4.23, N 11.76.; found C 70.59, H 4.25, N 11.75.

2-Cyclohexyl-5-phenyl-1,3,4-oxadiazole (9a):



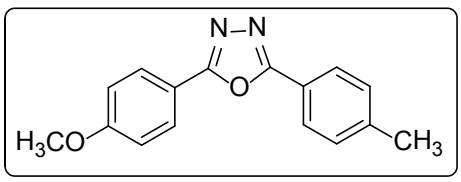
Brown solid; M.p. 107-109 ^{o}C (Lit.[8] 104 ^{o}C); ^{1}H NMR (400 MHz, $CDCl_3$): δ 1.23-1.46 (m, 3H), 1.61-1.71 (m, 3H) 1.83-1.87 (m, 2H), 2.11-2.14 (m, 2H), 2.94-2.99 (m, 1H), 7.46-7.48 (m, 3H), 8.00-8.02 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 25.4, 25.6, 30.2, 35.2, 124.1, 126.7, 128.9, 131.4, 164.4, 170.0.; IR (KBr): 3058, 2923, 2855, 1565, 1552, 1485, 1448, 1021, 768, 709, 688cm^{-1}. HRMS (m/z) (M+1) calcd for $C_{14}H_{16}N_2O$: 229.1335, found: 229.1340.

2-Phenyl-5-propyl-1,3,4-oxadiazole (10a):



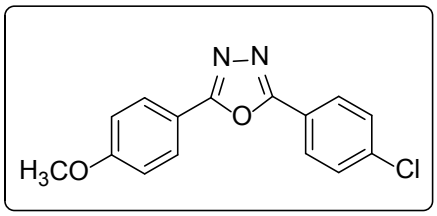
Yellow gummy, M.p. (Lit.[9] 75-76 ^{o}C); ^{1}H NMR (400 MHz, $CDCl_3$): δ 1.03 (t, 3H, J = 14.8 Hz), 1.83-1.89 (m, 2H), 2.89 (t, 2H, J = 15.2 Hz), 7.42-7.52 (m, 3H), 8.00-8.02 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 13.7, 20.2, 27.4, 126.9, 128.5, 129.1, 133.4, 164.8, 167.0.; IR (KBr): 2964, 2929, 2873, 1717, 1573, 1450, 1253, 1069, 1006, 776, 710, 691cm^{-1}. Anal calcd for $C_{11}H_{12}N_2O$ (188.09): C 70.19, H 6.43, N 14.88.; found C 70.22, H 6.44, N 14.86.

2-(4-Methoxyphenyl)-5-p-tolyl-1,3,4-oxadiazole (11a):



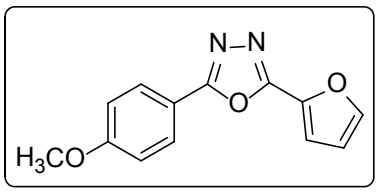
Yellow solid; M.p. 137-139 °C (Lit.[1] 137-138 °C); ^{1}H NMR (400 MHz, $CDCl_3$): δ 2.42 (s, 3H), 3.87 (s, 3H), 7.01 (d, 2H, *J* = 11.6 Hz), 7.31 (d, 2H, *J* = 10.4 Hz), 7.98-8.07 (m, 4H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 21.8, 55.6, 114.7, 116.7, 121.5, 127.0, 128.8, 129.9, 142.2, 162.4, 164.5.; IR (KBr): 2928, 2829, 1612, 1492, 1304, 1254, 1170, 1033, 835, 822, 744 cm^{-1}. Anal calcd for $C_{16}H_{14}N_2O_2$ (266.11): C 72.16, H 5.30, N 10.52.; found C 72.24, H 5.33, N 10.47.

2-(4-Chlorophenyl)-5-(4-methoxyphenyl)-1,3,4-oxadiazole (12a):



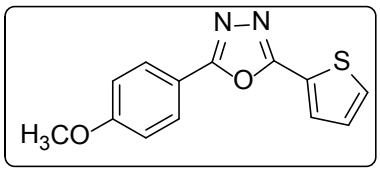
White solid; M.p. 164-165 °C (Lit.[4] 166-167 °C); ^{1}H NMR (400 MHz, $CDCl_3$): δ 3.85 (s, 3H), 6.99 (d, 2H, *J* = 11.6 Hz), 7.46 (d, 2H, *J* = 11.2 Hz), 8.01 (d, 4H, *J* = 11.6 Hz); ^{13}C NMR (100 MHz, $CDCl_3$): δ 55.6, 114.7, 116.3, 122.6, 128.2, 128.8, 129.5, 137.9, 162.6, 163.4, 164.8.; IR (KBr): 2929, 2829, 1611, 1495, 1479, 1305, 1252, 1170, 1089, 1028, 834, 743 cm^{-1}. HRMS (m/z) (M+1) calcd for $C_{15}H_{11}N_2O_2Cl$: 287.0582, found 287.0582.

2-Furan-2-yl-5-(4-methoxy-phenyl)-1,3,4-oxadiazole (13a):



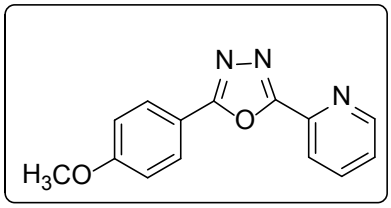
Brown solid; M.p. 128-130 °C (Lit.[3] 129-130 °C); ^{1}H NMR (400 MHz, $CDCl_3$): δ 3.86 (s, 3H), 6.58-6.59 (m, 1H) 6.99 (d, 2H, *J* = 8.8 Hz), 7.18 (d, 1H, *J* = 3.6 Hz), 7.63 (m, 1H), 8.03 (d, 2H, *J* = 8.8 Hz); ^{13}C NMR (100 MHz, $CDCl_3$): δ 55.5, 112.2, 113.8, 114.5, 115.9, 128.7, 139.6, 145.6, 157.0, 162.5, 163.9.; IR (KBr): 3126, 3111, 2924, 1633, 1617, 1504, 1454, 1312, 1265, 1180, 1106, 1083, 1018, 832, 758, 740, 638 cm^{-1}. HRMS (m/z) (M+1) calcd for $C_{13}H_{10}N_2O_3$: 243.0764, found: 243.0767.

2-(4-Methoxy-phenyl)-5-thiophen-2-yl-1,3,4-oxadiazole (14a):



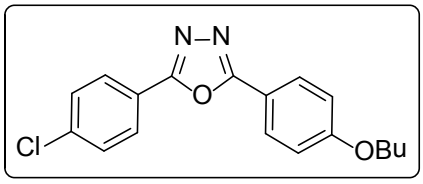
Brown solid; M.p. 136-137 ^{o}C (Lit.[10] 139-141 ^{o}C); ^{1}H NMR (400 MHz, $CDCl_3$): δ 3.86 (s, 3H), 7.00 (d, 2H, *J* = 8.8 Hz), 7.15-7.17 (m, 1H), 7.53 (d, 1H, *J* = 5.2 Hz), 7.78 (d, 1H, *J* = 3.6 Hz), 8.02 (d, 2H, *J* = 8.4 Hz);^{13}C NMR (100 MHz, $CDCl_3$): δ 55.6, 114.6, 116.2, 125.5, 128.2, 128.8, 129.6, 130.0, 160.5, 162.5, 164.1.; IR (KBr): 3102, 2939, 2829, 1611, 1592, 1497, 1421, 1251, 1186, 1026, 836, 739, 720 cm^{-1}. Anal calcd for $C_{13}H_{10}N_2O_2S$ (258.05): C 60.45, H 3.90, N 10.85.; found C 60.49, H 3.95, N 10.83.

2-[5-(4-Methoxy-phenyl)-1,3,4-oxadiazole-2-yl]-pyridine (15a):



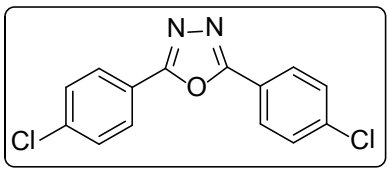
White solid; M.p. 155-156 ^{o}C (Lit.[11] 154-156 ^{o}C); ^{1}H NMR (400 MHz, $CDCl_3$): δ 3.85 (s, 3H), 6.99 (d, 2H, *J* = 8.8 Hz), 7.41-7.45 (m, 1H), 7.86 (t, 1H, *J* = 16 Hz), 8.12 (d, 2H, *J* = 8.8 Hz), 8.26 (d, 1H, *J* = 7.6 Hz), 8.77 (d, 1H, *J* = 7.6 Hz); ^{13}C NMR (100 MHz, $CDCl_3$): δ 55.5, 114.5, 116.1, 123.1, 125.7, 129.1, 137.3, 143.7, 150.3, 162.6, 163.5, 165.6.; IR (KBr): 3053, 2926, 2847, 1614, 1586, 1498, 1458, 1268, 1086, 1020, 832, 741 cm^{-1}. Anal calcd for $C_{14}H_{11}N_3O_2$ (253.09): C 66.40, H 4.38, N 16.59.; found C 66.43, H 4.43, N 16.56.

2-(4-Butoxyphenyl)-5-(4-chlorophenyl)-1,3,4-oxadiazole (16a):



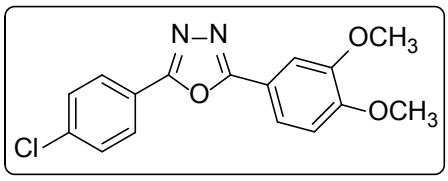
White solid; M.p. 132-133 ^{o}C (Lit.[2] 132-133 ^{o}C); ^{1}H NMR (400 MHz, $CDCl_3$): δ 1.00 (t, 3H, *J* = 9.6 Hz), 1.50-1.56 (m, 2H), 1.78-1.83 (m, 2H), 4.04 (t, 2H, *J* = 8.4 Hz), 7.01 (d, 2H, *J* = 11.6 Hz), 7.50 (d, 2H, *J* = 11.2 Hz), 8.03-8.07 (m, 4H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 14.0, 19.4, 31.3, 68.2, 115.2, 116.1, 122.8, 128.2, 128.9, 129.6, 137.9, 162.3, 163.4, 164.9.; IR (KBr): 3082, 2957, 2872, 1612, 1492, 1483, 1254, 1177, 1088, 1008, 839, 740 cm^{-1}. Anal calcd for $C_{18}H_{17}N_2O_2Cl$ (328.10): C 65.75, H 5.21, N 8.52.; found C 65.79, H 5.23, N 8.48.

2,5-Bis(4-chlorophenyl)-1,3,4-oxadiazole (17a):



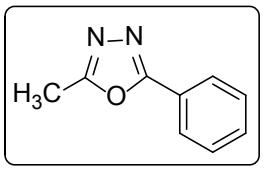
White solid; M.p. 250-251 ^{o}C (Lit.[2] 250-251 ^{o}C); ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.52 (d, 4H, *J* = 11.2 Hz), 8.07 (d, 4H, *J* = 11.6 Hz); ^{13}C NMR (100 MHz, $CDCl_3$): δ 122.4, 128.4, 129.7, 138.4, 164.2.; IR (KBr): 3084, 2956, .2924, 2853, 1605, 1478, 1461, 1261, 1091, 1073, 1011, 838, 738 cm^{-1}. Anal calcd for $C_{14}H_8N_2OCl_2$ (290.00): C 57.76, H 2.77, N 9.62.; found C 57.79, H 2.80, N 9.57.

2-(4-Chloro-phenyl)-5-(3,4-dimethoxy-phenyl)-1,3,4-oxadiazole (18a):



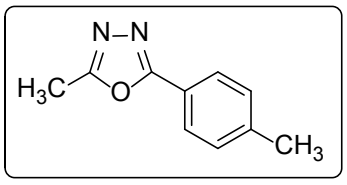
White solid; M.p. 170-171 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$): δ 3.95 (s, 3H), 3.98 (s, 3H), 6.97 (d, 1H, *J* = 8 Hz), 7.49 (d, 2H, *J* = 8.4 Hz), 7.63 (s, 1H), 7.67 (d, 1H, *J* = 8.2 Hz), 8.05 (d, 2H, *J* = 8.8 Hz); ^{13}C NMR (100 MHz, $CDCl_3$): δ 56.3, 56.4, 109.7, 111.3, 120.7, 122.7, 128.3, 129.7, 138.0, 141.2, 149.6, 152.4, 164.9, 169.3.; IR (KBr): 2923, 2852, 1607, 1509, 1498, 1482, 1274, 1255, 1179, 1141, 1090, 1016, 736, 640, 501 cm^{-1}.

2-Methyl-5-phenyl-1,3,4-oxadiazole (19a):



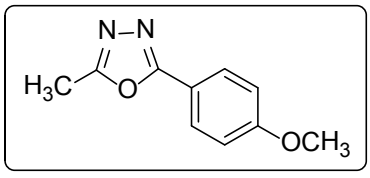
Brown solid; M.p. 60-61 °C (Lit.[12] 61-64 °C); ^{1}H NMR (400 MHz, $CDCl_3$): δ 2.60 (s, 3H), 7.45-7.51 (m, 3H), 8.01 (d, 2H, *J* = 6 Hz); ^{13}C NMR (100 MHz, $CDCl_3$): δ 11.1, 123.9, 126.7, 129.0, 131.5, 163.7, 164.8.; IR (KBr): 2958, 2870, 1679, 1612, 1591, 1500, 1474, 1296, 1249, 1175, 1032, 836, 740, 701, 527 cm^{-1}. HRMS (m/z) (M+1) calcd for $C_9H_8N_2O$: 161.0709, found: 161.0712.

2-Methyl-5-p-tolyl-1,3,4-oxadiazole (20a):



White solid; M.p.107-108 °C (Lit.[13] 134-135 °C); ^{1}H NMR (400 MHz, $CDCl_3$): δ 2.42 (s, 3H), 2.60 (s, 3H), 7.29 (d, 2H, *J* = 8.4 Hz), 7.91 (d, 2H, *J* = 8 Hz); ^{13}C NMR (100 MHz, $CDCl_3$): δ 11.2, 21.8, 121.3, 126.8, 129.9, 142.2, 163.5, 165.2.; IR (KBr): 3038, 2924, 2851, 2340, 1593, 1577, 1498, 1348, 1247, 1088, 1032, 861, 829, 733, 700, 508 cm^{-1}. HRMS (m/z) (M+1) calcd for $C_{10}H_{10}N_2O$: 175.0866, found: 175.0864.

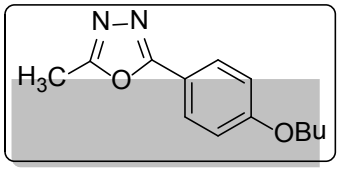
2-(4-Methoxy-phenyl)-5-methyl-1,3,4-oxadiazole (21a):



Yellow solid; M.p. 87-88 °C (Lit.[14] 88 °C); ^{1}H NMR (400 MHz, $CDCl_3$): δ 2.50 (s, 3H), 3.77 (s, 3H), 6.89 (d, 2H, *J* = 8.8 Hz), 7.85 (d, 2H, *J* = 8.8 Hz); ^{13}C NMR (100 MHz, $CDCl_3$): δ 11.1, 55.5, 114.5, 116.5, 128.5, 162.2, 163.2, 164.8.; IR (KBr): 3079, 2924, 2852, 1615, 1594, 1500, 1425, 1308, 1254,

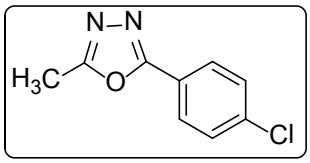
1177, 1087, 1017, 959, 844, 837, 739, 699, 528 cm^{-1}. HRMS (m/z) (M+1) calcd for $C_{10}H_{10}N_2O_2$: 191.0815, found: 191.0817.

2-(4-Butoxy-phenyl)-5-methyl-1,3,4-oxadiazole (22a):[15]



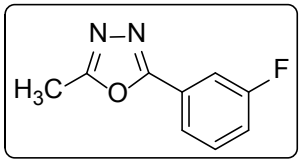
Brown solid; M.p. 58-59 °C; ^{1}H NMR (400 MHz, $CDCl_3$): δ 0.98 (t, 3H, *J* = 14.8 Hz), 1.47-1.53 (m, 2H), 1.77-1.80 (m, 2H), 2.58 (s, 3H), 4.00 (t, 2H, *J* = 13.2 Hz), 6.97 (d, 2H, *J* = 8.8 Hz), 7.93 (d, 2H, *J* = 8.8 Hz); ^{13}C NMR (100 MHz, $CDCl_3$): δ 11.1, 13.9, 19.3, 31.2, 68.0, 114.9, 116.2, 128.5, 161.8, 163.1, 164.9.; IR (KBr): 3055, 2925, 2853, 1724, 1581, 1556, 1450, 1350, 1248, 1073, 960, 781, 709, 692 cm^{-1}. Anal calcd for $C_{14}H_{19}N_2O_2$ (232.12): C 67.22, H 6.94, N 12.06.; found C 67.28, H 6.96, N 12.01.

2-(4-Chloro-phenyl)-5-methyl-1,3,4-oxadiazole (23a):



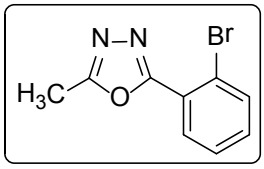
Brown solid; M.p. 96-98 °C (Lit.[16] 106-107 °C); ^{1}H NMR (400 MHz, $CDCl_3$): δ 2.56 (s, 3H), 7.40 (d, 2H, *J* = 8.8 Hz), 7.89 (d, 2H, *J* = 8.8 Hz); ^{13}C NMR (100 MHz, $CDCl_3$): δ 11.2, 122.5, 128.1, 129.5, 137.9, 164.0, 164.2.; IR (KBr): 3071, 2925, 2853, 1607, 1588, 1478, 1408, 1246, 1094, 1009, 848, 819, 730, 687, 507 cm^{-1}. HRMS (m/z) (M+1) calcd for $C_9H_7N_2OCl$: 195.0320, found: 195.0322.

2-(3-Fluoro-phenyl)-5-methyl-1,3,4-oxadiazole (24a):



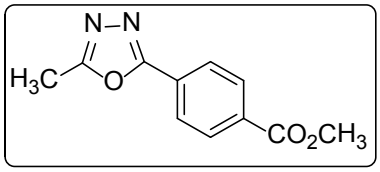
White solid; M.p.81-82 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$): δ 2.63 (s, 3H), 7.21-7.24 (m, 1H), 7.45-7.50 (m, 1H), 7.68-7.72 (m, 1H), 7.79-7.82 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 11.0, 113.6, 113.8, 118.5, 118.7, 122.4, 122.5, 125.7, 125.8, 130.9, 131.0, 161.5, 163.8, 163.9, 164.0, 164.0.; IR (KBr): 2926, 1703, 1578, 1558, 1458, 1436, 1307, 1262, 1197, 1083, 867, 800, 726, 680 cm^{-1}. HRMS (m/z) (M+1) calcd for $C_9H_7N_2OF$: 179.0615, found: 179.0617.

2-(2-Bromo-phenyl)-5-methyl-1,3,4-oxadiazole (25a):[17]



Yellow solid; M.p. 80-81 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$): δ 2.62 (s, 3H), 7.35 (t, 1H, *J* = 16 Hz), 7.42 (t, 1H, *J* = 12 Hz), 7.71 (d, 1H, *J* = 8 Hz), 7.86 (d, 1H, *J* = 8 Hz); ^{13}C NMR (100 MHz, $CDCl_3$): δ 11.3, 121.6, 125.5, 127.7, 131.6, 132.5, 134.6, 163.9, 164.3.; IR (KBr): 3062, 2927, 1577, 1566, 1548, 1471, 1427, 1239, 1022, 773, 730, 697cm^{-1}. Anal calcd for $C_9H_7N_2OBr$ (237.97): C 45.22, H 2.95, N 11.72.; found C 45.25, H 2.99, N 11.67.

4-(5-Methyl-[1,3,4]oxadiazol-2-yl)-benzoic acid methyl ester (26a):[18]



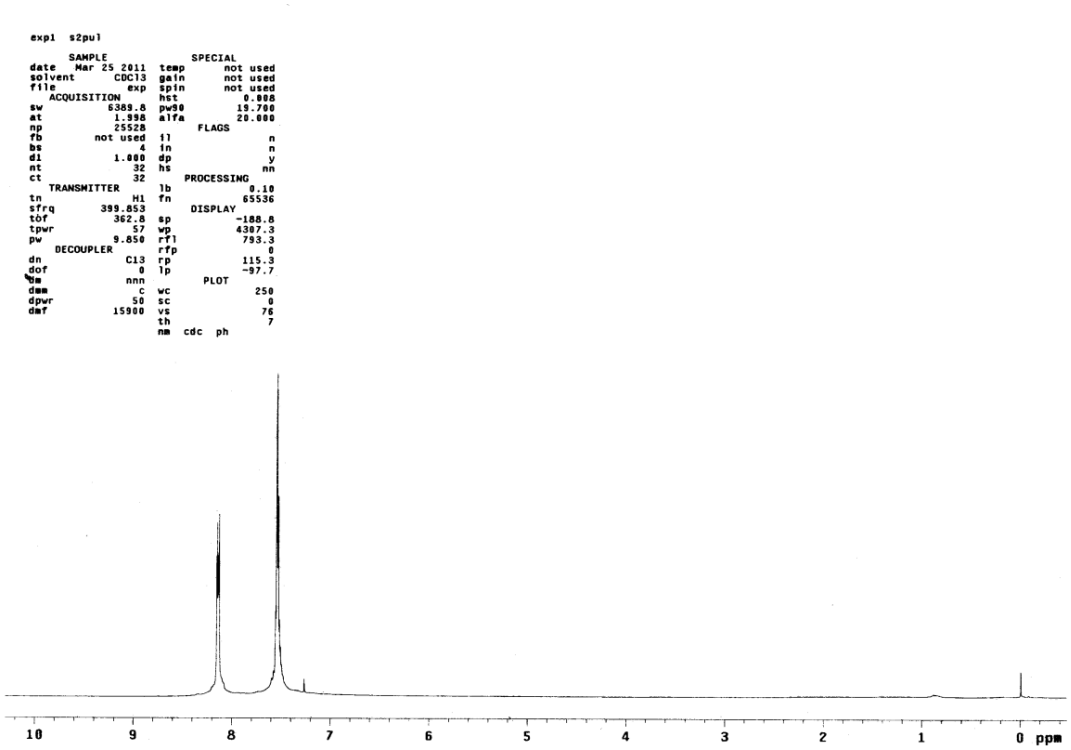
White solid; M.p.162-163 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$): δ 2.59 (s, 3H), 3.90 (s, 3H), 8.04 (d, 2H, *J* = 8.8 Hz), 8.1 (d, 2H, *J* = 8.8 Hz); ^{13}C NMR (100 MHz, $CDCl_3$): δ 11.3, 52.6, 126.8, 127.8, 130.4, 132.8, 164.3, 164.3, 166.2.; IR (KBr): 3064, 2962, 1717, 1571, 1430, 1413, 1275, 1240, 1106, 1014, 956, 868, 718, 482 cm^{-1}. Anal calcd for $C_{11}H_{10}N_2O_3$ (218.07): C 60.55, H 4.62, N 12.84.; found C 60.57, H 4.66, N 12.81.

References:

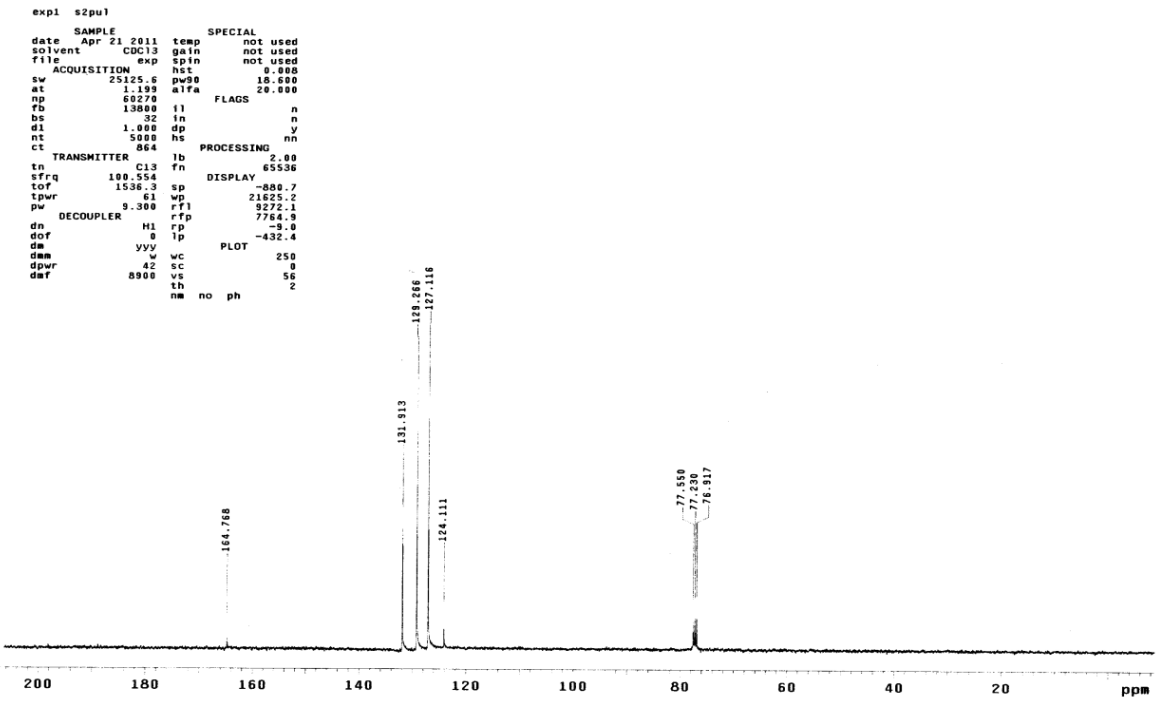
1. Z. Shang, J. Reiner, J. Chang and K. Zhao, *Tetrahedron Lett.,* 2005, **46**, 2701.
2. S. Guin, T. Ghosh, S. K. Rout, A. Banerjee and B. K. Patel, *Org. Lett.*, 2011, **13**, 5976.
3. Z. Shang, *Synth. Commun.*, 2006, **36**, 2927.
4. T. Kawano, T. Yoshizumi, K. Hirano, T. Satoh and M. Miura, *Org. Lett.,* 2009, **11**, 3072.
5. T. Huaijun, T. Hao, Z. Zhiguo, Y. Jibing, C. Changjie and Z. Keli, *Synthetic Met.*, 2009, **159**, 72.
6. F. N. Hayes, B. S. Rogers and D. G. Ott, *J. Am. Chem. Soc.,* 1955, **77**, 1850.
7. S. R. Pattan, P. A. Rabara, J. S. Pattan, A. A. Bukitagar, V. S. Wakale and D. S. Musmade, *Indian J. Chem. B*, 2009, **48B**, 1453.
8. S. Paolo, L. Alessandro, R. Arianna, C. Damiano, G. Giuseppe and C. Ornella, *Tetrahedron Lett.*, 2010, **51**, 4801.
9. D. Minoo, S. Peyman, B. Mostafa, Z. M. Ali and B. Mahboobeh, *Synth. Commun.*, 2007, **37**, 1201.
10. D. M. Pore, S. M. Mahadik and U. V. Desai, *Synth. Commun.*, 2008, **38**, 3121.
11. L. Yu, X. K. Qiang, D. J. Yong, Z. M. Xiang, W. X. Yu and Z. W. Guo, *Chinese Chem. Lett.*, 2007, **18**, 573.
12. W. Hans and K. Joachim, *Chem. Ber.*, 1963, **96**, 1049.
13. G. Nurhan, S. Mevlut, C. Elif, S. Ali and D. N. Turkish, *J. Chem.*, 2007, **31**, 335.
14. S. Bassem and F. K. M. Salem, *Molecules*, 2011, **16**, 4339.
15. B.-L. Wang, Z.-M. Li, Y.-H. Li, S.-H. Wang, *Gaodeng Xuexiao Huaxue Xuebao*, 2008, **29**, 90.
16. M. Nasser and R.-M. Kurosh, *Chinese Chem. Lett.*, 2008, **19**, 1143.
17. D. Daniel, D. Laurence, G. Michel, L. Patrick, D. Denis and M. Dwight, *PCT Int. Appl.*, WO 2004096220, 2004.
18. N. A. Popova, B. M. Krasovitskii, N. S. Pivnenko and Y. N. Surov, *Chem. Heterocycl. Comp.*, 1997, **33**, 712.

Spectra

2,5-Diphenyl-1,3,4-oxadiazole (1a): ^{1}H NMR (400 MHz, $CDCl_3$)

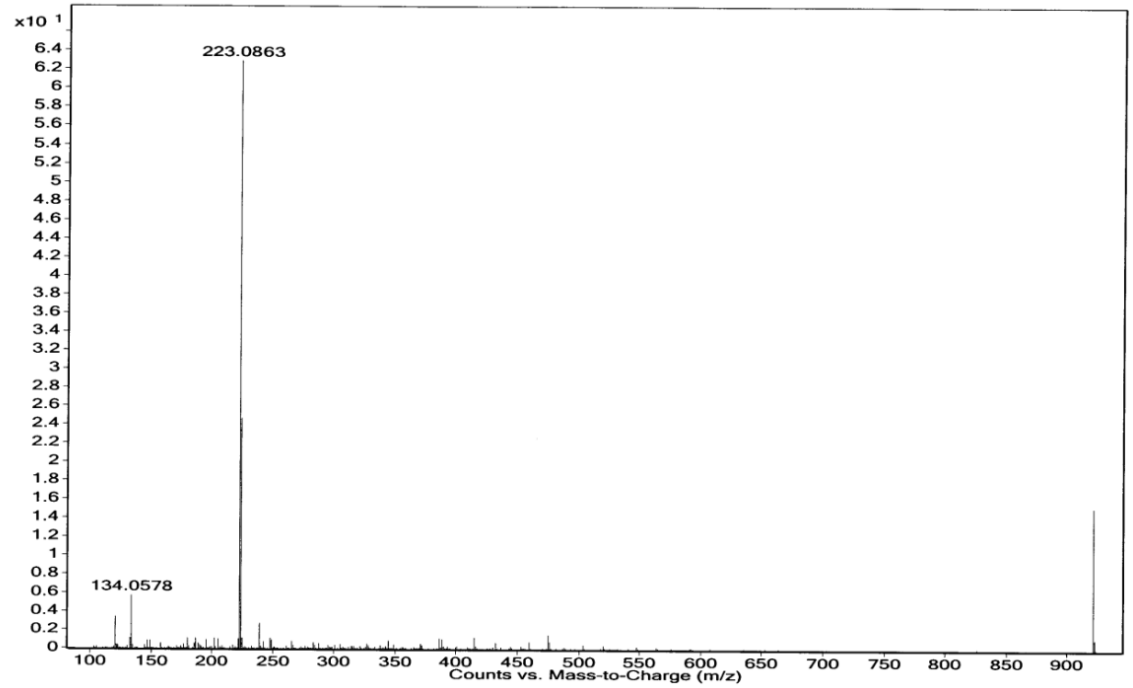


2,5-Diphenyl-1,3,4-oxadiazole (1a): ^{13}C NMR (100 MHz, $CDCl_3$)



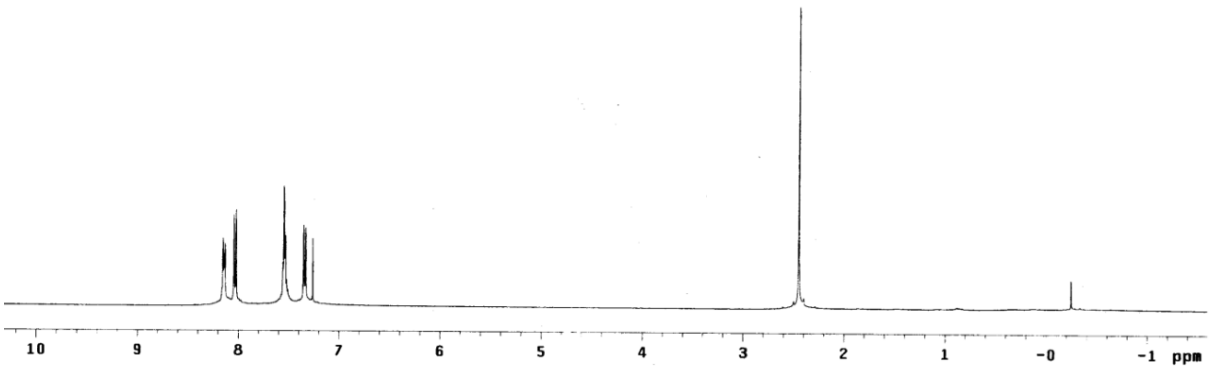
2,5-Diphenyl-1,3,4-oxadiazole (1a): HRMS

Sample Name	**Position**	**Instrument Name**	**User Name**
Inj Vol	**InjPosition**	**SampleType**	**IRM Calibration Status**
Data Filename	**ACQ Method**	**Comment**	**Acquired Time**

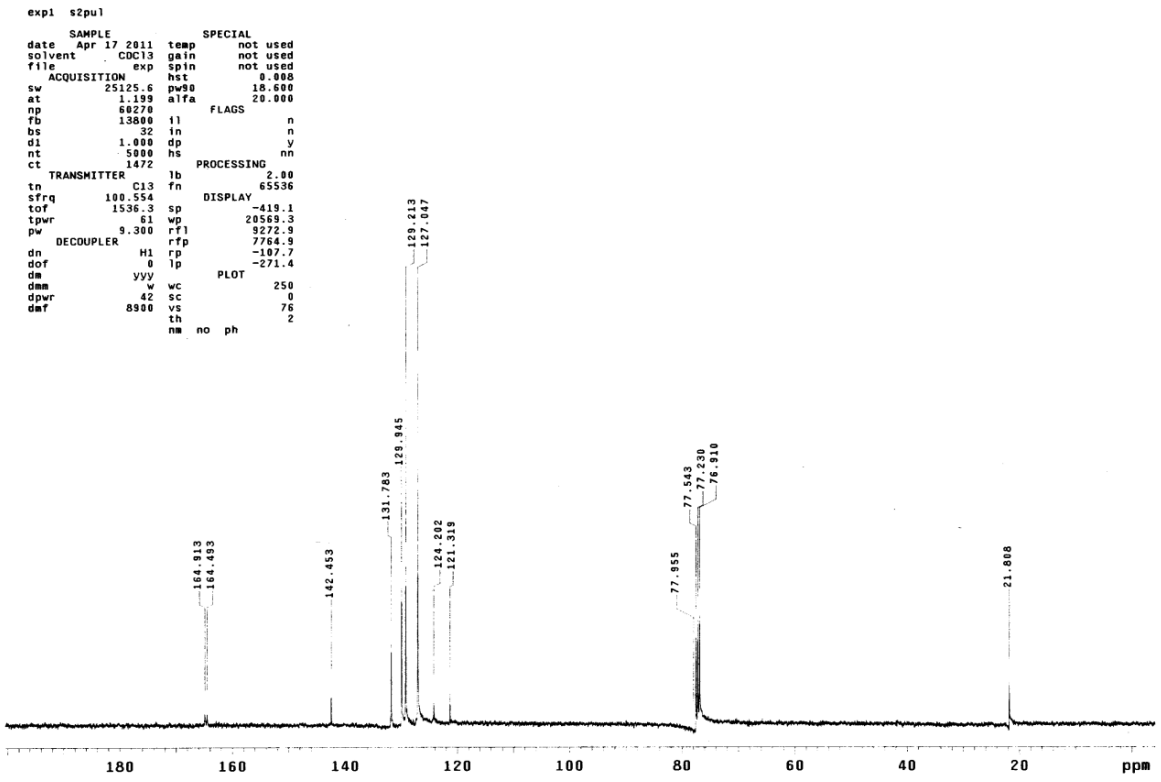


2-Phenyl-5-*p*-tolyl-1,3,4-oxadiazole (2a): ^{1}H NMR (400 MHz, $CDCl_3$)

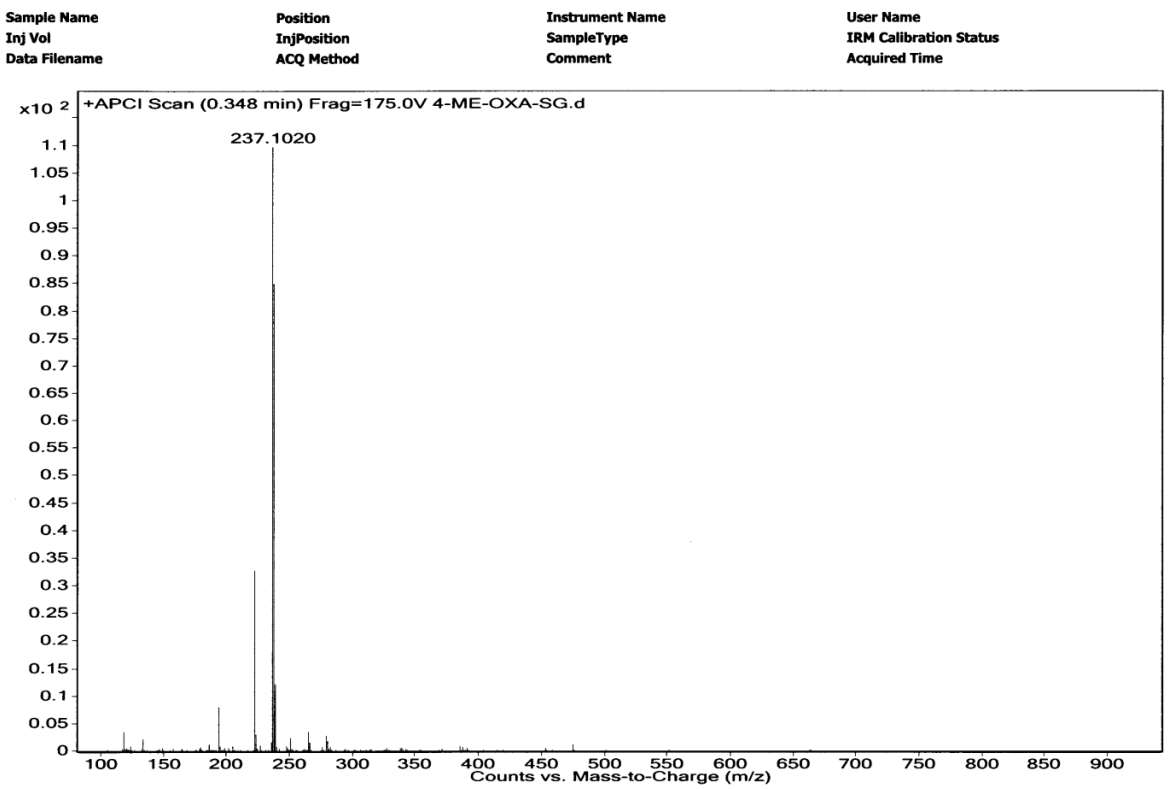
```
expl  s2pul

      SAMPLE                SPECIAL
date    Apr  1 2011  temp       not used
solvent      CDCl3   gain       not used
file          exp    spin       not used
   ACQUISITION       hst          0.008
sw          6389.8   pw90        15.700
at             1.998 alfa        20.000
np           25528        FLAGS
fb       not used   il                 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
sfrq       399.853       DISPLAY
tof          362.8   sp           -638.3
tpwr            57   wp           4770.1
pw           9.850   rfl           794.1
      DECOUPLER      rfp              0
dn             C13   rp            113.1
dof              0   lp            -92.9
dm             nnn         PLOT
dmm              c   wc              250
dpwr            50   sc                0
dmf          15900   vs              426
                     th               20
                     nm  cdc  ph
```



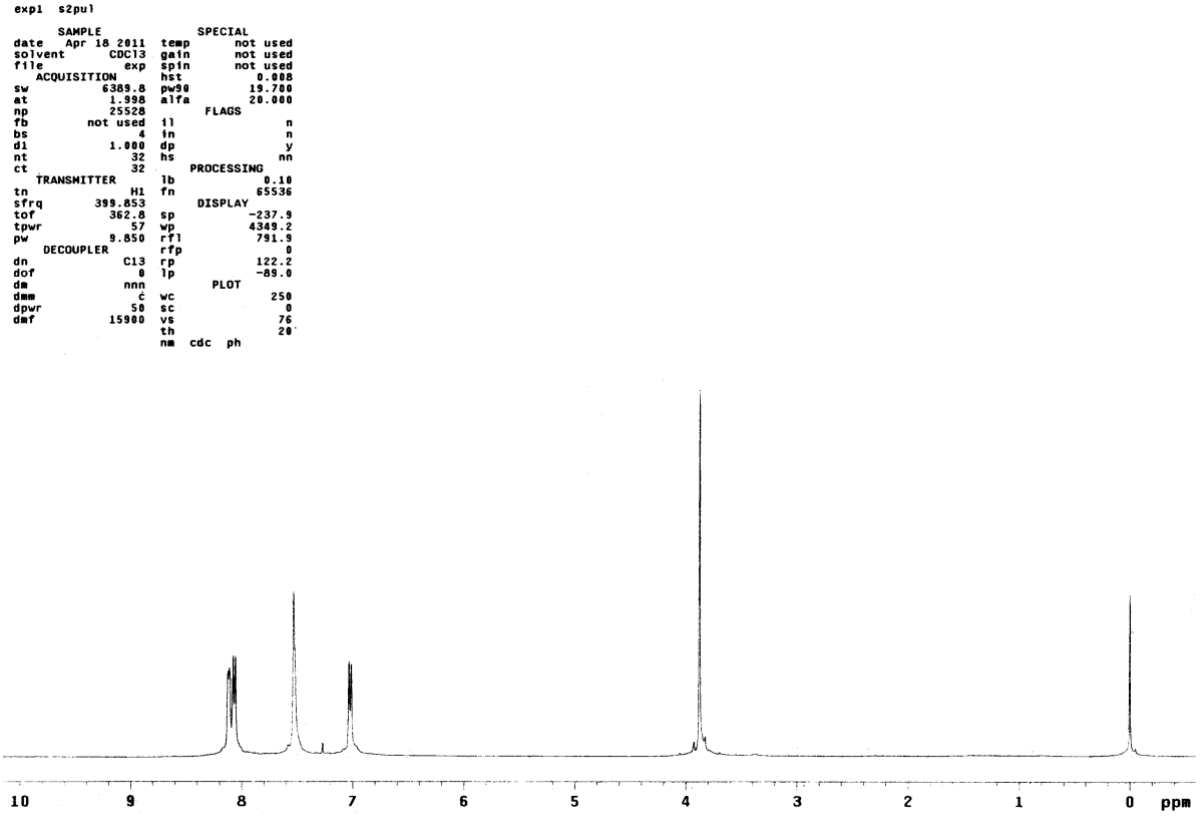
2-Phenyl-5-*p*-tolyl-1,3,4-oxadiazole (2a): ^{13}C NMR (100 MHz, $CDCl_3$)



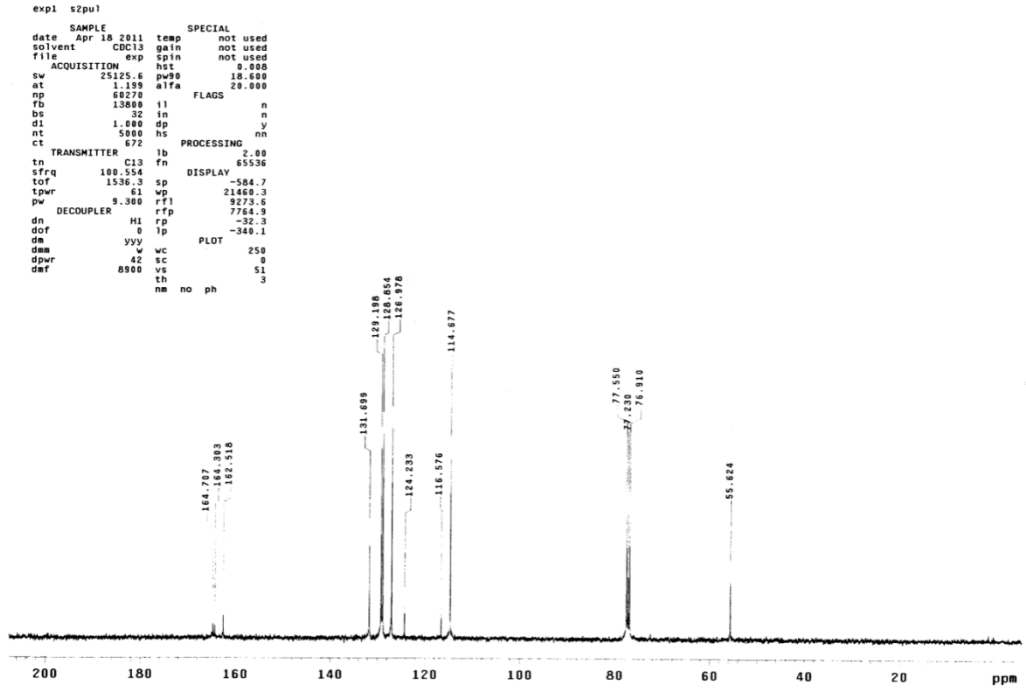
2-Phenyl-5-*p*-tolyl-1,3,4-oxadiazole (2a): HRMS



2-(4-Methoxyphenyl)-5-phenyl-1,3,4-oxadiazole (3a): ^{1}H NMR (400 MHz, $CDCl_3$)

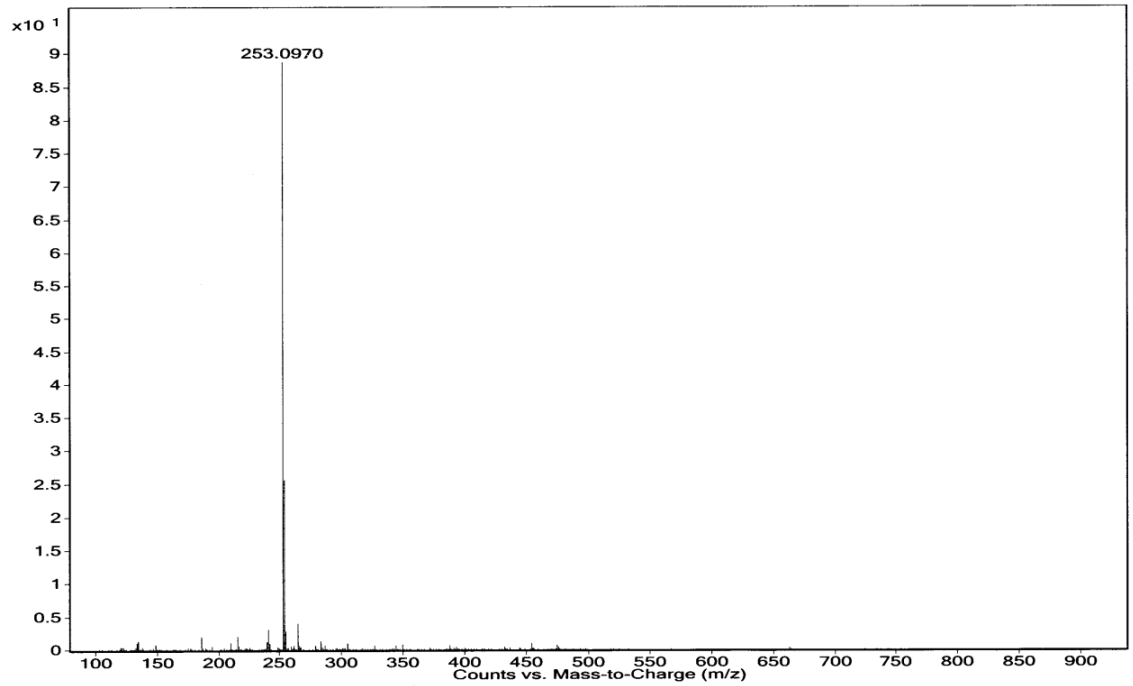


2-(4-Methoxyphenyl)-5-phenyl-1,3,4-oxadiazole (3a): ^{13}C NMR (100 MHz, $CDCl_3$)



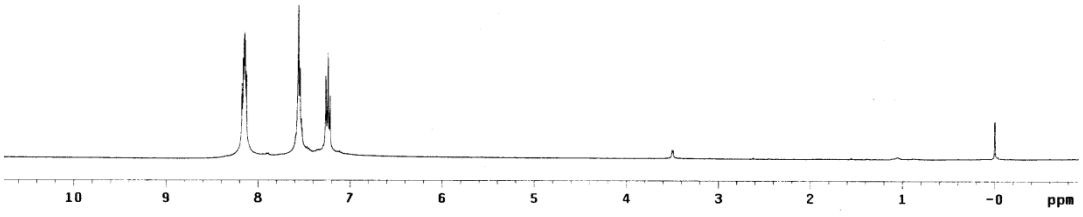
2-(4-Methoxyphenyl)-5-phenyl-1,3,4-oxadiazole (3a): HRMS

Sample Name	**Position**	**Instrument Name**	**User Name**
Inj Vol	**InjPosition**	**SampleType**	**IRM Calibration Status**
Data Filename	**ACQ Method**	**Comment**	**Acquired Time**

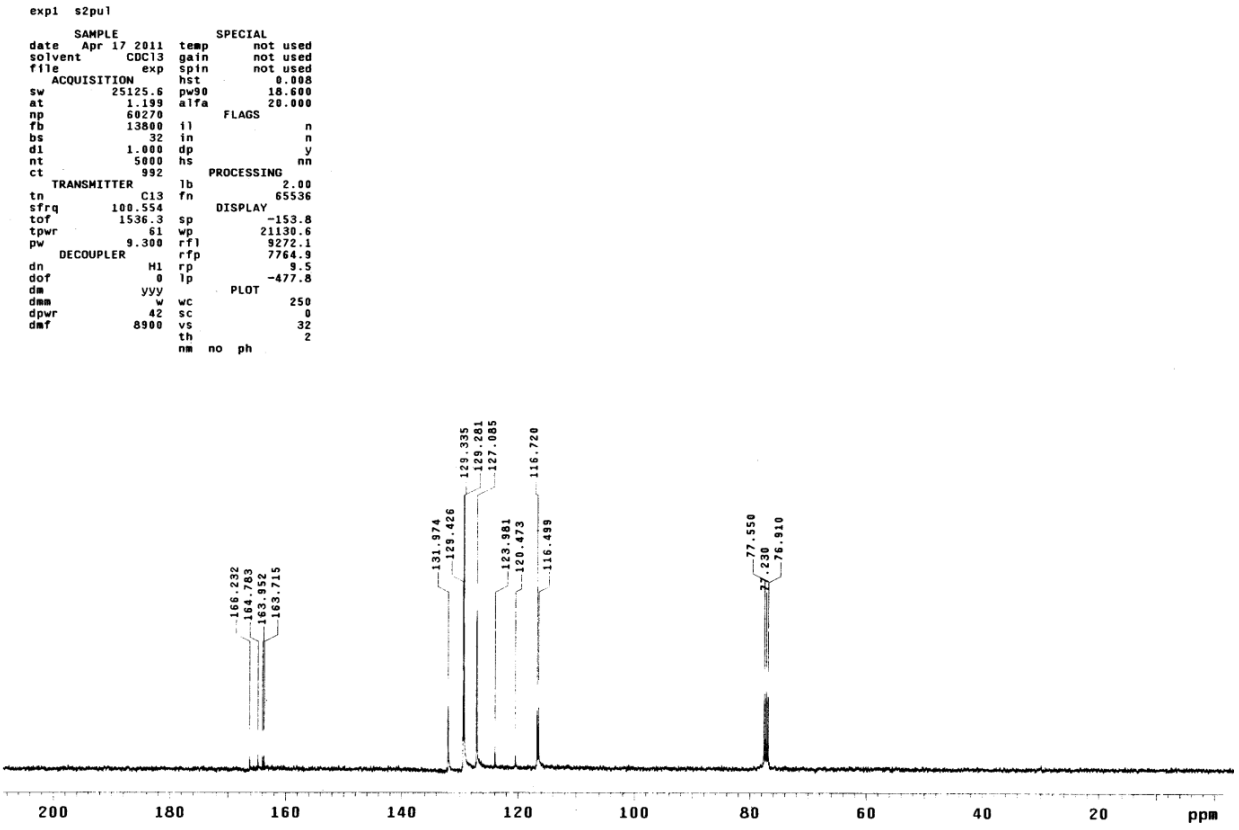


2-(4-Fluorophenyl)-5-phenyl-1,3,4-oxadiazole (4a): ^{1}H NMR (400 MHz, $CDCl_3$)

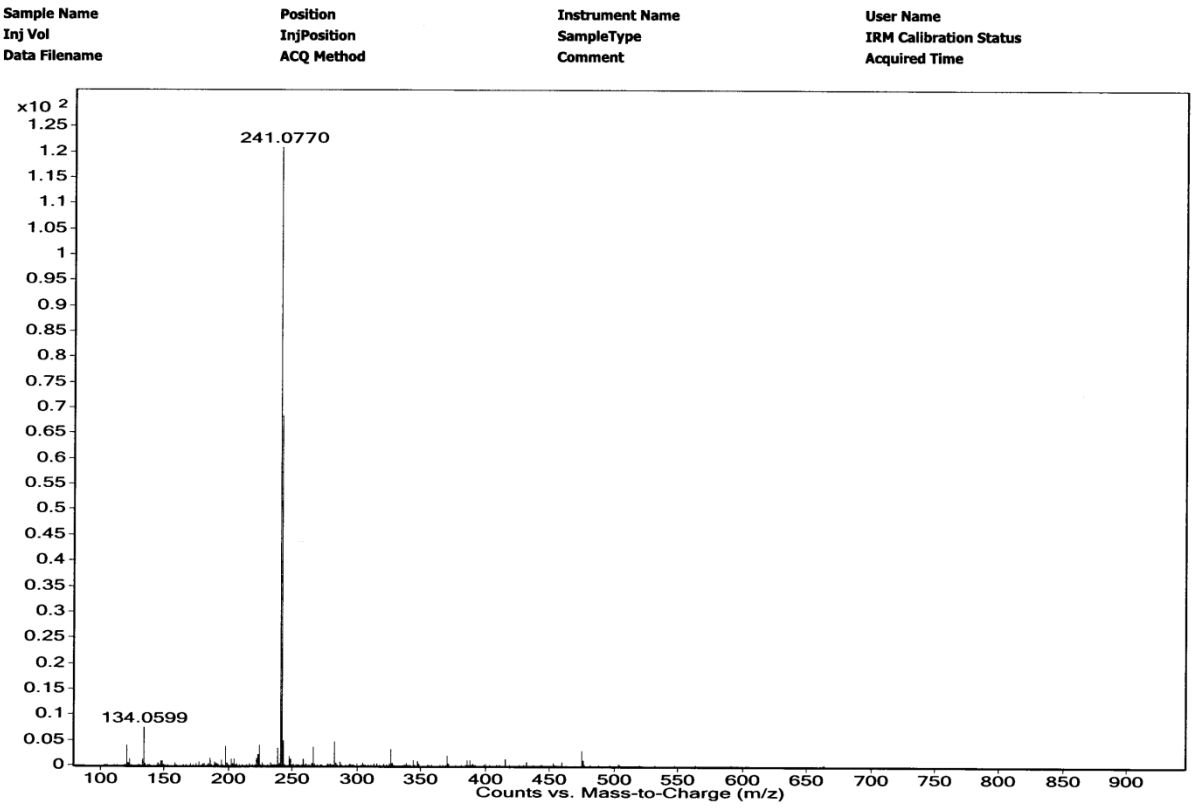
```
expl  s2pul

      SAMPLE                    SPECIAL
date    Apr  6 2011   temp       not used
solvent      CDCl3    gain       not used
file           exp    spin       not used
   ACQUISITION         hst            0.008
sw            6389.8   pw90          19.700
at             1.998   alfa          20.000
np            25528        FLAGS
fb        not used     il                n
bs               4     in                n
di           1.880     dp                y
nt              32     hs               nn
ct              32        PROCESSING
   TRANSMITTER          lb             0.10
tn               H1     fn            65536
sfrq       399.853          DISPLAY
tof            362.8     sp           -365.8
tpwr              57     wp           4710.4
pw             9.850     rfl           793.9
    DECOUPLER            rfp               0
dn               C13     rp            108.2
dof                0     lp            -90.4
dm               nnn          PLOT
dmm                c     wc               250
dpwr              50     sc                 0
dmf            15900     vs               336
                         th                20
                         nm  cdc  ph
```



2-(4-Fluorophenyl)-5-phenyl-1,3,4-oxadiazole (4a): ^{13}C NMR (100 MHz, $CDCl_3$)

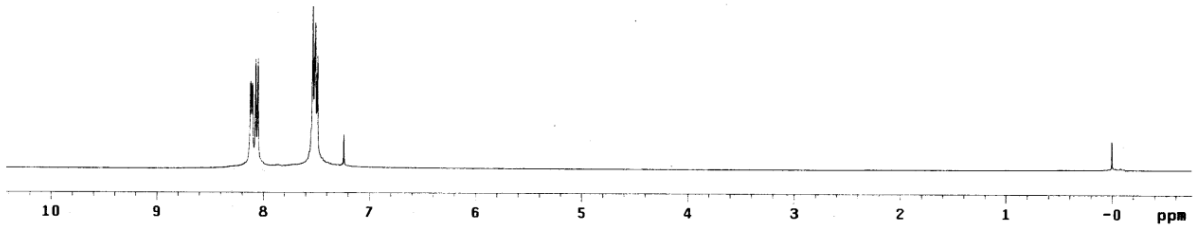


2-(4-Fluorophenyl)-5-phenyl-1,3,4-oxadiazole (4a): HRMS



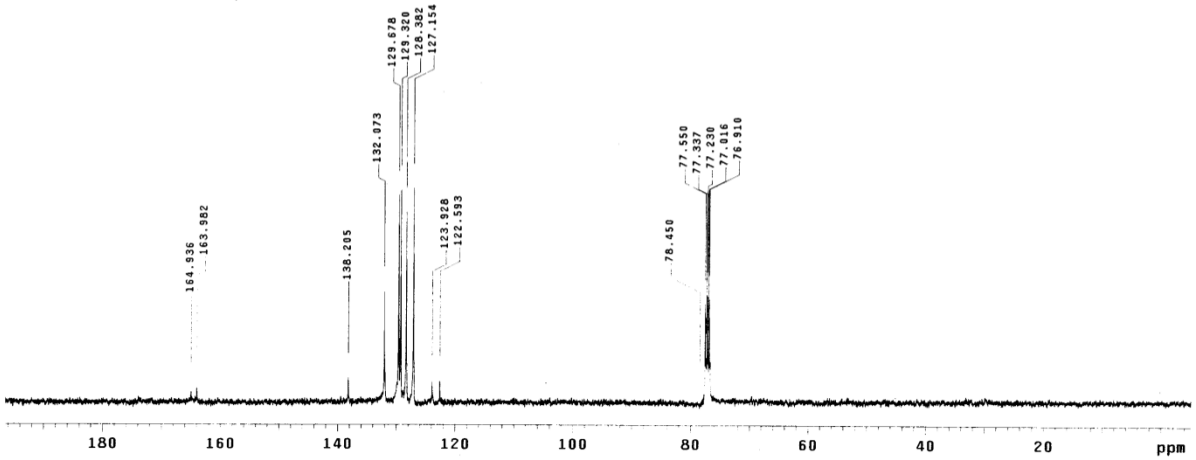
2-(4-Chlorophenyl)-5-phenyl-1,3,4-oxadiazole (5a): ^{1}H NMR (400 MHz, $CDCl_3$)

```
expl  s2pul

      SAMPLE                  SPECIAL
date    Mar 31 2011   temp       not used
solvent       CDCl3   gain       not used
file            exp   spin       not used
   ACQUISITION        hst           0.008
sw           6389.8   pw90         19.700
at            1.398   alfa         20.000
np            25528        FLAGS
fb        not used    il                n
bs               4    in                n
d1           1.000    dp                y
nt              32    hs               nn
ct              32        PROCESSING
   TRANSMITTER       lb             0.10
tn               H1   fn            65536
sfrq        399.853        DISPLAY
tof           362.8   sp           -289.1
tpwr             57   wp           4466.8
pw            9.850   rfl          3697.7
    DECOUPLER         rfp          2894.9
dn              C13   rp            117.8
dof               0   lp            -94.0
dm              nnn        PLOT
dmm               c   wc              250
dpwr             50   sc                0
dmf           15900   vs              147
                      th               20
                      nm  cdc  ph
```



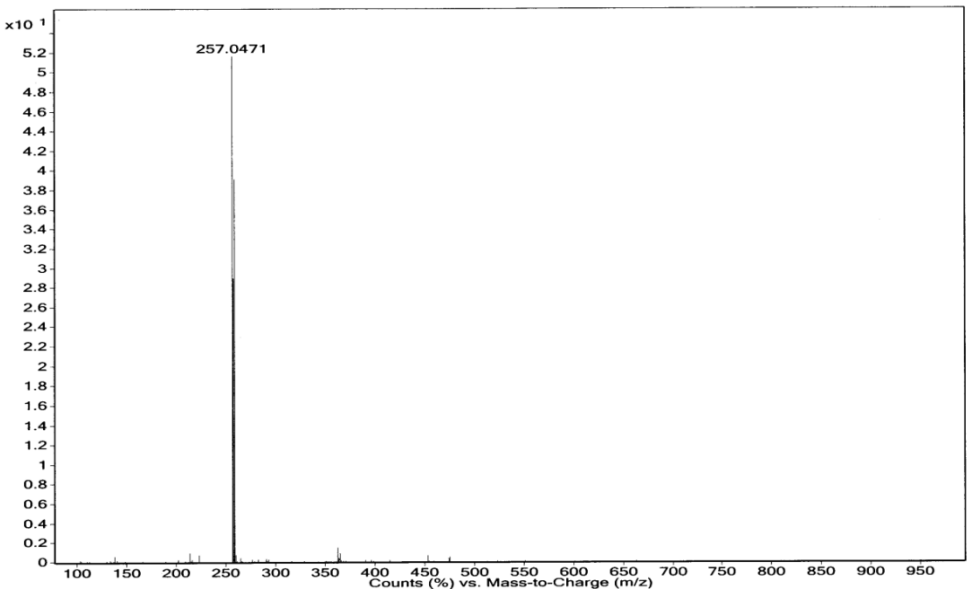
2-(4-Chlorophenyl)-5-phenyl-1,3,4-oxadiazole (5a): ^{13}C NMR (100 MHz, $CDCl_3$)

```
expl  s2pul

      SAMPLE                  SPECIAL
date    Apr  5 2011   temp       not used
solvent       CDCl3   gain       not used
file            exp   spin       not used
   ACQUISITION        hst           0.008
sw          25125.6   pw90         18.600
at            1.199   alfa         20.000
np            60270        FLAGS
fb            13800   il                n
bs               32   in                n
d1            1.000   dp                y
nt             5000   hs               nn
ct             2144        PROCESSING
   TRANSMITTER       lb             2.00
tn              C13   fn            65536
sfrq        100.554        DISPLAY
tof          1536.3   sp           -515.7
tpwr             61   wp          20271.8
pw            9.300   rfl          9270.6
    DECOUPLER         rfp          7764.9
dn               H1   rp            -59.8
dof               0   lp           -271.4
dm              yyy        PLOT
dmm               w   wc              250
dpwr             42   sc                0
dmf            8900   vs               45
                      th                2
                      nm  no  ph
```



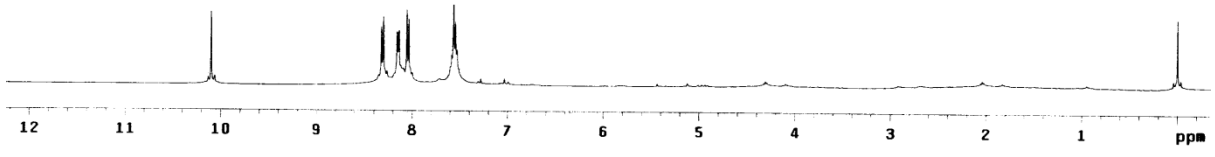
2-(4-Chlorophenyl)-5-phenyl-1,3,4-oxadiazole (5a): HRMS

Sample Name		**Position**	Vial 1	**Instrument Name**	Instrument 1	**User Name**	
Inj Vol	-1	**InjPosition**		**SampleType**	Sample	**IRM Calibration Status**	Success
Data Filename		**ACQ Method**		**Comment**		**Acquired Time**	8/29/2011 12:35:37

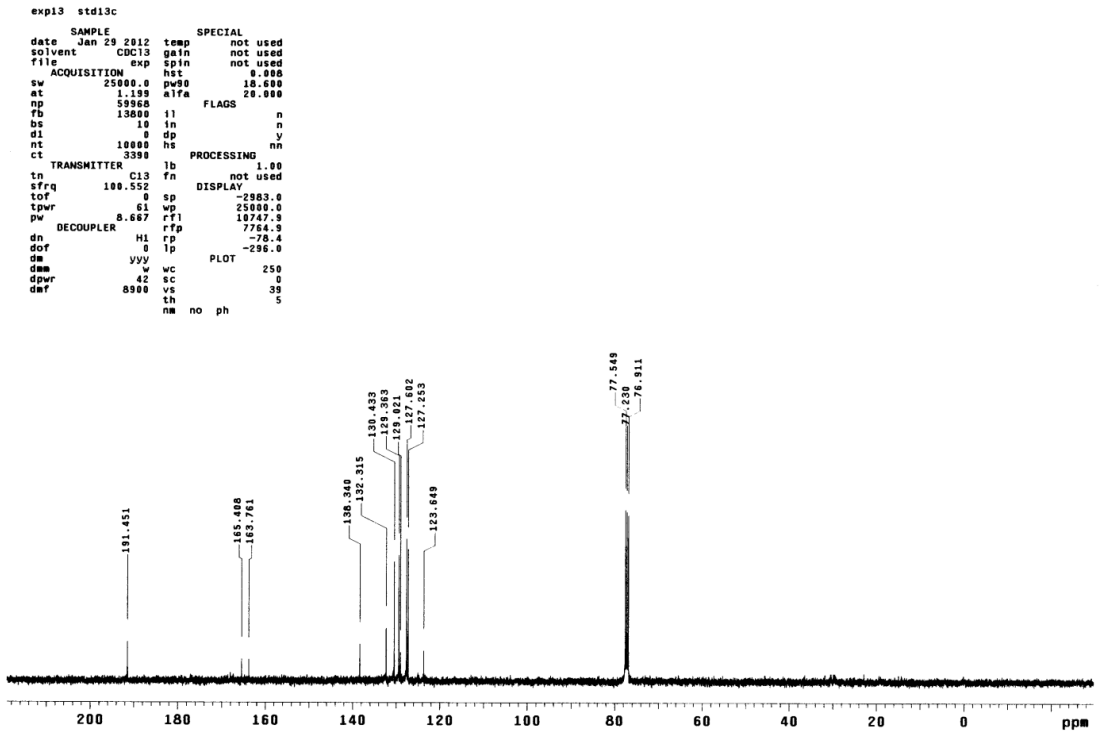


4-(5-Phenyl-1,3,4-oxadiazol-2-yl)-benzaldehyde (6a): ^{1}H NMR (400 MHz, $CDCl_3$)

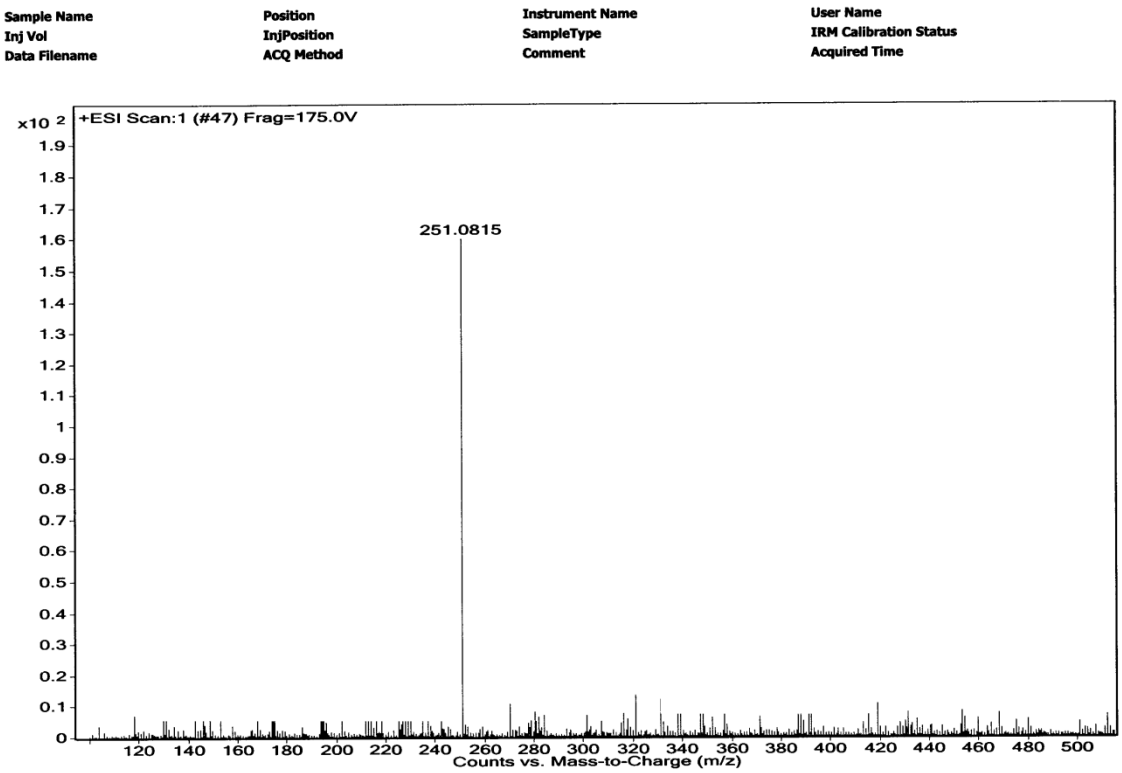
```
expl  s2pul

      SAMPLE                 SPECIAL
date    Dec 27 2011   temp        not used
solvent       CDCl3   gain        not used
file            exp   spin        not used
   ACQUISITION        hst             0.008
sw            6389.8   pw90         19.700
at             1.998   alfa         20.000
np             25528          FLAGS
fb         not used   il                n
bs                4   in                n
d1            1.000   dp                y
nt               32   hs               nn
ct               32      PROCESSING
   TRANSMITTER         lb             0.10
tn               H1   fn            65536
sfrq        399.853         DISPLAY
tof            362.8   sp           -140.8
tpwr              57   wp           5063.0
pw             9.850   rfl           787.2
   DECOUPLER           rfp               0
dn               C13   rp            105.2
dof                0   lp            -90.2
dm               nnn          PLOT
dmm                C   wc              250
dpwr              50   sc                0
dmf            15900   vs               38
                       th               20
                       nm  cdc  ph
```



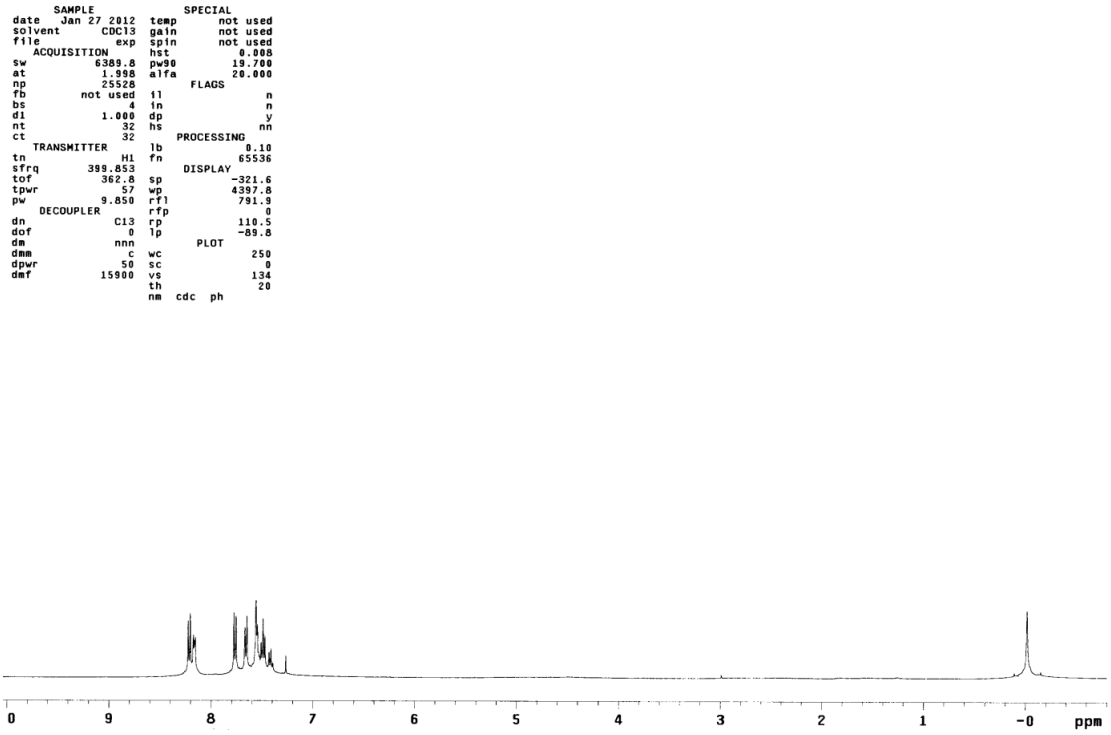
4-(5-Phenyl-1,3,4-oxadiazol-2-yl)-benzaldehyde (6a): ^{13}C NMR (100 MHz, $CDCl_3$)



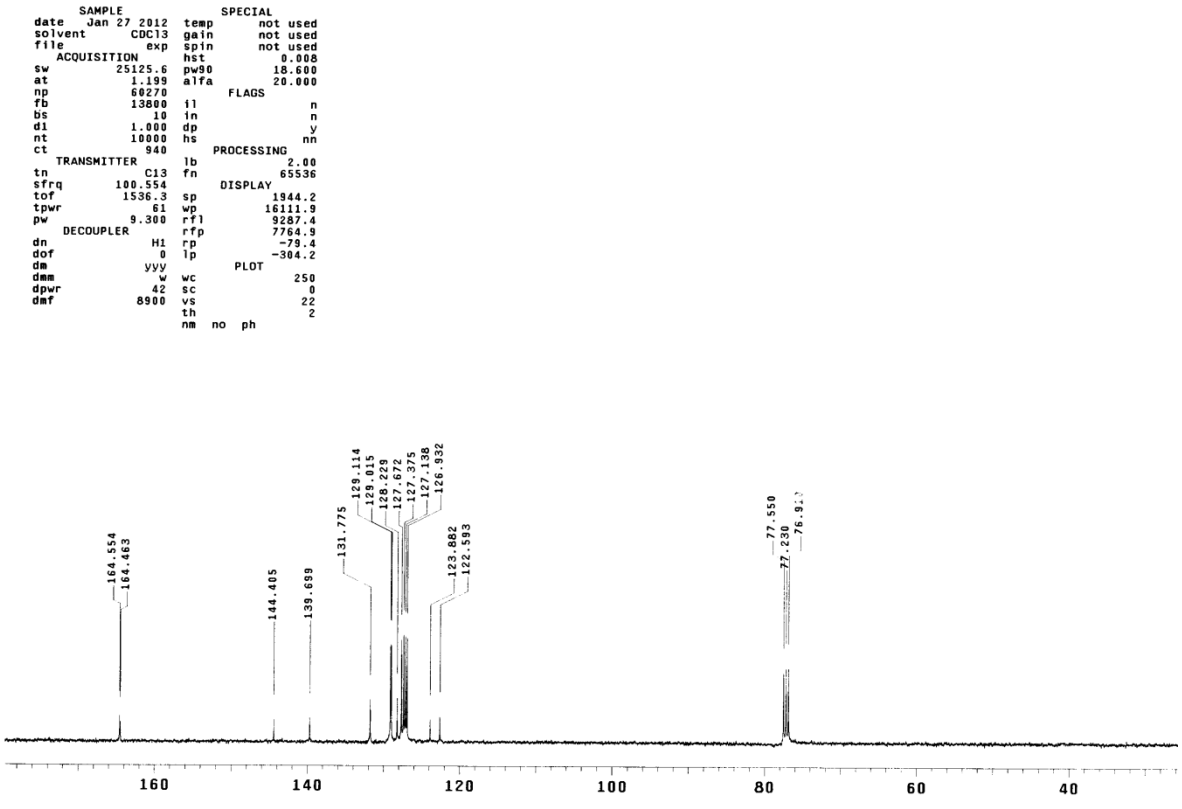
4-(5-Phenyl-1,3,4-oxadiazol-2-yl)-benzaldehyde (6a): HRMS



2-Biphenyl-4-yl-5-phenyl-1,3,4-oxadiazole (7a): ^{1}H NMR (400 MHz, $CDCl_3$)

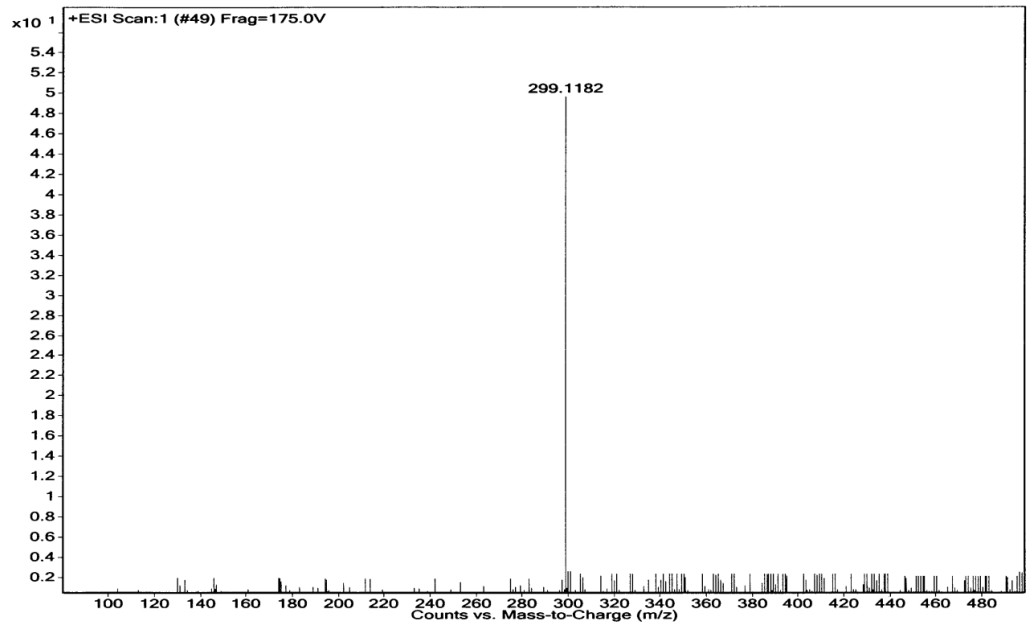


2-Biphenyl-4-yl-5-phenyl-1,3,4-oxadiazole (7a): ^{13}C NMR (100 MHz, $CDCl_3$)



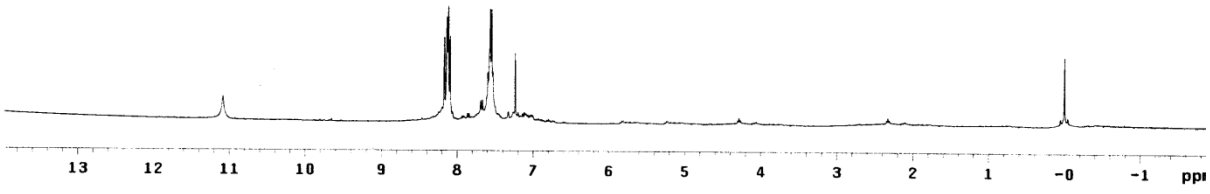
2-Biphenyl-4-yl-5-phenyl-1,3,4-oxadiazole (7a): HRMS

Sample Name	**Position**	**Instrument Name**	**User Name**
Inj Vol	**InjPosition**	**SampleType**	**IRM Calibration Status**
Data Filename	**ACQ Method**	**Comment**	**Acquired Time**

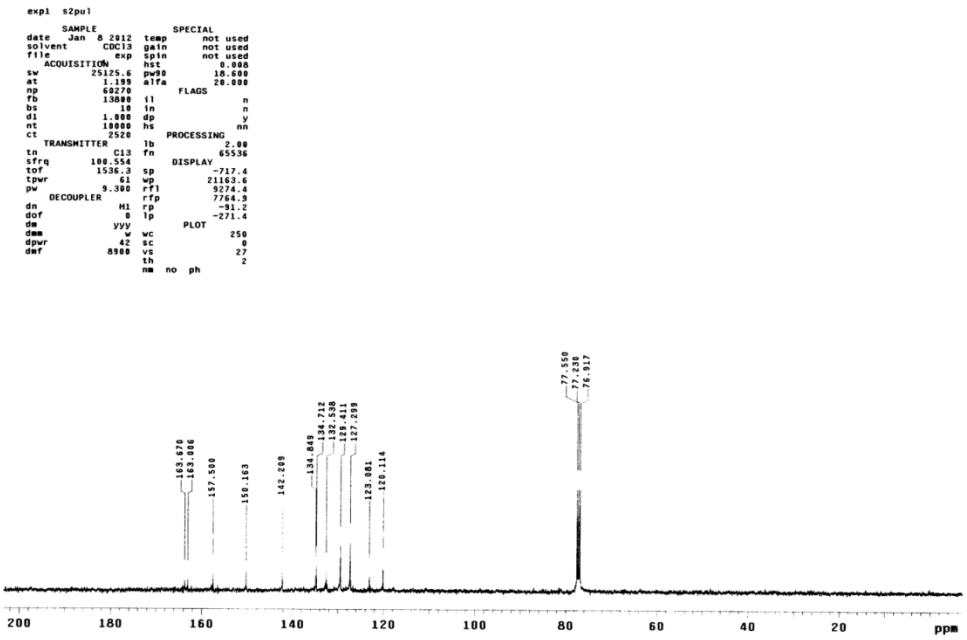


2-(5-Phenyl-1,3,4-oxadiazol-2-yl)-phenol (8a): ^{1}H NMR (400 MHz, $CDCl_3$)

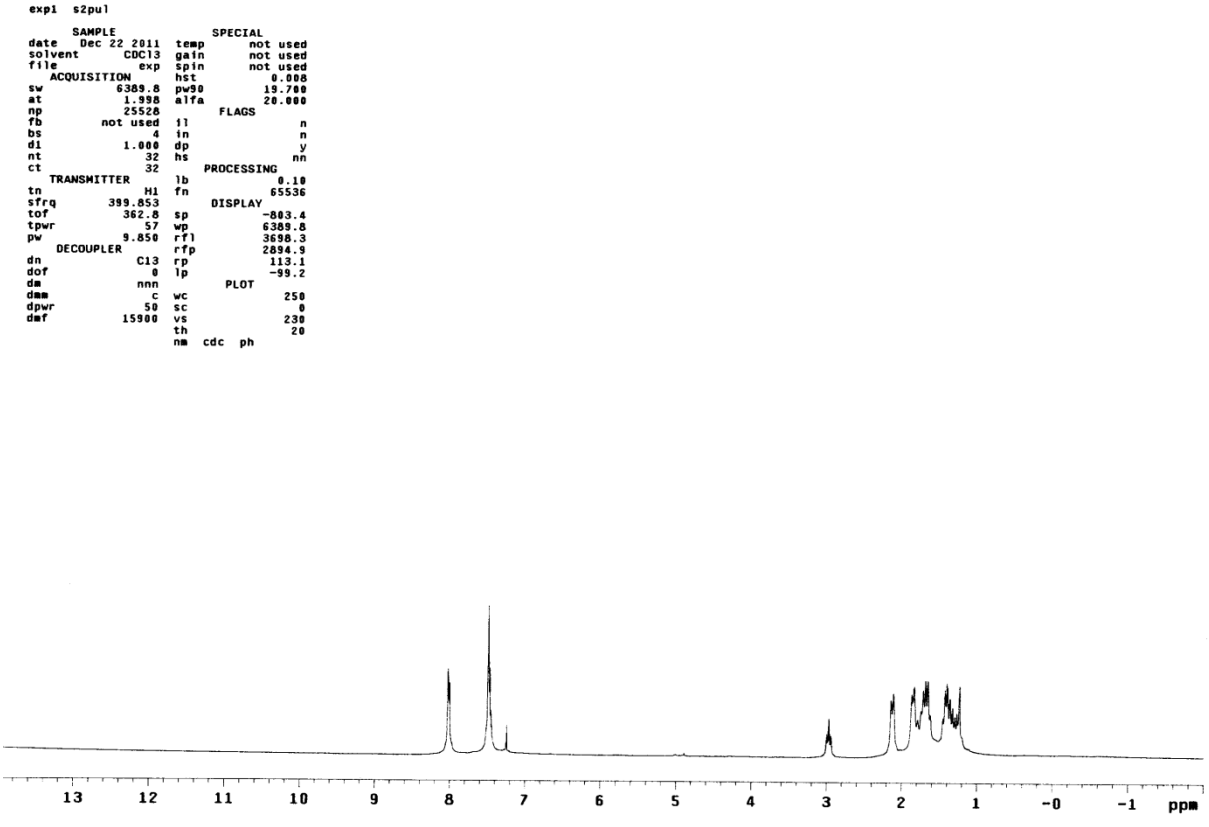
```
exp1  s2pul

      SAMPLE                SPECIAL
date   Jan  3 2012  temp       not used
solvent      CDCl3  gain       not used
file           exp  spin       not used
   ACQUISITION       hst          0.008
sw          6389.8  pw90        19.700
at           1.998  alfa        20.000
np           25528        FLAGS
fb       not used  il               n
bs              4  in               n
d1          1.000  dp               y
nt             32  hs              nn
ct             32      PROCESSING
   TRANSMITTER       lb           0.10
tn              H1  fn          65536
sfrq       399.853      DISPLAY
tof          362.8  sp         -804.7
tpwr            57  wp         6389.8
pw           9.850  rfl        3699.7
    DECOUPLER       rfp        2894.9
dn             C13  rp          115.1
dof              0  lp          -84.2
dm             nnn       PLOT
dmm              c  wc            250
dpwr            50  sc              0
dmf          15900  vs            301
                    th              9
                    nm  cdc  ph
```



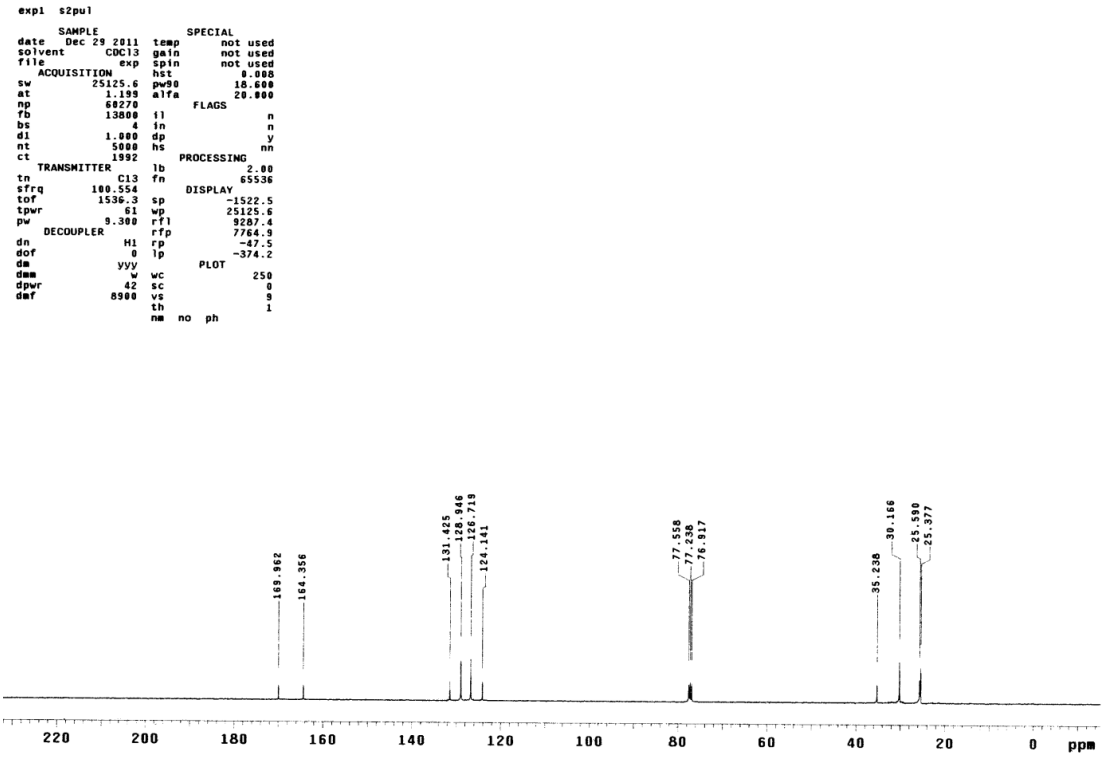
2-(5-Phenyl-1,3,4-oxadiazol-2-yl)-phenol (8a): ^{13}C NMR (100 MHz, $CDCl_3$)



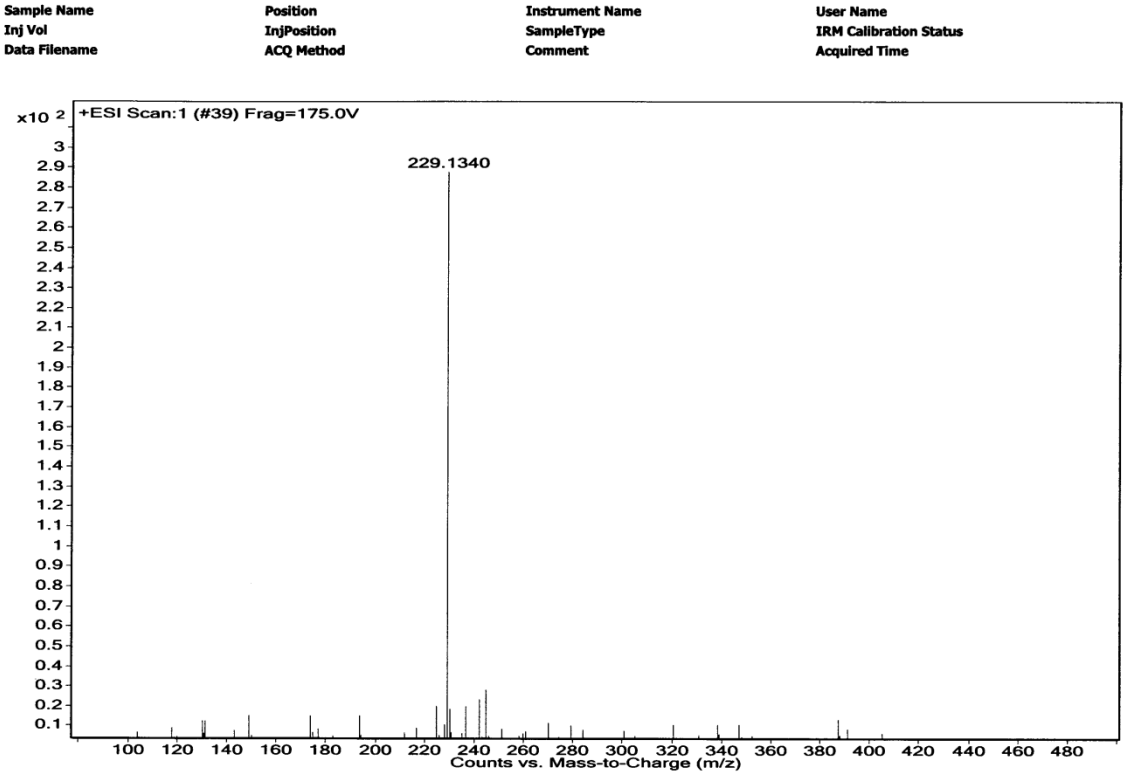
2-Cyclohexyl-5-phenyl-1,3,4-oxadiazole (9a): ^{1}H NMR (400 MHz, $CDCl_3$)



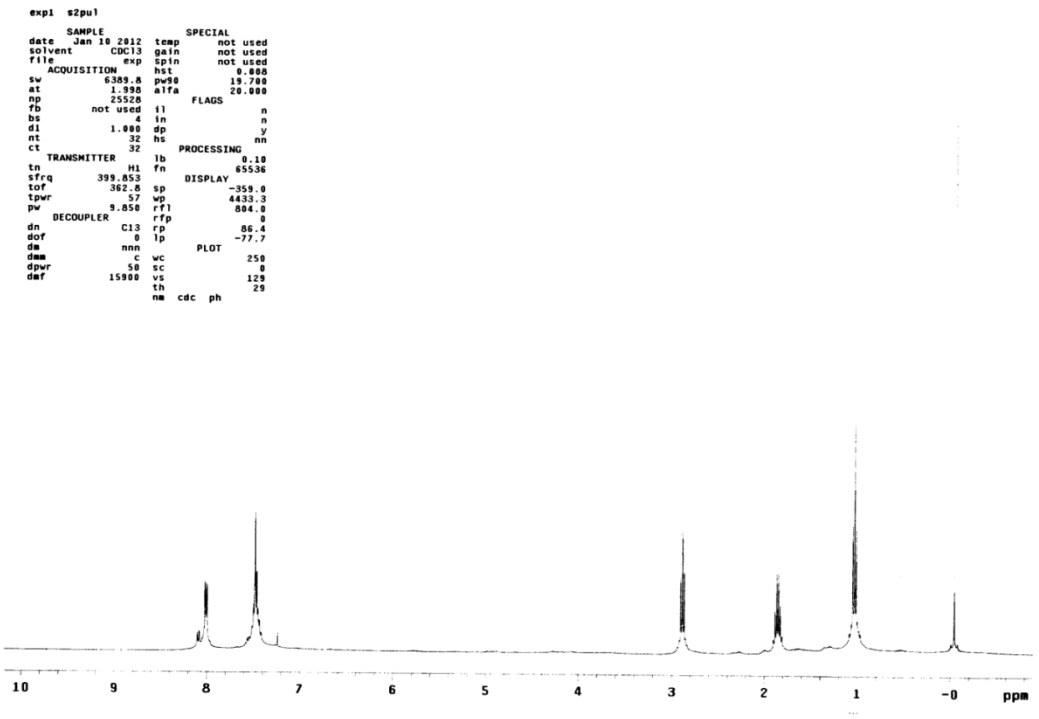
2-Cyclohexyl-5-phenyl-1,3,4-oxadiazole (9a): ^{13}C NMR (100 MHz, $CDCl_3$)



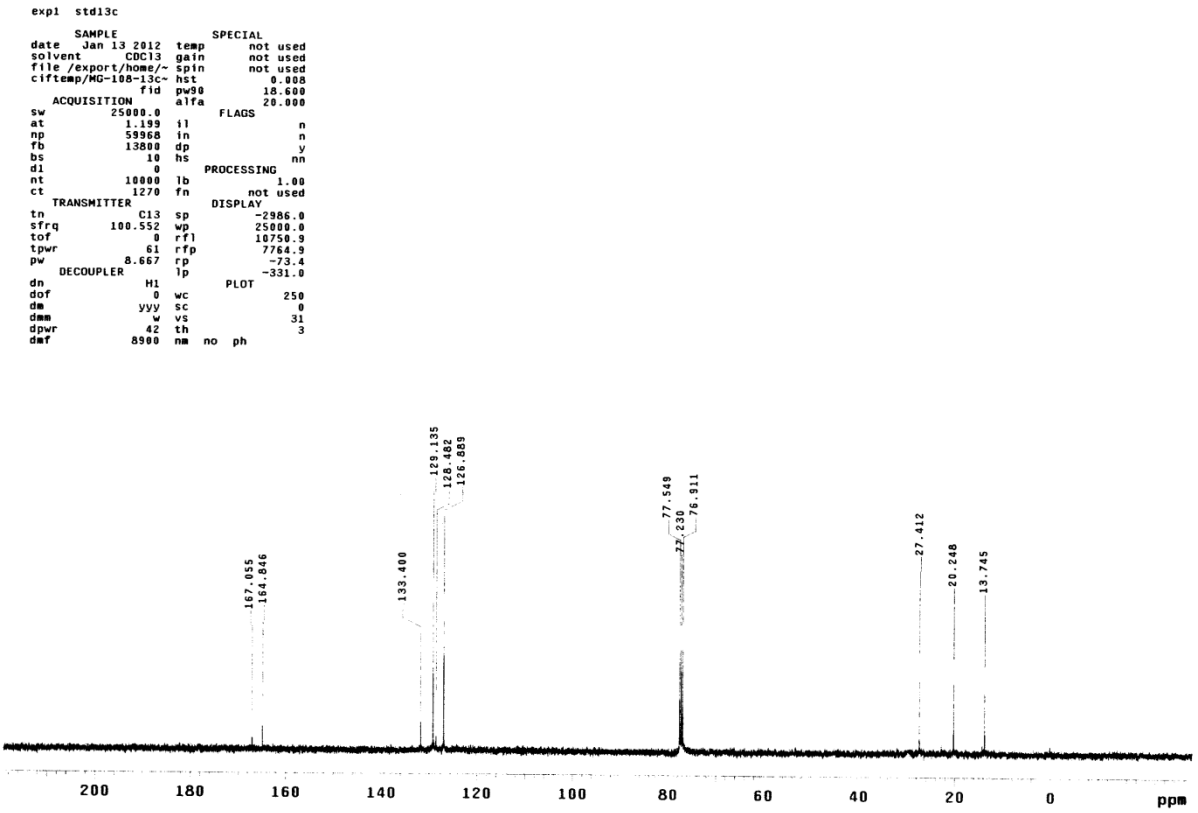
2-Cyclohexyl-5-phenyl-1,3,4-oxadiazole (9a): HRMS



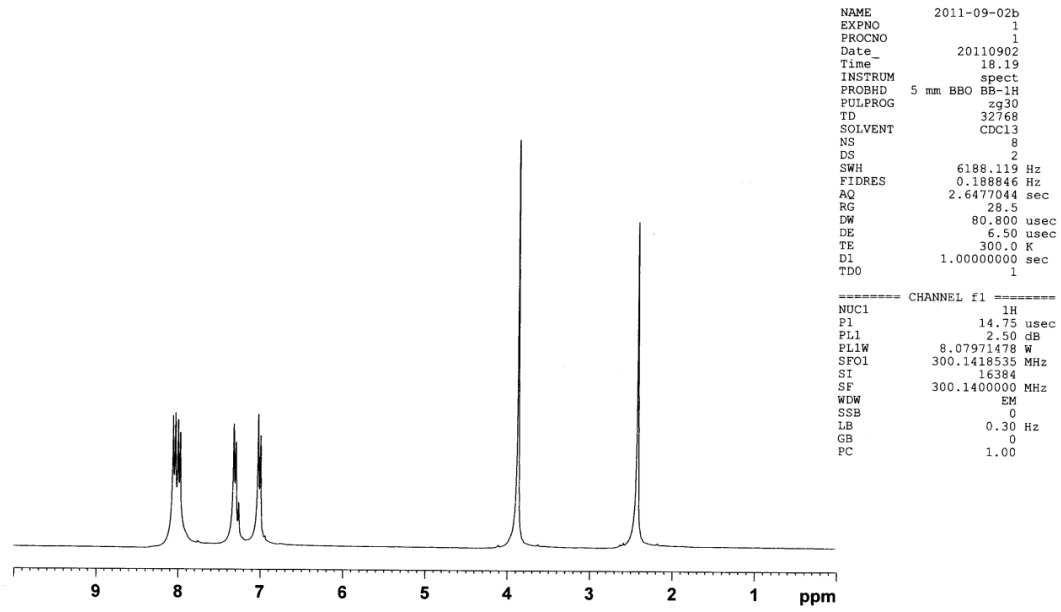
2-Phenyl-5-propyl-1,3,4-oxadiazole (10a): ^{1}H NMR (400 MHz, $CDCl_3$)



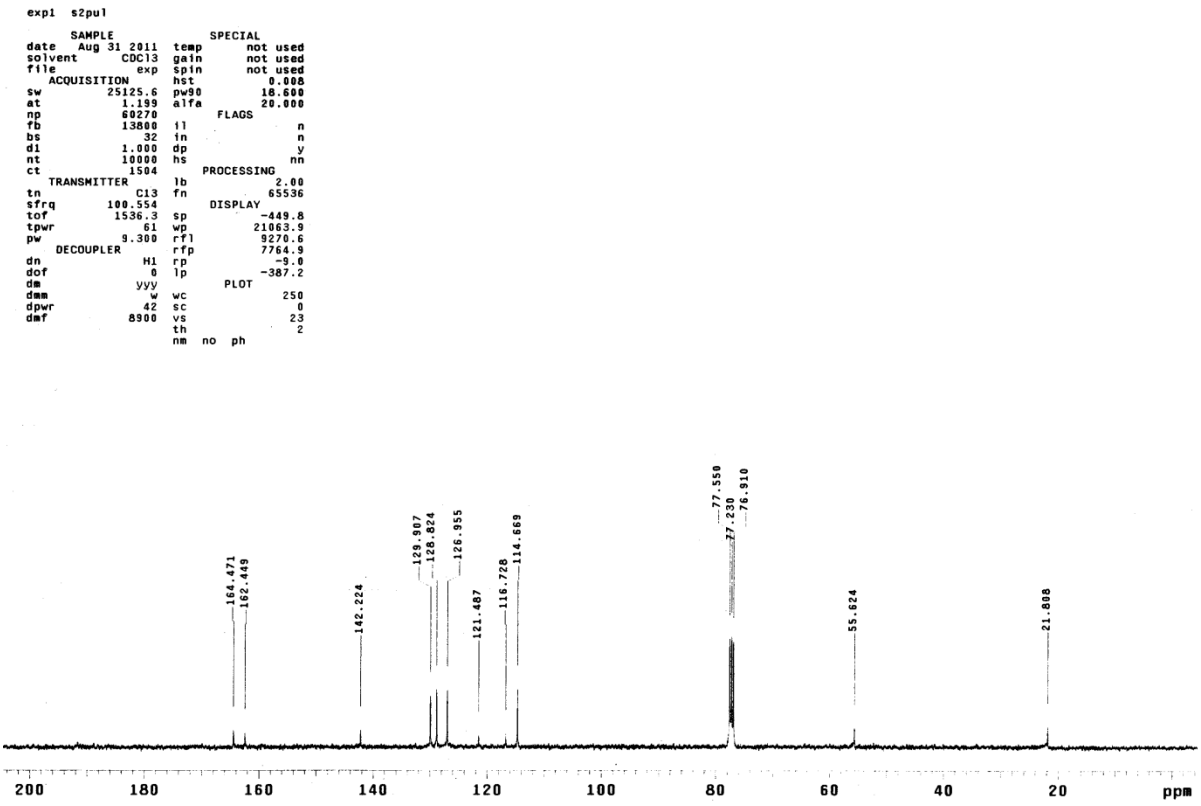
2-Phenyl-5-propyl-1,3,4-oxadiazole (10a): ^{13}C NMR (100 MHz, $CDCl_3$)



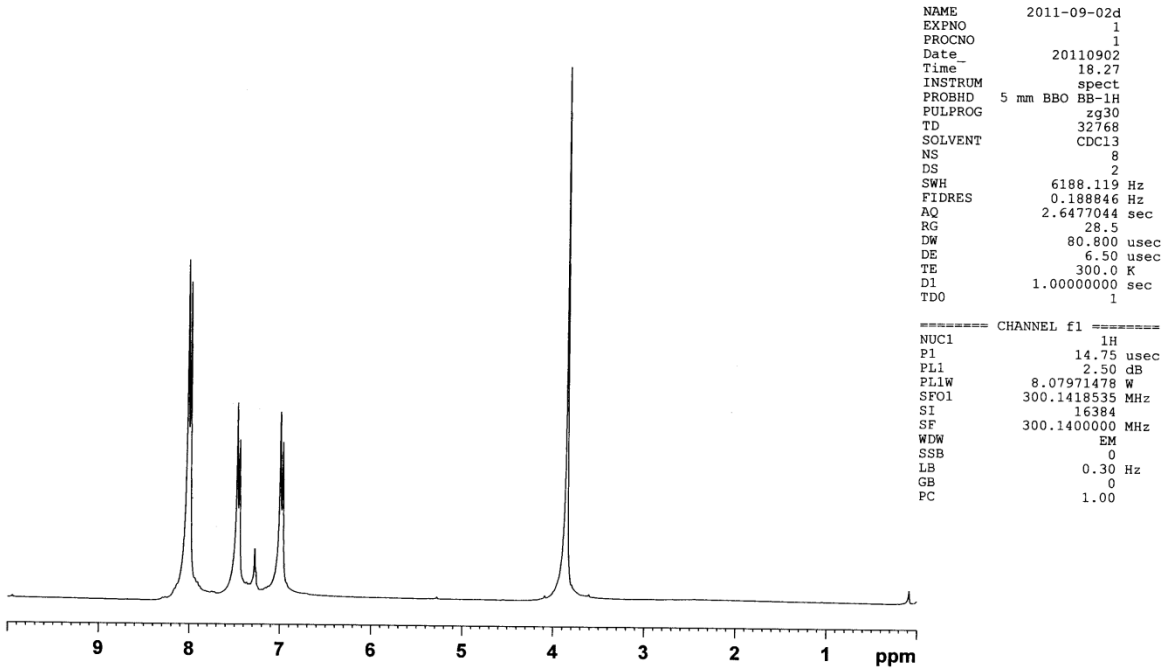
2-(4-Methoxyphenyl)-5-p-tolyl-1,3,4-oxadiazole (11a): ^{1}H NMR (400 MHz, $CDCl_3$)



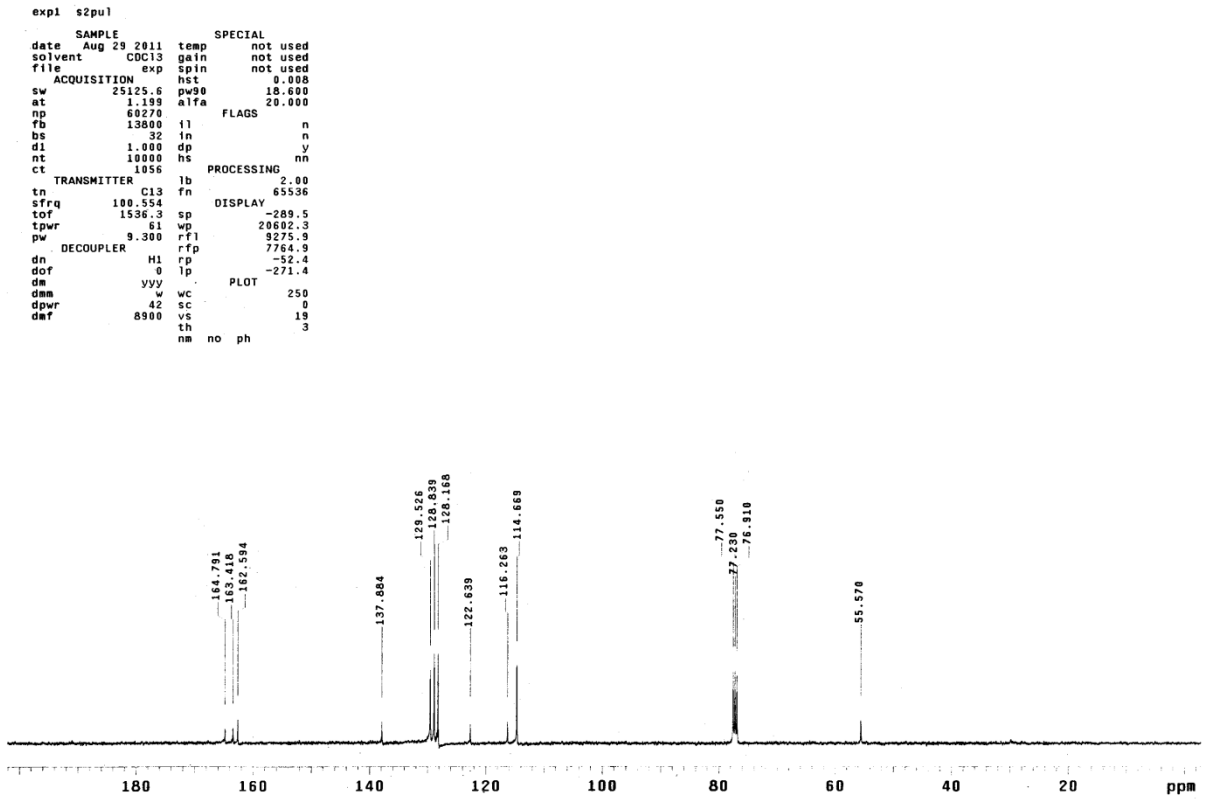
2-(4-Methoxyphenyl)-5-p-tolyl-1,3,4-oxadiazole (11a): ^{13}C NMR (100 MHz, $CDCl_3$)



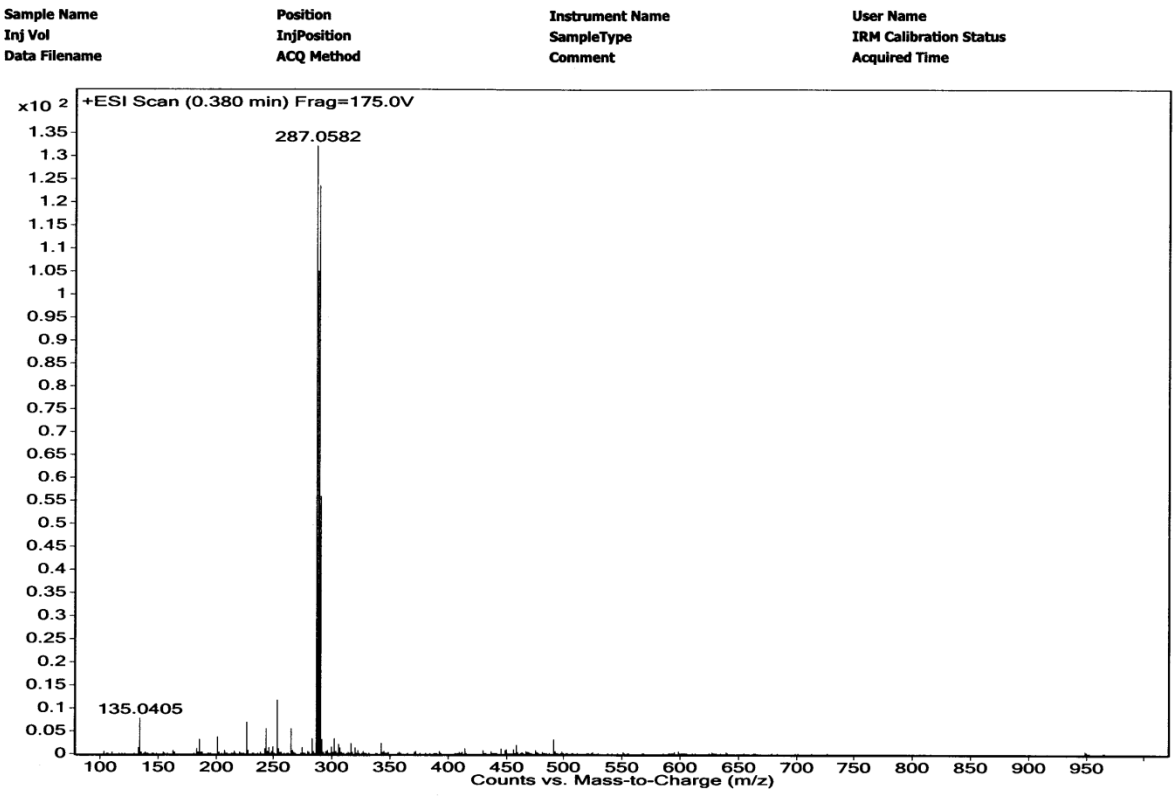
2-(4-Chlorophenyl)-5-(4-methoxyphenyl)-1,3,4-oxadiazole (12a): ^{1}H NMR (400 MHz, $CDCl_3$)



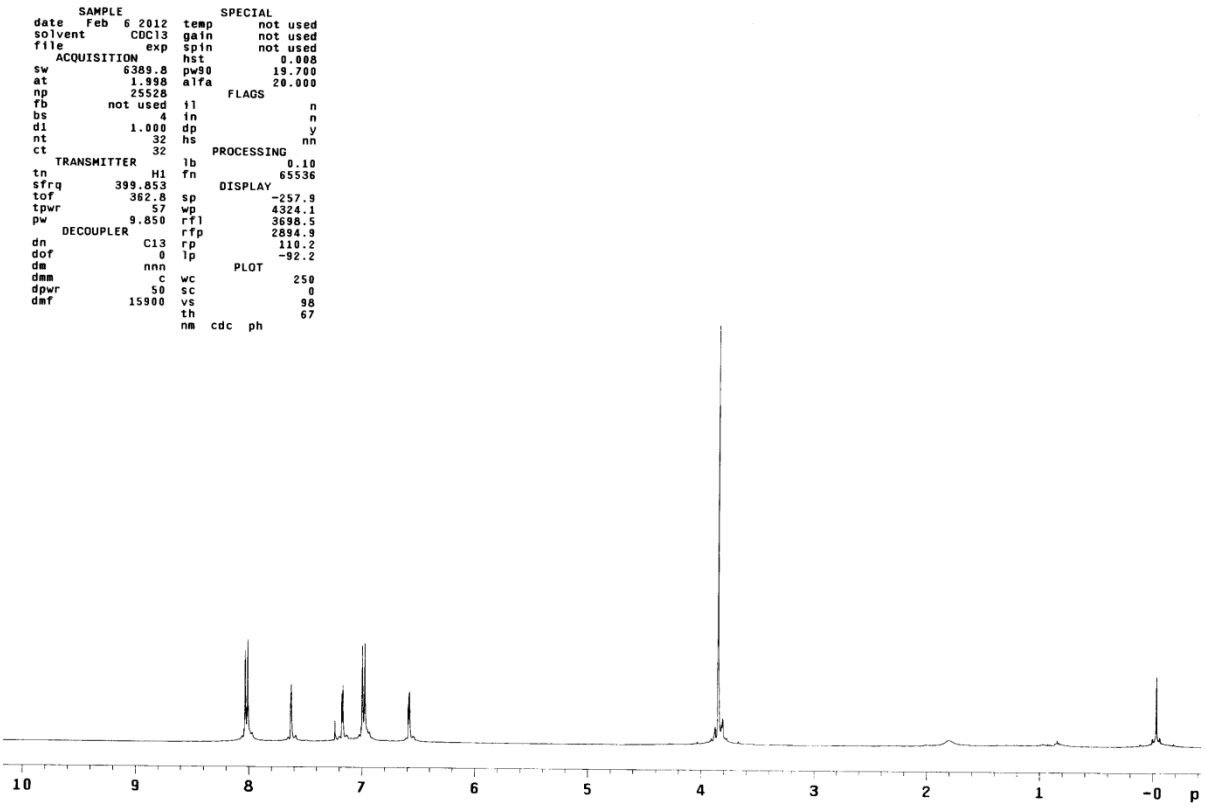
2-(4-Chlorophenyl)-5-(4-methoxyphenyl)-1,3,4-oxadiazole (12a): ^{13}C NMR (100 MHz, $CDCl_3$)



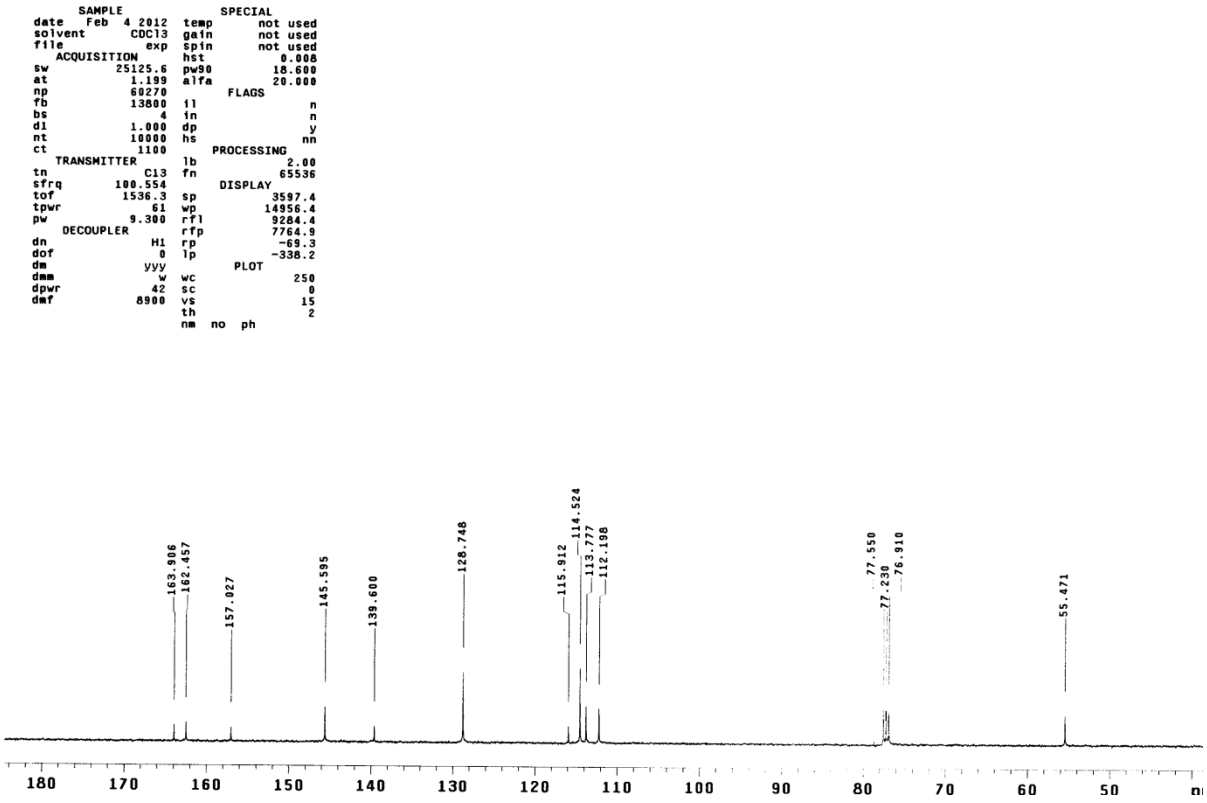
2-(4-Chlorophenyl)-5-(4-methoxyphenyl)-1,3,4-oxadiazole (12a): HRMS



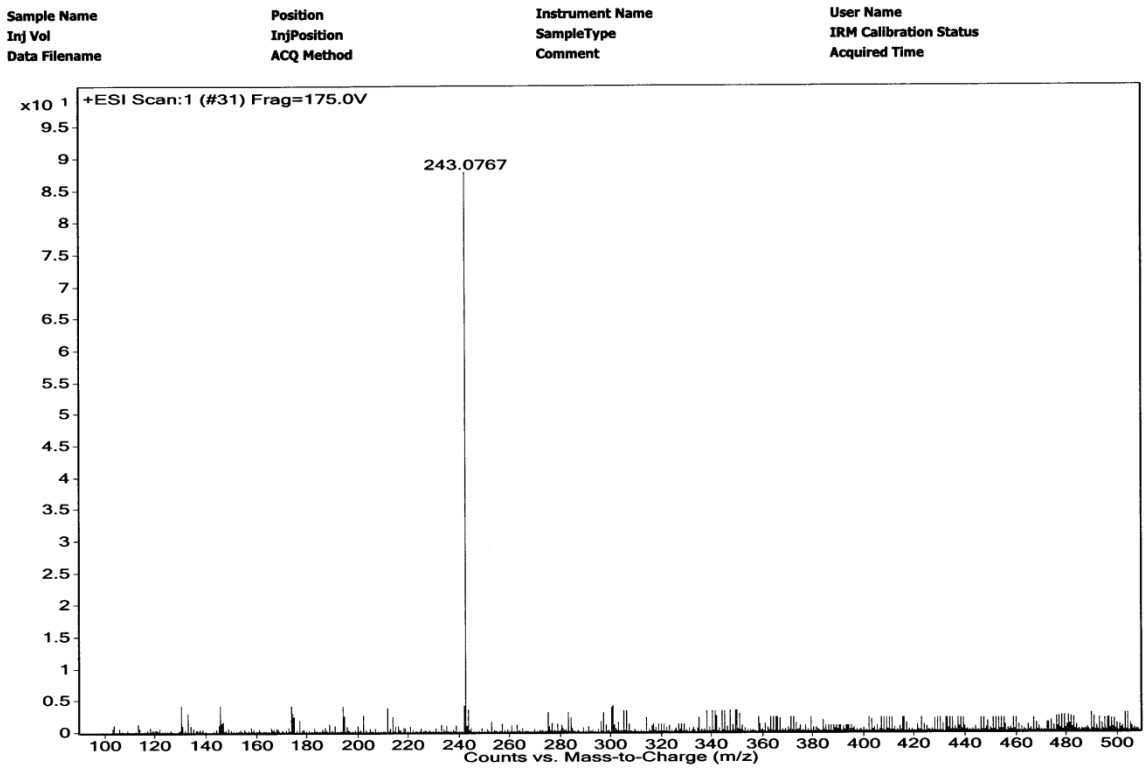
2-Furan-2-yl-5-(4-methoxy-phenyl)-1,3,4-oxadiazole (13a): ^{1}H NMR (400 MHz, $CDCl_3$)



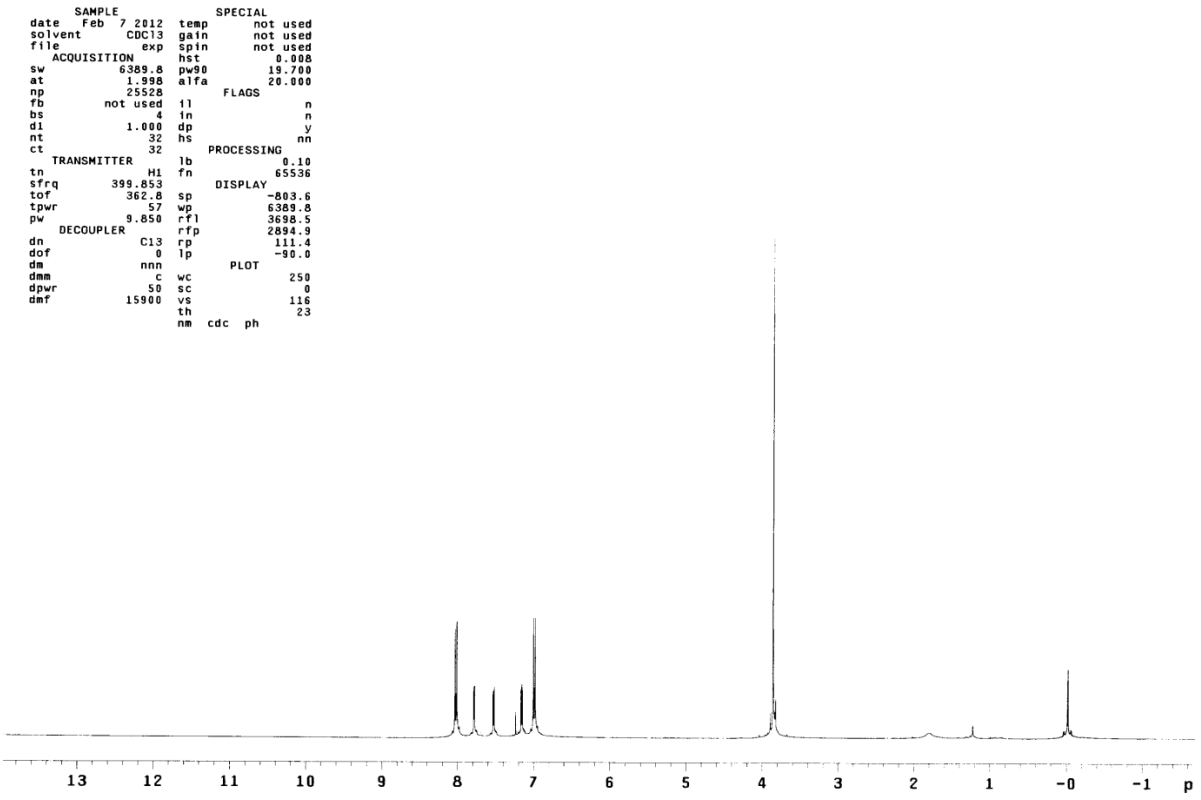
2-Furan-2-yl-5-(4-methoxy-phenyl)-1,3,4-oxadiazole (13a): ^{13}C NMR (100 MHz, $CDCl_3$)



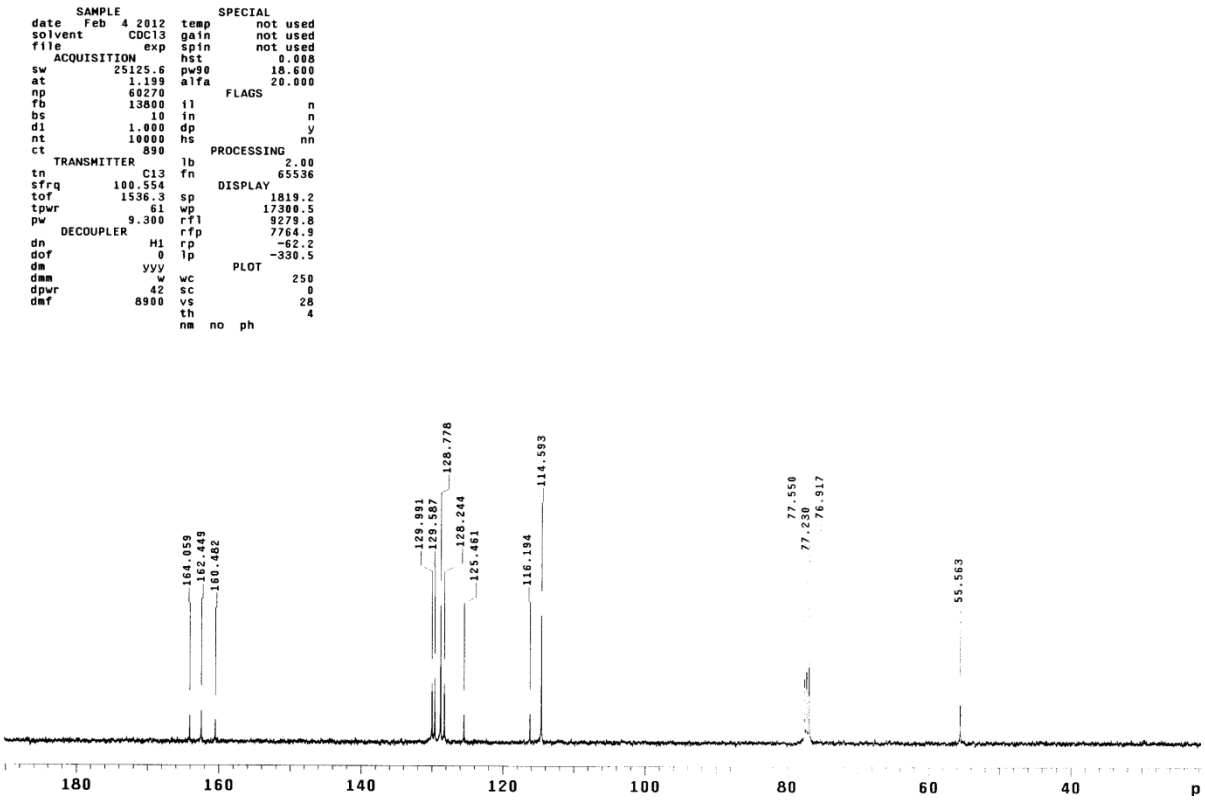
2-Furan-2-yl-5-(4-methoxy-phenyl)-1,3,4-oxadiazole (13a): HRMS



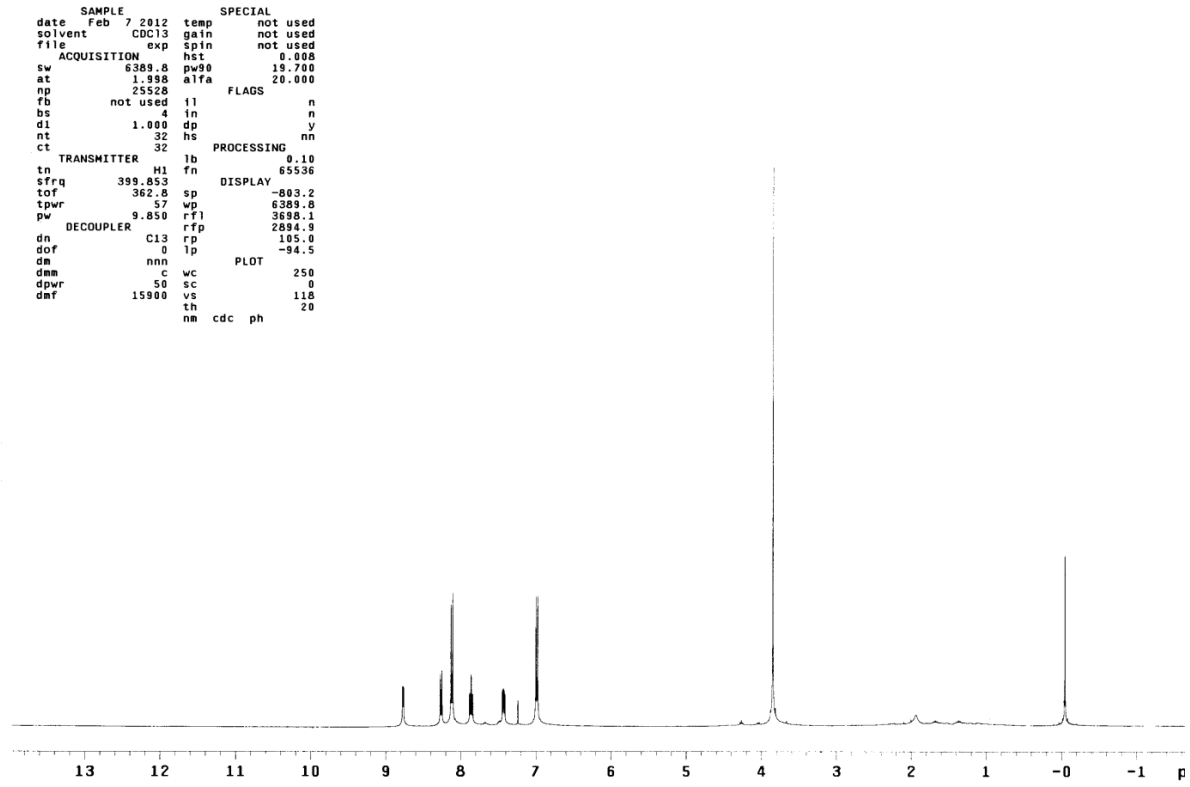
2-(4-Methoxy-phenyl)-5-thiophen-2-yl-1,3,4-oxadiazole (14a): ^{1}H NMR (400 MHz, $CDCl_3$)



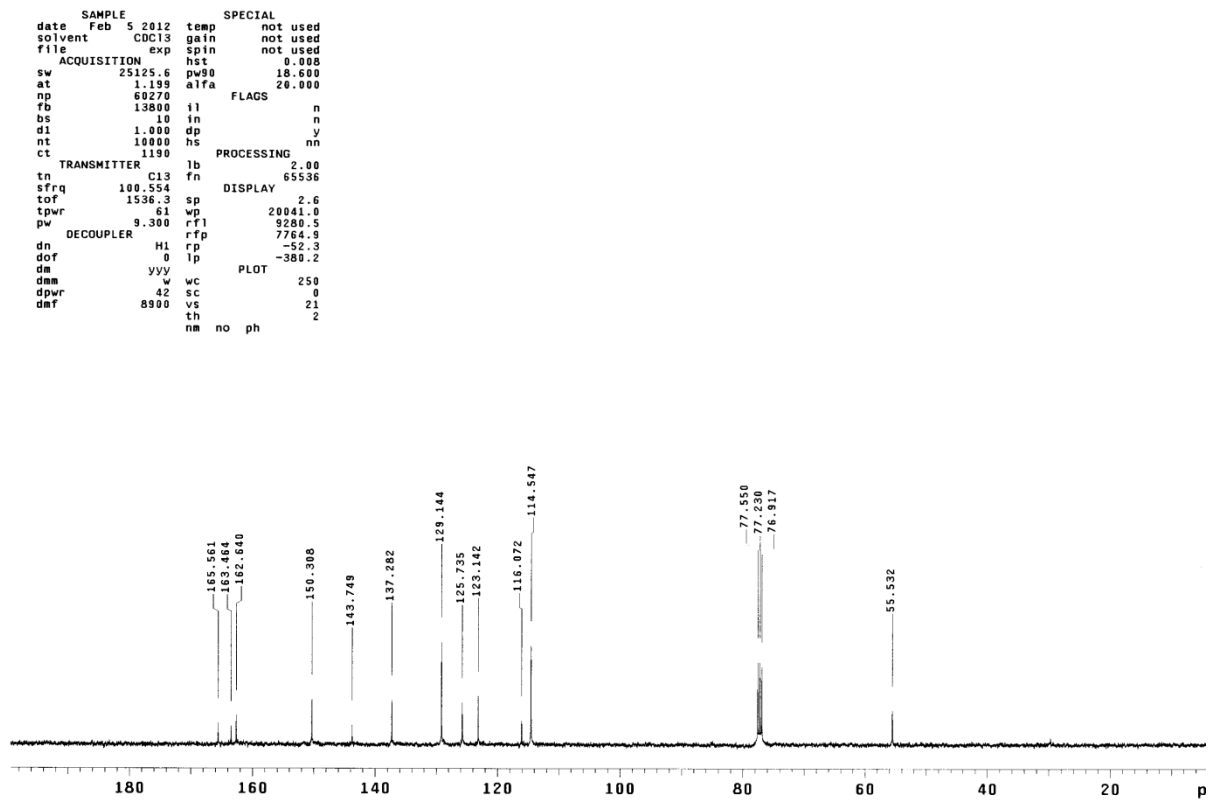
2-(4-Methoxy-phenyl)-5-thiophen-2-yl-1,3,4-oxadiazole (14a): ^{13}C NMR (100 MHz, $CDCl_3$)



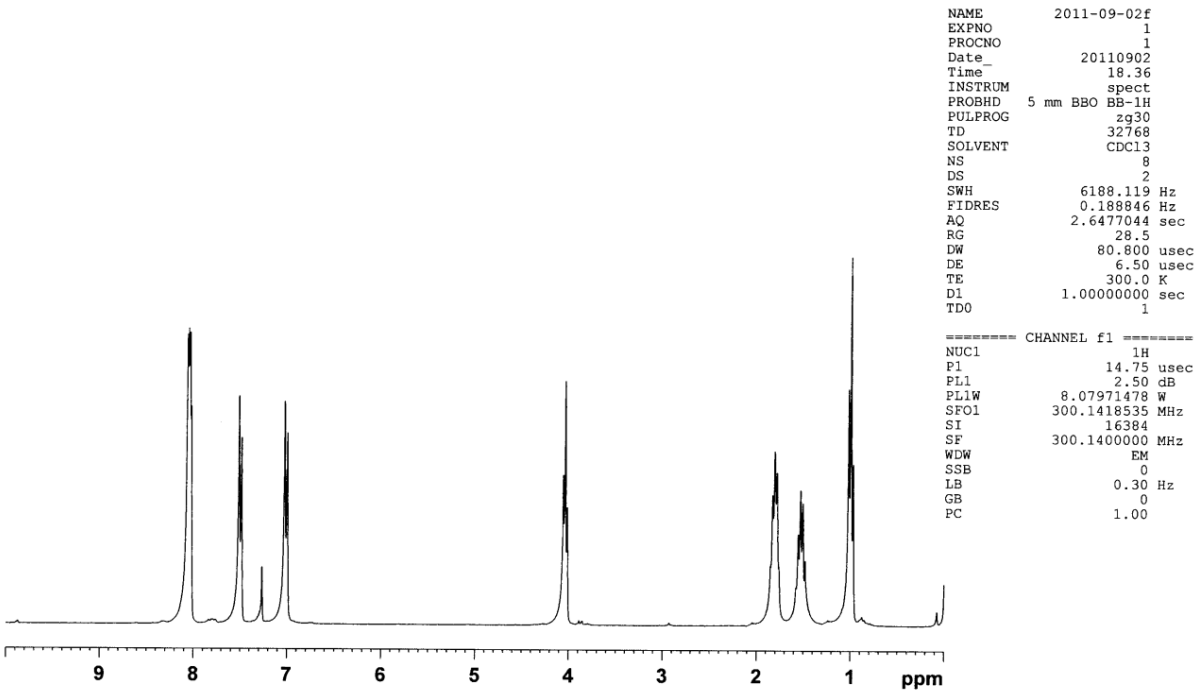
2-[5-(4-Methoxy-phenyl)-1,3,4-oxadiazole-2-yl]-pyridine (15a): ^{1}H NMR (400 MHz, $CDCl_3$)



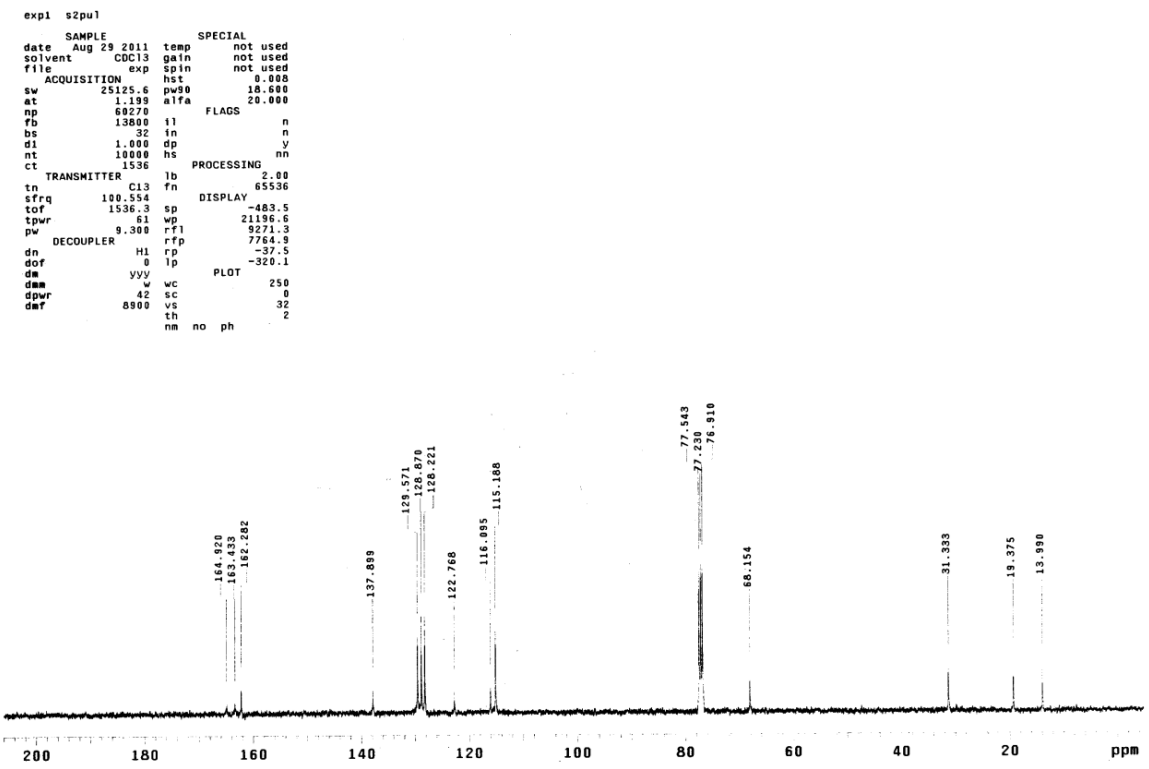
2-[5-(4-Methoxy-phenyl)-1,3,4-oxadiazole-2-yl]-pyridine (15a): ^{13}C NMR (100 MHz, $CDCl_3$)



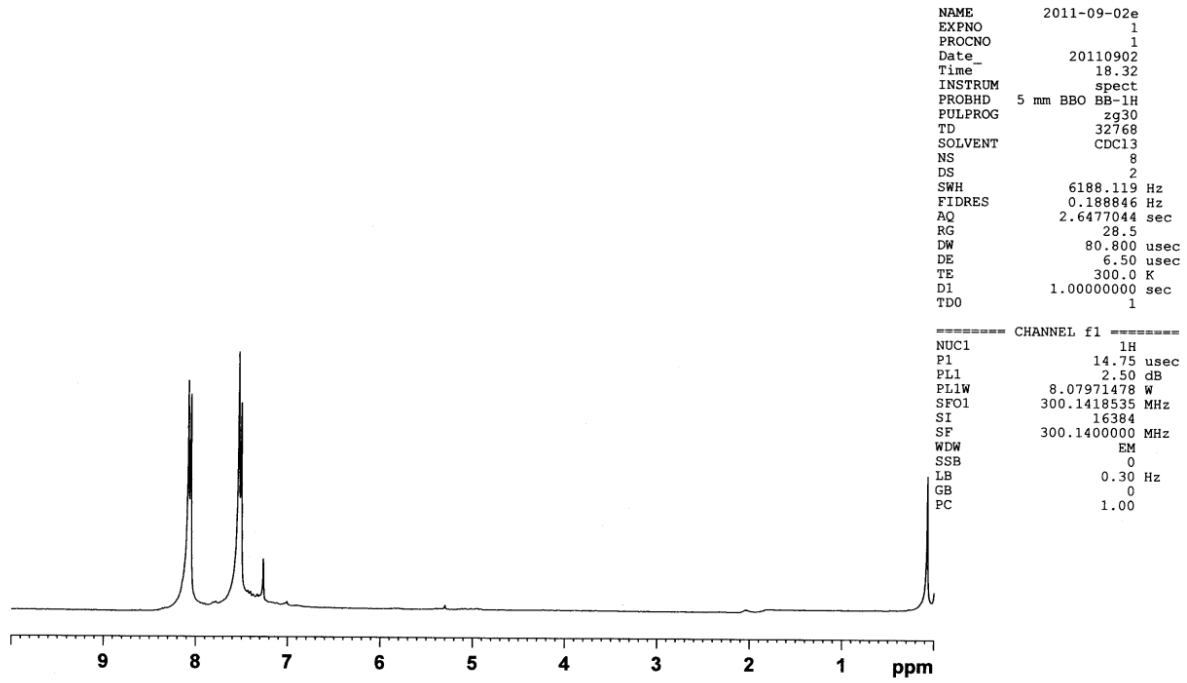
2-(4-Butoxyphenyl)-5-(4-chlorophenyl)-1,3,4-oxadiazole (16a): ^{1}H NMR (400 MHz, $CDCl_3$)



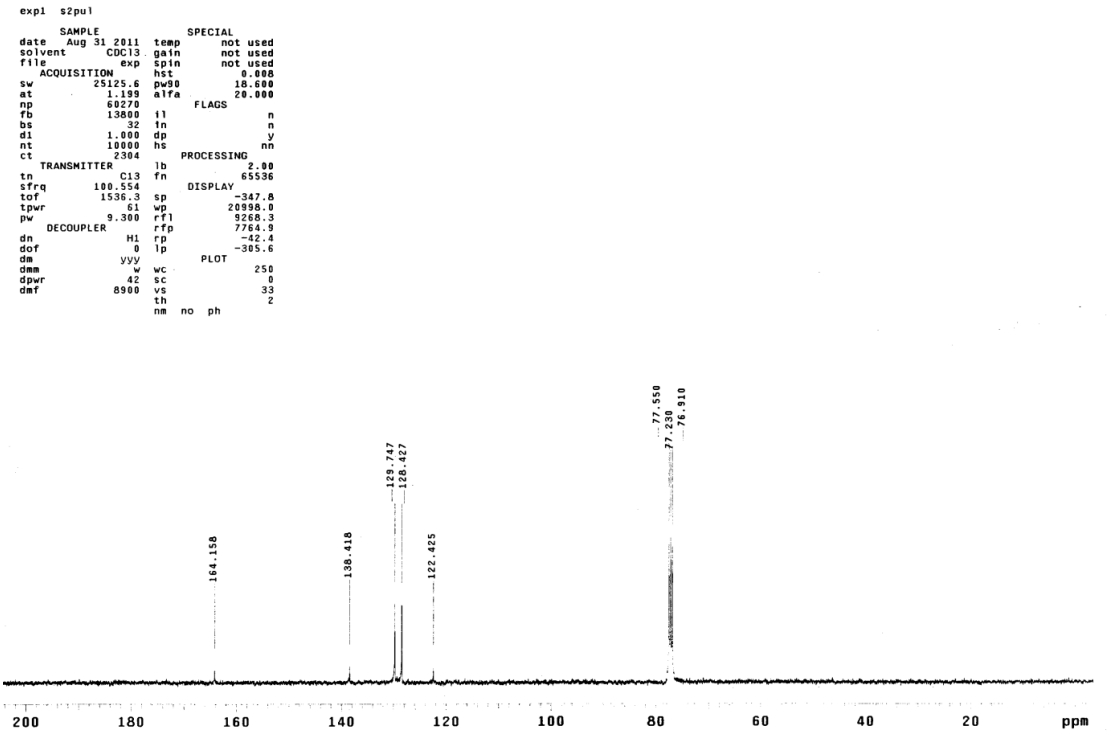
2-(4-Butoxyphenyl)-5-(4-chlorophenyl)-1,3,4-oxadiazole (16a): ^{13}C NMR (100 MHz, $CDCl_3$)



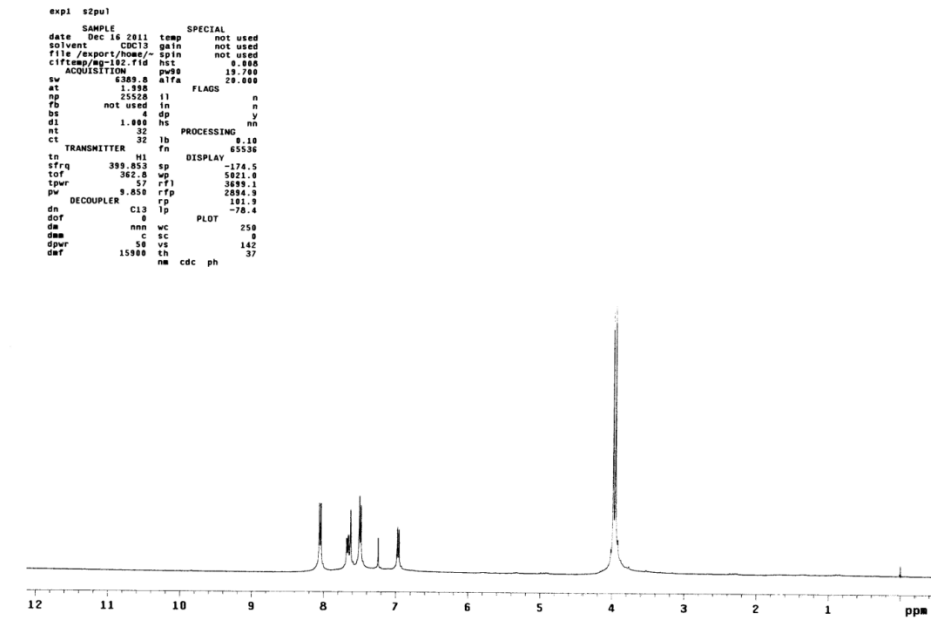
2,5-Bis(4-chlorophenyl)-1,3,4-oxadiazole (17a): ^{1}H NMR (400 MHz, $CDCl_3$)



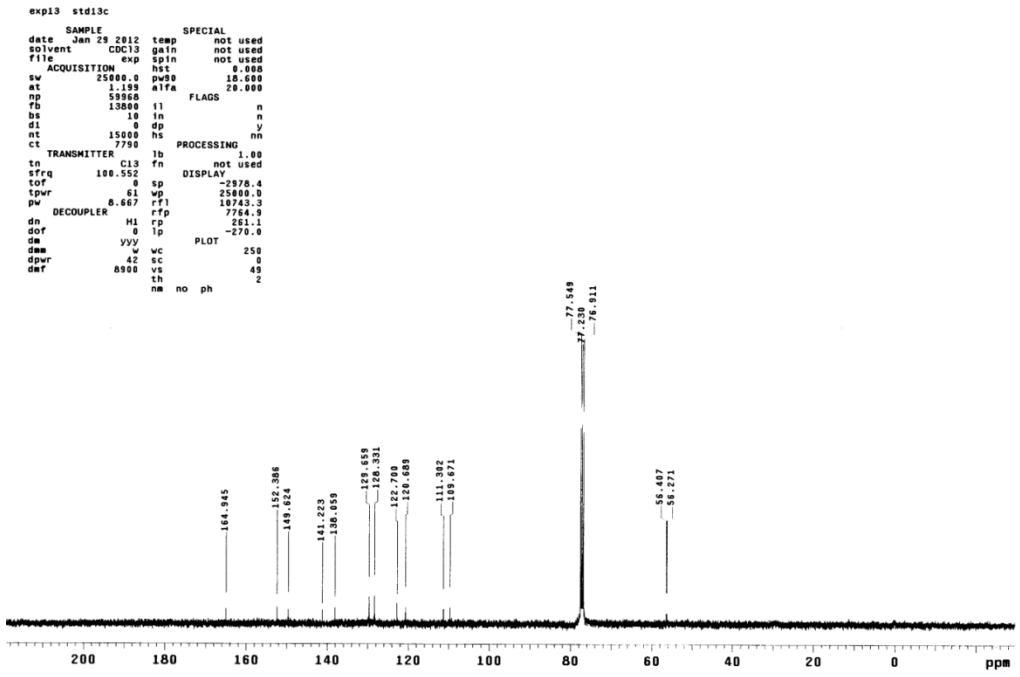
2,5-Bis(4-chlorophenyl)-1,3,4-oxadiazole (17a): ^{13}C NMR (100 MHz, $CDCl_3$)



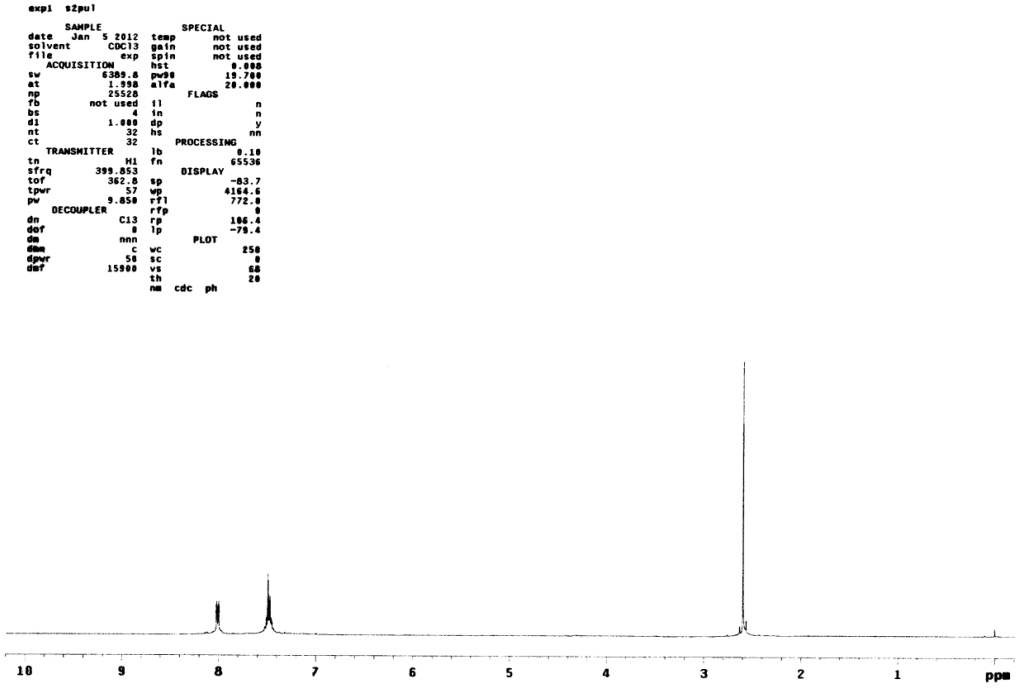
2-(4-Chloro-phenyl)-5-(3,4-dimethoxy-phenyl)-1,3,4-oxadiazole (18a): ^{1}H NMR (400 MHz, $CDCl_3$)



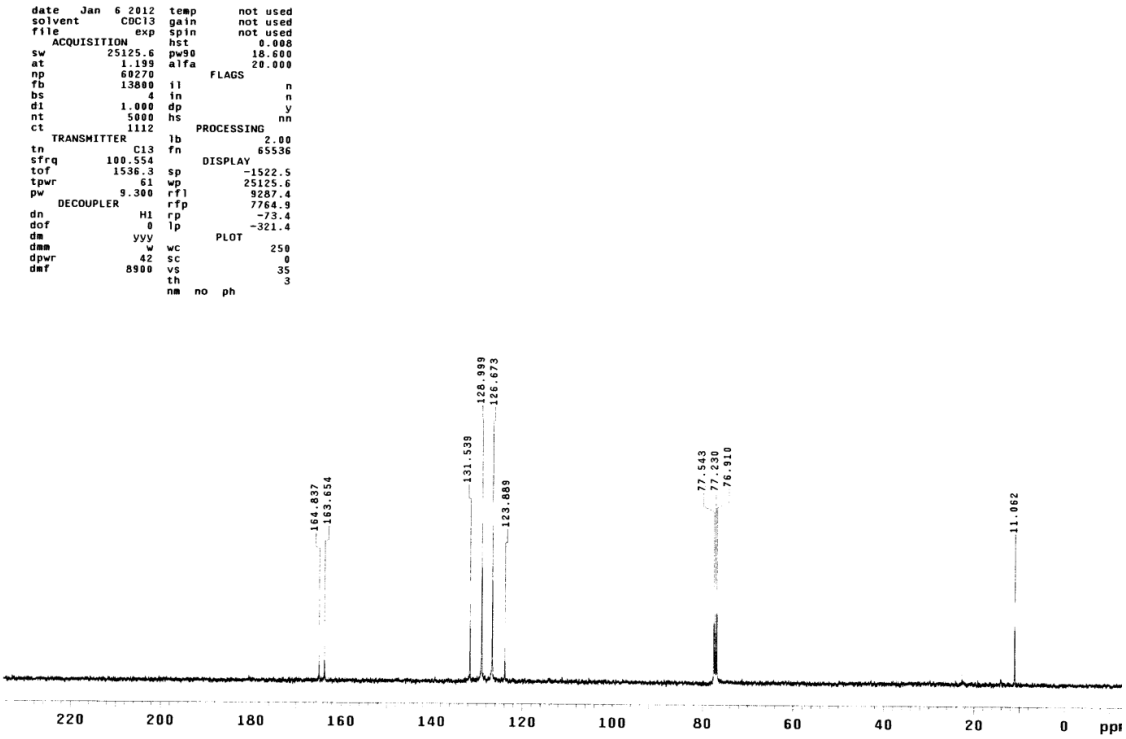
2-(4-Chloro-phenyl)-5-(3,4-dimethoxy-phenyl)-1,3,4-oxadiazole (18a): ^{13}C NMR (100 MHz, $CDCl_3$)



2-Methyl-5-phenyl-1,3,4-oxadiazole (19a): ^{1}H NMR (400 MHz, $CDCl_3$)

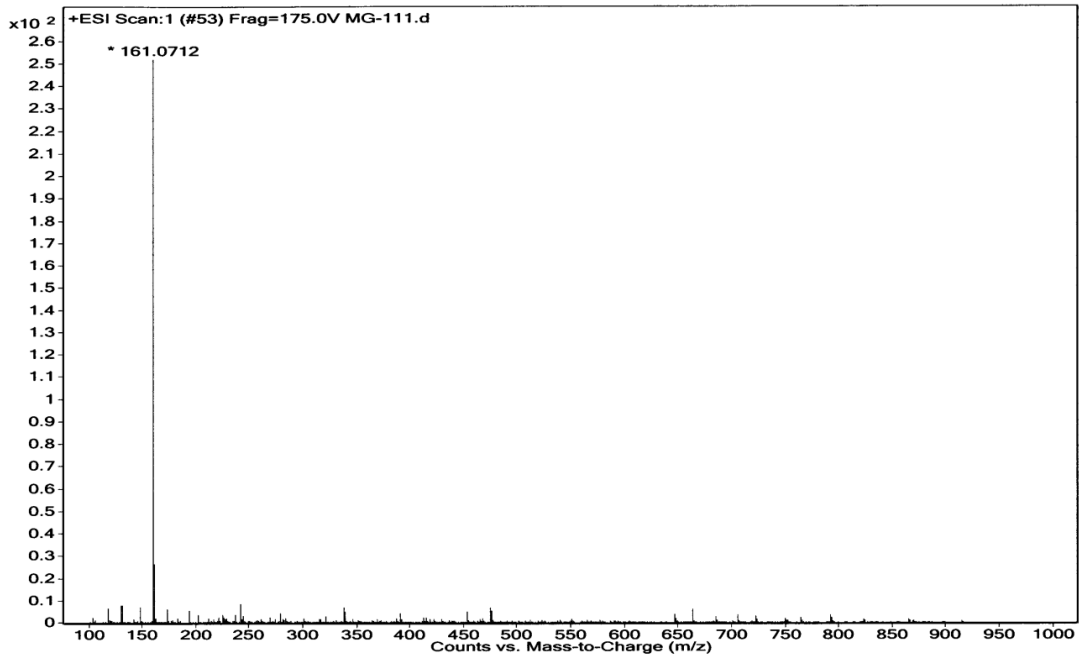


2-Methyl-5-phenyl-1,3,4-oxadiazole (19a): ^{13}C NMR (100 MHz, $CDCl_3$)

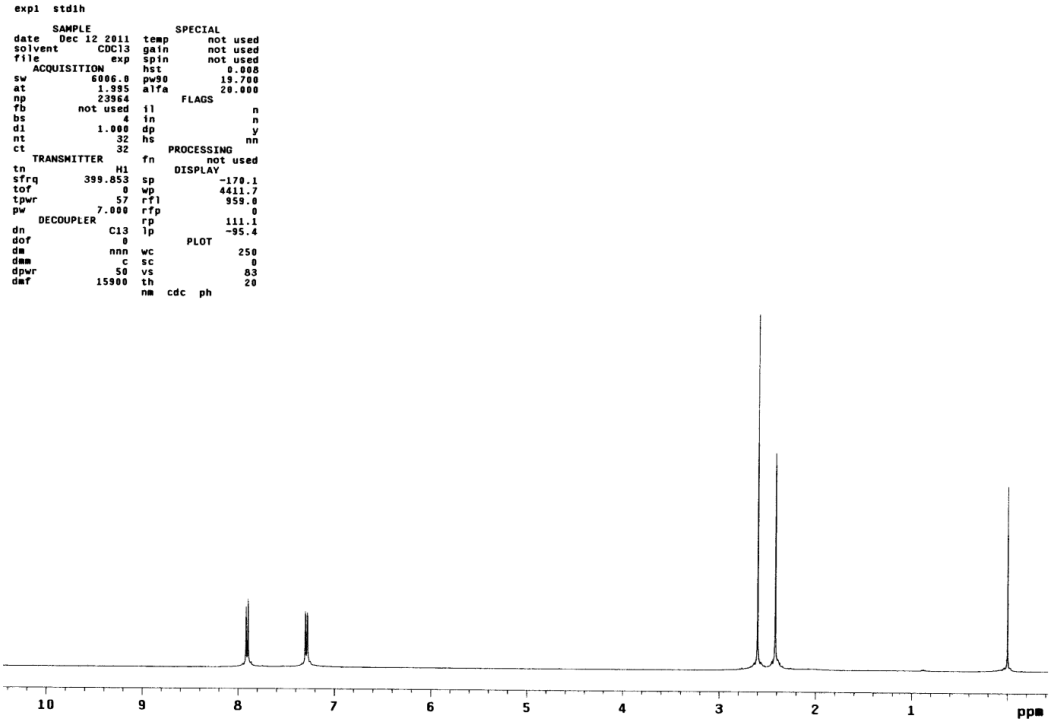


2-Methyl-5-phenyl-1,3,4-oxadiazole (19a): HRMS

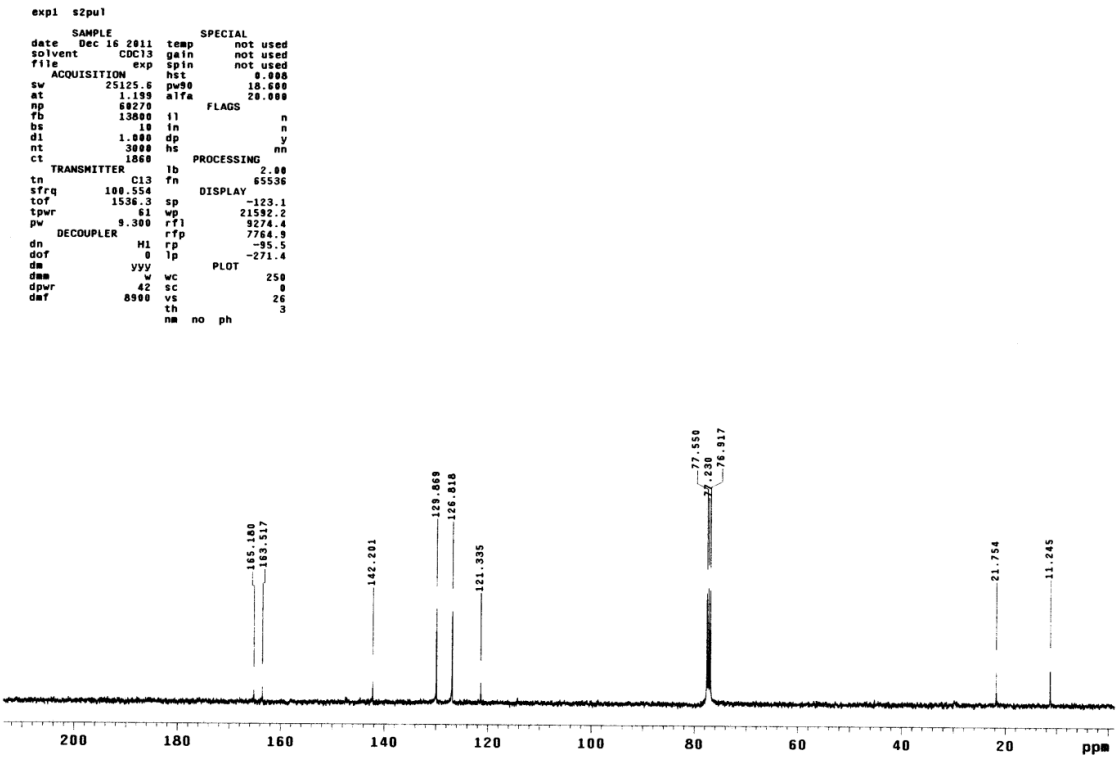
Sample Name	**Position**	**Instrument Name**	**User Name**
Inj Vol	**InjPosition**	**SampleType**	**IRM Calibration Status**
Data Filename	**ACQ Method**	**Comment**	**Acquired Time**



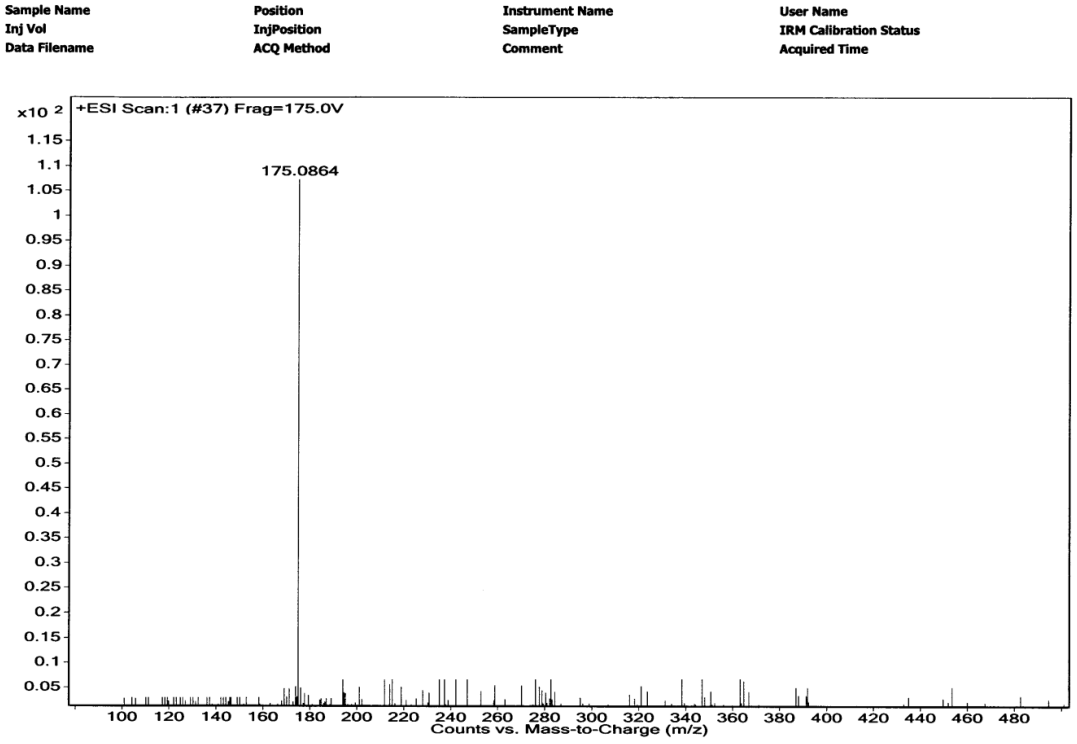
2-Methyl-5-p-tolyl-1,3,4-oxadiazole (20a): ^{1}H NMR (400 MHz, $CDCl_3$)



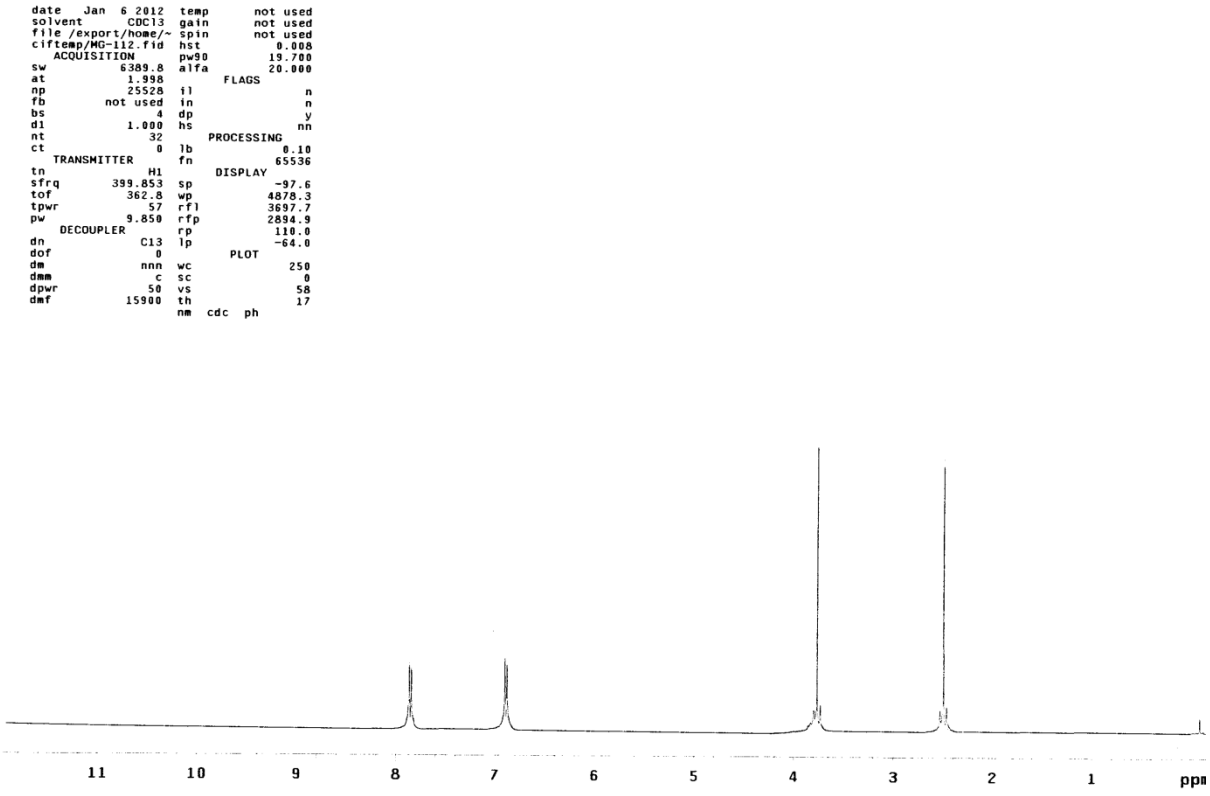
2-Methyl-5-p-tolyl-1,3,4-oxadiazole (20a): ^{13}C NMR (100 MHz, $CDCl_3$)



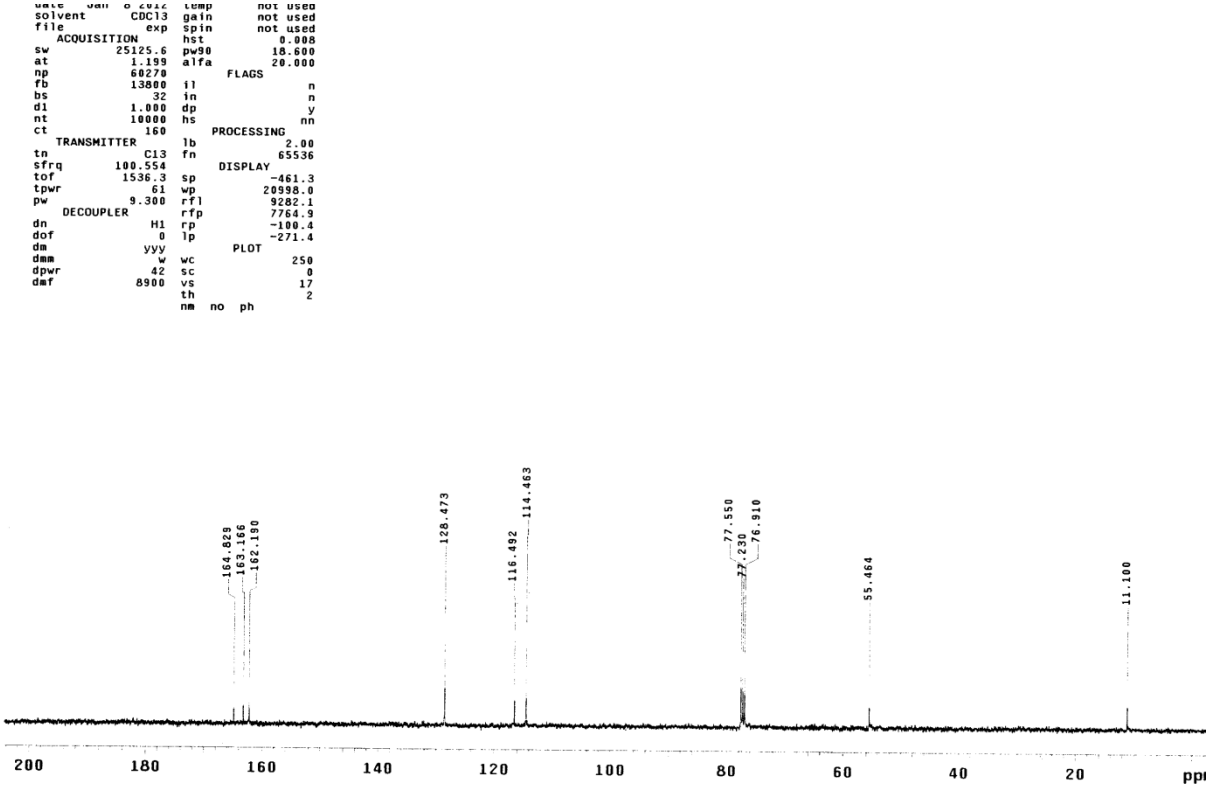
2-Methyl-5-p-tolyl-1,3,4-oxadiazole (20a): HRMS



2-(4-Methoxy-phenyl)-5-methyl-1,3,4-oxadiazole (21a): ^{1}H NMR (400 MHz, $CDCl_3$)

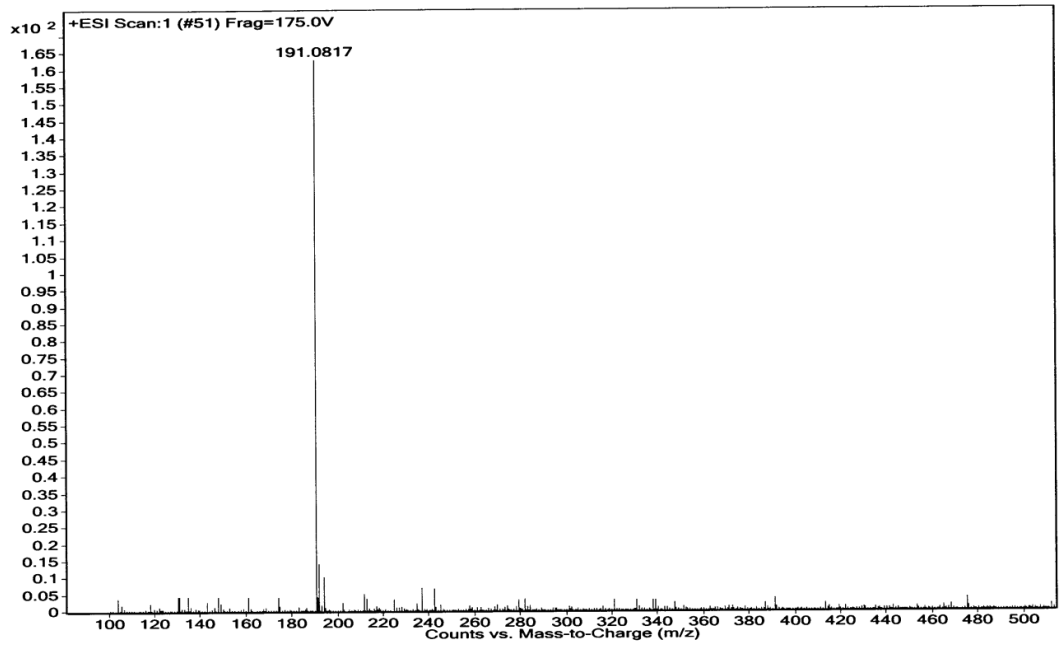


2-(4-Methoxy-phenyl)-5-methyl-1,3,4-oxadiazole (21a): ^{13}C NMR (100 MHz, $CDCl_3$)



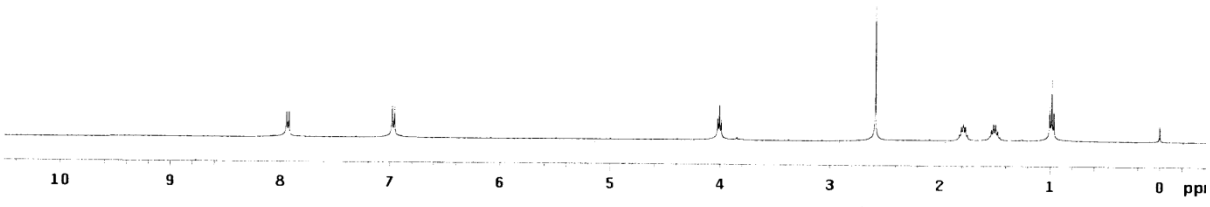
2-(4-Methoxy-phenyl)-5-methyl-1,3,4-oxadiazole (21a): HRMS

Sample Name	**Position**	**Instrument Name**	**User Name**
Inj Vol	**InjPosition**	**SampleType**	**IRM Calibration Status**
Data Filename	**ACQ Method**	**Comment**	**Acquired Time**

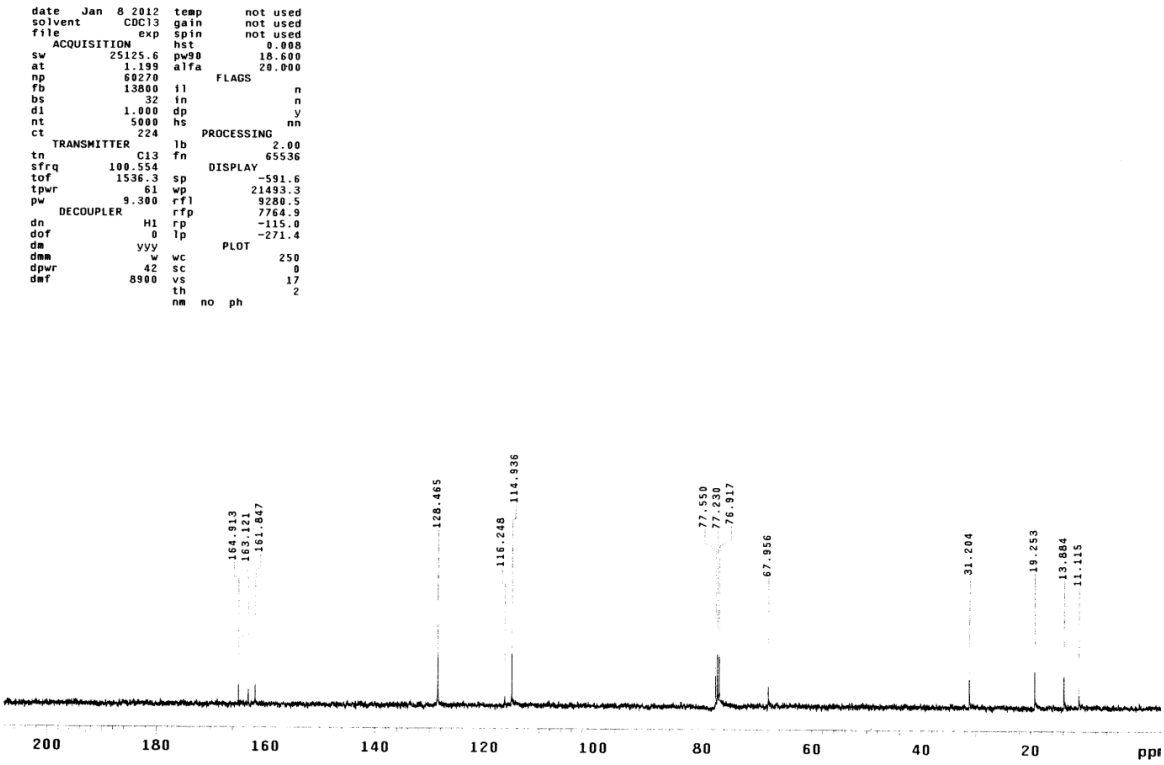


2-(4-Butoxy-phenyl)-5-methyl-1,3,4-oxadiazole (22a): ^{1}H NMR (400 MHz, $CDCl_3$)

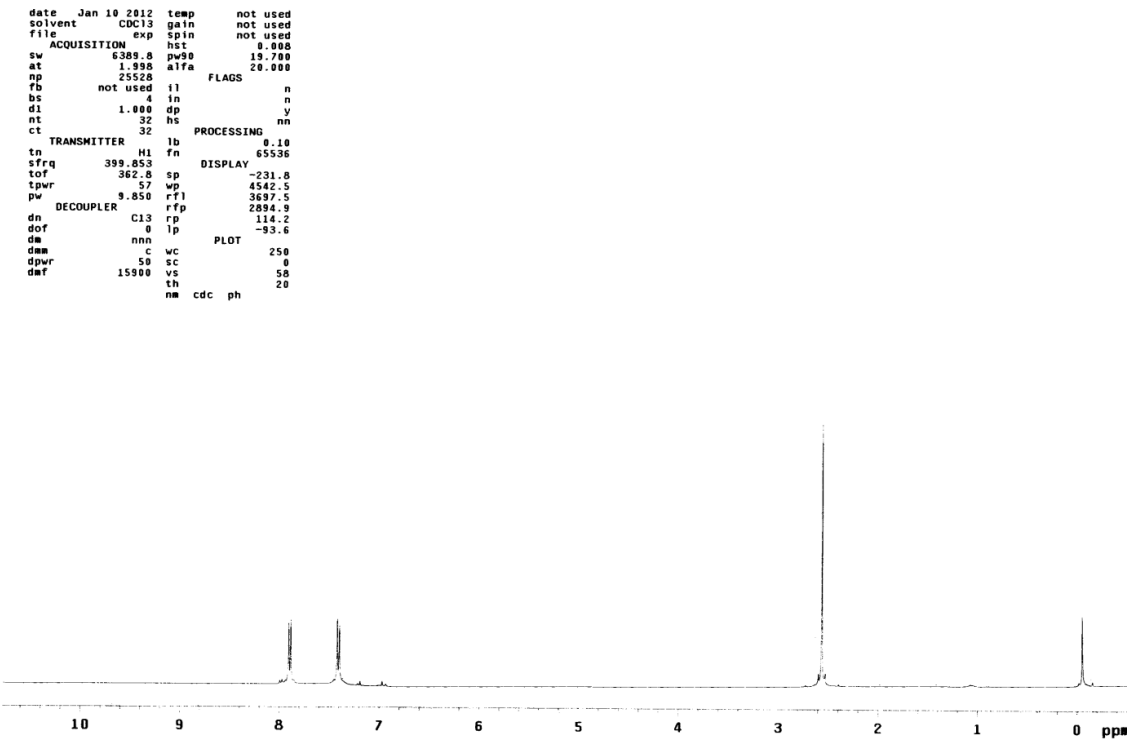
date	Jan 8 2012	temp	not used
solvent	CDCl3	gain	not used
file	exp	spin	not used
ACQUISITION		hst	9.008
sw	6389.8	pw90	19.700
at	1.998	alfa	20.000
np	25528	FLAGS	
fb	not used	il	n
bs	4	in	n
d1	1.000	dp	y
nt	32	hs	nn
ct	32	PROCESSING	
TRANSMITTER		lb	0.10
tn	H1	fn	65536
sfrq	399.853	DISPLAY	
tof	362.8	sp	-214.1
tpwr	57	wp	4416.5
pw	9.850	rfl	776.5
DECOUPLER		rfp	0
dn	C13	rp	108.1
dof	0	lp	-82.7
dm	nnn	PLOT	
dmm	c	wc	250
dpwr	50	sc	0
dmf	15900	vs	27
		th	20
		nm	cdc ph



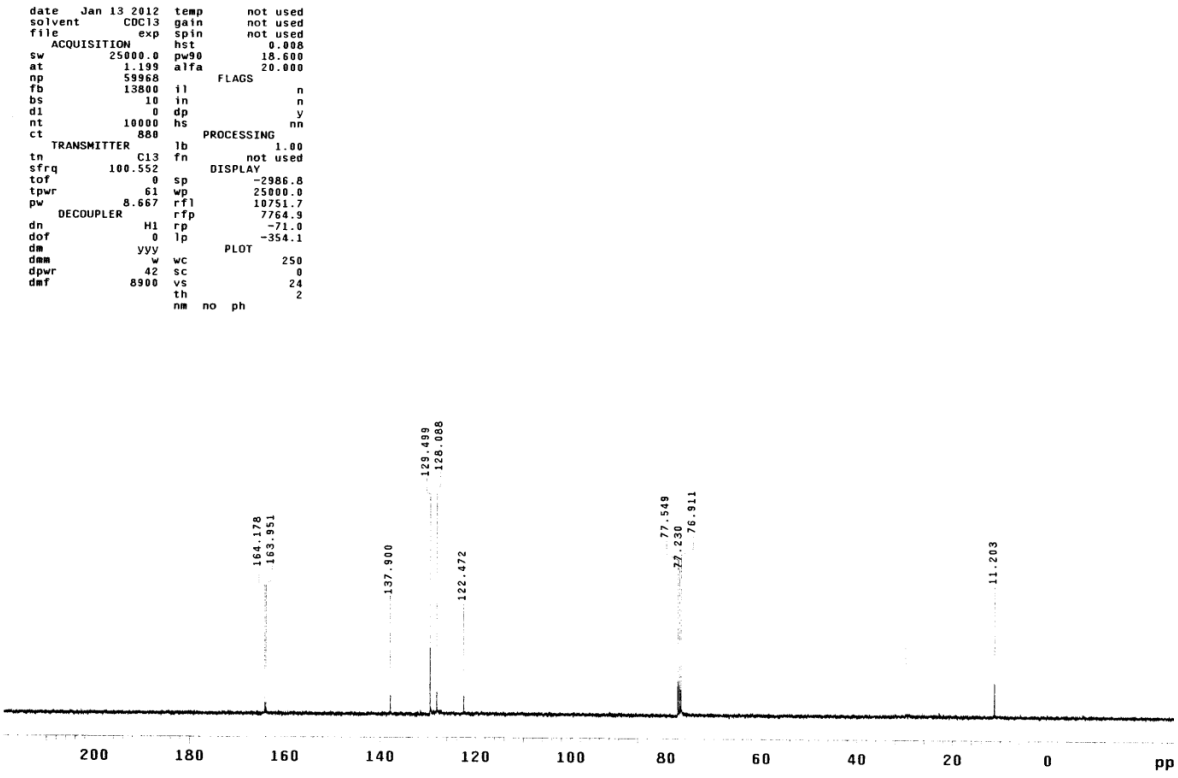
2-(4-Butoxy-phenyl)-5-methyl-1,3,4-oxadiazole (22a): ^{13}C NMR (100 MHz, $CDCl_3$)



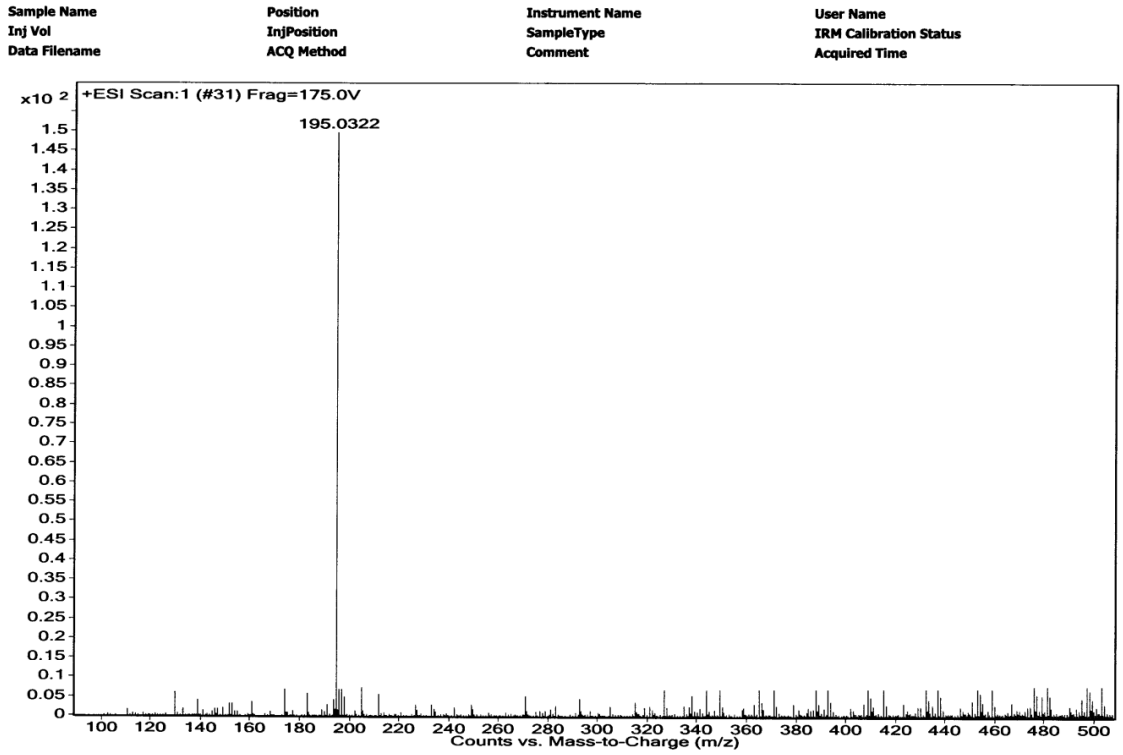
2-(4-Chloro-phenyl)-5-methyl-1,3,4-oxadiazole (23a): ^{1}H NMR (400 MHz, $CDCl_3$)



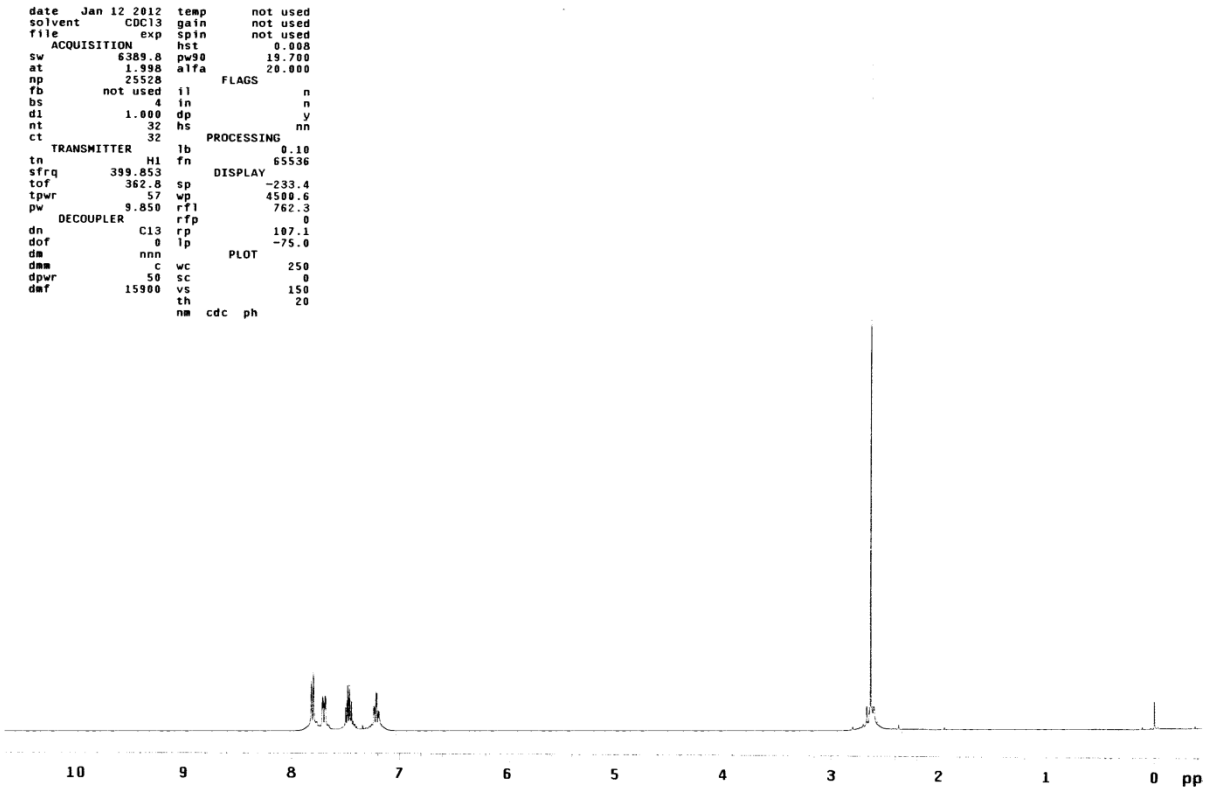
2-(4-Chloro-phenyl)-5-methyl-1,3,4-oxadiazole (23a): ^{13}C NMR (100 MHz, $CDCl_3$)



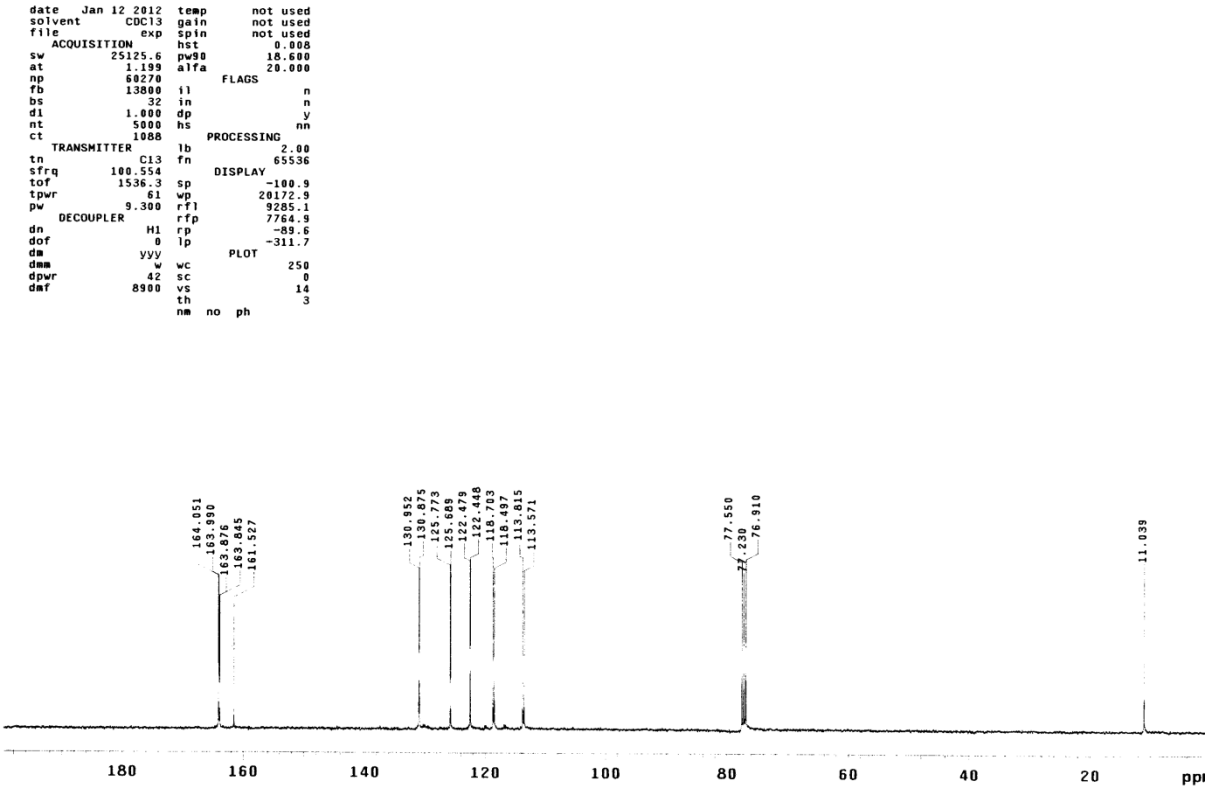
2-(4-Chloro-phenyl)-5-methyl-1,3,4-oxadiazole (23a): HRMS



2-(3-Fluoro-phenyl)-5-methyl-1,3,4-oxadiazole (24a): ^{1}H NMR (400 MHz, $CDCl_3$)

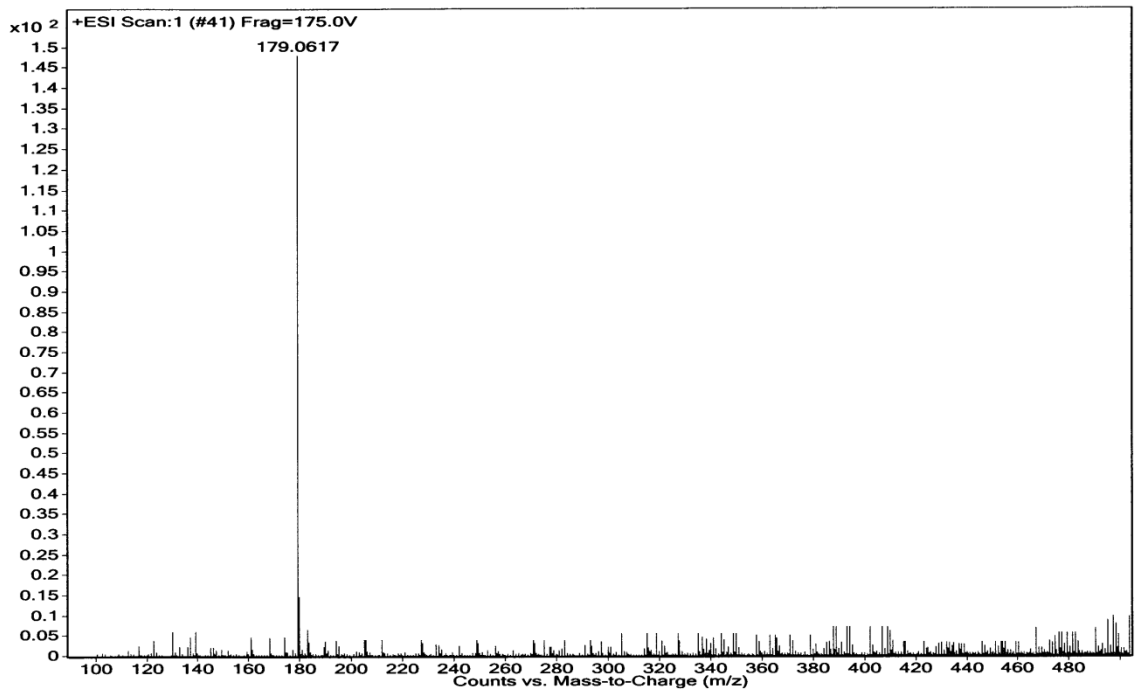


2-(3-Fluoro-phenyl)-5-methyl-1,3,4-oxadiazole (24a): ^{13}C NMR (100 MHz, $CDCl_3$)

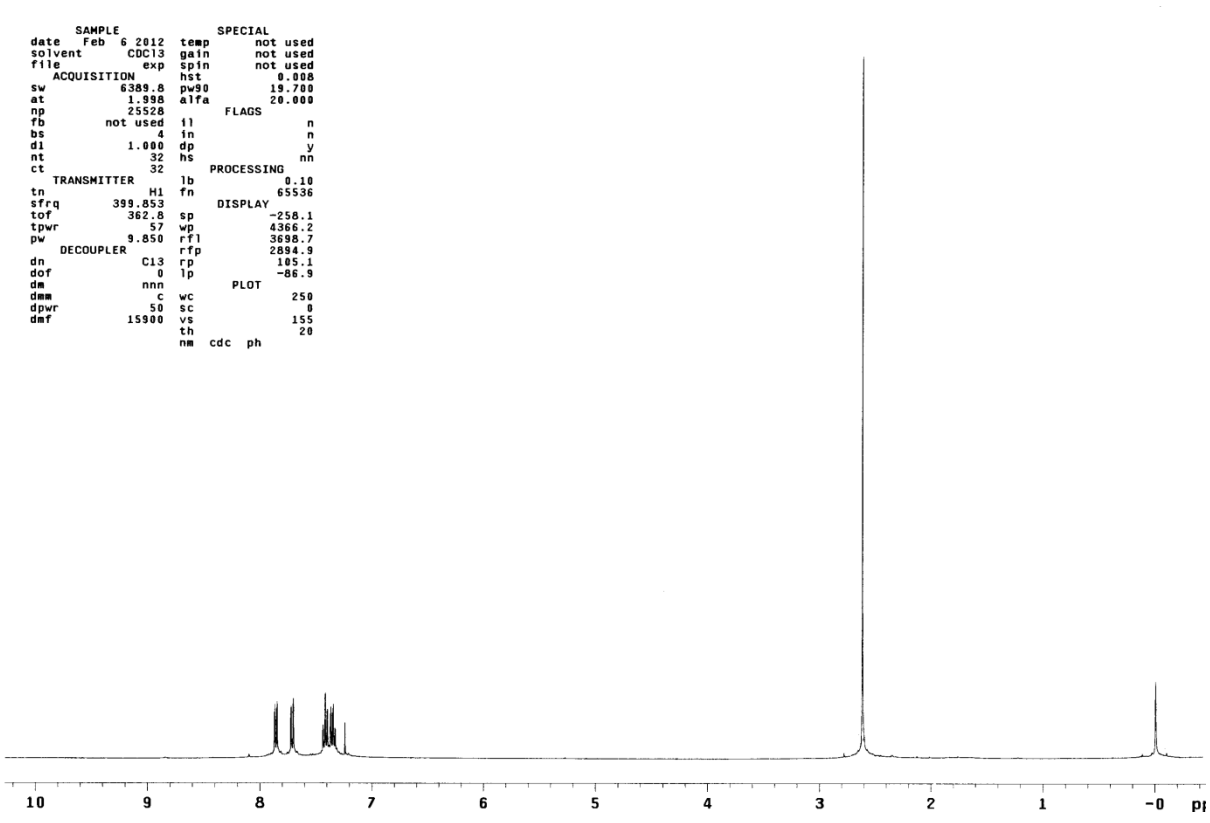


2-(3-Fluoro-phenyl)-5-methyl-1,3,4-oxadiazole (24a): HRMS

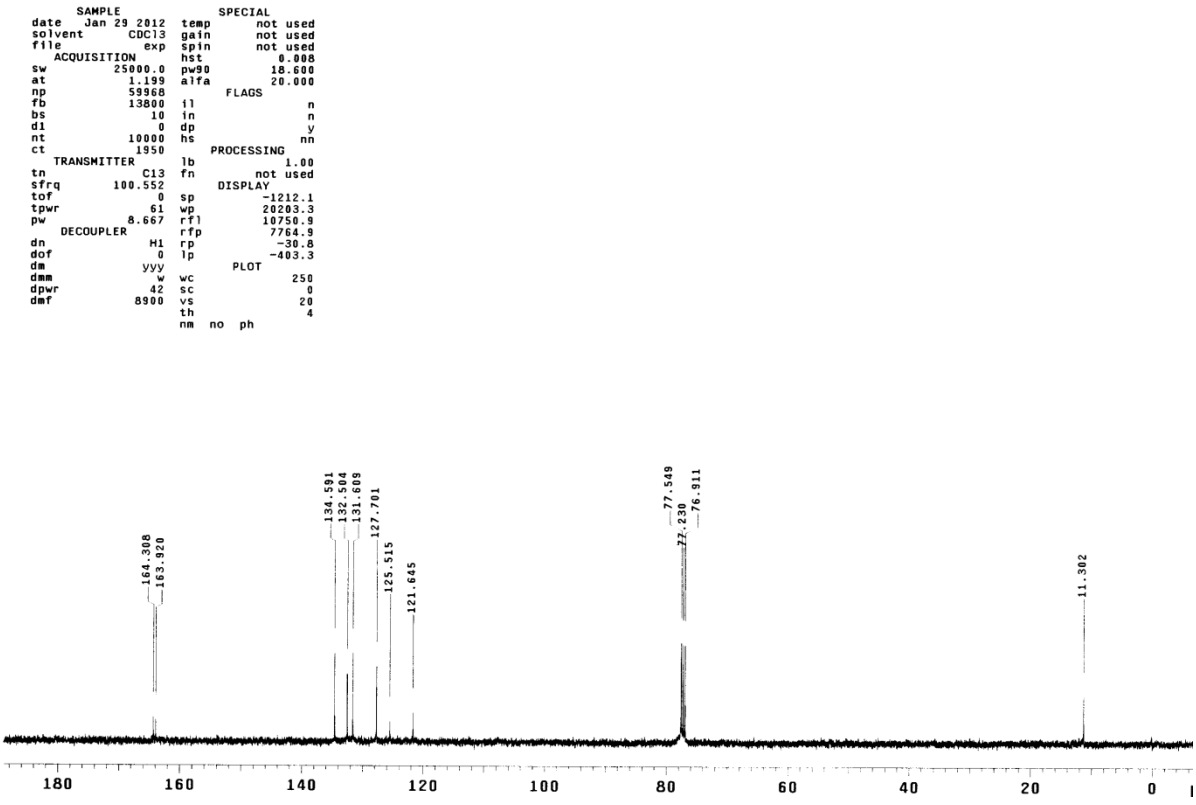
Sample Name	**Position**	**Instrument Name**	**User Name**
Inj Vol	**InjPosition**	**SampleType**	**IRM Calibration Status**
Data Filename	**ACQ Method**	**Comment**	**Acquired Time**



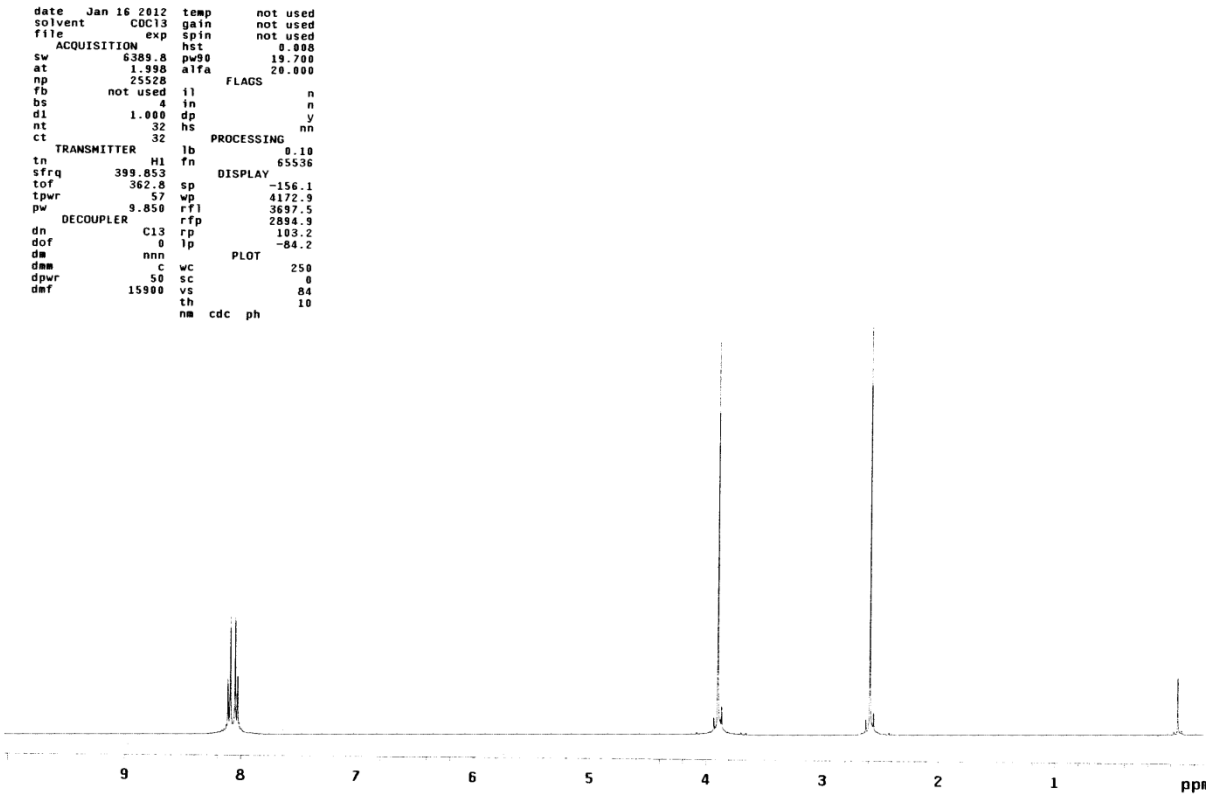
2-(2-Bromo-phenyl)-5-methyl-1,3,4-oxadiazole (25a): ^{1}H NMR (400 MHz, $CDCl_3$)



2-(2-Bromo-phenyl)-5-methyl-1,3,4-oxadiazole (25a): ^{13}C NMR (100 MHz, $CDCl_3$)



4-(5-Methyl-[1,3,4]oxadiazol-2-yl)-benzoic acid methyl ester (26a): ^{1}H NMR (400 MHz, $CDCl_3$)



4-(5-Methyl-[1,3,4]oxadiazol-2-yl)-benzoic acid methyl ester (26a): ^{13}C NMR (100 MHz, $CDCl_3$)