

Supporting Information

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

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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 F₂₅₄ (0.25mm). NMR spectra were recorded in CDCl₃ with tetramethylsilane as the internal standard for ¹H NMR (400 MHz), CDCl₃ solvent as the internal standard for ¹³C NMR (100 MHz). HRMS spectra were recorded using ESI mode. IR spectra were recorded in KBr or neat. The arylidenearylhydrazides, alkylidenearylhydrazides 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 MoK α radiation ($\lambda = 0.71073 \text{ \AA}$) 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.

- SMART V 4.043 Software for the CCD Detector System; Siemens Analytical Instruments Division: Madison, WI, 1995.
- SAINT V 4.035 Software for the CCD Detector System; Siemens Analytical Instruments Division: Madison, WI, 1995.
- 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.

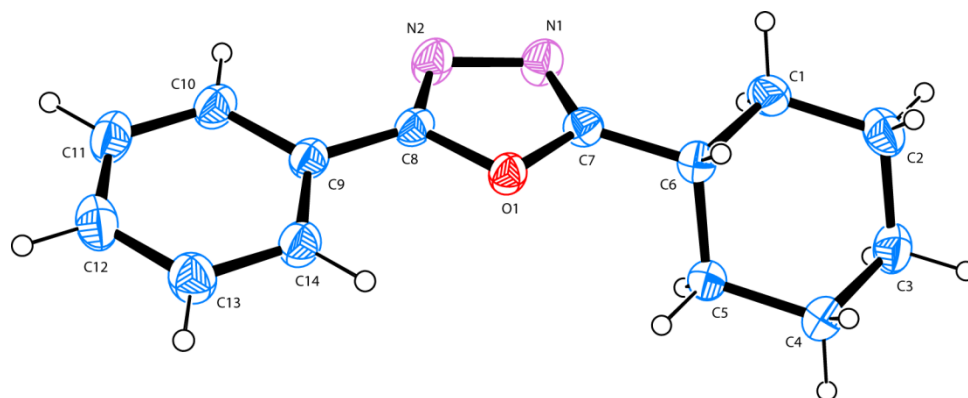
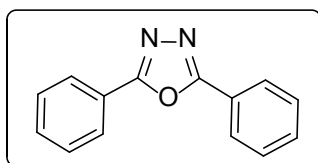


Figure S1: ORTEP view of **9a**

Crystallographic description of 9a: Crystal dimension (mm): 0.42 x 0.35 x 0.26. C₁₄H₁₆N₂O, 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) Å³; Z = 2; ρ_{cal} = 1.259 mg/m³; 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 [$I > 2\sigma_I$] R1 = 0.0384, wR2 = 0.1139, R indices (all data) R1 = 0.0483, wR2 = 0.1213; goodness of fit = 1.062.

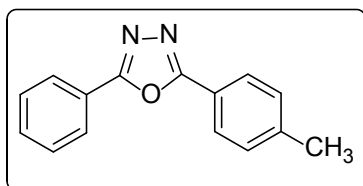
Spectral Data

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



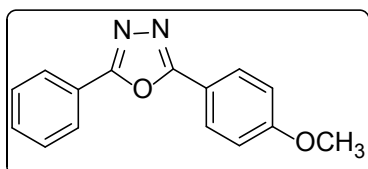
White Solid; M.p. 136-138 °C (Lit.¹ 138 °C); ¹H NMR (400 MHz, CDCl₃): δ 7.53-7.55 (m, 6H), 8.13-8.15 (m, 4H); ¹³C NMR (100 MHz, CDCl₃): δ 124.1, 127.1, 129.3, 131.9, 164.8.; IR (KBr): 3058, 2919, 1547, 1484, 1445, 1268, 1155, 1068, 1019, 964, 922, 782, 710, 686 cm⁻¹. HRMS (*m/z*) (M+1) calcd for C₁₄H₁₀N₂O: 223.0866, found 223.0863.

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



White solid; M.p. 121-122 °C (Lit.² 121-122 °C); ¹H NMR (400 MHz, CDCl₃): 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); ¹³C NMR (100 MHz, CDCl₃): 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 C₁₅H₁₂N₂O: 237.1022, found 237.1020.

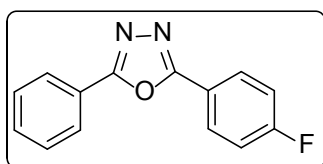
2-(4-Methoxy-phenyl)-5-phenyl-1,3,4-oxadiazole (3a):



White solid; M.p. 149-150 °C (Lit.¹ 148-150 °C); ¹H NMR (400 MHz, CDCl₃): 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); ¹³C NMR (100

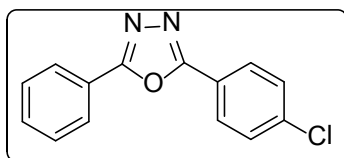
MHz, CDCl₃): δ 55.6, 114.7, 116.6, 124.2, 127.0, 128.9, 129.2, 131.7, 162.5, 164.3, 164.7.; IR (KBr): 2956, 2923, 2848, 1616, 1503, 1262, 1066, 1017, 831, 737, 706, 684 cm⁻¹. HRMS (*m/z*) (M+1) calcd for C₁₅H₁₂N₂O₂: 253.0972, found 253.0970.

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



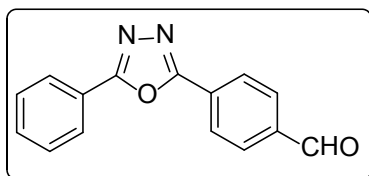
White solid; M.p. 151-152 °C (Lit.³ 151-152 °C); ¹H NMR (400 MHz, CDCl₃): δ 7.22-7.27 (m, 2H), 7.54-7.57 (m, 3H), 8.13-8.18 (m, 4H); ¹³C NMR (100 MHz, CDCl₃): δ 116.5, 116.7, 120.5, 124.0, 127.1, 129.28, 129.33, 129.4, 132.0, 163.7, 164.0, 164.8, 166.2.; IR (KBr): 3061, 2921, 1606, 1549, 1496, 1221, 1149, 1069, 841, 733, 703, 687 cm⁻¹. HRMS (*m/z*) (M+1) calcd for C₁₄H₉N₂OF: 241.0772, found 241.0770.

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



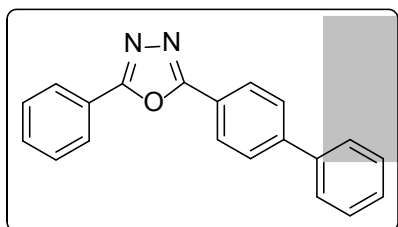
White solid; M.p. 161-162 °C (Lit.⁴ 162-163 °C); ¹H NMR (400 MHz, CDCl₃): δ 7.49-7.53 (m, 5H), 8.06 (d, 2H, *J* = 8.0 Hz), 8.11 (d, 2H, *J* = 6.6 Hz); ¹³C NMR (100 MHz, CDCl₃): δ 122.6, 123.9, 127.2, 128.4, 129.3, 129.7, 132.1, 138.2, 164.0, 164.9.; IR (KBr): 3061, 2920, 1605, 1550, 1478, 1406, 1086, 1074, 839, 730, 702, 687 cm⁻¹. HRMS (*m/z*) (M+1) calcd for C₁₄H₉N₂OCl: 257.0476, found: 257.0471.

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



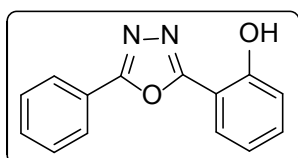
White solid; M.p. 168-169 °C (lit.⁵ 162.7 °C); ¹H NMR (400 MHz, CDCl₃): δ 7.53-7.59 (m, 3H), 8.05 (d, 2H, *J* = 8.4 Hz), 8.15 (d, 2H, *J* = 8 Hz), 8.31 (d, 2H, *J* = 8 Hz), 10.10 (s, 1H); ¹³C NMR (100 MHz, CDCl₃): δ 123.6, 127.3, 127.6, 129.0, 129.4, 130.4, 132.3, 138.3, 163.8, 165.4, 191.5.; IR (KBr): 3060, 2925, 2853, 1703, 1547, 1446, 1271, 1204, 1075, 833, 729, 704, 685 cm⁻¹. HRMS (*m/z*) (M+1) calcd for C₁₅H₁₀N₂O₂: 251.0815, found: 251.0815.

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



White solid; M.p. 164-166 °C (Lit.⁶ 166-167 °C); ¹H NMR (400 MHz, CDCl₃): 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); ¹³C NMR (100 MHz, CDCl₃): 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 C₂₀H₁₄N₂O: 299.1179, found: 299.1182.

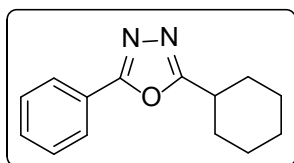
2-(5-Phenyl-1,3,4-oxadiazol-2-yl)-phenol (8a):



White solid; M.p. 185-187 °C (Lit.⁷ 183-185 °C); ¹H NMR (400 MHz, CDCl₃): δ 7.55-7.69 (m, 4H), 8.10-8.18 (m, 5H), 11.08 (s, 1H); ¹³C NMR (100 MHz, CDCl₃): δ 120.1, 123.1, 127.3, 129.4, 132.5,

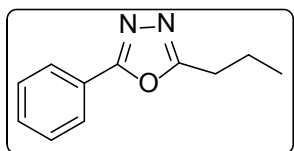
134.7, 134.8, 142.2, 150.2, 157.5, 163.0, 163.7.; IR (KBr): 3152, 2917, 1535, 1487, 1447, 1377, 1248, 1232, 1066, 823, 749, 707, 683 cm^{-1} . Anal calcd for $\text{C}_{14}\text{H}_{10}\text{N}_2\text{O}_2$ (238.07): C 70.58, H 4.23, N 11.76.; found C 70.59, H 4.25, N 11.75.

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



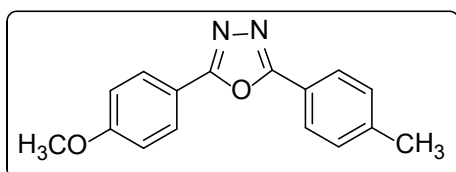
Brown solid; M.p. 107-109 °C (Lit.⁸ 104 °C); ^1H NMR (400 MHz, CDCl_3): δ 1.23-1.46 (m, 3H), 1.61-1.71 (m, 3H) 1.83-1.87 (m, 2H), 2.11-2.14 (m, 2H), 2.94-2.99 (m, 1H), 7.46-7.48 (m, 3H), 8.00-8.02 (m, 2H); ^{13}C NMR (100 MHz, CDCl_3): δ 25.4, 25.6, 30.2, 35.2, 124.1, 126.7, 128.9, 131.4, 164.4, 170.0.; IR (KBr): 3058, 2923, 2855, 1565, 1552, 1485, 1448, 1021, 768, 709, 688 cm^{-1} . HRMS (m/z) (M+1) calcd for $\text{C}_{14}\text{H}_{16}\text{N}_2\text{O}$: 229.1335, found: 229.1340.

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



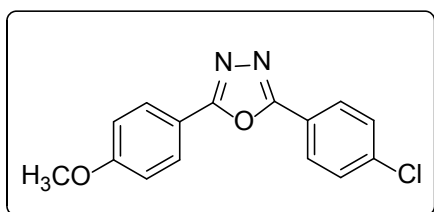
Yellow gummy, M.p. (Lit.⁹ 75-76 °C); ^1H NMR (400 MHz, CDCl_3): δ 1.03 (t, 3H, $J = 14.8$ Hz), 1.83-1.89 (m, 2H), 2.89 (t, 2H, $J = 15.2$ Hz), 7.42-7.52 (m, 3H), 8.00-8.02 (m, 2H); ^{13}C NMR (100 MHz, CDCl_3): δ 13.7, 20.2, 27.4, 126.9, 128.5, 129.1, 133.4, 164.8, 167.0.; IR (KBr): 2964, 2929, 2873, 1717, 1573, 1450, 1253, 1069, 1006, 776, 710, 691 cm^{-1} . Anal calcd for $\text{C}_{11}\text{H}_{12}\text{N}_2\text{O}$ (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):



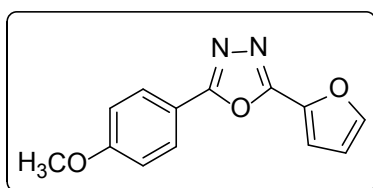
Yellow solid; M.p. 137-139 °C (Lit.¹ 137-138 °C); ¹H NMR (400 MHz, CDCl₃): δ 2.42 (s, 3H), 3.87 (s, 3H), 7.01 (d, 2H, *J* = 11.6 Hz), 7.31 (d, 2H, *J* = 10.4 Hz), 7.98-8.07 (m, 4H); ¹³C NMR (100 MHz, CDCl₃): δ 21.8, 55.6, 114.7, 116.7, 121.5, 127.0, 128.8, 129.9, 142.2, 162.4, 164.5.; IR (KBr): 2928, 2829, 1612, 1492, 1304, 1254, 1170, 1033, 835, 822, 744 cm⁻¹. Anal calcd for C₁₆H₁₄N₂O₂ (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):



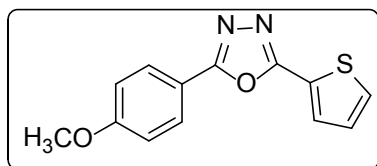
White solid; M.p. 164-165 °C (Lit.⁴ 166-167 °C); ¹H NMR (400 MHz, CDCl₃): δ 3.85 (s, 3H), 6.99 (d, 2H, *J* = 11.6 Hz), 7.46 (d, 2H, *J* = 11.2 Hz), 8.01 (d, 4H, *J* = 11.6 Hz); ¹³C NMR (100 MHz, CDCl₃): δ 55.6, 114.7, 116.3, 122.6, 128.2, 128.8, 129.5, 137.9, 162.6, 163.4, 164.8.; IR (KBr): 2929, 2829, 1611, 1495, 1479, 1305, 1252, 1170, 1089, 1028, 834, 743 cm⁻¹. HRMS (*m/z*) (*M*+1) calcd for C₁₅H₁₁N₂O₂Cl: 287.0582, found 287.0582.

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



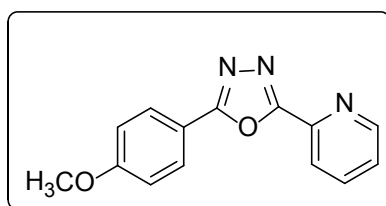
Brown solid; M.p. 128-130 °C (Lit.³ 129-130 °C); ¹H NMR (400 MHz, CDCl₃): δ 3.86 (s, 3H), 6.58-6.59 (m, 1H), 6.99 (d, 2H, *J* = 8.8 Hz), 7.18 (d, 1H, *J* = 3.6 Hz), 7.63 (m, 1H), 8.03 (d, 2H, *J* = 8.8 Hz); ¹³C NMR (100 MHz, CDCl₃): δ 55.5, 112.2, 113.8, 114.5, 115.9, 128.7, 139.6, 145.6, 157.0, 162.5, 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 C₁₃H₁₀N₂O₃: 243.0764, found: 243.0767.

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



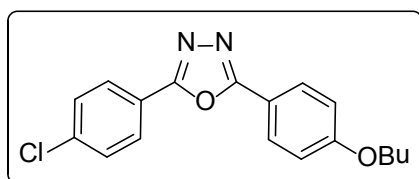
Brown solid; M.p. 136-137 °C (Lit.¹⁰ 139-141 °C); ¹H NMR (400 MHz, CDCl₃): δ 3.86 (s, 3H), 7.00 (d, 2H, *J* = 8.8 Hz), 7.15-7.17 (m, 1H), 7.53 (d, 1H, *J* = 5.2 Hz), 7.78 (d, 1H, *J* = 3.6 Hz), 8.02 (d, 2H, *J* = 8.4 Hz); ¹³C NMR (100 MHz, CDCl₃): δ 55.6, 114.6, 116.2, 125.5, 128.2, 128.8, 129.6, 130.0, 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 C₁₃H₁₀N₂O₂S (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):



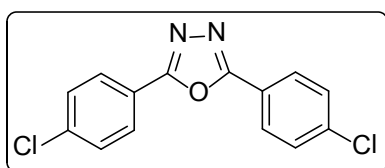
White solid; M.p. 155-156 °C (Lit.¹¹ 154-156 °C); ¹H NMR (400 MHz, CDCl₃): δ 3.85 (s, 3H), 6.99 (d, 2H, *J* = 8.8 Hz), 7.41-7.45 (m, 1H), 7.86 (t, 1H, *J* = 16 Hz), 8.12 (d, 2H, *J* = 8.8 Hz), 8.26 (d, 1H, *J* = 7.6 Hz), 8.77 (d, 1H, *J* = 7.6 Hz); ¹³C NMR (100 MHz, CDCl₃): δ 55.5, 114.5, 116.1, 123.1, 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 C₁₄H₁₁N₃O₂ (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):



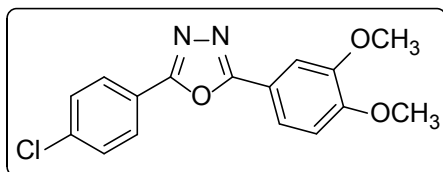
White solid; M.p. 132-133 °C (Lit.² 132-133 °C); ¹H NMR (400 MHz, CDCl₃): δ 1.00 (t, 3H, *J* = 9.6 Hz), 1.50-1.56 (m, 2H), 1.78-1.83 (m, 2H), 4.04 (t, 2H, *J* = 8.4 Hz), 7.01 (d, 2H, *J* = 11.6 Hz), 7.50 (d, 2H, *J* = 11.2 Hz), 8.03-8.07 (m, 4H); ¹³C NMR (100 MHz, CDCl₃): δ 14.0, 19.4, 31.3, 68.2, 115.2, 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 C₁₈H₁₇N₂O₂Cl (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):



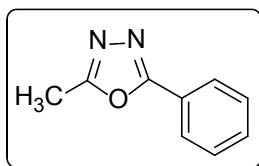
White solid; M.p. 250-251 °C (Lit.² 250-251 °C); ¹H NMR (400 MHz, CDCl₃): δ 7.52 (d, 4H, *J* = 11.2 Hz), 8.07 (d, 4H, *J* = 11.6 Hz); ¹³C NMR (100 MHz, CDCl₃): δ 122.4, 128.4, 129.7, 138.4, 164.2.; IR (KBr): 3084, 2956, 2924, 2853, 1605, 1478, 1461, 1261, 1091, 1073, 1011, 838, 738 cm⁻¹. Anal calcd for C₁₄H₈N₂OCl₂ (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):



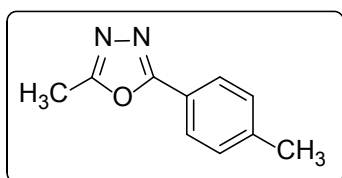
White solid; M.p. 170-171 °C; ¹H NMR (400 MHz, CDCl₃): δ 3.95 (s, 3H), 3.98 (s, 3H), 6.97 (d, 1H, *J* = 8 Hz), 7.49 (d, 2H, *J* = 8.4 Hz), 7.63 (s, 1H), 7.67 (d, 1H, *J* = 8.2 Hz), 8.05 (d, 2H, *J* = 8.8 Hz); ¹³C NMR (100 MHz, CDCl₃): δ 56.3, 56.4, 109.7, 111.3, 120.7, 122.7, 128.3, 129.7, 138.0, 141.2, 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):



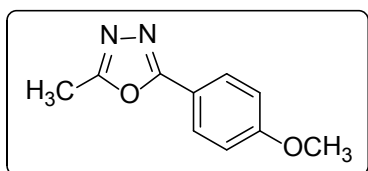
Brown solid; M.p. 60-61 °C (Lit.¹² 61-64 °C); ¹H NMR (400 MHz, CDCl₃): δ 2.60 (s, 3H), 7.45-7.51 (m, 3H), 8.01 (d, 2H, *J* = 6 Hz); ¹³C NMR (100 MHz, CDCl₃): δ 11.1, 123.9, 126.7, 129.0, 131.5, 163.7, 164.8.; IR (KBr): 2958, 2870, 1679, 1612, 1591, 1500, 1474, 1296, 1249, 1175, 1032, 836, 740, 701, 527 cm⁻¹. HRMS (*m/z*) (*M*+1) calcd for C₉H₈N₂O: 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); ¹H NMR (400 MHz, CDCl₃): δ 2.42 (s, 3H), 2.60 (s, 3H), 7.29 (d, 2H, *J* = 8.4 Hz), 7.91 (d, 2H, *J* = 8 Hz); ¹³C NMR (100 MHz, CDCl₃): 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 C₁₀H₁₀N₂O: 175.0866, found: 175.0864.

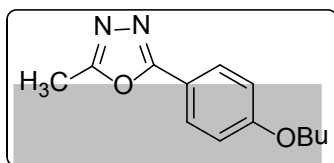
2-(4-Methoxy-phenyl)-5-methyl-1,3,4-oxadiazole (21a):



Yellow solid; M.p. 87-88 °C (Lit.¹⁴ 88 °C); ¹H NMR (400 MHz, CDCl₃): 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); ¹³C NMR (100 MHz, CDCl₃): 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,

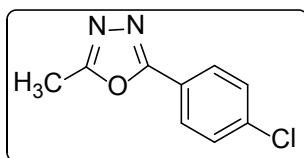
1177, 1087, 1017, 959, 844, 837, 739, 699, 528 cm^{-1} . HRMS (m/z) (M+1) calcd for $\text{C}_{10}\text{H}_{10}\text{N}_2\text{O}_2$: 191.0815, found: 191.0817.

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



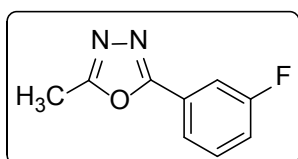
Brown solid; M.p. 58-59 °C; ^1H NMR (400 MHz, CDCl_3): δ 0.98 (t, 3H, $J = 14.8$ Hz), 1.47-1.53 (m, 2H), 1.77-1.80 (m, 2H), 2.58 (s, 3H), 4.00 (t, 2H, $J = 13.2$ Hz), 6.97 (d, 2H, $J = 8.8$ Hz), 7.93 (d, 2H, $J = 8.8$ Hz); ^{13}C NMR (100 MHz, CDCl_3): δ 11.1, 13.9, 19.3, 31.2, 68.0, 114.9, 116.2, 128.5, 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 $\text{C}_{14}\text{H}_{19}\text{N}_2\text{O}_2$ (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):



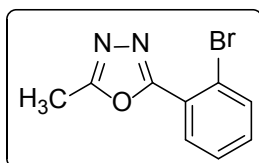
Brown solid; M.p. 96-98 °C (Lit.¹⁶ 106-107 °C); ^1H NMR (400 MHz, CDCl_3): δ 2.56 (s, 3H), 7.40 (d, 2H, $J = 8.8$ Hz), 7.89 (d, 2H, $J = 8.8$ Hz); ^{13}C NMR (100 MHz, CDCl_3): δ 11.2, 122.5, 128.1, 129.5, 137.9, 164.0, 164.2.; IR (KBr): 3071, 2925, 2853, 1607, 1588, 1478, 1408, 1246, 1094, 1009, 848, 819, 730, 687, 507 cm^{-1} . HRMS (m/z) (M+1) calcd for $\text{C}_9\text{H}_7\text{N}_2\text{OCl}$: 195.0320, found: 195.0322.

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



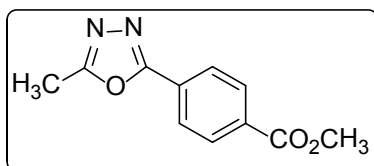
White solid; M.p. 81-82 °C; ^1H NMR (400 MHz, CDCl_3): δ 2.63 (s, 3H), 7.21-7.24 (m, 1H), 7.45-7.50 (m, 1H), 7.68-7.72 (m, 1H), 7.79-7.82 (m, 1H); ^{13}C NMR (100 MHz, CDCl_3): δ 11.0, 113.6, 113.8, 118.5, 118.7, 122.4, 122.5, 125.7, 125.8, 130.9, 131.0, 161.5, 163.8, 163.9, 164.0, 164.0.; IR (KBr): 2926, 1703, 1578, 1558, 1458, 1436, 1307, 1262, 1197, 1083, 867, 800, 726, 680 cm^{-1} . HRMS (m/z) (M+1) calcd for $\text{C}_9\text{H}_7\text{N}_2\text{OF}$: 179.0615, found: 179.0617.

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



Yellow solid; M.p. 80-81 °C; ^1H 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, 697 cm^{-1} . Anal calcd for $\text{C}_9\text{H}_7\text{N}_2\text{OBr}$ (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 °C; ^1H 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 $\text{C}_{11}\text{H}_{10}\text{N}_2\text{O}_3$ (218.07): C 60.55, H 4.62, N 12.84.; found C 60.57, H 4.66, N 12.81.

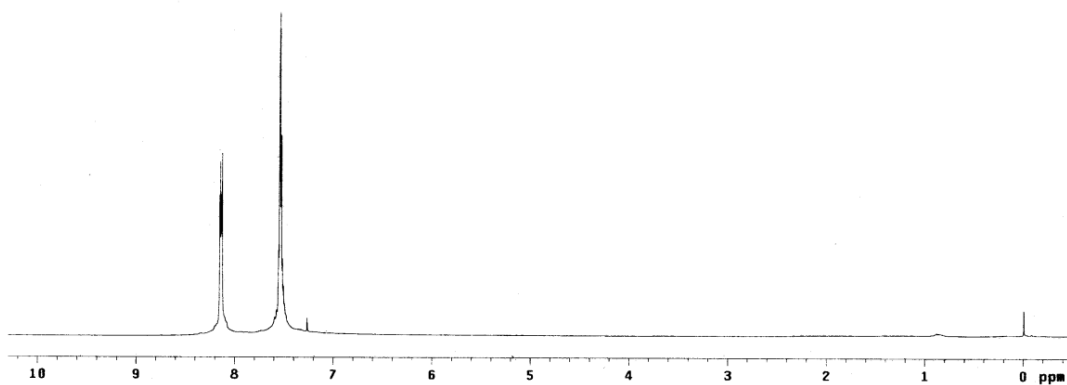
References:

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Spectra

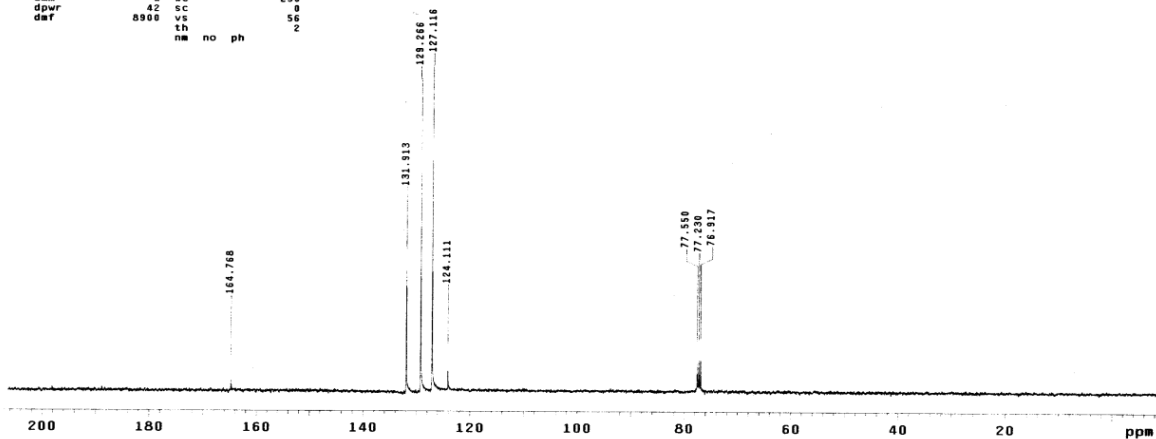
2,5-Diphenyl-1,3,4-oxadiazole (1a): ¹H NMR (400 MHz, CDCl₃)

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SAMPLE
date Mar 25 2011 temp SPECIAL
solvent CDC13 gain not used
file exp sp1n not used
ACQUISITION hst 0.000
sw 6389.6 pw90 19.700
at 1.390 alfa 20.000
np 25520 FLAGS
fb not used f1 n
bs 4 in n
d1 1.000 dp y
nt 32 hs nn
ct 32
TRANSMITTER Tn 0.10
tn H1 Tn 65536
sfrq 399.853 DISPLAY
tof 362.8 ep -188.6
tpwr 57 wp 4387.3
pw 9.850 rf1 793.3
DECOUPLER C13 rfp 0
dn 0 rp 115.3
dof 0 lp -97.7
nm nnn PLOT
dwm c wc 250
dpwr 50 sc 0
dwt 15900 vs 75
nm cdc ph 7
```

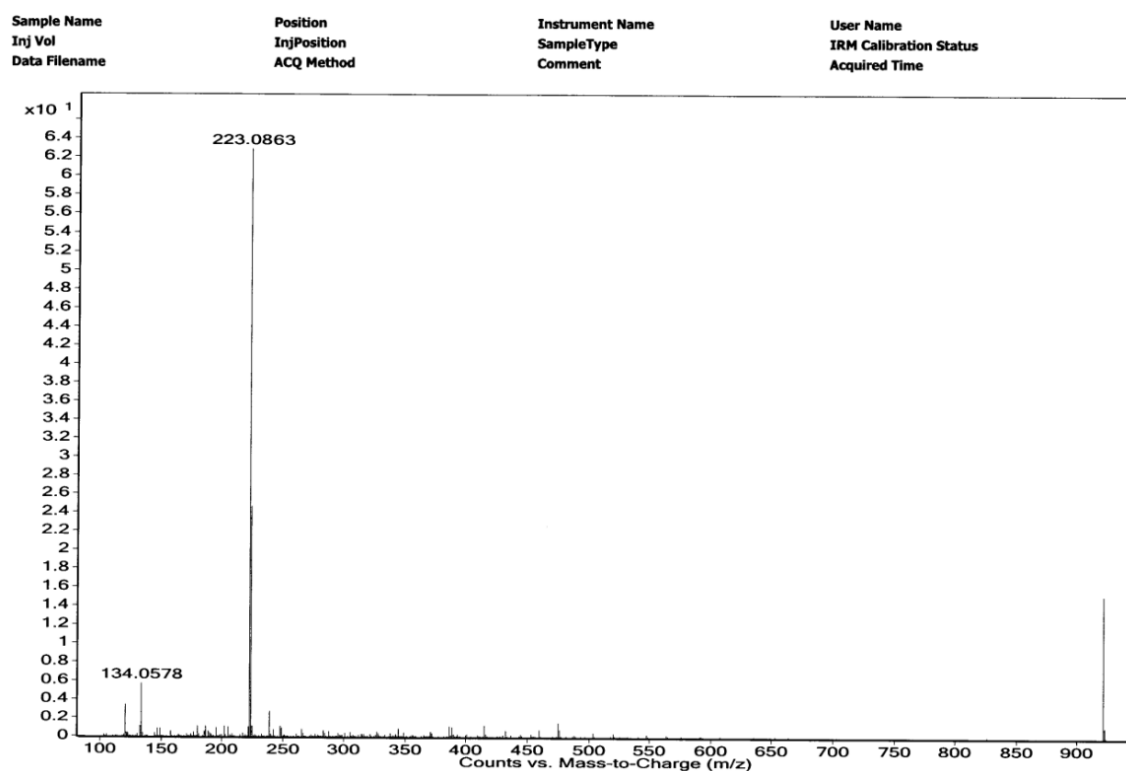


2,5-Diphenyl-1,3,4-oxadiazole (1a): ¹³C NMR (100 MHz, CDCl₃)

```
exp1 s2pu1
SAMPLE
date Apr 21 2011 temp SPECIAL
solvent CDC13 gain not used
file exp sp1n not used
ACQUISITION hst 0.000
sw 25125.6 pw90 18.600
at 1.199 alfa 20.000
np 60270 FLAGS
fb 13600 f1 n
bs 32 in n
d1 1.000 dp y
nt 5000 hs nn
ct 864
TRANSMITTER Tn 2.00
tn C13 Tn 65536
sfrq 100.554 DISPLAY
tof 1536.3 sp -888.7
tpwr 61 wp 21625.2
pw 9.300 rf1 9272.1
DECOUPLER H1 rfp 7764.9
dn 8 rp -9.0
dof 8 lp -432.4
nm vvv PLOT
dwm w wc 250
dpwr 42 sc 0
dwt 8900 vs 56
nm no ph 2
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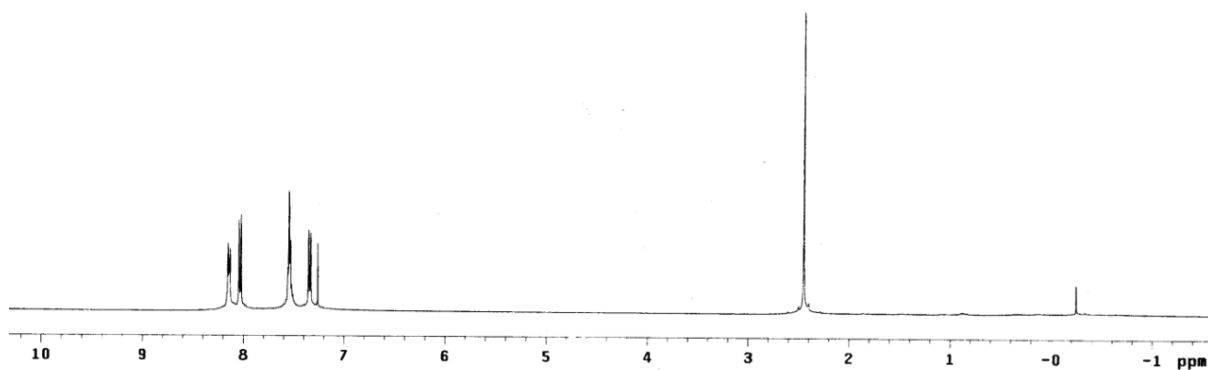


2,5-Diphenyl-1,3,4-oxadiazole (1a): HRMS

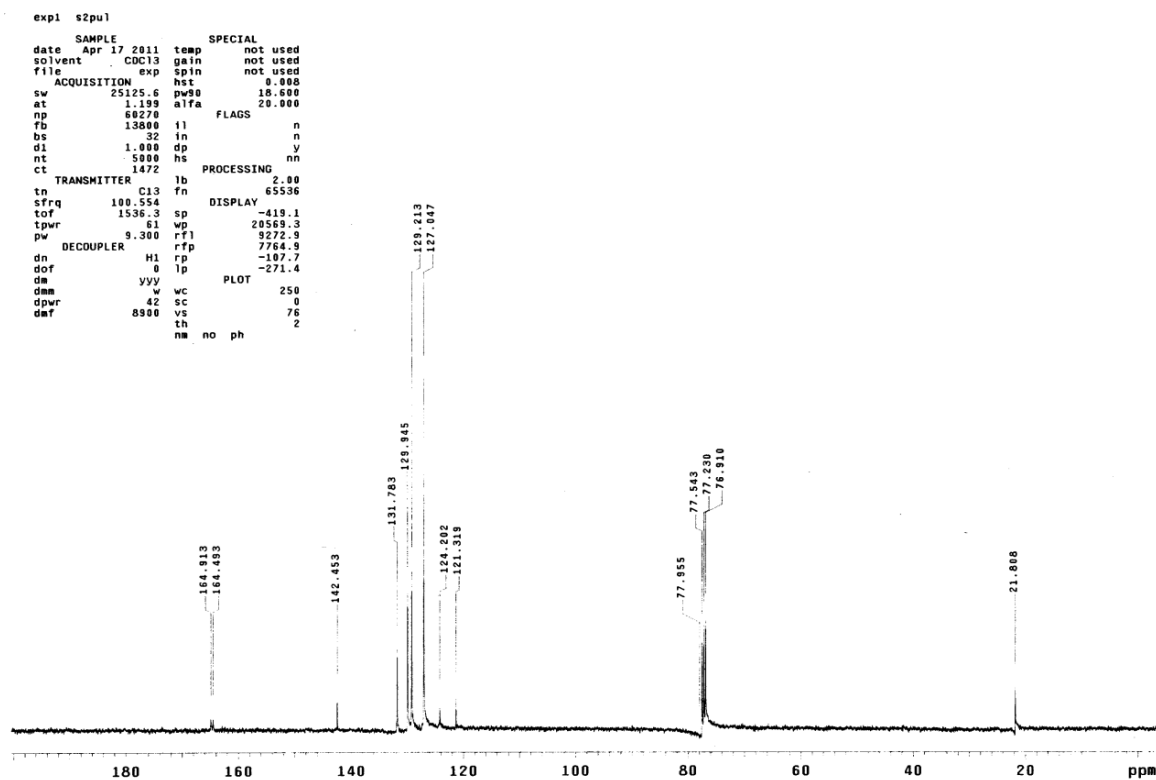


2-Phenyl-5-*p*-tolyl-1,3,4-oxadiazole (2a): ¹H NMR (400 MHz, CDCl₃)

```
exp1 s2pu1
SAMPLE
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 19.700
at 1.998 alfa 20.000
np 25528 FLAGS
fb not used il n
ds 4 in n
d1 1.000 dp y
nt 32 hs nn
ct 32
TRANSMITTER lb 0.10
tn H1 fn 65536
sfrq 399.853 DISPLAY
tof 362.8 sp -638.3
tpwr 57 wp 4779.1
pv 9.850 rfp 794.1
DECOUPLER c13 rp 113.1
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dpcr 50 sc 0
dmf 15900 vs 426
th 20
nm cdc ph
```

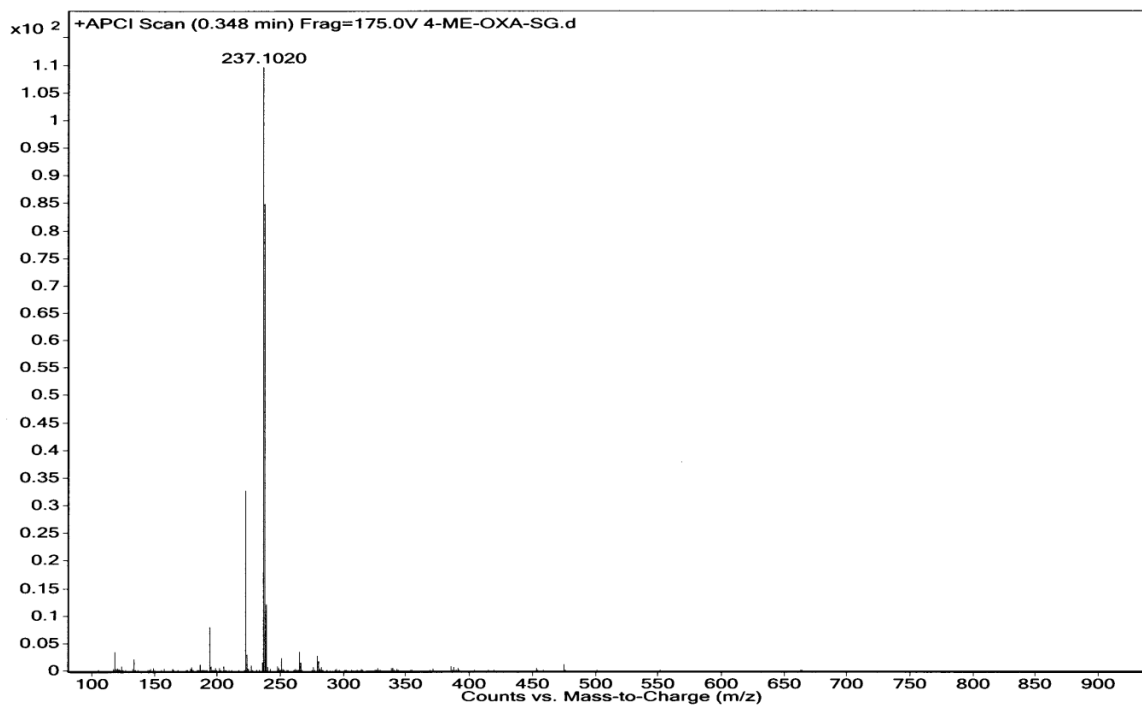


2-Phenyl-5-*p*-tolyl-1,3,4-oxadiazole (2a): ^{13}C NMR (100 MHz, CDCl_3)



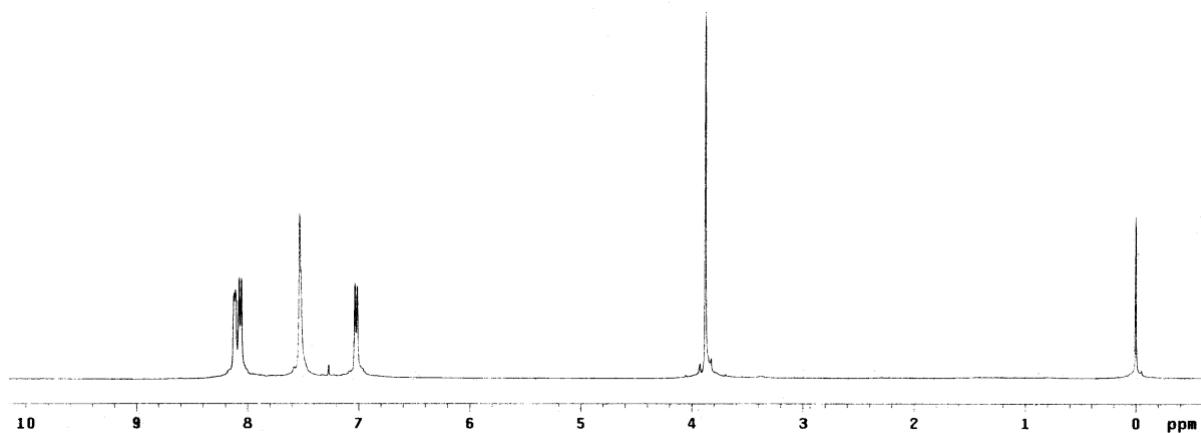
2-Phenyl-5-*p*-tolyl-1,3,4-oxadiazole (2a): HRMS

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



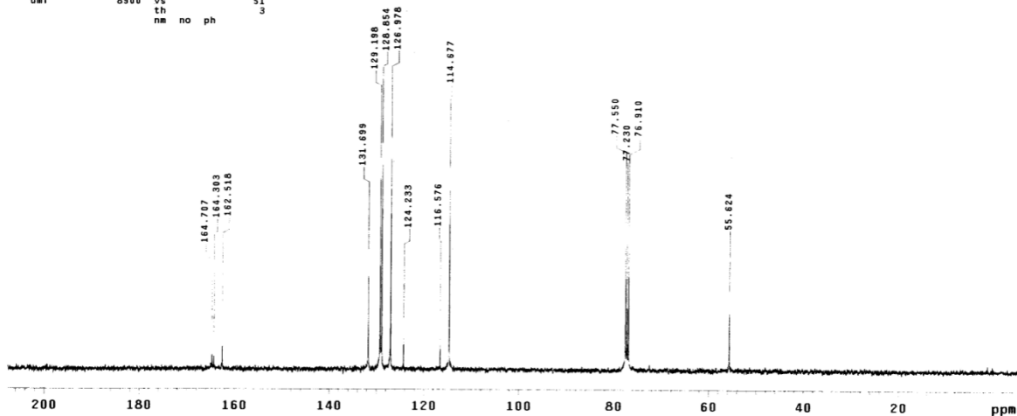
2-(4-Methoxyphenyl)-5-phenyl-1,3,4-oxadiazole (3a): ^1H NMR (400 MHz, CDCl_3)

```
expl s2pu1
SAMPLE
date Apr 18 2011 temp not used
solvent CDCl3 gain not used
file exp spin not used
ACQUISITION hst 0.000
sw 6389.8 pu90 19.700
at 1.998 a1fa 20.000
np 25528 FLAGS
fb not used i1 n
bs 4 in n
d1 1.000 dp y
nt 32 hs nn
ct
TRANSMITTER lb 0.10
tn H1 fn 65536
sfrq 399.853 DISPLAY
tof 362.8 sp -237.9
tpwr 57 wp 4349.2
pw 9.850 rF1 791.9
DECOUPLER rfp 0
dn C13 rp 122.2
dof 0 lp -89.0
dm nnn WC PLOT 250
dmm c
dpwr 50 sc 0
dmf 15900 vs 76
th 20
nm cdc ph
```

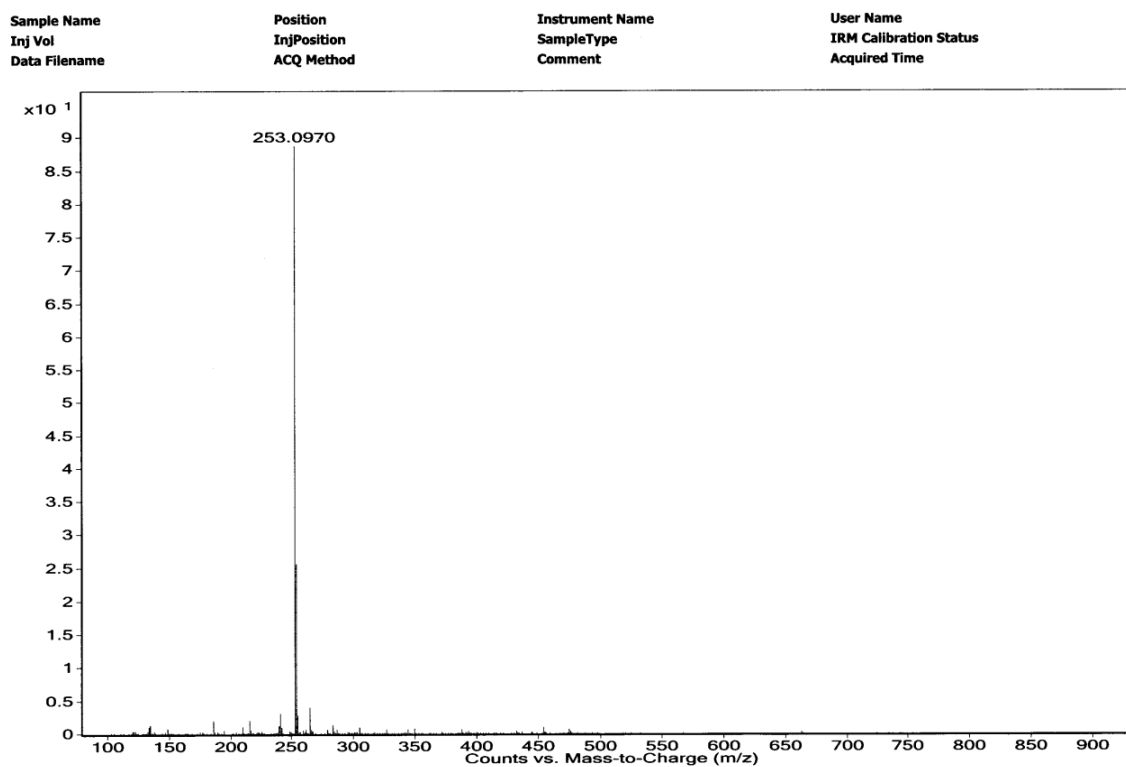


2-(4-Methoxyphenyl)-5-phenyl-1,3,4-oxadiazole (3a): ^{13}C NMR (100 MHz, CDCl_3)

```
expl s2pu1
SAMPLE
date Apr 18 2011 temp not used
solvent CDCl3 gain not used
file exp spin not used
ACQUISITION hst 0.000
sw 25125.6 pu90 18.000
at 1.199 a1fa 20.000
np 88270 FLAGS
fb 13800 i1 n
bs 32 in n
d1 1.000 dp y
nt 5000 hs nn
ct
TRANSMITTER lb 2.00
tn C13 fn 65536
sfrq 100.554 DISPLAY
tof 1536.3 sp -584.7
tpwr 61 wp 21469.3
pw 9.300 rF1 9273.6
DECOUPLER rfp 7764.9
dn H1 rp -32.3
dof 0 lp -340.1
dm yyy WC PLOT 250
dmm v
dpwr 42 sc 0
dmf 8900 vs 51
th 3
nm no ph
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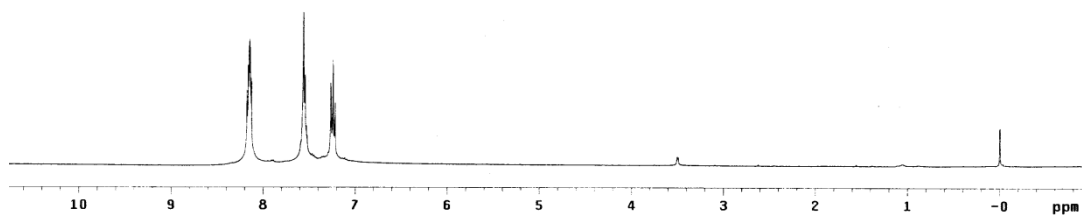


2-(4-Methoxyphenyl)-5-phenyl-1,3,4-oxadiazole (3a): HRMS



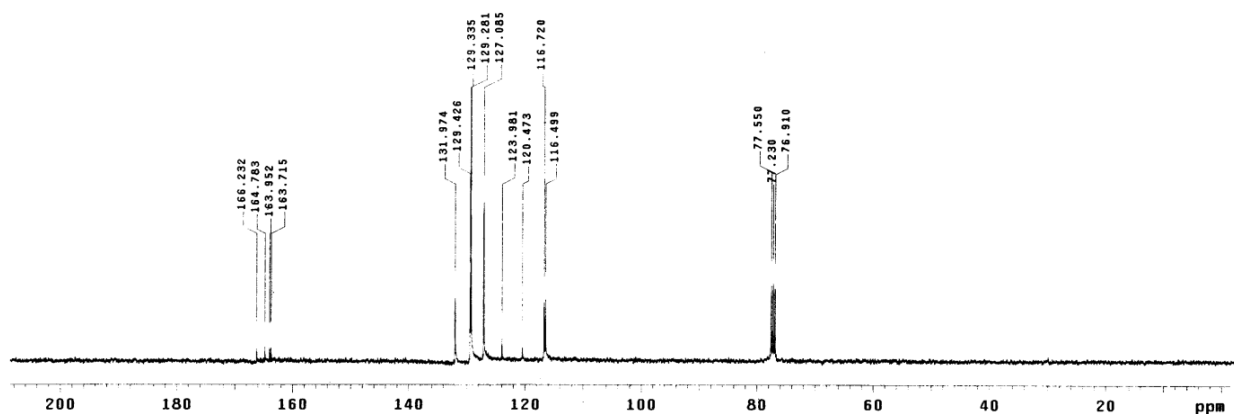
2-(4-Fluorophenyl)-5-phenyl-1,3,4-oxadiazole (4a): ¹H NMR (400 MHz, CDCl₃)

```
expt s2pu1
SAMPLE
date Apr 6 2011 temp not used
solvent CDCl3 gain not used
file exp spin not used
ACQUISITION hst 0.985
sv 6389.8 pw90 19.700
at 1.390 alfa 20.000
np 25528
fb not used il
bs 4 in n
d1 1.000 dp y
nt 32 hs nn
ct 32 PROCESSING 0.10
TRANSMITTER lb fn 65536
tn 399.853
sfrq 362.8 sp DISPLAY -365.8
tof 57 wp 4719.4
pw 9.850 rfl 783.9
DECOUPLER rfp 0
dn C13 rp 100.2
dor 0 lp -90.4
dm nnn PLDT 250
dmc c wc 336
dpwr 50 sc 0
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nm cdc ph 20
```



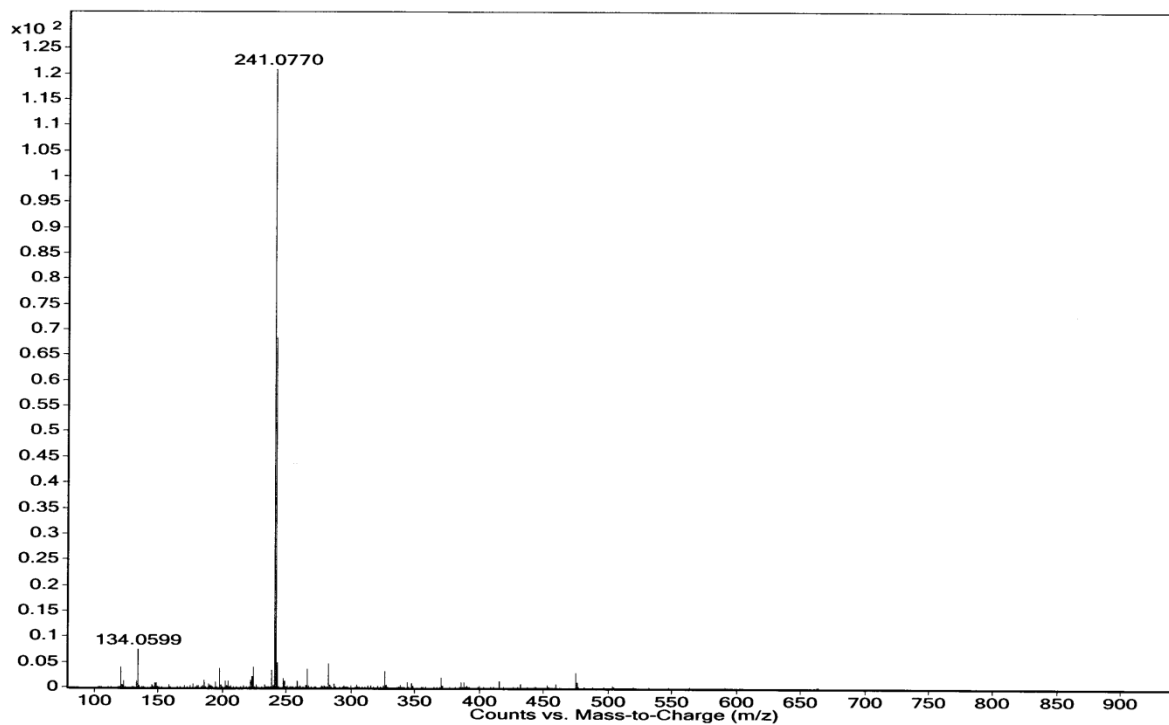
2-(4-Fluorophenyl)-5-phenyl-1,3,4-oxadiazole (4a): ^{13}C NMR (100 MHz, CDCl_3)

```
exp1 s2pu1
SAMPLE          SPECIAL
date Apr 17 2011 temp not used
solvent CDCl3 gain not used
file           exp spin not used
ACQUISITION    hst 0.008
sw 25125.6 pw90 18.800
at 1.189 a17a 20.000
np 60270 FLAGS
fb 13800 tl n
bs 32 in n
dl 1.000 dp y
nt 5000 hs nn
ct 992 PROCESSING
TRANSMITTER    tb 2.00
tn C13 fn 65536
sfrq 100.554 DISPLAY
tof 1536.3 sp -153.8
tpwr 61 wp 21130.6
pw 9.300 rfp 9272.1
DECOUPLER      H1 rfp 7764.9
dn 0 lp 9.5
dof 0 tp -477.8
dm yyy PLOT
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nm no ph 2
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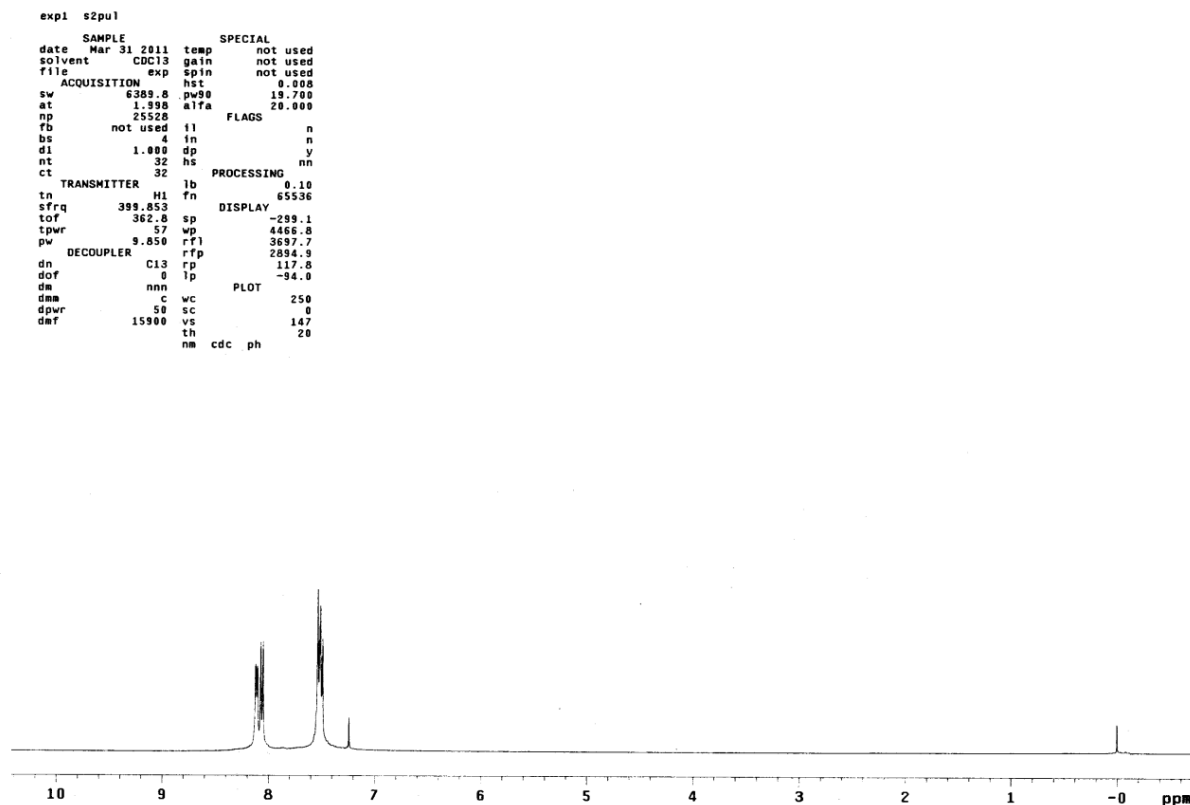


2-(4-Fluorophenyl)-5-phenyl-1,3,4-oxadiazole (4a): HRMS

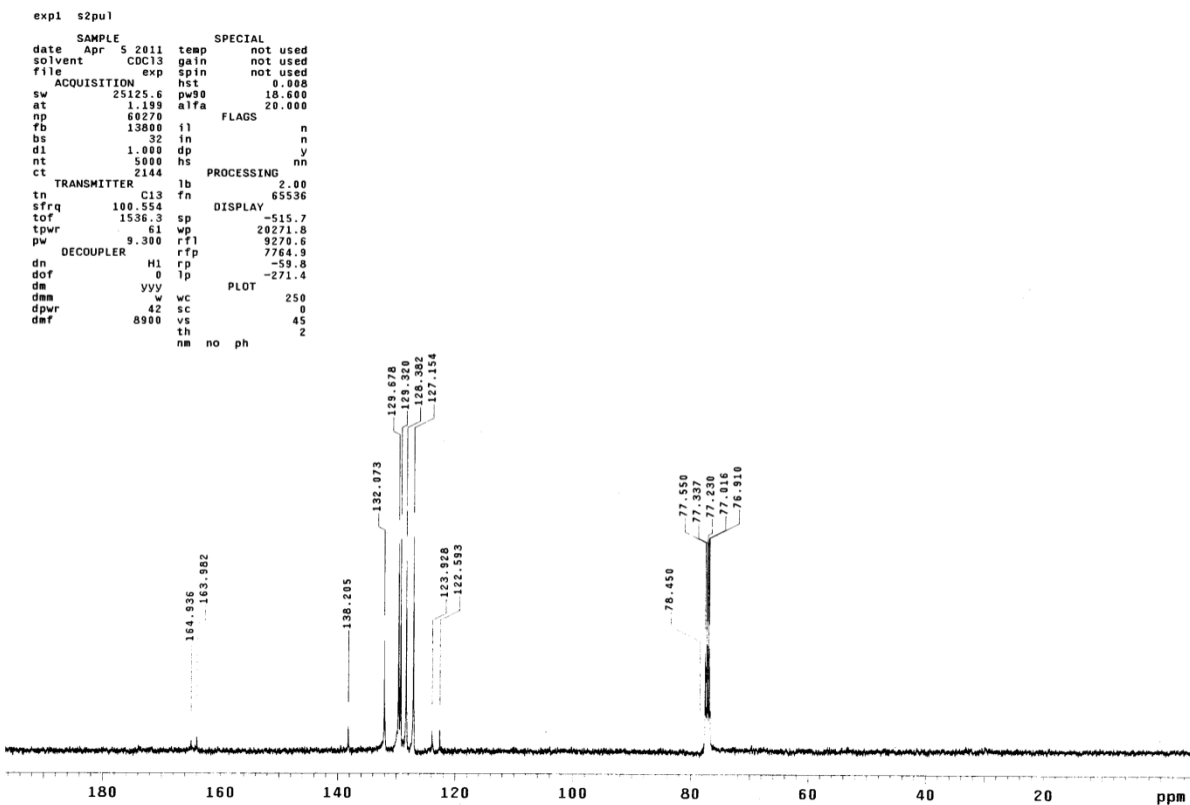
Sample Name	Position	Instrument Name	User Name
Inj Vol	InjPosition	SampleType	IRM Calibration Status
Data Filename	ACQ Method	Comment	Acquired Time



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



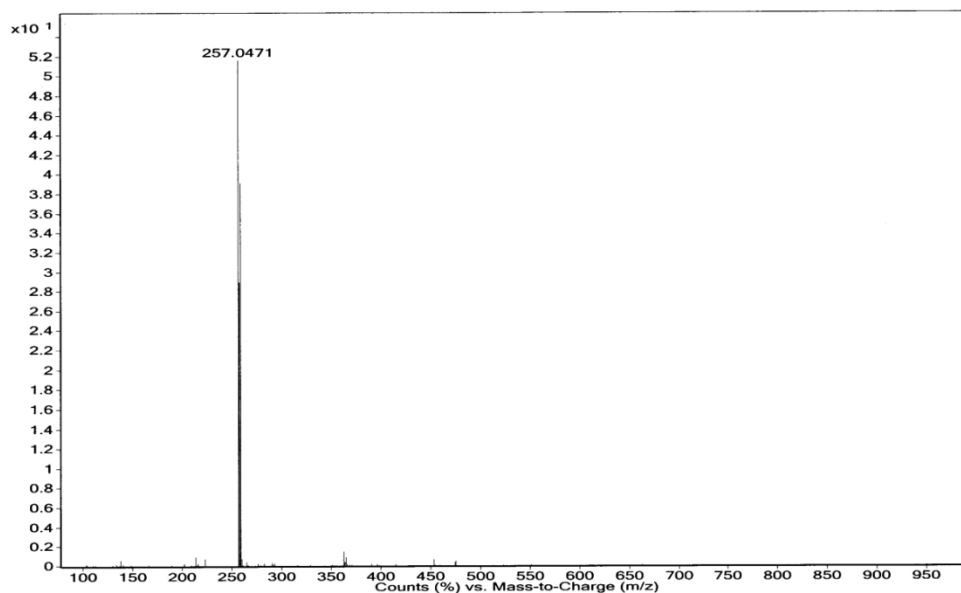
2-(4-Chlorophenyl)-5-phenyl-1,3,4-oxadiazole (5a): ^{13}C NMR (100 MHz, CDCl_3)



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

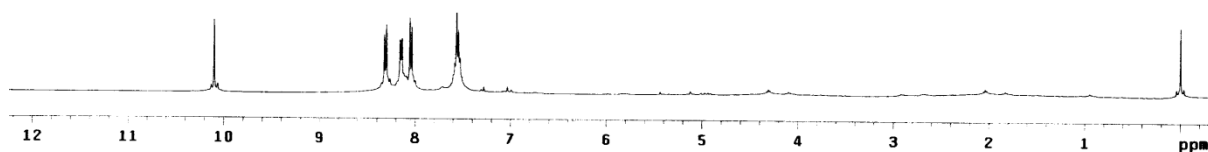
Sample Name	Position	Vial	Instrument Name	Instrument 1	User Name
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Data Filename		ACQ Method	Comment		Acquired Time

Success
8/29/2011 12:35:33



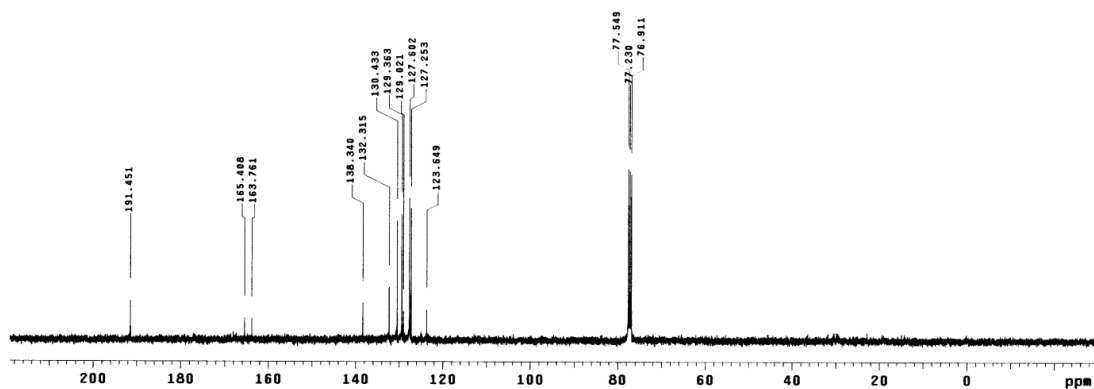
4-(5-Phenyl-1,3,4-oxadiazol-2-yl)-benzaldehyde (6a): ¹H NMR (400 MHz, CDCl₃)

```
#exp1 s2pu1
SAMPLE
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
fb not used il
bs 4 in n
d1 1.000 dp y
nt 32 hs nn
ct 32
TRANSMITTER lb 0.10
tn H1 fn 65536
sfrq 399.853
tof 362.8 sp DISPLAY -140.8
tpwr 57 wp 5063.0
pw 9.850 rfl 787.2
DECOUPLER rfp
dn C13 fp 105.2
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dm nnn PLOT
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dpwr 50 sc 0
dmf 15900 vs 38
th 20
na cdc ph
```



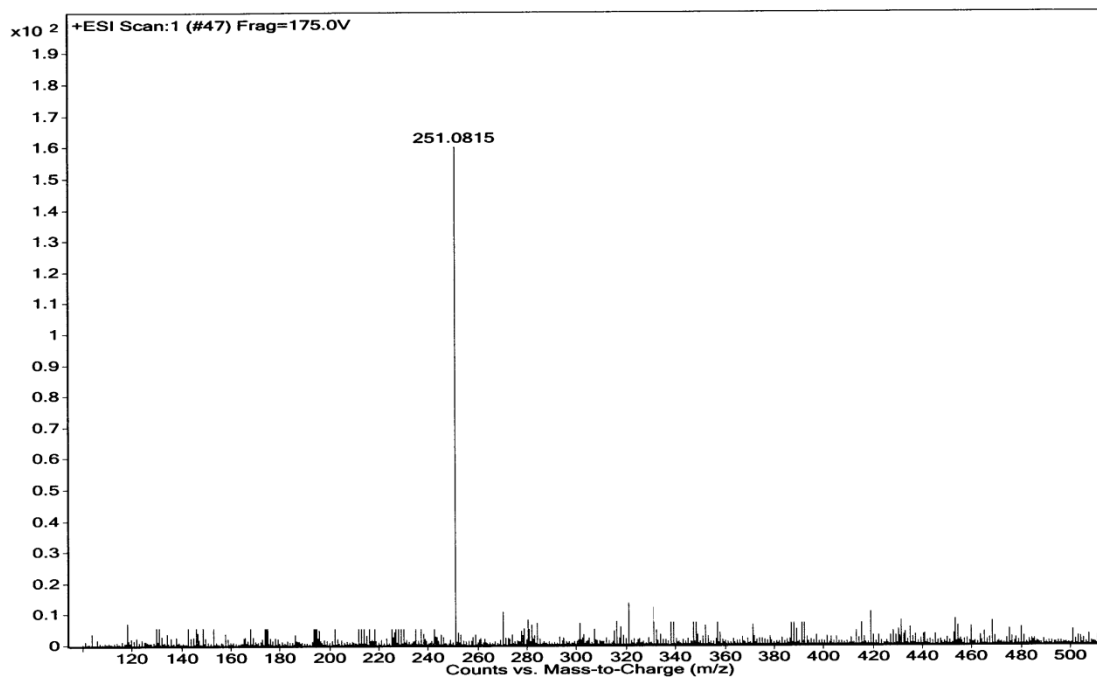
4-(5-Phenyl-1,3,4-oxadiazol-2-yl)-benzaldehyde (6a): ^{13}C NMR (100 MHz, CDCl_3)

```
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date Jan 29 2012 temp not used
solvent CDCl3 gain not used
file exp spin not used
ACQUISITION
sw 25000.0 hst 0.000
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np 59868
fb 13500
bs 10
dl 0
nt 10000
ct 3390
TRANSMITTER C13
tn C13
sfrq 100.552
tof 0
tpwr 61
pw 8.667
DECOUPLER H1
dn 0
dm yyv
dpr 42
def 8000
SPECIAL
temp not used
gain not used
spin not used
hst 0.000
pwr 18.500
atfa 20.000
FLAGS
i1 n
in n
dp y
hs nn
PROCESSING
fb 1.00
fn not used
DISPLAY
sp -2883.0
wp 25000.0
rf1 10747.9
rfp 7764.9
rp -78.4
lp -296.0
PLOT
wc 250
sc 0
vs 38
th 5
nm no ph
```



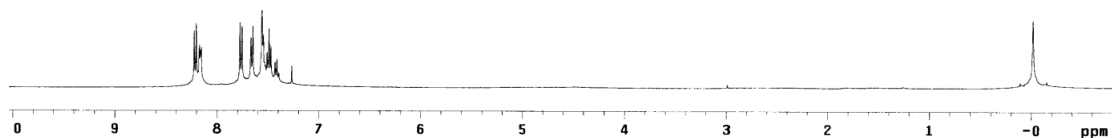
4-(5-Phenyl-1,3,4-oxadiazol-2-yl)-benzaldehyde (6a): HRMS

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



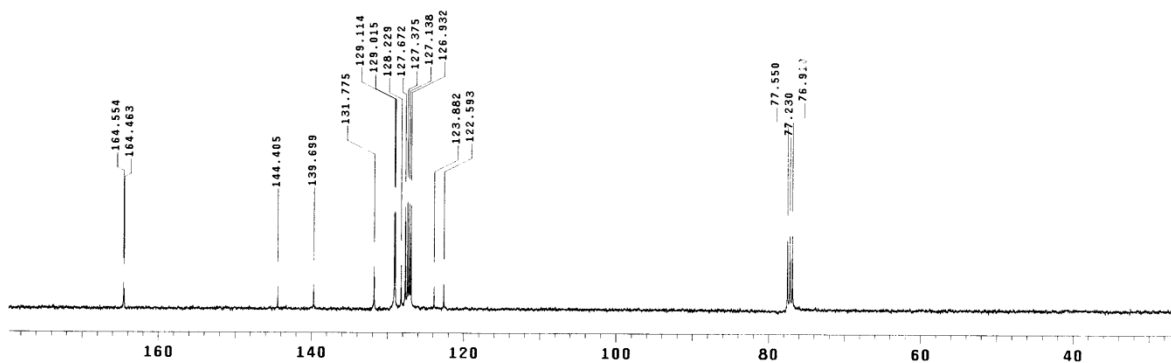
2-Biphenyl-4-yl-5-phenyl-1,3,4-oxadiazole (7a): ¹H NMR (400 MHz, CDCl₃)

```
SAMPLE          SPECIAL
date Jan 27 2012 temp not used
solvent CDC13 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
fb not used i1 n
bs 4 in n
d1 1.000 dp y
nt 32 hs nn
ct
TRANSMITTER lb 0.10
tn H1 fn 65536
sfrq 399.853 DISPLAY
tof 362.8 sp -321.6
tpwr 57 wp 4397.8
pw 9.850 rf1 791.3
DECOUPLER rfp 0
dn C13 rp 110.5
dot 0 lp -89.8
dm nnn PLOT
dmm c wc 250
dpwr 50 sc 0
dmf 15900 vs 134
nm cdc ph 20
```



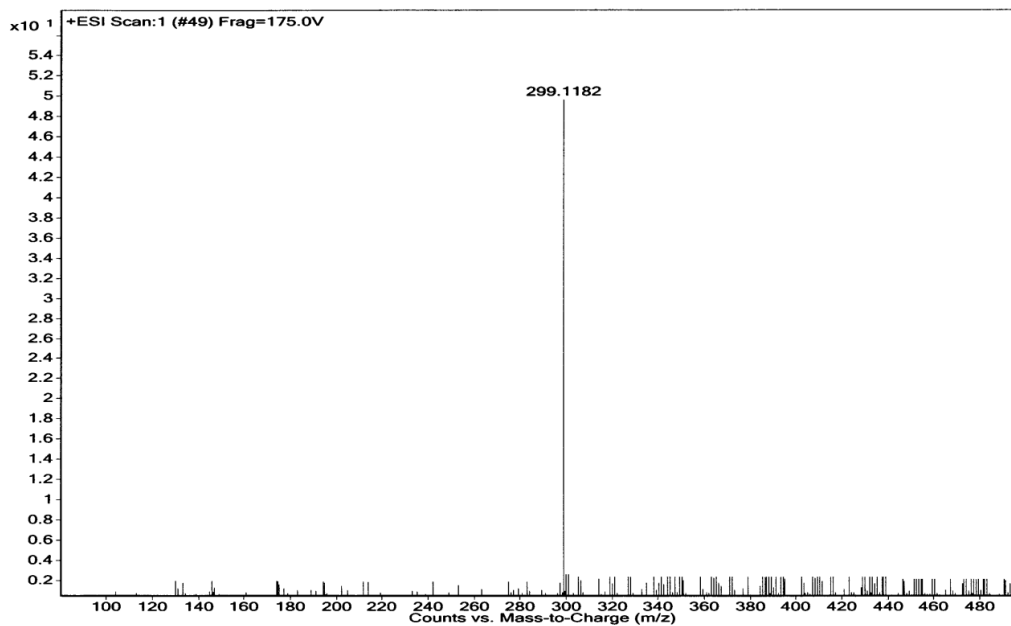
2-Biphenyl-4-yl-5-phenyl-1,3,4-oxadiazole (7a): ¹³C NMR (100 MHz, CDCl₃)

```
SAMPLE          SPECIAL
date Jan 27 2012 temp not used
solvent CDC13 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
fb 13800 i1 n
bs 10 in n
d1 1.000 dp y
nt 10000 hs nn
ct
TRANSMITTER lb 2.00
tn C13 fn 65536
sfrq 100.554 DISPLAY
tof 1536.3 sp 1944.2
tpwr 61 wp 16111.9
pw 9.300 rf1 9287.4
DECOUPLER rfp 7764.9
dn H1 rp -79.4
dot 0 lp -304.2
dm VVV PLOT
dmm w wc 250
dpwr 42 sc 0
dmf 8900 vs 22
nm no ph 2
```



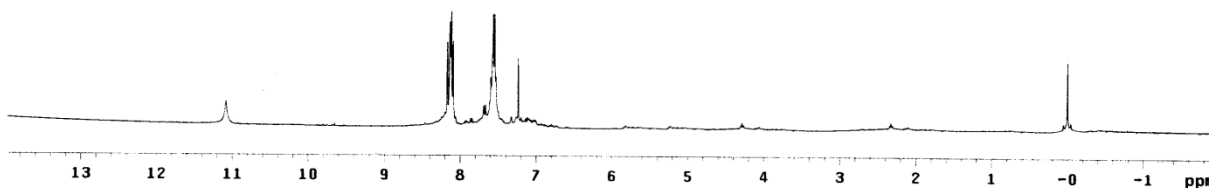
2-Biphenyl-4-yl-5-phenyl-1,3,4-oxadiazole (7a): HRMS

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

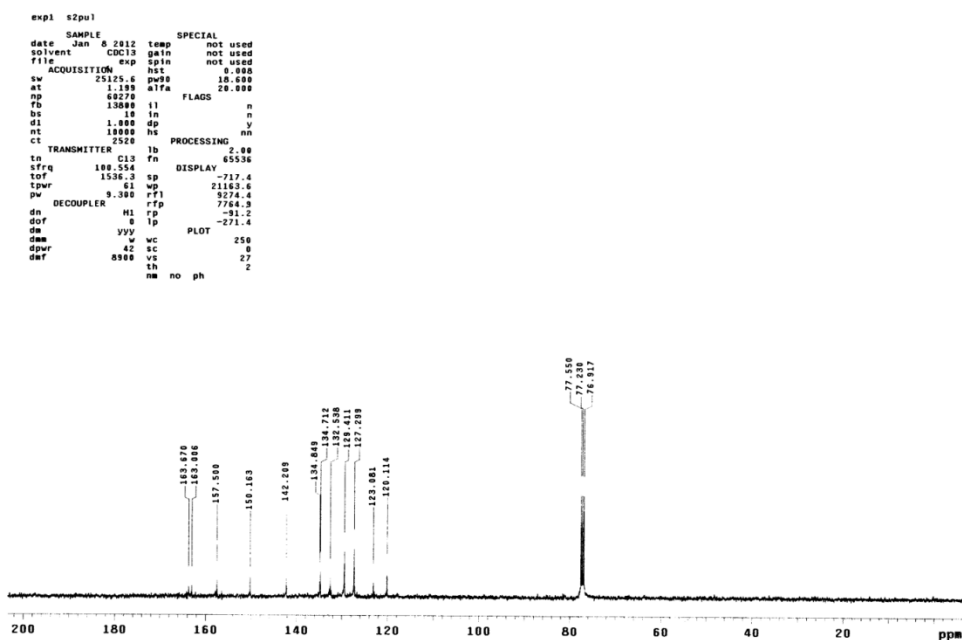


2-(5-Phenyl-1,3,4-oxadiazol-2-yl)-phenol (8a): ¹H NMR (400 MHz, CDCl₃)

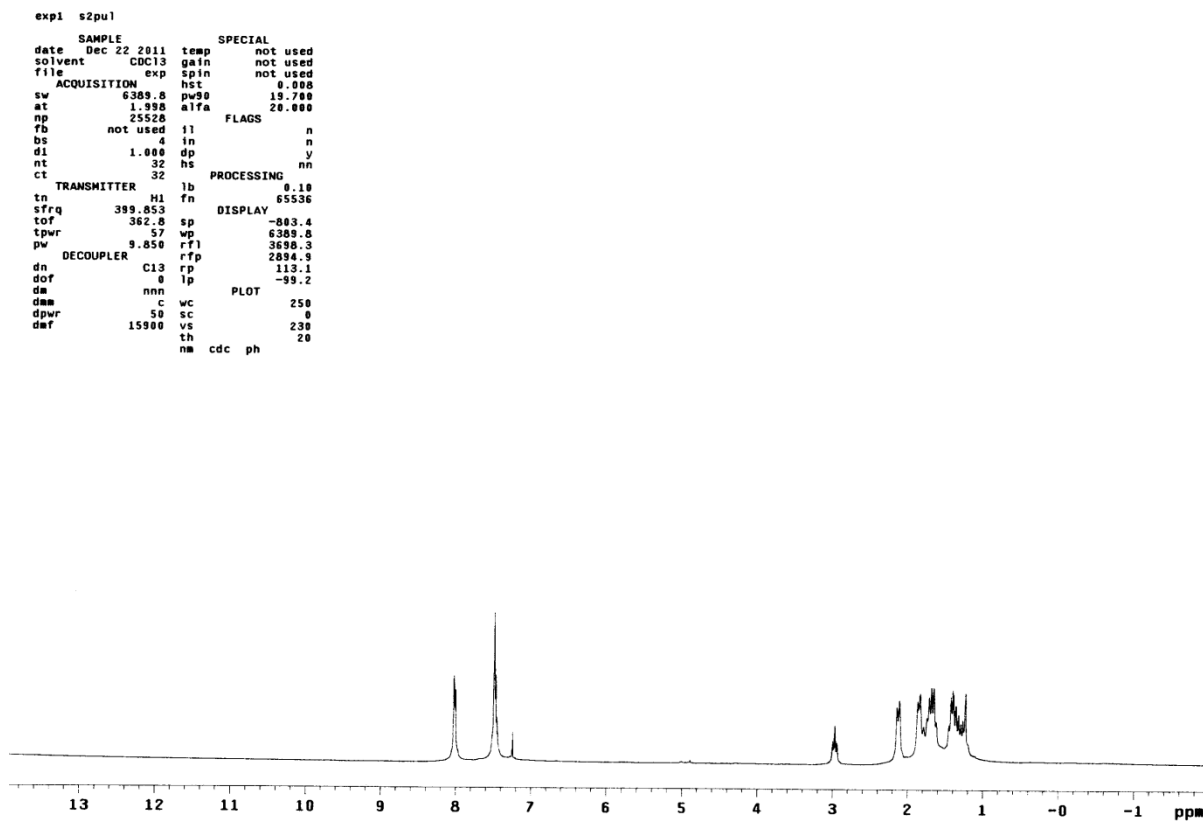
```
exp1 s2pu1
SAMPLE
date Jan 3 2012 temp not used
solvent CDCl3 gain not used
file exp spin not used
ACQUISITION
sw 6389.8 pw90 19.700
at 1.998 alfa 20.000
np 25528 FLAGS
fb not used i1 n
bs 4 in n
dl 1.000 dp y
nt 32 hs nn
ct 32 PROCESSING
TRANSMITTER lb 0.10
tn H1 rn 65536
sfrq 399.853 DISPLAY
tof 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
da nnn PLOT
dam c wc 250
dpwr 50 sc 0
def 15980 vs 301
nm cdc ph 9
```



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

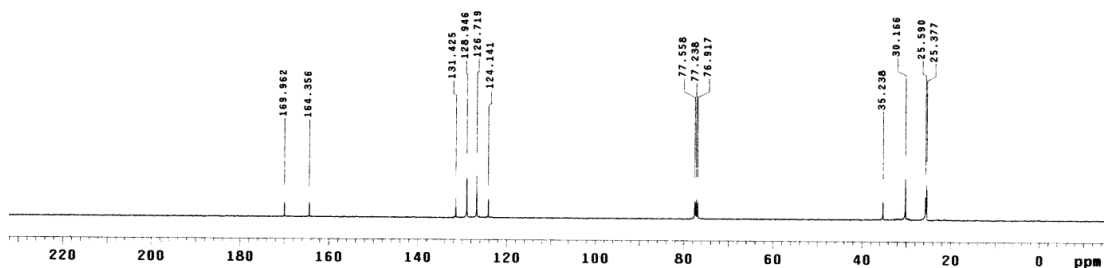


2-Cyclohexyl-5-phenyl-1,3,4-oxadiazole (9a): ^1H NMR (400 MHz, CDCl_3)



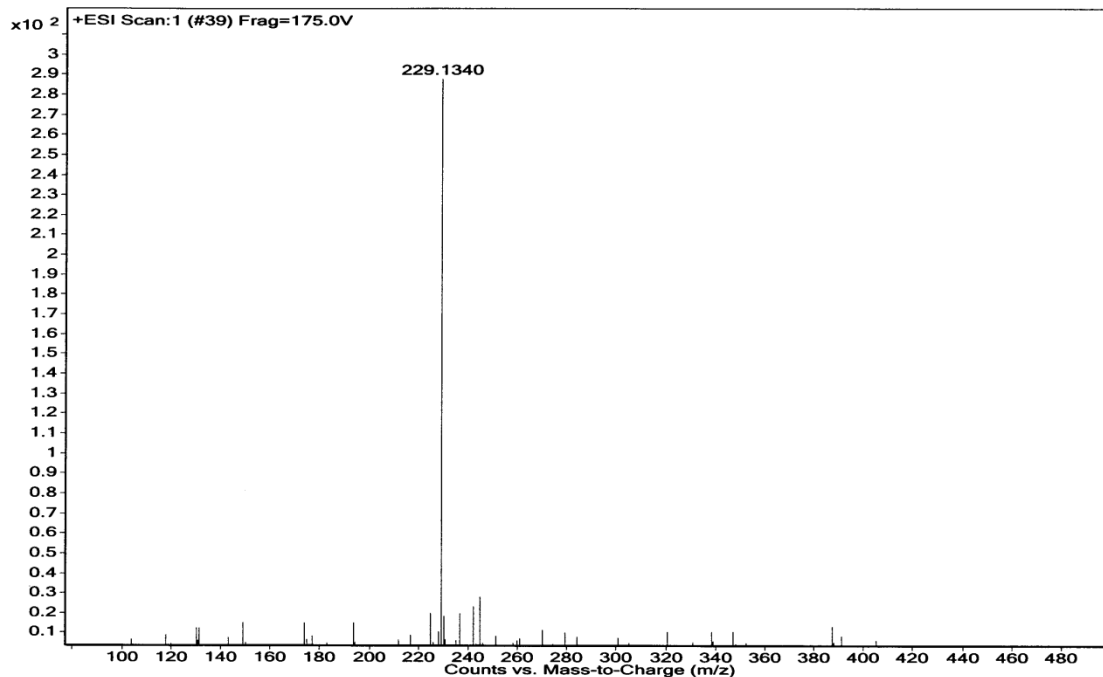
2-Cyclohexyl-5-phenyl-1,3,4-oxadiazole (9a): ^{13}C NMR (100 MHz, CDCl_3)

```
expl s2pu1
SAMPLE
date Dec 29 2011 temp not used
solvent CDCl3 gain not used
file exp spin not used
ACQUISITION hsc 8.000
sw 25125.6 pw90 18.000
at 1.199 a1fa 20.000
np 60270
fb 13800 f1 n
bs 4 f2 n
d1 1.000 dp y
nt 5000 hs nn
ct 1992
TRANSMITTER lb 2.00
tn C13 fn 65536
sfreq 100.554 DISPLAY
tof 1536.3 sp -1522.5
tpwr 61 wp 25125.6
pw 9.300 rf1 3207.4
DECOUPLER rfp 7764.9
dn H1 rp -47.5
dof 0 lp -374.2
da yyy PLOT
dme w wc 250
dper 42 sc 0
daf 8900 vs 9
th 1
nm no ph 1
```

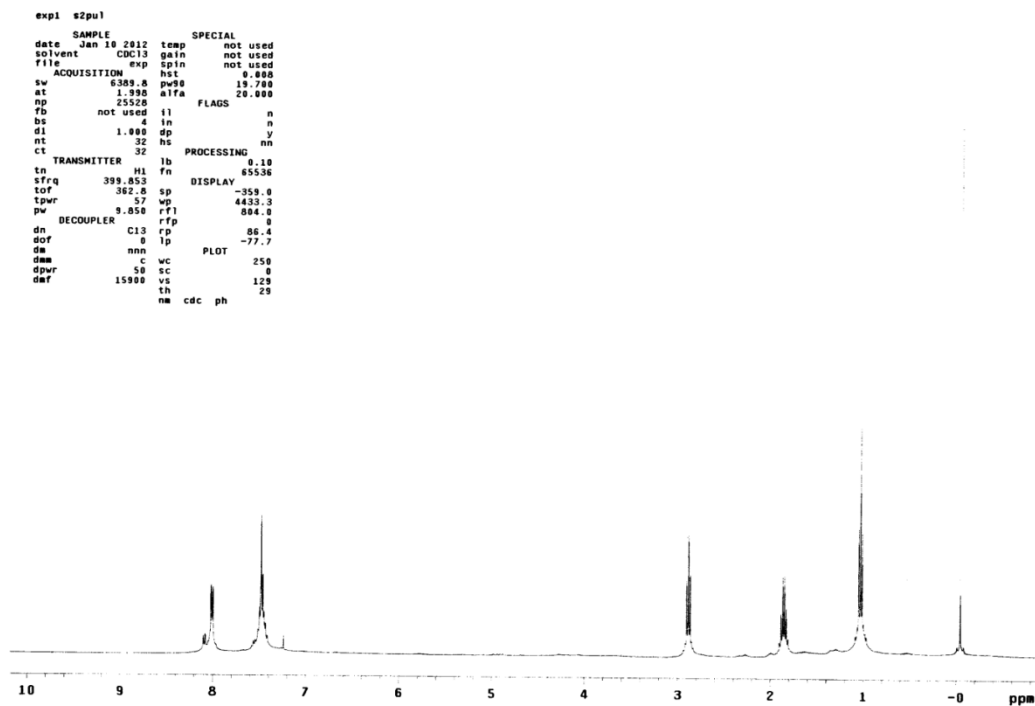


2-Cyclohexyl-5-phenyl-1,3,4-oxadiazole (9a): HRMS

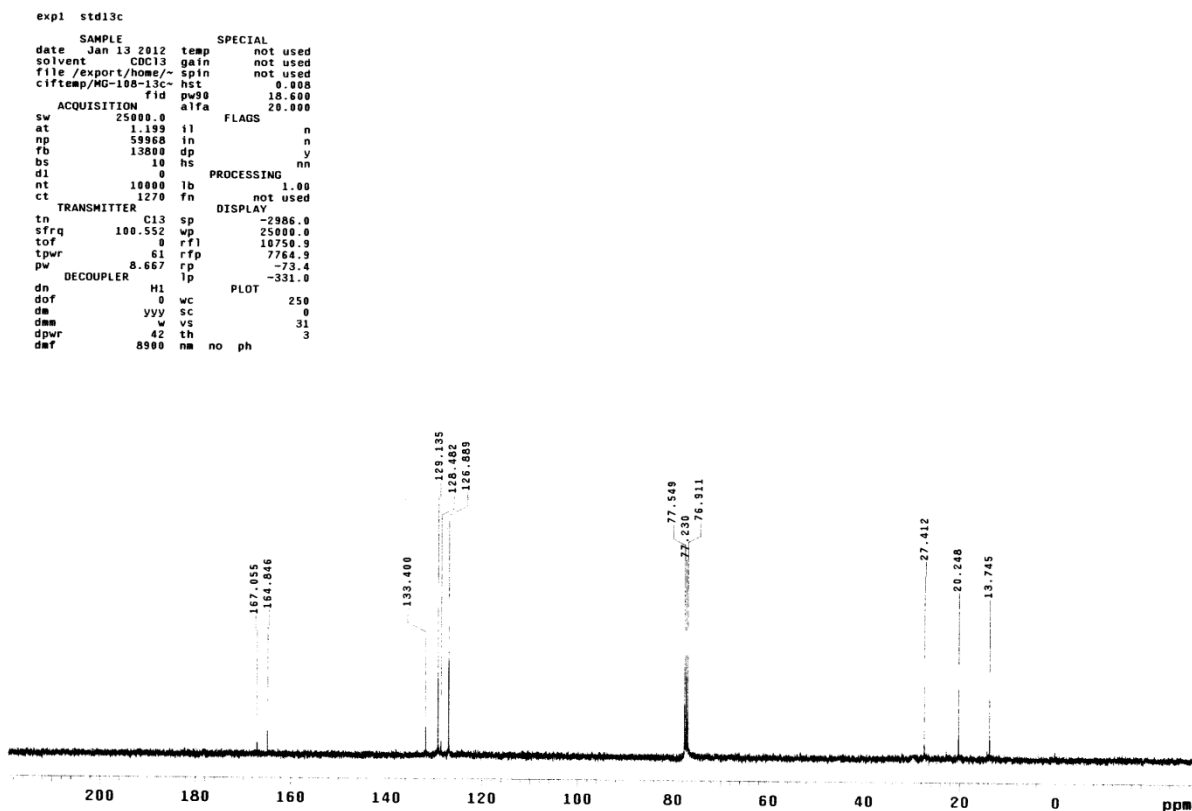
Sample Name	Position	Instrument Name	User Name
Inj Vol	InjPosition	SampleType	IRM Calibration Status
Data Filename	ACQ Method	Comment	Acquired Time



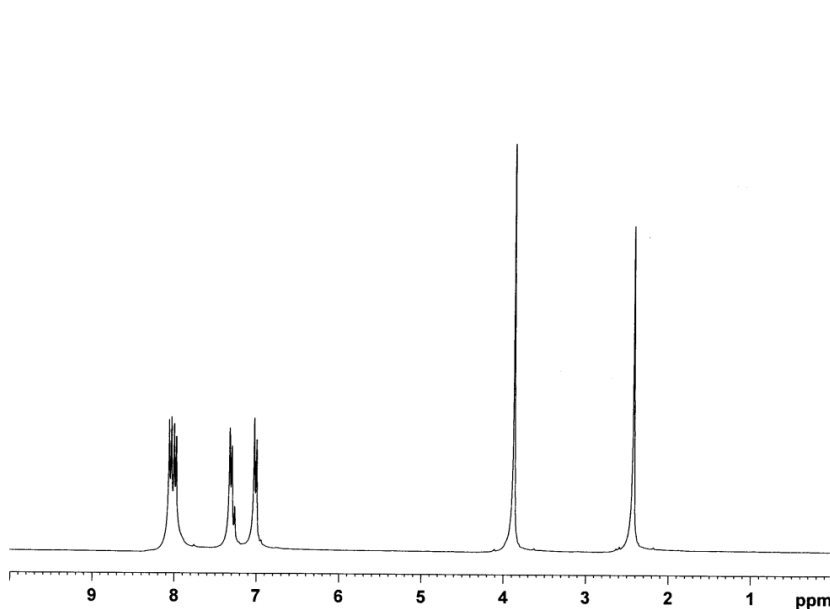
2-Phenyl-5-propyl-1,3,4-oxadiazole (10a): ^1H NMR (400 MHz, CDCl_3)



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



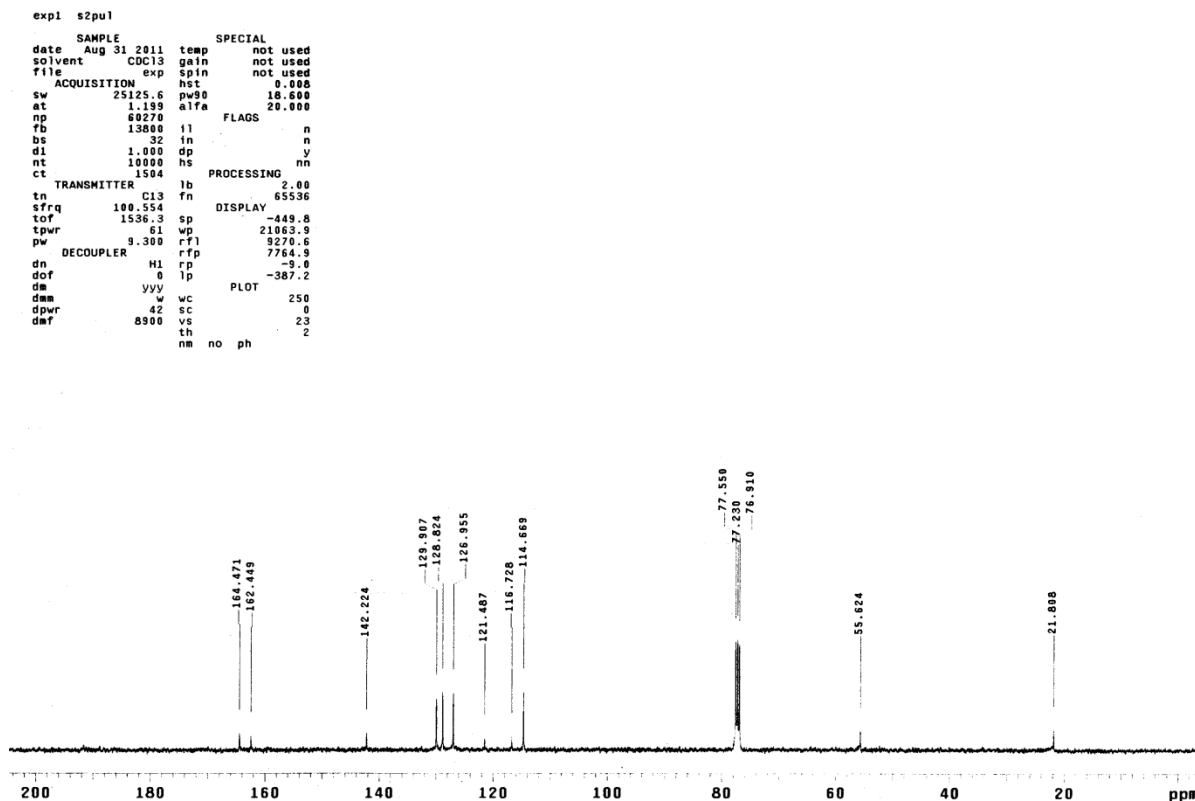
2-(4-Methoxyphenyl)-5-p-tolyl-1,3,4-oxadiazole (11a): ¹H NMR (400 MHz, CDCl₃)



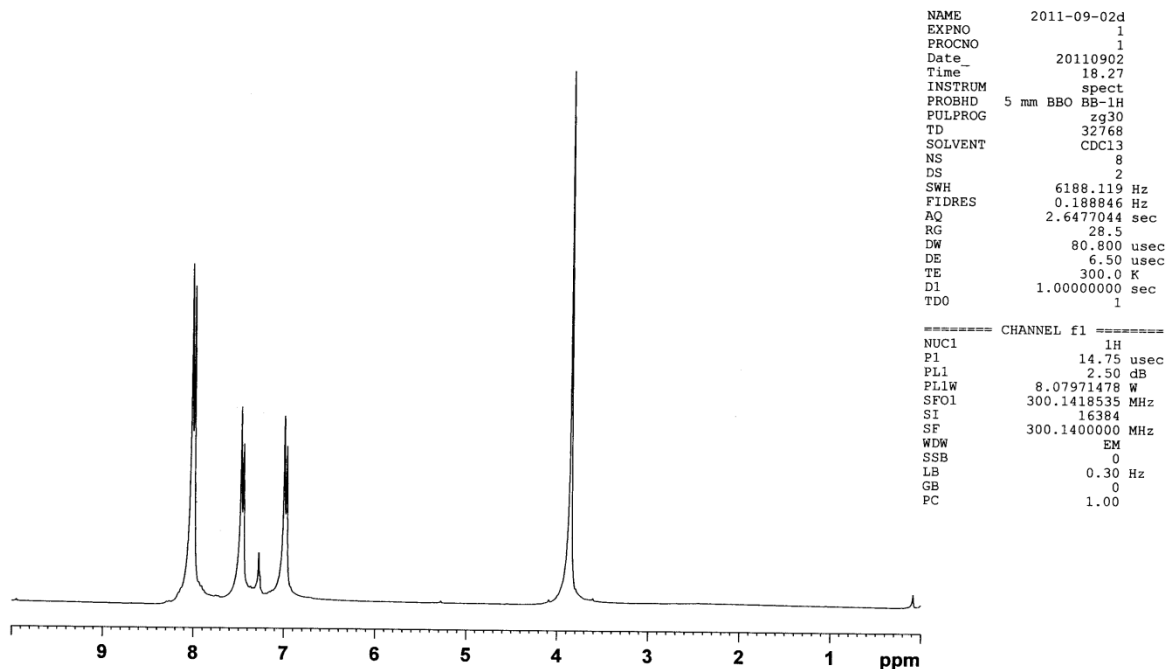
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NAME          2011-09-02b
EXPNO         1
PROCNO        1
Date_         20110902
Time         18.19
INSTRUM      spect
PROBHD       5 mm BBO BB-1H
PULPROG      zg30
TD           32768
SOLVENT      CDCl3
NS           8
DS           2
SWH          6188.119 Hz
FIDRES       0.188846 Hz
AQ           2.6477044 sec
RG           28.5
DW           80.800 usec
DE           6.50 usec
TE           300.0 K
D1           1.00000000 sec
TD0          1

===== CHANNEL f1 =====
NUC1          1H
P1           14.75 usec
PL1          2.50 dB
PL1W         8.07971478 W
SFO1         300.1418535 MHz
SI           16384
SF           300.1400000 MHz
WDW          EM
SSB          0
LB           0.30 Hz
GB           0
PC           1.00
```

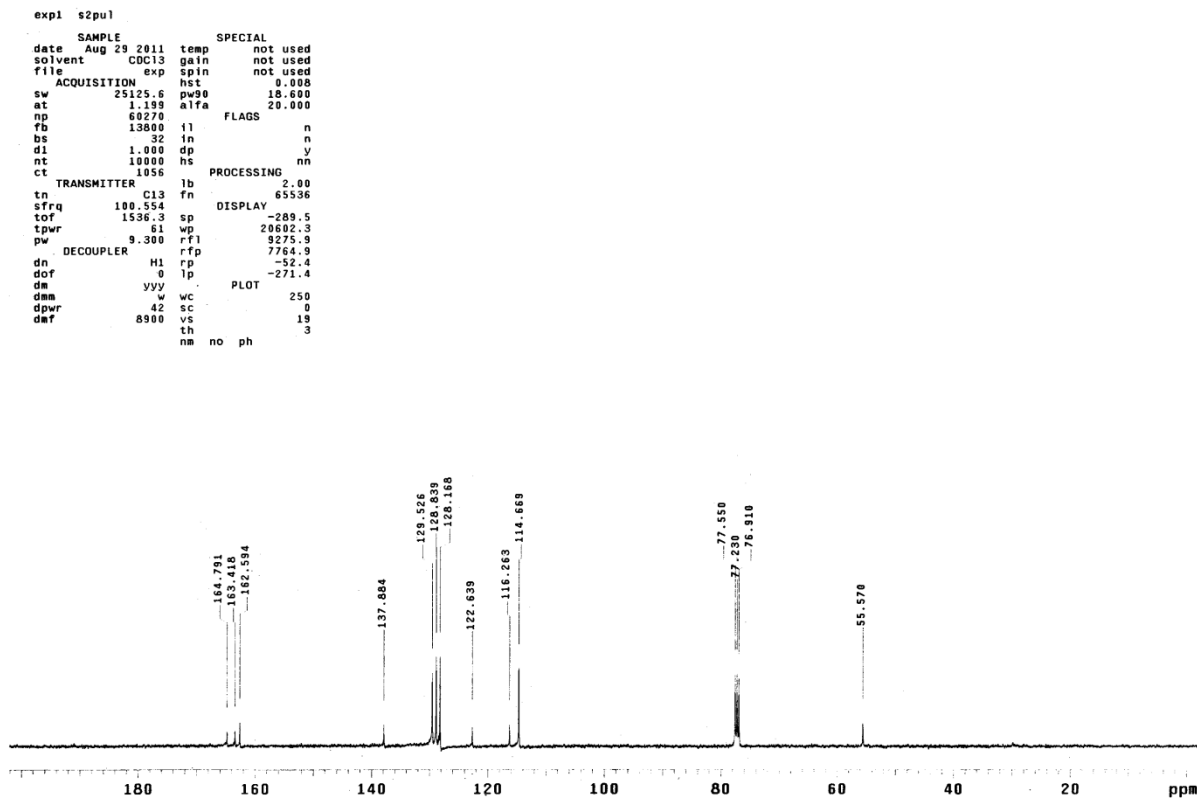
2-(4-Methoxyphenyl)-5-p-tolyl-1,3,4-oxadiazole (11a): ¹³C NMR (100 MHz, CDCl₃)



2-(4-Chlorophenyl)-5-(4-methoxyphenyl)-1,3,4-oxadiazole (12a): ¹H NMR (400 MHz, CDCl₃)

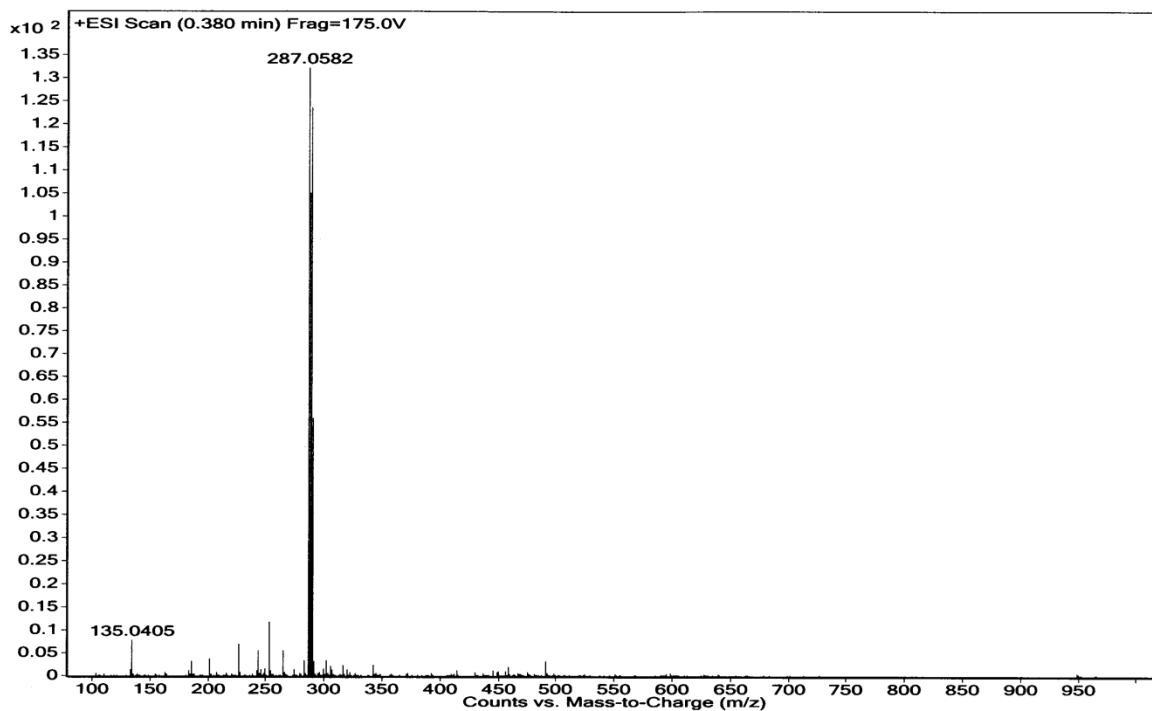


2-(4-Chlorophenyl)-5-(4-methoxyphenyl)-1,3,4-oxadiazole (12a): ¹³C NMR (100 MHz, CDCl₃)



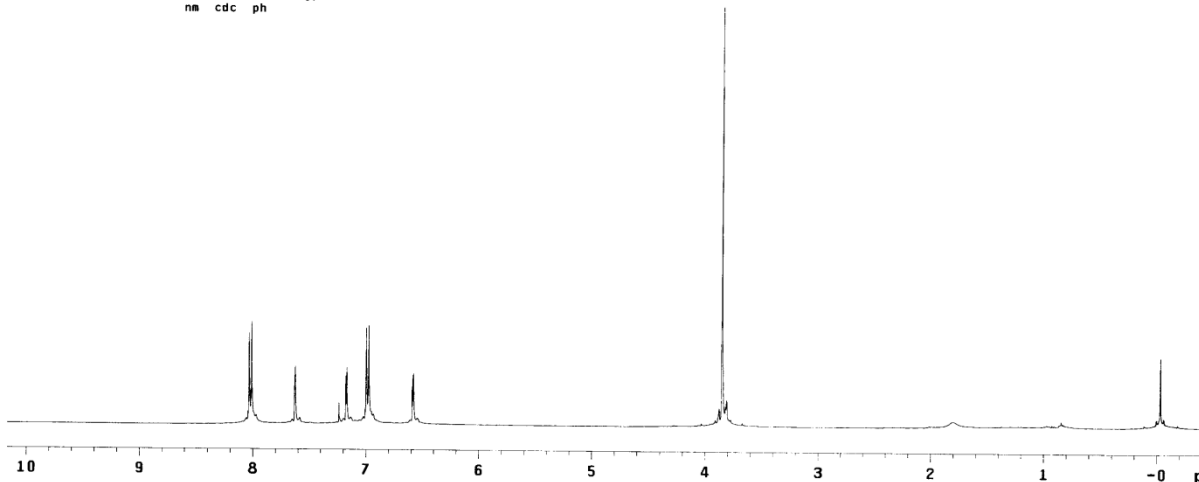
2-(4-Chlorophenyl)-5-(4-methoxyphenyl)-1,3,4-oxadiazole (12a): HRMS

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



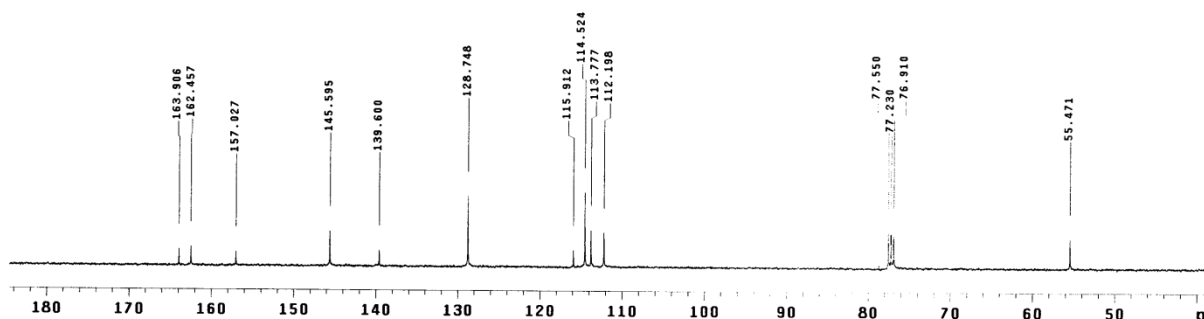
2-Furan-2-yl-5-(4-methoxy-phenyl)-1,3,4-oxadiazole (13a): ¹H NMR (400 MHz, CDCl₃)

```
SAMPLE          SPECIAL
date Feb 6 2012 temp not used
solvent CDC13 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
fb not used i1 FLAGS
bs 4 in n
dl 1.000 dp y
nt 32 hs n
ct 32 hs n
TRANSMITTER H1 lb 0.10
tn H1 fn 65536
sfrq 399.853 DISPLAY
tof 362.8 sp -257.9
tpwr 57 wp 4324.1
pw 9.850 rfl 3698.5
DECOUPLER C13 rfp 2894.9
dn C13 rp 110.2
dof 0 lp -92.2
da nnn PLOT
dmm c wc 250
dpwr 50 sc 0
dmf 15900 vs 98
nm cdc ph 67
```



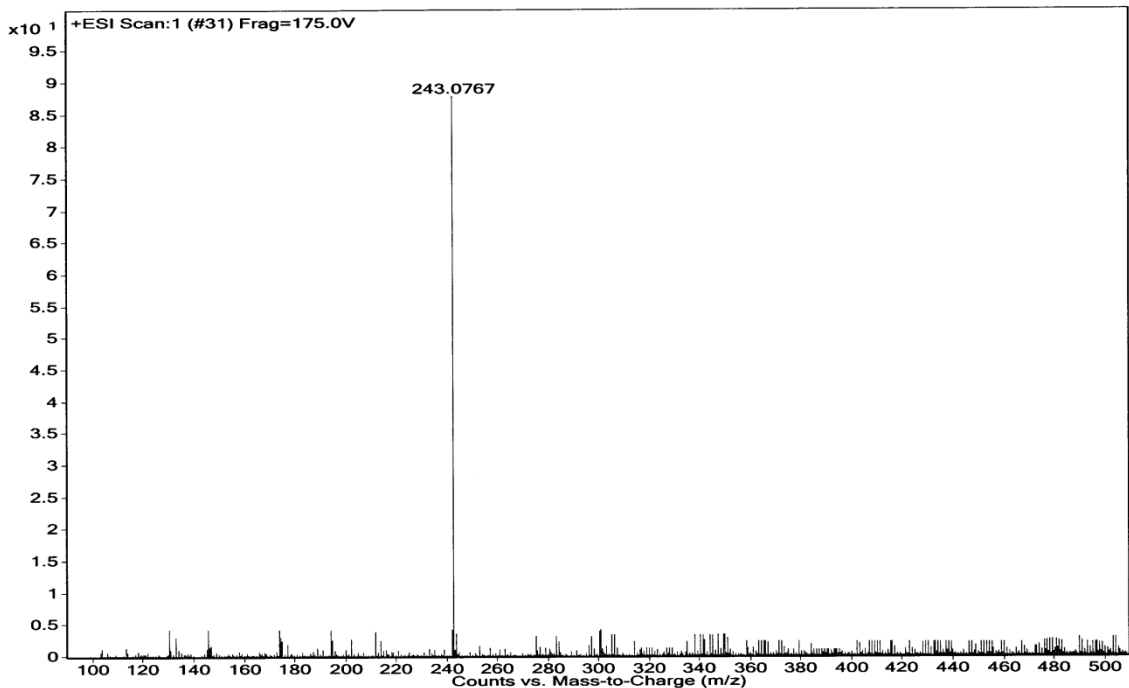
2-Furan-2-yl-5-(4-methoxy-phenyl)-1,3,4-oxadiazole (13a): ^{13}C NMR (100 MHz, CDCl_3)

```
SAMPLE          SPECIAL
date    Feb 4 2012    temp    not used
solvent  CDCl3      gain    not used
file
ACQUISITION  exp    spin    not used
sw       25125.6    hst     0.008
at       1.199     pwr     18.000
np       60270     alfa    20.000
fb       13800     FLAGS
bs       4        in      n
dl       1.000    dp      y
nt       10000   hs      nn
ct       1100
TRANSMITTER  fb      2.00
tn          C13   fn      65536
sfrq       100.554  DISPLAY
tof        1536.3  sp      3597.4
tpwr       61     wp      14956.4
pw         9.300   rfl     9284.4
DECOUPLER  H1     rfp     7764.9
dn         0      rp      -69.3
dof        0      lp      -338.2
dm         yyy    PLOT
dmm        w     wc      250
dpvr       42    sc      0
daf        8900  vs      15
           th      2
           nm    no  ph
```

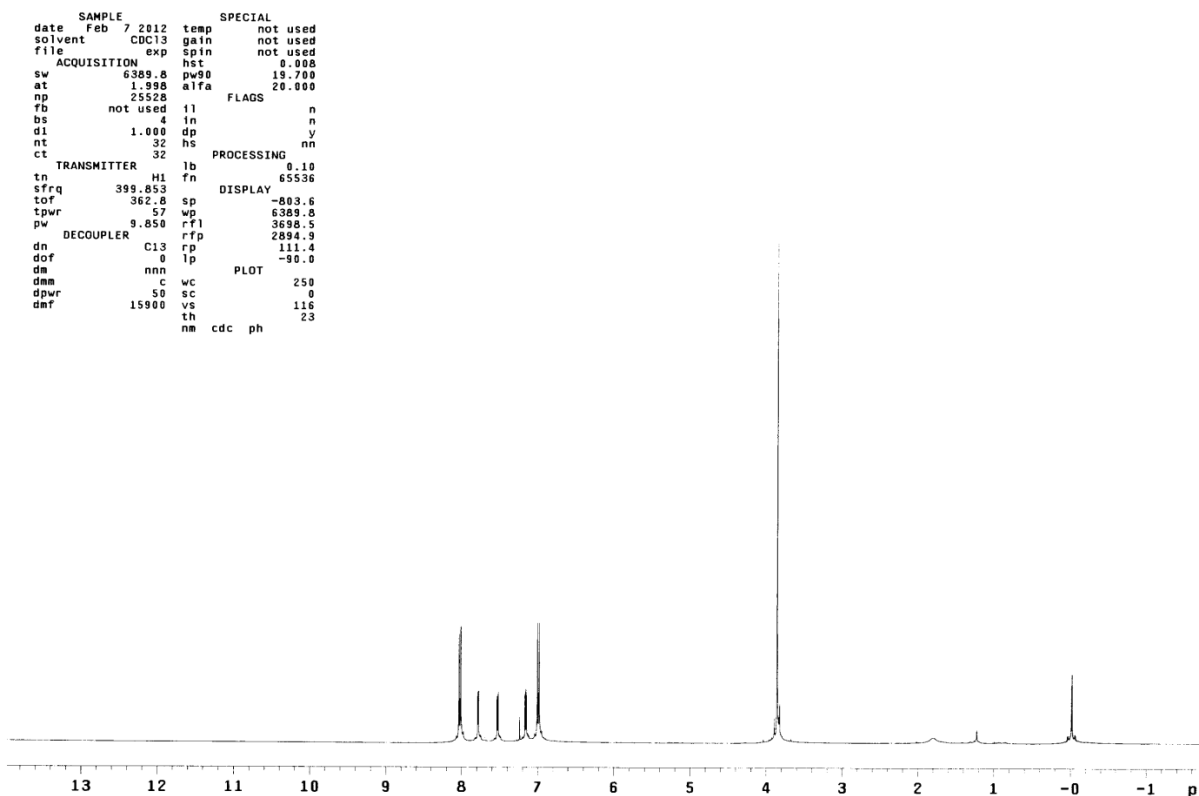


2-Furan-2-yl-5-(4-methoxy-phenyl)-1,3,4-oxadiazole (13a): HRMS

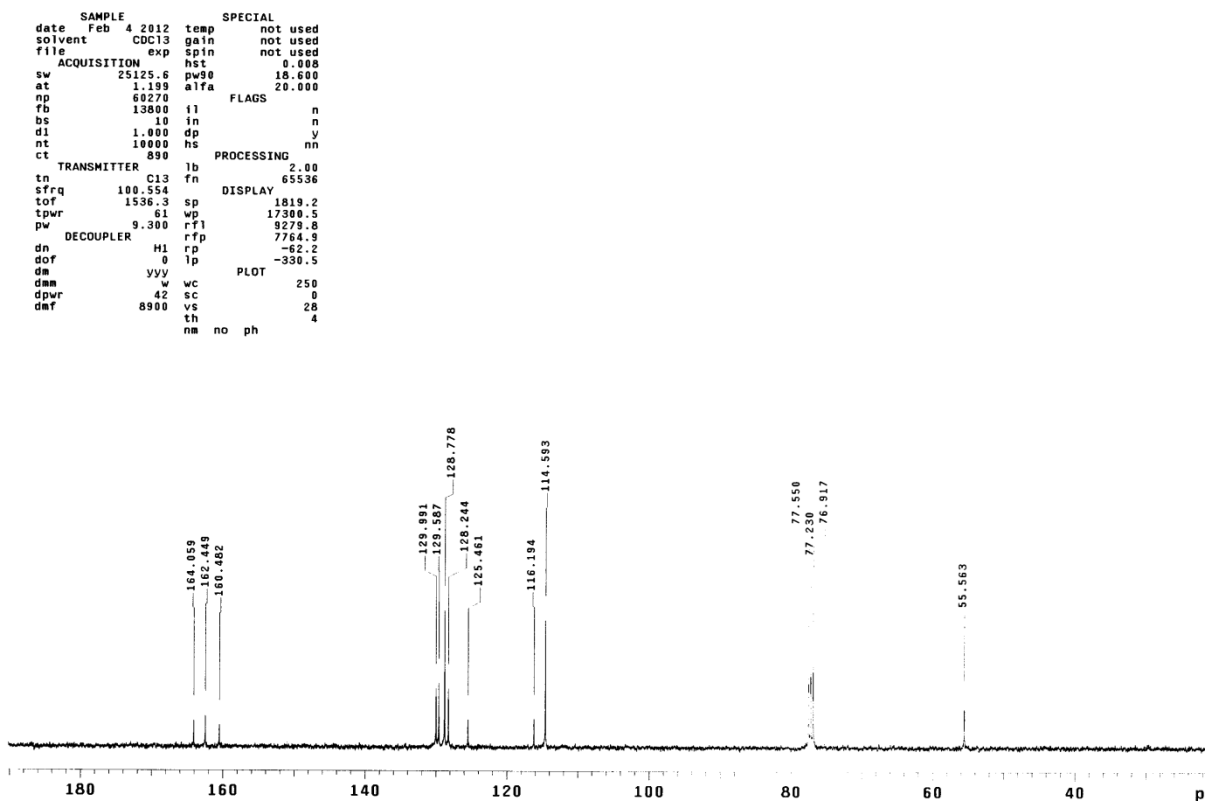
Sample Name	Position	Instrument Name	User Name
Inj Vol	InjPosition	SampleType	IRM Calibration Status
Data Filename	ACQ Method	Comment	Acquired Time



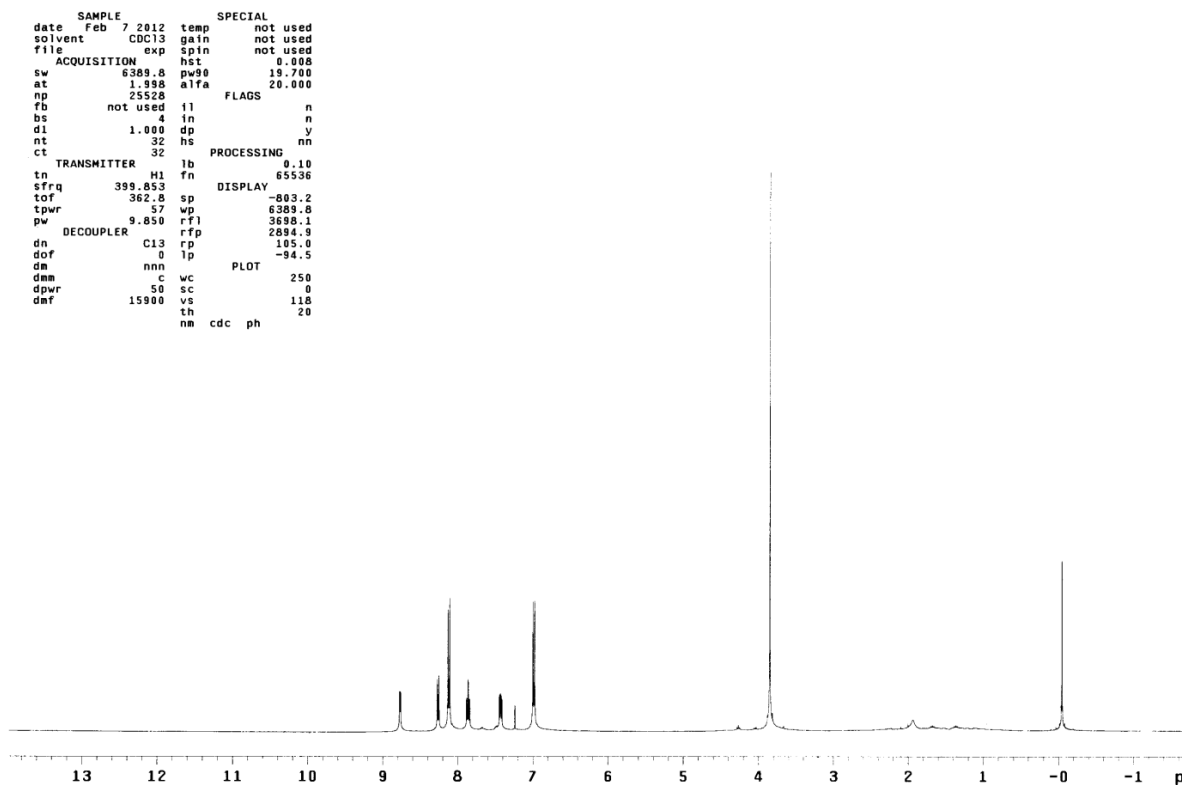
2-(4-Methoxy-phenyl)-5-thiophen-2-yl-1,3,4-oxadiazole (14a): ^1H NMR (400 MHz, CDCl_3)



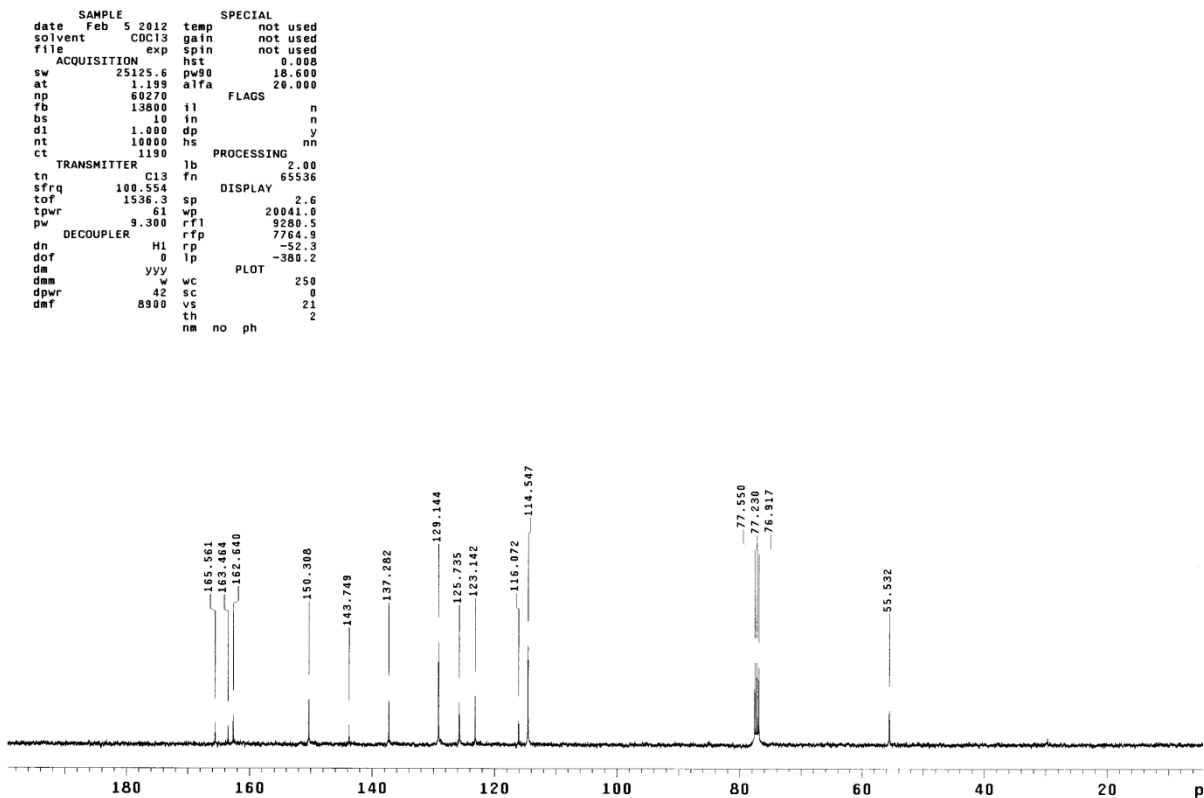
2-(4-Methoxy-phenyl)-5-thiophen-2-yl-1,3,4-oxadiazole (14a): ^{13}C NMR (100 MHz, CDCl_3)



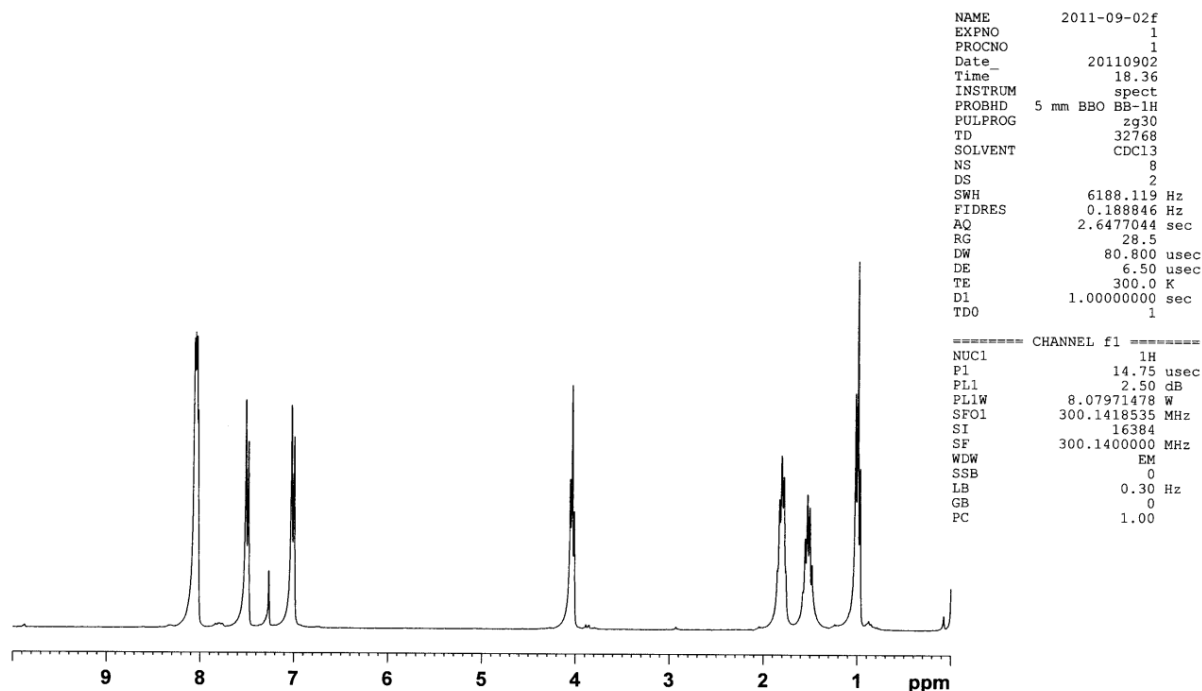
2-[5-(4-Methoxy-phenyl)-1,3,4-oxadiazole-2-yl]-pyridine (15a): ¹H NMR (400 MHz, CDCl₃)



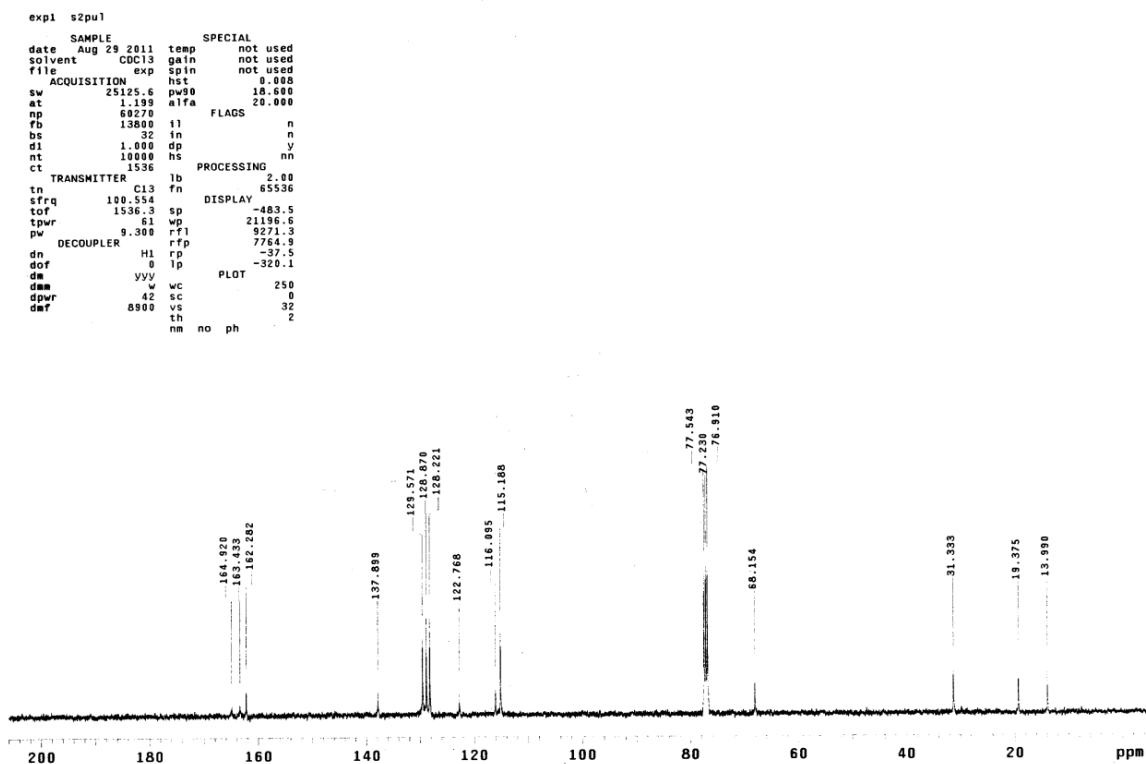
2-[5-(4-Methoxy-phenyl)-1,3,4-oxadiazole-2-yl]-pyridine (15a): ¹³C NMR (100 MHz, CDCl₃)



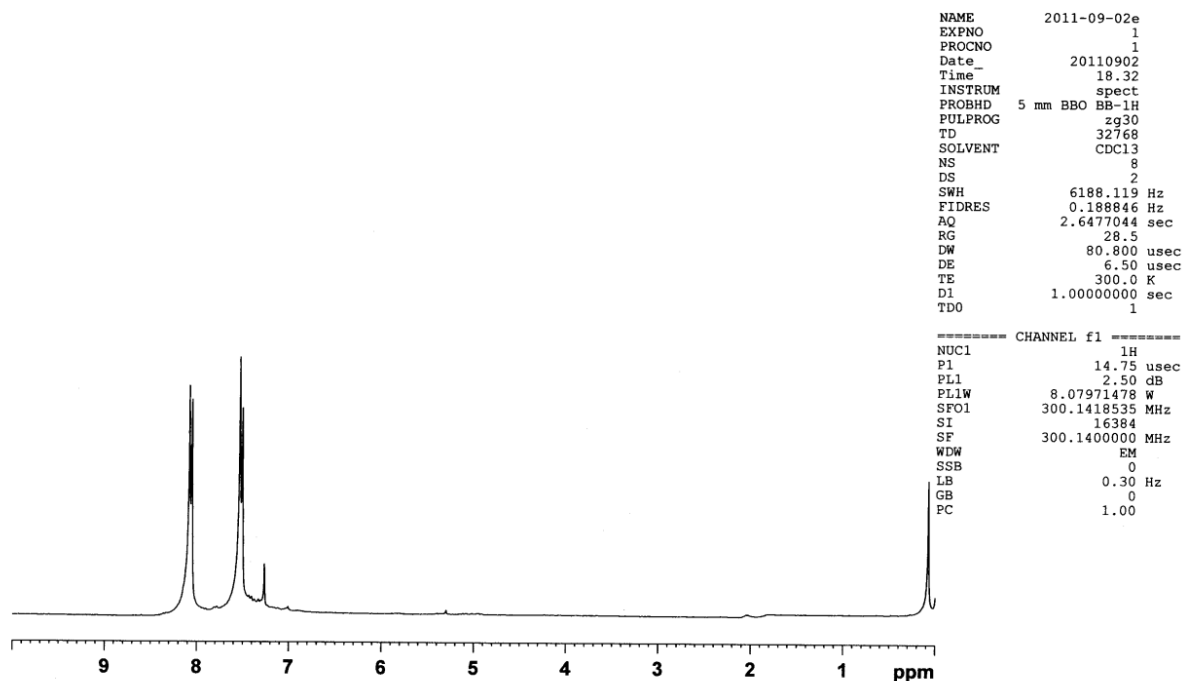
2-(4-Butoxyphenyl)-5-(4-chlorophenyl)-1,3,4-oxadiazole (16a): ¹H NMR (400 MHz, CDCl₃)



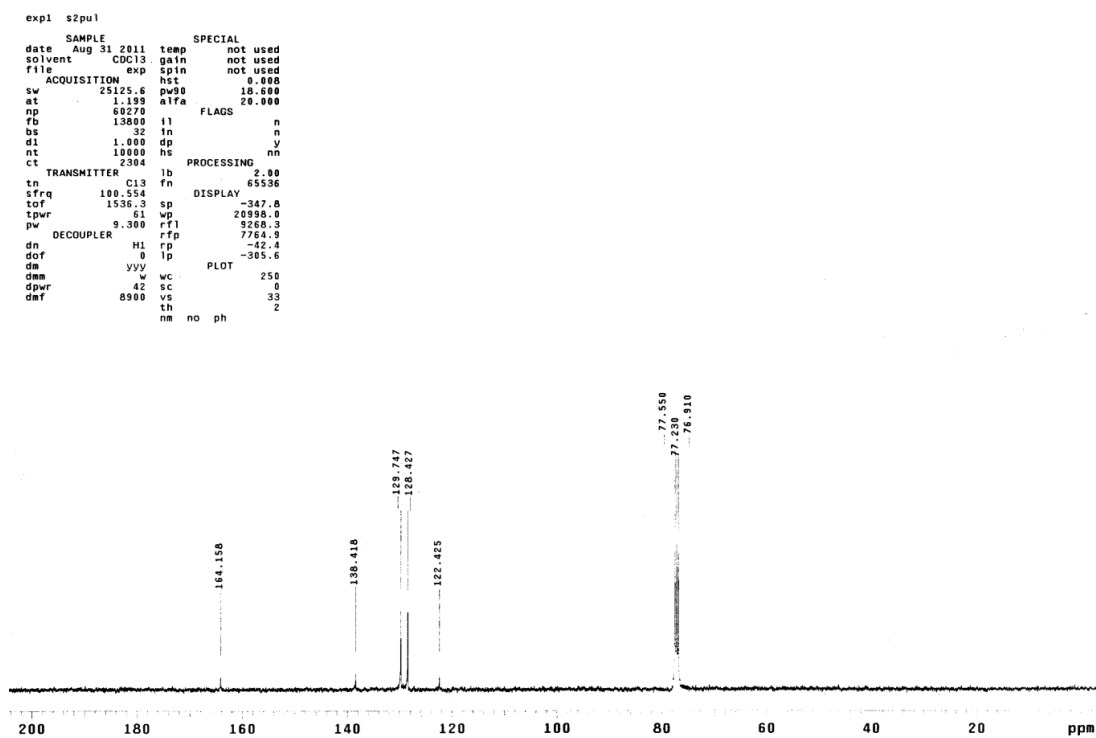
2-(4-Butoxyphenyl)-5-(4-chlorophenyl)-1,3,4-oxadiazole (16a): ¹³C NMR (100 MHz, CDCl₃)



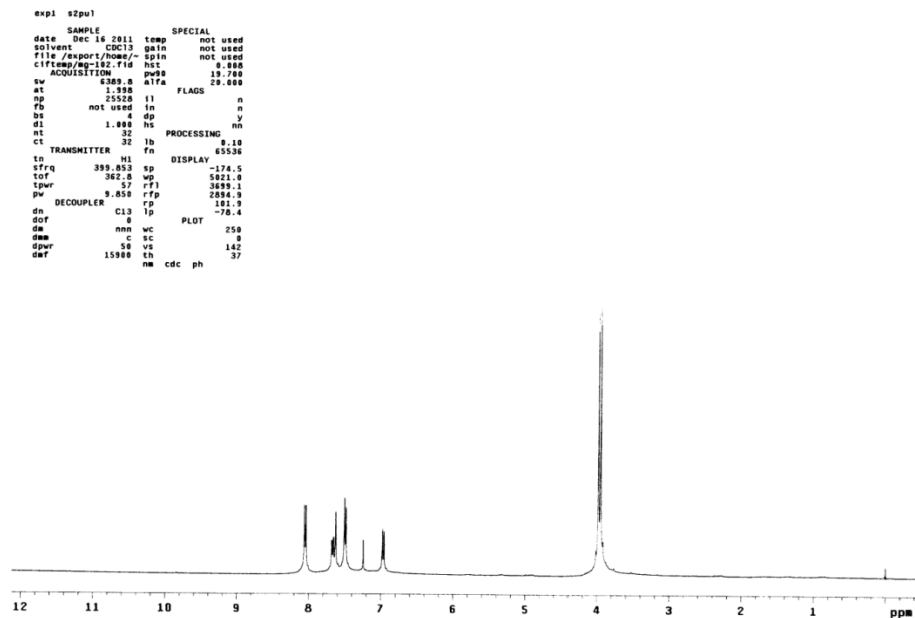
2,5-Bis(4-chlorophenyl)-1,3,4-oxadiazole (17a): ¹H NMR (400 MHz, CDCl₃)



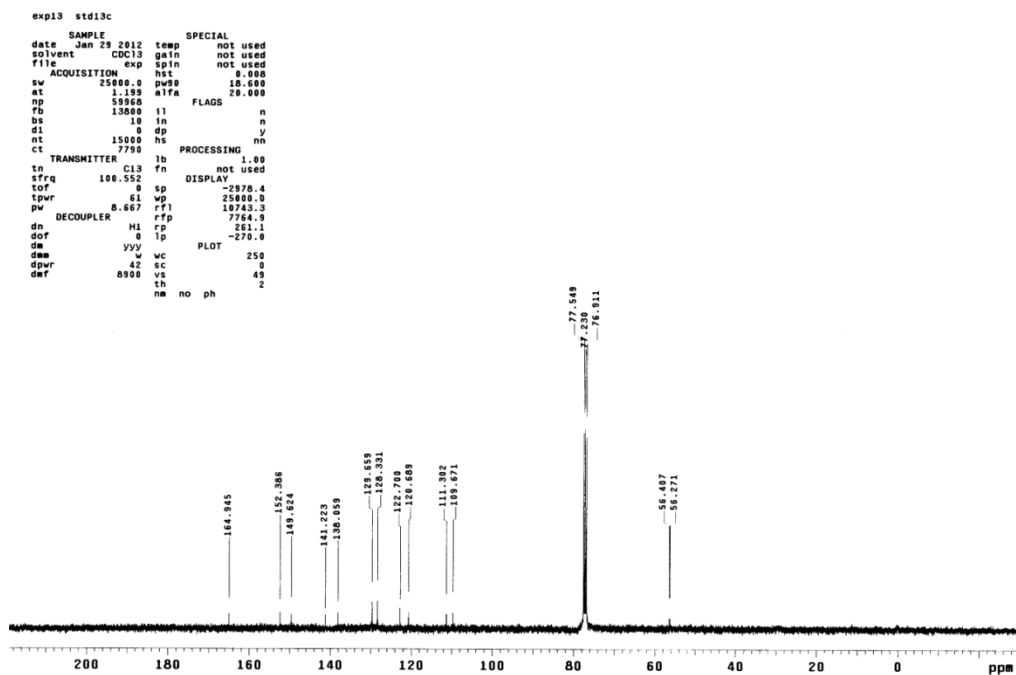
2,5-Bis(4-chlorophenyl)-1,3,4-oxadiazole (17a): ¹³C NMR (100 MHz, CDCl₃)



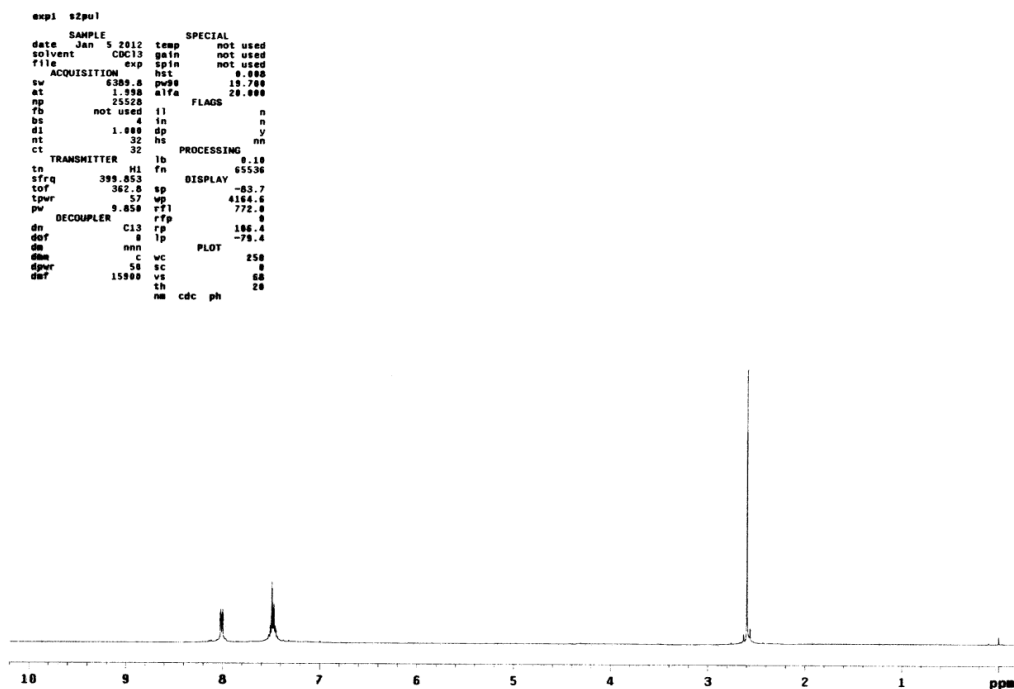
2-(4-Chloro-phenyl)-5-(3,4-dimethoxy-phenyl)-1,3,4-oxadiazole (18a): ^1H NMR (400 MHz, CDCl_3)



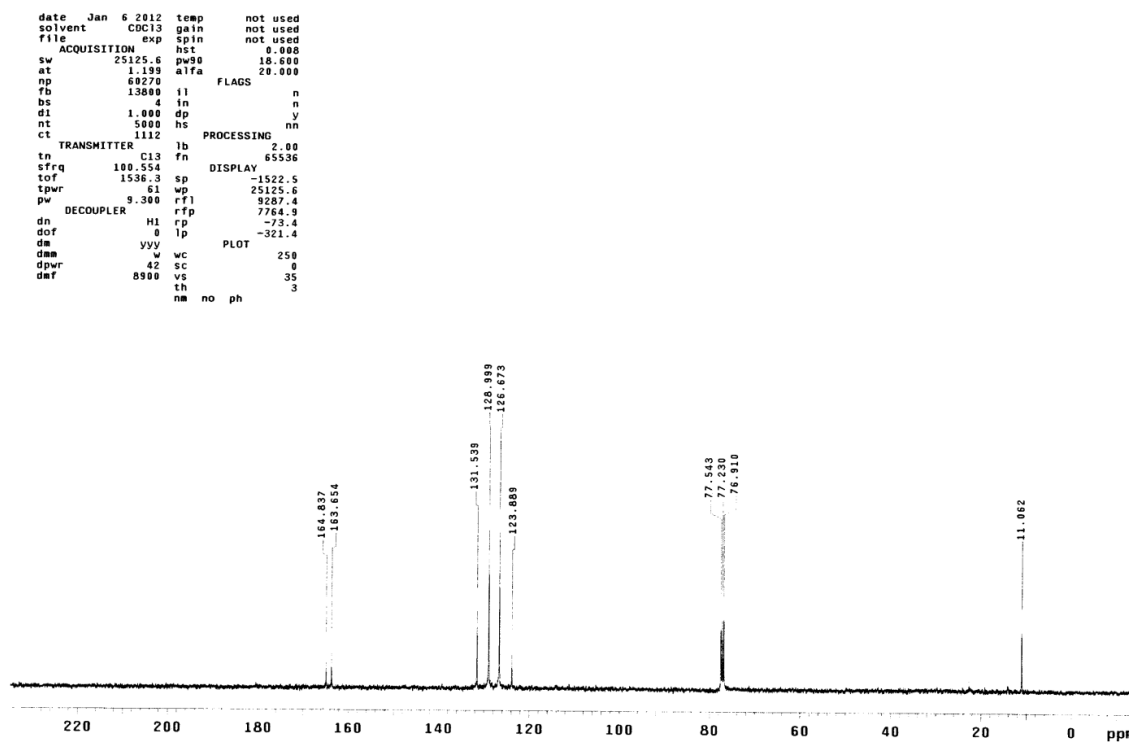
2-(4-Chloro-phenyl)-5-(3,4-dimethoxy-phenyl)-1,3,4-oxadiazole (18a): ^{13}C NMR (100 MHz, CDCl_3)



2-Methyl-5-phenyl-1,3,4-oxadiazole (19a): ¹H NMR (400 MHz, CDCl₃)

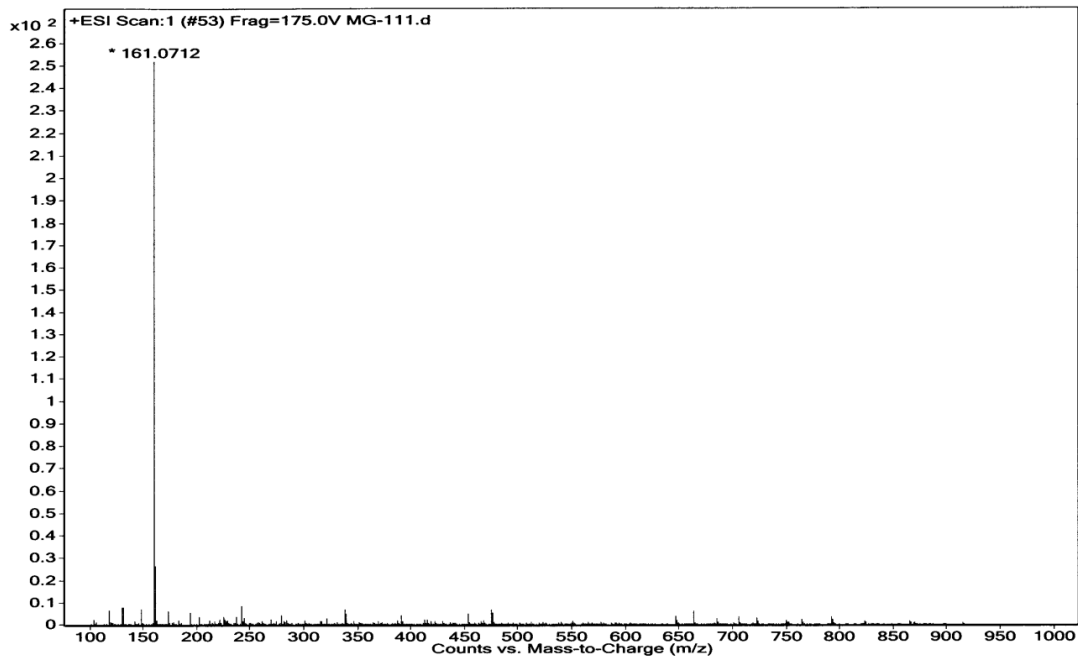


2-Methyl-5-phenyl-1,3,4-oxadiazole (19a): ¹³C NMR (100 MHz, CDCl₃)



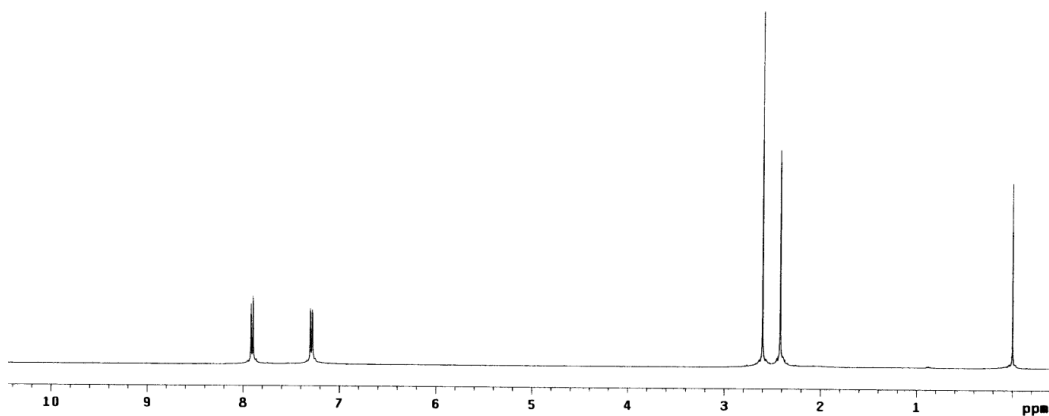
2-Methyl-5-phenyl-1,3,4-oxadiazole (19a): HRMS

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



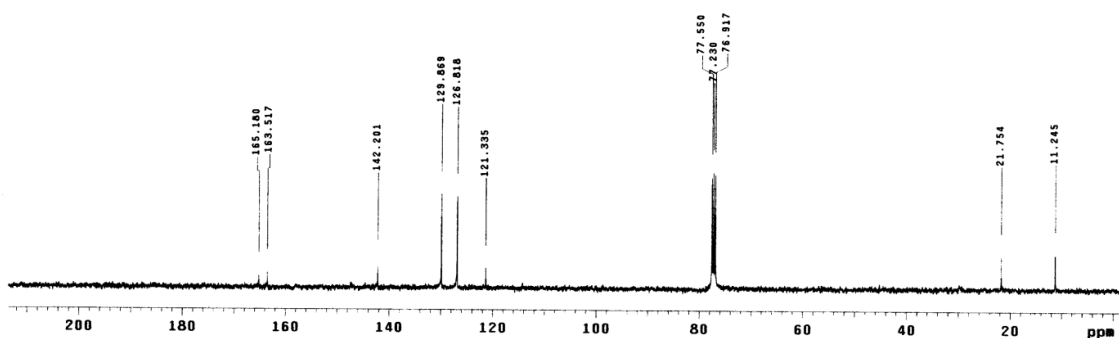
2-Methyl-5-p-tolyl-1,3,4-oxadiazole (20a): ¹H NMR (400 MHz, CDCl₃)

```
expl stdih
SAMPLE
date Dec 12 2011 temp SPECIAL
solvent CDCl3 gain not used
file exp spin not used
ACQUISITION hst 0.000
sw 6006.0 pw90 19.700
at 1.985 a1fa 20.000
np 23964
fb not used il
bs 4 ln n
d1 1.000 dp y
nt 32 hs
ct 32 PROCESSING nn
TRANSMITTER fn not used
tn H1 DISPLAY
sfrq 399.853 sp -170.1
tof 0 wp 4411.7
tpwr 57 rfl 959.0
pw 7.000 rfp 0
DECOUPLER C13 rp 111.1
dn 0 tp PLOT -95.4
da nnn wc 250
dwm c sc 0
dpwr 50 vs 83
def 15900 th cdc ph 20
```



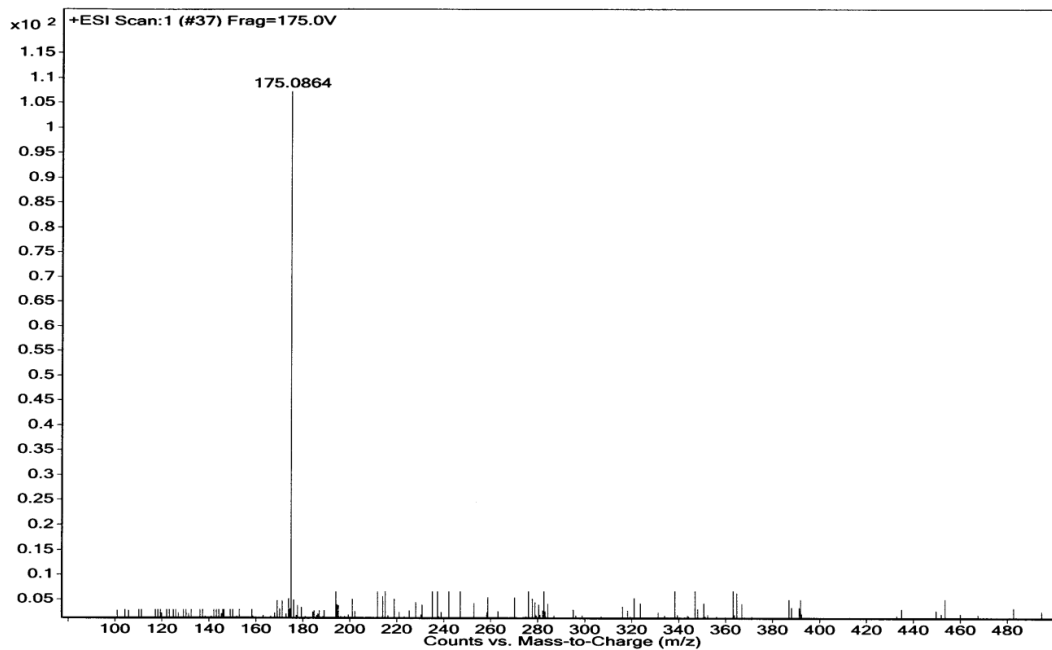
2-Methyl-5-p-tolyl-1,3,4-oxadiazole (20a): ^{13}C NMR (100 MHz, CDCl_3)

```
exp1 s2pu1
SAMPLE
date Dec 16 2011 temp not used
solvent CDCl3 gain not used
file ACQUISITION exp spin not used
sw 25125.6 pu90 18.600
at 1.139 hst 20.000
np 88270 a17a
fb 13000 f1
bs 10 fn
d1 1.000 dp
nt 3000 hs
ct 1860
SPECIAL
FLAGS
n
n
y
nn
TRANSMITTER
tn C13 fn 2.00
sfrq 100.554 DISPLAY 65536
tof 1536.3 sp -123.1
tpwr 61 wp 21592.2
pw 9.300 rF1 9274.4
DECOUPLER rfp 7564.8
dn H1 rp -95.5
dof 0 lp -271.4
dm vvv PLOT
dmm w wc 250
dpuv 42 sc 0
def 8900 vs 26
th 3
na no ph
```



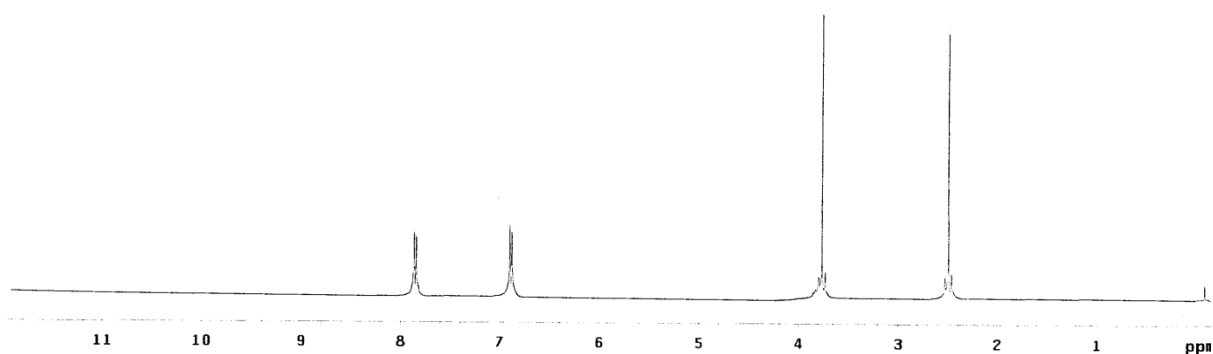
2-Methyl-5-p-tolyl-1,3,4-oxadiazole (20a): HRMS

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



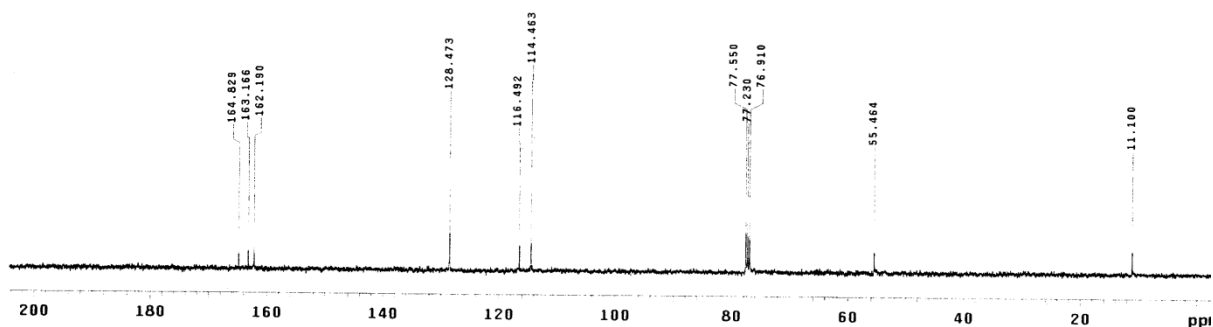
2-(4-Methoxy-phenyl)-5-methyl-1,3,4-oxadiazole (21a): ^1H NMR (400 MHz, CDCl_3)

```
date Jan 6 2012 temp not used
solvent CDCl3 gain not used
file /export/home/~ spin not used
ciftemp/MG-112.fid hst 0.008
ACQUISITION pw90 19.700
sw 6399.8 alfa 20.000
at 1.998 FLAGS
np 25528 fl n
fb not used in n
bs 4 dp y
d1 1.000 hs nn
nt 32 PROCESSING
ct 0 lb 0.10
TRANSMITTER fn 65536
tn H1 DISPLAY
sfrq 399.853 sp -97.6
tof 362.8 wp 4878.3
tpwr 57 rfl 3697.7
pw 9.850 rfp 2894.9
DECOUPLER rp 110.0
dn C13 lp -64.0
dof 0 PLOT
dm nnn wc 250
dmm c sc 0
dpwr 50 vs 58
dmf 15900 th 17
nm cdc ph
```



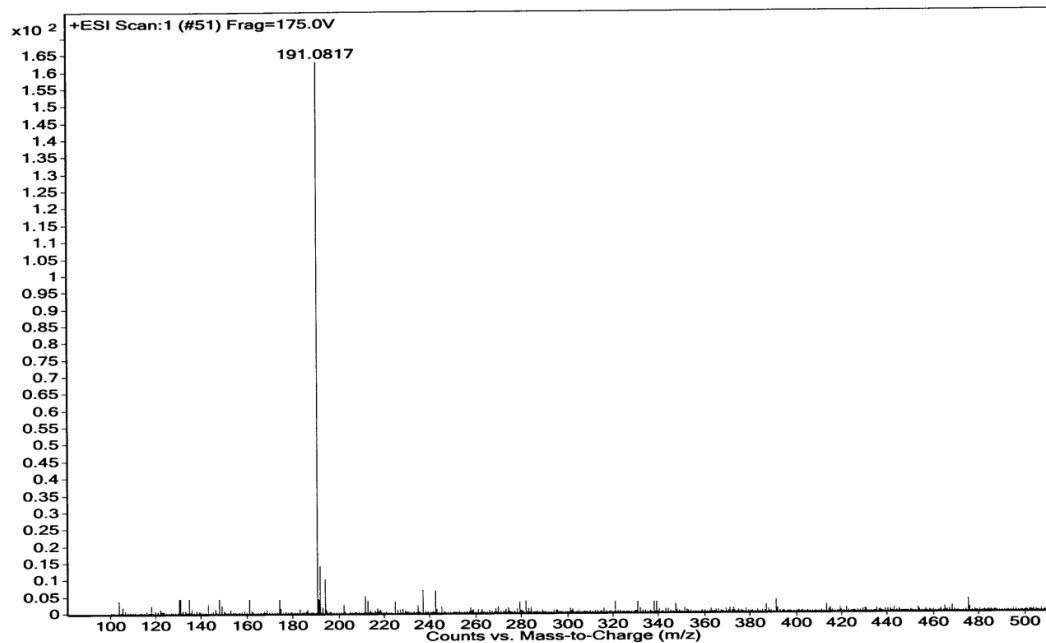
2-(4-Methoxy-phenyl)-5-methyl-1,3,4-oxadiazole (21a): ^{13}C NMR (100 MHz, CDCl_3)

```
date Jan 6 2012 temp not used
solvent CDCl3 gain not used
file /export/home/~ exp not used
ACQUISITION hst 0.008
sw 25125.6 pw90 18.600
at 1.199 alfa 20.000
np 60279 FLAGS
fb 13800 fl n
bs 32 in n
d1 1.000 dp y
nt 18000 hs nn
ct 160 PROCESSING
TRANSMITTER lb 2.00
tn C13 fn 65536
sfrq 100.554 DISPLAY
tof 1536.3 sp -461.3
tpwr 61 wp 20998.0
pw 9.300 rfl 9282.1
DECOUPLER rfp 7764.9
dn H1 rp -100.4
dof 0 lp -271.4
dm yyy PLOT
dmm w wc 250
dpwr 42 sc 0
dmf 8900 th 17
nm no ph
```



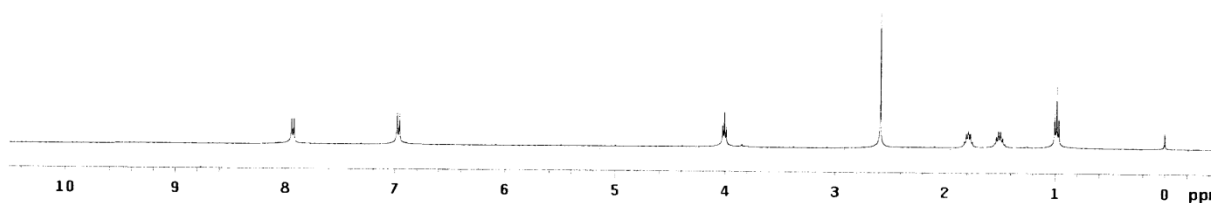
2-(4-Methoxy-phenyl)-5-methyl-1,3,4-oxadiazole (21a): HRMS

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



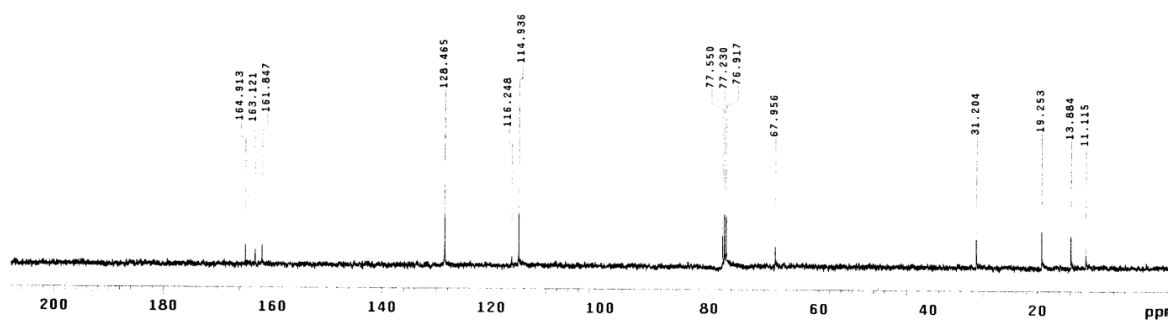
2-(4-Butoxy-phenyl)-5-methyl-1,3,4-oxadiazole (22a): ¹H NMR (400 MHz, CDCl₃)

```
date Jan 8 2012 temp not used
solvent CDCl3 gain not used
file exp spin not used
ACQUISITION hst 0.000
sw 6389.8 pw90 19.700
at 1.998 alfa 20.000
np 25528
fb not used fl FLAGS n
bs 4 in n
d1 1.000 dp y
nt 32 hs nn
ct 32
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 rf1 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
dof 15900 vs 27
nm th 20
nm cdc ph
```



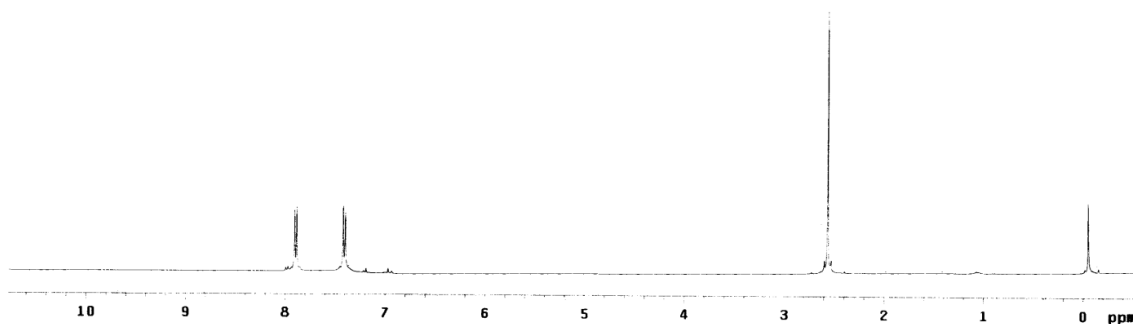
2-(4-Butoxy-phenyl)-5-methyl-1,3,4-oxadiazole (22a): ^{13}C NMR (100 MHz, CDCl_3)

```
date Jan 8 2012 temp not used
solvent CDCl3 gain not used
file exp spin not used
ACQUISITION hst 0.008
sw 25125.6 pw90 18.000
at 1.199 alfa 20.000
np 60270 FLAGS
fb 13000 i1 n
bs 32 in n
d1 1.000 dp y
nt 5000 hs nn
ct 224 PROCESSING
tn 224 lb 2.00
tn C13 fn 65536
sfrq 100.554 DISPLAY -591.6
tof 1536.3 sp 21493.3
tpwr 61 wp 9280.5
pw 9.300 rfp 7764.9
DECOUPLER H1 rfp -115.0
dn 0 lp -271.4
dm yvy PLOT 250
dmm w wc 0
dpwr 42 sc 17
dntf 8900 vs th 2
nm no ph
```



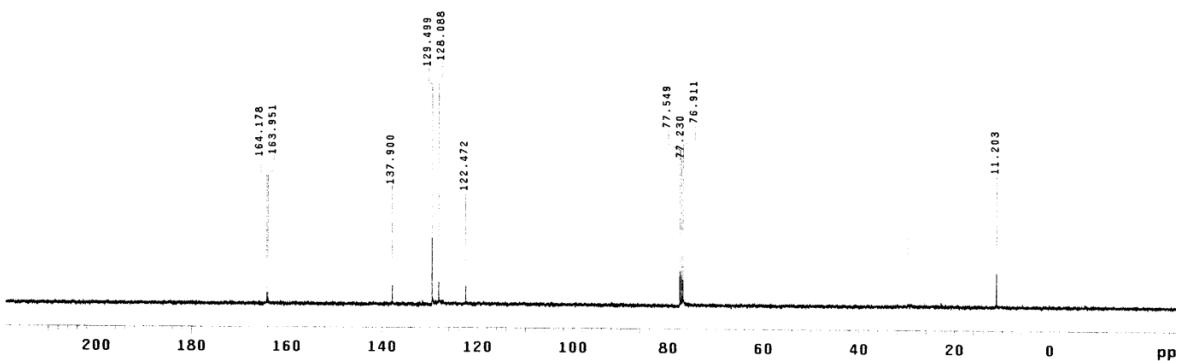
2-(4-Chloro-phenyl)-5-methyl-1,3,4-oxadiazole (23a): ^1H NMR (400 MHz, CDCl_3)

```
date Jan 10 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 i1 n
bs 4 in n
d1 1.000 dp y
nt 32 hs nn
ct 32 PROCESSING
tn H1 lb 0.10
tn 399.853 fn 65536
sfrq 362.8 sp -231.8
tpwr 57 wp 4542.5
pw 9.850 rfp 2894.9
DECOUPLER C13 rfp 114.2
dn 0 lp -93.6
dm nnn PLOT 250
dmm c wc 0
dpwr 50 sc 58
dntf 15900 vs th 20
nm cdc ph
```



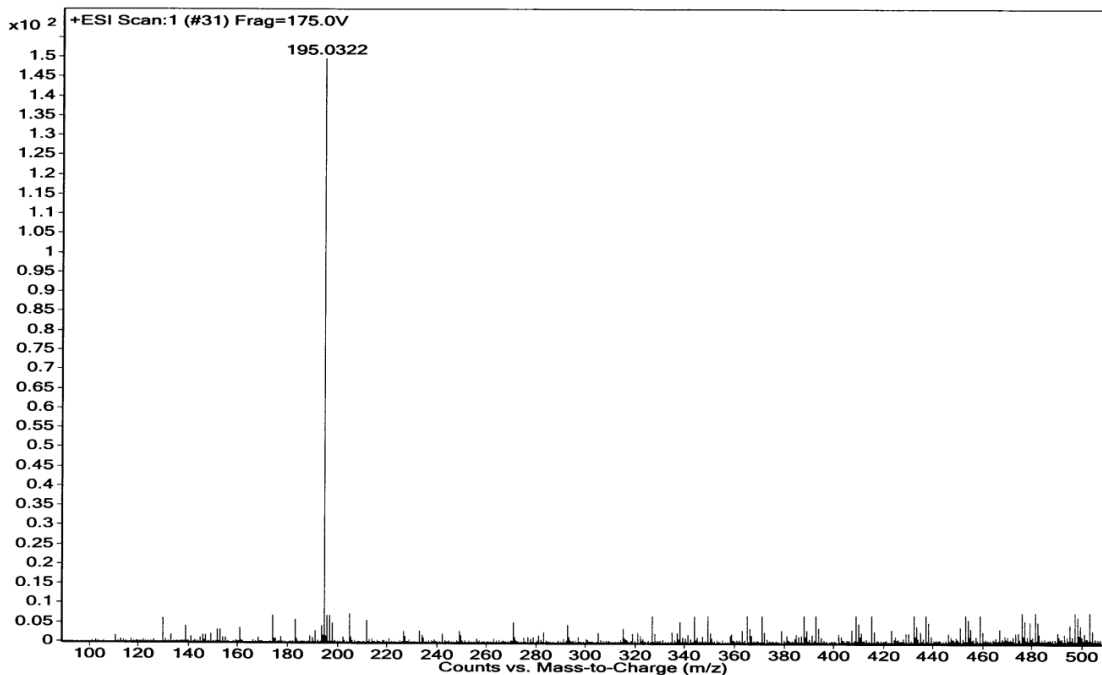
2-(4-Chloro-phenyl)-5-methyl-1,3,4-oxadiazole (23a): ¹³C NMR (100 MHz, CDCl₃)

```
date Jan 13 2012 temp not used
solvent CDCl3 gain not used
file exp spin not used
ACQUISITION hst 0.008
sw 25000.0 pw90 18.500
at 1.199 alfa 20.000
np 59968 FLAGS
fb 13800 il n
bs 10 in n
dl 0 dp y
nt 10000 hs nn
ct 800 PROCESSING
TRANSMITTER lb 1.00
tn C13 fn not used
sfrq 100.552 DISPLAY
tof 0 sp -2986.8
tpwr 61 wp 25000.0
pw 8.667 rf1 10751.7
DECOUPLER rfp 7754.9
dn H1 rp -71.0
dof 0 lp -354.1
da yy w PLOT
dwm yyc wc 250
dpwr 42 sc 0
dof 8900 vs 24
dof th 2
nm no ph
```

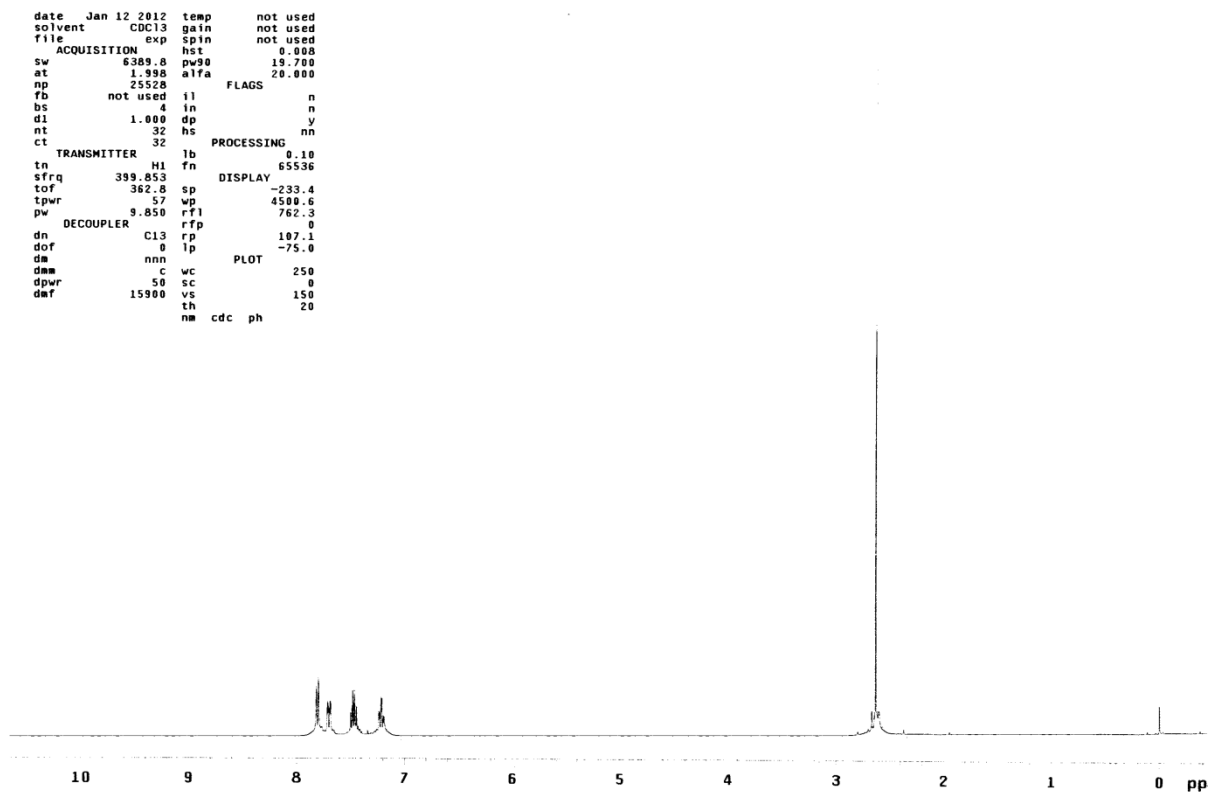


2-(4-Chloro-phenyl)-5-methyl-1,3,4-oxadiazole (23a): HRMS

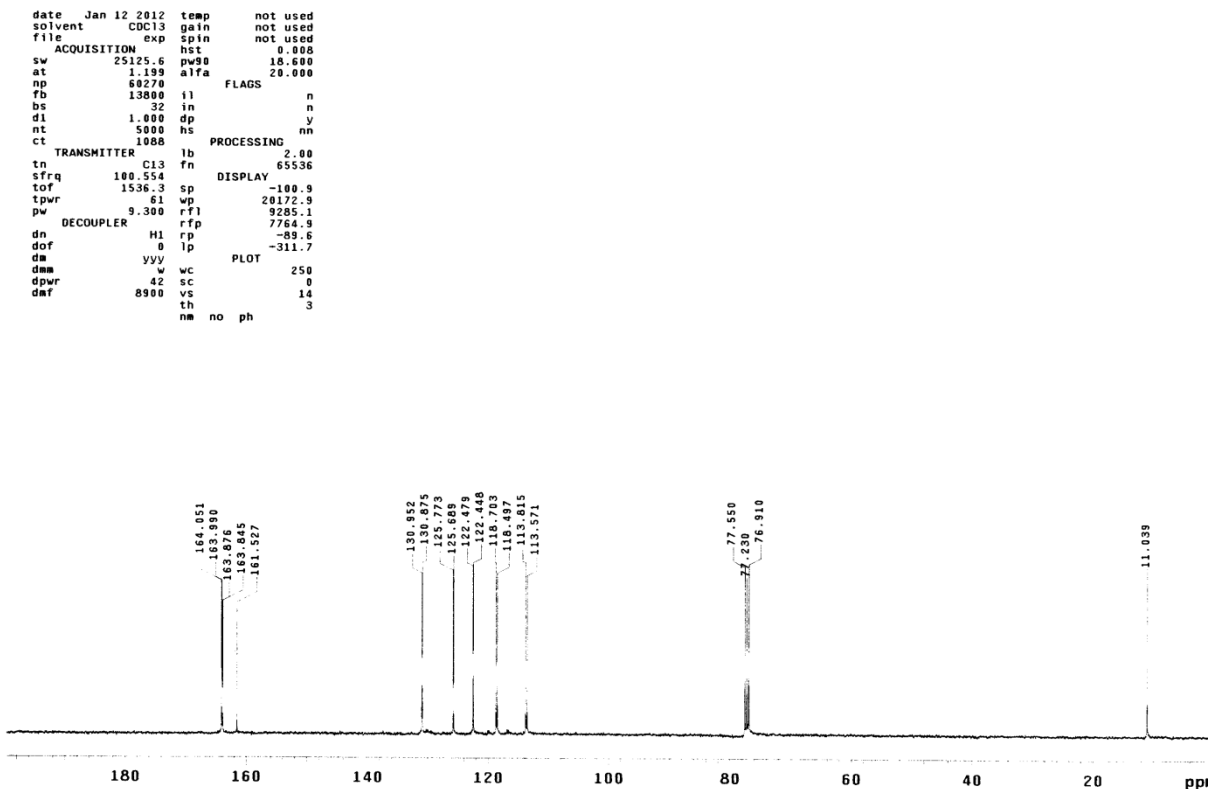
Sample Name	Position	Instrument Name	User Name
Inj Vol	InjPosition	SampleType	IRM Calibration Status
Data Filename	ACQ Method	Comment	Acquired Time



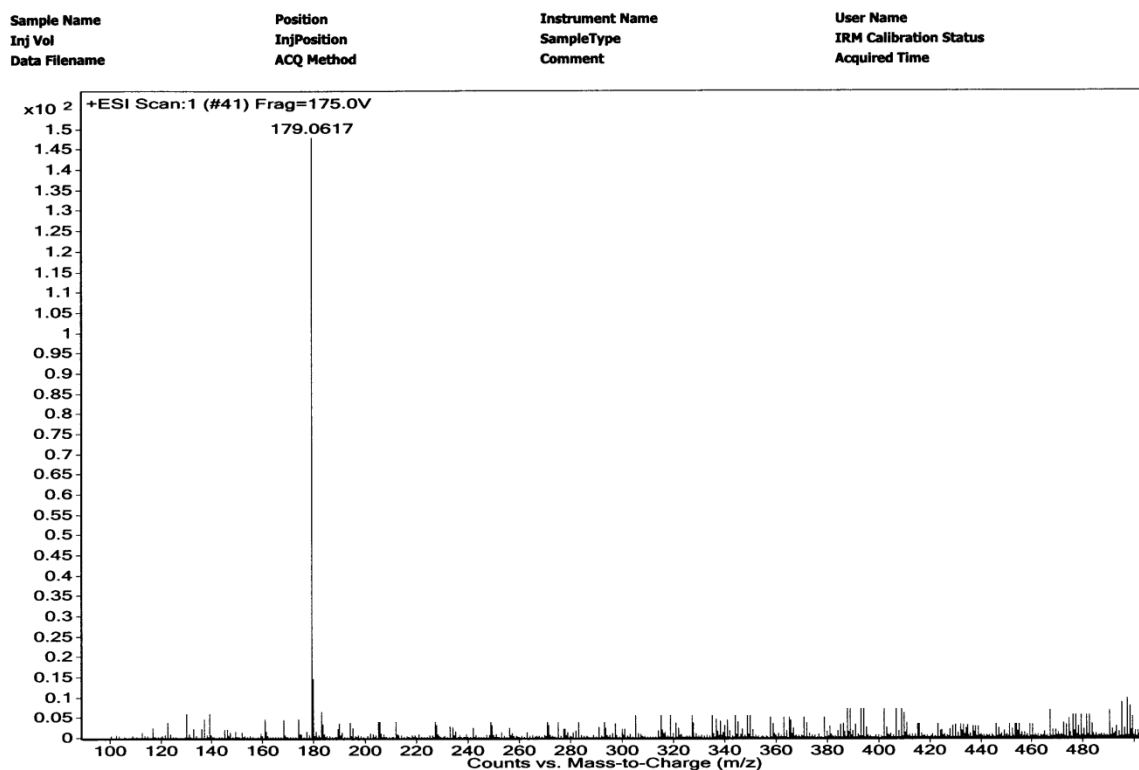
2-(3-Fluoro-phenyl)-5-methyl-1,3,4-oxadiazole (24a): ¹H NMR (400 MHz, CDCl₃)



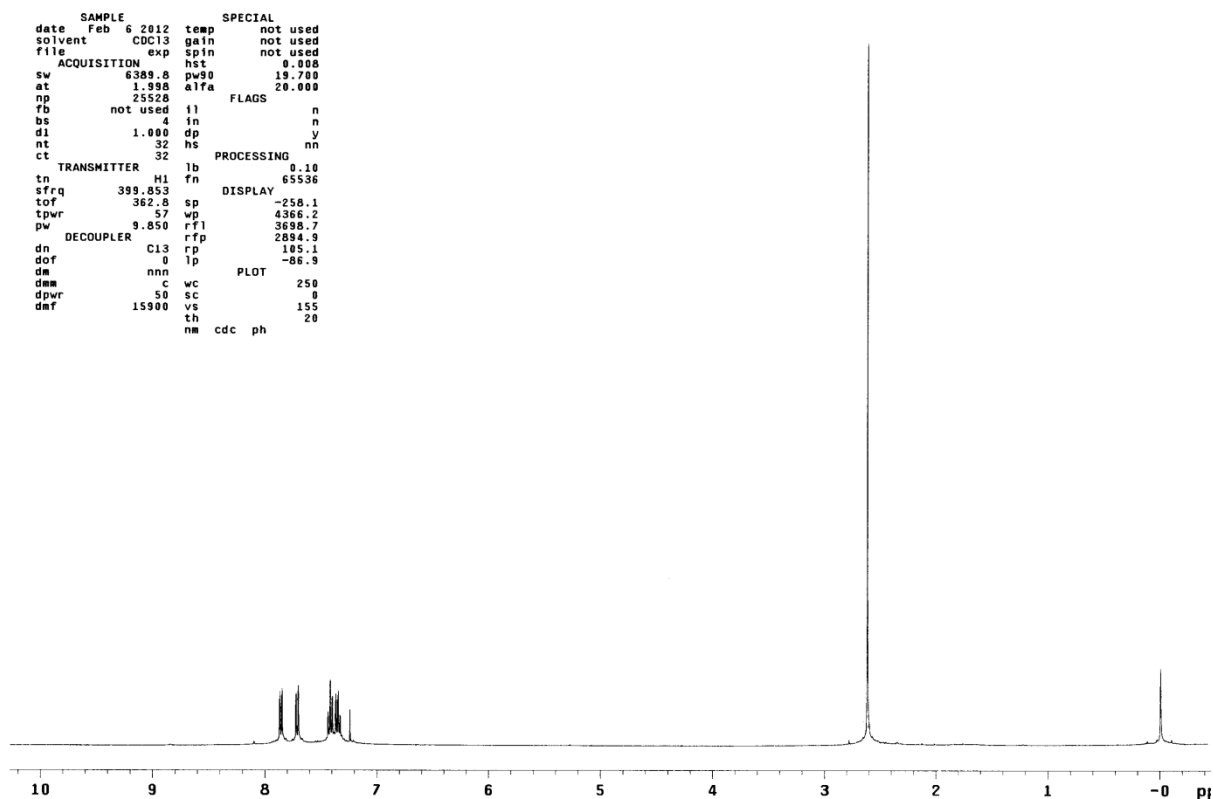
2-(3-Fluoro-phenyl)-5-methyl-1,3,4-oxadiazole (24a): ¹³C NMR (100 MHz, CDCl₃)



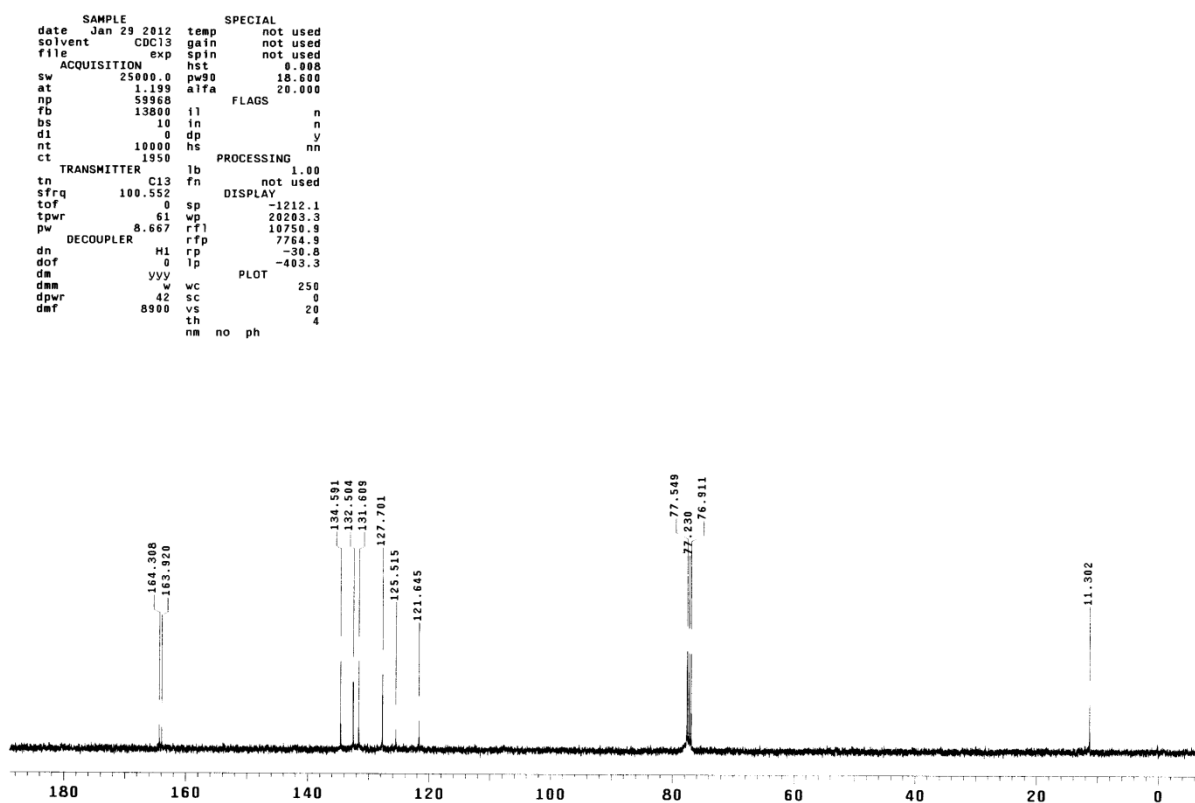
2-(3-Fluoro-phenyl)-5-methyl-1,3,4-oxadiazole (24a): HRMS



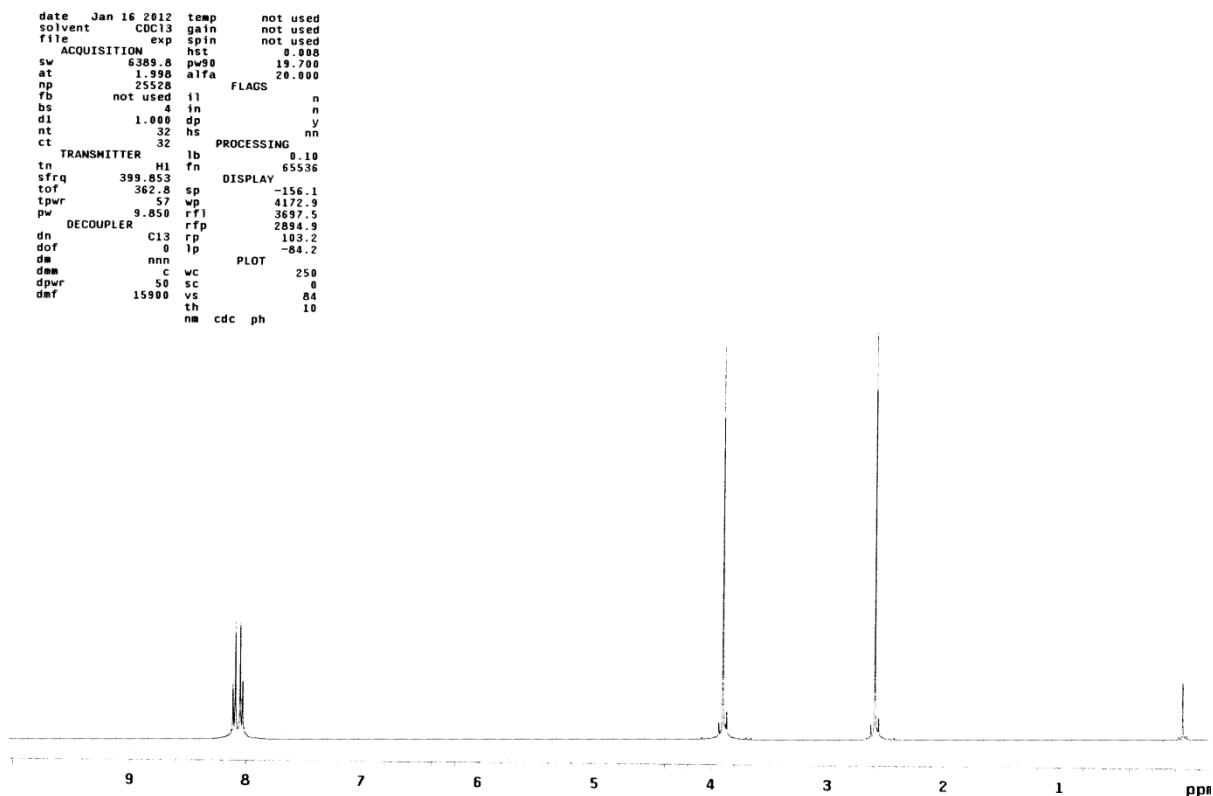
2-(2-Bromo-phenyl)-5-methyl-1,3,4-oxadiazole (25a): ¹H NMR (400 MHz, CDCl₃)



2-(2-Bromo-phenyl)-5-methyl-1,3,4-oxadiazole (25a): ¹³C NMR (100 MHz, CDCl₃)



4-(5-Methyl-[1,3,4]oxadiazol-2-yl)-benzoic acid methyl ester (26a): ¹H NMR (400 MHz, CDCl₃)



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

```
exp13 s2pu1
SAMPLE
date Jan 28 2012 temp not used
solvent CDCl3 gain not used
file exp sp1n not used
ACQUISITION hst 0.000
sw 25125.6 pw90 18.600
at 1.199 alfa 20.000
np 60270
fb 13800 il
bs 10 in
di 1.000 dp
nt 10000 hs
ct 1450
TRANSMITTER lb 2.00
tn C13 fn 65536
sfrq 100.554
tof 1536.3 sp -1510.3
tpwr 61 wp 25125.6
pw 9.300 rfl 9275.2
DECOUPLER H1 rfp 7764.9
dn 0 lp -58.9
dof 0 lp -358.3
dm yyy
dmm w wc 250
dpr 42 sc 0
dmf 8900 vs 22
th 3
nm no ph
```

