Supporting Information

Divergent reactivities of *o*-halo anilides with CuO nanoparticle in water: A green synthesis of benzoxazoles and *o*-hydroxy anilides

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Experimental:

General remarks

Unless otherwise stated, all reagents were purchased from commercial sources and used without further purification. Reaction progress was monitored by TLC using Merck silica gel 60 F_{254} (0.25mm) with detection by UV or iodine. Chromatography was performed using Merck silica gel (60-120) mesh size with freshly distilled solvents. Columns were typically packed as slurry and equilibrated with the appropriate solvent system prior to use. ^{1}H NMR (400 MHz and 600 MHz) and ^{13}C NMR (100 MHz and 150 Hz) spectra were recorded on a Varian FT-400 MHz and Bruker FT-600 MHz instrument using TMS as an internal standard. Data are presented as follows: chemical shift (ppm), multiplicity (s = singlet, d = doublet, t = triplet, q = quartet, m = multiplet, b = broad, brs = broad singlet, brm= broad multiplet, coupling constant *J* (Hz). Elemental analyses were carried out on a Perkin–Elmer 2400 automatic carbon, hydrogen, nitrogen and sulfur analyser. Melting points were recorded on Buchi B-545 melting point apparatus and are

uncorrected. IR spectra were recorded in KBr or neat on a Nicolet Impact 410 spectrophotometer. Mass data were obtained with a WATERS MS system, Q-tof premier and data analyzed using Mass Lynx4.1.

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

References

1 SMART, SAINT and XPREP, Siemens Analytical X-ray Instruments Inc., Madison,Wisconsin.

2 G. M. Sheldrick, *SADABS: Empirical Absorption and Correction Software*, University of Gottingen, Institut fur Anorganische Chemieder Universitat, Tammanstrasse 4, D-3400 Gottingen, Germany, 1999–2003.

3 G. M. Sheldrick, SHELXS-97, University of Gottingen, Germany, 1997.

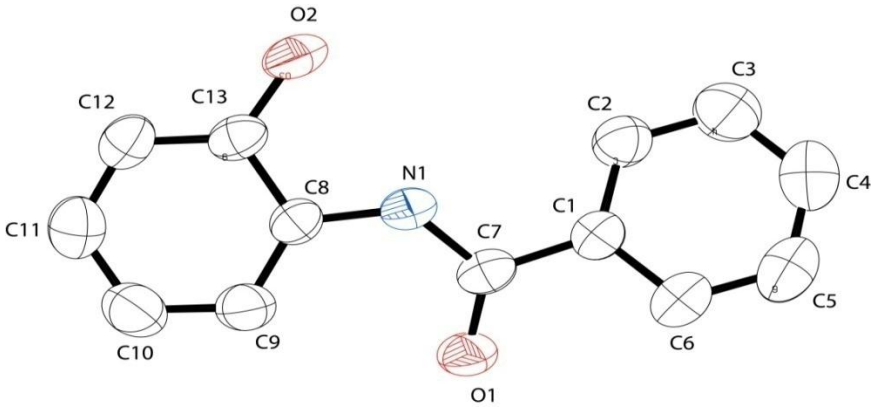


Figure 1. ORTEP views of *N*-(2-Hydroxyphenyl)benzamide (**2a′**)

Crystallographic description of *N*-(2-Hydroxyphenyl)benzamide (2a′): $C_{13}H_{11}NO_2$, crystal dimension 0.28 x 0.26 x 0.24 mm, M_r = 213.23, Monoclinic, Space group P $2_1/c$, a = 10.9246(10) Å, b = 7.0228(6) Å, c = 14.1338(12) Å, α = 90.00, β = 90.645(6), γ = 90.00, V = 1084.29(16) Å^3, Z = 4, ρ_{calcd} = 1.306 mg/m^3, μ = 0.089 mm^{-1}, F(000) = 448, reflection collected / unique = 2385 / 1350, refinement method = full-matrix least-squares on F^2, final R indices [$I > 2\sigma(I)$]: R_1 = 0.0789, wR_2 = 0.2155, R indices (all data): R_1 = 0.1433, wR_2 = 0.2512, goodness of fit = 1.174. CCDC-919286 (for *N*-(2-hydroxyphenyl)benzamide) contains the supplementary crystallographic data for this paper. These data can be obtained free of charge from The Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/data_request/cif.

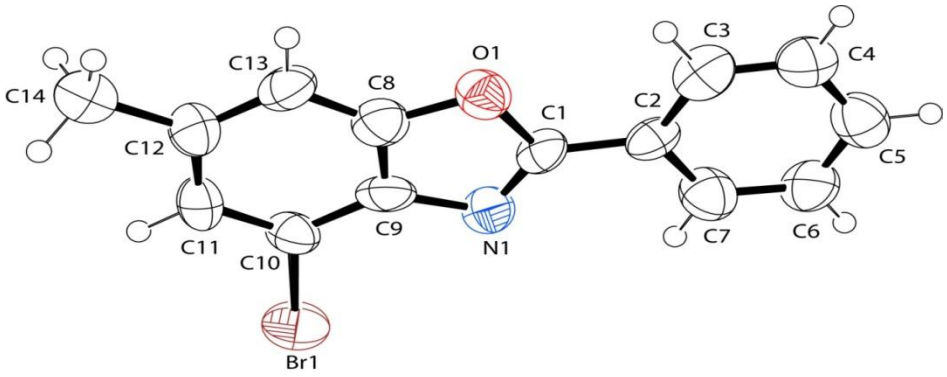
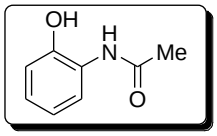


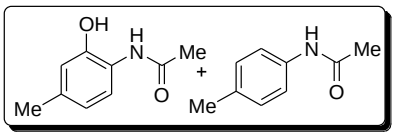
Figure 2 ORTEP views of 4-Bromo-6-methyl-2-phenylbenzo[d]oxazole (**21aa**)

Crystallographic description of 4-Bromo-6-methyl-2-phenylbenzo[d]oxazole (21aa): $C_{14}H_{10}BrNO$, crystal dimensions 0.28 x 0.26 x 0.24 mm, M_r = 288.13, Monoclinic, Space group P $2/_1$, a = 10.3512(8) Å, b = 14.0265(11) Å, c = 12.8571(10) Å, α = 90.00, β = 105.177(5), γ = 90.00, V = 1801.6(2) Å^3, Z = 6, ρ_{calcd} = 1.593 mg/m^3, μ = 3.403 mm^{-1}, F(000) = 760, reflection collected / unique = 7274 / 3248 , refinement method = full-matrix least-squares on F^2, final R indices [$I > 2\sigma(I)$]: R_1 = 0.0552, wR_2 = 0.1374, R indices (all data): R_1 = 0.1695, wR_2 = 0.1897, goodness of fit = 0.890. CCDC - 919285 (for 4-Bromo-6-methyl-2-phenylbenzo[d]oxazole) contains the supplementary crystallographic data for this paper. These data can be obtained free of charge from The Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/data_request/cif.

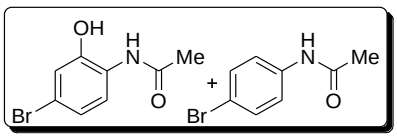
Spectal Data



***N*-(2-Hydroxyphenyl)acetamide** (**1a′**): Brown solid; M.p. 199-201 ^{o}C (lit.[4] 201 ^{o}C); ^{1}H NMR (DMSO-d_6, 400 MHz): δ (ppm) 2.09 (s, 3H), 6.73-6.77 (m, 1H), 6.85 (d, 1H, *J* = 7.6 Hz), 6.91-6.95 (m, 1H), 7.66 (d, 1H, *J* = 7.6 Hz), 9.31 (brs, 1H), 9.76 (s, 1H); ^{13}C NMR (DMSO-d_6, 100 MHz): δ (ppm) 18.7, 111.1, 114.1, 117.5, 119.8, 121.5, 143.0, 164.2; IR (KBr): 3403, 2925, 2617, 1658, 1595, 1542, 1455, 1380, 1282, 1240, 1106, 1037, 1016, 765, 660 cm^{-1}; HRMS (ESI): calcd. for ($C_8H_9NO_2$) (MH^+) 152.0706; found 152.0693.

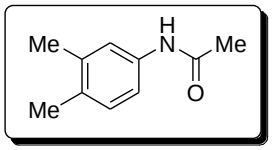


Mixture of *N*-(2-Hydroxy-4-methylphenyl)acetamide and *N*-*p*-Tolylacetamide (**2a′+2a′′**): Off white solid; ^{1}H NMR (DMSO-d_6, 400 MHz): δ (ppm) 2.01 (s, 3H), 2.06 (s, 3H), 2.18 (s, 3H), 2.23 (s, 3H), 6.56 (d, 2H, *J* = 8.4 Hz), 6.66 (s, 1H), 7.07 (d, 2H, *J* = 8.4 Hz), 7.45 (t, 2H, *J* = 8 Hz), 9.29 (s, 1H), 9.65 (s, 1H), 9.83 (s, 1H); ^{13}C NMR (DMSO-d_6, 100 MHz): δ (ppm) 20.5, 20.6, 23.5, 23.96, 116.7, 119.1, 119.6, 122.5, 123.8, 129.1, 131.9, 134.2, 136.8, 147.9, 168.2, 169.1; IR (KBr): 3431, 3270, 3073, 2919, 1661, 1639, 1621, 1550, 1415, 1383, 1301, 1268, 1250, 1160, 1119, 1045, 1015, 973, 945, 860, 797 cm^{-1}.

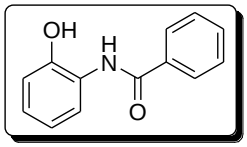


Mixture of *N*-(4-Bromo-2-hydroxyphenyl)acetamide and *N*-(4-Bromophenyl)acetamide (**3a′+3a′′**): Brown solid; ^{1}H NMR (DMSO-d_6, 400 MHz): δ (ppm) 2.07 (s, 3H), 2.02 (s, 3H), 6.93 (d, 1H, *J* = 8.8 Hz), 7.00 (s, 1H), 7.46 (d, 2H, *J* = 7.6 Hz), 7.54 (d, 2H, *J* = 8.4 Hz), 7.73 (d, 1H, *J* = 8.8 Hz), 9.26 (s, 1H), 10.1 (s, 1H), 10.4 (s, 1H); ^{13}C NMR (DMSO-d_6, 100 MHz): δ (ppm) 23.7, 24.0, 114.6,

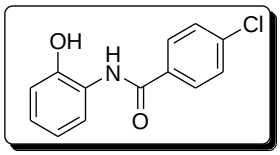
115.6, 118.0, 120.9, 121.6, 123.7, 126.1, 131.5, 138.7, 149.0, 168.6, 169.1; IR (KBr): 3390, 2704, 1658, 1604, 1586, 1534, 1407, 1366, 1270, 1235, 1197, 1118, 1010, 966, 877, 848, 796 cm^{-1}.



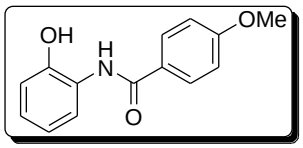
***N*-(3,4-Dimethylphenyl)acetamide** (**4a′′**): Brown solid; M.p. 83–85^{o}C; ^{1}H NMR ($CDCl_3$, 400 MHz): δ (ppm) 2.11 (s, 3H), 2.18 (s, 6H), 7.01 (d, 1H, *J* = 8 Hz), 7.21 (d, 1H, *J* = 8 Hz), 7.26 (s, 1H), 8.06 (brs, 1H); ^{13}C NMR ($CDCl_3$, 100 MHz): δ (ppm) 19.3, 19.9, 24.4, 117.9, 121.8, 129.96, 132.7, 135.9, 137.2, 169.1; IR (KBr): 2922, 2858, 1600, 1592, 1539, 1505, 1448, 1408, 1371, 1317, 1263, 1208, 1164, 1120, 1022, 875 cm^{-1}; elemental analysis calcd (%) for $C_{10}H_{13}NO$ (163.2163) C 73.59, H 8.03, N 8.58; found C 73.67, H 7.99, N 8.51.



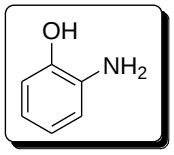
***N*-(2-Hydroxyphenyl)benzamide** (**2a′**): Brown solid; M.p. 145-148 ^{o}C; ^{1}H NMR (DMSO-d_6, 400 MHz): δ (ppm) 6.84 (t, 1H, *J* = 7.6 Hz), 6.93 (d, 1H, *J* = 8 Hz), 7.02-7.06 (m, 1H), 7.53-7.59 (m, 3H), 7.68 (d, 1H, *J* = 8 Hz), 7.97 (d, 2H, *J* = 6.8 Hz), 9.53 (s, 1H), 9.78 (s, 1H); ^{13}C NMR (DMSO-d_6, 100 MHz): δ (ppm) 116.0, 119.1, 124.1, 125.7, 127.5, 127.6, 128.5, 131.7, 134.4, 149.3, 165.8; IR (KBr): 3048, 3026, 2923, 2850, 1645, 1575, 1542, 1452, 1367, 1286, 1238, 1094, 748, 703 cm^{-1}; HRMS (ESI): calcd. for ($C_{13}H_{11}NO_2$) (MH^+) 214.0863; found 214.0848.



4-Chloro-*N*-(2-hydroxyphenyl)benzamide (**3a′**): Brown solid; M.p. 164-166.5 ^{o}C; ^{1}H NMR (DMSO-d_6, 400 MHz): δ (ppm) 6.83 (t, 1H, *J* = 7.6 Hz), 6.92 (d, 1H, *J* = 8 Hz), 7.05 (t, 1H, *J* = 7.6 Hz), 7.60 (d, 3H, *J* = 7.6 Hz), 7.99 (d, 2H, *J* = 7.6 Hz), 9.62 (s, 1H), 9.74 (s, 1H); ^{13}C NMR (DMSO-d_6, 100 MHz): δ (ppm) 115.9, 118.9, 124.7, 125.5, 126.0, 128.5, 129.5, 133.2, 136.4, 149.7, 164.3; IR (KBr): 3211, 2923, 2853, 1732, 1633, 1596, 1528, 1484, 1455, 1329, 1292, 1096, 913, 746 cm^{-1}; HRMS (ESI): calcd. for ($C_{13}H_{10}ClNO_2$) (MH^+) 248.0473; found 248.0461.

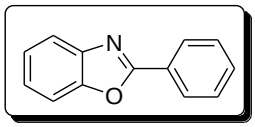


***N*-(2-Hydroxyphenyl)-4-methoxybenzamide** (**4a′**): Brown solid; M.p. 170-172 ^{o}C; ^{1}H NMR (DMSO-d_6, 400 MHz): δ (ppm) 3.84 (s, 3H), 6.83 (t, 1H, *J* = 7.2 Hz), 6.91 (d, 1H, *J* = 8 Hz), 6.99-7.07 (m, 3H), 7.66 (d, 1H, *J* = 8 Hz), 7.96 (d, 2H, *J* = 8.8 Hz), 9.43 (s, 1H), 9.74 (brs, 1H); ^{13}NMR (DMSO-d_6, 100 MHz): δ (ppm) 55.5, 113.8, 116.2, 119.1, 123.9, 125.6, 126.2, 126.4, 129.5, 149.2, 162.0, 164.9; IR (KBr): 3262, 2959, 2389, 1628, 1604, 1508, 1486, 1327, 1291, 1262, 1235, 1174, 1027, 910, 843, 757 cm^{-1}; elemental analysis calcd (%) for $C_{14}H_{13}NO_3$ (243.2574) C 69.12, H 5.39, N 5.76; found C 69.19, H 5.32, N 5.71.

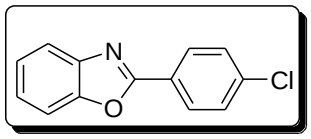


2-Hydroxyaniline: M.p. 216-218 ^{o}C, ^{1}H NMR (DMSO-d_6, 400 MHz): δ (ppm) 4.36 (brs, 2H), 6.27 (t, 1H, *J* = 7.6 Hz), 6.39-6.47 (m, 2H), 6.52 (1H, d, *J* = 7.6 Hz), 8.81 (brs, 1H); ^{13}C NMR (DMSO-d_6, 100 MHz): δ (ppm) 114.4, 114.5, 116.4, 119.5,

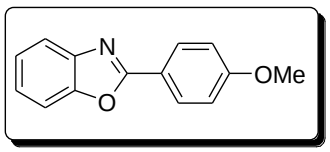
136.5, 143.9; IR (KBr): 3376, 3305, 1605, 1511, 1459, 1402, 1267, 1216, 1075, 1031, 896, 846, 741 cm^{-1}; elemental analysis calcd (%) for C_6H_7NO (109.1256): C 66.04, H 6.47, N 12.84; found C 66.09, H 6.43, N 12.73.



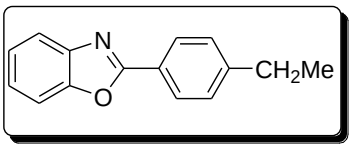
2-Phenylbenzo[*d*]oxazole (**2aa**): White solid; M.p. 101-103 ^oC (lit.[5] 103-104 ^oC); ^1H NMR ($CDCl_3$, 400 MHz): δ (ppm) 7.33-7.35 (m, 2H), 7.51-7.52 (m, 3H), 7.56-7.58 (m, 1H), 7.75-7.78 (m, 1H), 8.23-8.26 (m, 2H); ^{13}C NMR ($CDCl_3$, 100 MHz): δ (ppm) 110.8, 120.2, 124.8, 125.3, 127.3, 127.8, 129.1, 131.7, 142.3, 150.9, 163.2; IR (KBr): 2927, 2851, 1635, 1618, 1553, 1448, 1242, 1053, 924, 806, 745, 704 cm^{-1}; elemental analysis calcd (%) for $C_{13}H_9NO$ (195.2163): C 79.98, H 7.17, N 4.65; found C 80.05, H 4.62, N 7.09.



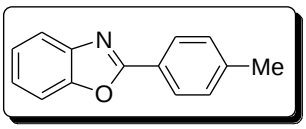
2-(4-Chlorophenyl)benzo[*d*]oxazole (**3aa**): White solid; M.p. 149-151 ^oC (lit.[5] 153-154 ^oC); ^1H NMR ($CDCl_3$, 400 MHz): δ (ppm) 7.32-7.36 (m, 2H), 7.48 (d, 2H, J = 8.8 Hz), 7.55-7.57 (m, 1H), 7.73-7.76 (m, 1H), 8.17 (d, 2H, J = 8.8 Hz); ^{13}C NMR ($CDCl_3$, 100 MHz): δ (ppm) 110.8, 120.2, 124.9, 125.5, 125.8, 128.9, 129.4, 137.9, 142.1, 150.9, 162.2; IR (KBr): 3054, 1616, 1481, 1452, 1404, 1243, 1091, 1055, 1009, 924, 832, 738 cm^{-1}; HRMS (ESI): calcd. for ($C_{13}H_8ClNO$) (MH^+) 230.0367; found 230.0355.



2-(4-Methoxyphenyl)benzo[*d*]oxazole (**4aa**): White solid; M.p. 103-105 ^{o}C (lit.[5] 103-105 ^{o}C); ^{1}H NMR ($CDCl_3$, 400 MHz): δ (ppm) 3.86 (s, 3H), 7.01 (d, 2H, *J* = 9.2 Hz), 7.79-7.33 (m, 2H), 7.53-7.55 (m, 1H), 7.22-7.25 (m, 1H), 8.19 (d, 2H, *J* = 9.2 Hz); ^{13}C NMR ($CDCl_3$, 100 MHz): δ (ppm) 55.4, 110.4, 114.4, 119.67, 119.71, 124.5, 124.6, 129.4, 142.4, 150.7, 162.4, 163.2; IR (KBr): 2923, 1617, 1604, 1503, 1454, 1253, 1242, 1169, 1105, 1059, 1017, 919, 831, 740, 729 cm^{-1}; HRMS (ESI): calcd. for ($C_{14}H_{11}NO_2$) (MH^+) 226.0863; found 226.0877.

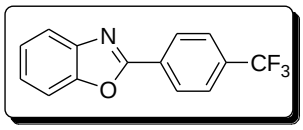


2-(4-Ethylphenyl)benzo[*d*]oxazole (**5aa**): White solid; M.p. 83-85 ^{o}C (lit.[6] 84-86 ^{o}C); ^{1}H NMR ($CDCl_3$, 400 MHz): δ (ppm) 1.18 (t, 3H, *J* = 8 Hz), 2.62 (q, 2H, *J* = 7.6 Hz), 7.22-7.25 (m, 4H), 7.44-7.47 (m, 1H), 7.65-7.67 (m, 1H), 8.07 (d, 2H, *J* = 8 Hz); ^{13}C NMR ($CDCl_3$, 100MHz): δ (ppm) 15.3, 29.0, 110.6, 119.9, 124.6, 124.7, 124.9, 127.8, 128.5, 142.3, 148.3, 150.8, 163.4; IR (KBr): 2954, 2928, 2862, 1618, 1552, 1496, 1453, 1414, 1286, 1244, 1168, 1053, 1009, 922 cm^{-1}; elemental analysis calcd (%) for $C_{15}H_{13}NO$ (223.2693): C 80.69, H 5.87, N 6.27; found C 80.77, H 5.93, N 6.20.

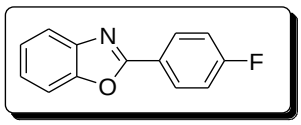


2-p-Tolylbenzo[d]oxazole (**6aa**): White Solid; M.p. 111-113 ^{o}C (lit.[7] 110-112 ^{o}C); ^{1}H NMR ($CDCl_3$, 400 MHz): δ (ppm) 2.38 (s, 3H), 7.27-7.31 (m, 4H), 7.51-7.53 (m, 1H), 7.73-7.75 (m, 1H), 8.11 (d, 2H, *J* = 7.6 Hz); ^{13}C NMR ($CDCl_3$, 100 MHz): δ (ppm) 21.7, 110.6, 119.9, 124.5, 124.6, 124.9, 127.7, 129.7, 142.1, 142.3, 105.8, 163.4; IR (KBr): 3054, 2917, 1621, 1552, 1500, 1450, 1242, 1196, 1172, 1054, 1015, 820, 745, 724 cm^{-1}; HRMS (ESI): calcd. for ($C_{14}H_{11}NO$) (MH^+) 210.0935; found 210.0947.

2-(4-(Methylthio)phenyl)benzo[*d*]oxazole (**7aa**): Yellowish-white solid; M.p. 103-106 ^{o}C; ^{1}H NMR ($CDCl_3$, 400 MHz): δ (ppm) 2.53 (s, 3H), 7.32 (d, 4H, *J* = 6.8 Hz), 7.53-7.56 (m, 1H), 7.72-7.74 (m, 1H), 8.13 (d, 2H, *J* = 8 Hz); ^{13}C NMR ($CDCl_3$, 100 MHz): δ (ppm) 15.1, 110.6, 119.9, 123.4, 124.7, 125.1, 125.8, 127.9, 142.3, 143.8, 150.8, 162.9; IR (KBr): 2916, 1923, 1614, 1594, 1484, 1453, 1404, 1242, 1177, 1094, 1051, 1007, 941, 742 cm^{-1}; elemental analysis calcd (%) for $C_{14}H_{11}NOS$ (241.3088): C 69.68, H 4.59, N 5.80, S 13.29; found C 69.77, H 4.51, N 5.72, S 13.40.

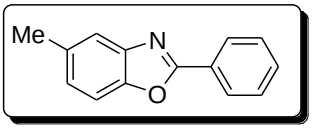


2-(4-(Trifluoromethyl)phenyl)benzo[*d*]oxazole (**8aa**): White solid; M.p. 148-150 ^{o}C (lit.[8] 146-147 ^{o}C); ^{1}H NMR ($CDCl_3$, 400 MHz): δ (ppm) 7.36-7.39 (m, 2H), 7.58-7.60 (m, 1H), 7.77 (d, 3H, *J* = 8.4 Hz), 8.35 (d, 2H, *J* = 8 Hz); ^{13}C NMR ($CDCl_3$, 100 MHz): δ (ppm) 110.9, 120.6, 122.6, 125.1, 125.9, 126.02, 126.05, 127.9, 130.6, 142.1, 151.0, 161.6; IR (KBr): 2958, 1933, 1608, 1558, 1453, 1415, 1321, 1244, 1167, 1116, 1069, 846, 815, 743 cm^{-1}; elemental analysis calcd (%) for $C_{14}H_8F_3NO$ (263.2143): C 63.88, H 3.06, N 5.32; found C 63.97, H 3.11, N 5.24.

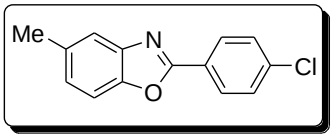


2-(4-Fluorophenyl)benzo[*d*]oxazole (**9aa**): White solid; M.p. 106-108 ^{o}C; ^{1}H NMR ($CDCl_3$, 400 MHz): δ (ppm) 7.11-7.16 (m, 2H), 7.27-7.29 (m, 2H), 7.49-7.51 (m, 1H), 7.68-7.69 (m, 1H), 8.16-8.20 (m, 2H); ^{13}C NMR ($CDCl_3$, 100 MHz): δ (ppm)

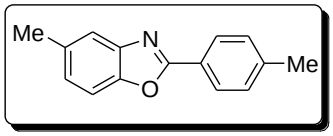
110.7, 116.3 (d, 1C, *J* = 22.1 Hz), 120.1, 123.6, 125.0 (d, 1C, *J* = 47.3 Hz), 129.9 (d, 1C, *J* = 9.2 Hz), 142.2, 150.9, 162.3, 163.7, 162.2; IR (KBr): 3054, 2923, 1895, 1600, 1498, 1472, 1451, 1412, 1230, 1152, 1053, 834, 761 cm^{-1}; elemental analysis calcd (%) for $C_{13}H_8FNO$ (213.2068): C 73.23, H 3.78, N 6.57; found C 73.29, H 3.72, N 6.51.



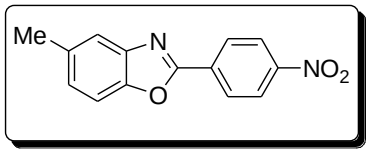
5-Methyl-2-phenylbenzo[*d*]oxazole (**10aa**): White solid; M.p. 103-105 ºC (lit.[9] 103-105 ºC); ^1H NMR ($CDCl_3$, 400 MHz): δ (ppm) 2.45 (s, 3H), 7.14 (d, 1H, *J* = 8.4 Hz), 7.43 (d, 1H, *J* = 8 Hz), 7.49-7.51 (m, 3H), 7.54 (s, 1H), 8.21-8.24 (m, 2H); ^{13}C NMR ($CDCl_3$, 100 MHz): δ (ppm) 21.6, 109.9, 119.9, 126.3, 127.4, 127.6, 128.9, 131.4, 134.4, 142.4, 149.1, 163.1; IR (KBr): 3032, 2920, 2857, 1551, 1474, 1445, 1334, 1263, 1198, 1053, 1021, 925, 825, 795, 775, 700 cm^{-1}; HRMS (ESI): calcd. for ($C_{14}H_{11}NO$) (MH^+) 210.0913; found 210.0925.



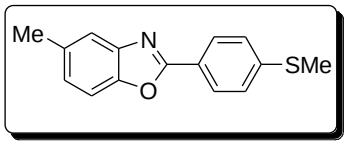
2-(4-Chlorophenyl)-5-methylbenzo[*d*]oxazole (**11aa**): White solid; M.p. 148-150 ºC (lit.[9] 148-150 ºC); ^1H NMR ($CDCl_3$, 400 MHz): δ (ppm) 2.46 (s, 3H), 7.14 (d, 1H, *J* = 7.6 Hz), 7.42 (d, 1H, *J* = 8.4 Hz), 7.46 (d, 2H, *J* = 8.4 Hz), 7.52 (s, 1H), 8.14 (d, 2H, *J* = 8.4 Hz); ^{13}C NMR ($CDCl_3$, 400 MHz): δ (ppm) 21.7, 110.1, 120.1, 125.9, 126.6, 128.9, 129.3, 134.7, 137.7, 142.4, 149.1, 162.3; IR (KBr): 2917, 2857, 1596, 1552, 1476, 1456, 1401, 1260, 1201, 1089, 1050, 1006, 825, 796 cm^{-1}; HRMS (ESI): calcd. for $C_{14}H_{10}ClNO$ (MH^+) 244.0524; found 244.0524.



5-Methyl-2-p-tolylbenzo[*d*]oxazole (**12aa**): White Solid; M.p. 137-139 ^{o}C (lit.[9] 138-141 ^{o}C); ^{1}H NMR ($CDCl_3$, 400 MHz): δ (ppm) 2.41 (s, 3H), 2.46 (s, 3H), 7.12 (d, 1H, *J* = 8 Hz), 7.30 (d, 2H, *J* = 8 Hz), 7.41 (d, 1H, *J* = 8.4 Hz), 7.52 (s, 1H), 8.11 (d, 2H, *J* = 8 Hz); ^{13}C NMR ($CDCl_3$, 100 MHz): δ (ppm) 21.7, 21.8, 109.9, 119.9, 124.7, 126.1, 127.6, 129.7, 134.4, 141.9, 142.5, 149.0, 163.5; IR (KBr): 2917, 2857, 1610, 1577, 1555, 1498, 1473, 1426, 1330, 1261, 1179, 1054, 1012, 924, 825, 796 cm^{-1}; HRMS (ESI): calcd. for $C_{15}H_{13}NO$ (MH^+) 224.107; found 224.1067.

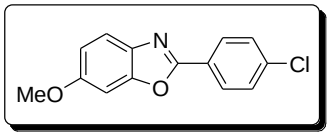


5-Methyl-2-(4-nitrophenyl)benzo[*d*]oxazole (**13aa**): Yellow solid; M.p. 204-206 ^{o}C; ^{1}H NMR ($CDCl_3$, 400 MHz): δ (ppm): 2.51 (s, 3H), 7.23-7.26 (m, 1H), 7.49 (d, 1H, *J* = 8 Hz), 7.59 (s, 1H), 8.35-8.42 (m, 4H); ^{13}C NMR ($CDCl_3$, 100 MHz): δ (ppm) 21.7, 110.4, 120.6, 124.3, 127.7, 128.4, 133.1, 135.4, 142.3, 149.4, 160.8; IR (KBr): 2923, 1599, 1555, 1520, 1481, 1342, 1196, 1105, 1060, 853, 798, 707 cm^{-1}; HRMS (ESI): calcd. for $C_{14}H_{10}N_2O_3$ (MH^+) 255.0764; found 255.0760.

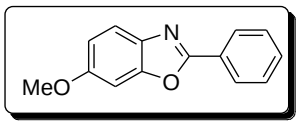


5-Methyl-2-(4-(methylthio)phenyl)benzo[*d*]oxazole (**14aa**): Yellowish solid; M.p 116-118 ^{o}C; ^{1}H NMR ($CDCl_3$, 400 MHz): δ (ppm) 2.46 (s, 3H), 2.52 (s, 3H), 7.11-7.13 (m, 1H), 7.32 (d, 2H, *J* = 8.8 Hz), 7.41 (d, 1H, *J* = 8.4 Hz), 7.51 (s, 1H), 8.11 (d, 2H, *J* = 8.8 Hz); ^{13}C NMR ($CDCl_3$, 100 MHz): δ (ppm) 15.1, 21.7, 109.9, 119.9, 123.7, 125.8, 126.2, 127.9, 134.5, 142.5, 143.6, 149.0, 163.1; IR (KBr): 2923, 1596, 1541, 1481, 1451, 1404, 1289, 1259, 1179, 1116, 1094, 1050, 820, 790, 728 cm^{-1};

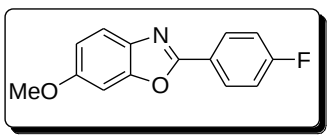
elemental analysis calcd (%) for $C_{15}H_{13}NOS$ (255.3353): C 70.56, H 5.13, N 5.49, S 12.56; found C 70.65, H 5.21, N 5.41, S 12.63.



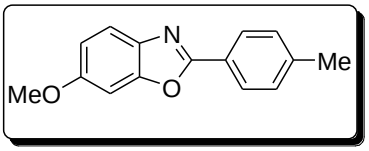
2-(4-Chlorophenyl)-6-methoxybenzo[*d*]oxazole (**15aa**): White solid; M.p. 134-136 ^{o}C; ^{1}H NMR ($CDCl_3$, 400 MHz): δ (ppm) 3.86 (s, 3H), 6.94 (dd, 1H, J_1 = 2.4 Hz, J_2 = 8.8 Hz), 7.077-7.083 (m, 1H), 7.46 (d, 2H, J = 8.4 Hz), 7.61 (d, 1H, J = 8.8 Hz), 8.11 (d, 2H, J = 8.4 Hz); ^{13}C NMR ($CDCl_3$, 100 MHz): δ (ppm) 56.1, 95.5, 113.1, 120.2, 125.9, 128.5, 129.3, 135.9, 137.3, 151.8, 158.6, 161.3; IR (KBr): 2934, 2829, 1618, 1484, 1317, 1292, 1220, 1146, 1113, 1089, 1050, 1020, 815, 762 cm^{-1}; elemental analysis calcd (%) for $C_{14}H_{10}ClNO_2$ (259.687): C 64.75, H 3.88, N 5.39; found C 64.81, H 3.94, N 5.31.



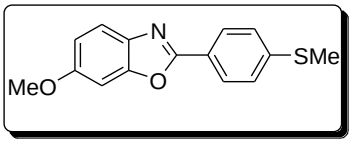
6-Methoxy-2-phenylbenzo[*d*]oxazole (**16aa**): Off-white solid; M. p 63-66 ^{o}C (lit.[10] 65-66 ^{o}C); ^{1}H NMR ($CDCl_3$, 400 MHz,): δ (ppm) 3.86 (s, 3H), 6.94 (dd, 1H, J_1 = 2.4 Hz, J_2 = 8.8 Hz), 7.086-7.092 (m, 1H), 7.48-7.49 (m, 3H), 7.62 (d, 1H, J = 8.8 Hz), 8.17-8.19 (m, 2H); ^{13}C NMR ($CDCl_3$, 100 MHz): δ (ppm) 56.96, 95.5, 112.9, 120.0, 127.3, 127.4, 128.9, 131.1, 135.9, 151.7, 158.4, 162.3; IR (KBr): 2934, 2921, 1620, 1488, 1448, 1347, 1273, 1215, 1176, 1144, 1127, 1053, 1023, 838, 814 cm^{-1}; HRMS (ESI): calcd. for ($C_{14}H_{11}NO_2$) (MH^+) 226.0863; found 226.0874.



2-(4-Fluorophenyl)-6-methoxybenzo[*d*]oxazole (**17aa**): White Solid; M.p. 105-107 ^{o}C; ^{1}H NMR ($CDCl_3$, 400 MHz): δ (ppm) 3.89 (s, 3H), 6.96 (dd, 1H, J_1 = 2.4 Hz, J_2 = 8.4 Hz), 7.105-7.111 (m, 1H), 7.19 (t, 2H, J = 8.8 Hz), 7.63 (d, 1H, J = 8.8 Hz), 8.18-8.22 (m, 2H); ^{13}C NMR ($CDCl_3$, 100 MHz): δ (ppm) 56.1, 95.6, 112.9, 116.2 (d, 1C, J = 22.1 Hz), 120.1, 123.8, 129.5 (d, 1C, J = 9.2 Hz), 135.9, 151.8, 158.4, 161.5, 164.7 (d, 1C, J = 51 Hz); IR (KBr): 2941, 2835, 1620, 1599, 1496, 1465, 1349, 1278, 1221, 1147, 1132, 1051, 831, 803 cm^{-1}; elemental analysis calcd (%) for $C_{14}H_{10}FNO_2$ (243.2327): C 69.13, H 4.14, N 5.76; found C 69.22, H 4.18, N 5.70.

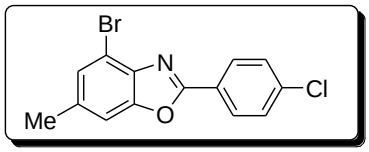


6-Methoxy-2-p-tolylbenzo[*d*]oxazole (**18aa**): White solid; M.p. 94-96 ^{o}C; ^{1}H NMR ($CDCl_3$, 400 MHz): δ (ppm) 2.39 (s, 3H), 3.85 (s, 3H), 6.92 (dd, 1H, J_1 = 2.8 Hz, J_2 = 8.8 Hz), 7.067-7.072 (m, 1H), 7.28 (d, 2H, J = 8 Hz), 7.33 (1H, d, J = 8.8 Hz), 8.06 (d, 2H, J = 8.4 Hz); ^{13}C NMR ($CDCl_3$, 100 MHz): δ (ppm) 21.6, 55.9, 95.5, 112.6, 119.8, 124.6, 127.2, 129.6, 135.9, 141.5, 151.6, 158.2, 162.5; IR (KBr): 3001, 2928, 1862, 1626, 1486, 1462, 1347, 1272, 1212, 1178, 1143, 1126, 1056, 1019, 826, 801, 724 cm^{-1}; elemental analysis calcd (%) for $C_{15}H_{13}NO_2$: C 75.30, H 5.48, N 5.85; found C 75.38, H 5.41, N 5.79.

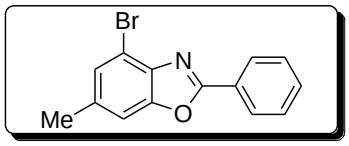


6-Methoxy-2-(4-(methylthio)phenyl)benzo[*d*]oxazole (**19aa**): Yellowish solid; M.p. 128–130 ^{o}C; ^{1}H NMR ($CDCl_3$, 400 MHz): δ (ppm) 2.52 (s, 3H), 3.86 (s, 3H), 6.93 (dd, 1H, J_1 = 2.0 Hz, J_2 = 8.4 Hz), 7.075-7.08 (m, 1H), 7.31 (d, 2H, J = 8.8 Hz), 7.59 (d, 1H, J = 8.8 Hz), 8.07 (d, 2H, J = 8.4 Hz); ^{13}C NMR ($CDCl_3$, 100 MHz): δ (ppm) 15.1, 56.0, 95.5, 112.8, 119.8, 123.7, 125.8, 127.5, 136.0, 143.1, 151.6, 158.2, 162.1; IR (KBr): 2959, 2923, 2830, 1617, 1595, 1571, 1429, 1404, 1338, 1325,

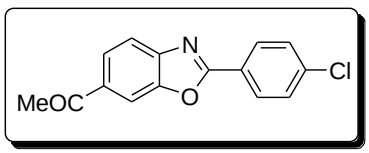
1297, 1266, 1190, 1145, 1095, 1044, 1028, 1008, 983, 959, 841 cm^{-1}; HRMS (ESI): calcd. for (MH^+) 272.074; found 272.0738.



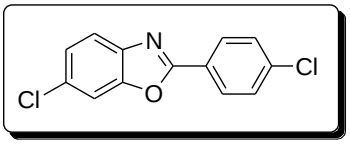
4-Bromo-2-(4-chlorophenyl)-6-methylbenzo[*d*]oxazole (**20aa**): White solid; M.p. 184–186 ^oC; ^1H NMR ($CDCl_3$, 400 MHz): δ (ppm) 2.49 (s, 3H), 7.32-7.33 (m, 1H), 7.37-7.38 (m, 1H), 7.49 (d, 2H, J = 9.2 Hz), 8.21 (d, 2H, J = 8.8 Hz); ^{13}C NMR ($CDCl_3$, 100 MHz): δ (ppm) 21.7, 110.2, 112.2, 125.3, 129.2, 129.3, 137.2, 138.1, 139.5, 151.1, 162.1; IR (KBr): 2917, 2819, 1612, 1588, 1484, 1407, 1331, 1251, 1198, 1088, 1053, 1011, 976, 926, 871, 838, 818 cm^{-1}; HRMS (ESI): calcd. for ($C_{14}H_9BrClNO$) (MH^+) 321.9629; found 321.9640.



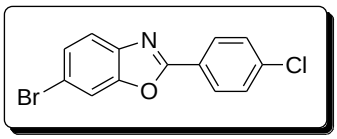
4-Bromo-6-methyl-2-phenylbenzo[*d*]oxazole (**21aa**): Yellowish-white solid; M.p. 135–137 ^oC; ^1H NMR ($CDCl_3$, 400 MHz): δ (ppm) 2.48 (s, 3H), 7.32 (s, 1H), 7.36 (s, 1H), 7.49-7.54 (m, 3H), 8.27 (dd, 2H, J_1 = 1.6 Hz, J_2 = 8.0 Hz); ^{13}C NMR ($CDCl_3$, 100 MHz): δ (ppm) 21.6, 110.1, 112.0, 126.8, 127.9, 128.89, 129.94, 131.8, 136.8, 139.6, 151.0, 163.1; IR (KBr): 3054, 2915, 2893, 1611, 1550, 1473, 1447, 1399, 1333, 1287, 1198, 1255, 1198, 1055, 1022, 976, 928, 866, 846 cm^{-1}; elemental analysis calcd (%) for $C_{14}H_{10}BrNO$ (288.1389): C 58.36, H 3.50, N 4.86; found C 58.42, H 3.55, N 4.81.



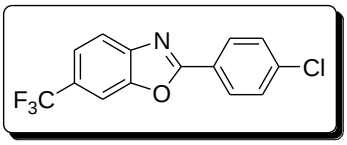
1-(2-(4-Chlorophenyl)benzo[*d*]oxazol-6-yl)ethanone (**22aa**): White solid; M.p. 185–187 ^{o}C; ^{1}H NMR ($CDCl_3$, 400 MHz): δ (ppm) 2.67 (s, 3H), 7.50 (d, 2H, J = 8.4 Hz), 7.78 (d, 1H, J = 8.4 Hz), 7.99 (dd, 1H, J_1 = 1.6 Hz, J_2 = 8.4 Hz), 8.18 (d, 3H, J = 8.8 Hz); ^{13}C NMR ($CDCl_3$, 100 MHz): δ (ppm) 26.9, 110.9, 119.8, 125.1, 125.7, 129.3, 129.5, 134.6, 138.7, 146.0, 150.8, 164.9, 169.9; IR (KBr): 3065, 1674, 1613, 1595, 1548, 1482, 1425, 1405, 1347, 1282, 1257, 1222, 1095, 1056, 826, 728 cm^{-1}; elemental analysis calcd (%) for $C_{15}H_{10}ClNO_2$ (271.6977): C 66.31, H 3.71, N 5.16; found C 66.38, H 3.78, N 5.10.



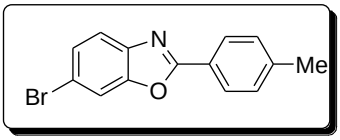
6-Chloro-2-(4-chlorophenyl)benzo[*d*]oxazole (**23aa**): White solid; M.p. 148–150 ^{o}C (lit.[11] 148-150 ^{o}C); ^{1}H NMR ($CDCl_3$, 400 MHz): δ (ppm) 7.32 (dd, 1H, J_1 = 2.0 Hz, J_2 = 8.4 Hz), 7.48 (d, 2H, J = 8.8 Hz), 7.56 (s, 1H), 7.64 (d, 1H, J = 8.0 Hz), 8.13 (s, 2H, J = 8.8 Hz); ^{13}C NMR ($CDCl_3$, 100 MHz): δ (ppm) 111.4, 120.7, 125.3, 125.6, 129.0, 129.5, 131.1, 138.3, 140.9, 151.0, 162.8; IR (KBr): 3083, 1982, 1615, 1591, 1548, 1482, 1461, 1425, 1401, 1326, 1259, 1239, 1124, 1094, 1009, 918, 854, 841 cm^{-1}; HRMS (ESI): calcd. for ($C_{13}H_7Cl_2NO$) (MH^+) 263.9977; found 263.9989.



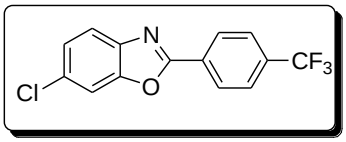
6-Bromo-2-(4-chlorophenyl)benzo[*d*]oxazole (**24aa**): White solid; M.p. 157–160 ^{o}C; ^{1}H NMR ($CDCl_3$, 400 MHz): δ (ppm) 7.49-7.47 (m, 3H), 7.60 (d, 1H, J = 8.4 Hz), 7.22 (s, 1H), 8.14 (d, 2H, J = 8.8 Hz); ^{13}C NMR ($CDCl_3$, 100 MHz): δ (ppm) 114.3, 118.4, 121.2, 125.3, 128.4, 129.1, 129.5, 138.3, 141.4, 151.4, 162.7; IR (KBr): 3082, 2928, 1925, 1614, 1547, 1478, 1459, 1399, 1325, 1258, 1084, 1051, 1009, 906, 812, 728 cm^{-1}; HRMS (ESI): calcd. for ($C_{13}H_7BrClNO$) (MH^+) 307.9472; found 307.9487.



2-(4-Chlorophenyl)-6-(trifluoromethyl)benzo[*d*]oxazole (**25aa**): White solid; M.p. 114–116 ^{o}C; ^{1}H NMR ($CDCl_3$, 400 MHz): δ (ppm) 7.51 (d, 2H, J = 8.4 Hz), 7.62 (d, 1H, J = 8.4 Hz), 7.83 (d, 2H, J = 8.8 Hz), 8.18 (d, 2H, J = 8.4 Hz); ^{13}C NMR ($CDCl_3$, 100 MHz): δ (ppm) 108.6, 120.6, 122.2, 125.0, 129.3, 129.6, 138.8, 144.9, 150.3, 164.5; IR (KBr): 3092, 1912, 1616, 1597, 1552, 1483, 1434, 1333, 1305, 1263, 1166, 1119, 1047, 927, 828 cm^{-1}; HRMS (ESI): calcd. for ($C_{14}H_7F_3ClNO$) (MH^+) 298.0241; found 298.0251.

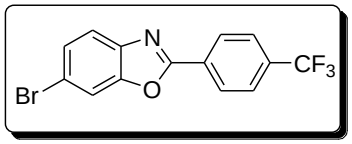


6-Bromo-2-p-tolylbenzo[d]oxazole (**26aa**): White solid; M.p. 127–129 ^{o}C; ^{1}H NMR ($CDCl_3$, 400 MHz): δ (ppm) 2.42 (s, 3H), 7.30 (d, 2H, J = 8.0 Hz)7.44 (dd, 1H, J_1 = 2.0 Hz, J_2 = 8.8 Hz), 7.58 (d, 1H, J = 8.0 Hz), 7.71 (s, 1H), 8.09 (d, 2H, J = 8.0 Hz); ^{13}C NMR ($CDCl_3$, 100 MHz): δ (ppm) 21.9, 114.2, 117.8, 120.9, 124.1, 127.8, 128.1, 129.9, 141.6, 142.6, 151.3, 163.9; IR (KBr): 3027, 2917, 1613, 1497, 1456, 1437, 1325, 1255, 1182, 1118, 1050, 907, 830 cm^{-1}; elemental analysis calcd (%) for $C_{14}H_{10}BrNO$ (288.1389): C 58.36, H 3.50, N 4.86; found C 58.45, H 3.44, N 4.81.

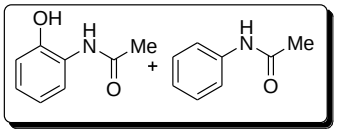


6-Chloro-2-(4-(trifluoromethyl)phenyl)benzo[d]oxazole (**27aa**): White solid; M.p. 120–123 ^{o}C; ^{1}H NMR ($CDCl_3$, 400 MHz): δ (ppm) 7.34 (dd, 1H, J_1 = 2.0 Hz, J_2 =

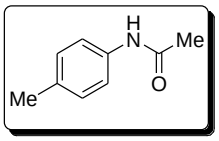
8.4 Hz), 7.59 (s, 1H), 7.67 (d, 1H, *J* = 8.8 Hz), 7.76 (d, 2H, *J* = 8.4 Hz), 8.31 (d, 2H, *J* = 8.0 Hz); ^{13}C NMR ($CDCl_3$, 100 MHz): δ (ppm) 111.6, 121.0, 125.9, 126.1, 128.0, 130.1, 131.7, 140.8, 151.1, 162.2; IR (KBr): 2958, 1614, 1558, 1500, 1461, 1426, 1409, 1323, 1159, 1108, 1067, 922, 817 cm^{-1}; HRMS (ESI): calcd. for ($C_{14}H_7F_3ClNO$) (MH^+) 298.0241; found 298.0255.



6-Bromo-2-(4-(trifluoromethyl)phenyl)benzo[d]oxazole (**28aa**): White solid; M.p. 106–108 ^{o}C; ^{1}H NMR ($CDCl_3$, 400 MHz): δ (ppm) 7.49 (dd, 1H, J_1 = 1.6 Hz, J_2 = 8.4 Hz), 7.64 (d, 1H, *J* = 8.8 Hz), 7.77 (d, 3H, *J* = 8.0 Hz), 8.33 (d, 2H, *J* = 8.0 Hz); ^{13}C NMR ($CDCl_3$, 100 MHz): δ (ppm) 114.5, 118.9, 121.5, 126.2, 127.8, 128.1, 128.6, 130.1, 141.3, 151.4, 162.1; IR (KBr): 3090, 2922, 1899, 1651, 1606, 1556, 1523, 1504, 1459, 1414, 1379, 1320, 1259, 1171, 1124, 1068, 1052, 1013, 966, 907, 847, 819 cm^{-1}; elemental analysis calcd (%) for $C_{14}H_7BrF_3NO$ (342.1104): C 49.15, H 2.06, N 4.09; found C 49.23, H 2.11, N 4.01.



Mixture of *N*-(2-Hydroxyphenyl)acetamide (1a′) and N-phenylacetamide (**1a**″): Brown solid; ^{1}H NMR (DMSO-d_6, 600 MHz): δ (ppm) 2.09 (s, 3H), 2.15 (s, 3H), 6.81 (t, 1H, *J* = 7.8 Hz), 6.91 (d, 1H, *J* = 7.8 Hz), 6.99 (t, 1H, *J* = 7.2 Hz), 7.07 (t, 1H, *J* = 7.8 Hz), 7.34 (t, 2H, *J* = 7.8 Hz), 7.62 (d, 2H, *J* = 7.8 Hz), 7.72 (d, 1H, *J* = 7.8 Hz), 9.35 (s, 1H), 9.78 (s, 1H), 9.97 (s, 1H); ^{13}C NMR (DMSO-d_6, 150 MHz): δ (ppm) 23.9, 24.3, 116.4, 119.6, 119.8, 123.3, 123.9, 125.6, 126.5, 129.2, 139.4, 148.5, 169.5, 170.1; IR (KBr): 3481, 3403, 3295, 2966, 1661, 1596, 1556, 1500, 1453, 1368, 1322, 1284, 1263, 1106, 1038, 1014, 966, 844 cm^{-1}.



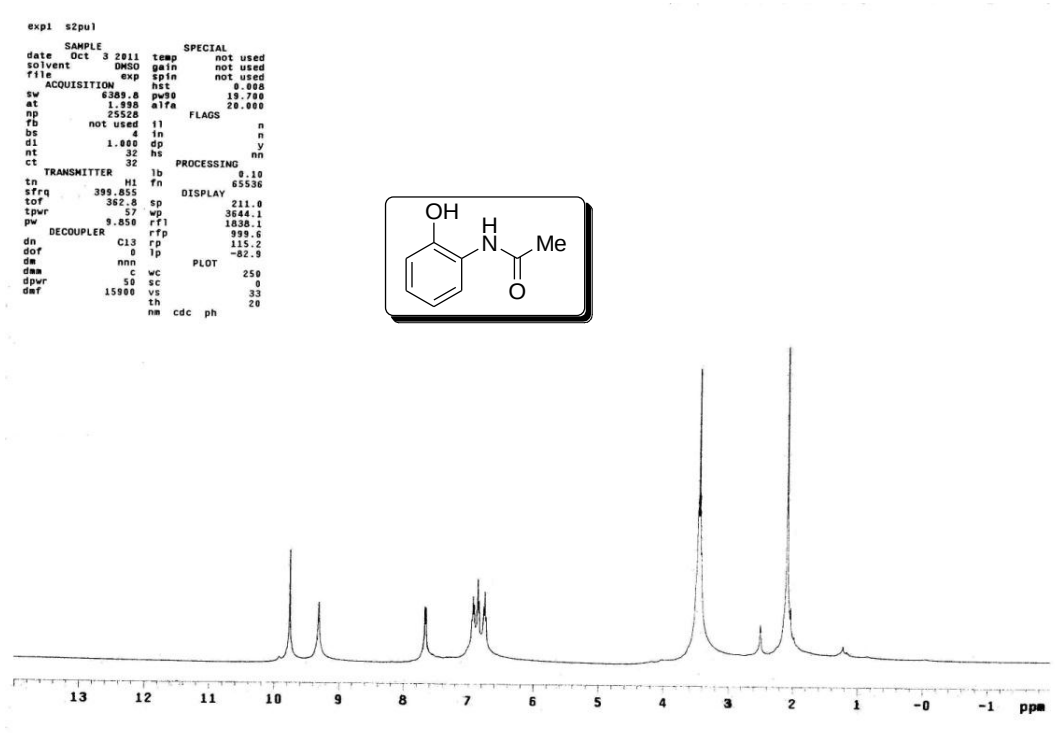
***N*-*p*-Tolylacetamide** (**2a′′**): Brown solid, M.p. 134–137^{o}C; ^{1}H NMR ($CDCl_3$, 600 MHz): δ (ppm) 2.14 (s, 3H), 2.30 (s, 3H), 7.098-7.108 (m, 2H), 7.359-7.369 (m, 2H), 7.42 (brs, 1H); ^{13}C NMR ($CDCl_3$, 150 MHz): δ (ppm) 21.0, 24.6, 120.3, 129.6, 134.2, 135.5, 168.7; IR (KBr): 2920, 2850, 1662, 1602, 1551, 1511, 1445, 1378, 1365, 1322, 1264, 1040, 819, 752 cm^{-1}; elemental analysis calcd (%) for $C_9H_{11}NO$ (149.1897) C 72.46, H 7.43, N 9.39; found C 72.39, H 7.45, N 9.31.

References

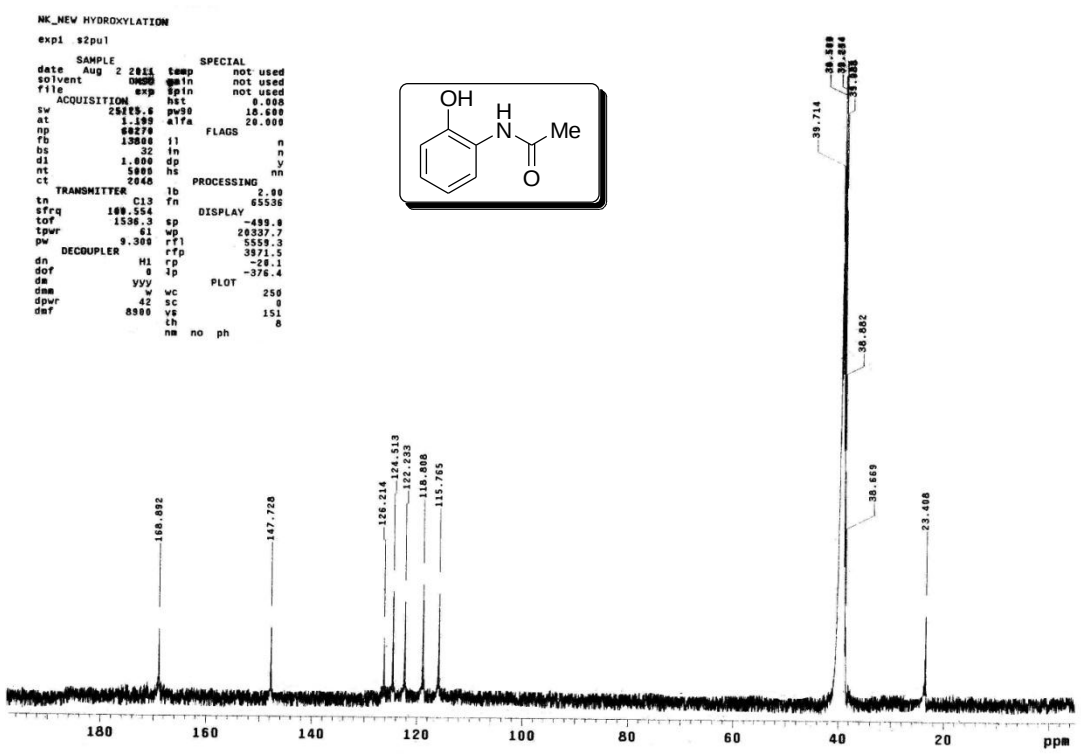
4. L. Chas Raiford, *J. Am. Chem. Soc.*, **1919**, *41*, 2068.
5. M. M. Guru, M. A. Ali and T. Punniyamurthy, *Org. Lett.*, **2011**, *13*, 1194.
6. S. Ueda and H. Nagasawa, *Angew. Chem. Int. Ed.*, **2008**, *47*, 6411.
7. M. Kidwai, V. Bansal, A. Saxena, S. Aery and S. Mozumdar, *Tetrahedron Lett.*, **2006**, *47*, 8049.
8. D. Subhas Bose and M. Idrees, *Synthesis*, **2010**, *3*, 398.
9. R. H. Shoar, M. Heidary, M. Farzaneh and R. Malakouti, *Synthetic Commun.*, **2009**, *39*, 1742.
10. M. I. El-Sheikh , A. Marks and E. R. Biehl, *J. Org. Chem.*, **1981**, *46*, 3256.
11. Y. Leng, F. Yang, W. Zhu, Y. Wu and X. Li, *Org. Biomol. Chem.*, **2011**, *9*, 5288.

SPECTRA

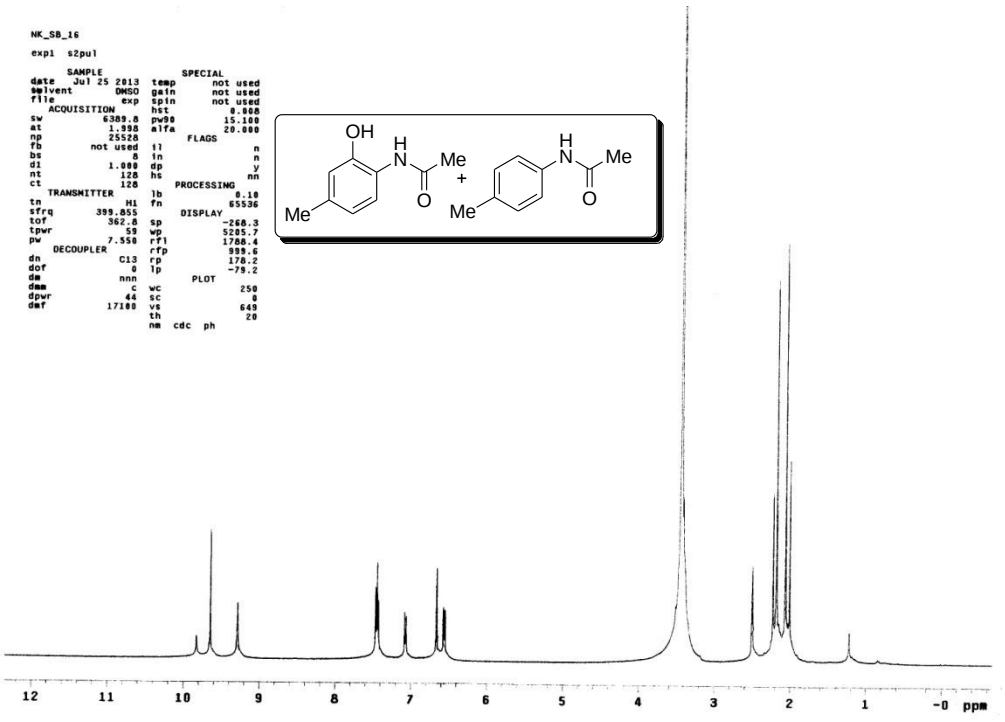
N-(2-Hydroxyphenyl)acetamide (1a′): ^{1}H NMR (DMSO-d_6, 400 MHz)



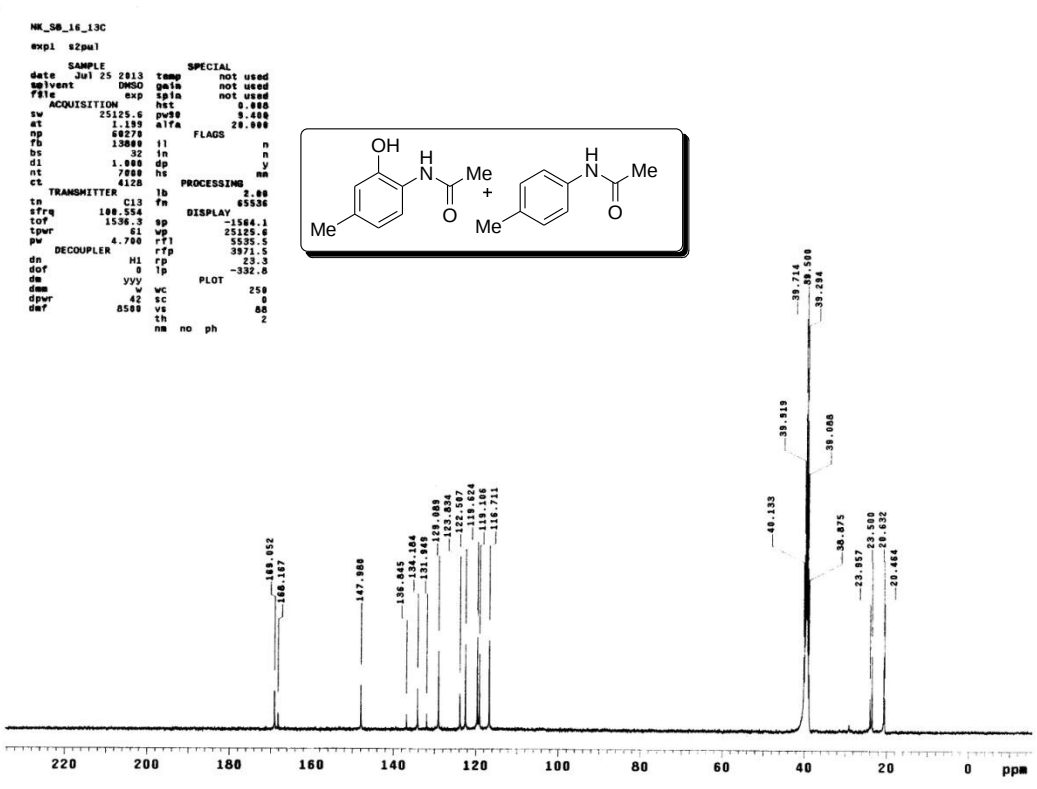
N-(2-Hydroxyphenyl)acetamide (1a′): ^{13}C NMR (DMSO-d_6, 100 MHz)



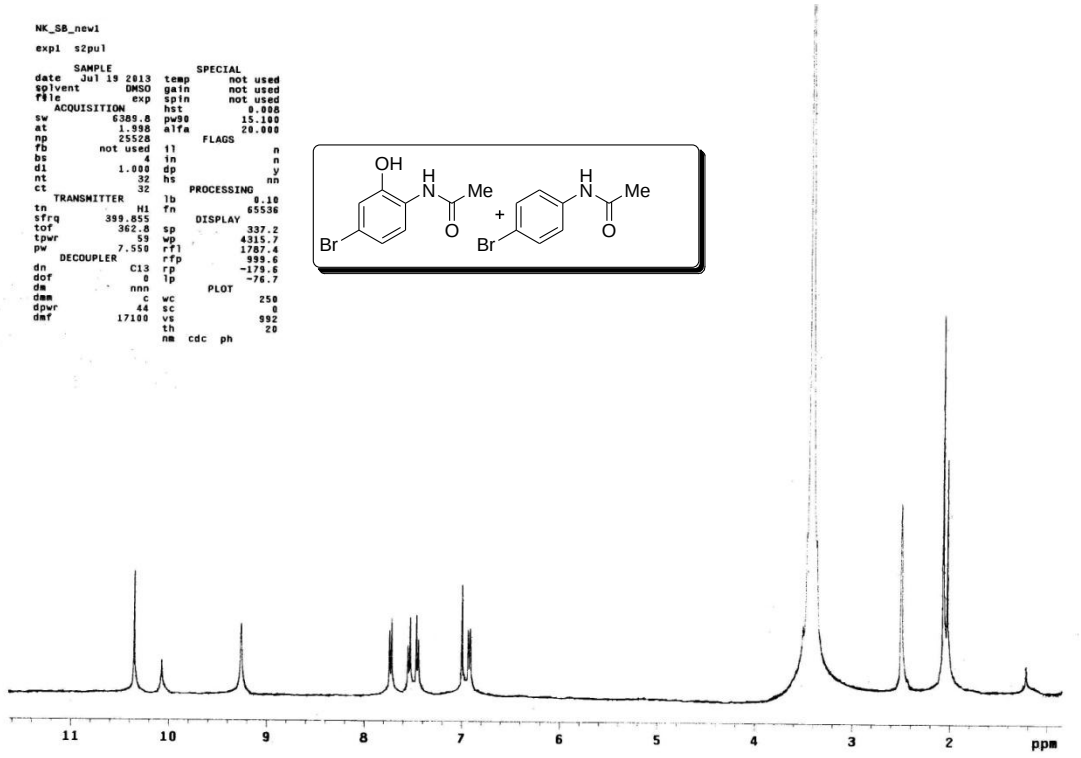
Mixture of *N*-(2-Hydroxy-4-methylphenyl)acetamide and *N*-*p*-Tolylacetamide (2a′+2a′′): ^{1}H NMR (DMSO-d_6, 400 MHz)



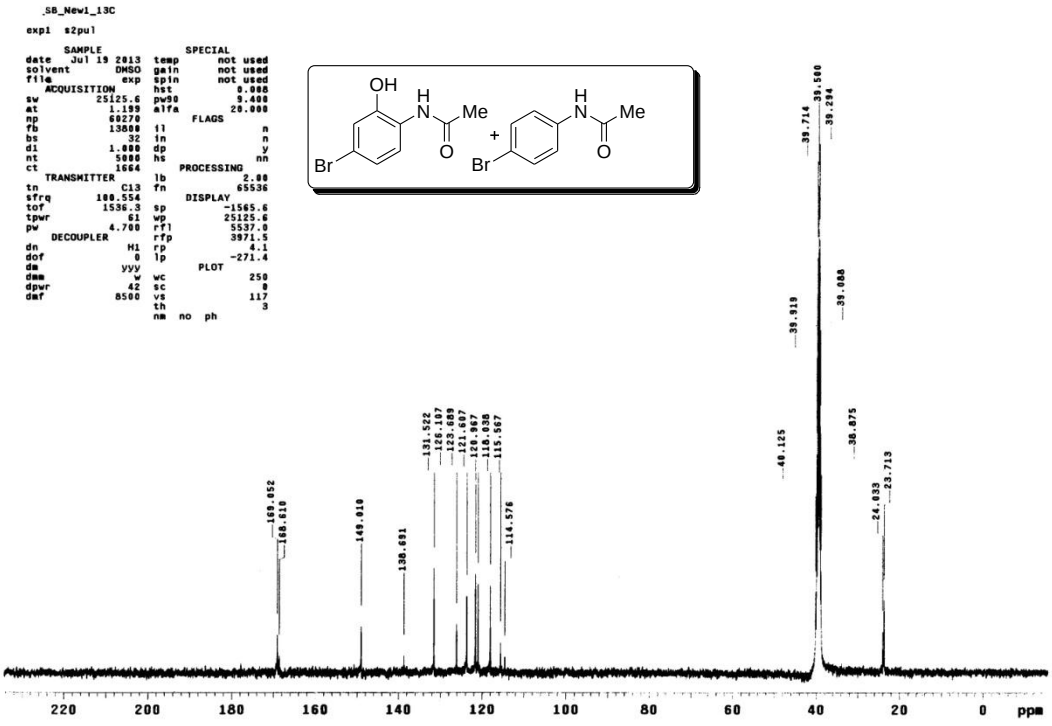
Mixture of *N*-(2-Hydroxy-4-methylphenyl)acetamide and *N*-*p*-Tolylacetamide (2a′+2a′′): ^{13}C NMR (DMSO-d_6, 100 MHz)



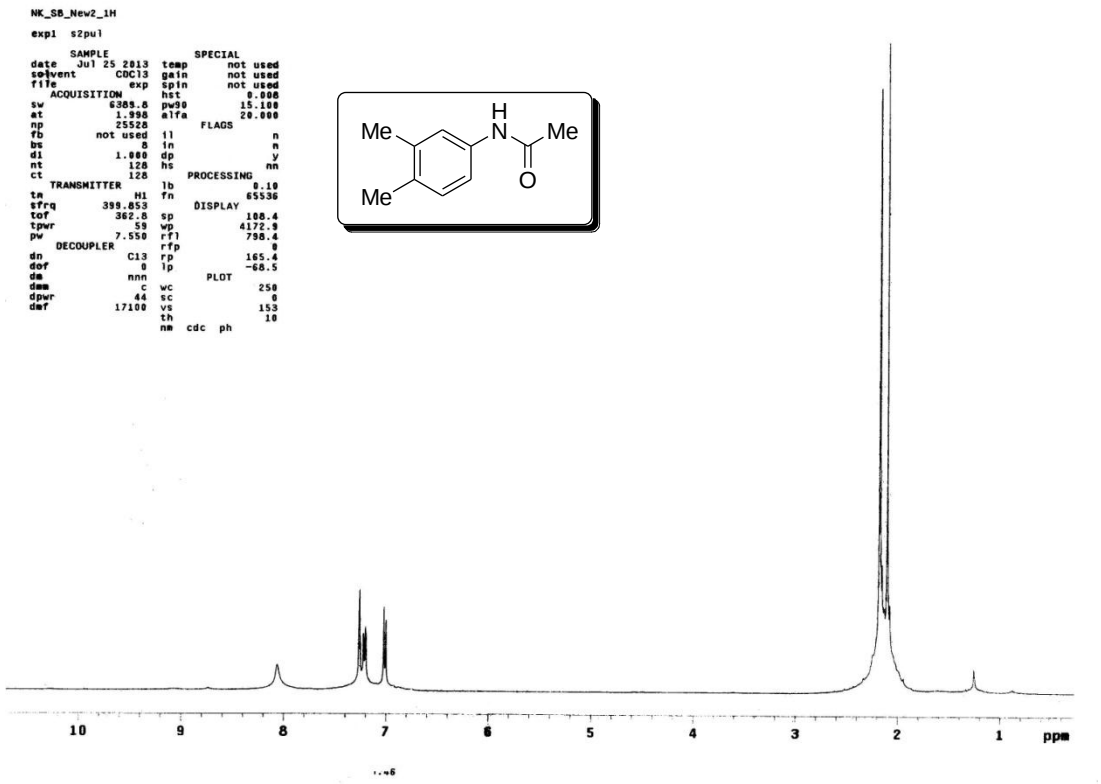
Mixture of *N*-(4-Bromo-2-hydroxyphenyl)acetamide and *N*-(4-Bromophenyl)acetamide (3a′+3a′′): ^{1}H NMR (DMSO-d_6, 400 MHz)



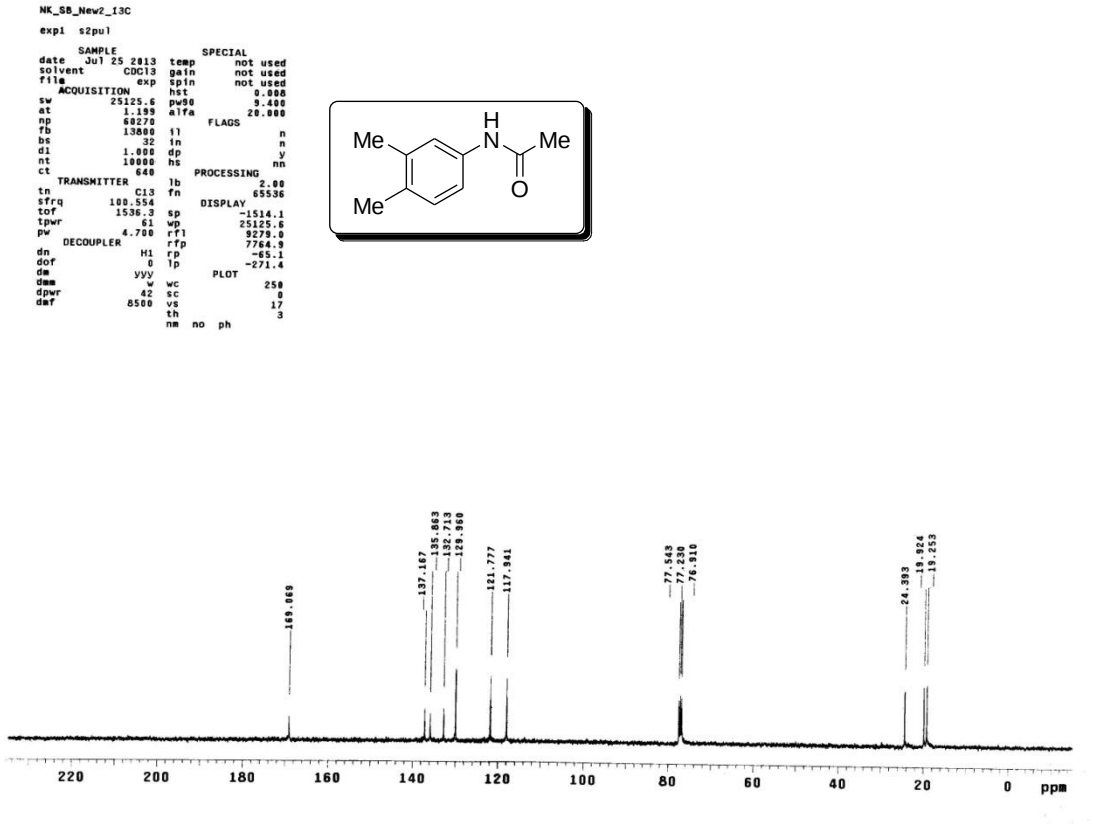
Mixture of *N*-(4-Bromo-2-hydroxyphenyl)acetamide and *N*-(4-Bromophenyl)acetamide (3a′+3a′′): ^{13}C NMR (DMSO-d_6, 100 MHz)



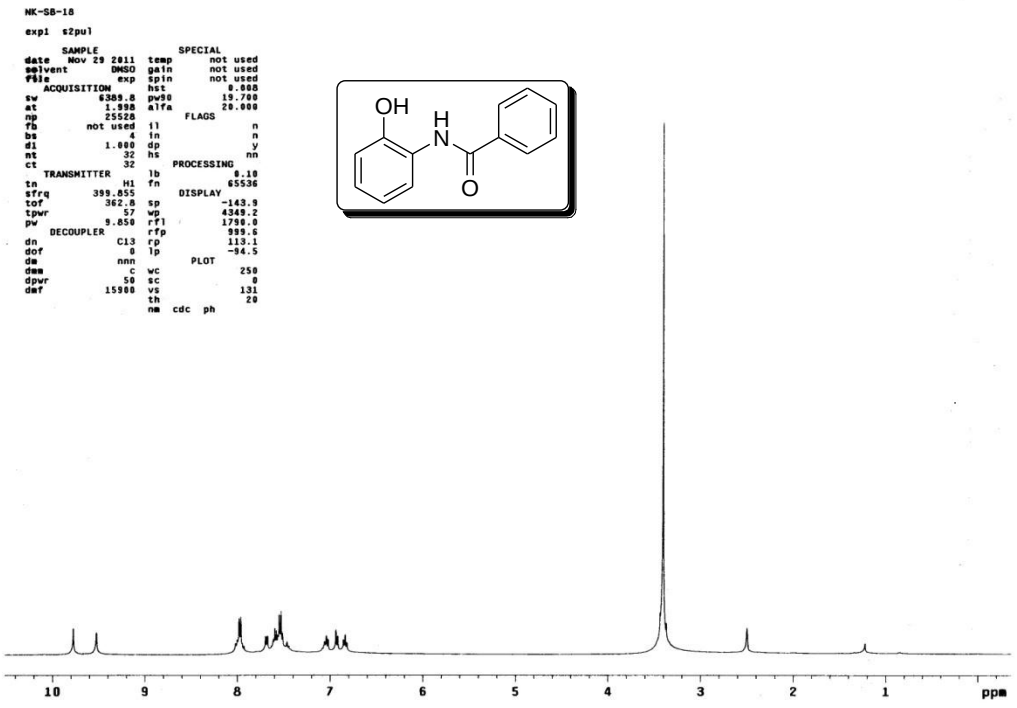
_N_-(3,4-Dimethylphenyl)acetamide (4a′′): ^{1}H NMR ($CDCl_3$, 400 MHz)



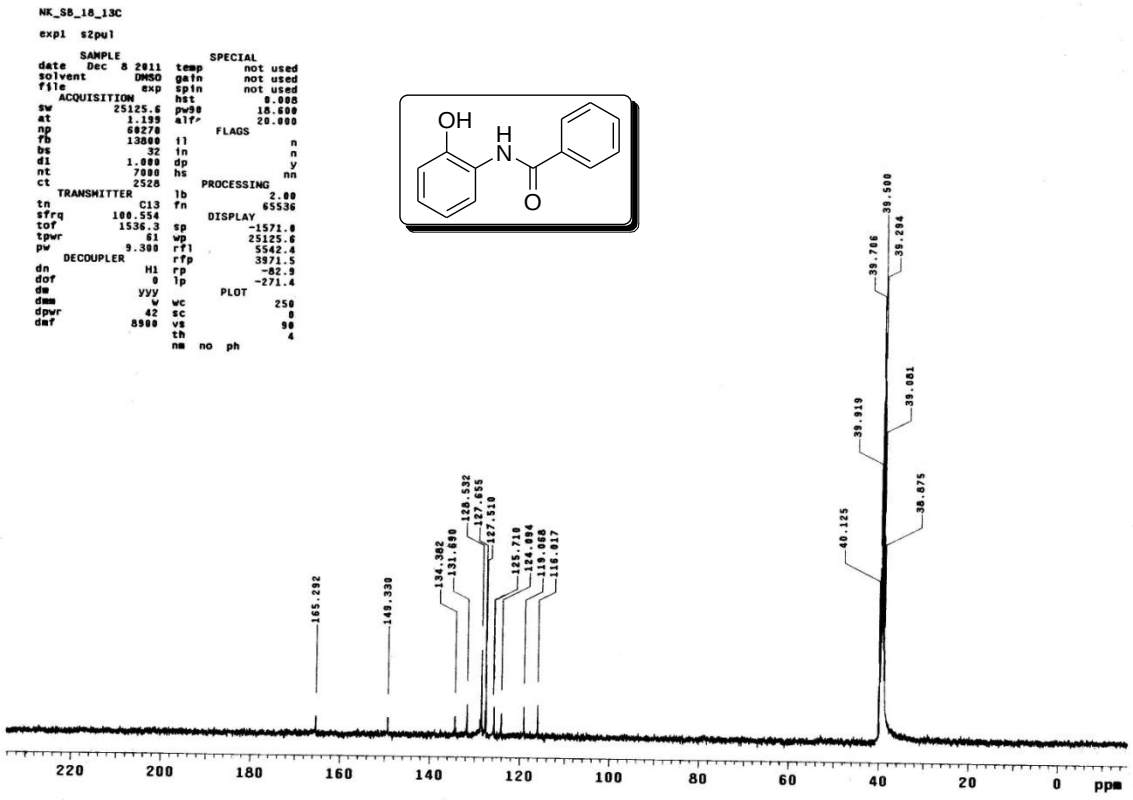
_N_-(3,4-Dimethylphenyl)acetamide (4a′′): ^{13}C NMR ($CDCl_3$, 100 MHz)



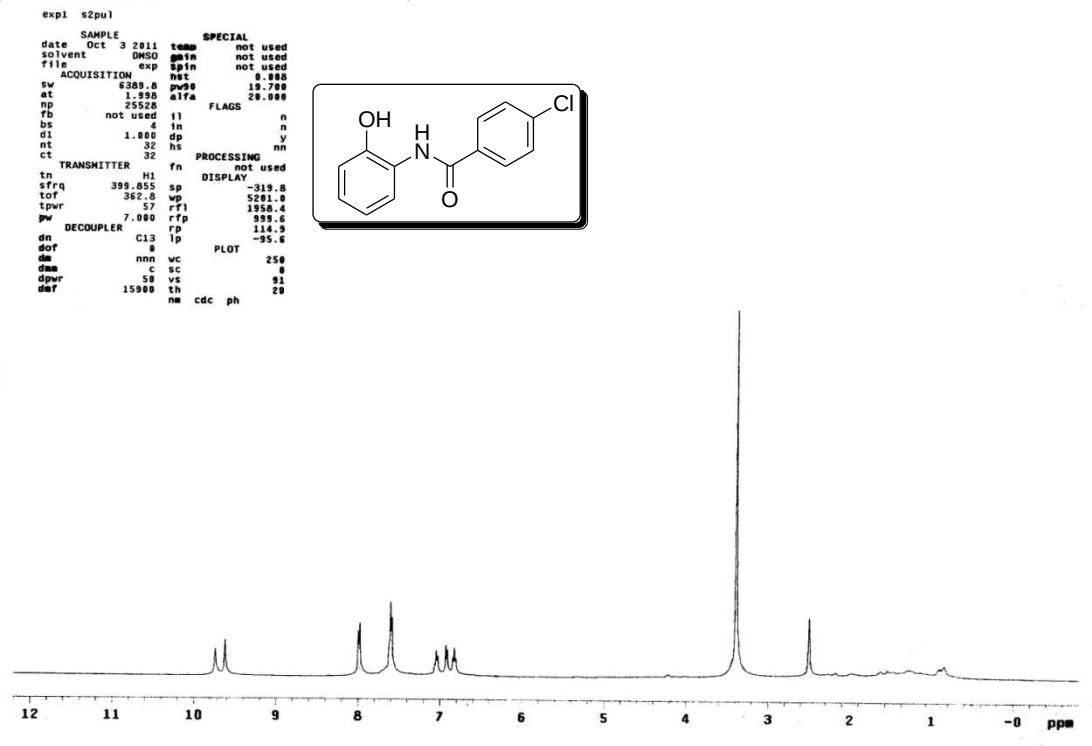
_N_-(2-Hydroxyphenyl)benzamide (2a′): ^{1}H NMR (DMSO-d_6, 400 MHz)



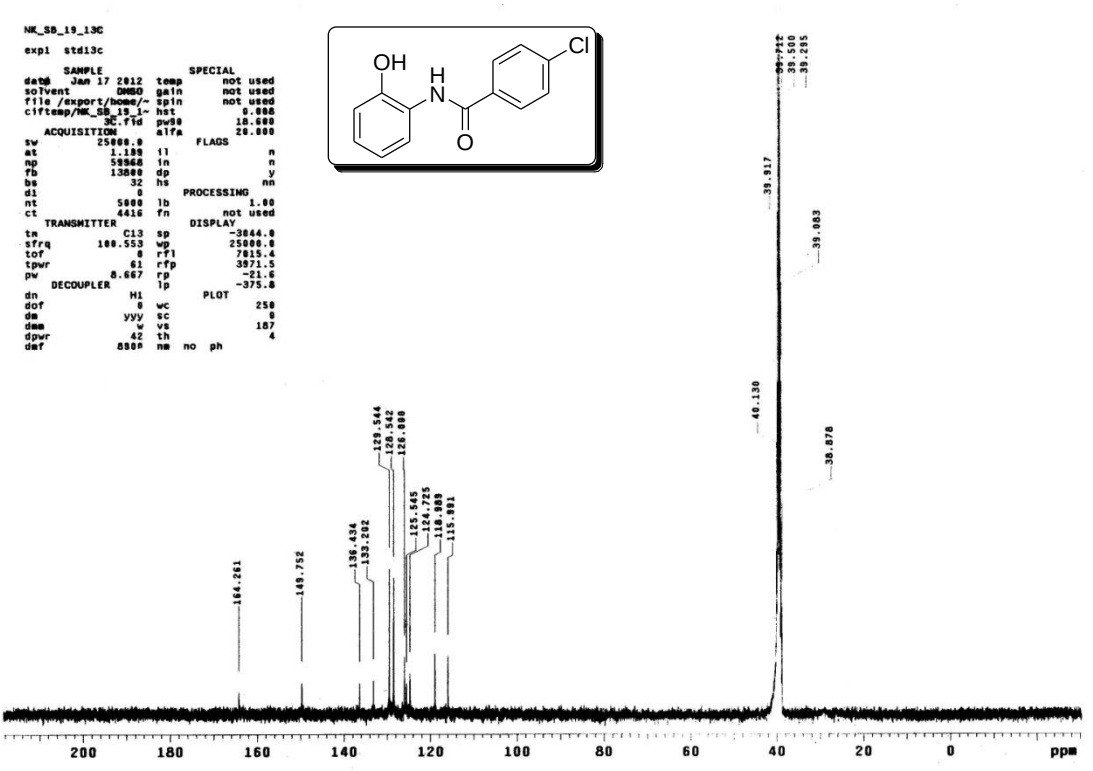
_N_-(2-Hydroxyphenyl)benzamide (2a′): ^{13}C NMR (DMSO-d_6, 100 MHz)



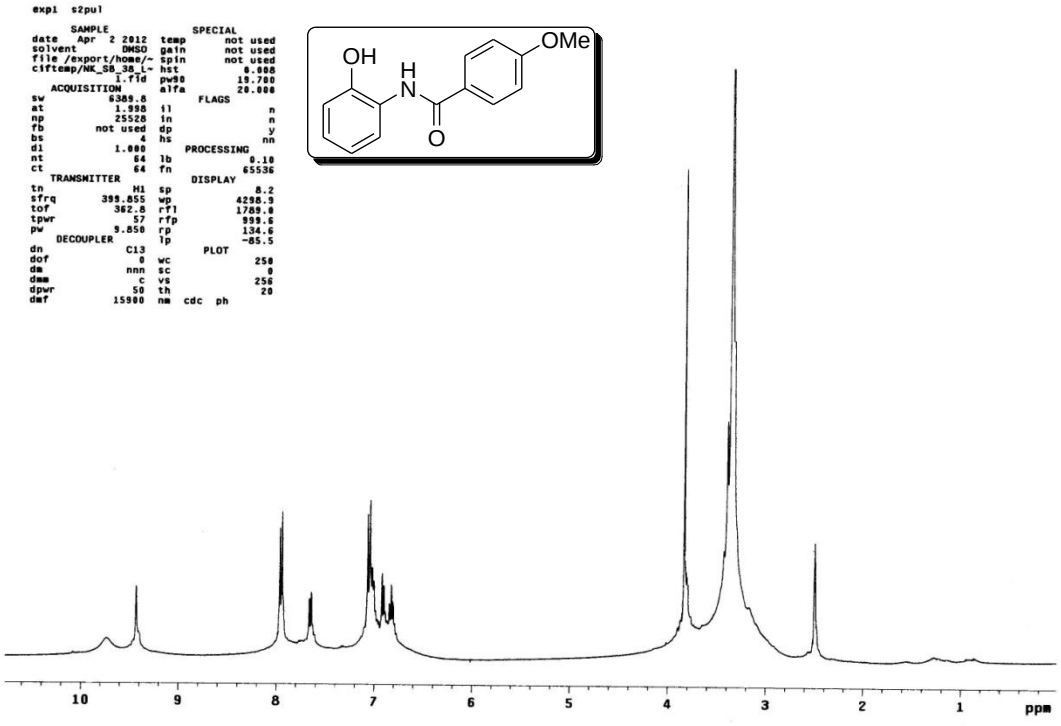
4-Chloro-*N*-(2-hydroxyphenyl)benzamide (3a′): ^{1}H NMR (DMSO-d_6, 400 MHz)



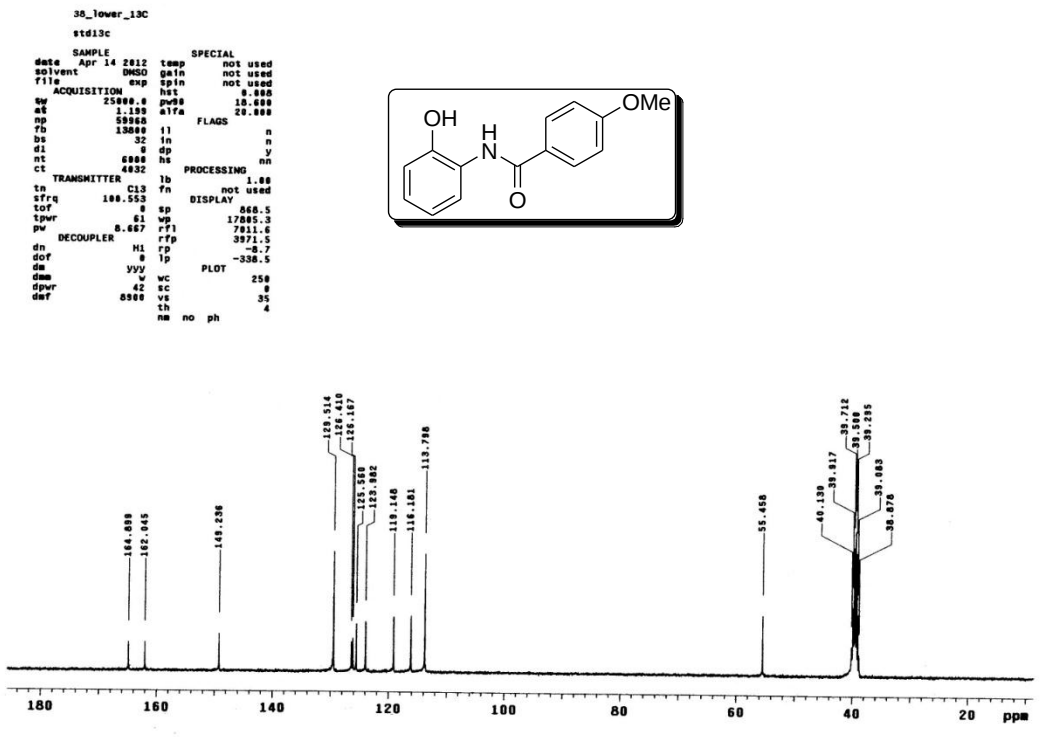
4-Chloro-*N*-(2-hydroxyphenyl)benzamide (3a′): ^{13}C NMR (DMSO-d_6, 100 MHz)



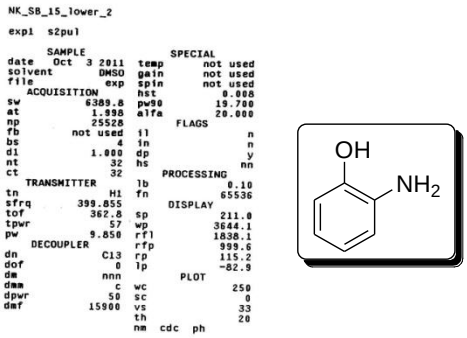
***N*-(2-Hydroxyphenyl)-4-methoxybenzamide (4a′): ^{1}H NMR (DMSO-d_6, 400 MHz)**

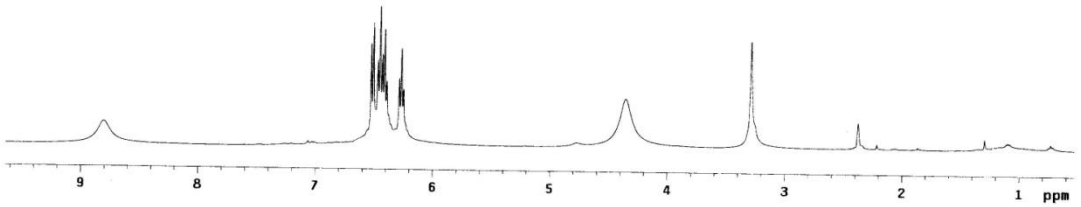


***N*-(2-Hydroxyphenyl)-4-methoxybenzamide (4a′): ^{13}C NMR (DMSO-d_6, 100 MHz)**

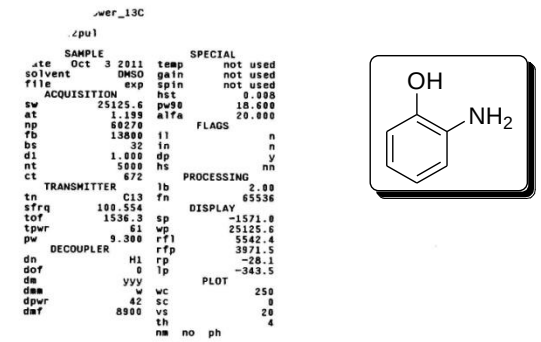


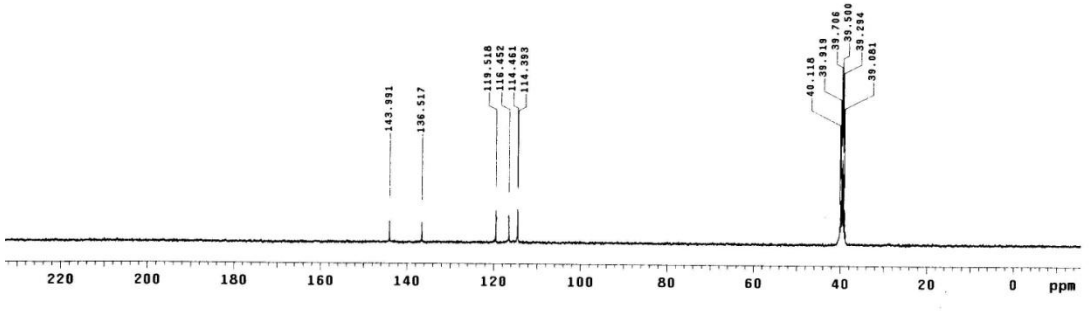
2-Hydroxyaniline: ^{1}H NMR (DMSO-d_6, 400 MHz)



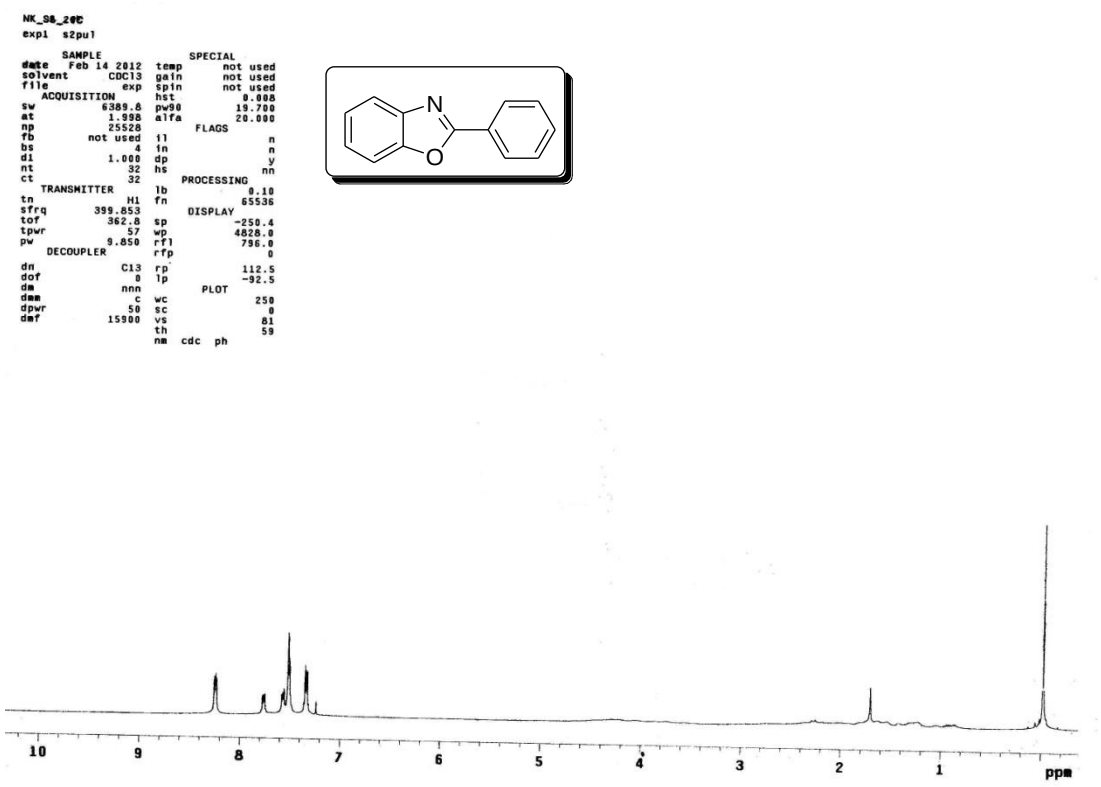


2-Hydroxyaniline: ^{13}C NMR (DMSO-d_6, 100 MHz)

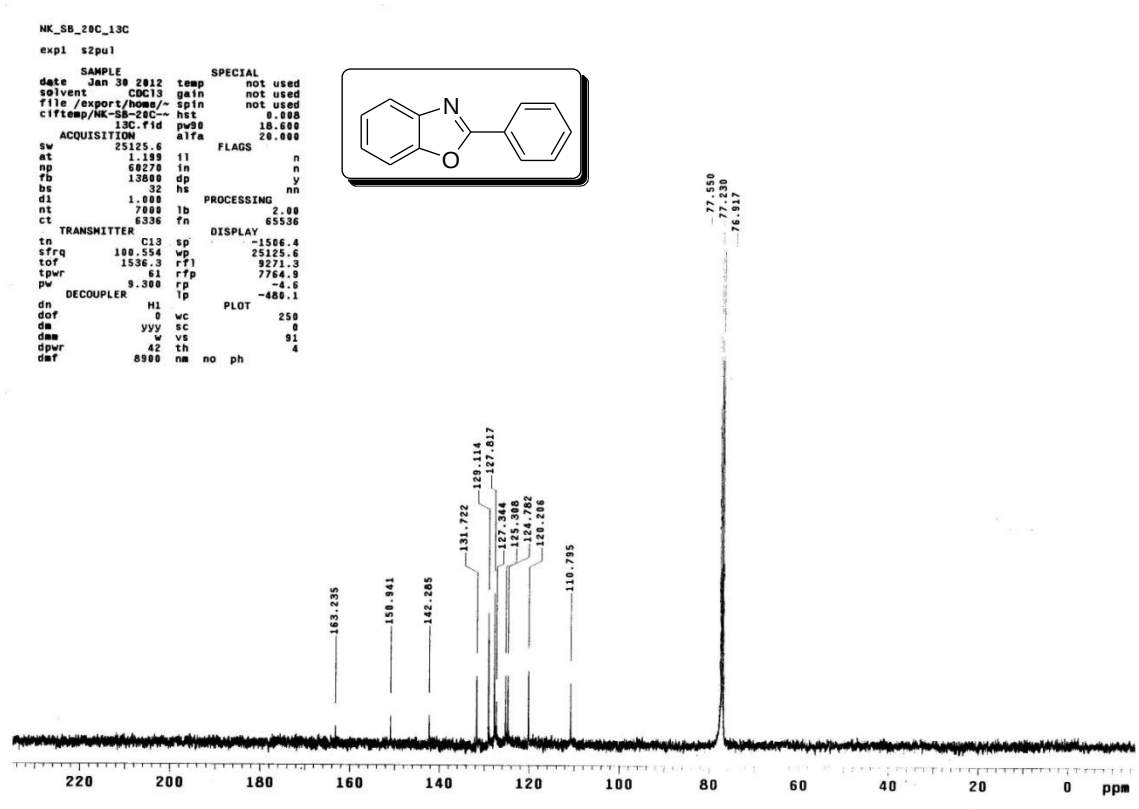




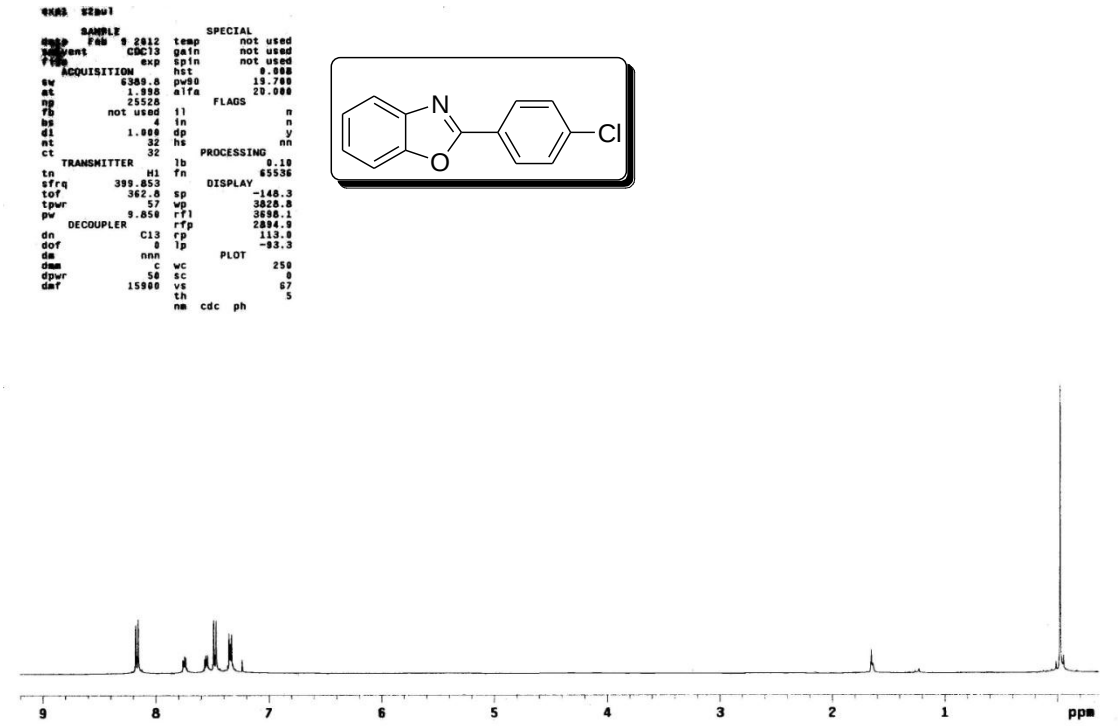
2-Phenylbenzo[*d*]oxazole (2aa): ^{1}H NMR ($CDCl_3$, 400 MHz)



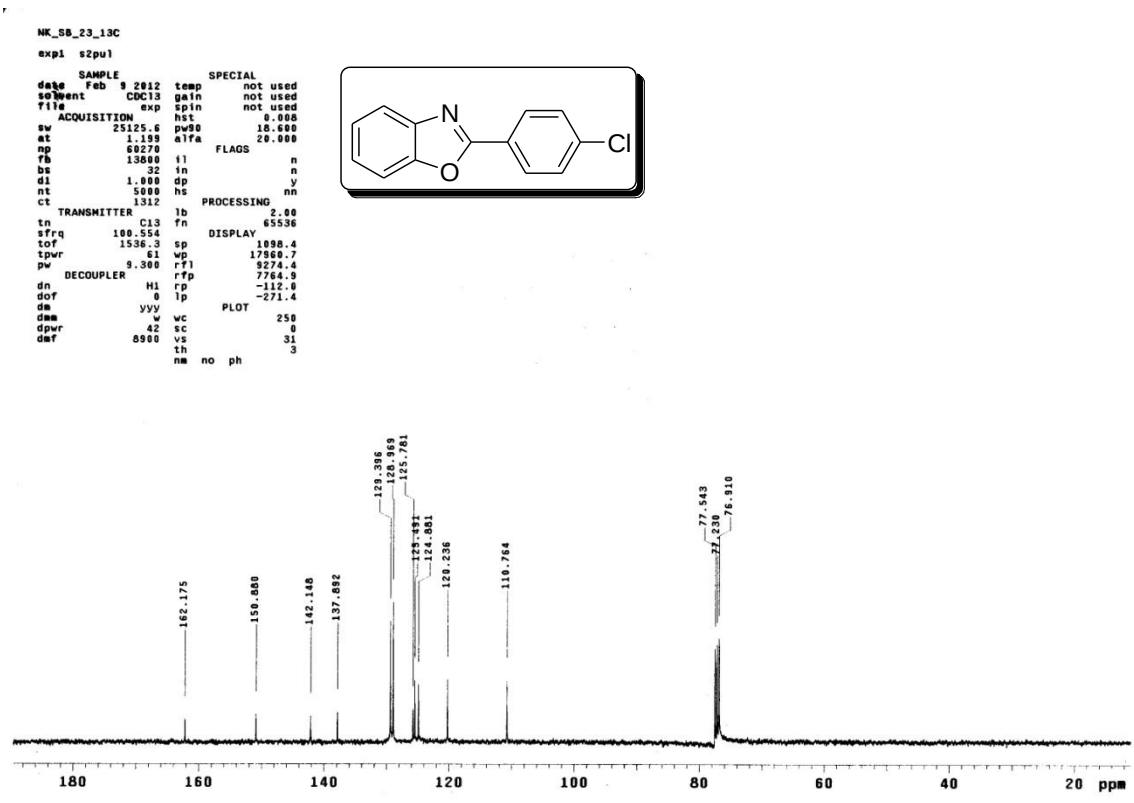
2-Phenylbenzo[*d*]oxazole (2aa): ^{13}C NMR ($CDCl_3$, 100 MHz)



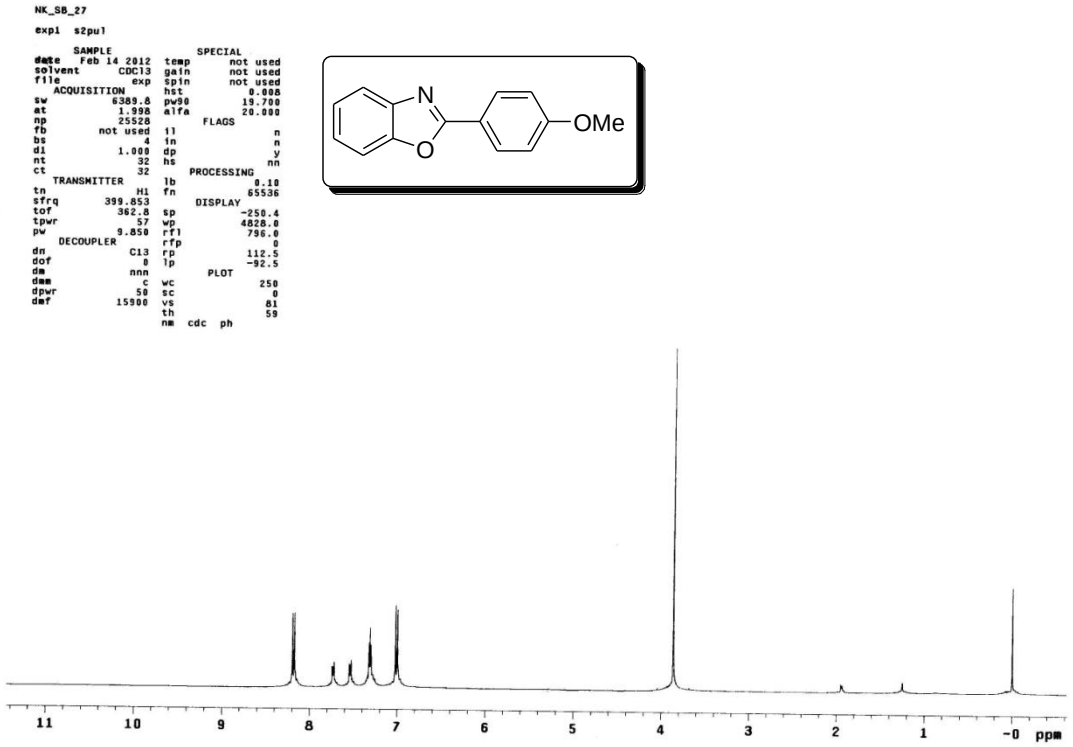
2-(4-Chlorophenyl)benzo[*d*]oxazole (3aa): ^{1}H NMR ($CDCl_3$, 400 MHz)



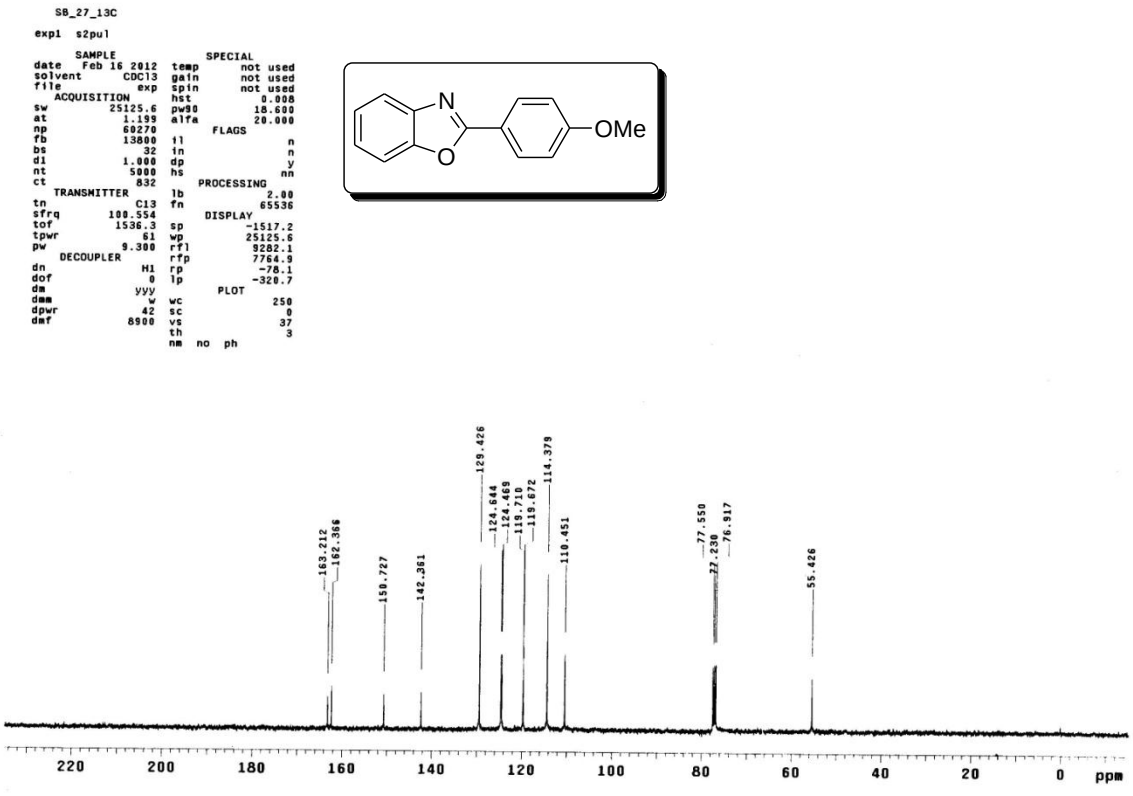
2-(4-Chlorophenyl)benzo[*d*]oxazole (3aa): ^{13}C NMR ($CDCl_3$, 100 MHz)



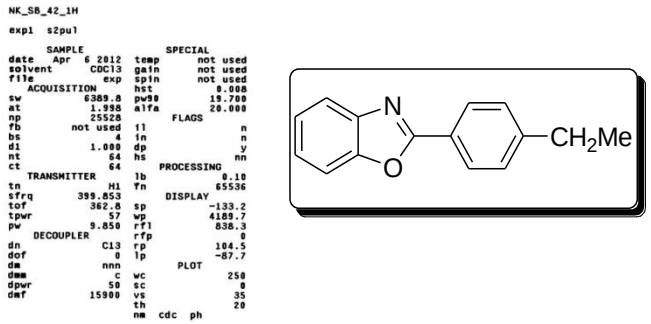
2-(4-Methoxyphenyl)benzo[*d*]oxazole (4aa): ^{1}H NMR ($CDCl_3$, 400 MHz)

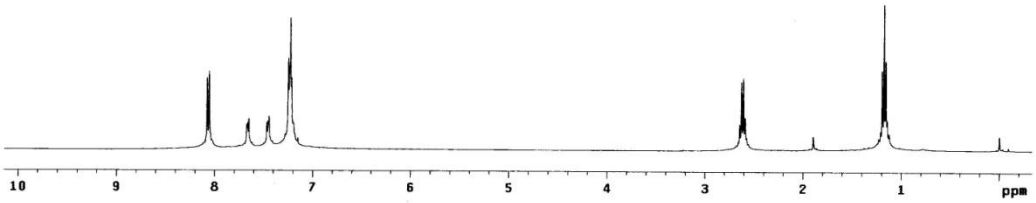


2-(4-Methoxyphenyl)benzo[*d*]oxazole (4aa): ^{13}C NMR ($CDCl_3$, 100 MHz)

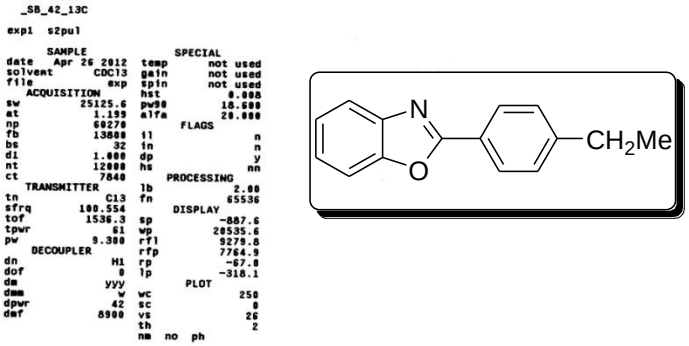


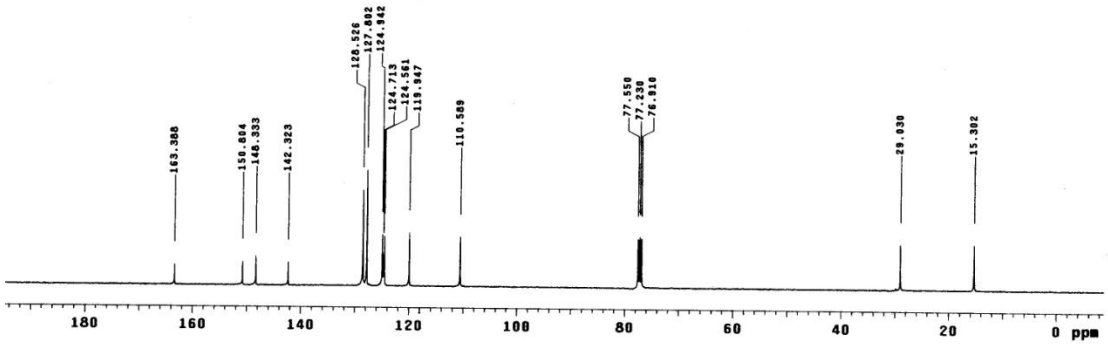
2-(4-Ethylphenyl)benzo[*d*]oxazole (5aa): ^{1}H NMR (CDCl$_3$, 400 MHz)



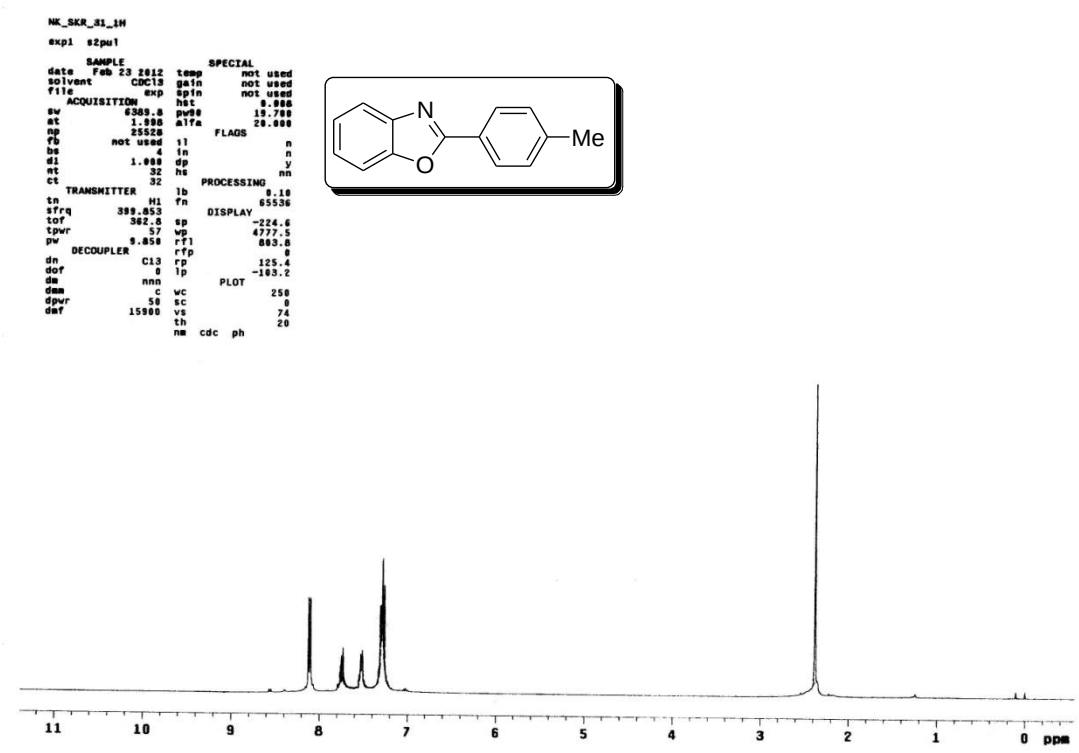


2-(4-Ethylphenyl)benzo[*d*]oxazole (5aa): ^{13}C NMR (CDCl$_3$, 100 MHz)

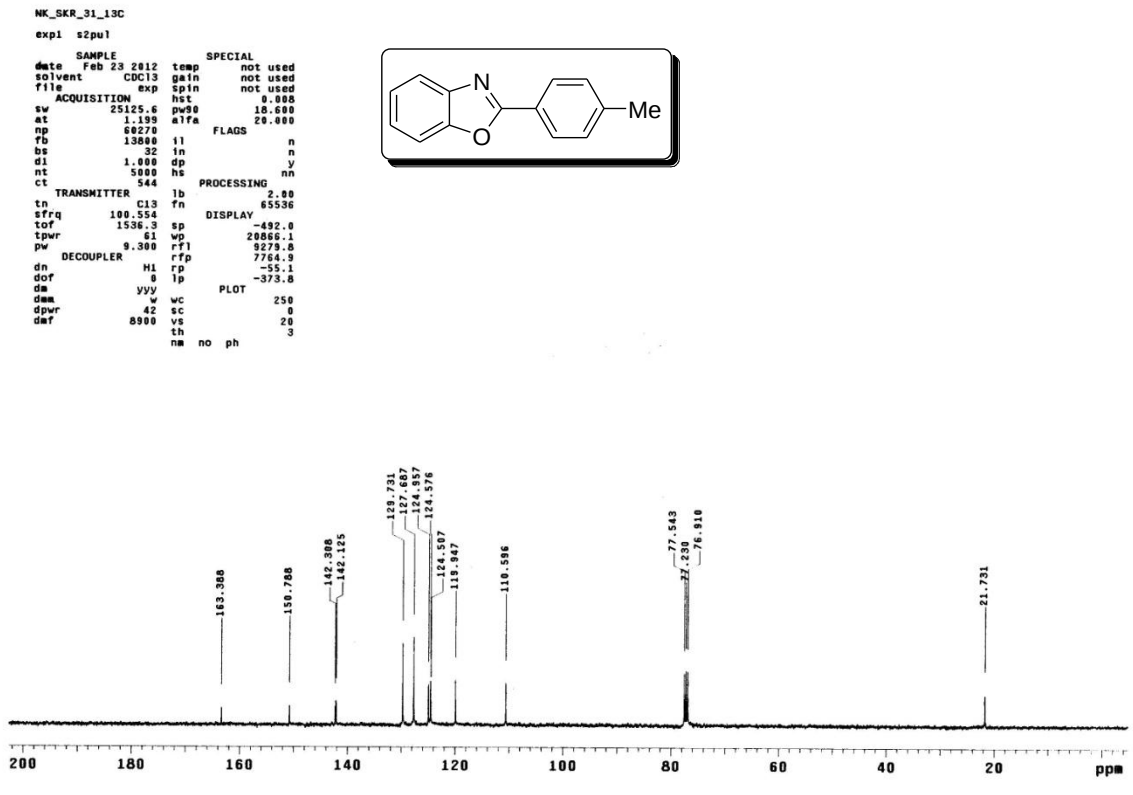




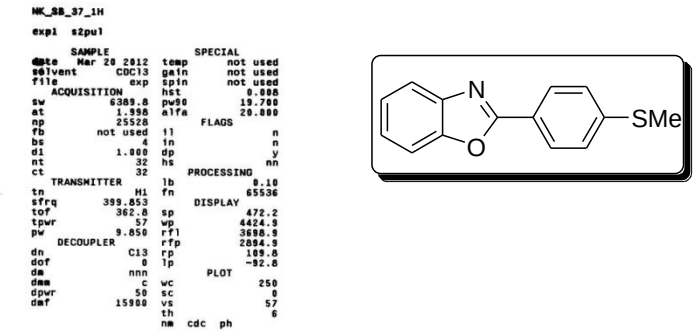
2-p-Tolylbenzo[d]oxazole (6aa): ^{1}H NMR ($CDCl_3$, 400 MHz)

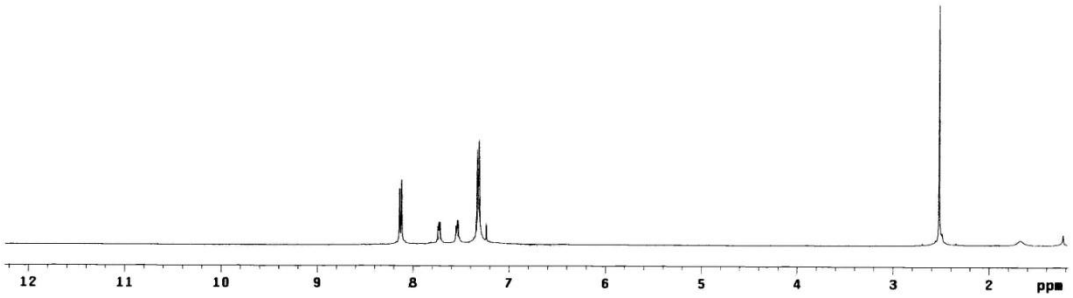


2-p-Tolylbenzo[d]oxazole (6aa): ^{13}C NMR ($CDCl_3$, 100 MHz)

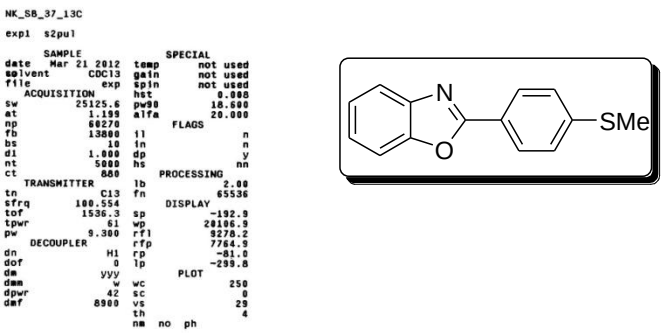


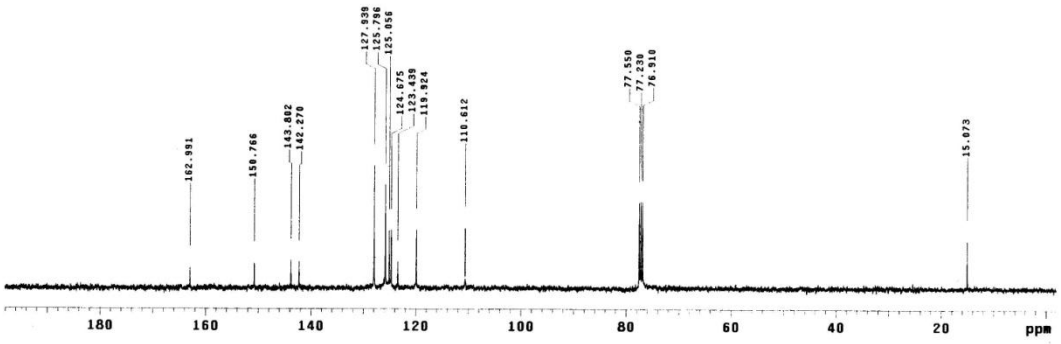
2-(4-(Methylthio)phenyl)benzo[*d*]oxazole (7aa): ^{1}H NMR (CDCl$_3$, 400 MHz)



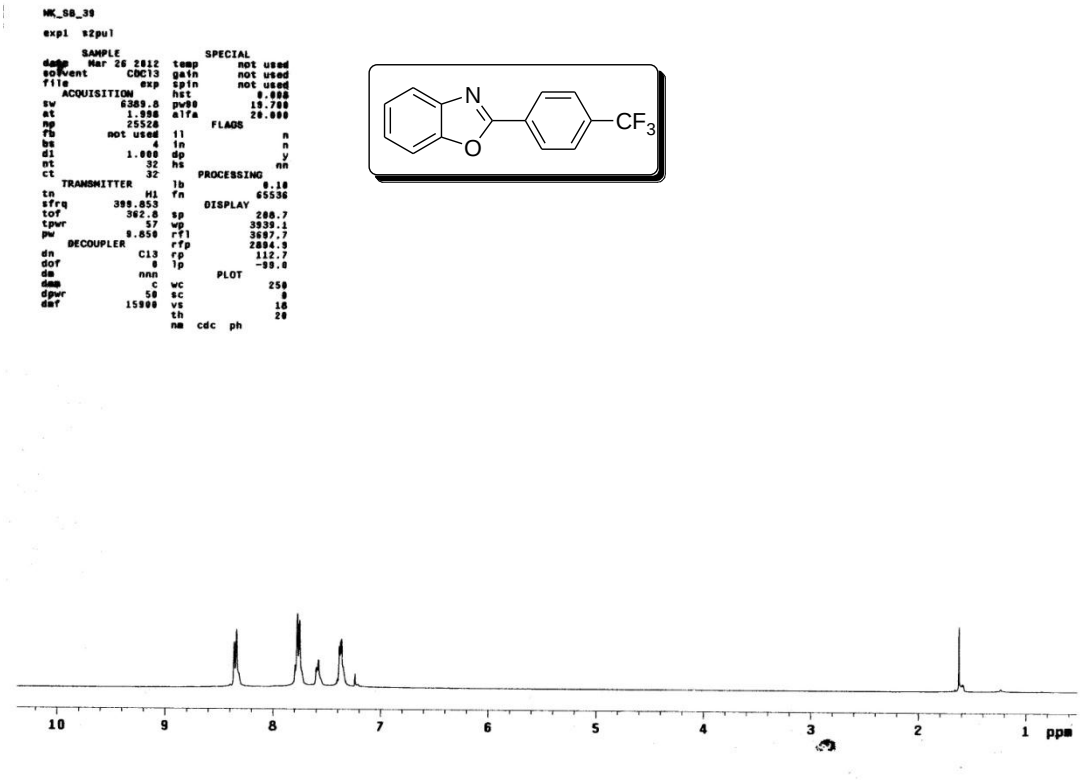


2-(4-(Methylthio)phenyl)benzo[*d*]oxazole (7aa): ^{13}C NMR (CDCl$_3$, 100 MHz)

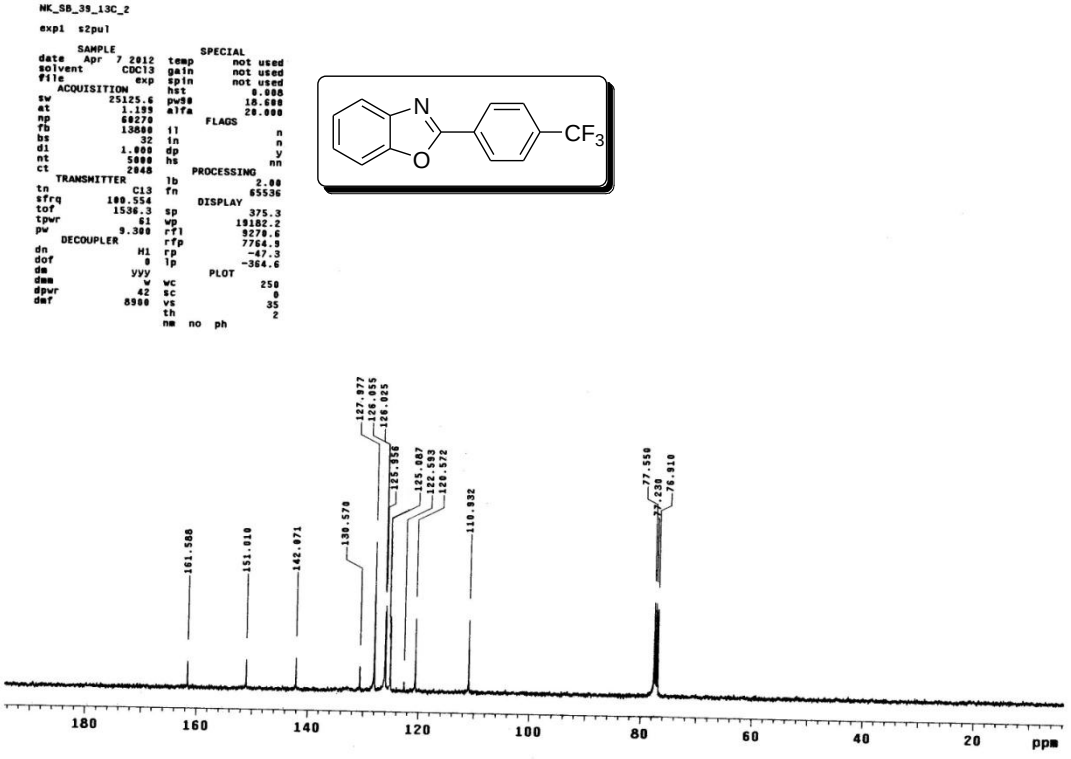




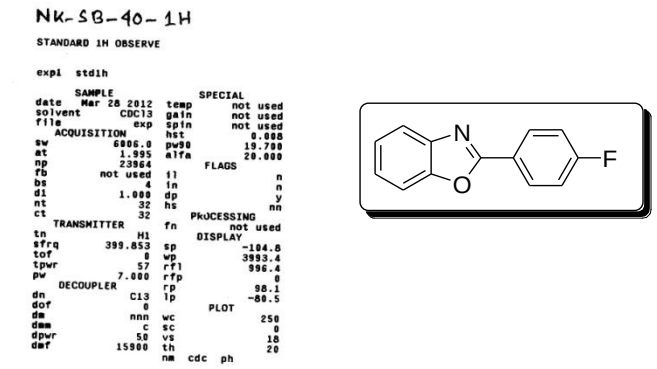
2-(4-(Trifluoromethyl)phenyl)benzo[*d*]oxazole (8aa): ^{1}H NMR ($CDCl_3$, 400 MHz)

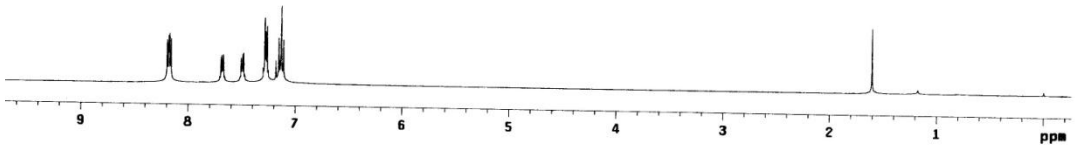


2-(4-(Trifluoromethyl)phenyl)benzo[*d*]oxazole (8aa): ^{13}C NMR ($CDCl_3$, 100 MHz)

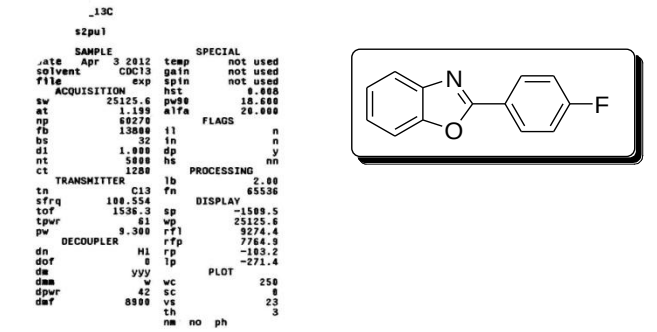


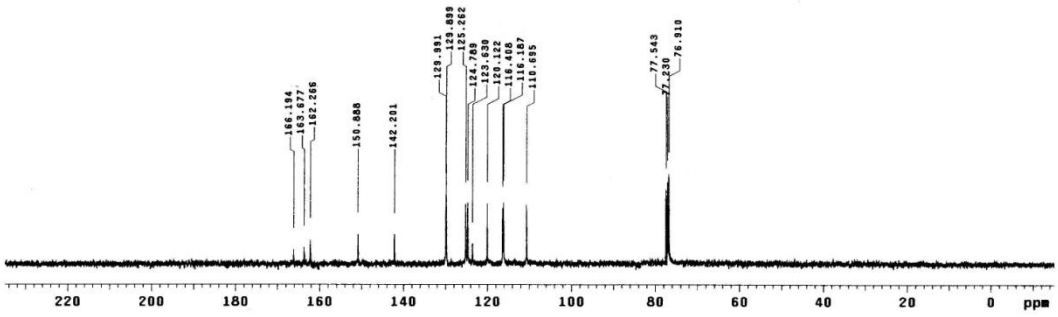
2-(4-Fluorophenyl)benzo[*d*]oxazole (9aa): ^{1}H NMR ($CDCl_3$, 400 MHz)



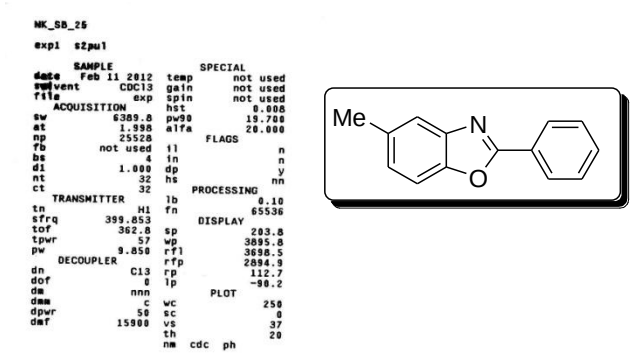


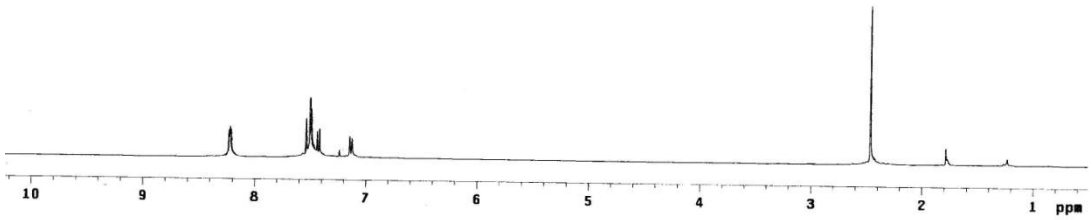
2-(4-Fluorophenyl)benzo[*d*]oxazole (9aa): ^{13}C NMR ($CDCl_3$, 100 MHz)



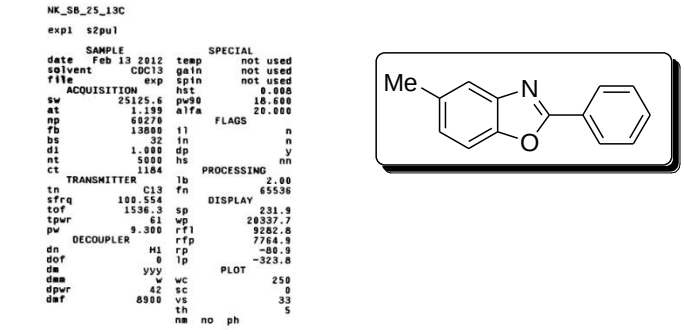


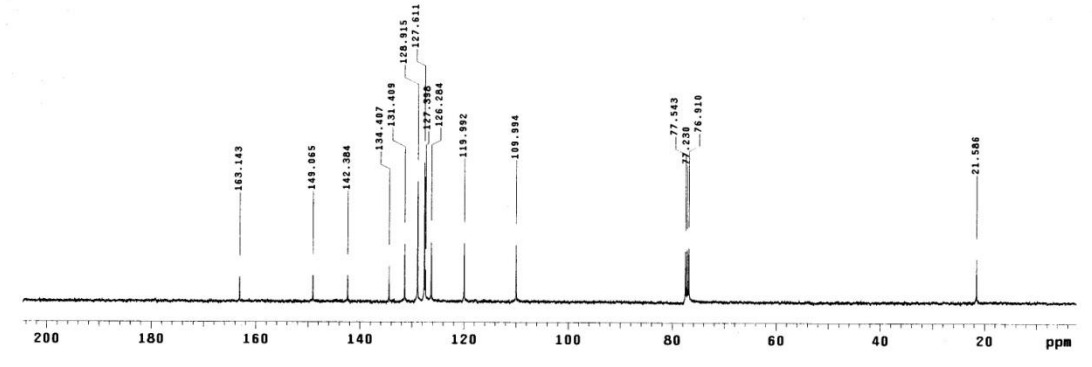
5-Methyl-2-phenylbenzo[*d*]oxazole (10aa): ^{1}H NMR ($CDCl_3$, 400 MHz)



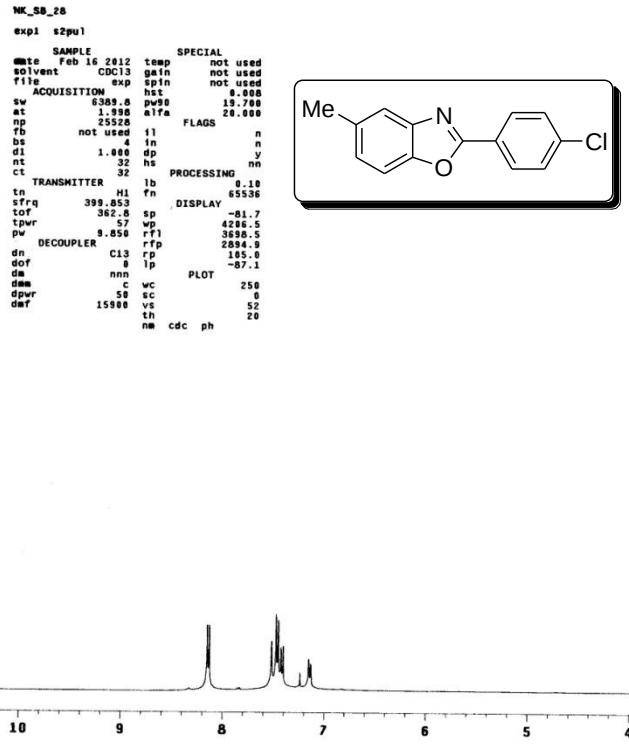


5-Methyl-2-phenylbenzo[*d*]oxazole (10aa): ^{13}C NMR ($CDCl_3$, 100 MHz)

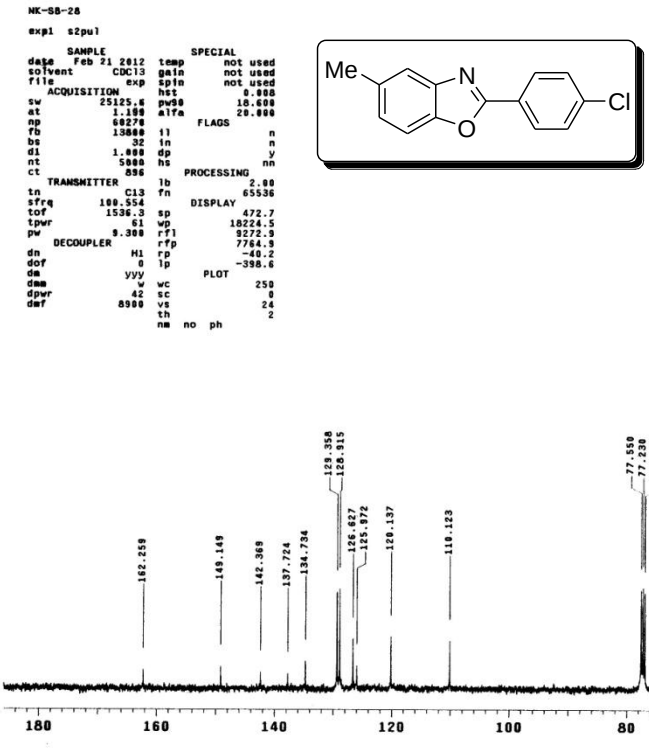




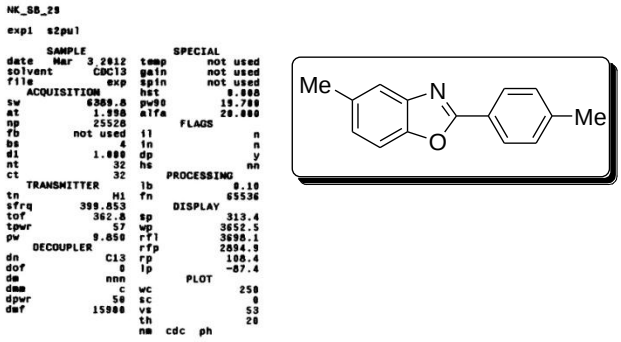
2-(4-Chlorophenyl)-5-methylbenzo[*d*]oxazole (11aa): ^{1}H NMR ($CDCl_3$, 400 MHz)

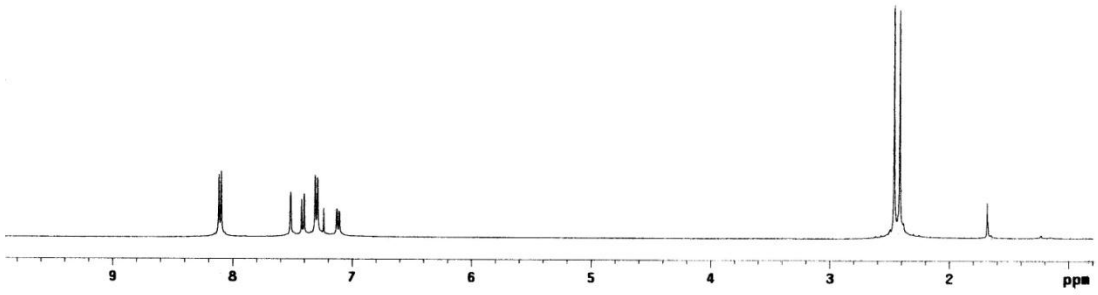


2-(4-Chlorophenyl)-5-methylbenzo[*d*]oxazole (11aa): ^{13}C NMR ($CDCl_3$, 100 MHz)

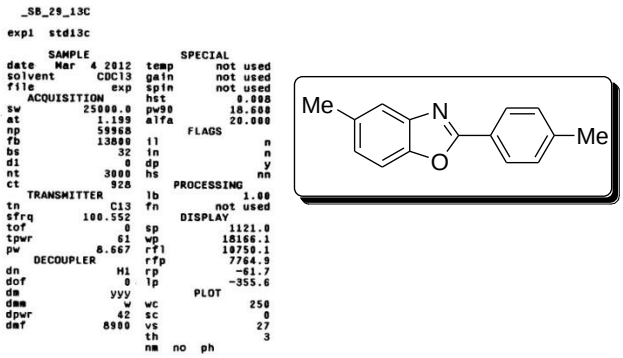


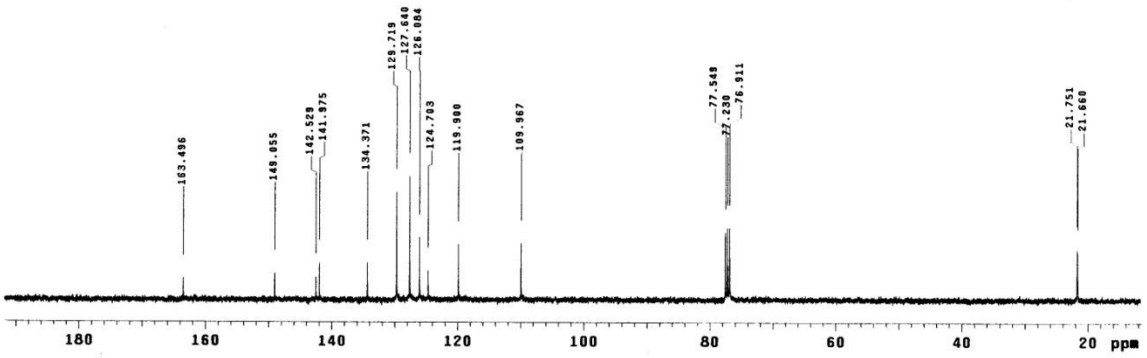
5-Methyl-2-p-tolylbenzo[*d*]oxazole (12aa): ^{1}H NMR ($CDCl_3$, 400 MHz)



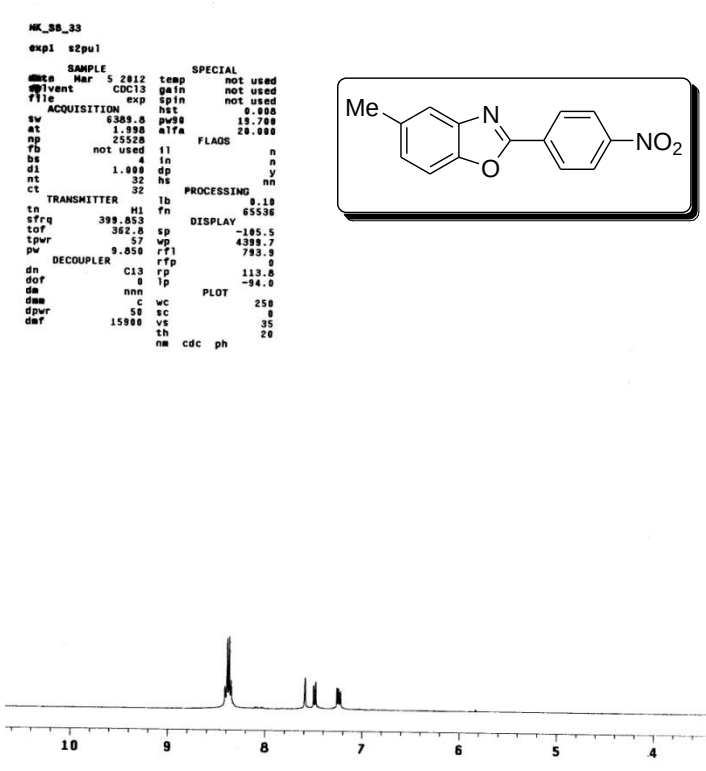


5-Methyl-2-p-tolylbenzo[*d*]oxazole (12aa): ^{13}C NMR ($CDCl_3$, 100 MHz)

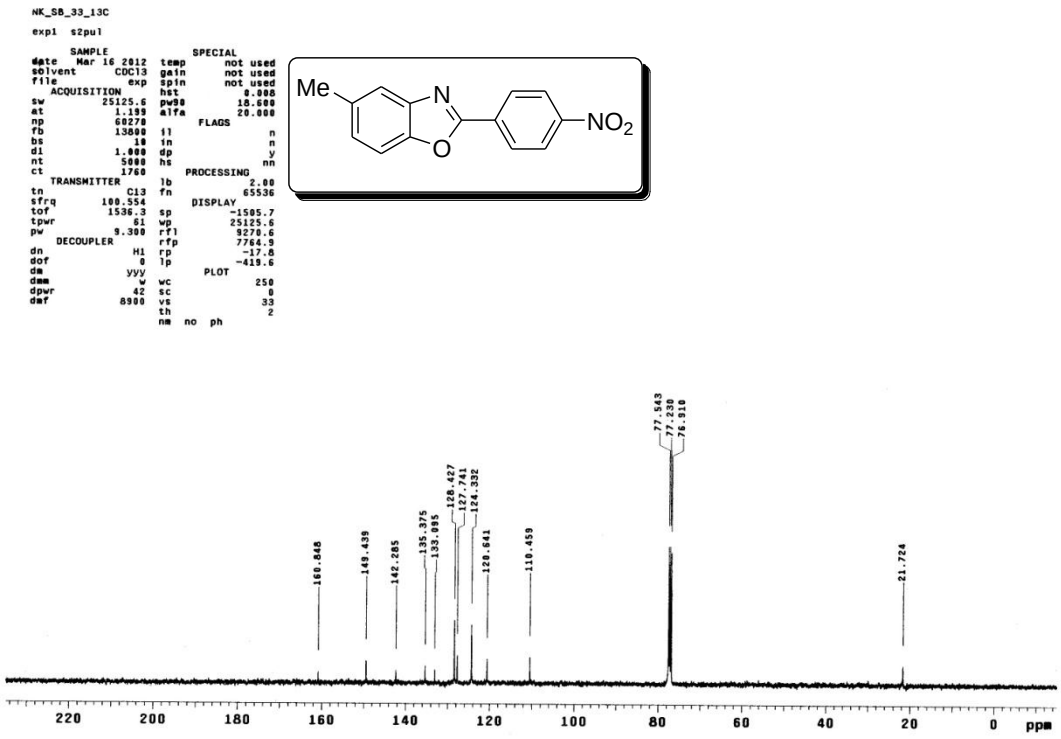




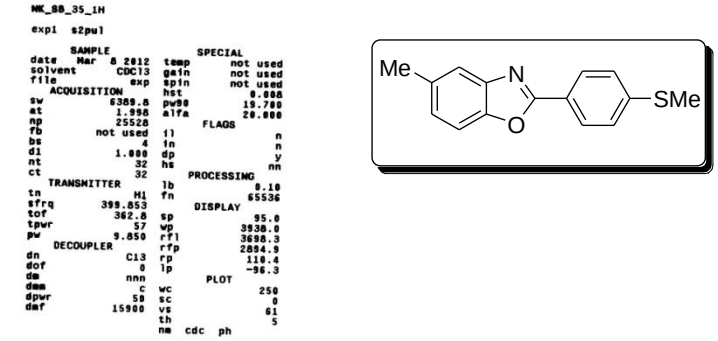
5-Methyl-2-(4-nitrophenyl)benzo[*d*]oxazole (13aa): ^{1}H NMR ($CDCl_3$, 400 MHz)

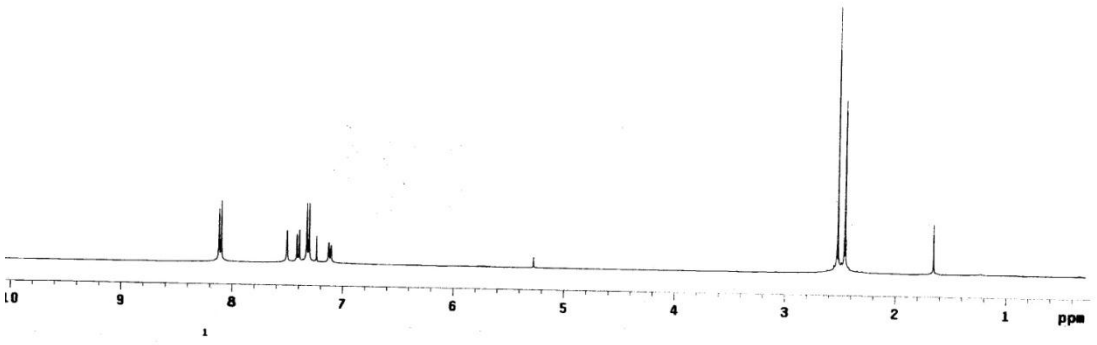


5-Methyl-2-(4-nitrophenyl)benzo[*d*]oxazole (13aa): ^{13}C NMR ($CDCl_3$, 100 MHz)

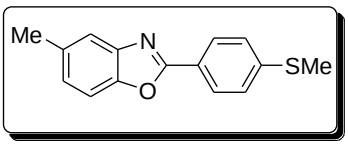


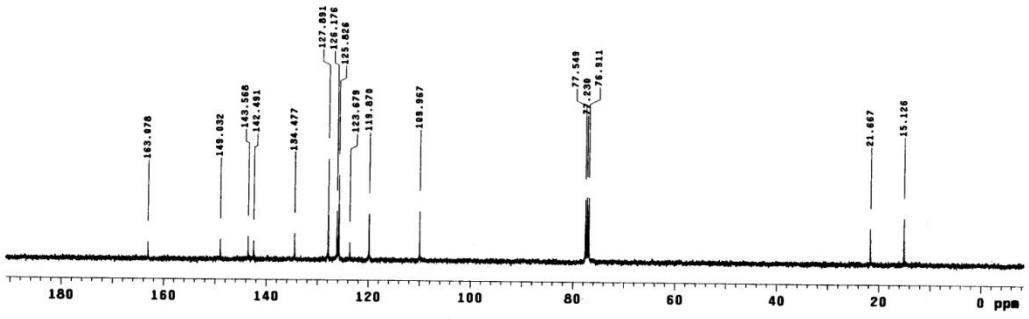
5-Methyl-2-(4-(methylthio)phenyl)benzo[*d*]oxazole (14aa): ^{1}H NMR ($CDCl_3$, 400 MHz)



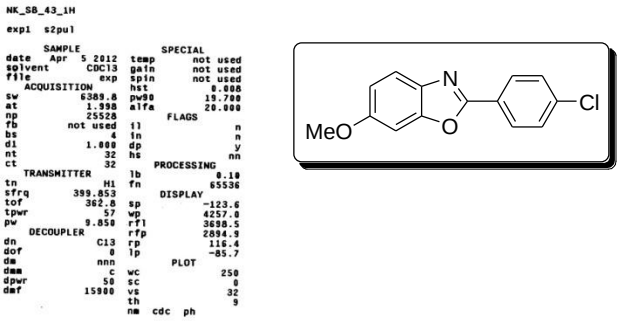


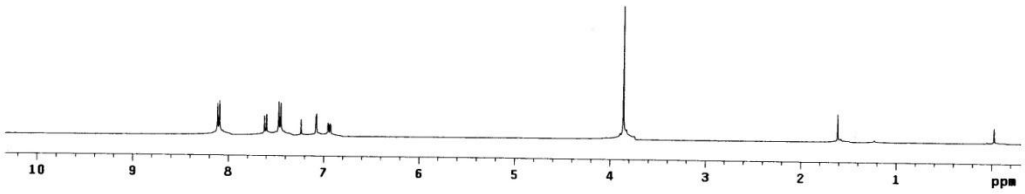
5-Methyl-2-(4-(methylthio)phenyl)benzo[*d*]oxazole (14aa): ^{13}C NMR ($CDCl_3$, 100 MHz)



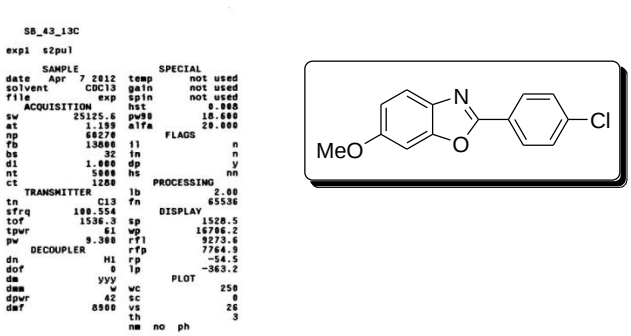


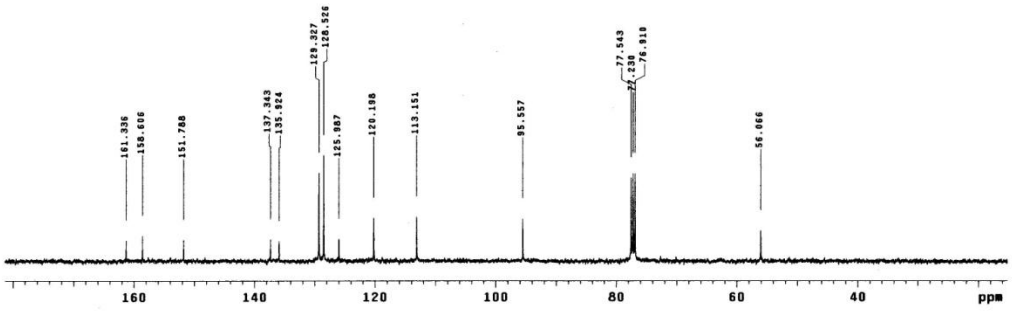
2-(4-Chlorophenyl)-6-methoxybenzo[*d*]oxazole (15aa): ^{1}H NMR ($CDCl_3$, 400 MHz)



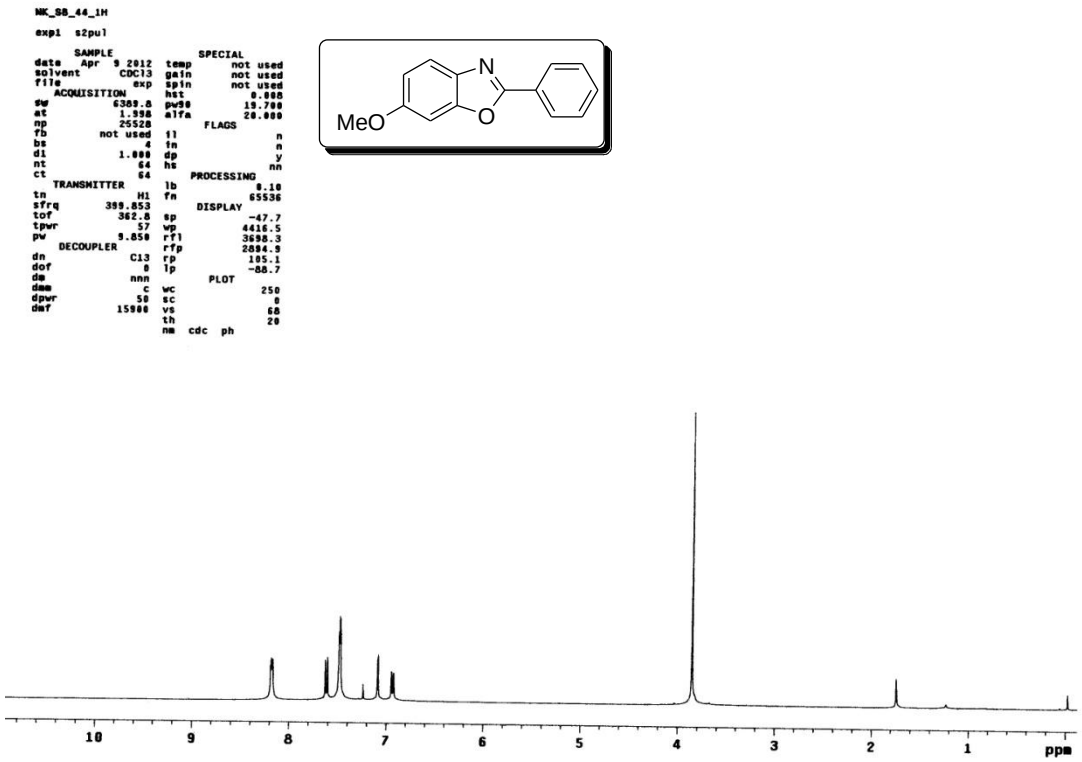


2-(4-Chlorophenyl)-6-methoxybenzo[*d*]oxazole (15aa): ^{13}C NMR ($CDCl_3$, 100 MHz)

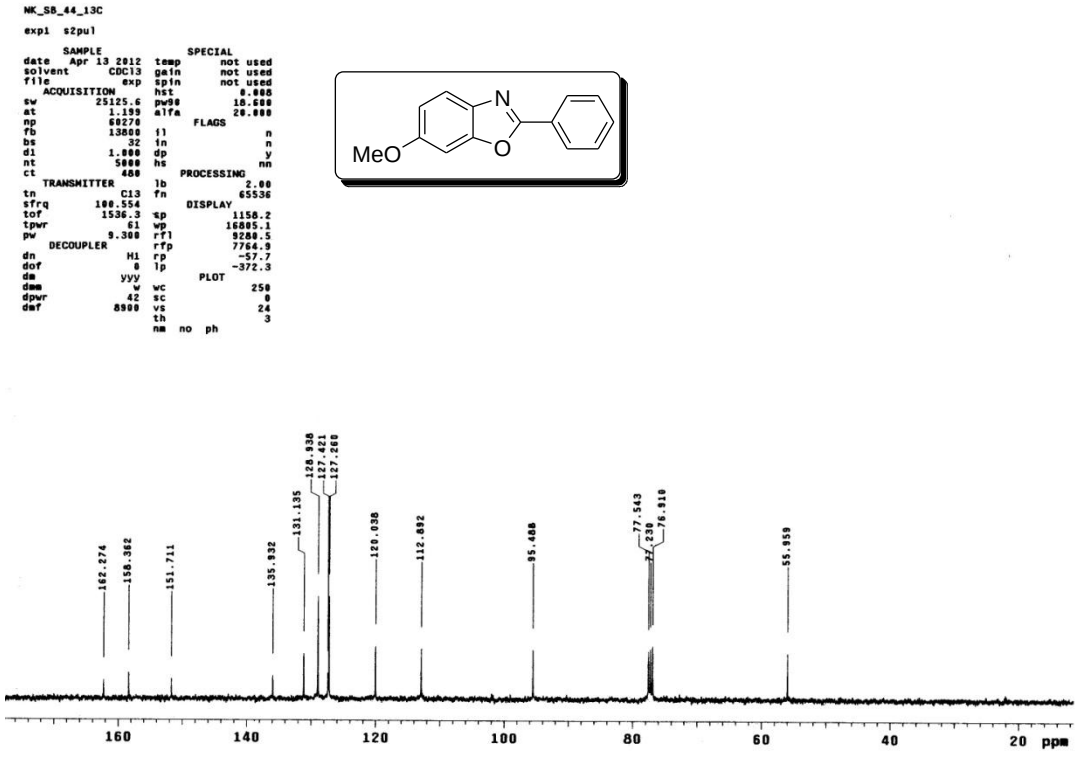




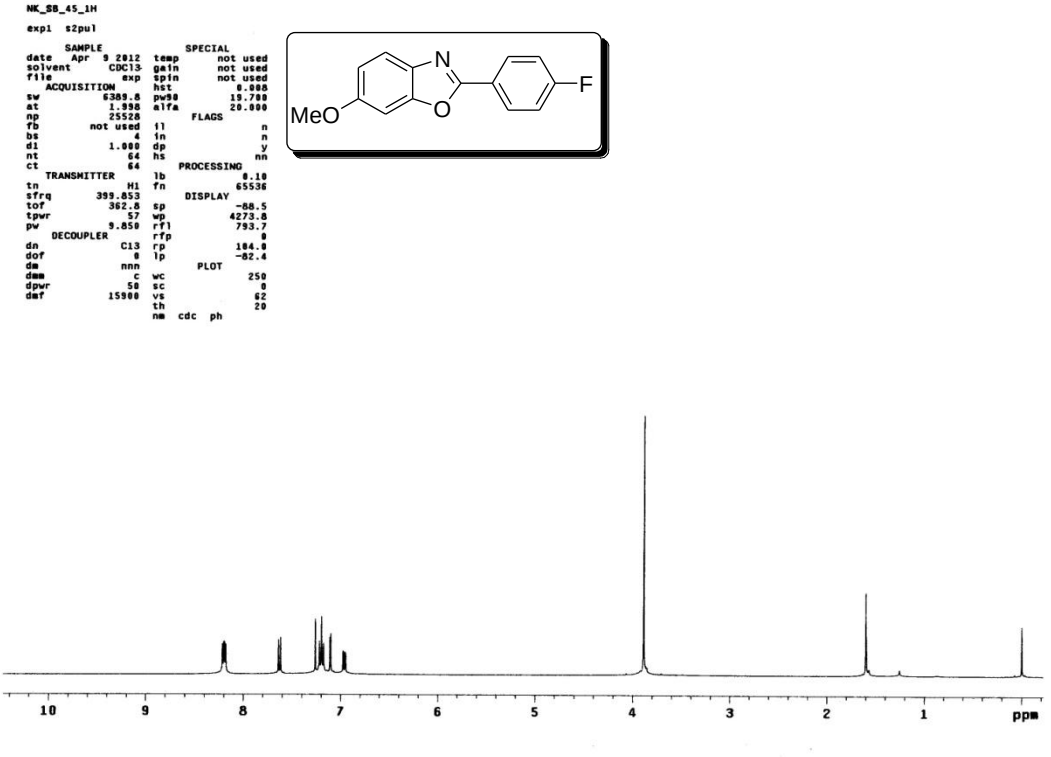
6-Methoxy-2-phenylbenzo[*d*]oxazole (16aa): ^{1}H NMR ($CDCl_3$, 400 MHz)



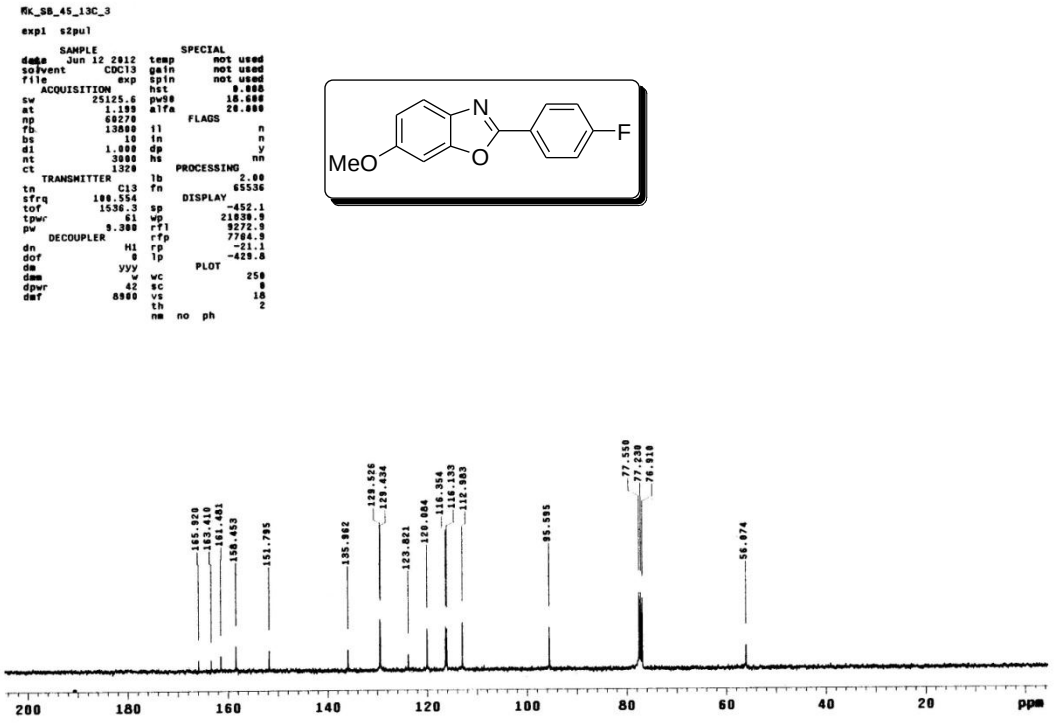
6-Methoxy-2-phenylbenzo[*d*]oxazole (16aa): ^{13}C NMR ($CDCl_3$, 100 MHz)



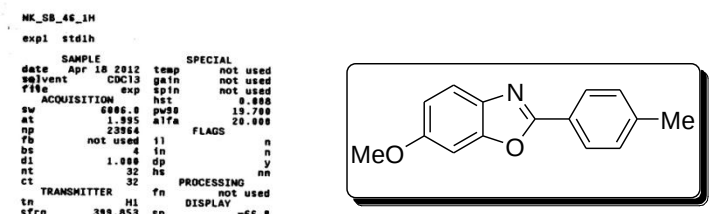
2-(4-Fluorophenyl)-6-methoxybenzo[*d*]oxazole (17aa): ^{1}H NMR ($CDCl_3$, 400 MHz)

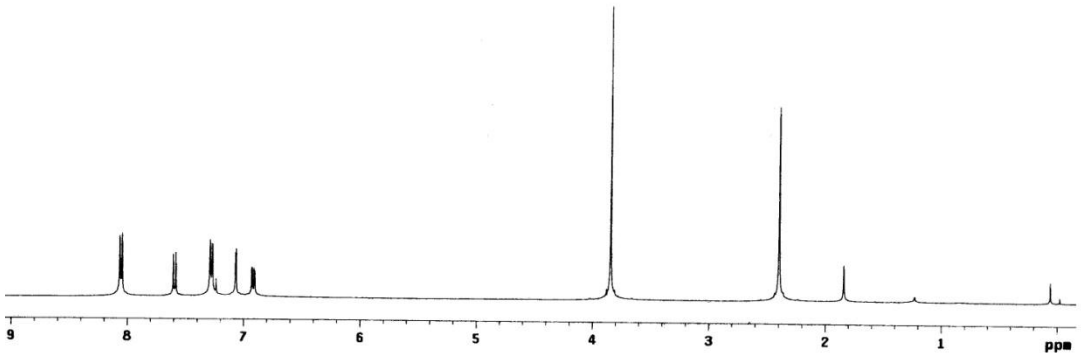


2-(4-Fluorophenyl)-6-methoxybenzo[*d*]oxazole (17aa): ^{13}C NMR ($CDCl_3$, 100 MHz)

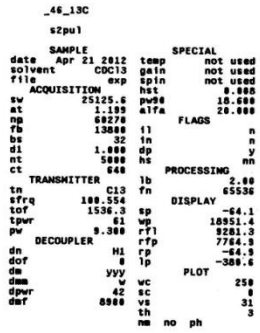


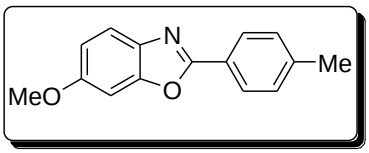
6-Methoxy-2-p-tolylbenzo[*d*]oxazole (18aa): ^{1}H NMR ($CDCl_3$, 400 MHz)

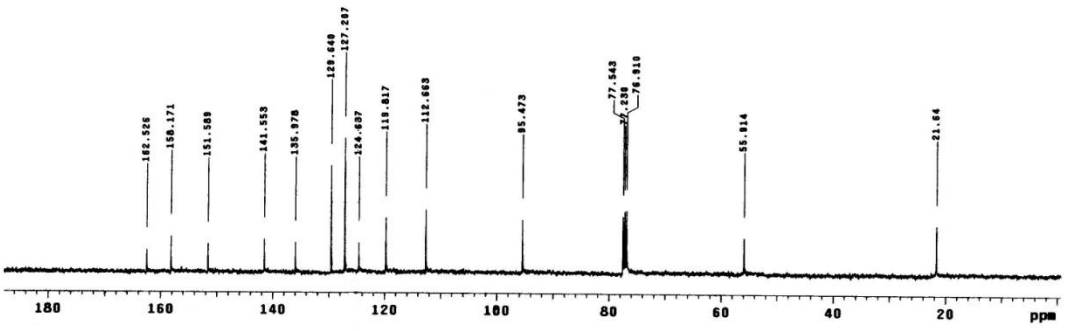




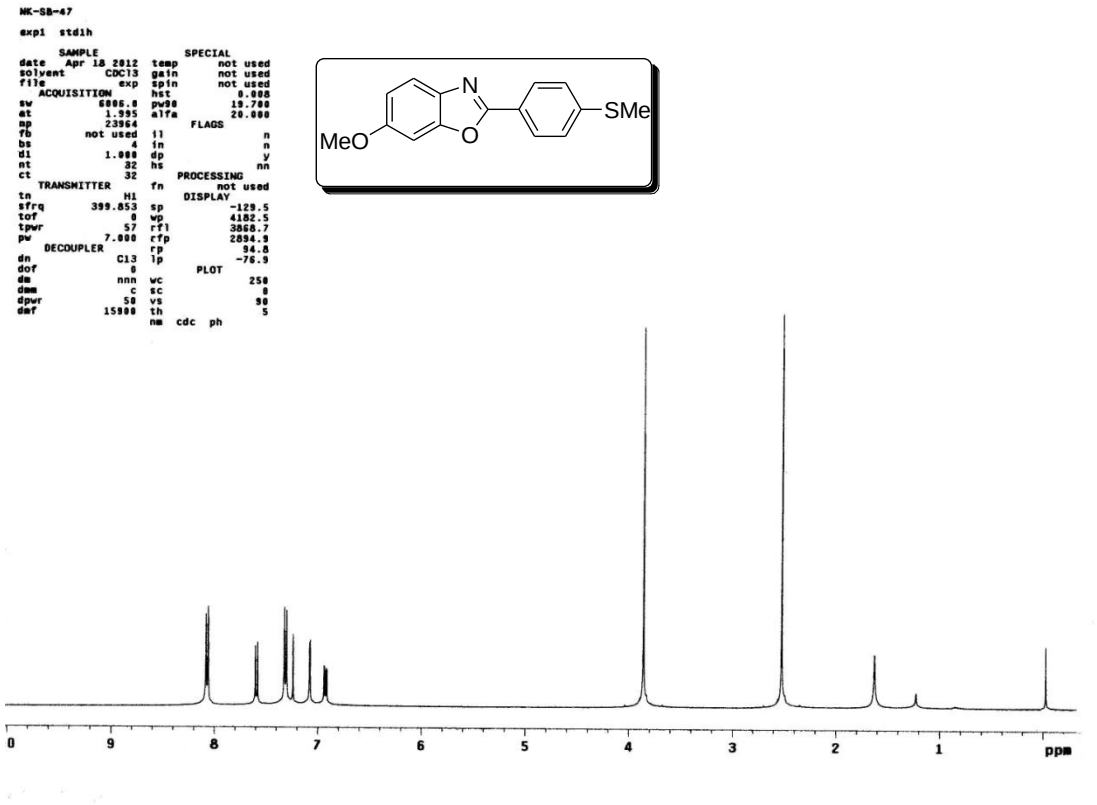
6-Methoxy-2-p-tolylbenzo[*d*]oxazole (18aa): ^{13}C NMR ($CDCl_3$, 100 MHz)



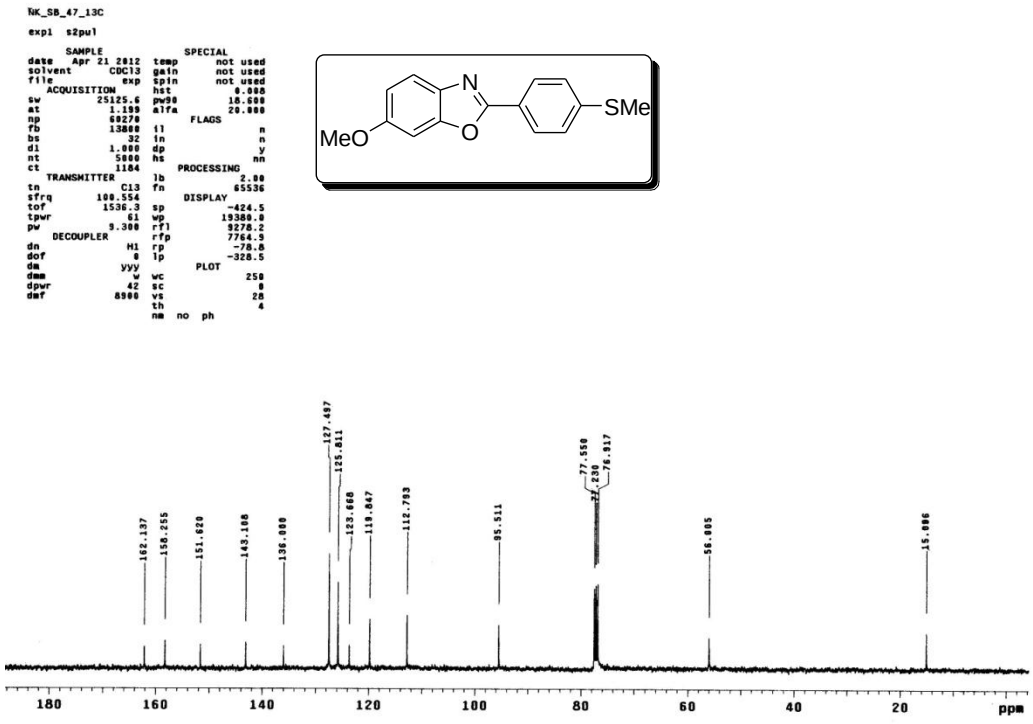




6-Methoxy-2-(4-(methylthio)phenyl)benzo[*d*]oxazole (19aa): ^{1}H NMR ($CDCl_3$, 400 MHz)

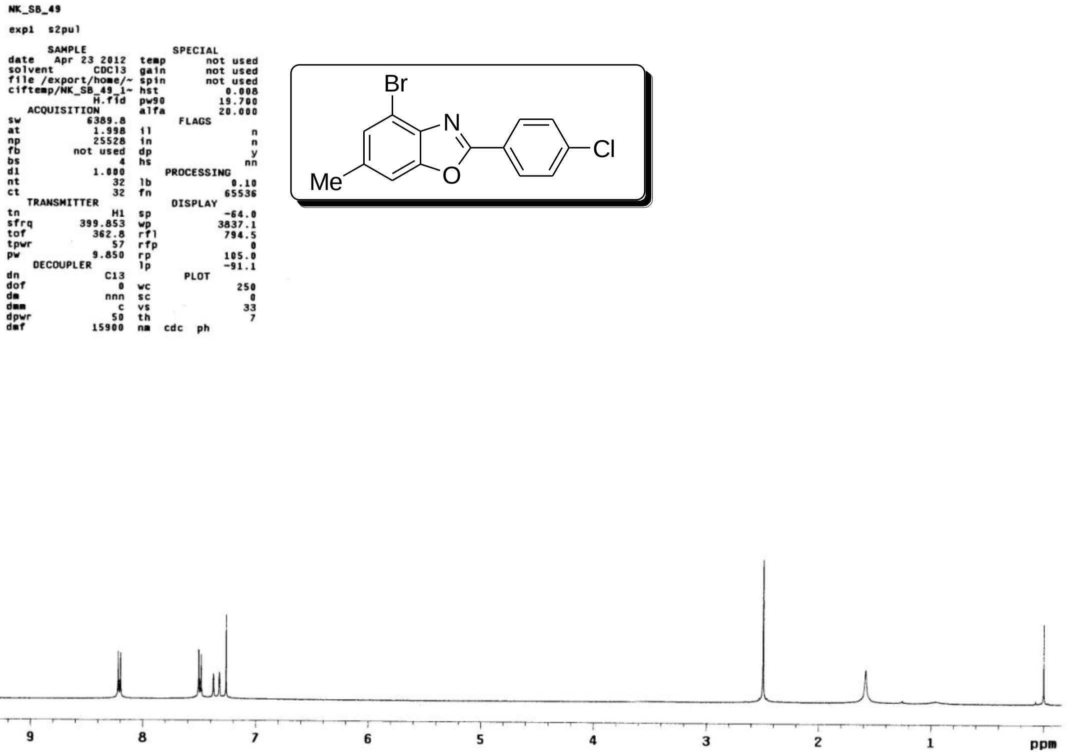


6-Methoxy-2-(4-(methylthio)phenyl)benzo[*d*]oxazole (19aa): ^{13}C NMR ($CDCl_3$, 100 MHz)

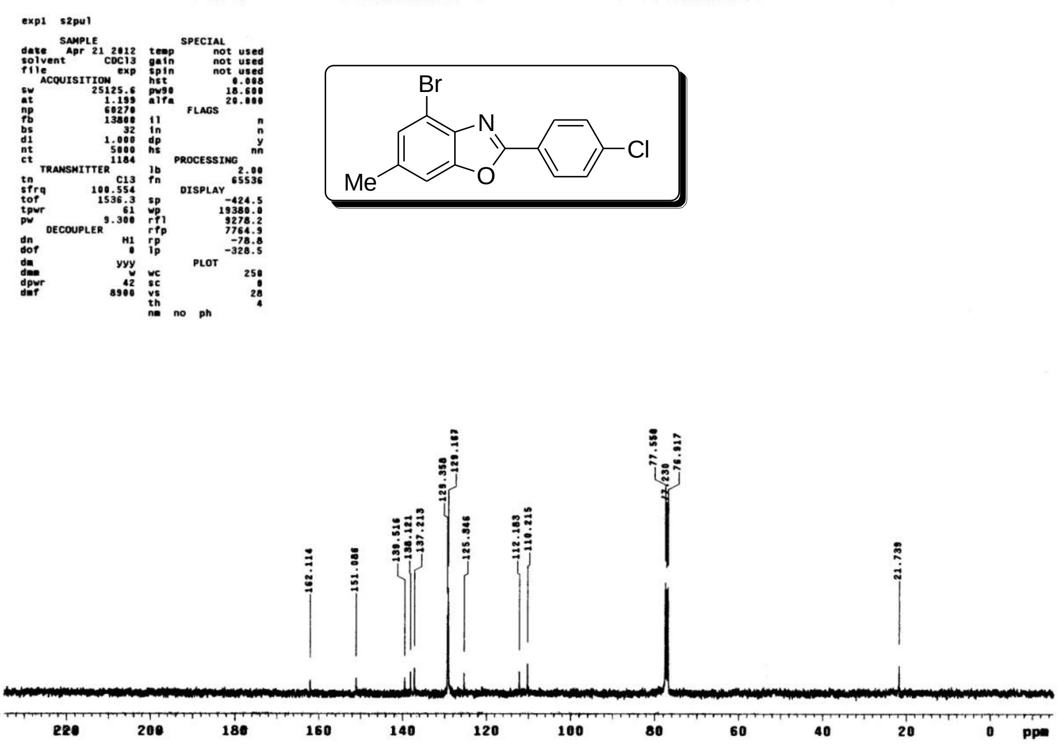


Electronic Supplementary Material (ESI) for RSC Advances

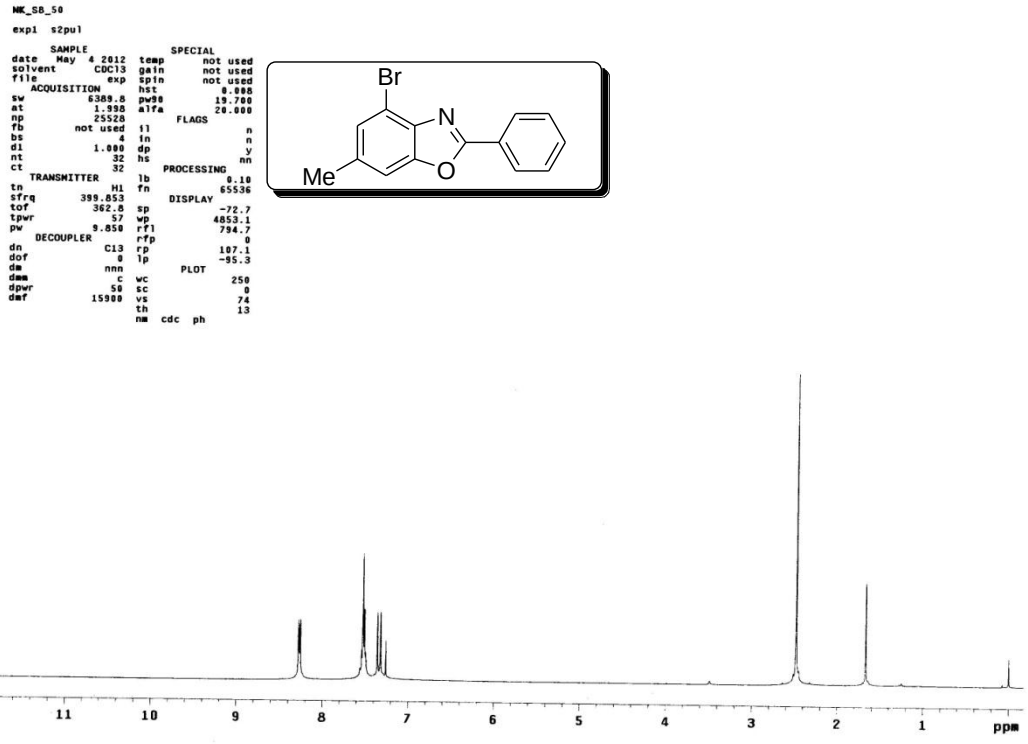
4-Bromo-2-(4-chlorophenyl)-6-methylbenzo[*d*]oxazole (20aa): ^{1}H NMR (CDCl$_3$, 400 MHz)



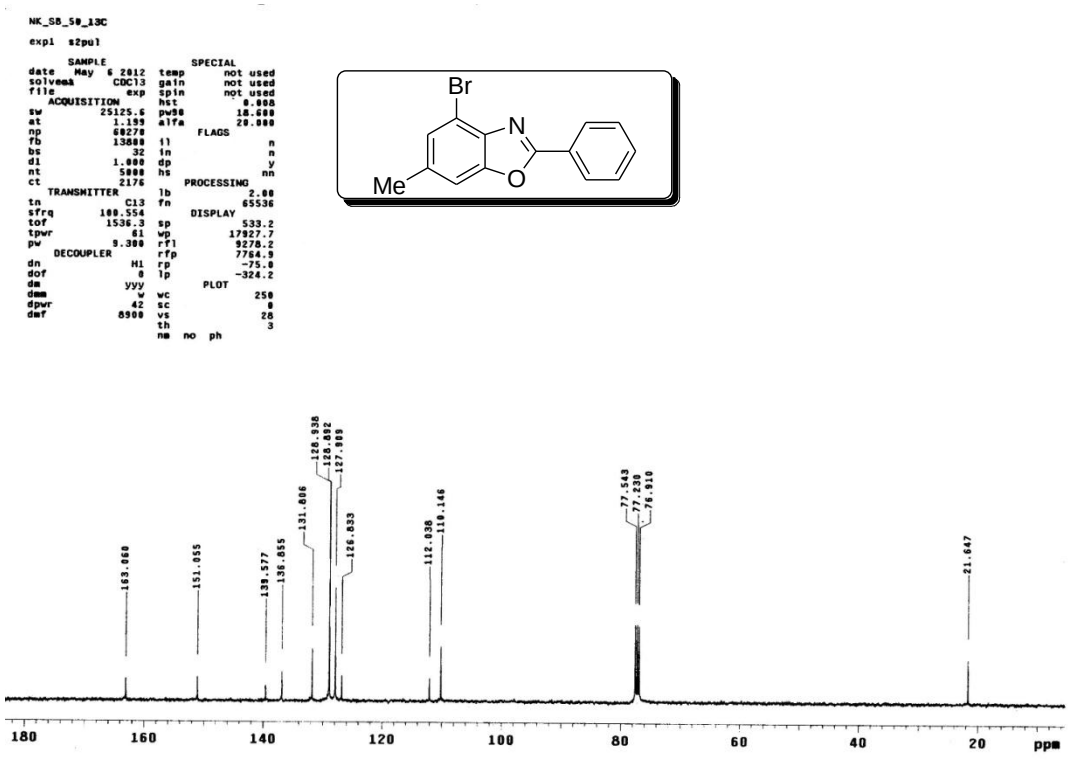
4-Bromo-2-(4-chlorophenyl)-6-methylbenzo[*d*]oxazole (20aa): ^{13}C NMR (CDCl$_3$, 100 MHz)



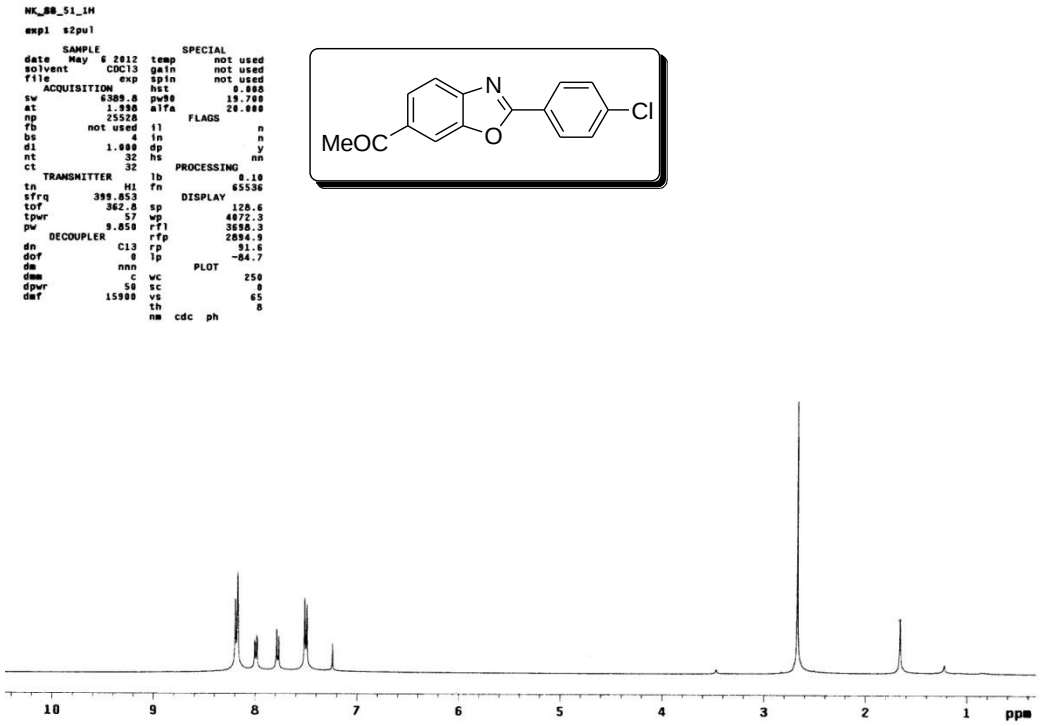
4-Bromo-6-methyl-2-phenylbenzo[*d*]oxazole (21aa): ^{1}H NMR ($CDCl_3$, 400 MHz)



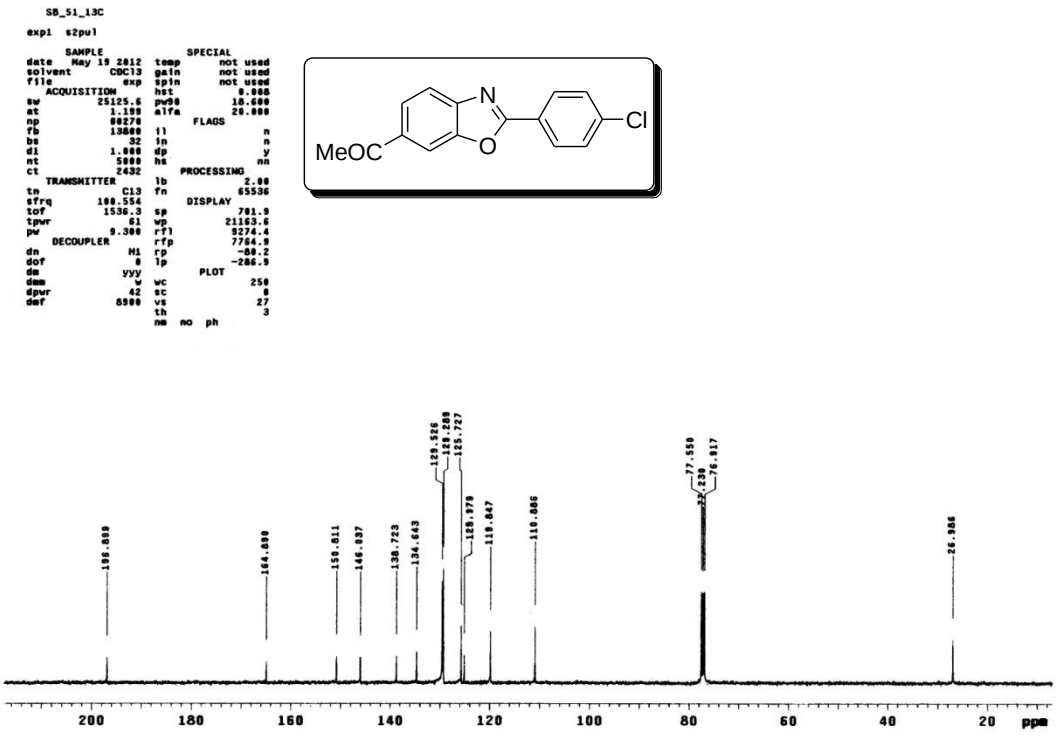
4-Bromo-6-methyl-2-phenylbenzo[*d*]oxazole (21aa): ^{13}C NMR: ($CDCl_3$, 100 MHz)



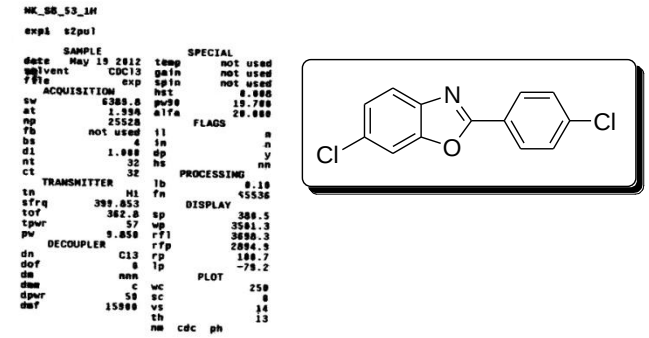
1-(2-(4-Chlorophenyl)benzo[*d*]oxazol-6-yl)ethanone (22aa): ^{1}H NMR ($CDCl_3$, 400 MHz)

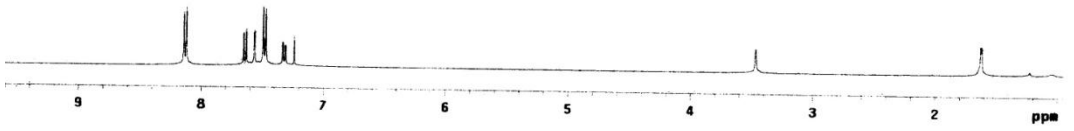


1-(2-(4-Chlorophenyl)benzo[*d*]oxazol-6-yl)ethanone (22aa): ^{13}C NMR ($CDCl_3$, 100 MHz)

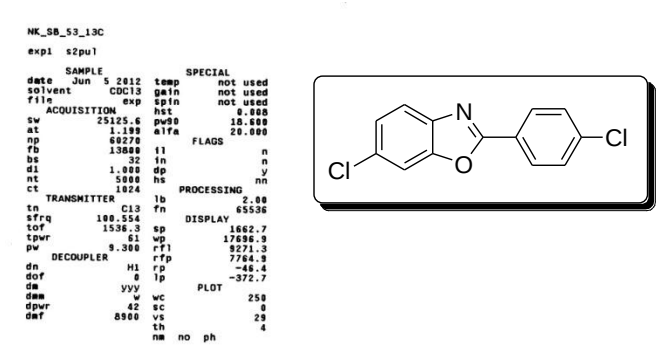


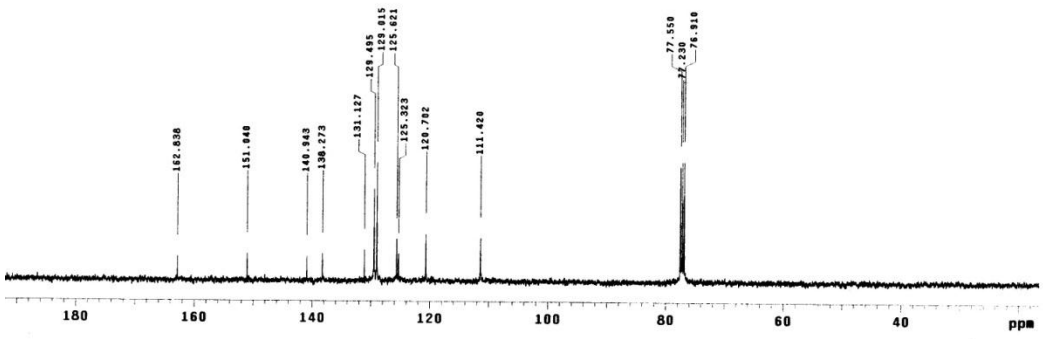
6-Chloro-2-(4-chlorophenyl)benzo[*d*]oxazole (23aa): ^{1}H NMR ($CDCl_3$, 400 MHz)



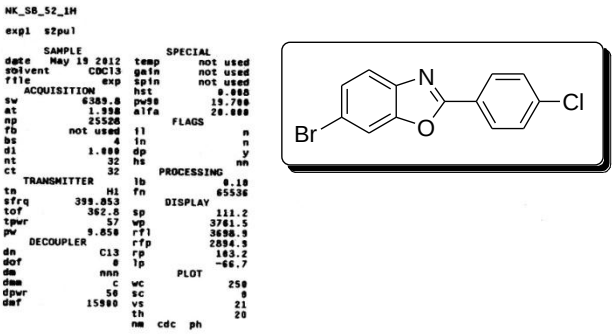


6-Chloro-2-(4-chlorophenyl)benzo[*d*]oxazole (23aa): ^{13}C NMR ($CDCl_3$, 100 MHz)

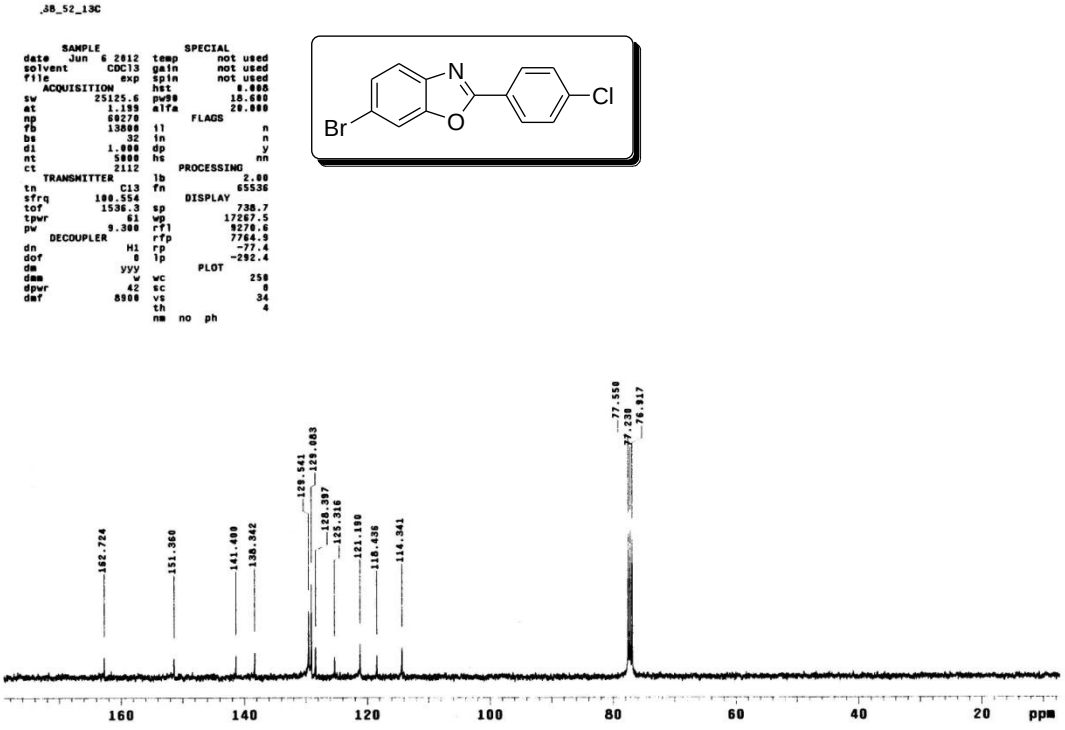




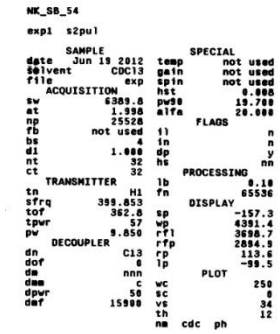
6-Bromo-2-(4-chlorophenyl)benzo[*d*]oxazole (24aa): ^{1}H NMR ($CDCl_3$, 400 MHz)

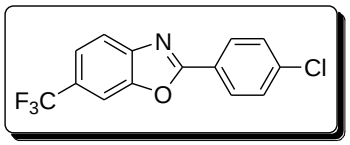


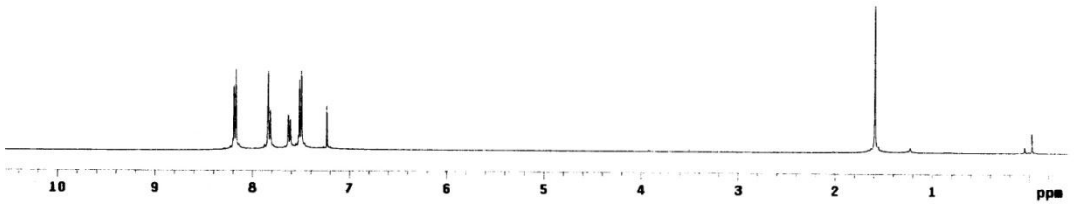
6-Bromo-2-(4-chlorophenyl)benzo[*d*]oxazole (24aa): ^{13}C NMR ($CDCl_3$, 100 MHz)



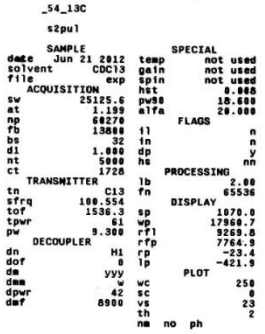
2-(4-Chlorophenyl)-6-(trifluoromethyl)benzo[*d*]oxazole (25aa): ^{1}H NMR ($CDCl_3$, 400 MHz)

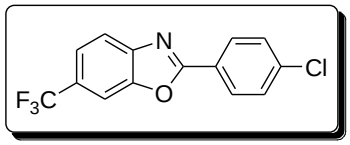


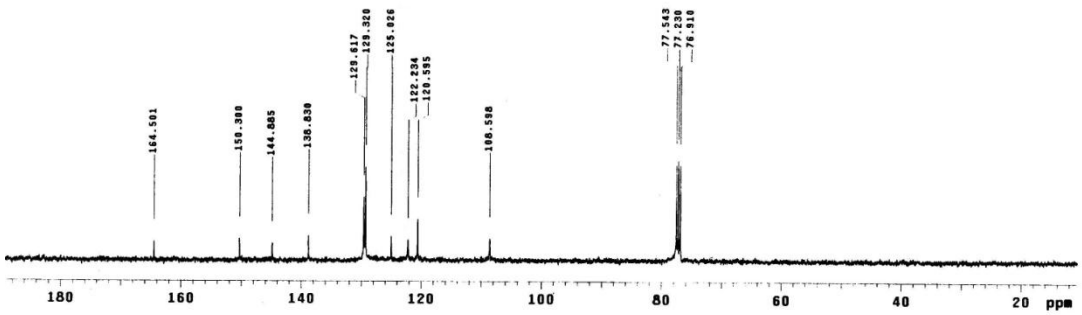




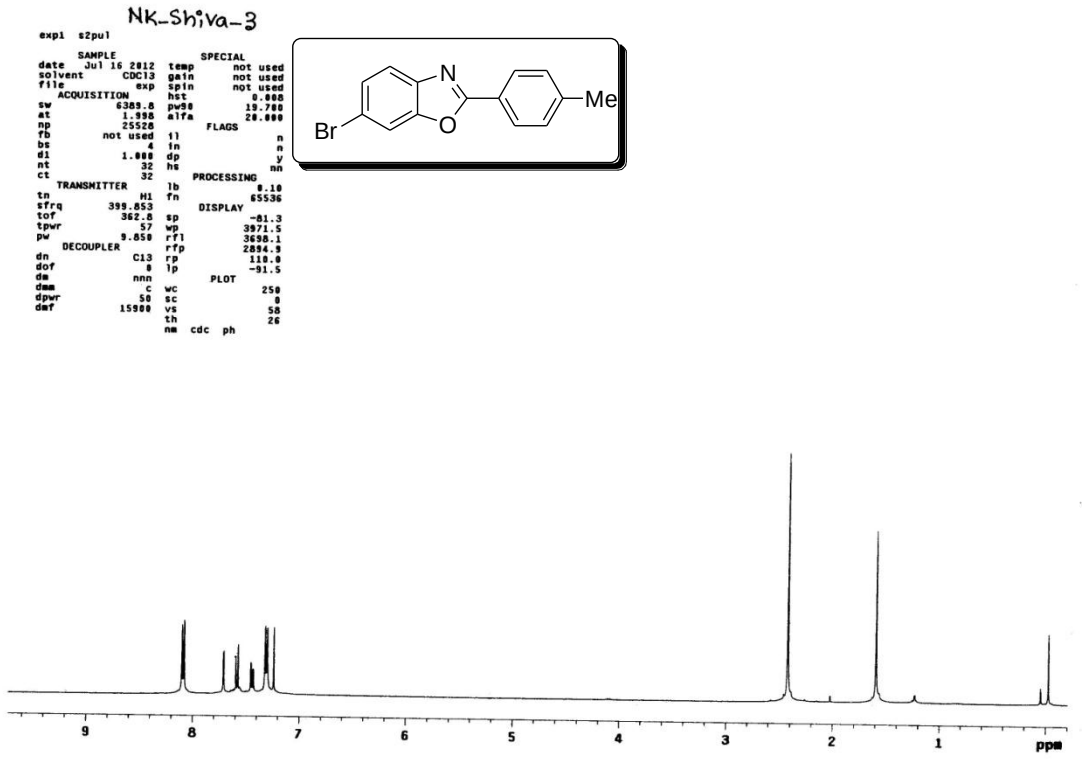
2-(4-Chlorophenyl)-6-(trifluoromethyl)benzo[*d*]oxazole (25aa): ^{13}C NMR ($CDCl_3$, 100 MHz)



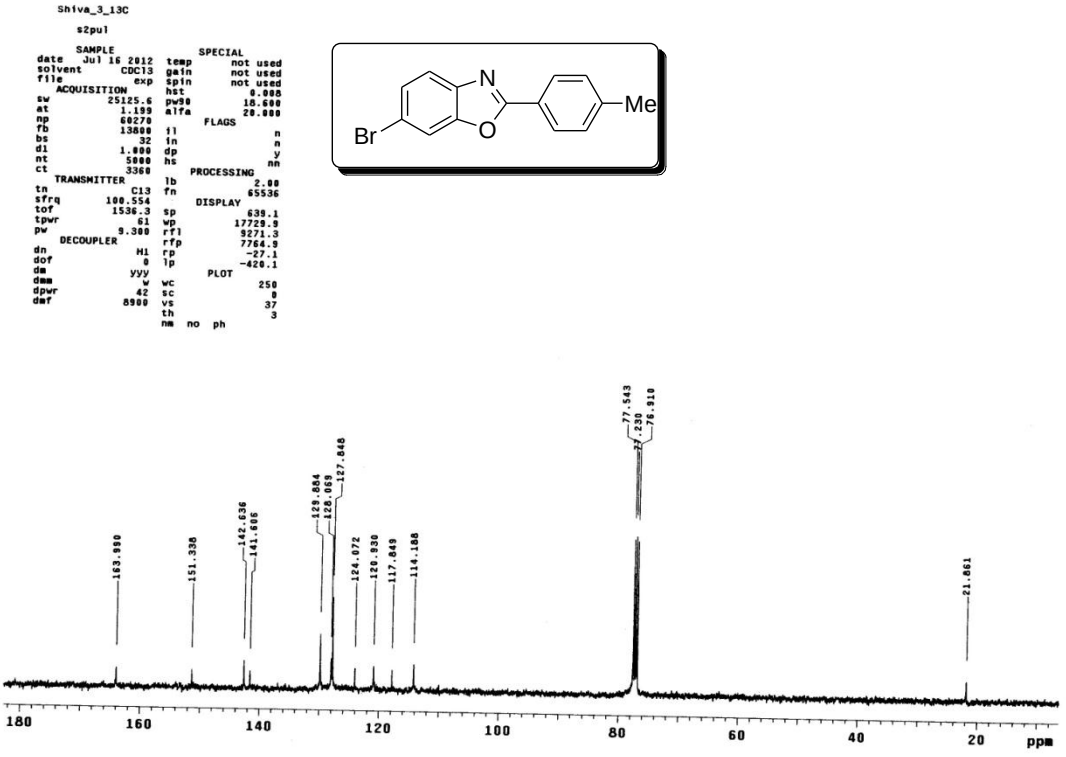




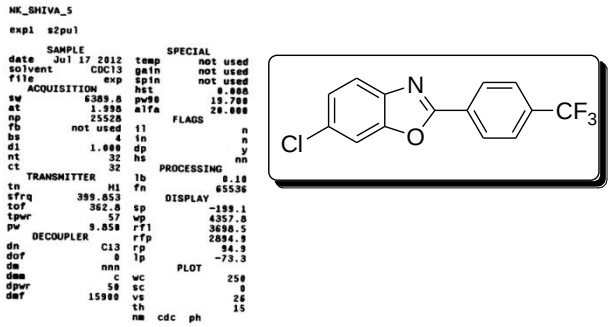
6-Bromo-2-p-tolylbenzo[d]oxazole (26aa): ^{1}H NMR ($CDCl_3$, 400 MHz)

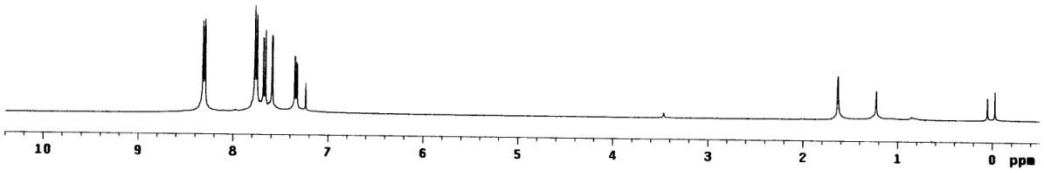


6-Bromo-2-p-tolylbenzo[d]oxazole (26aa): ^{13}C NMR ($CDCl_3$, 100 MHz)

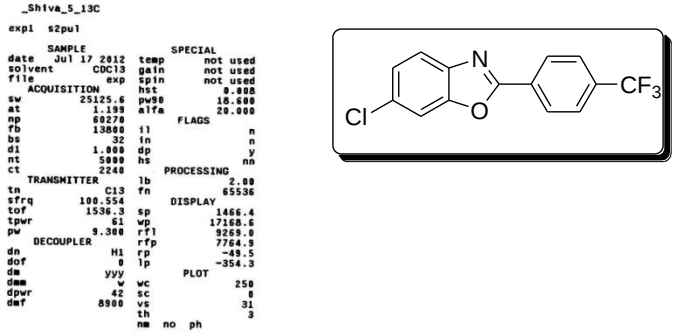


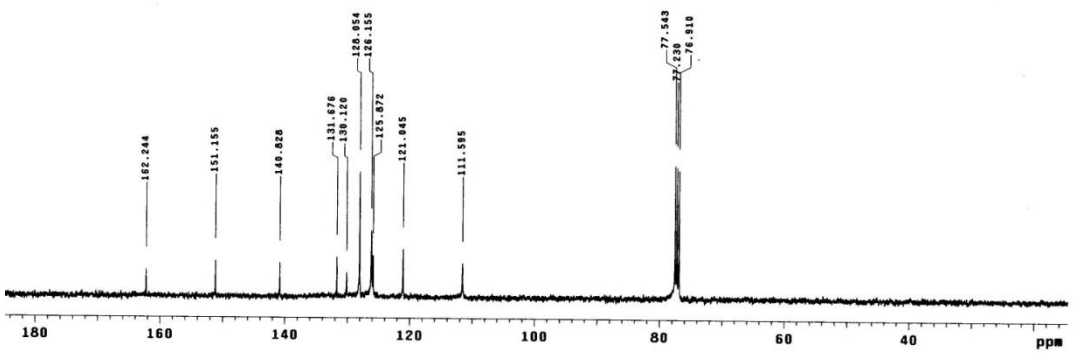
6-Chloro-2-(4-(trifluoromethyl)phenyl)benzo[d]oxazole (27aa): ^{1}H NMR ($CDCl_3$, 400 MHz)



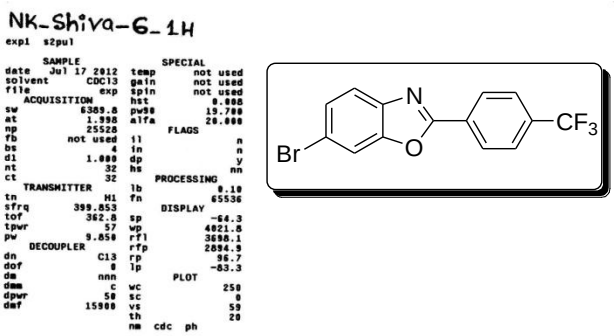


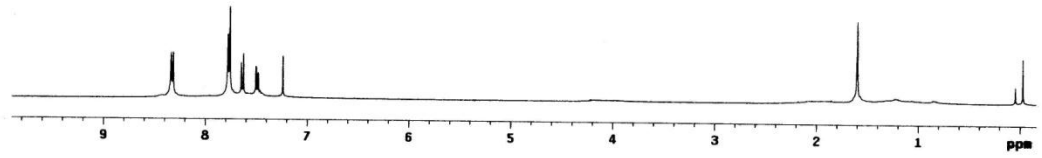
6-Chloro-2-(4-(trifluoromethyl)phenyl)benzo[d]oxazole (27aa): ^{13}C NMR ($CDCl_3$, 100 MHz)



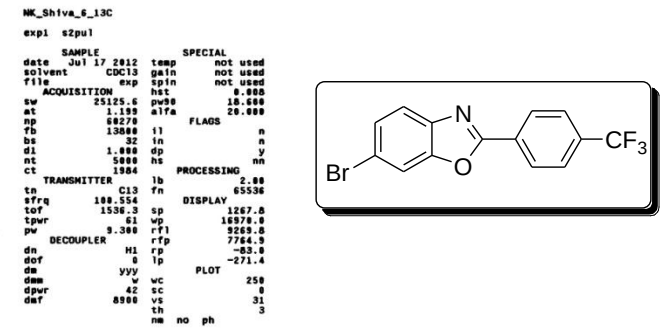


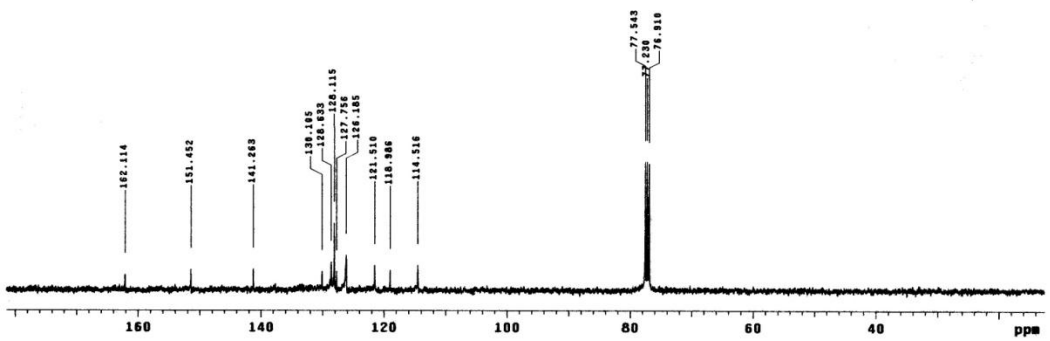
6-Bromo-2-(4-(trifluoromethyl)phenyl)benzo[d]oxazole (28aa): ^{1}H NMR ($CDCl_3$, 400 MHz)



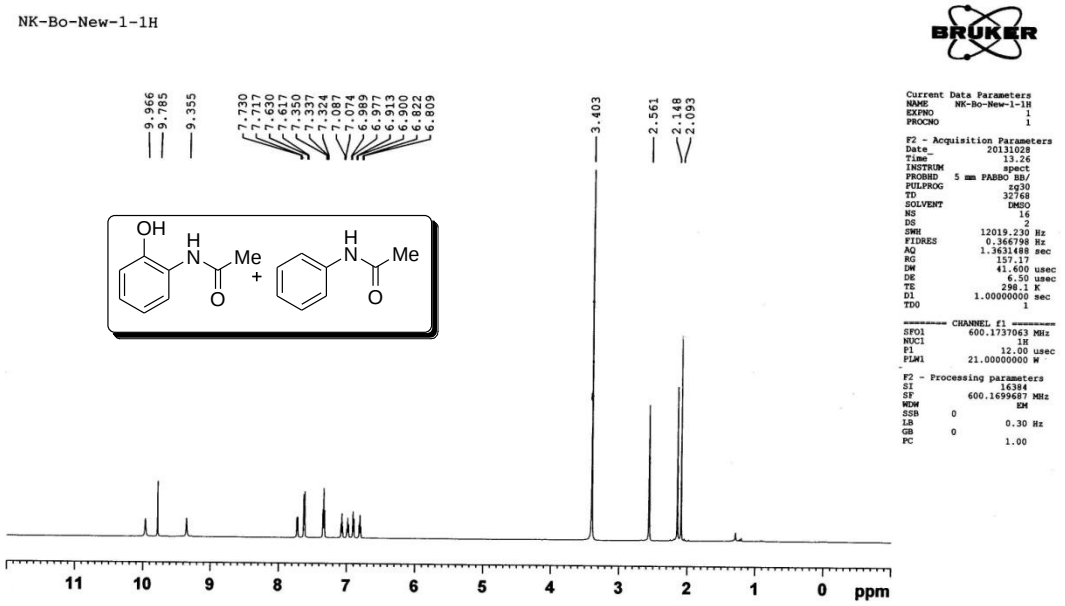


6-Bromo-2-(4-(trifluoromethyl)phenyl)benzo[d]oxazole (28aa): ^{13}C NMR ($CDCl_3$, 100 MHz)

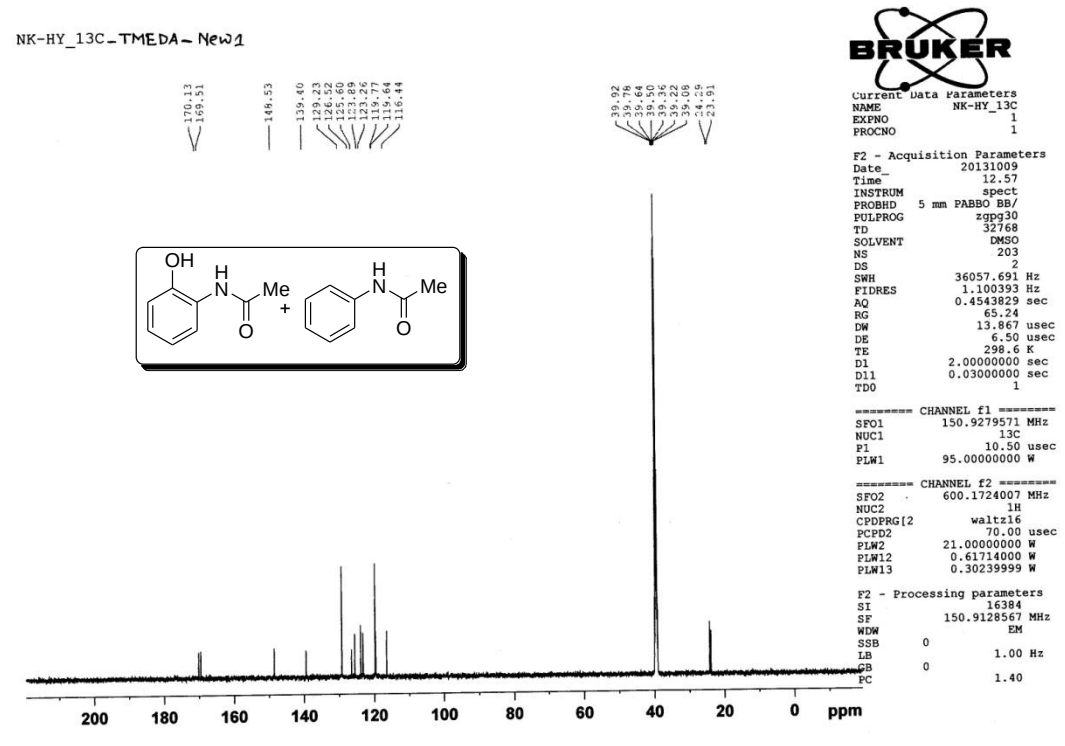




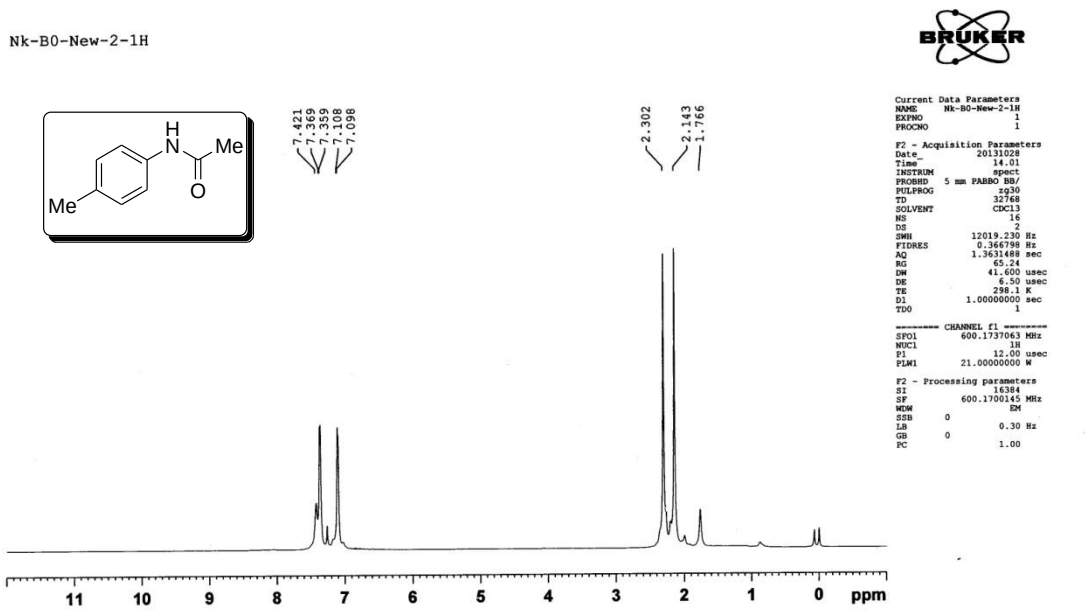
Mixture of *N*-(2-Hydroxyphenyl)acetamide (1a′) and N-phenylacetamide (1a″): ^{1}H NMR (DMSO-d_6, 600 MHz)



Mixture of *N*-(2-Hydroxyphenyl)acetamide (1a′) and N-phenylacetamide (1a″): ^{13}C NMR (DMSO-d_6, 150 MHz)



N-*p*-Tolylacetamide (2a′′): ^{1}H NMR ($CDCl_3$, 600 MHz)



N-*p*-Tolylacetamide (2a′′): ^{13}C NMR ($CDCl_3$, 150 MHz)