

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 F₂₅₄ (0.25mm) with detection by UV or iodine. Chromatography was performed using Merck silica gel (60-120) mesh size with freshly distilled solvents. Columns were typically packed as slurry and equilibrated with the appropriate solvent system prior to use. ¹H NMR (400 MHz and 600 MHz) and ¹³C 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 ($\lambda = 0.71073 \text{ \AA}$) at 298 K. Cell parameters were retrieved using SMART ¹USA, 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 program³ 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 Chemie der Universitat, Tammanstrasse 4, D-3400 Gottingen, Germany, 1999–2003.
- 3 G. M. Sheldrick, SHELXS-97, University of Gottingen, Germany, 1997.

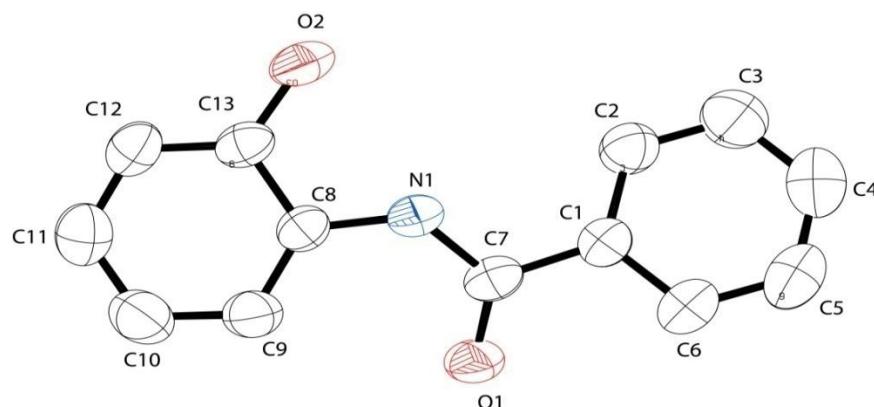


Figure 1. ORTEP views of *N*-(2-Hydroxyphenyl)benzamide (**2a'**)

Crystallographic description of *N*-(2-Hydroxyphenyl)benzamide (2a'):

$C_{13}H_{11}NO_2$, crystal dimension $0.28 \times 0.26 \times 0.24$ mm, $M_r = 213.23$, Monoclinic, Space group P 2₁/c, $a = 10.9246(10)$ Å, $b = 7.0228(6)$ Å, $c = 14.1338(12)$ Å, $\alpha = 90.00$, $\beta = 90.645(6)$, $\gamma = 90.00$, $V = 1084.29(16)$ Å³, $Z = 4$, $\rho_{\text{calcd}} = 1.306$ mg/m³, $\mu = 0.089$ 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.

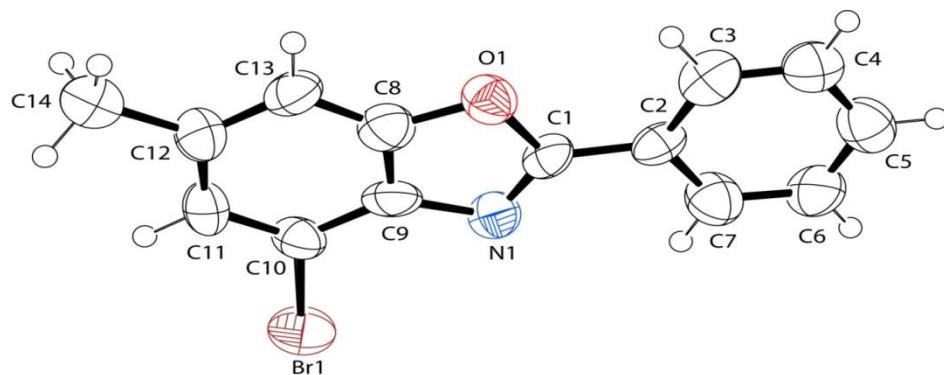
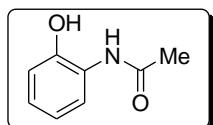


Figure 2 ORTEP views of 4-Bromo-6-methyl-2-phenylbenzo[d]oxazole (**21aa**)

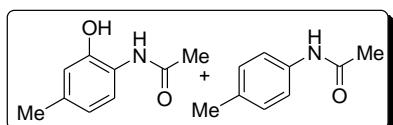
Crystallographic description of 4-Bromo-6-methyl-2-phenylbenzo[d]oxazole (21aa):

$C_{14}H_{10}BrNO$, crystal dimensions $0.28 \times 0.26 \times 0.24$ mm, $M_r = 288.13$, Monoclinic, Space group P 2₁, $a = 10.3512(8)$ Å, $b = 14.0265(11)$ Å, $c = 12.8571(10)$ Å, $\alpha = 90.00$, $\beta = 105.177(5)$, $\gamma = 90.00$, $V = 1801.6(2)$ Å³, $Z = 6$, $\rho_{\text{calcd}} = 1.593$ mg/m³, $\mu = 3.403$ 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.

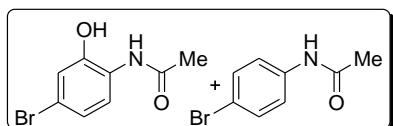
Spectral Data



***N*-(2-Hydroxyphenyl)acetamide (**1a'**):** Brown solid; M.p. 199-201 °C (lit.⁴ 201 °C);
¹H 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); ¹³C 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 (C₈H₉NO₂) (MH⁺) 152.0706; found 152.0693.

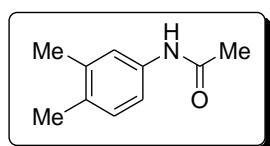


Mixture of *N*-(2-Hydroxy-4-methylphenyl)acetamide and *N*-*p*-Tolylacetamide (2a'+2a''**):** Off white solid; ¹H NMR (DMSO-*d*₆, 400 MHz): δ (ppm) 2.01 (s, 3H), 2.06 (s, 3H), 2.18 (s, 3H), 2.23 (s, 3H), 6.56 (d, 2H, *J* = 8.4 Hz), 6.66 (s, 1H), 7.07 (d, 2H, *J* = 8.4 Hz), 7.45 (t, 2H, *J* = 8 Hz), 9.29 (s, 1H), 9.65 (s, 1H), 9.83 (s, 1H); ¹³C 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.

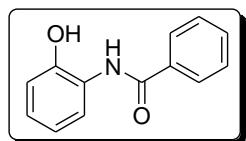


Mixture of *N*-(4-Bromo-2-hydroxyphenyl)acetamide and *N*-(4-Bromophenyl)acetamide (3a'+3a''**):** Brown solid; ¹H NMR (DMSO-*d*₆, 400 MHz): δ (ppm) 2.07 (s, 3H), 2.02 (s, 3H), 6.93 (d, 1H, *J* = 8.8 Hz), 7.00 (s, 1H), 7.46 (d, 2H, *J* = 7.6 Hz), 7.54 (d, 2H, *J* = 8.4 Hz), 7.73 (d, 1H, *J* = 8.8 Hz), 9.26 (s, 1H), 10.1 (s, 1H), 10.4 (s, 1H); ¹³C NMR (DMSO-*d*₆, 100 MHz): δ (ppm) 23.7, 24.0, 114.6,

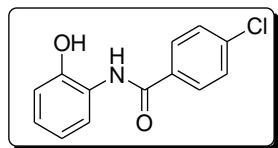
115.6, 118.0, 120.9, 121.6, 123.7, 126.1, 131.5, 138.7, 149.0, 168.6, 169.1; IR (KBr): 3390, 2704, 1658, 1604, 1586, 1534, 1407, 1366, 1270, 1235, 1197, 1118, 1010, 966, 877, 848, 796 cm⁻¹.



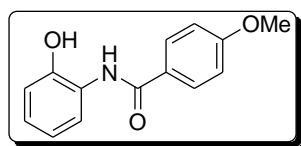
N-(3,4-Dimethylphenyl)acetamide (4a''): Brown solid; M.p. 83–85°C; ¹H NMR (CDCl₃, 400 MHz): δ (ppm) 2.11 (s, 3H), 2.18 (s, 6H), 7.01 (d, 1H, *J* = 8 Hz), 7.21 (d, 1H, *J* = 8 Hz), 7.26 (s, 1H), 8.06 (brs, 1H); ¹³C NMR (CDCl₃, 100 MHz): δ (ppm) 19.3, 19.9, 24.4, 117.9, 121.8, 129.96, 132.7, 135.9, 137.2, 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 C₁₀H₁₃NO (163.2163) C 73.59, H 8.03, N 8.58; found C 73.67, H 7.99, N 8.51.



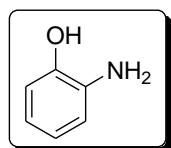
N-(2-Hydroxyphenyl)benzamide (2a'): Brown solid; M.p. 145-148 °C; ¹H NMR (DMSO-*d*₆, 400 MHz): δ (ppm) 6.84 (t, 1H, *J* = 7.6 Hz), 6.93 (d, 1H, *J* = 8 Hz), 7.02-7.06 (m, 1H), 7.53-7.59 (m, 3H), 7.68 (d, 1H, *J* = 8 Hz), 7.97 (d, 2H, *J* = 6.8 Hz), 9.53 (s, 1H), 9.78 (s, 1H); ¹³C NMR (DMSO-*d*₆, 100 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 (C₁₃H₁₁NO₂) (MH⁺) 214.0863; found 214.0848.



4-Chloro-N-(2-hydroxyphenyl)benzamide (3a'): Brown solid; M.p. 164-166.5 °C;
¹H 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); ¹³C 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 (C₁₃H₁₀ClNO₂) (MH⁺) 248.0473; found 248.0461.

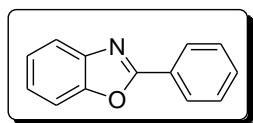


N-(2-Hydroxyphenyl)-4-methoxybenzamide (4a'): Brown solid; M.p. 170-172 °C; ¹H NMR (DMSO-*d*₆, 400 MHz): δ (ppm) 3.84 (s, 3H), 6.83 (t, 1H, *J* = 7.2 Hz), 6.91 (d, 1H, *J* = 8 Hz), 6.99-7.07 (m, 3H), 7.66 (d, 1H, *J* = 8 Hz), 7.96 (d, 2H, *J* = 8.8 Hz), 9.43 (s, 1H), 9.74 (brs, 1H); ¹³NMR (DMSO-*d*₆, 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 C₁₄H₁₃NO₃ (243.2574) C 69.12, H 5.39, N 5.76; found C 69.19, H 5.32, N 5.71.

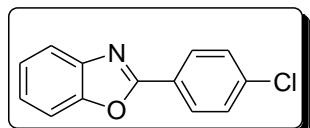


2-Hydroxyaniline: M.p. 216-218 °C, ¹H NMR (DMSO-*d*₆, 400 MHz): δ (ppm) 4.36 (brs, 2H), 6.27 (t, 1H, *J* = 7.6 Hz), 6.39-6.47 (m, 2H), 6.52 (1H, d, *J* = 7.6 Hz), 8.81 (brs, 1H); ¹³C NMR (DMSO-*d*₆, 100 MHz): δ (ppm) 114.4, 114.5, 116.4, 119.5,

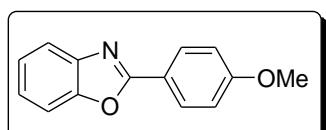
136.5, 143.9; IR (KBr): 3376, 3305, 1605, 1511, 1459, 1402, 1267, 1216, 1075, 1031, 896, 846, 741 cm⁻¹; elemental analysis calcd (%) for C₆H₇NO (109.1256): C 66.04, H 6.47, N 12.84; found C 66.09, H 6.43, N 12.73.



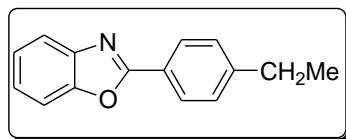
2-Phenylbenzo[*d*]oxazole (2aa): White solid; M.p. 101-103 °C (lit.⁵ 103-104 °C); ¹H NMR (CDCl₃, 400 MHz): δ (ppm) 7.33-7.35 (m, 2H), 7.51-7.52 (m, 3H), 7.56-7.58 (m, 1H), 7.75-7.78 (m, 1H), 8.23-8.26 (m, 2H); ¹³C NMR (CDCl₃, 100 MHz): δ (ppm) 110.8, 120.2, 124.8, 125.3, 127.3, 127.8, 129.1, 131.7, 142.3, 150.9, 163.2; IR (KBr): 2927, 2851, 1635, 1618, 1553, 1448, 1242, 1053, 924, 806, 745, 704 cm⁻¹; elemental analysis calcd (%) for C₁₃H₉NO (195.2163): C 79.98, H 7.17, N 4.65; found C 80.05, H 4.62, N 7.09.



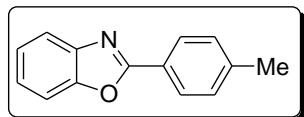
2-(4-Chlorophenyl)benzo[*d*]oxazole (3aa): White solid; M.p. 149-151 °C (lit.⁵ 153-154 °C); ¹H NMR (CDCl₃, 400 MHz): δ (ppm) 7.32-7.36 (m, 2H), 7.48 (d, 2H, *J* = 8.8 Hz), 7.55-7.57 (m, 1H), 7.73-7.76 (m, 1H), 8.17 (d, 2H, *J* = 8.8 Hz); ¹³C NMR (CDCl₃, 100 MHz): δ (ppm) 110.8, 120.2, 124.9, 125.5, 125.8, 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 (C₁₃H₈ClNO) (MH⁺) 230.0367; found 230.0355.



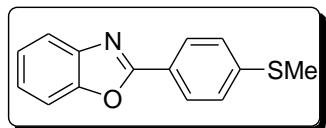
2-(4-Methoxyphenyl)benzo[d]oxazole (4aa): White solid; M.p. 103-105 °C (lit.⁵ 103-105 °C); ¹H NMR (CDCl₃, 400 MHz): δ (ppm) 3.86 (s, 3H), 7.01 (d, 2H, *J* = 9.2 Hz), 7.79-7.33 (m, 2H), 7.53-7.55 (m, 1H), 7.22-7.25 (m, 1H), 8.19 (d, 2H, *J* = 9.2 Hz); ¹³C NMR (CDCl₃, 100 MHz): δ (ppm) 55.4, 110.4, 114.4, 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 (C₁₄H₁₁NO₂) (MH⁺) 226.0863; found 226.0877.



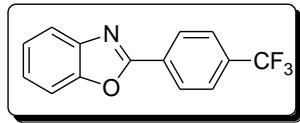
2-(4-Ethylphenyl)benzo[d]oxazole (5aa): White solid; M.p. 83-85 °C (lit.⁶ 84-86 °C); ¹H NMR (CDCl₃, 400 MHz): δ (ppm) 1.18 (t, 3H, *J* = 8 Hz), 2.62 (q, 2H, *J* = 7.6 Hz), 7.22-7.25 (m, 4H), 7.44-7.47 (m, 1H), 7.65-7.67 (m, 1H), 8.07 (d, 2H, *J* = 8 Hz); ¹³C NMR (CDCl₃, 100MHz): δ (ppm) 15.3, 29.0, 110.6, 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 C₁₅H₁₃NO (223.2693): C 80.69, H 5.87, N 6.27; found C 80.77, H 5.93, N 6.20.



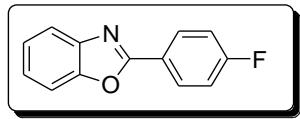
2-p-Tolylbenzo[d]oxazole (6aa): White Solid; M.p. 111-113 °C (lit.⁷ 110-112 °C); ¹H NMR (CDCl₃, 400 MHz): δ (ppm) 2.38 (s, 3H), 7.27-7.31 (m, 4H), 7.51-7.53 (m, 1H), 7.73-7.75 (m, 1H), 8.11 (d, 2H, *J* = 7.6 Hz); ¹³C NMR (CDCl₃, 100 MHz): δ (ppm) 21.7, 110.6, 119.9, 124.5, 124.6, 124.9, 127.7, 129.7, 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 (C₁₄H₁₁NO) (MH⁺) 210.0935; found 210.0947.



2-(4-(Methylthio)phenyl)benzo[d]oxazole (7aa): Yellowish-white solid; M.p. 103–106 °C; ^1H 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 $\text{C}_{14}\text{H}_{11}\text{NOS}$ (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.

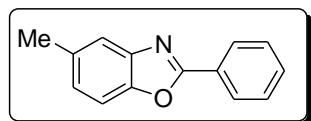


2-(4-(Trifluoromethyl)phenyl)benzo[d]oxazole (8aa): White solid; M.p. 148–150 °C (lit.⁸ 146–147 °C); ^1H NMR (CDCl_3 , 400 MHz): δ (ppm) 7.36–7.39 (m, 2H), 7.58–7.60 (m, 1H), 7.77 (d, 3H, J = 8.4 Hz), 8.35 (d, 2H, J = 8 Hz); ^{13}C NMR (CDCl_3 , 100 MHz): δ (ppm) 110.9, 120.6, 122.6, 125.1, 125.9, 126.02, 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 $\text{C}_{14}\text{H}_8\text{F}_3\text{NO}$ (263.2143): C 63.88, H 3.06, N 5.32; found C 63.97, H 3.11, N 5.24.

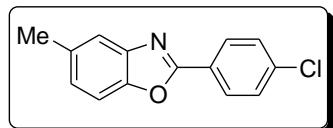


2-(4-Fluorophenyl)benzo[d]oxazole (9aa): White solid; M.p. 106–108 °C; ^1H NMR (CDCl_3 , 400 MHz): δ (ppm) 7.11–7.16 (m, 2H), 7.27–7.29 (m, 2H), 7.49–7.51 (m, 1H), 7.68–7.69 (m, 1H), 8.16–8.20 (m, 2H); ^{13}C NMR (CDCl_3 , 100 MHz): δ (ppm)

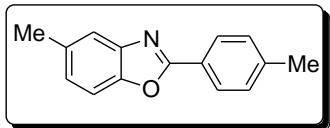
110.7, 116.3 (d, 1C, $J = 22.1$ Hz), 120.1, 123.6, 125.0 (d, 1C, $J = 47.3$ Hz), 129.9 (d, 1C, $J = 9.2$ Hz), 142.2, 150.9, 162.3, 163.7, 162.2; IR (KBr): 3054, 2923, 1895, 1600, 1498, 1472, 1451, 1412, 1230, 1152, 1053, 834, 761 cm^{-1} ; elemental analysis calcd (%) for $\text{C}_{13}\text{H}_8\text{FNO}$ (213.2068): C 73.23, H 3.78, N 6.57; found C 73.29, H 3.72, N 6.51.



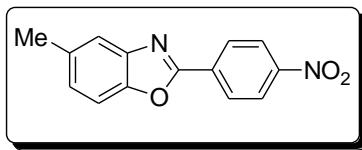
5-Methyl-2-phenylbenzo[d]oxazole (10aa): White solid; M.p. 103-105 °C (lit.⁹ 103-105 °C); ^1H NMR (CDCl_3 , 400 MHz): δ (ppm) 2.45 (s, 3H), 7.14 (d, 1H, $J = 8.4$ Hz), 7.43 (d, 1H, $J = 8$ Hz), 7.49-7.51 (m, 3H), 7.54 (s, 1H), 8.21-8.24 (m, 2H); ^{13}C NMR (CDCl_3 , 100 MHz): δ (ppm) 21.6, 109.9, 119.9, 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 $(\text{C}_{14}\text{H}_{11}\text{NO})(\text{MH}^+)$ 210.0913; found 210.0925.



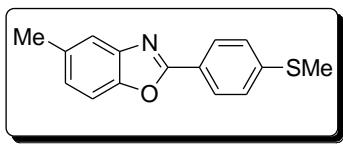
2-(4-Chlorophenyl)-5-methylbenzo[d]oxazole (11aa): White solid; M.p. 148-150 °C (lit.⁹ 148-150 °C); ^1H NMR (CDCl_3 , 400 MHz): δ (ppm) 2.46 (s, 3H), 7.14 (d, 1H, $J = 7.6$ Hz), 7.42 (d, 1H, $J = 8.4$ Hz), 7.46 (d, 2H, $J = 8.4$ Hz), 7.52 (s, 1H), 8.14 (d, 2H, $J = 8.4$ Hz); ^{13}C NMR (CDCl_3 , 400 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 $\text{C}_{14}\text{H}_{10}\text{ClNO}(\text{MH}^+)$ 244.0524; found 244.0524.



5-Methyl-2-p-tolylbenzo[*d*]oxazole (12aa): White Solid; M.p. 137-139 °C (lit.⁹ 138-141 °C); ¹H NMR (CDCl₃, 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); ¹³C NMR (CDCl₃, 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 C₁₅H₁₃NO (MH⁺) 224.107; found 224.1067.

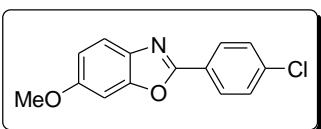


5-Methyl-2-(4-nitrophenyl)benzo[*d*]oxazole (13aa): Yellow solid; M.p. 204-206 °C; ¹H NMR (CDCl₃, 400 MHz): δ (ppm): 2.51 (s, 3H), 7.23-7.26 (m, 1H), 7.49 (d, 1H, *J* = 8 Hz), 7.59 (s, 1H), 8.35-8.42 (m, 4H); ¹³C NMR (CDCl₃, 100 MHz): δ (ppm) 21.7, 110.4, 120.6, 124.3, 127.7, 128.4, 133.1, 135.4, 142.3, 149.4, 160.8; IR (KBr): 2923, 1599, 1555, 1520, 1481, 1342, 1196, 1105, 1060, 853, 798, 707 cm⁻¹; HRMS (ESI): calcd. for C₁₄H₁₀N₂O₃ (MH⁺) 255.0764; found 255.0760.

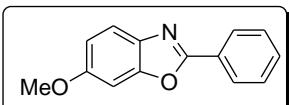


5-Methyl-2-(4-(methylthio)phenyl)benzo[*d*]oxazole (14aa): Yellowish solid; M.p 116-118 °C; ¹H NMR (CDCl₃, 400 MHz): δ (ppm) 2.46 (s, 3H), 2.52 (s, 3H), 7.11-7.13 (m, 1H), 7.32 (d, 2H, *J* = 8.8 Hz), 7.41 (d, 1H, *J* = 8.4 Hz), 7.51 (s, 1H), 8.11 (d, 2H, *J* = 8.8 Hz); ¹³C NMR (CDCl₃, 100 MHz): δ (ppm) 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;

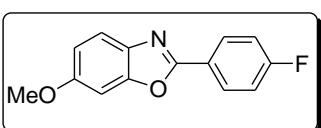
elemental analysis calcd (%) for C₁₅H₁₃NOS (255.3353): C 70.56, H 5.13, N 5.49, S 12.56; found C 70.65, H 5.21, N 5.41, S 12.63.



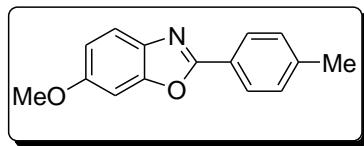
2-(4-Chlorophenyl)-6-methoxybenzo[d]oxazole (15aa): White solid; M.p. 134-136 °C; ¹H NMR (CDCl₃, 400 MHz): δ (ppm) 3.86 (s, 3H), 6.94 (dd, 1H, *J*₁ = 2.4 Hz, *J*₂ = 8.8 Hz), 7.077-7.083 (m, 1H), 7.46 (d, 2H, *J* = 8.4 Hz), 7.61 (d, 1H, *J* = 8.8 Hz), 8.11 (d, 2H, *J* = 8.4 Hz); ¹³C NMR (CDCl₃, 100 MHz): 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 C₁₄H₁₀ClNO₂ (259.687): C 64.75, H 3.88, N 5.39; found C 64.81, H 3.94, N 5.31.



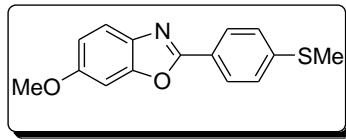
6-Methoxy-2-phenylbenzo[d]oxazole (16aa): Off-white solid; M. p 63-66 °C (lit.¹⁰ 65-66 °C); ¹H NMR (CDCl₃, 400 MHz): δ (ppm) 3.86 (s, 3H), 6.94 (dd, 1H, *J*₁ = 2.4 Hz, *J*₂ = 8.8 Hz), 7.086-7.092 (m, 1H), 7.48-7.49 (m, 3H), 7.62 (d, 1H, *J* = 8.8 Hz), 8.17-8.19 (m, 2H); ¹³C NMR (CDCl₃, 100 MHz): δ (ppm) 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 (C₁₄H₁₁NO₂) (MH⁺) 226.0863; found 226.0874.



2-(4-Fluorophenyl)-6-methoxybenzo[d]oxazole (17aa): White Solid; M.p. 105-107 °C; ^1H 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 $\text{C}_{14}\text{H}_{10}\text{FNO}_2$ (243.2327): C 69.13, H 4.14, N 5.76; found C 69.22, H 4.18, N 5.70.

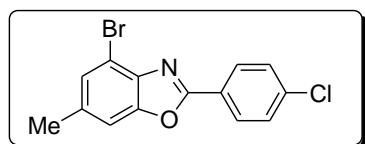


6-Methoxy-2-p-tolylbenzo[d]oxazole (18aa): White solid; M.p. 94-96 °C; ^1H NMR (CDCl_3 , 400 MHz): δ (ppm) 2.39 (s, 3H), 3.85 (s, 3H), 6.92 (dd, 1H, $J_1 = 2.8$ Hz, $J_2 = 8.8$ Hz), 7.067-7.072 (m, 1H), 7.28 (d, 2H, $J = 8$ Hz), 7.33 (1H, d, $J = 8.8$ Hz), 8.06 (d, 2H, $J = 8.4$ Hz); ^{13}C NMR (CDCl_3 , 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 $\text{C}_{15}\text{H}_{13}\text{NO}_2$: C 75.30, H 5.48, N 5.85; found C 75.38, H 5.41, N 5.79.

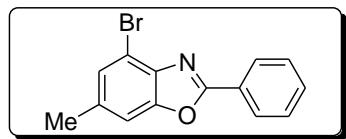


6-Methoxy-2-(4-(methylthio)phenyl)benzo[d]oxazole (19aa): Yellowish solid; M.p. 128–130 °C; ^1H NMR (CDCl_3 , 400 MHz): δ (ppm) 2.52 (s, 3H), 3.86 (s, 3H), 6.93 (dd, 1H, $J_1 = 2.0$ Hz, $J_2 = 8.4$ Hz), 7.075-7.08 (m, 1H), 7.31 (d, 2H, $J = 8.8$ Hz), 7.59 (d, 1H, $J = 8.8$ Hz), 8.07 (d, 2H, $J = 8.4$ 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,

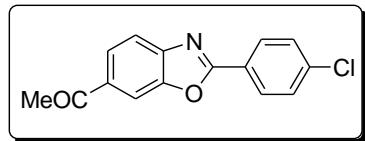
1297, 1266, 1190, 1145, 1095, 1044, 1028, 1008, 983, 959, 841 cm⁻¹; HRMS (ESI): calcd. for (MH⁺) 272.074; found 272.0738.



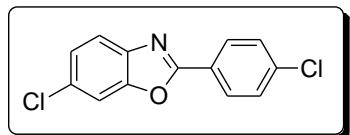
4-Bromo-2-(4-chlorophenyl)-6-methylbenzo[d]oxazole (20aa): White solid; M.p. 184–186 °C; ¹H NMR (CDCl₃, 400 MHz): δ (ppm) 2.49 (s, 3H), 7.32-7.33 (m, 1H), 7.37-7.38 (m, 1H), 7.49 (d, 2H, *J* = 9.2 Hz), 8.21 (d, 2H, *J* = 8.8 Hz); ¹³C NMR (CDCl₃, 100 MHz): δ (ppm) 21.7, 110.2, 112.2, 125.3, 129.2, 129.3, 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 (C₁₄H₉BrClNO) (MH⁺) 321.9629; found 321.9640.



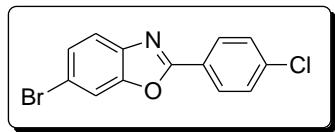
4-Bromo-6-methyl-2-phenylbenzo[d]oxazole (21aa): Yellowish-white solid; M.p. 135–137 °C; ¹H NMR (CDCl₃, 400 MHz): δ (ppm) 2.48 (s, 3H), 7.32 (s, 1H), 7.36 (s, 1H), 7.49-7.54 (m, 3H), 8.27 (dd, 2H, *J*₁ = 1.6 Hz, *J*₂ = 8.0 Hz); ¹³C NMR (CDCl₃, 100 MHz): δ (ppm) 21.6, 110.1, 112.0, 126.8, 127.9, 128.89, 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 C₁₄H₁₀BrNO (288.1389): C 58.36, H 3.50, N 4.86; found C 58.42, H 3.55, N 4.81.



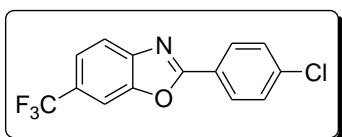
1-(2-(4-Chlorophenyl)benzo[d]oxazol-6-yl)ethanone (22aa): White solid; M.p. 185–187 °C; ^1H NMR (CDCl_3 , 400 MHz): δ (ppm) 2.67 (s, 3H), 7.50 (d, 2H, J = 8.4 Hz), 7.78 (d, 1H, J = 8.4 Hz), 7.99 (dd, 1H, J_1 = 1.6 Hz, J_2 = 8.4 Hz), 8.18 (d, 3H, J = 8.8 Hz); ^{13}C NMR (CDCl_3 , 100 MHz): δ (ppm) 26.9, 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 $\text{C}_{15}\text{H}_{10}\text{ClNO}_2$ (271.6977): C 66.31, H 3.71, N 5.16; found C 66.38, H 3.78, N 5.10.



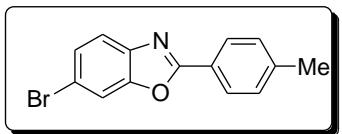
6-Chloro-2-(4-chlorophenyl)benzo[d]oxazole (23aa): White solid; M.p. 148–150 °C (lit.¹¹ 148–150 °C); ^1H NMR (CDCl_3 , 400 MHz): δ (ppm) 7.32 (dd, 1H, J_1 = 2.0 Hz, J_2 = 8.4 Hz), 7.48 (d, 2H, J = 8.8 Hz), 7.56 (s, 1H), 7.64 (d, 1H, J = 8.0 Hz), 8.13 (s, 2H, J = 8.8 Hz); ^{13}C NMR (CDCl_3 , 100 MHz): 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 ($\text{C}_{13}\text{H}_7\text{Cl}_2\text{NO}$) (MH^+) 263.9977; found 263.9989.



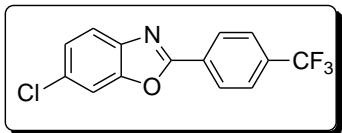
6-Bromo-2-(4-chlorophenyl)benzo[d]oxazole (24aa): White solid; M.p. 157–160 °C; ^1H NMR (CDCl_3 , 400 MHz): δ (ppm) 7.49–7.47 (m, 3H), 7.60 (d, 1H, J = 8.4 Hz), 7.22 (s, 1H), 8.14 (d, 2H, J = 8.8 Hz); ^{13}C NMR (CDCl_3 , 100 MHz): δ (ppm) 114.3, 118.4, 121.2, 125.3, 128.4, 129.1, 129.5, 138.3, 141.4, 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 ($\text{C}_{13}\text{H}_7\text{BrClNO}$) (MH^+) 307.9472; found 307.9487.



2-(4-Chlorophenyl)-6-(trifluoromethyl)benzo[d]oxazole (25aa): White solid; M.p. 114–116 °C; ^1H 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 ($\text{C}_{14}\text{H}_7\text{F}_3\text{ClNO}$) (MH^+) 298.0241; found 298.0251.

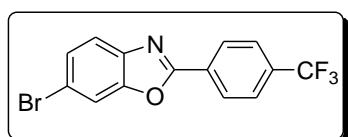


6-Bromo-2-p-tolylbenzo[d]oxazole (26aa): White solid; M.p. 127–129 °C; ^1H NMR (CDCl_3 , 400 MHz): δ (ppm) 2.42 (s, 3H), 7.30 (d, 2H, J = 8.0 Hz), 7.44 (dd, 1H, J_1 = 2.0 Hz, J_2 = 8.8 Hz), 7.58 (d, 1H, J = 8.0 Hz), 7.71 (s, 1H), 8.09 (d, 2H, J = 8.0 Hz); ^{13}C NMR (CDCl_3 , 100 MHz): δ (ppm) 21.9, 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 $\text{C}_{14}\text{H}_{10}\text{BrNO}$ (288.1389): C 58.36, H 3.50, N 4.86; found C 58.45, H 3.44, N 4.81.

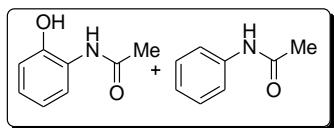


6-Chloro-2-(4-(trifluoromethyl)phenyl)benzo[d]oxazole (27aa): White solid; M.p. 120–123 °C; ^1H NMR (CDCl_3 , 400 MHz): δ (ppm) 7.34 (dd, 1H, J_1 = 2.0 Hz, J_2 =

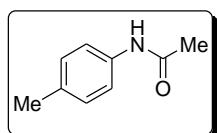
8.4 Hz), 7.59 (s, 1H), 7.67 (d, 1H, J = 8.8 Hz), 7.76 (d, 2H, J = 8.4 Hz), 8.31 (d, 2H, J = 8.0 Hz); ^{13}C NMR (CDCl_3 , 100 MHz): δ (ppm) 111.6, 121.0, 125.9, 126.1, 128.0, 130.1, 131.7, 140.8, 151.1, 162.2; IR (KBr): 2958, 1614, 1558, 1500, 1461, 1426, 1409, 1323, 1159, 1108, 1067, 922, 817 cm^{-1} ; HRMS (ESI): calcd. for ($\text{C}_{14}\text{H}_7\text{F}_3\text{ClNO}$) (MH^+) 298.0241; found 298.0255.



6-Bromo-2-(4-(trifluoromethyl)phenyl)benzo[d]oxazole (28aa): White solid; M.p. 106–108 °C; ^1H 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 $\text{C}_{14}\text{H}_7\text{BrF}_3\text{NO}$ (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; ^1H NMR ($\text{DMSO}-d_6$, 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 ($\text{DMSO}-d_6$, 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°C; ^1H 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 $\text{C}_9\text{H}_{11}\text{NO}$ (149.1897) C 72.46, H 7.43, N 9.39; found C 72.39, H 7.45, N 9.31.

References

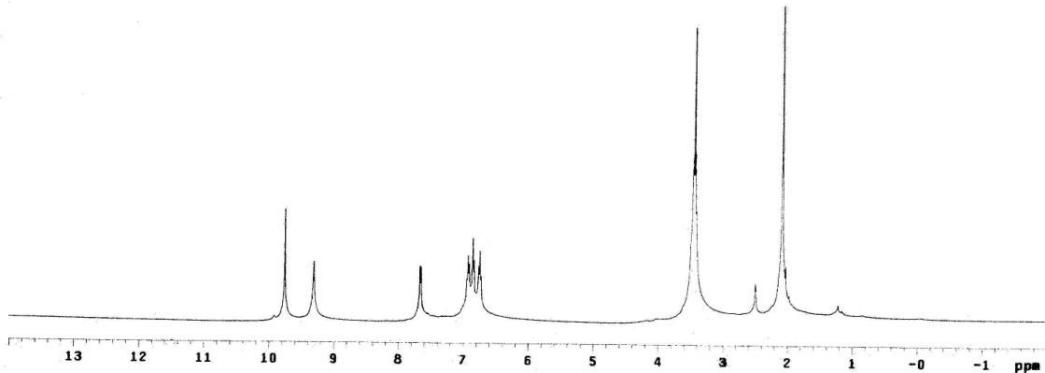
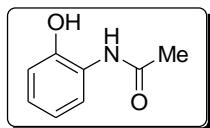
4. L. Chas Raiford, *J. Am. Chem. Soc.*, **1919**, *41*, 2068.
5. M. M. Guru, M. A. Ali and T. Punniyamurthy, *Org. Lett.*, **2011**, *13*, 1194.
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8. D. Subhas Bose and M. Idrees, *Synthesis*, **2010**, *3*, 398.

9. R. H. Shoar, M. Heidary, M. Farzaneh and R. Malakouti, *Synthetic Commun.*, **2009**, *39*, 1742.
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11. Y. Leng, F. Yang, W. Zhu, Y. Wu and X. Li, *Org. Biomol. Chem.*, **2011**, *9*, 5288.

SPECTRA

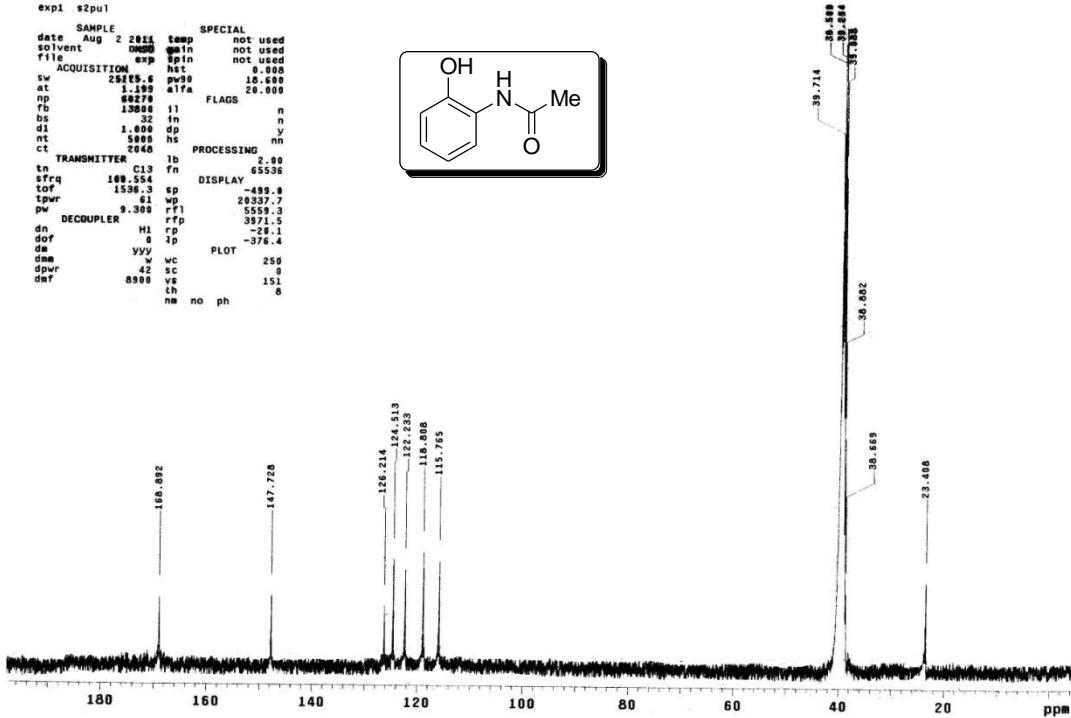
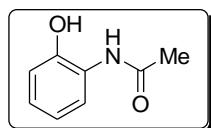
N-(2-Hydroxyphenyl)acetamide (1a'): ^1H NMR (DMSO- d_6 , 400 MHz)

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solvent   DMSO gain  not used
file      exp spin  not used
ACQUISITION exp spin  not used
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at        1.398 alfa  20.000
tpw     25000    flags
fb      not used 11   n
bs        4   in    n
di      1.60   dp    y
nt      32   hs    nn
ct      32   PROCESSING
TRANSMITTER C13  lb   0.10
tn      H1   fn  65536
sfreq  399.855 DISPLAY
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tpw    57   wp   363.1
pw     9.800 r1   1636.1
DECOUPLER   rfp   999.6
dn      C13 rfp  115.2
dof      0   lp   -82.9
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dfr    15900  vs   33
nm   cdc ph   20
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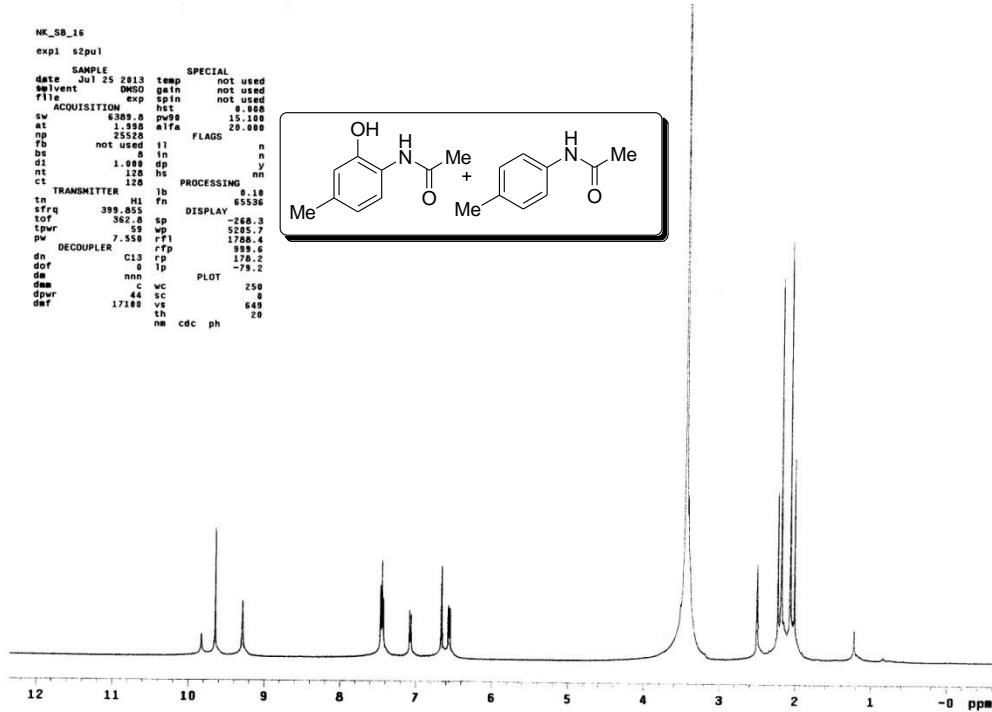


N-(2-Hydroxyphenyl)acetamide (1a'): ^{13}C NMR (DMSO- d_6 , 100 MHz)

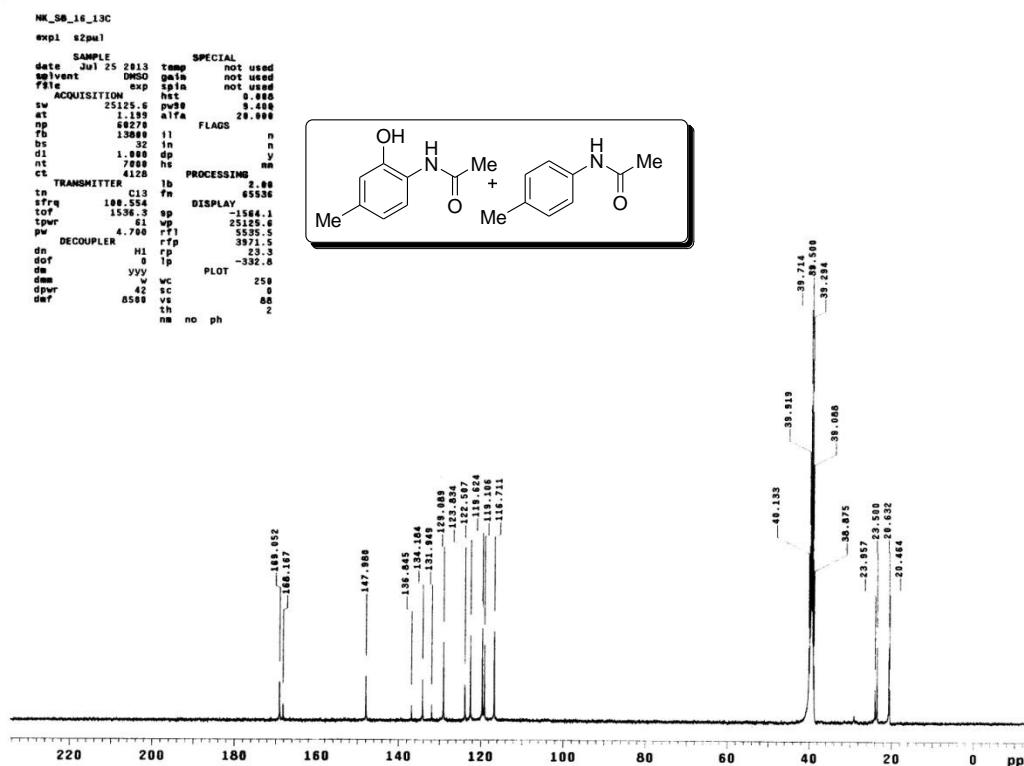
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file      exp spin  not used
ACQUISITION exp spin  not used
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at        1.398 alfa  20.000
tpw     15300    flags
fb      13800  11   n
bs        32   in    n
di      1.800   dp    y
nt      51   hs    nn
ct      2640  PROCESSING 2.00
TRANSMITTER C13  lb   2.00
tn      H1   fn  65536
sfreq  109.554 DISPLAY
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tpw    61   wp   20337.7
pw     9.300 r1   5371.5
DECOUPLER   rfp  3371.5
dof      0   lp   -28.1
dm      yyy   PLOT
das    w   wc   250
dpwr  42   sc   0
dfr    8900  vs   151
nm   no ph   6
```



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

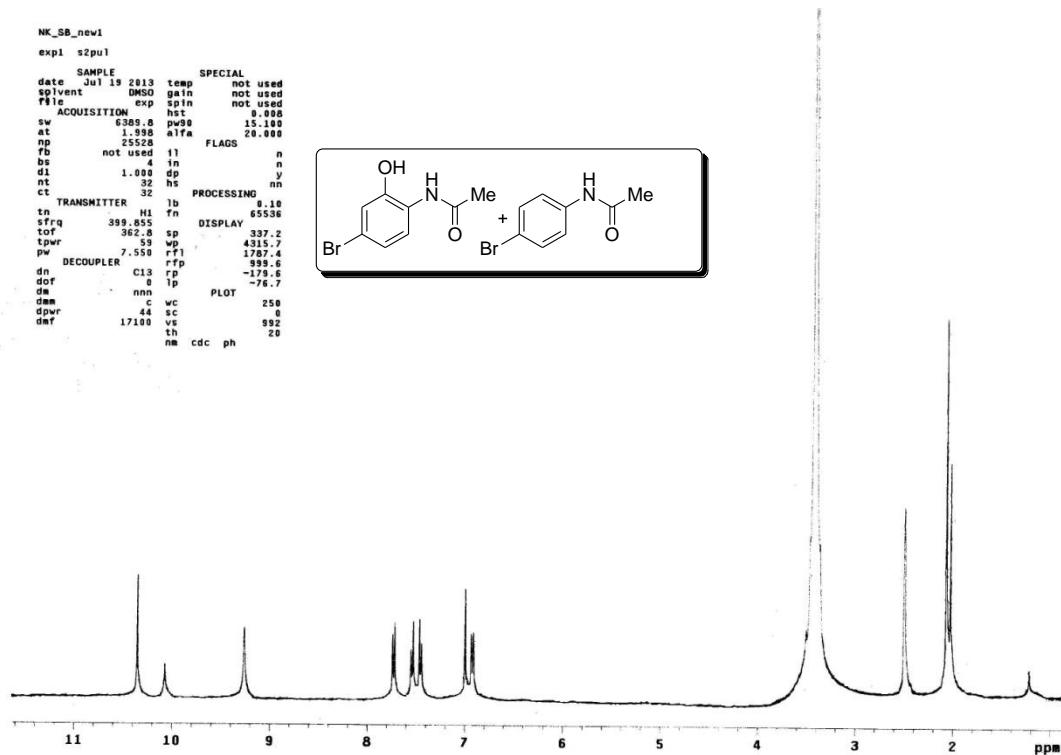
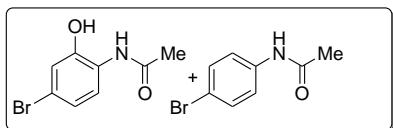


Mixture of *N*-(2-Hydroxy-4-methylphenyl)acetamide and *N*-*p*-Tolylacetamide ($2\mathbf{a}' + 2\mathbf{a}''$): ^{13}C NMR (DMSO- d_6 , 100 MHz)



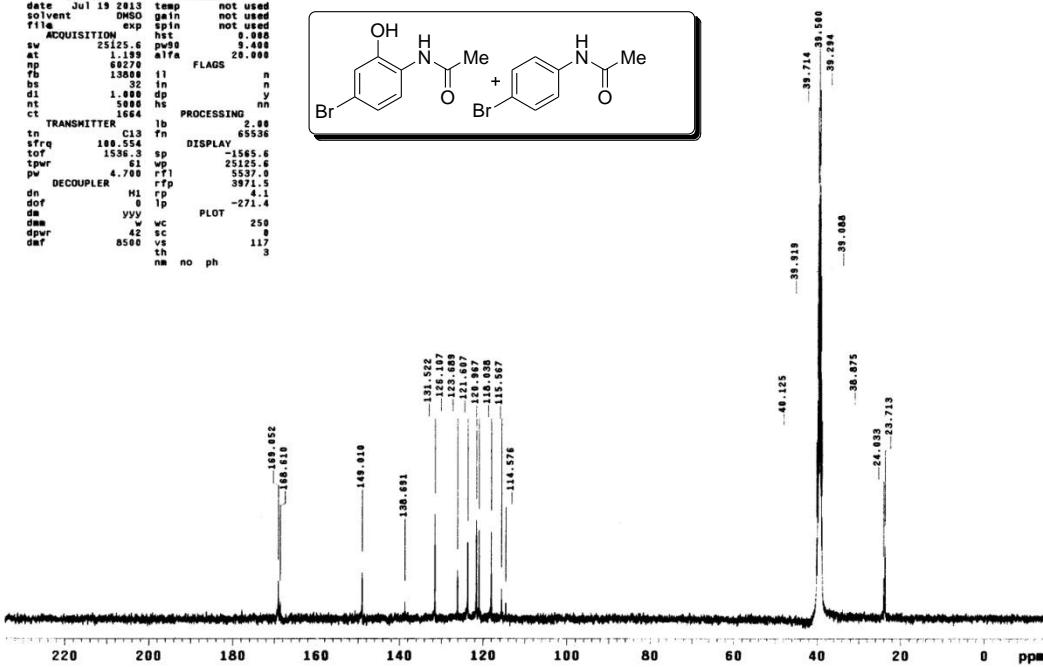
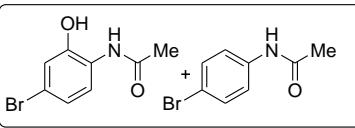
Mixture of *N*-(4-Bromo-2-hydroxyphenyl)acetamide and *N*-(4-Bromophenyl)acetamide ($3\text{a}' + 3\text{a}''$): ^1H NMR (DMSO- d_6 , 400 MHz)

```
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expt s2pul
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date Jul 19 2013 temp not used
solvent DMSO gain not used
file exp spin not used
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sw 6389.8 pw90 11.100
at 1.998 alfa 20.000
np 25528 flags
rb not used 11 n
bs 4 in n
di 1.000 dp y
nt 32 hs nn
ct 32 PROCESSING nn
TRANSMITTER lb 0.10
tn H1 fn 65536
sfrq 399.855 DISPLAY 65536
t0f 362.8 sp 337.2
tpwr 59 wp 4315.7
pw 7.558 rf1 177.4
DECOUPLER C13 rfp 999.6
dof C13 rp -179.6
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nm cdc ph 20
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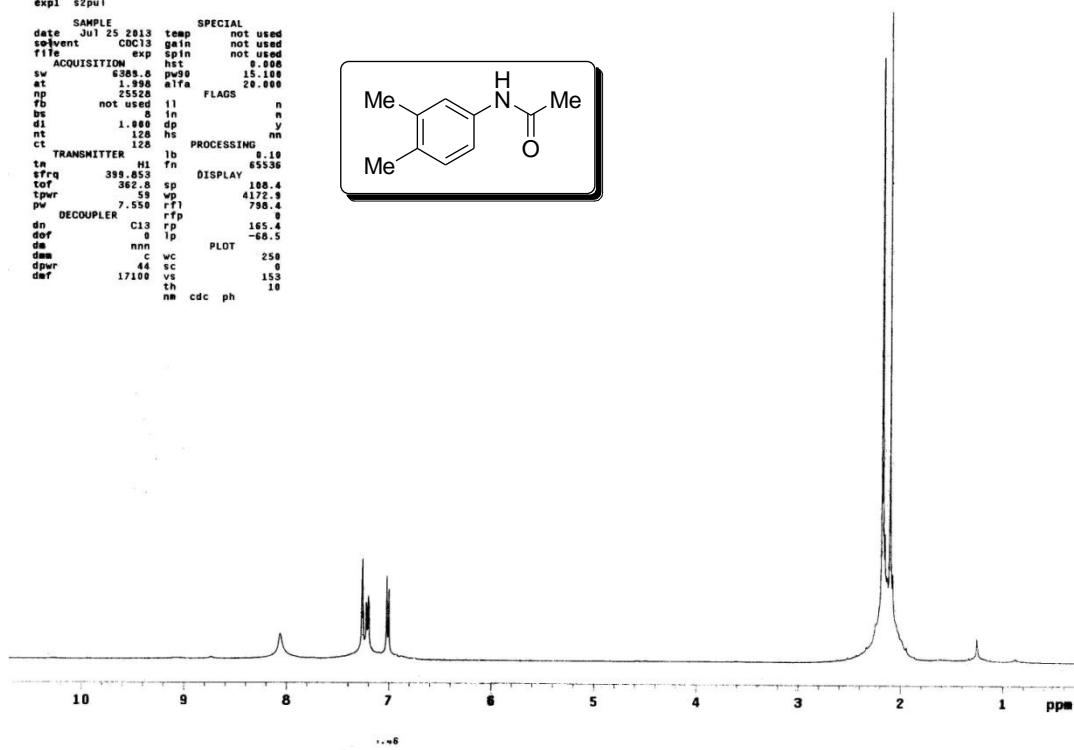
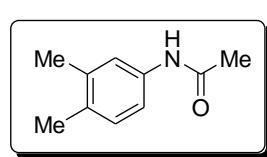
Mixture of *N*-(4-Bromo-2-hydroxyphenyl)acetamide and *N*-(4-Bromophenyl)acetamide ($3\text{a}' + 3\text{a}''$): ^{13}C NMR (DMSO- d_6 , 100 MHz)

```
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expt s2pul
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solvent DMSO gain not used
file exp spin not used
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np 60270 flags
rb 13800 11 n
bs 32 in n
di 1.000 dp y
nt 5884 hs nn
ct 1564 PROCESSING nn
TRANSMITTER lb 2.00
tn C13 fm 65536
sfrq 108.470 DISPLAY 65536
t0f 1536.3 sp -1565.6
tpwr 61 wp 25125.6
pw 4.760 rf1 5530.0
DECOUPLER C13 rfp 3971.5
dn H1 rp 4.1
dof 0 lp -271.4
de yy w PLOT 250
dmm v wc 250
dpwr 42 sc 0
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nm no ph 3
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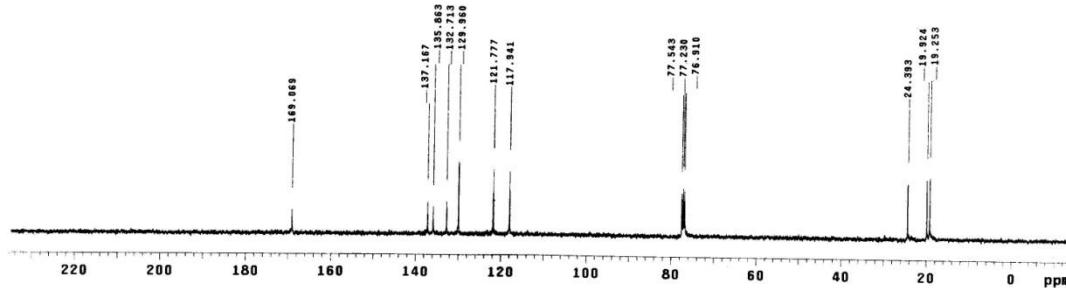
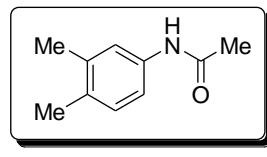
N-(3,4-Dimethylphenyl)acetamide (4a''): ^1H NMR (CDCl_3 , 400 MHz)

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solvent CDCl3 gain not used
file exp spin not used
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at 1.998 pw1 20.000
np 25528 FLAGS
td not used 11 n
bs 8 in
di 1.000 dp y
nt 128 nn
ct 128 PROCESSING
TRANSMITTER lb 0.10
tn H1 fn 65536
sfrq 399.854 DISPLAY
t0f 362.0 sp 100.4
tpwr 59 vp 4172.9
pw 7.550 rfp 798.4
DECOUPLER rfp 0
dn C13 rp 165.4
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nm cdc ph
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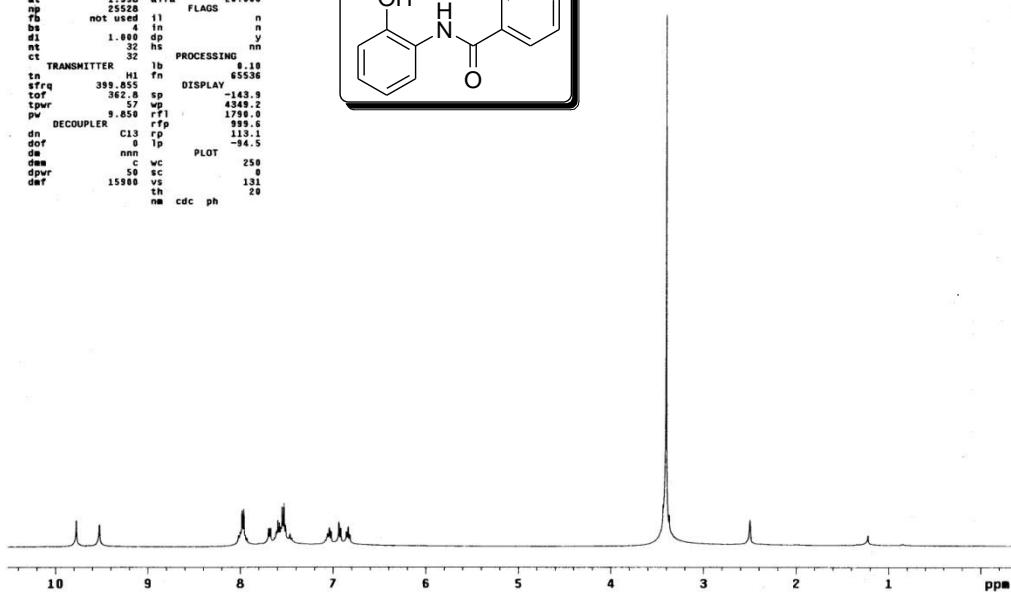
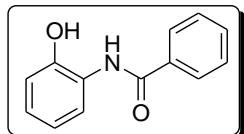
N-(3,4-Dimethylphenyl)acetamide (4a''): ^{13}C NMR (CDCl_3 , 100 MHz)

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date Jul 25 2013 temp not used
solvent CDCl3 gain not used
file exp spin not used
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sw 25125.6 pw0 5.400
at 68270 alfa 20.000
np 68270 FLAGS
fb 13600 11 n
bs 32 in
di 1.000 dp y
nt 10000 ns nn
ct 640 PROCESSING
TRANSMITTER lb 2.00
tn C13 1p fn 65536
sfrq 100.554 DISPLAY
t0f 1536.3 sp -1514.1
tpwr 61 rp 2515.6
pw 4.700 rfp 9278.0
DECOUPLER rfp 7764.9
dn H1 rp -65.1
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nm no ph 3
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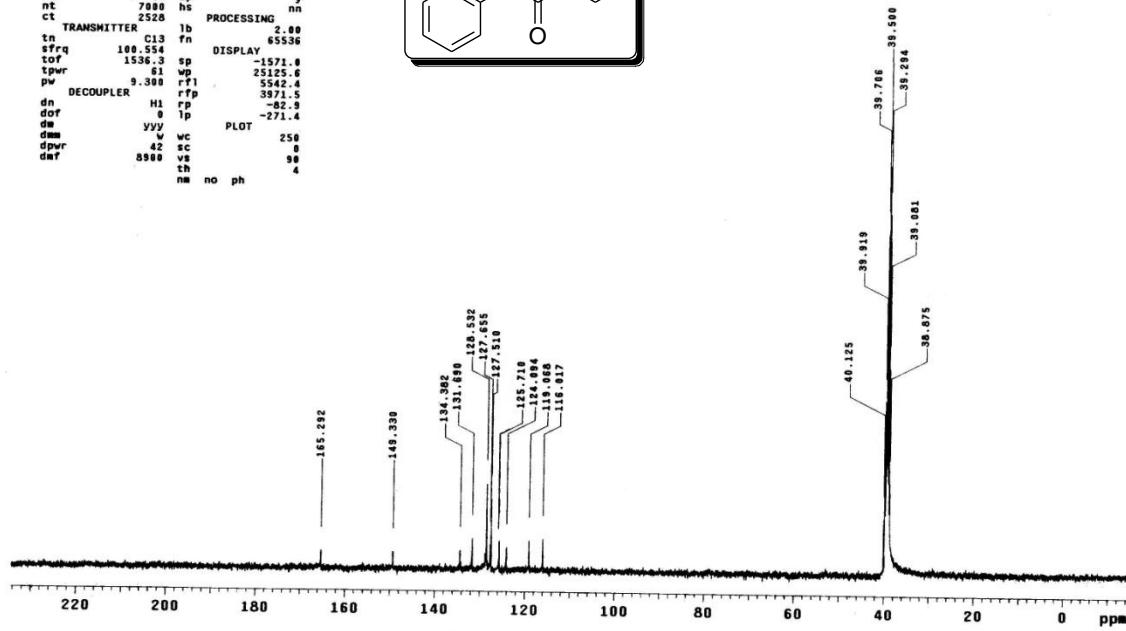
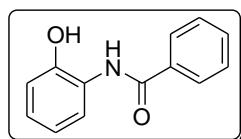
N-(2-Hydroxyphenyl)benzamide (2a'): ^1H NMR (DMSO- d_6 , 400 MHz)

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solvent DMSO gain not used
file exp spin not used
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at 1.998 np 20.000
np 25528 FLAGS
rf0 not used 11 n
bs 4 in n
di 1.000 dp y
nt 32 hs nn
ct 32 PROCESSING
TRANSMITTER lb 0.10
tn HI 65536
sfreq 399.855 DISPLAY
tot 362.8 sp -143.9
tpwr 57 w 400.2
pw 9.650 r1 1750.0
DECOUPLER rfp 999.6
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dav th 20
nm cdc ph



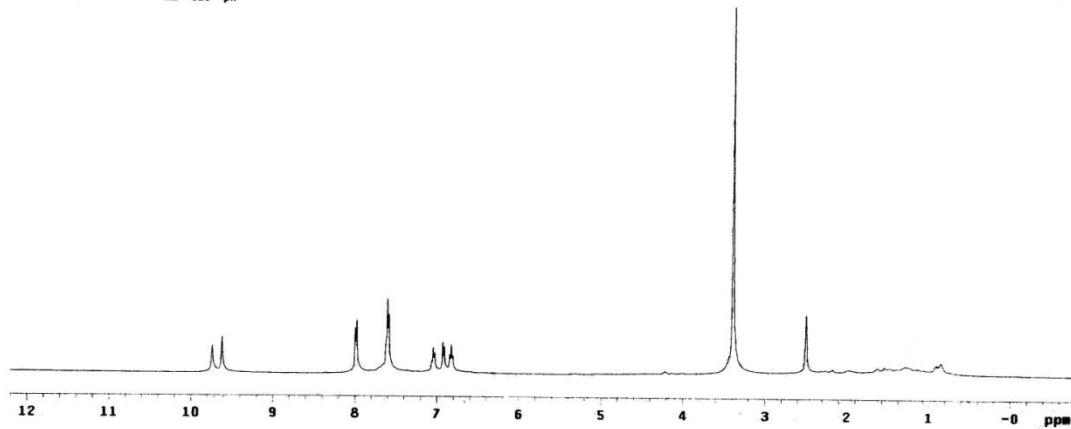
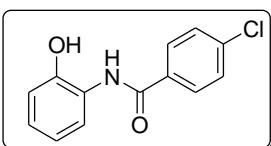
N-(2-Hydroxyphenyl)benzamide (2a'): ^{13}C NMR (DMSO- d_6 , 100 MHz)

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SAMPLE SPECIAL
date Dec 8 2011 temp not used
solvent DMSO gain not used
file exp spin not used
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at 1.199 al7 20.000
np 68278 FLAGS
rf0 13841 11 n
bs 32 in n
di 1.000 dp y
nt 7900 hs nn
ct 2528 PROCESSING
TRANSMITTER lb 2.00
tn C13 fn 65536
sfreq 100.554 DISPLAY
tot 153.8 sp -1571.0
tpwr 61 w 25125.6
pw 9.300 r1 5542.4
DECOUPLER rfp 3971.5
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de VVY PLOT
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nm no ph



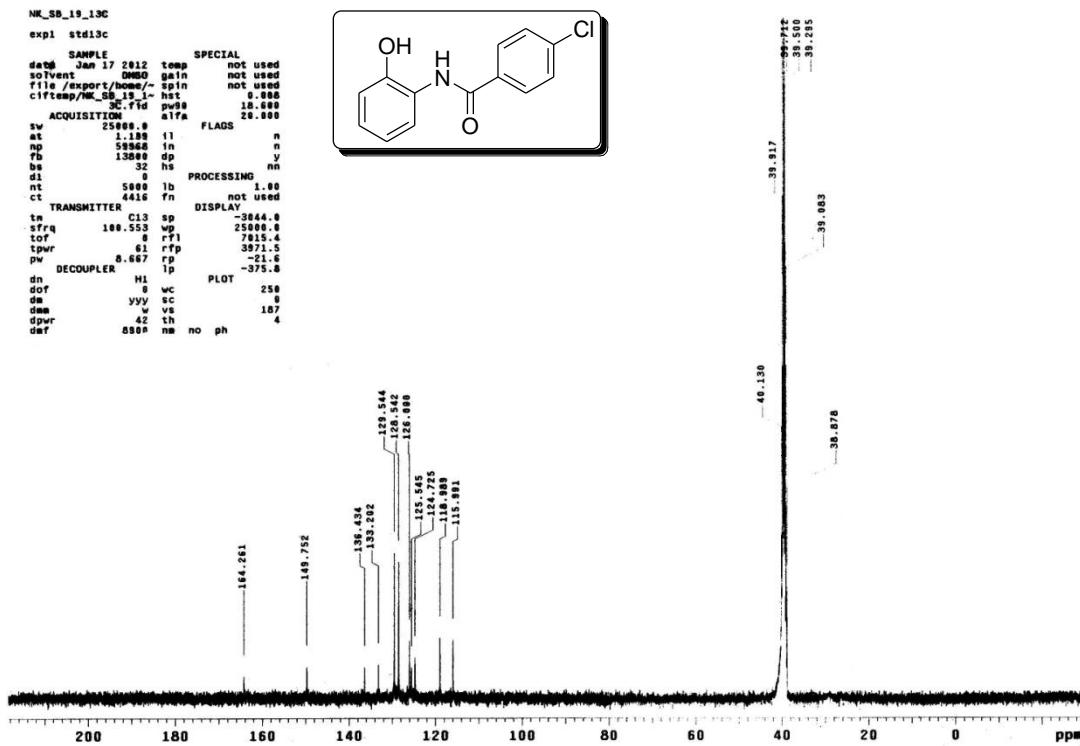
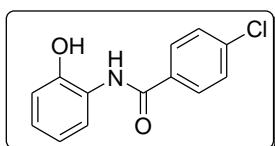
4-Chloro-N-(2-hydroxyphenyl)benzamide (3a'): ^1H NMR (DMSO- d_6 , 400 MHz)

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np 25528 FLAGS
fb not used 11 n
bs 4 in n
d1 1.000 dp y
nt 32 hs nn
ct 32 PROCESSING nn
TRANSMITTER fn not used
tr H1 DISPLAY
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tof 362.8 wp 5281.0
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pw 7.000 rfp 595.6
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dsc cdc ph

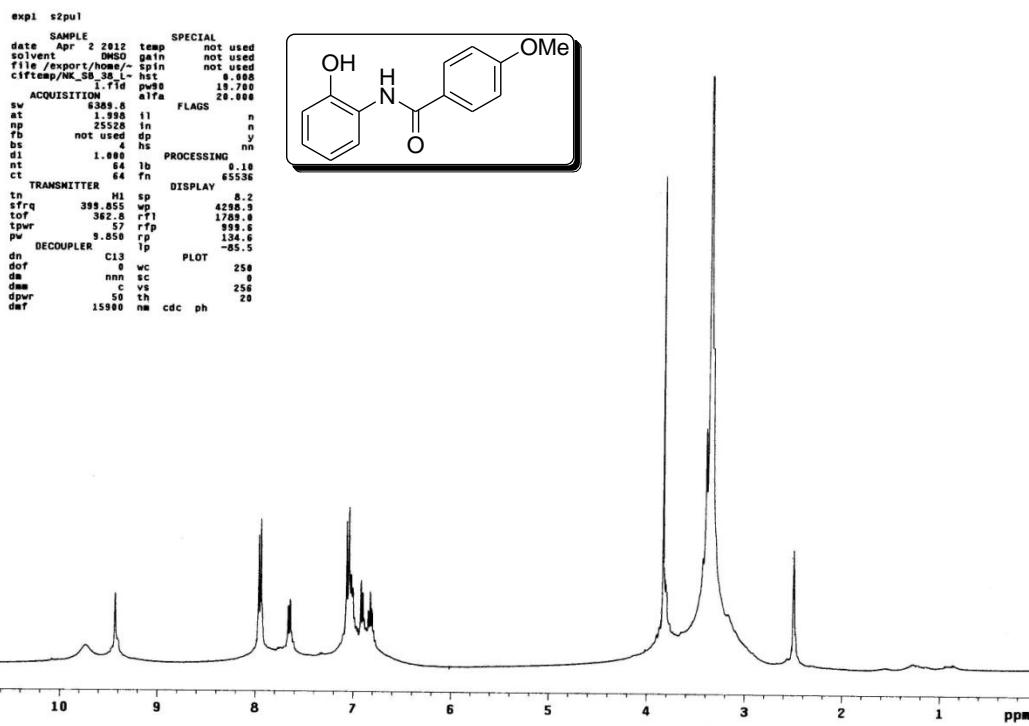


4-Chloro-N-(2-hydroxyphenyl)benzamide (3a'): ^{13}C NMR (DMSO- d_6 , 100 MHz)

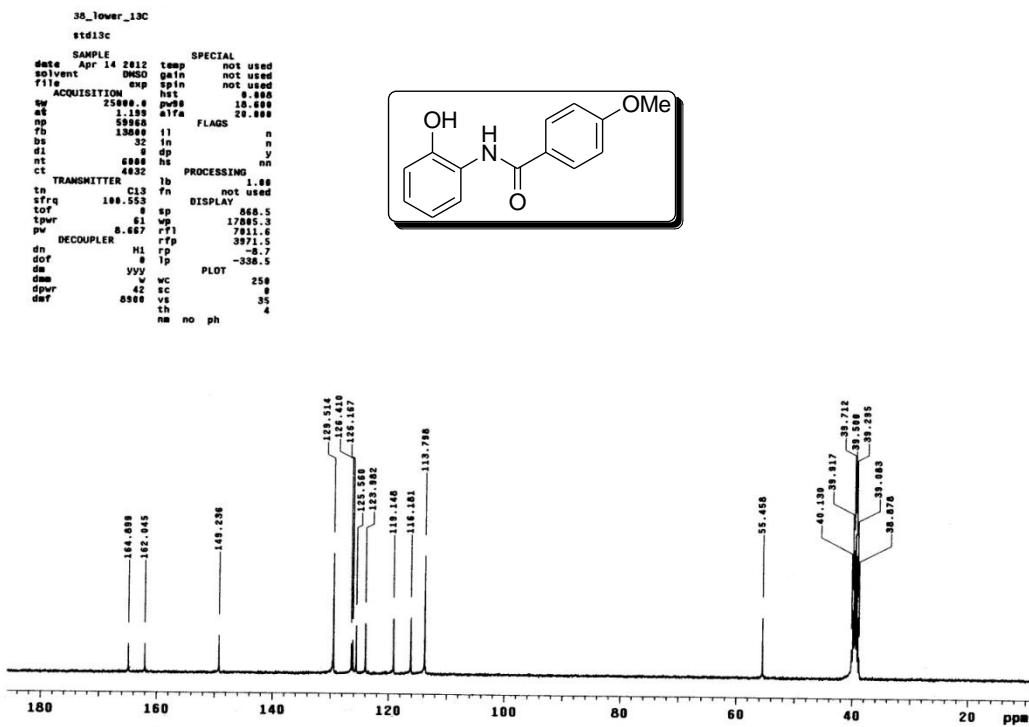
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DC_Tfd pw90 18.000
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sw 25000.0 FLAGS
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np 5000 n n
fb 13000 dp y
bs 32 hs nn
d1 0 PROCESSING
nt 5000 1b 1.00
ct 4416 fn not used
TRANSMITTER H1 DISPLAY
tr C13 sp -3844.8
sfrq 100.553 wp 25000.0
tof 8 rf1 7815.4
tpwr 61 rfp 3971.5
pw 8.667 rfp -21.4
DECOUPLER C13 1p -375.8
dn H1 PLOT
dof 8 wc 258
de ywc 8
dss w vs 107
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dft 8500 nm no ph



N-(2-Hydroxyphenyl)-4-methoxybenzamide (4a'): ^1H NMR (DMSO- d_6 , 400 MHz)

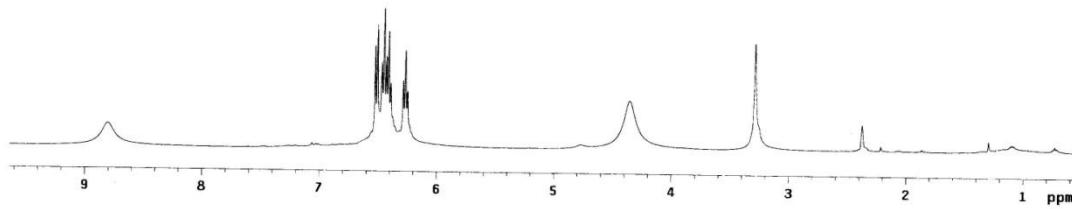
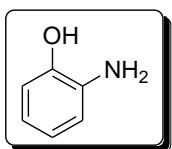


N-(2-Hydroxyphenyl)-4-methoxybenzamide (4a'): ^{13}C NMR (DMSO- d_6 , 100 MHz)



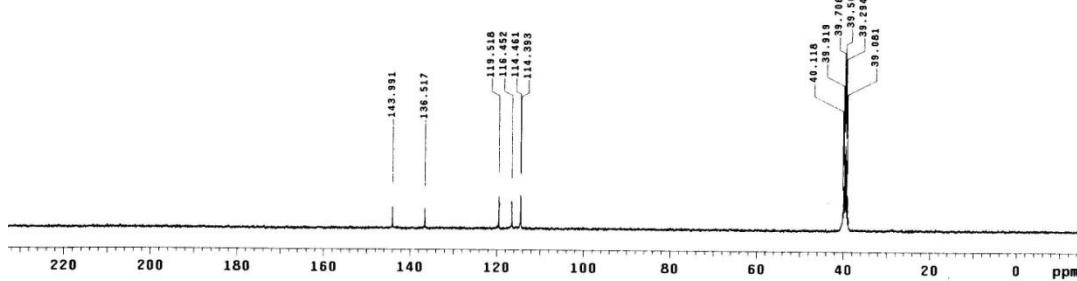
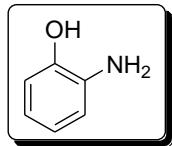
2-Hydroxyaniline: ^1H NMR (DMSO- d_6 , 400 MHz)

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solvent DMSO-d6 spin  not used
file   exp      spin  not used
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at     1.390 alfa  20.000
np     25528 flags
fb     not used 11  n
bs     1.000 dp   n
dl     1.000 0.1  y
nt     32 hs   nm
ct     32 PROCESSING nn
TRANSMITTER 1b   0.10
tn     H1 fn   65536
sfrq  399.855 DISPLAY
t0f    362.000
tpwr  57.000
pw    9.850 rfp  999.6
DECOUPLER   rfp  999.6
dn     C13 tp   115.2
dof    0 lp   -32.5
dm     nnn p   250
dss   c wc   250
dpwr  50 sc   0
dswf  15900 vs   33
th    nm cdc ph  20
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2-Hydroxyaniline: ^{13}C NMR (DMSO- d_6 , 100 MHz)

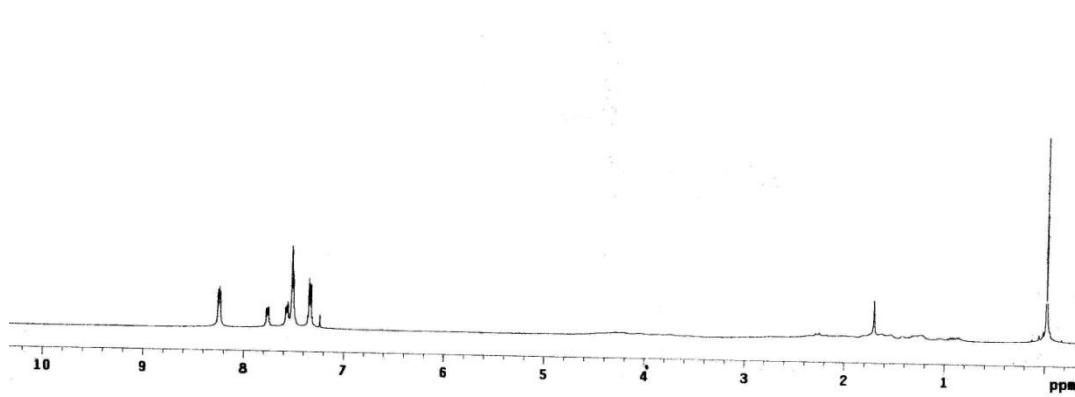
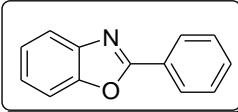
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over_13C
zpu1
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solvent DMSO-d6 spin  not used
file   exp      spin  not used
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np     50000 flags
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bs     300 0.1  n
dl     1.000 0.1  y
nt     5000 hs   nn
ct     672 PROCESSING nn
TRANSMITTER 1b   2.00
tn     C13 fn   65536
sfrq  100.554 DISPLAY
t0f    1536.3 sp   -1571.0
tpwr  65.000 rfp  25125.6
pw    9.300 rfp  3971.5
DECOUPLER   rfp  3971.5
dn     H1 rp   -28.1
dof    0 lp   -343.5
de     yyy w   250
dss   c wc   250
dpwr  42 sc   0
dswf  8900 vs   20
th    nm no ph  4
```



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

NK_SB_20C
expi s2pul

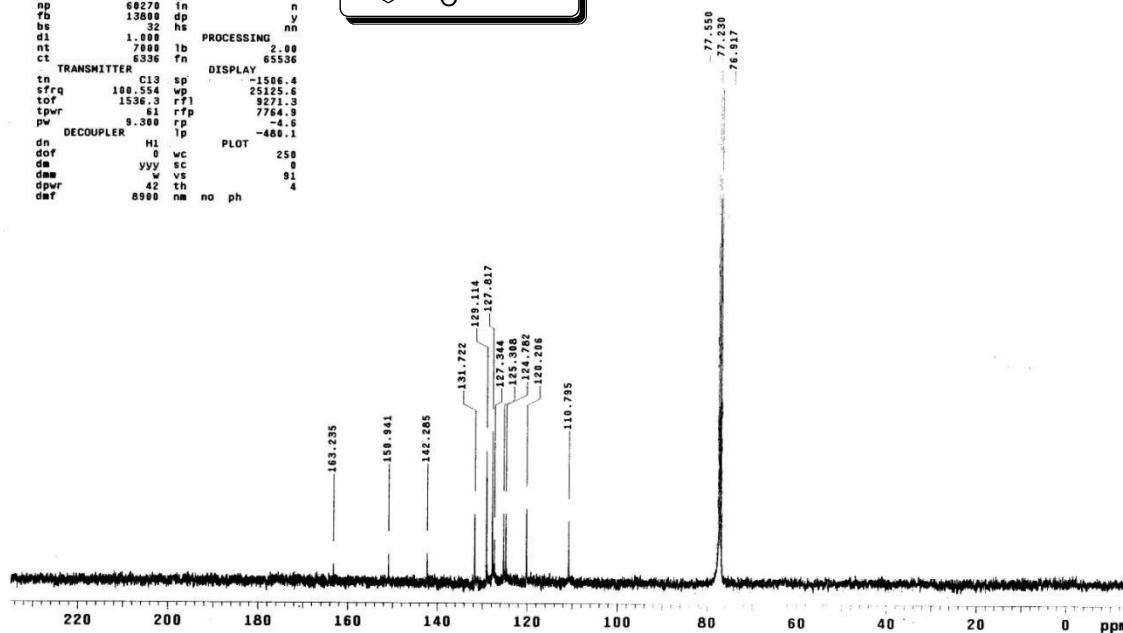
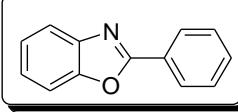
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date Feb 14 2012 temp not used
solvent CDCl₃ gain not used
file expi spin not used
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sw 6389.8 pw0 19.700
at 1.998 alfa 20.000
np 25528 FLAGS
fb not used 11 n
bs 4 in n
di 1.000 dp y
nt 32 hs nn
ct 32 PROCESSING nn
tn TRANSMITTER 1b 0.10
tn HI fn 65536
sfrq 398.453 DISPLAY
tot 362.8 sp -250.4
tpwr 57 wp 4828.0
pw 9.850 rfp 756.0
DECOUPLER C13 rfp 0
dn C13 rp 112.5
dof 0 rp -92.5
dm nnn PLOT
dme c wc 250
dpwr 50 sc 0
dfr 15900 vs 81
nm cdc ph 59



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

NK_SB_20C_13C
expi s2pul

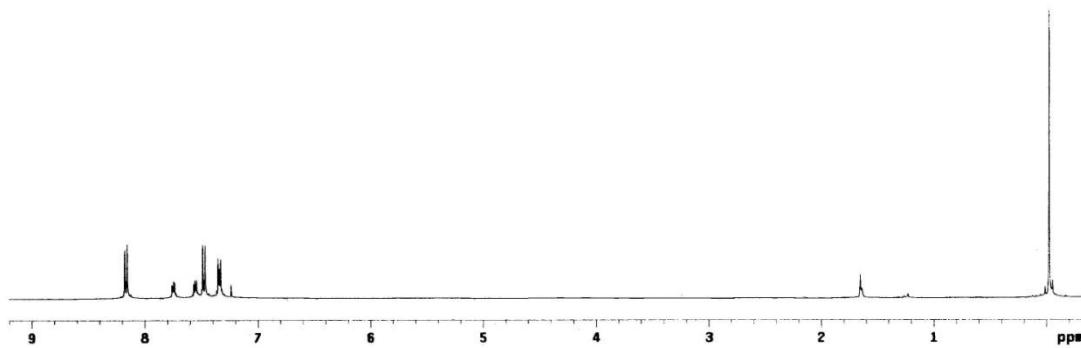
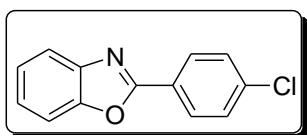
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date Jan 30 2012 temp not used
solvent CDCl₃ gain not used
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c13temp/NK_SB_20C-.hst 0.000
13C.fid pw0 18.600
ACQUISITION time 20.000
sw 25125.6 FLAGS
at 1.189 11 n
np 68270
nt 13800 dp n
bs 32 hs nn
di 1.000 PROCESSING
nt 7000 1b 2.00
ct 6336 fn 65536
tn TRANSMITTER 1b DISPLAY
sfrq 100.554 wp 25125.6
tot 1536.0 rfp 9271.3
tpwr 61 rfp 7700.0
pw 9.300 ip -44.6
DECOUPLER C13 sp -1506.4
dof 0 wc 250
dm vyy sc 0
dme w vs 91
dpwr 42 th 4
dfr 8900 nm no ph



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

```
HKRS_S2B11
SAMPLE   9_2812 temp    not used
solvent   CDCl3 gain     not used
file      exp spin    not used
ACQUISITION hst pw00    0.008
av        256.0 pw90    13.700
at        1.000 alfa   20.000
np        255.6   FLAGS
rb        not used 11    n
bs        4       in
dt        1.000 dp    y
nt        32      hs
ct        32      nn
PROCESSING
TRANSMITTER Cl3 rfp   0.10
tn        H1 fn    65536
sfrq    399.853 DISPLAY
tof      362.8 sp    -148.3
tpwr    57    wp    3828.5
pw      9.858 t1    3890.1
DECOUPLER C13 rfp   2894.0
dn        C13 rfp   113.0
dof      0    ip    -93.3
de        nuc   PLOT
dme      c    wc    250
dpwr    58    sc    0
dsf      15900 th    5
nm      cdc ph

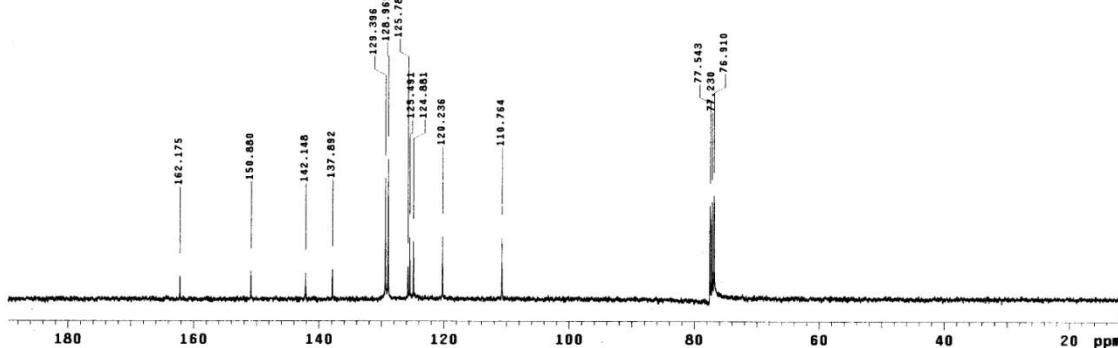
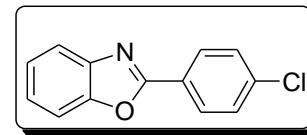
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2-(4-Chlorophenyl)benzo[d]oxazole (3aa): ^{13}C NMR (CDCl_3 , 100 MHz)

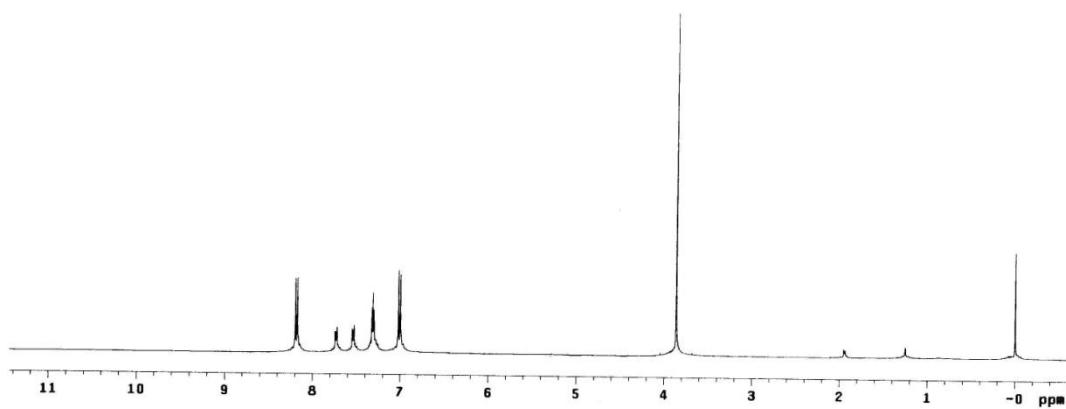
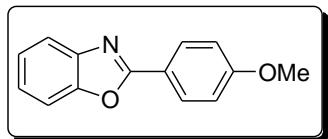
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expi s2pul
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date     Feb 9 2012  tof      16.600
solvent  CDCl3 gain     not used
file      exp spin    not used
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av        256.0 pw90    20.000
at        1.159 alfa   16.600
np        60270   FLAGS
rb        13800 11    n
bs        32      in
dt        1.000 dp    y
nt        5000 hs
ct        1312   PROCESSING
TRANSMITTER Cl3 rfp   2.00
tn        H1 fn    65536
sfrq    100.554 DISPLAY
tof      1536.3 sp    1098.4
tpwr    61    wp    1729.7
pw      9.300 t1    927.4
DECOUPLER C13 rfp   7764.9
dn        H1 rfp   -112.0
dof      0    ip    -271.4
de        yyy   PLOT
dme      w    wc    250
dpwr    42    sc    0
dsf      8900 vs    31
nm      no ph

```



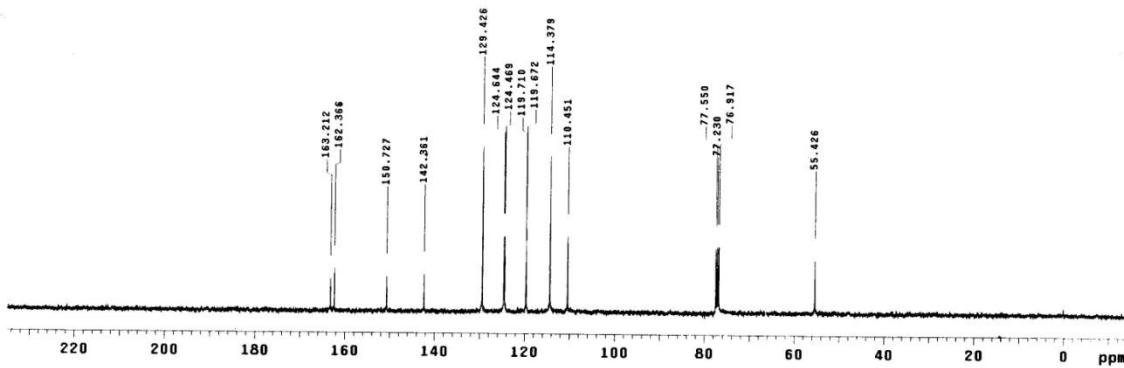
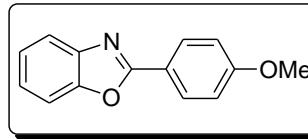
2-(4-Methoxyphenyl)benzo[d]oxazole (4aa): ^1H NMR (CDCl_3 , 400 MHz)

NK_SB_27
expi s2pul
SAMPLE SPECIAL
date Feb 14 2012 temp not used
solvent CDCl₃ gain not used
file exp spin not used
ACQUISITION hst 0.008
sw 6389.8 pw0 15.700
at 1.998 alfa 20.000
np 256 flags
fb not used 11 n
bs 4 in n
dt 1.000 dp y
nt 32 hs nn
ct 32 PROCESSING 0.10
tn TRANSMITTER 1b 0.10
tn H1 fn 65536
sfrq 399.853 DISPLAY -250.4
tof 362.8 sp
tpwr 57 wp 4828.0
pw 9.450 v1 796.0
DECOUPLER rfp 0
dn C13 rp 112.5
dof 0 ip -92.5
de nnn PLOT
dss c wc 250
dpwr 50 sc 0
dprv 15900 vs 81
th 59 nm cdc ph



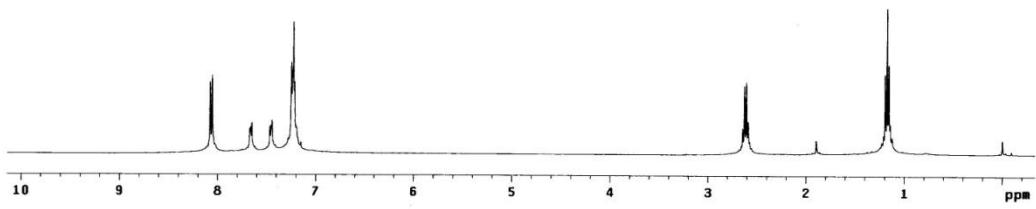
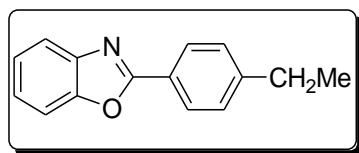
2-(4-Methoxyphenyl)benzo[d]oxazole (4aa): ^{13}C NMR (CDCl_3 , 100 MHz)

SB_27_13C
expi s2pul
SAMPLE SPECIAL
date Feb 16 2012 temp 2.00
solvent CDCl₃ gain not used
file exp spin not used
ACQUISITION hst 0.008
sw 2025.6 pw0 18.600
at 1.159 alfa 20.000
np 60270 flags
fb 13800 11 n
bs 32 in n
dt 1.000 dp y
nt 5000 hs nn
ct 832 PROCESSING 2.00
tn TRANSMITTER 13C 1b 65536
tn H1 fn 65536
sfrq 100.554 DISPLAY -1517.2
tof 1536.3 sp 25125.6
tpwr 61 wp 5221.1
pw 9.300 v1 7764.9
DECOUPLER rfp -78.1
dn 0 ip -320.7
dss yw PLOT
dss yw wc 250
dpwr 42 sc 0
dprv 8500 vs 37
th 3 nm no ph



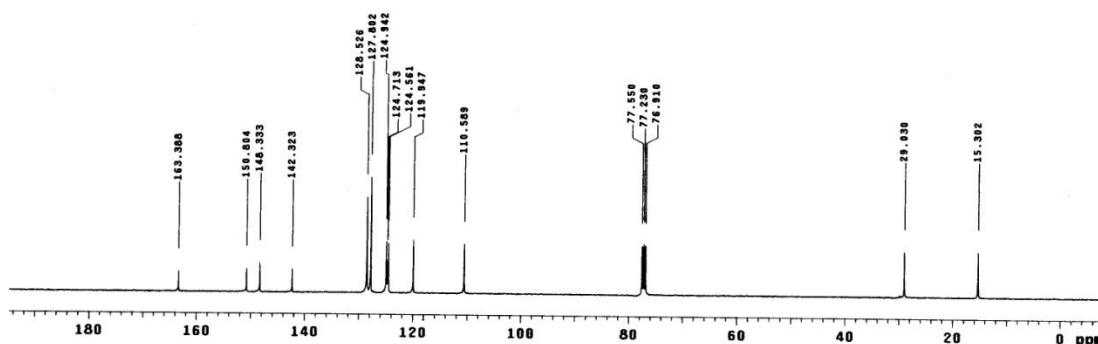
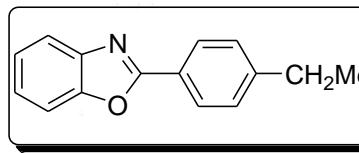
2-(4-Ethylphenyl)benzo[d]oxazole (5aa): ^1H NMR (CDCl_3 , 400 MHz)

```
NK_SB_42_1H
exptl s2pul
SAMPLE SPECIAL
date Apr 6 2012 temp not used
solvent CDCl3 gain not used
filet EXP in not used
ACQUISITION hst 0.008
sw 6388.8 pw90 15.700
at 1.000 25520 alfa FLAGS
np 64 ns nm
rb not used 11 n
dec 1.000 0.00 y
dt 1.000 0.00 y
nt 64 ns nm
ct 64 PROCESSING
TRANSMITTER H1 fn 0.10
tn H1 fn 65536
sfrq 399.853 DISPLAY
tot 362.5 sp -133.2
tpwr 57 wp 4189.7
pw 9.859 rfp 838.3
DECOUPLER C13 rp 104.5
dn C13 rp 104.5
dof 0 1p -67.7
dss mnn wc PLOT
dss 0 250
dpwr 50 sc 0
dmf 15900 vs 35
dmf 15900 th 26
nm cdc ph
```



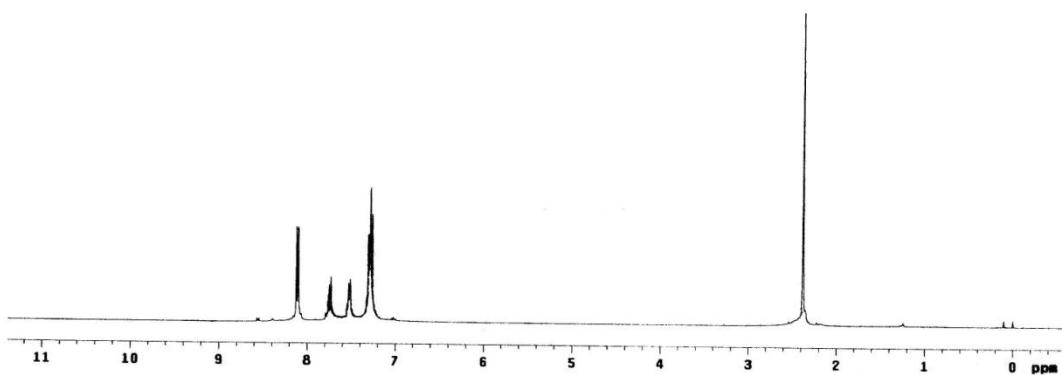
2-(4-Ethylphenyl)benzo[d]oxazole (5aa): ^{13}C NMR (CDCl_3 , 100 MHz)

```
_SB_42_13C
exptl s2pul
SAMPLE SPECIAL
date Apr 26 2012 temp not used
solvent CDCl3 gain not used
filet EXP in not used
ACQUISITION hst 0.008
sw 25125.6 pw90 15.698
at 1.000 25520 alfa FLAGS
np 60278 11 n
rb 13000 32 in n
dec 1.000 0.00 y
nt 12888 ns nm
ct 7840 PROCESSING
TRANSMITTER H1 fn 2.00
tn C13 fn 65536
sfrq 100.554 DISPLAY
tot 1536.3 sp -887.6
tpwr 61 wp 28535.6
pw 3.300 rfp 5279.8
DECOUPLER C13 rp 7744.9
dn H1 rp -67.0
dof 0 1p -318.1
dss y 1p PLOT
dss w wc 250
dpwr 42 sc 0
dmf 8500 vs 26
dmf 8500 th 2
nm no ph
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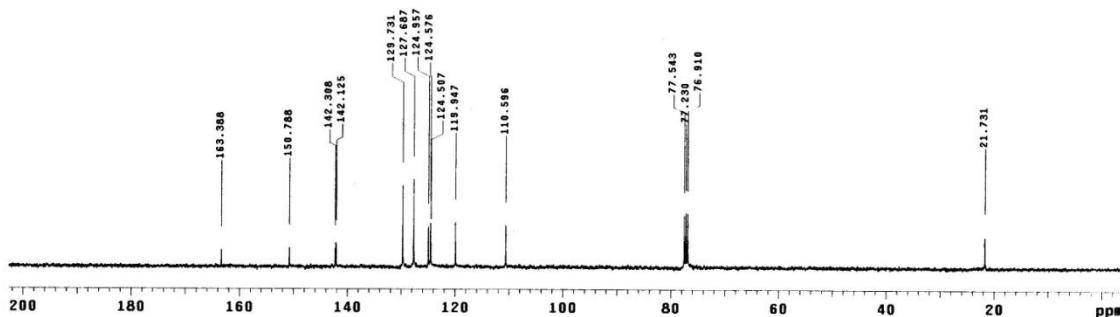
2-p-Tolylbenzo[d]oxazole (6aa): ^1H NMR (CDCl_3 , 400 MHz)

NK_SKR_31_1H
expt s2pu1
SAMPLE SPECIAL
date Feb 23 2012 temp not used
solvent CDCl₃ gain not used
file exp spin not used
ACQUISITION hst 20.000
sw 6389.8 pw08 19.700
et 1.580 alfa 20.000
np 32728 r1 20.000
fb not used 11 flags
bs 4 in n
sl 1.000 sp y
st 32 nn
ct 32 PROCESSING
TRANSMITTER H1 f1 0.10
tn H1 f1 0.536
sfrq 399.853 DISPLAY
tof 382.8 sp -224.6
tpwr 51 w0 477.5
pw 9.858 r1 0.000
DECOUPLER rfp 0
dn C13 rp 125.4
dof 0 ip -195.2
de nnn PLOT
dm c wc 250
dpwr 50 tc 0
dmt 15900 vs 74
nm cdc ph 20



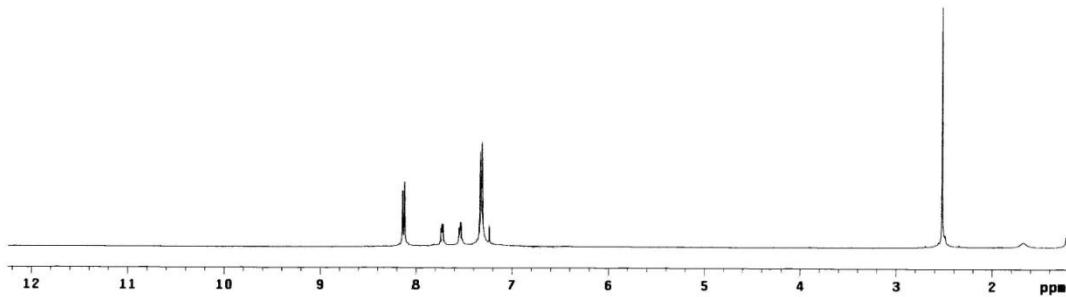
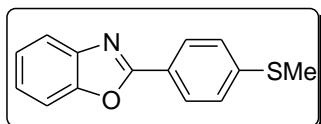
2-p-Tolylbenzo[d]oxazole (6aa): ^{13}C NMR (CDCl_3 , 100 MHz)

NK_SKR_31_13C
expt s2pu1
SAMPLE SPECIAL
date Feb 23 2012 temp not used
solvent CDCl₃ gain not used
file exp spin not used
ACQUISITION hst 0.000
sw 25125.6 pw08 18.600
et 1.189 alfa 20.000
np 66270 flags
fb 13800 11 n
bs 1.000 in n
sl 1.000 dp y
nt 5000 hs nn
ct 544 PROCESSING
TRANSMITTER H1 f1 2.00
tn C13 f1 0.536
sfrq 100.554 DISPLAY
tof 1536.3 sp -492.0
tpwr 61 w0 2000.1
pw 9.300 r1 9279.6
DECOUPLER rfp 7764.9
dn H1 rp -55.1
dof 0 ip -373.8
de vvy wc 250
dm 42 sc 0
dpwr 8900 vs 20
dmt 8900 th 3
nm no ph



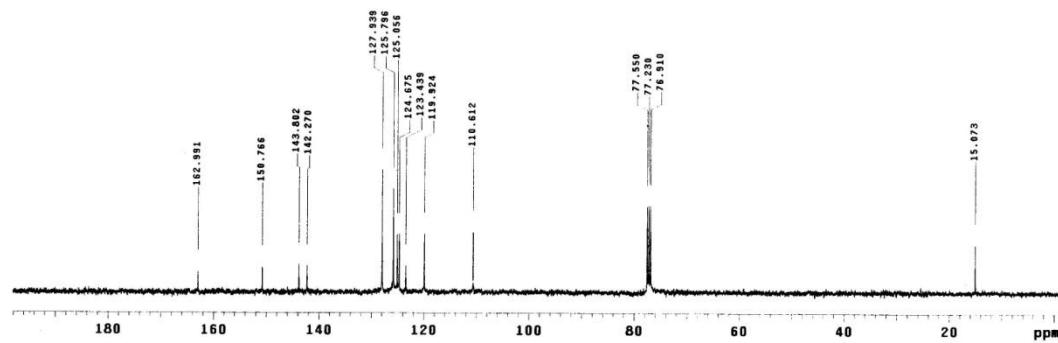
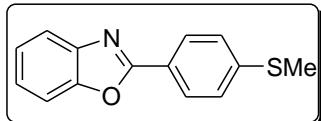
2-(4-(Methylthio)phenyl)benzo[d]oxazole (7aa): ^1H NMR (CDCl_3 , 400 MHz)

NK_SB_37_1H
expt s2pul
SAMPLE SPECIAL
date Mar 28 2012 temp not used
solvent CDCl₃ gain not used
file exp gain not used
ACQUISITION hst 0.000
sw 6389.8 pw0 19.700
at 25528 alfa 20.000
np 1 25528 FLAGS
fb not used 11 n
bs 1.000 ap n
dti 1.000 pp y
nt 32 hs nn
ct 32
PROCESSING
TRANSMITTER H1 fn 8.10
tn 399.853 DISPLAY
tot 367.5 sp 472.2
tpwr 57 442.5
pw 9.850 rfp 3698.9
DECOUPLER C13 fp 2894.9
dn C13 12 11.0
dof 0 -92.0
dm nnn 0 p
dss w 250
dpwv 50 c 0
def 15900 vs 57
nm cdc ph 6

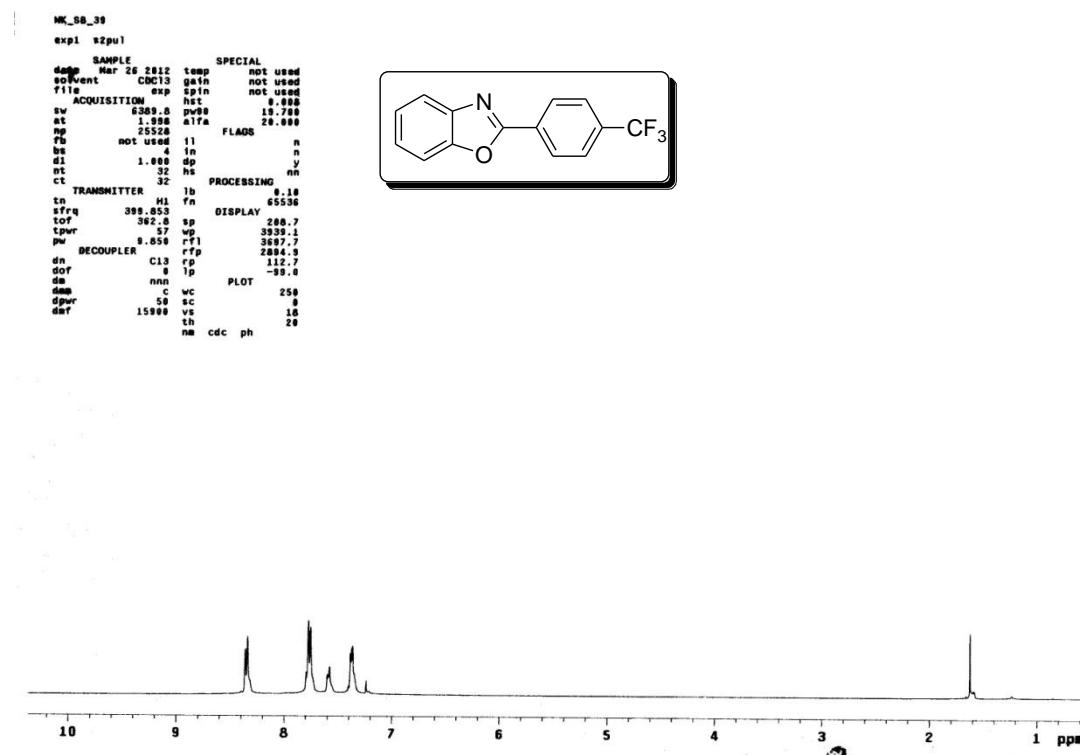


2-(4-(Methylthio)phenyl)benzo[d]oxazole (7aa): ^{13}C NMR (CDCl_3 , 100 MHz)

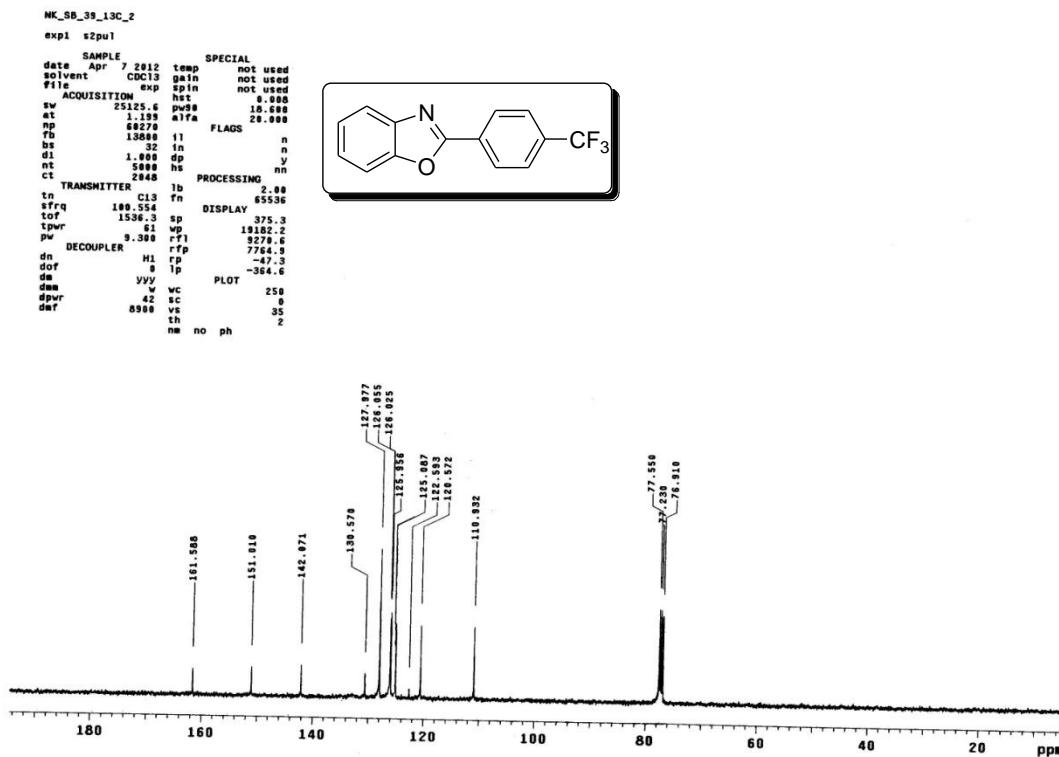
NK_SB_37_13C
expt s2pul
SAMPLE SPECIAL
date Mar 21 2012 temp not used
solvent CDCl₃ gain not used
file exp gain not used
ACQUISITION hst 0.000
sw 25125.6 pw0 16.600
at 1.125 20.000
np 6370 0.000
fb 13800 11 n
bs 10 in n n
dti 1.000 pp y
nt 5000 hs nn
ct 800
PROCESSING
TRANSMITTER C13 fn 2.00
tn 100.554 DISPLAY
tot 1536.3 sp -192.9
tpwr 40 200.9
pw 9.300 rfp 3270.2
DECOUPLER rfp 7764.9
dn H1 fp -81.0
dof 0 1p -299.0
dm vyy 0 p
dss w 250
dpwv 42 c 0
def 8900 vs 29
nm no ph 4



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



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

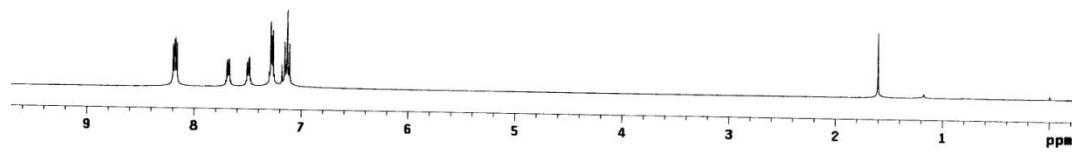
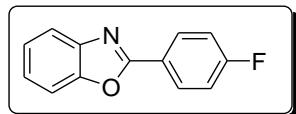


2-(4-Fluorophenyl)benzo[d]oxazole (9aa): ^1H NMR (CDCl_3 , 400 MHz)

NK-SB-40-1H

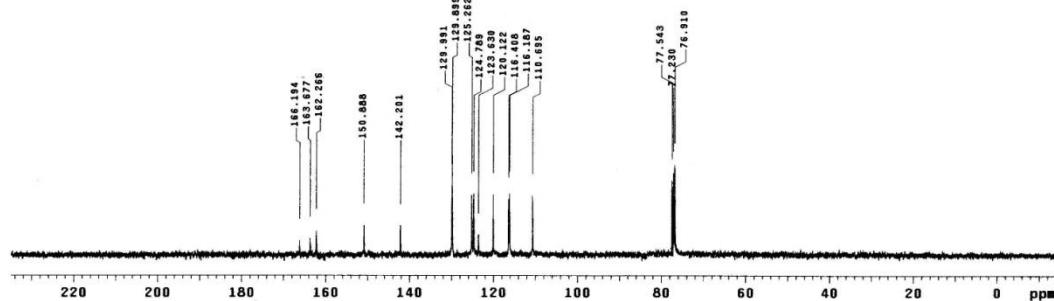
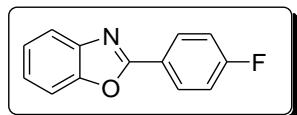
STANDARD IN OBSERVE

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solvent CDCl₃ gain not used
file exp spin not used
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at 1.995 alfa 20.000
nd 23864 flags
fb not used 11 n
bs 4 in n
di 1.000 dp y
nt 32 ns
ct 32 PkPROCESSING not used
tn TRANSMITTER H1 DISPLAY
sfrq 399.852 sp -104.8
t0f 8 wp 3993.4
tpwr 57 rrf1 996.4
pw 7.000 rfp 0
DECOUPLER C13 fp -98.1
dn 0 PLOT
d0f 0
ds nm wC 250
dss c sc 0
dpwr 50 vs 18
def 15900 th 20
nm cdc ph



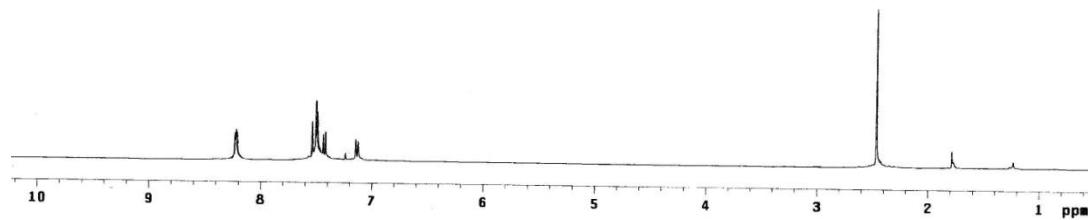
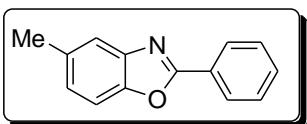
2-(4-Fluorophenyl)benzo[d]oxazole (9aa): ^{13}C NMR (CDCl_3 , 100 MHz)

_J3C
szpul
SAMPLE SPECIAL
date Apr 3 2012 temp not used
solvent CDCl₃ gain not used
file exp spin not used
ACQUISITION hst 0.008
sw 25125.6 pw98 18.680
at 1.995 alfa 20.000
nd 60270 flags
fb 13800 11 n
bs 32 in
di 1.000 dp y
nt 5000 hs nm
ct 1280 PROCESSING 0.00
tn TRANSMITTER C13 H1 65536
sfrq 108.554 DISPLAY
t0f 1538.3 sp 1589.5
tpwr 8.000 fp 25125.6
pw 9.300 rrf1 9274.4
DECOUPLER H1 rfp 7764.9
dn 8 YYY fp -183.2
d0f 8 PLOT
ds w wC 250
dpwr 8989 vs 23
def 8989 th 3
nm no ph



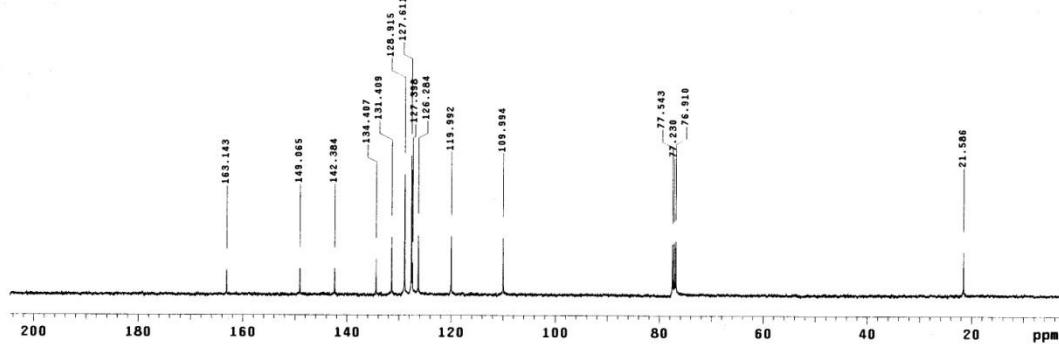
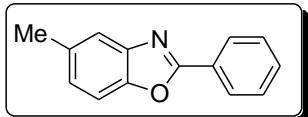
5-Methyl-2-phenylbenzo[*d*]oxazole (10aa): ^1H NMR (CDCl_3 , 400 MHz)

NK_SB_25
expt s2pul
SAMPLE SPECIAL
date Feb 11 2012 temp not used
solvent CDCl₃ gain not used
file exp in not used
ACQUISITION hst 0.006
sw 6389.8 pw90 19.700
at 1.000 25.280
np 25228 FLAGS
fb not used 11 n
bs 4 1.000
dt 1.000 32 y
nt 32 hs nn
ct 32 PROCESSING
TRANSMITTER lb 0.10
tn HI fn 65536
sfrq 399.853 DISPLAY
tof 362.8 sp 293.8
tpwr 57 wp 3895.8
pw 9.850 r71 3495.5
DECOUPLER rfp 2894.9
dn C13 rp 112.7
dof nnn lp -90.2
dm c wc 250
dpwr 59 sc 0
dmt 15900 vs 37
th 20
nm cdc ph



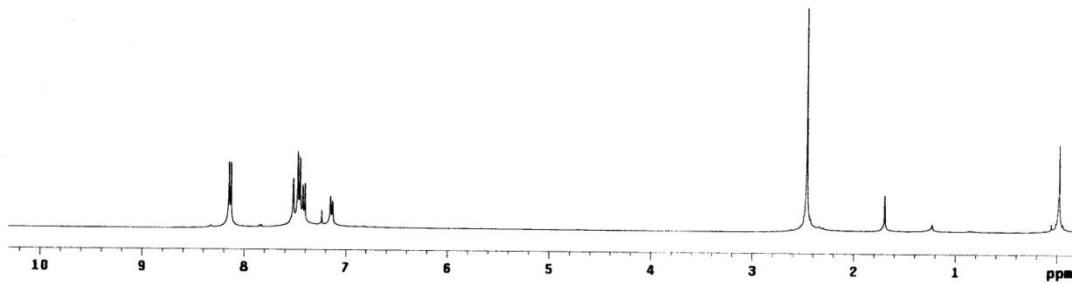
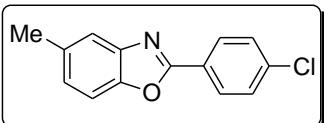
5-Methyl-2-phenylbenzo[*d*]oxazole (10aa): ^{13}C NMR (CDCl_3 , 100 MHz)

NK_SB_25_13C
expt s2pul
SAMPLE SPECIAL
date Feb 13 2012 temp not used
solvent CDCl₃ gain not used
file exp in not used
ACQUISITION hst 0.006
sw 25125.6 pw90 18.600
at 1.000 62.700
np 62.700 FLAGS
fb 13600 11 n
bs 32 in
dt 1.000 5000 y
nt 5000 hs nn
ct 1164 PROCESSING
TRANSMITTER lb 2.00
tn C13 rp 65536
sfrq 100.554 DISPLAY
tof 1536.3 sp 231.9
tpwr 57 wp 2895.8
pw 9.300 r71 9282.6
DECOUPLER rfp 7764.9
dn HI rp -86.9
dof 8 rp -525.0
dm vvv wc 250
dpwr 42 sc 0
dmt 6900 vs 33
th 5
nm no ph



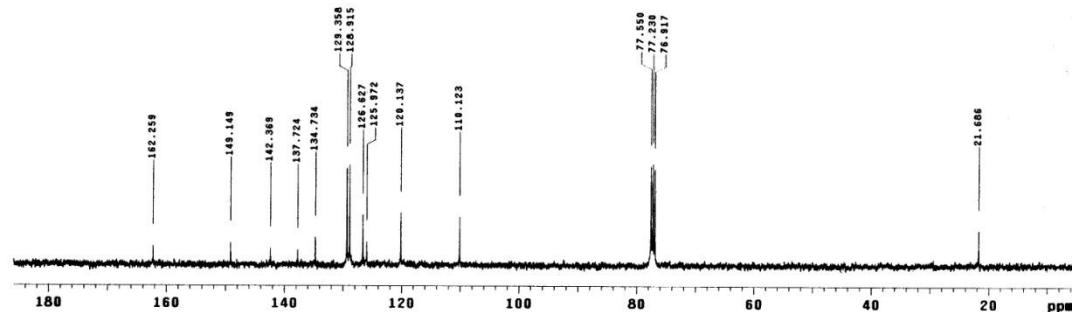
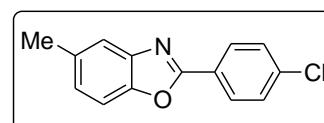
2-(4-Chlorophenyl)-5-methylbenzo[d]oxazole (11aa): ^1H NMR (CDCl_3 , 400 MHz)

NK-SB-26
exp1 s2pul
SAMPLE: 2-(4-Chlorophenyl)-5-methylbenzo[d]oxazole
SPECIAL:
date Feb 16 2012 temp not used
solvent CDCl₃ gain not used
file exp spin not used
ACQUISITION hst 0.008
sw 6383.5 pw0.5 15.788
at 1.000 3516 20.000
np 25528 flags
rb not used 11 n
bs 1.000 1m n
dt 1.000 dp y
nt 32 hs nn
ct 32 PROCESSING nn
TRANSMITTER lb 0.18
tn H1 fn 65536
sfrq 399.853 DISPLAY 65536
tot 360.0 sp -81.7
tpwr 9.850 rrf1 4286.5
pw 9.850 rrf1 3658.5
DECOUPLER C13 rrf1 2894.9
dn C13 0 185.0
dof 0 1p -07.1
de nnn PLOT
dme v c 250
dpwr 58 sc 0
dft 15900 vs 52
nm cdc ph 20
nm cdc ph



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

NK-SB-26
exp1 s2pul
SAMPLE: 2-(4-Chlorophenyl)-5-methylbenzo[d]oxazole
SPECIAL:
date Feb 21 2012 temp not used
solvent CDCl₃ gain not used
file exp spin not used
ACQUISITION hst 0.008
sw 25025.6 pw0.5 16.680
at 1.188 60278 flags
rs 13884 11 n
bs 32 1m n
dt 1.000 dp y
nt 58000 nn
ct 896 PROCESSING nn
TRANSMITTER lb 2.00
tn C13 fn 65536
sfrq 100.533 DISPLAY 472.7
tot 1532.3 sp 472.7
tpwr 61 rrf1 18224.5
pw 9.300 rrf1 9272.9
DECOUPLER C13 rrf1 7744.9
dn H1 0 40.2
dof 0 1p -398.6
de vvv PLOT
dme v c 250
dpwr 42 sc 0
dft 8900 vs 24
nm no ph 2

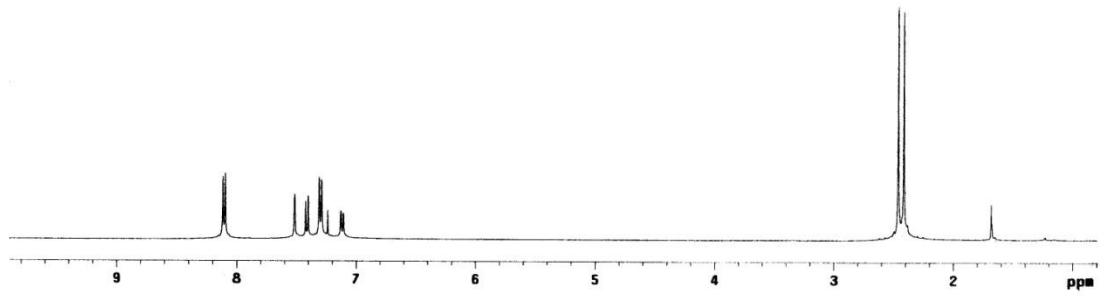
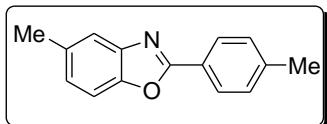


5-Methyl-2-p-tolylbenzo[d]oxazole (12aa): ^1H NMR (CDCl_3 , 400 MHz)

```
NK_BB_29
expl stdpp1

SAMPLE          SPECIAL
date  Mar 3 2012 temp  not used
solvent   CDCl3 gain  not used
file    exp spin  not used
      ACQUISITION hist  not used
      sw 6369.8 pw90 15.798
      at 1.998 alfa 28.880
      np 256sc 252sc FLAGS
      fb not used 1l n
      d1 4 in n
      dt 1.000 dp y
      nt 32 n n
      ct 32 PROCESSING nn

      TRANSMITTER 1b fn 0.10
      tn HI fn 65536
      sfrq 399.853 DISPLAY
      tof 362.8 sp 313.4
      tpowr 57 wp 3652.5
      pw 9.850 r1 3881.1
      DECOUPLER C13 rfp 2694.3
      dn C13 rfp 108.4
      dof 0 1p -87.4
      os nm not used
      ds c wc 250
      dpwr 50 sc 0
      daf 15888 vs 53
      th 20
      nm cdc ph
```

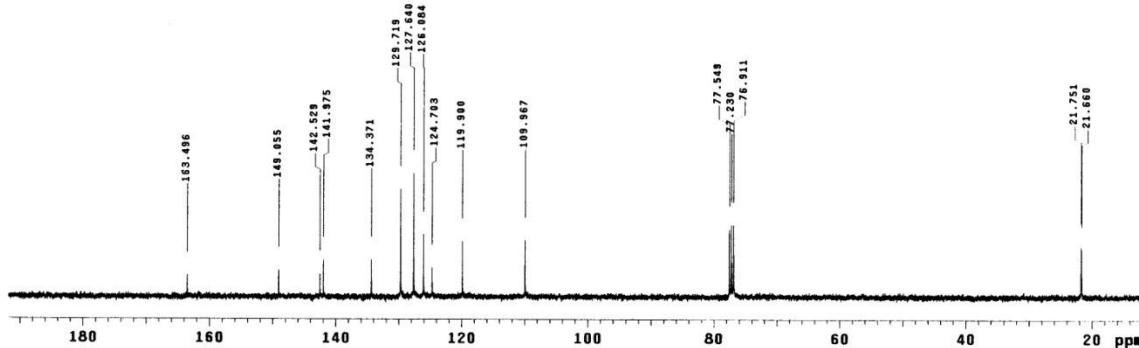
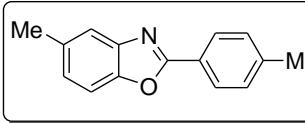


5-Methyl-2-p-tolylbenzo[d]oxazole (12aa): ^{13}C NMR (CDCl_3 , 100 MHz)

```
_SB_29_13C
expl std13c

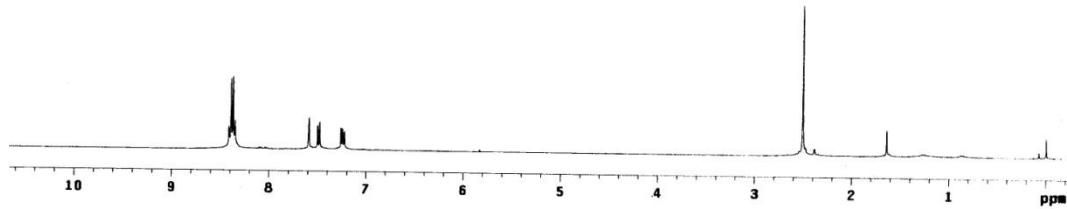
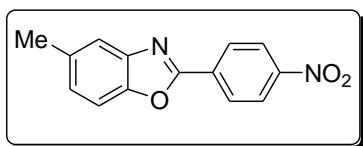
SAMPLE          SPECIAL
date  Mar 4 2012 temp  not used
solvent   CDCl3 gain  not used
file    exp spin  not used
      ACQUISITION hist  not used
      sw 25000.0 pw90 18.668
      at 1.193 alfa 20.080
      np 512sc 512sc FLAGS
      fb 13880 32 in n
      d1 3000 dp y
      nt 32 hs n
      ct 32 PROCESSING nn

      TRANSMITTER 1b fn 1.00
      tn C13 fn not used
      sfrq 100.552 DISPLAY
      tof 0 sp 1121.0
      tpowr 61 wp 18166.1
      pw 8.667 r1 10750.1
      DECOUPLER 8.667 rfp 7764.9
      dn HI rfp -41
      dof 0 1p -355.6
      os vyy not used
      ds v wc 250
      dpwr 42 sc 0
      daf 65880 vs 27
      th 3
      nm no ph
```



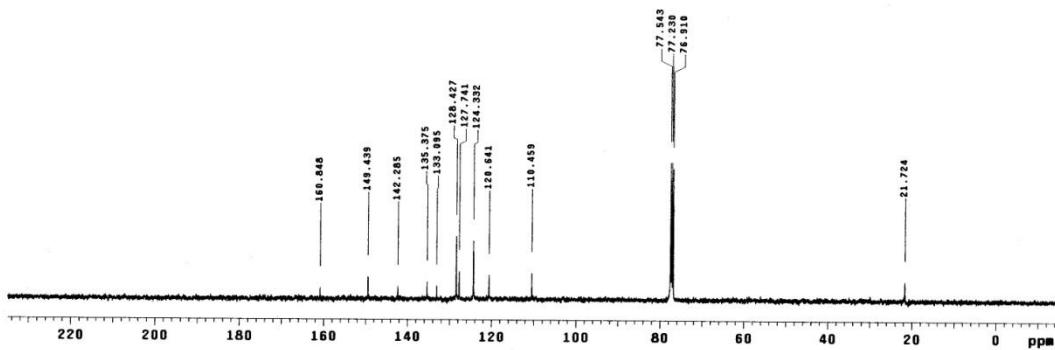
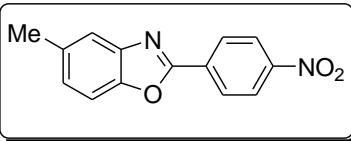
5-Methyl-2-(4-nitrophenyl)benzo[d]oxazole (13aa): ^1H NMR (CDCl_3 , 400 MHz)

```
NK_SB_33
expt s2pul
SAMPLE          SPECIAL
date  Mar  5 2012 temp  not used
solvent   CDCl3  gain  not used
file      exp spin  not used
ACQUISITION    pw100  time  0.008
sw       6389.5  pw90  15.700
at        1.998  alfa  28.000
np       256     t90p1  10
rb       not used  il   n
bs        4      in   n
nt       1.000  dp   y
nt       32    hs   nn
ct        32    PROCESSING
TRANSMITTER    lb   0.10
tn       C13  fn   65536
sfrq    399.853  DISPLAY
tof      362.8  sp   -105.5
tpwr    57    wp   4389.7
pw      9.050  r1   793.3
DECOUPLER     rfp  0
dn       C13  rp   113.8
dof      0      ip   -94.0
dme      c    wc   250
dpwr    50    sc   0
ddef    15900  tc   35
        th   20
        nm  cdc ph
```



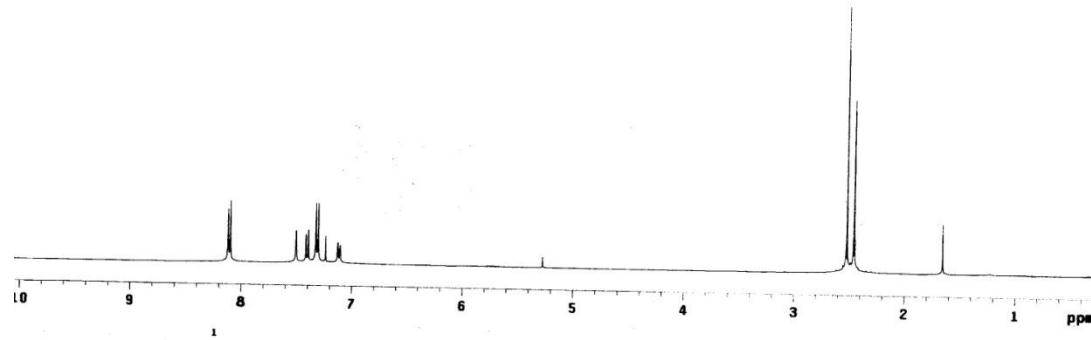
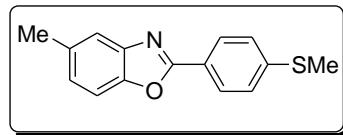
5-Methyl-2-(4-nitrophenyl)benzo[d]oxazole (13aa): ^{13}C NMR (CDCl_3 , 100 MHz)

```
NK_SB_33_13C
expt s2pul
SAMPLE          SPECIAL
date  Mar 16 2012 temp  not used
solvent   CDCl3  gain  not used
file      exp spin  not used
ACQUISITION    pw100  time  0.008
sw       25125.6  pw90  2.000
at        1.199  alfa  20.000
np       60278  t90p1  10
rb       not used  il   n
bs        4      in   n
nt       1.000  dp   y
nt       32    hs   nn
ct        1780  PROCESSING
TRANSMITTER    lb   2.00
tn       C13  fn   65536
sfrq    199.900  DISPLAY
tof      1536.3  sp   -1505.7
tpwr    61    wp   25125.6
pw      9.300  r1   7764.6
DECOUPLER     rfp  0
dn       H1  rp   -17.8
dof      0      ip   -419.6
dme      yw  wc   250
dpwr    42    sc   0
ddef    8900  tc   33
        th   20
        nm  no ph
```



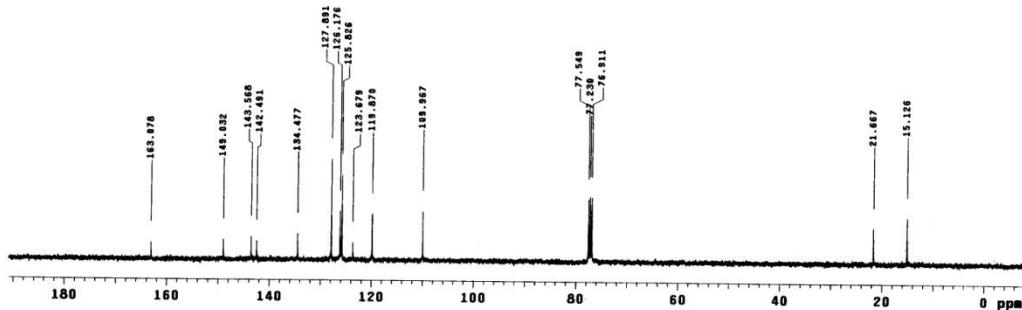
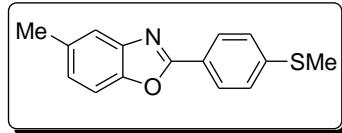
5-Methyl-2-(4-(methylthio)phenyl)benzo[d]oxazole (14aa): ^1H NMR (CDCl_3 , 400 MHz)

```
MM_08_35_1H
expt s2pul
SAMPLE      SPECIAL
date Mar 8 2012 temp    not used
solvent   CDCl3 gain    not used
file       exp spin    not used
ACQUISITION hst      0.005
sw        6380.5 pw1a   15.700
np        25528   flags
rf0      not used 11
bs        4   in     n
d1      1.000 dp     y
nt       32 hs     nn
ct        32 PROCESSING nn
TRANSMITTER lb      1.0
tn        H1 fn    65536
sfrq     399.853   DISPLAY
t0f      362.5   sp    95.0
t0vr    57.0   ap    50.0
pw       9.859   rfp   3698.3
DECOUPLER   C13 rfp   2894.9
dn        C13 rp    110.4
dof      8   ip    -36.3
da       nnn   PLOT
dme      c   wc    250
dpwr    50   tc    0
dmtf    15900 vs    61
        th    5
        nm cdc ph
```



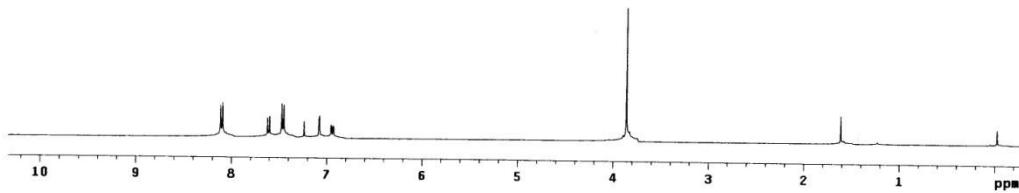
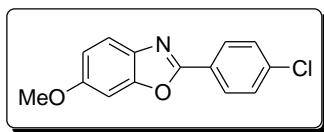
5-Methyl-2-(4-(methylthio)phenyl)benzo[d]oxazole (14aa): ^{13}C NMR (CDCl_3 , 100 MHz)

```
SB-35
expt std13c
SAMPLE      SPECIAL
date Mar 14 2012 temp    not used
solvent   CDCl3 gain    not used
file       exp spin    not used
ACQUISITION hst      0.005
sw        25000.0 pw1a   10.000
at       1.191   a1fa  25.000
np        55984   flags
rf0      13600.0   11    n
bs        10   in     n
d1      1.000 dp     y
nt       500 hs     nn
ct        2178 lb      1.00
TRANSMITTER C13 fn    not used
tn        H1 rp    -649.7
sfrq     100.552   DISPLAY
t0f      8   sp    -649.7
t0vr    61.0   wp    20835.2
pw       8.687   rfp   2884.5
DECOUPLER   C13 rfp   0
dn        H1 rp    -67.6
dof      8   ip    -323.6
da       vvv   PLOT
dme      w   wc    250
dpwr    40   tc    0
dmtf    8500 vs    25
        th    4
        nm no ph
```



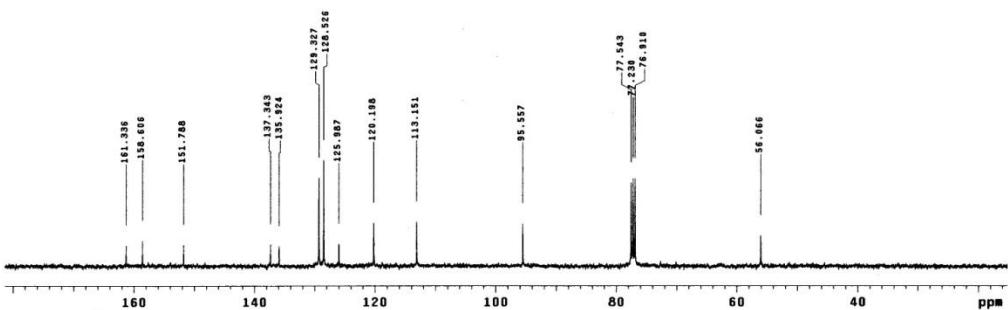
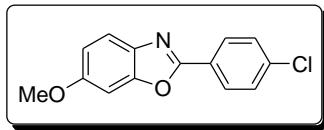
2-(4-Chlorophenyl)-6-methoxybenzo[d]oxazole (15aa): ^1H NMR (CDCl_3 , 400 MHz)

```
NK_SB_43_1H
exp1 s2pul
SAMPLE          SPECIAL
date   Apr  5 2012 temp    not used
solvent   CDCl3 gain    not used
file    exp spin   not used
ACQUISITION   hst    not used
sw      6389.8 pw90   19.798
at      1.100   alfa   0.008
np      25528   flags
fb      not used 11   n
bs      32      in     n
dl      1.000   dp     y
nt      32      hs     n
ct      32      PROCESSING
tn      TRANSMITTER lb     0.10
sfrq   399.0   H1    fm    65536
t0f    382.8   sp     -123.6
tpwr   57      wp    4257.0
pw     9.851   rF1    3698.5
        9.851   rF2    2891.1
decoupler C13   rFp   116.4
dof     0      ip     -85.7
da     3000   nme   PLOT
dme     0      wc    250
dpwr   50      sc     0
dref    15900  ve    32
        0      th     5
        nm cdc ph
```



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

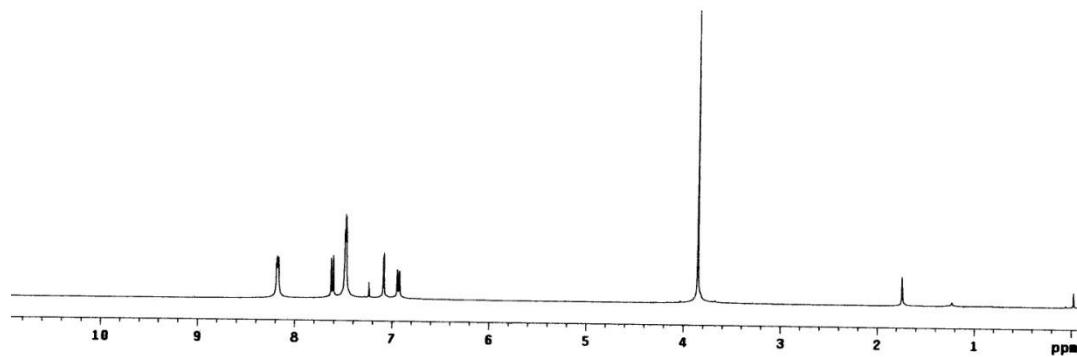
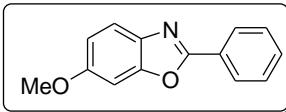
```
SB_43_13C
exp1 s2pul
SAMPLE          SPECIAL
date   Jul 28 2012 temp    not used
solvent   CDCl3 gain    not used
file    exp spin   not used
ACQUISITION   hst    not used
sw      25125.6 pw90   18.680
at      1.150   alfa   20.000
np      13600   flags
fb      32      in     n
bs      32      hs     n
dl      1.000   dp     y
nt      5000   hs     n
ct      1280   PROCESSING 2.00
tn      TRANSMITTER C13  fm    65536
sfrq   100.554   DISPLAY
t0f    1538.0   sp    1528.5
tpwr   51      wp    16796.2
pw     9.300   rF1    9273.6
        9.300   rF2    7749.9
decoupler C13   rFp   -54.5
dof     0      ip    -363.2
da     3000   vVY   PLOT
dme     0      wc    250
dpwr   42      sc     0
dref    8500  ve    26
        0      th     5
        nm no ph
```



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

NK_5B_44_1H
exp1 s2pul

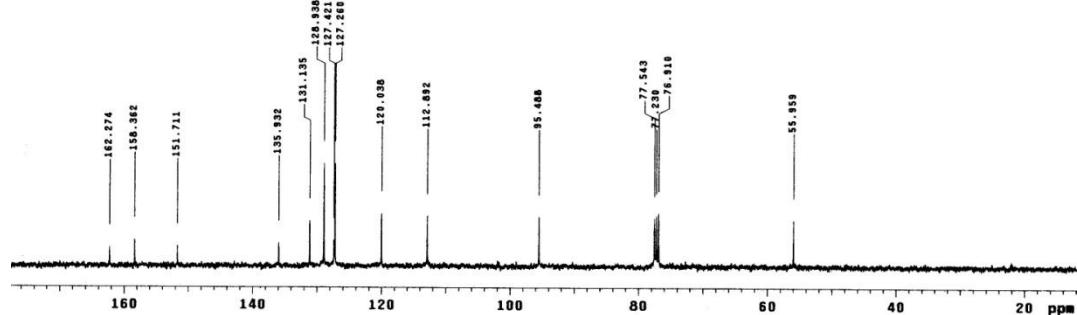
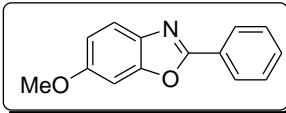
SAMPLE SPECIAL
date Apr 13 2012 temp not used
solvent CDCl₃ gain not used
file exp spin not used
ACQUISITION hz 6.400
sw 6389.8 pw98 15.700
at 1.199 alfa 20.000
np 25528 FLAGS
rb not used 11 n
bs 32 dp n
dt 1.000 y
nt 64 hs nn
ct 64 PROCESSING 2.00
TRANSMITTER lb 2.00
tn H1 fm 65536
sfrq 399.853 DISPLAY
tof 342.8 sp -47.7
tpwr 57 vp 4416.5
pv 8.858 rfp 3598.3
DECOUPLER C13 fp 2894.9
dn C13 ip 19.1
dof 8 lp -88.7
dss nnn PLOT
dme c wc 250
dpwr 42 sc 0
def 15988 vs 68
nm cdc ph 20



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

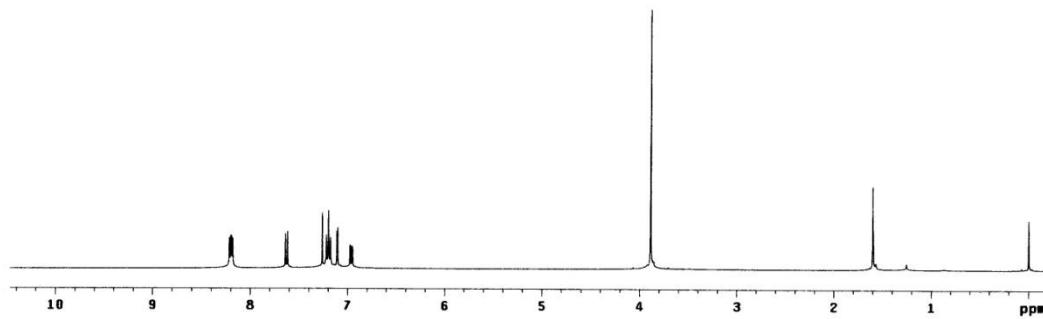
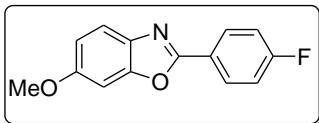
NK_5B_44_13C
exp1 s2pul

SAMPLE SPECIAL
date Apr 13 2012 temp 2.00
solvent CDCl₃ gain not used
file exp spin not used
ACQUISITION hz 6.400
sw 25125.6 pw98 10.000
at 1.199 alfa 20.000
np 4096 rfp 77.9
rb 13869 il n
bs 32 dp n
dt 1.000 y
nt 500 hs nn
ct 400 PROCESSING 2.00
TRANSMITTER C13 fm 65536
sfrq 100.554 DISPLAY
tof 1536.3 sp 1158.2
tpwr 61 vp 16805.1
pv 0.300 rfp 9248.5
DECOUPLER H1 fp 77.9
dn H1 ip -57.7
dof 8 lp -372.3
dss yyy PLOT
dme v wc 250
dpwr 42 sc 0
def 8988 vs 24
nm no ph 3



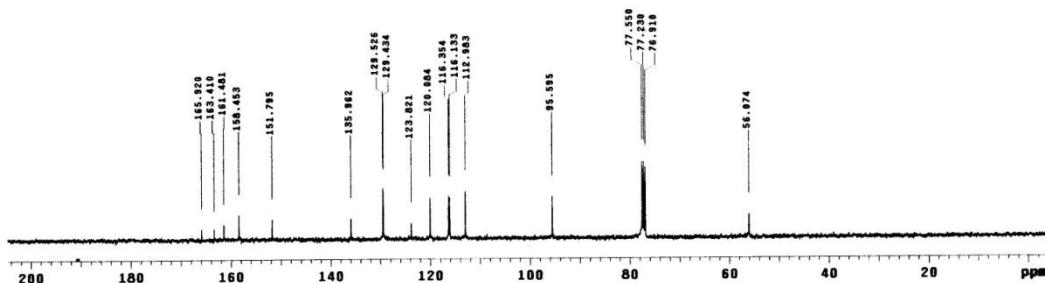
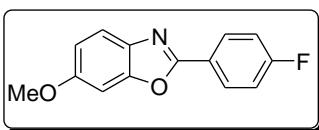
2-(4-Fluorophenyl)-6-methoxybenzo[d]oxazole (17aa): ^1H NMR (CDCl_3 , 400 MHz)

MR_08_45_1H
exp1 szpul
SAMPLE SPECIAL
date Apr 9 2012 temp not used
solvent CDCl₃ gain not used
file exp spin not used
ACQUISITION hst 8.888
sw 6389.0 pw90 19.700
at 1.000 alfa 20.000
np 25528 flags
fb not used 11 n
bs 1.000 dp y
dt 1.000 dp y
nt 64 hs nn
ct 64 PROCESSING nn
TRANSMITTER H1 fn 6.19
tn C13 rfp 65536
sfrq 399.853 DISPLAY
tot 362.6 sp -86.5
tpwr 57 wp 4273.8
pw 9.850 rf1 793.7
DECOUPLER C13 rfp 0
dn 0 1P 184.0
dof 0 1P -02.4
dm nnn PLOT
dme c wc 250
dpwr 50 sc 0
dmt 15900 vs 62
nm cdc ph 20



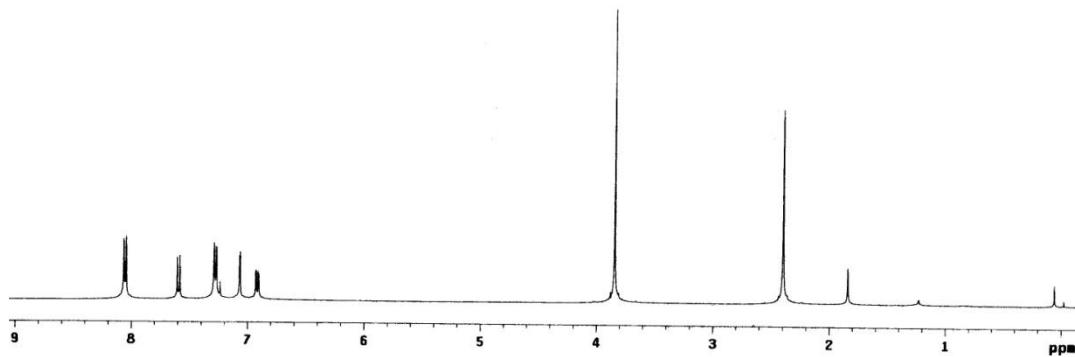
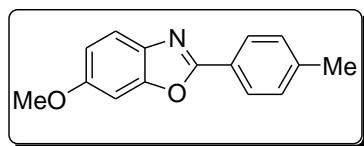
2-(4-Fluorophenyl)-6-methoxybenzo[d]oxazole (17aa): ^{13}C NMR (CDCl_3 , 100 MHz)

MR_08_45_13C_3
exp1 szpul
SAMPLE SPECIAL
date Jun 12 2012 temp not used
solvent CDCl₃ gain not used
file exp spin not used
ACQUISITION hst 8.888
sw 25125.6 pw90 19.888
at 60.199 pw16 25.000
np 60270 flags
fb 13880 11 n
bs 1.000 dp n
dt 1.000 dp y
nt 3800 hs nn
ct 1320 PROCESSING 2.00
TRANSMITTER H1 fn 65536
sfrq 100.550 DISPLAY
tot 1532.3 sp -452.1
tpwr 61 wp 21030.9
pw 9.390 rf1 7744.5
DECOUPLER C13 rfp 0
dn 0 1P -21.1
dof 0 1P -429.8
dm VVY PLOT
dme 42 wc 250
dpwr 8800 vs 18
dmt 8800 th 2
nm no ph



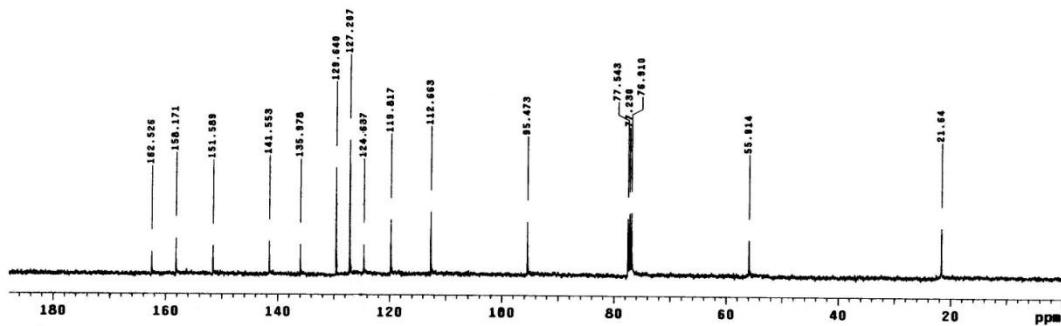
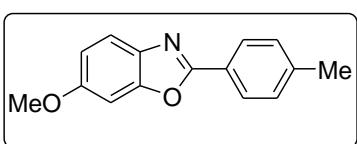
6-Methoxy-2-p-tolylbenzo[d]oxazole (18aa): ^1H NMR (CDCl_3 , 400 MHz)

```
MK_SB_40_1H
expi stdinh
SAMPLE          SPECIAL
date  Apr 18 2012 temp  not used
solvent   CDCl3  gain  not used
file    exp  spin  not used
        ACQUISITION het  8.000
        sw   6000.0  pw90  13.00
        at   1.395  201fa  20.00
        np   23984  FLAGs
        rb  not used  11  n
        bs   4  in  n
        di  1.000  dp  y
        nt   32  hs  nn
        ct   32  PROCESSING
        TRANSMITTER H1  not used
        tn   H1  DISPLAY
        sfrq  399.851  sp  -66.8
        tof   8  pw  371.0
        tpwr  57  rfp  3689.1
        pw   7.000  rfp  2894.9
        DECOUPLER C13  fp  87.5
        dn   C13  fp  -83.5
        dof   0  PLOT
        de   nnn  wc  250
        dmsc  c  sc  0
        dpwr  50  w  0
        def   15900  th  10
        nm  cdc  ph
```



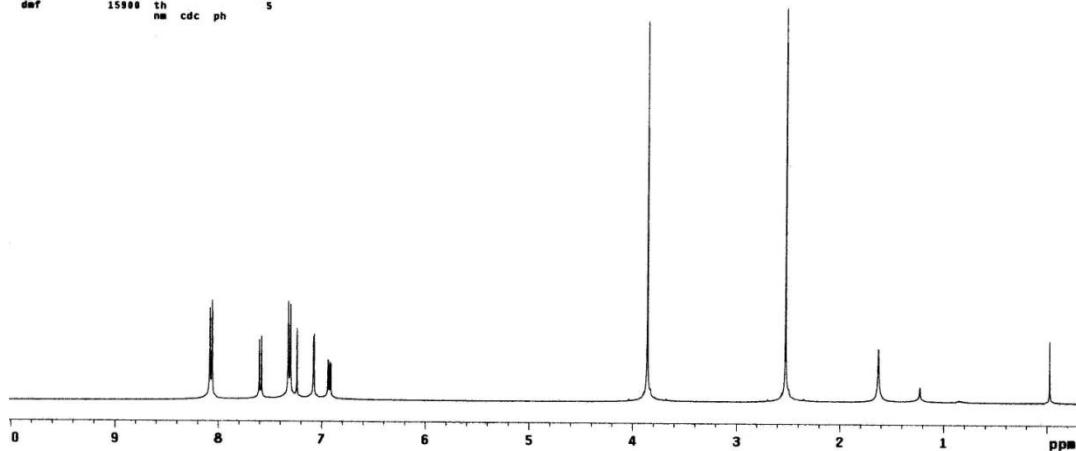
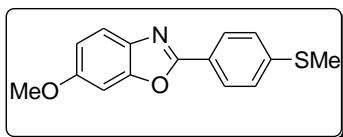
6-Methoxy-2-p-tolylbenzo[d]oxazole (18aa): ^{13}C NMR (CDCl_3 , 100 MHz)

```
_40_13C
s2pul
SAMPLE          SPECIAL
date  Apr 21 2012 temp  not used
solvent   CDCl3  gain  not used
file    exp  spin  not used
        ACQUISITION het  8.000
        sw   25125.6  pw90  10.000
        at   1.395  201fa  20.000
        np   64278  FLAGs
        rb  13888  11  n
        bs   32  in  n
        di  1.000  dp  y
        nt   32000  hs  nn
        ct   640  PROCESSING
        TRANSMITTER C13  1b  2.00
        tn   C13  fn  65536
        sfrq  100.554  DISPLAY
        tof   1536.3  sp  -64.1
        tpwr  62  wp  160.4
        pw   9.398  rfp  5221.3
        DECOUPLER H1  rfp  7784.9
        dn   H1  fp  -64.9
        dof   0  PLOT
        de   vvv  w  250
        dmsc  w  sc  0
        dpwr  42  w  0
        def   6500  th  31
        nm  no  ph
```



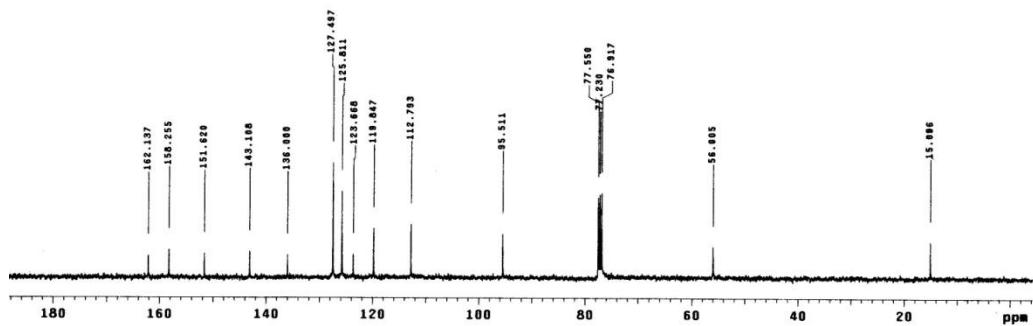
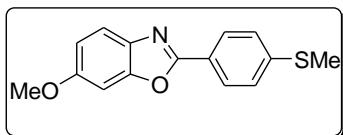
6-Methoxy-2-(4-(methylthio)phenyl)benzo[d]oxazole (19aa): ^1H NMR (CDCl_3 , 400 MHz)

NK_SB_47
expt stdih
SAMPLE SPECIAL
date Apr 18 2012 temp not used
solvent CDCl₃ gain not used
file exp spin not used
ACQUISITION hst 8.000
sw 6000.0 pw08 19.700
at 1.395 alfa 20.000
np 64 scan 128
fb not used 11 in n
bs 4 dp n
dt 1.800 dp y
nt 32 nn
ct 32 PROCESSING
TRANSMITTER fm not used
tn HI DISPLAY
sfrq 399.053 sp -129.5
tof 0 wp 4182.5
tpwr 57 rfp 3868.7
pw 7.000 rfp 20.000
DECOUPLER rfp 94.8
dn C13 1p -76.9
dof 0 PLOT
de mm wc 250
dme c sc 8
dpwr 50 vs 90
def 15000 th 5
nm cdc ph



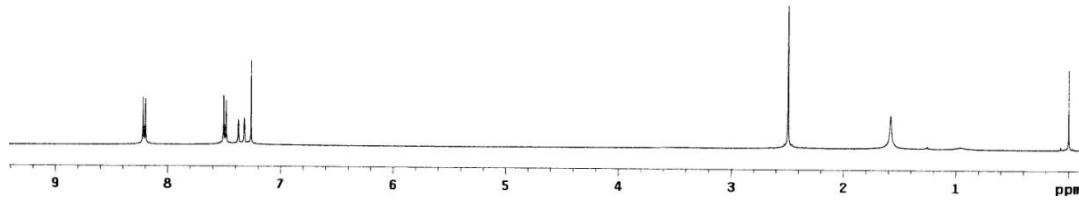
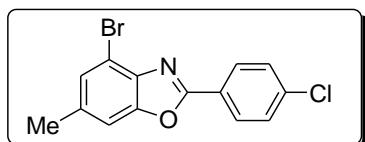
6-Methoxy-2-(4-(methylthio)phenyl)benzo[d]oxazole (19aa): ^{13}C NMR (CDCl_3 , 100 MHz)

NK_SB_47_13C
expt z2pu1
SAMPLE SPECIAL
date Apr 21 2012 temp not used
solvent CDCl₃ gain not used
file exp spin not used
ACQUISITION 25125.6 pw08 16.000
sw 6027.8 pw08 16.000
at 1.193 alfa 20.000
np 6027.8 scan 128
fb 1304 11 in n
bs 32 in n
dt 1.800 dp y
nt 512 nn
ct 1184 PROCESSING
TRANSMITTER lb 2.00
tn C13 fm 5536
sfrq 108.554 DISPLAY
tof 1536.3 sp -424.5
tpwr 61 wp 19390.0
pw 9.300 rfp 3774.5
DECOUPLER rfp 7764.5
dn HI rfp -78.8
dof 0 PLOT
de VVY wc 250
dme c sc 8
dpwr 42 vs 28
def 4500 th 4
nm no ph



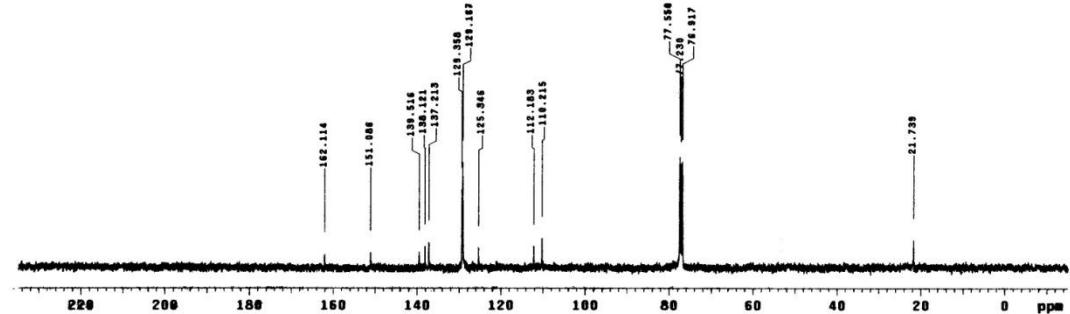
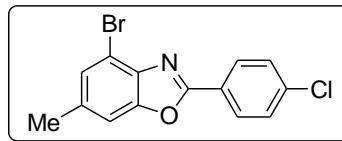
4-Bromo-2-(4-chlorophenyl)-6-methylbenzo[d]oxazole (20aa): ^1H NMR (CDCl_3 , 400 MHz)

```
NK_SB_49
exp1 s2pu1
SAMPLE          SPECIAL
date Apr 23 2012 temp not used
solvent CDCl3 gain not used
file /export/home-/spin not used
ciftemp/NK_SB_49_1- hst 0.008
      H.Tid pw90 19.700
      ACQUISITION alfa 20.000
sw 6389.8   FLAGS
at 1.998 1l n
np 25528 1p n
rb not used dp y
bs 4 hs nn
di 1.000 PROCESSING
nt 32 lb 0.10
ct 32 fn 65536
      32 th 7
      32 nm cdc ph
TRANSMITTER H1 sp -64.0
tn 399.03 1p 360.1
tfrq 362.8 rfp 794.5
tpwr 57 rfp 0
pw 9.850 rp 105.0
      DECOUPLER C13 1p -91.1
dn C13 PLOT
dof 0 wc 250
dm nnn sc 0
ds v vs 33
dpwr 50 th 7
dav 15900 nm cdc ph
```



4-Bromo-2-(4-chlorophenyl)-6-methylbenzo[d]oxazole (20aa): ^{13}C NMR (CDCl_3 , 100 MHz)

```
exp1 s2pu1
SAMPLE          SPECIAL
date Apr 21 2012 temp not used
solvent CDCl3 gain not used
file /exp1/home-/spin not used
ciftemp/NK_SB_49_1- hst 0.008
      ACQUISITION hst 20.000
sw 25125.6  alfa 20.000
at 1.199 1l 65536
np 69279   FLAGS
rb 13800 1l n
bs 92 1n n
di 1.000 dp y
nt 5000 hs nn
ct 1184 PROCESSING
      TRANSMITTER H1 1b 2.00
tn 100.593 1p 65536
tfrq 100.593 sp DISPLAY
      100.593 1p -424.5
tpwr 61 wp 19388.0
pw 9.300 rfp 9278.2
      DECOUPLER C13 1p 774.5
dn H1 rp -78.6
dof 0 1p -328.5
      0 wc 250
ds v vs 33
dpwr 42 sc 8
dav 8980 vs 28
      th 4
      nm no ph
```



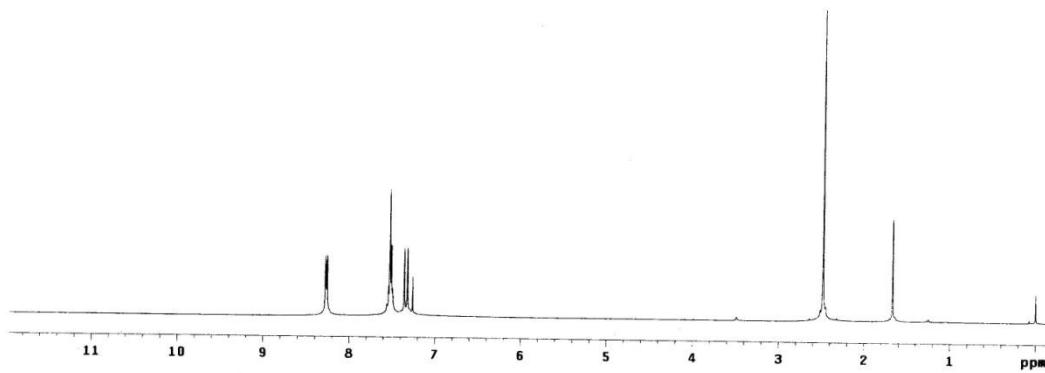
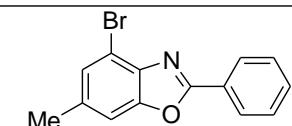
4-Bromo-6-methyl-2-phenylbenzo[*d*]oxazole (21aa): ^1H NMR (CDCl_3 , 400 MHz)

```

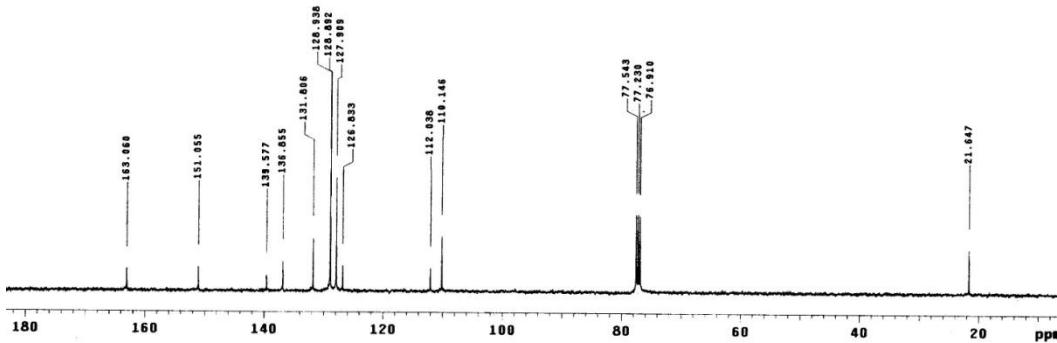
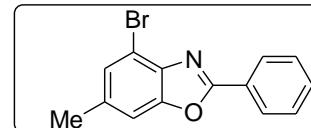
MK_S8_50
exp1 s2pul

          SAMPLE           SPECIAL
date May 4 2013 temp  not used
solvent CD13C gain  not used
          ACQUISITION    ipm  not used
          sw      6389.8 pw80 19.7000
          fb      1.938 alfa 20.0000
          ap      255.000
          n       not used il   n
          b       not used 4    n
          d1     1.000 dp   y
          d2     1.000 hs   y
          ct      32    PROCESSING
          TRANSMITTER lb   0.10
          sfrq  389.853 DISPLAY -72.7
          tfrq  362.8 sp   -72.7
          tpwr  57    wp   4853.1
          rfrq  57    rp   794.7
          pwr   57    rfp  107.1
          dncp   C13  rp   107.1
          dn     0    tp   -95.3
          dnm   nrm  PLOT
          dnmw   C  wc   250
          dpwr   50  sc   70
          dmfp  15900 vs   70
          dmfp  15900 vsp  70
          dm   cdc  ph

```



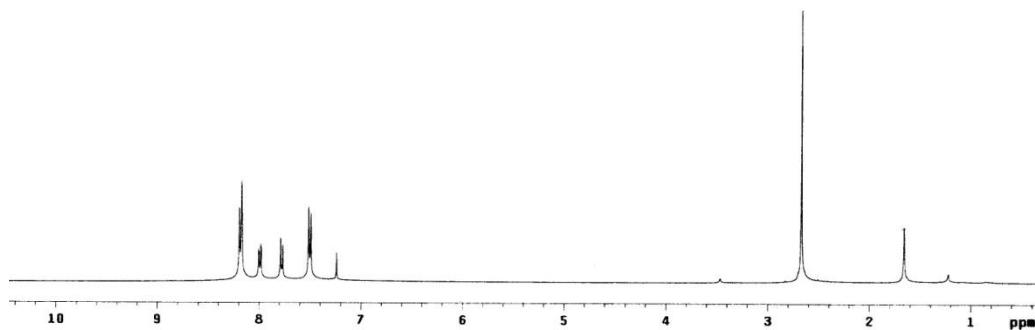
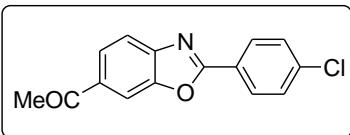
4-Bromo-6-methyl-2-phenylbenzo[*d*]oxazole (21aa): ^{13}C NMR: (CDCl_3 , 100 MHz)



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

SB_50_51_1H
exptl s2pul

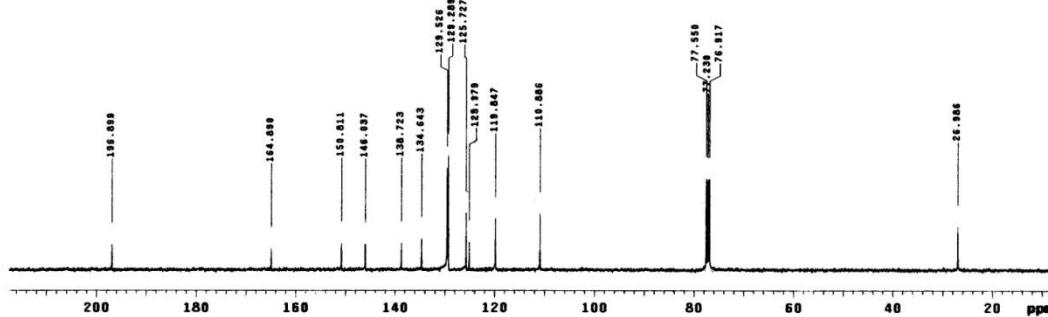
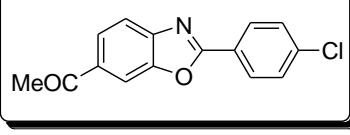
SAMPLE	SPECIAL
date May 6 2012	temp not used
solvent CDCl ₃	gain not used
file exp	spin not used
ACQUISITION	set
sw 6385.6	pw00 19.700
at 1.000	rtfa 20.000
nt 25528	flags
fb not used	i1 n
bs 32	in n
di 1.000	dp y
nt 32	hs nn
ct 32	PROCESSING
TRANSMITTER	lb 0.10
tn H1 fn 65536	
sfrq 399.853	DISPLAY
tot 362.0	sp 128.6
tpwr 57	wp 4872.3
pw 5.650	rf1 3856.3
DECOUPLER	C13 rfp 280.0
dn C13	rp 51.6
dof 0	ip -64.7
de mnn	PLOT
dm c	vc 250
dpwr 59	sc 0
defv 15900	vs 65
nm cdc ph	th 8



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

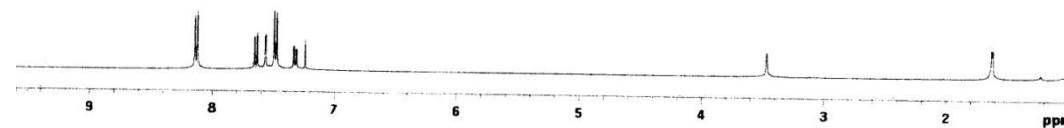
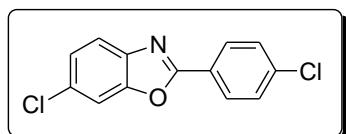
SB_51_13C
exptl s2pul

SAMPLE	SPECIAL
date May 18 2012	temp not used
solvent CDCl ₃	gain not used
file exp	spin not used
ACQUISITION	set
sw 25125.6	pw00 18.688
at 1.100	rtfa 20.000
nt 68278	flags
fb 1500.0	i1 n
bs 32	in n
di 1.000	dp y
nt 25528	hs nn
ct 2432	PROCESSING
TRANSMITTER	lb 2.00
tn C13 fn 65536	
sfrq 100.054	DISPLAY
tot 1536.3	sp 781.9
tpwr 61	wp 21163.6
pw 9.300	rf1 52.4
DECOUPLER	H1 rfp 7764.9
dn C13	rp -68.2
dof 0	ip -286.9
de yw	PLOT
dm v	vc 250
dpwr 42	sc 0
defv 8500	vs 27
nm no ph	th 3



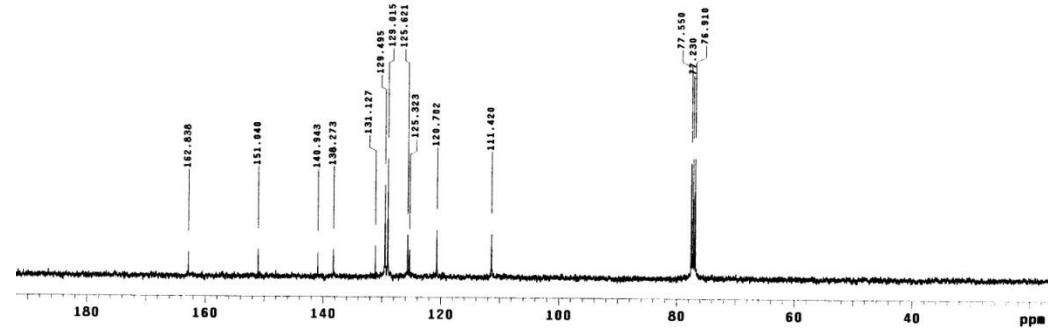
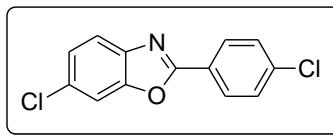
6-Chloro-2-(4-chlorophenyl)benzo[d]oxazole (23aa): ^1H NMR (CDCl_3 , 400 MHz)

```
NK_SS_53_1H
exp1 t2pu1
SAMPLE SPECIAL
date May 19 2012 temp not used
solvent CDCl3 gain not used
file exp spin not used
ACQUISITION hst 0.005
sw 6386.5 pw0 15.788
at 1.354 pw1a 20.000
np 25528 flags
fb not used 11 n
bs 4 n
di 1.000 dp y
nt 32 hs nn
ct 32 PROCESSING 0.10
TRANSMITTER lb fm 0.10
tn C13 fm 65536
stf/q 399.453 DISPLAY
tot 362.0 sp 388.5
tpwr 57 vp 3581.3
pw 9.850 r1 3680.3
DECOUPLER C13 rfp 2894.9
dn 25125.6 pw0 18.600
at 13680 alfa 20.000
np 69270 flags
fb 13680 11 n
bs 5000 n
di 1.000 dp y
nt 5000 hs ny
ct 1824 PROCESSING 0.10
TRANSMITTER lb fm 0.00
tn C13 fm 65536
stf/q 100.554 DISPLAY
tot 1536.3 sp 1662.7
tpwr 61 vp 17896.9
pw 9.380 r1 9271.3
DECOUPLER C13 rfp 7781.3
dn H1 rfp -46.4
dof 0 ip -372.7
de yyy wc 250
dpwr 42 sc 0
dmf 8980 vs 29
th no ph
```



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

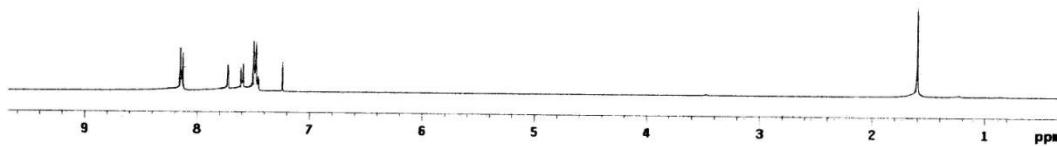
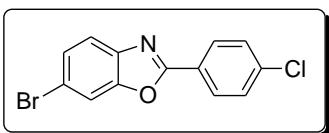
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NK_SS_53_13C
exp1 s2pu1
SAMPLE SPECIAL
date Jun 5 2012 temp not used
solvent CDCl3 gain not used
file exp spin not used
ACQUISITION hst 0.005
sw 25125.6 pw0 18.600
at 13680 alfa 20.000
np 69270 flags
fb 13680 11 n
bs 5000 n
di 1.000 dp y
nt 5000 hs ny
ct 1824 PROCESSING 0.00
TRANSMITTER lb fm 0.00
tn C13 fm 65536
stf/q 100.554 DISPLAY
tot 1536.3 sp 1662.7
tpwr 61 vp 17896.9
pw 9.380 r1 9271.3
DECOUPLER C13 rfp 7781.3
dn H1 rfp -46.4
dof 0 ip -372.7
de yyy wc 250
dpwr 42 sc 0
dmf 8980 vs 29
th no ph
```



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

NK_SB_52_1H
exp1 szpul

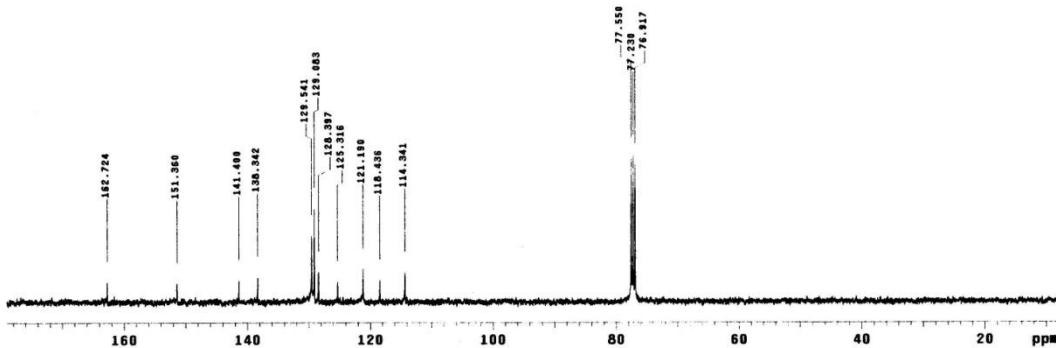
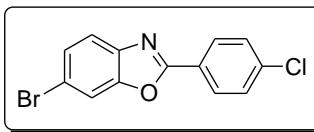
SAMPLE SPECIAL
date May 19 2012 temp not used
solvent CDCl₃ gain not used
file exp spin not used
ACQUISITION hst 8.000
sw 6385.8 pw8 15.750
at 1.958 alfa 28.000
np 25500 flags n
fb not used 11 n
bs 4 in
dl 1.000 dp y
nt 32 hs nn
ct 32 PROCESSING 0.10
TRANSMITTER lb 0.10
tn HI fn 65536
sfrq 399.853 DISPLAY
tof 362.8 sp 111.2
tpwr 57 vp 3781.5
pw 8.85 r1 314.5
DECOUPLER C13 rfp 2894.3
dn C13 rp 163.2
dof 8 tp -66.7
de nm PLOT
dme c wc 250
dpwr 50 sc 0
dfr 15900 vs 21
th 20
nm cdc ph



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

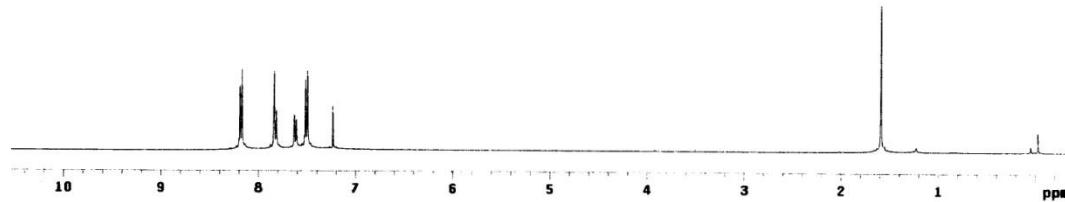
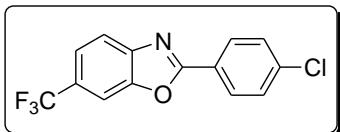
.38_52_13C

SAMPLE SPECIAL
date Jun 6 2012 temp not used
solvent CDCl₃ gain not used
file exp spin not used
ACQUISITION hst 8.000
sw 25125.6 pw8 15.600
at 68270 alfa 28.000
np 13860 flags n
fb 13860 11 n
bs 32 in n
dl 1.000 dp y
nt 5000 hs nn
ct 2112 PROCESSING 2.00
TRANSMITTER lb 2.00
tn C13 fn 65536
sfrq 100.554 DISPLAY
tof 1536.3 sp 728.7
tpwr 120 vc 120.5
pw 9.300 r1 8270.6
DECOUPLER rfp 7764.9
dn HI rp -77.4
dof 8 lp -292.4
de VVY PLOT
dme c wc 250
dpwr 42 tc 0
dfr 8500 vs 34
th 4
nm no ph



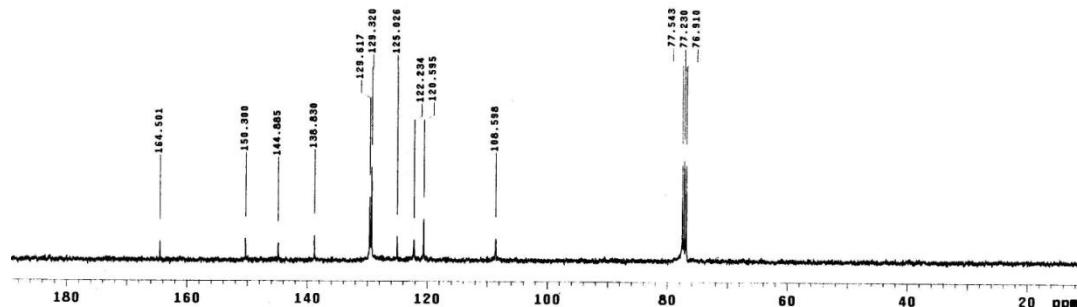
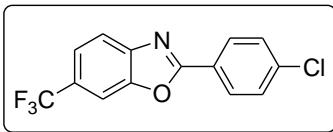
2-(4-Chlorophenyl)-6-(trifluoromethyl)benzo[d]oxazole (25aa): ^1H NMR (CDCl_3 , 400 MHz)

NK_S6_54
exp1 s2pu1
SAMPLE SPECIAL
date Jun 19 2012 temp not used
solvent CDCl₃ gain not used
file exp spin not used
ACQUISITION hst 0.008
sw 1289.8 117.0 28.000
at 1.000 117.0 28.000
np 25288 FLAGS
fb not used 11 n
bs 1.000 4 in n
di 1.000 dp y
nt 32 hs nn
ct 32 PROCESSING
TRANSMITTER lb 0.18
tn C13 fn 65536
s1rq 399.0 sp DISPLAY -157.3
tof 362.8 sp -157.3
tpwr 57 wp 4381.4
pw 9.850 r71 3699.7
DECOUPLER C13 r7 2800.0
dn 0 ip 113.6
dof 0 ip -99.5
ds nnn PLOT
dss c wc 250
dpw 50 sc 0
dpw 15998 vs 34
dft 15998 th 12
nm cdc ph

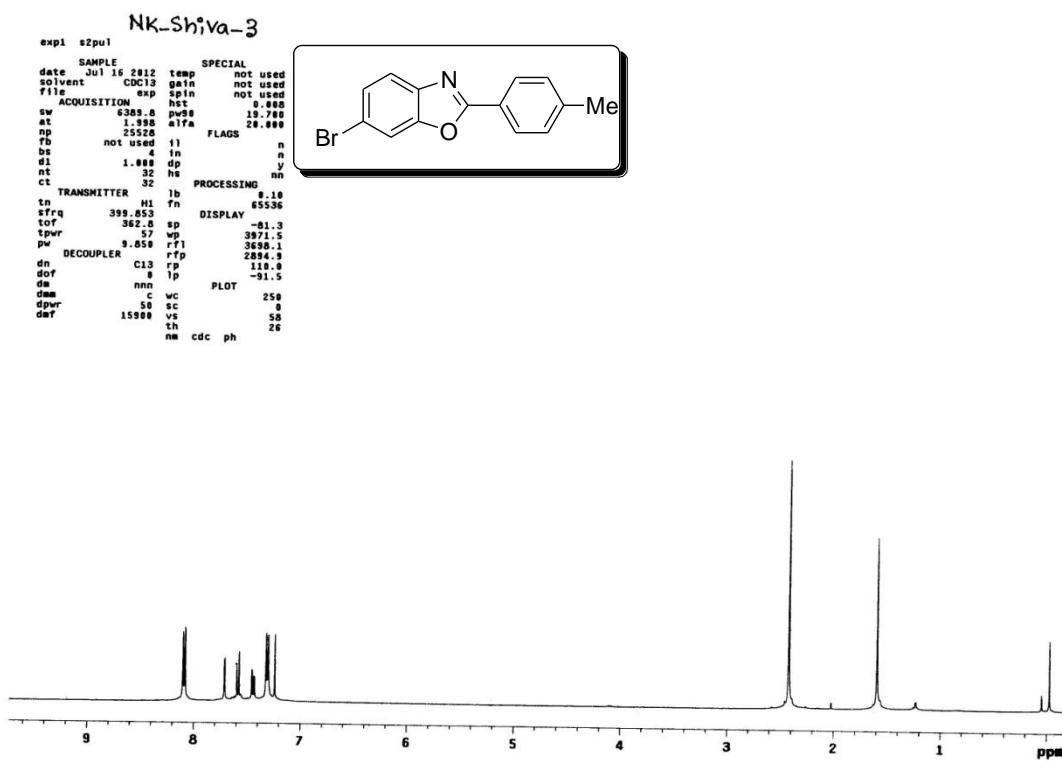


2-(4-Chlorophenyl)-6-(trifluoromethyl)benzo[d]oxazole (25aa): ^{13}C NMR (CDCl_3 , 100 MHz)

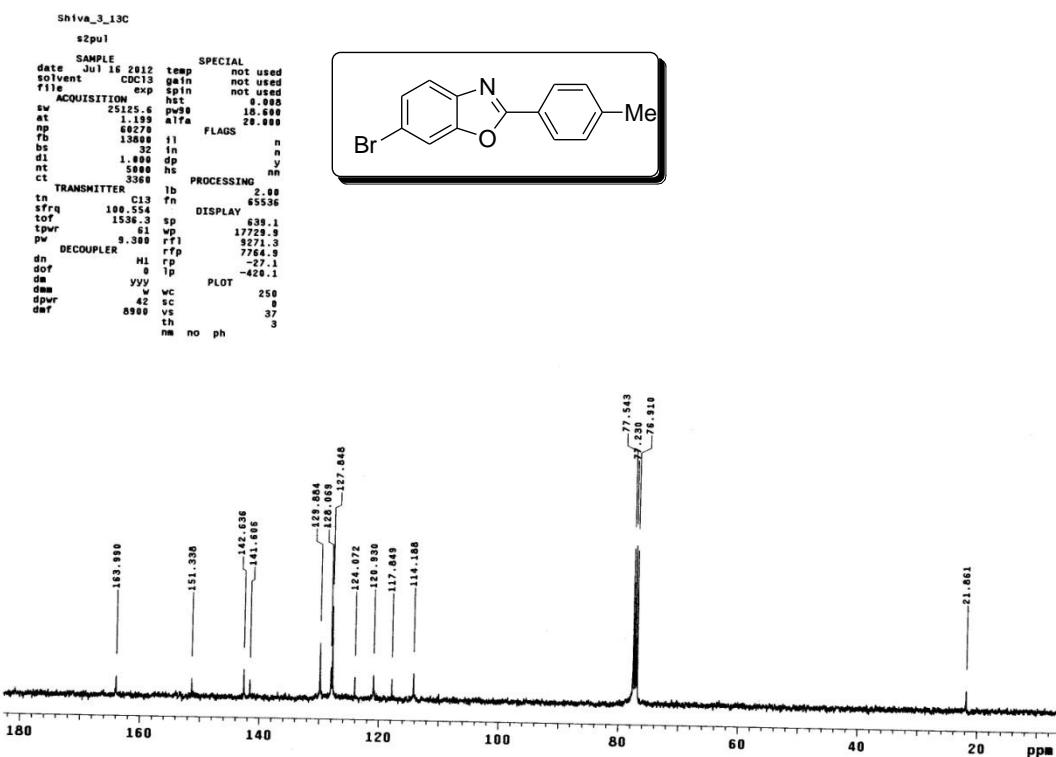
_54_13C
s2pu1
SAMPLE SPECIAL
date Jun 21 2012 temp not used
solvent CDCl₃ gain not used
file exp spin not used
ACQUISITION hst 10.000 18.000
sw 25125.6 6000 28.000
at 1.189 117.0 28.000
np 66270 FLAGS
fb 15800 11 n
bs 32 in n
di 1.000 dp y
nt 5998 hs nn
ct 1728 PROCESSING
TRANSMITTER lb 2.00
tn C13 fn 65536
s1rq 100.0 sp DISPLAY 1870.0
tof 1530.3 sp 1870.0
tpwr 61 wp 17968.7
pw 9.300 r71 9269.8
DECOUPLER C13 r7 7746.5
dn 0 rp -23.4
dof 0 ip -421.9
ds vvv PLOT
dss w wc 250
dpw 42 sc 0
dpw 8990 vs 23
dft 8990 th 23
nm no ph



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

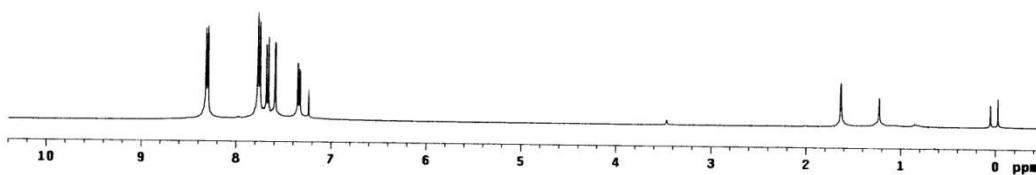
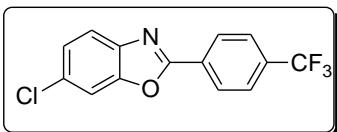


6-Bromo-2-p-tolylbenzo[d]oxazole (26aa): ^{13}C NMR (CDCl_3 , 100 MHz)



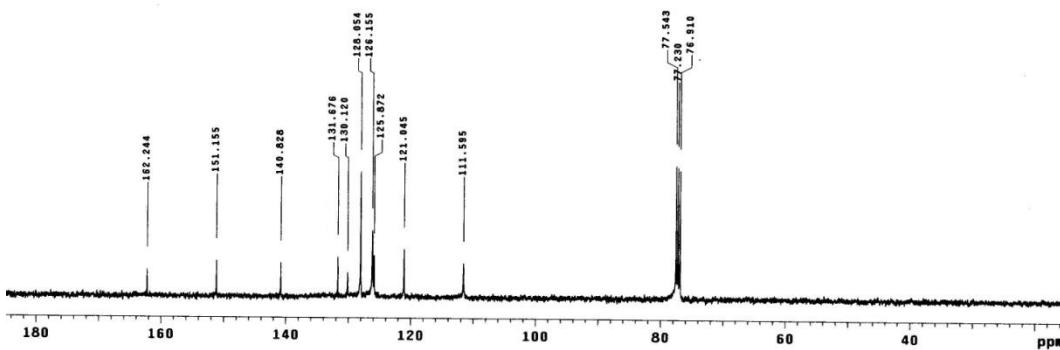
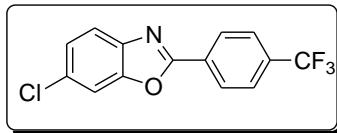
6-Chloro-2-(4-(trifluoromethyl)phenyl)benzo[d]oxazole (27aa): ^1H NMR (CDCl_3 , 400 MHz)

```
NK_SHIVA_5
expt1 s2pul
SAMPLE SPECIAL
date Jul 17 2012 temp not used
solvent CDCl3 gain not used
file exp1 t1 not used
ACQUISITION hst 8.888
sw 6389.8 pw90 15.788
at 1.000 t90 28.000
np 25528 flags
fb not used t1 n
bs 1.000 dp n
dl 1.000 dp y
nt 32 hs nn
ct 32 PROCESSING
TRANSMITTER lb 0.10
tn H1 fp 65536
sfrq 399.853 DISPLAY
tof 367.1 sp
tppr 57 vp -189.1
pw 9.858 r1 4357.8
DECOUPLER 9.858 r1 3698.5
dn C13 r1p 2854.9
dof 0 1p 5
dss nnn PLOT
dme c wc 250
dpwv 50 vs 0
dewf 15900 ts 26
nm cdc ph 15
```



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

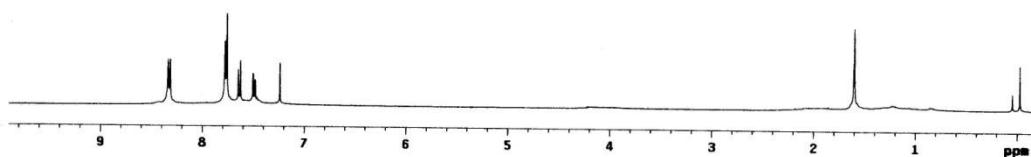
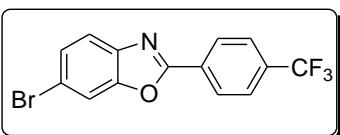
```
_Shiva_5_13C
expt1 s2pul
SAMPLE SPECIAL
date Jul 17 2012 temp not used
solvent CDCl3 gain not used
file exp1 t1 not used
ACQUISITION hst 8.888
sw 25125.6 pw90 18.688
at 1.139 t90 20.000
np 13880 flags
fb 13880 t1 n
bs 32 in n
dl 1.139 dp y
nt 5888 hs nn
ct 2240 PROCESSING
TRANSMITTER lb 2.00
tn C13 fp 65536
sfrq 100.554 DISPLAY
tof 1536.3 sp 1466.4
tppr 61 vp 17168.6
pw 9.388 r1 3252.9
DECOUPLER r1p 7764.9
dn H1 r1p -49.5
dof 0 1p -354.3
dss yw PLOT
dme vwc 250
dpwv 42 sc 0
dewf 8800 ts 31
nm no ph 3
```



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

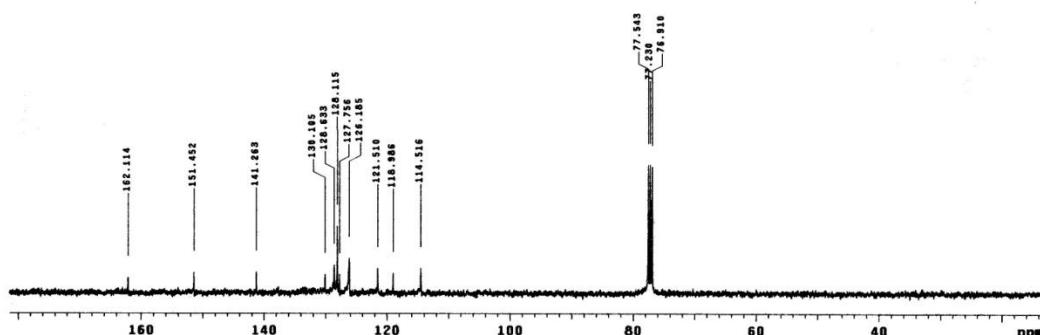
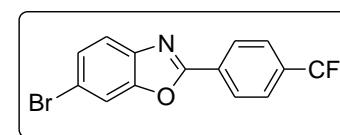
NK_Shiva-6_1H
expt s2pul

```
sample       SPECIAL
date Jul 17 2013 temp    not used
solvent   CDCl3  gain   not used
file      exp  spin  not used
          acq  pres  8.000
          sw   6399.8  tdec  12.0
          at   1.199  a1fa  28.000
          np   25528  flags
          fb   not used  il   n
          bs   not used  in   n
          di   1.000  dp   y
          nt   32      th   nn
          ct   32      ph
          tr   1b      processing 8.10
          trans H1  fm
          sfrq 399.853  display 65536
          tof   362.8  sp   -64.3
          tppw  57    wp   4821.5
          pw   9.850  rfp   2894.9
          decoupler C13 rfp   96.7
          dof   nnn ip   -83.3
          dm   c wc   250
          dppw  58    sc   0
          ddef  15900 th   50
          nm cdc ph   20
```

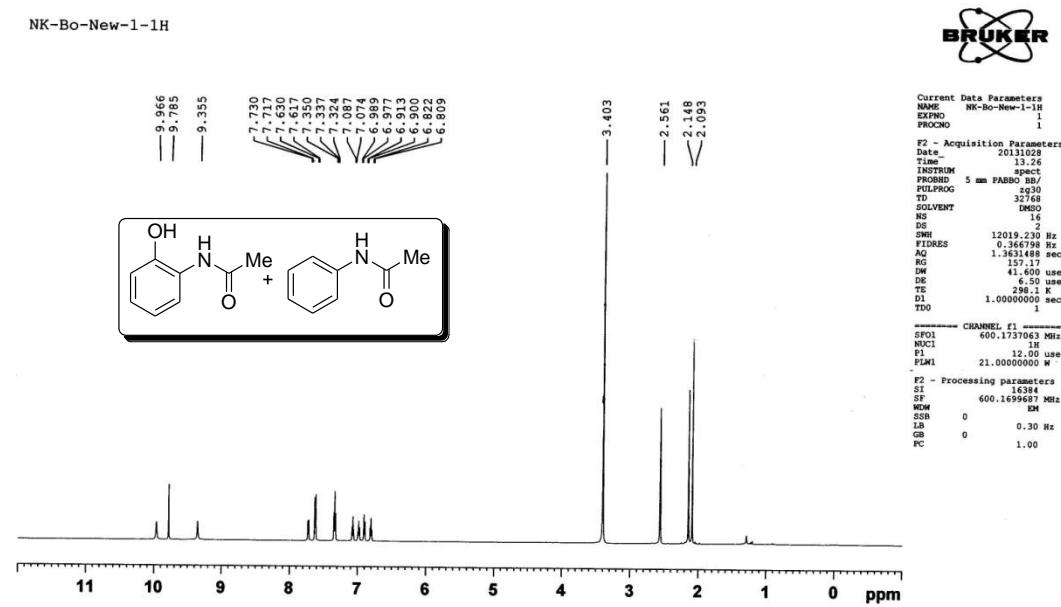


6-Bromo-2-(4-(trifluoromethyl)phenyl)benzo[d]oxazole (28aa): ^{13}C NMR (CDCl_3 , 100 MHz)

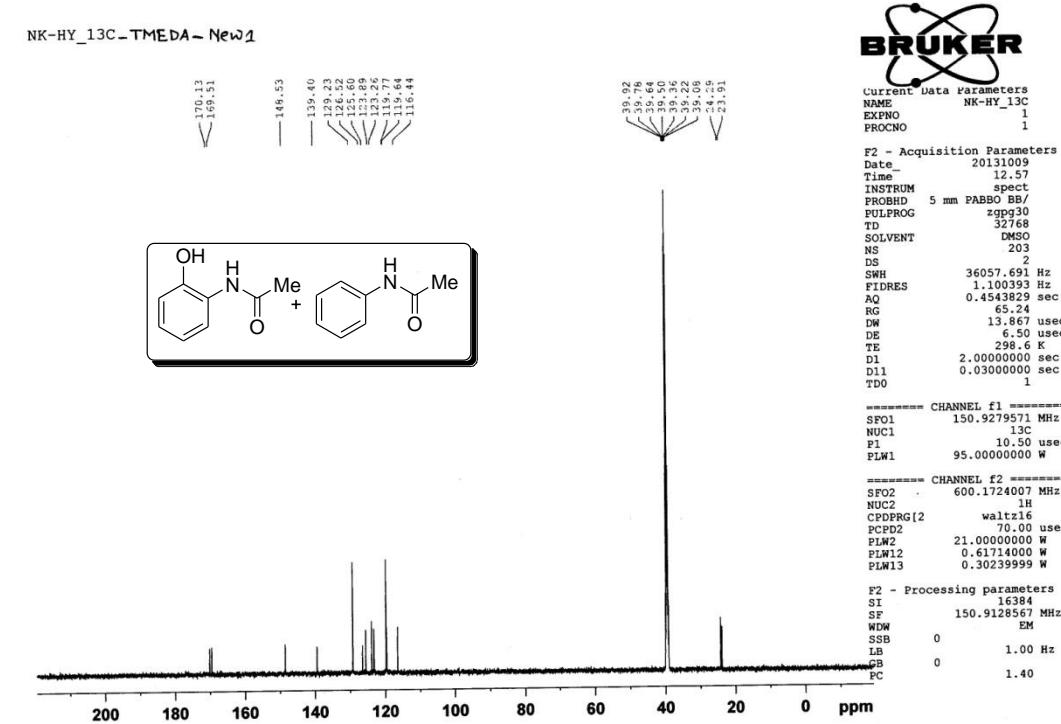
NK_Shiva_6_13C
expt s2pul
sample SPECIAL
date Jul 17 2013 temp not used
solvent CDCl3 gain not used
file exp spin not used
 acq pres 8.000
 sw 25125.6 tdec 10.000
 at 1.199 a1fa 28.000
 np 13048 flags
 fb 32 il n
 bs 32 in n
 di 1.000 dp y
 nt 1984 th nn
 ct 1984 processing 2.00
 trans C13 fn
 sfrq 100.554 display 65536
 tof 1536.3 sp 1267.0
 tppw 61 wp 1000.0
 pw 9.380 rfp 7764.0
 decoupler H1 rfp 96.0
 dof vvv ip -83.0
 dm v wc 250
 dppw 42 sc 0
 ddef 8900 vt 31
 nm no ph
 th 3



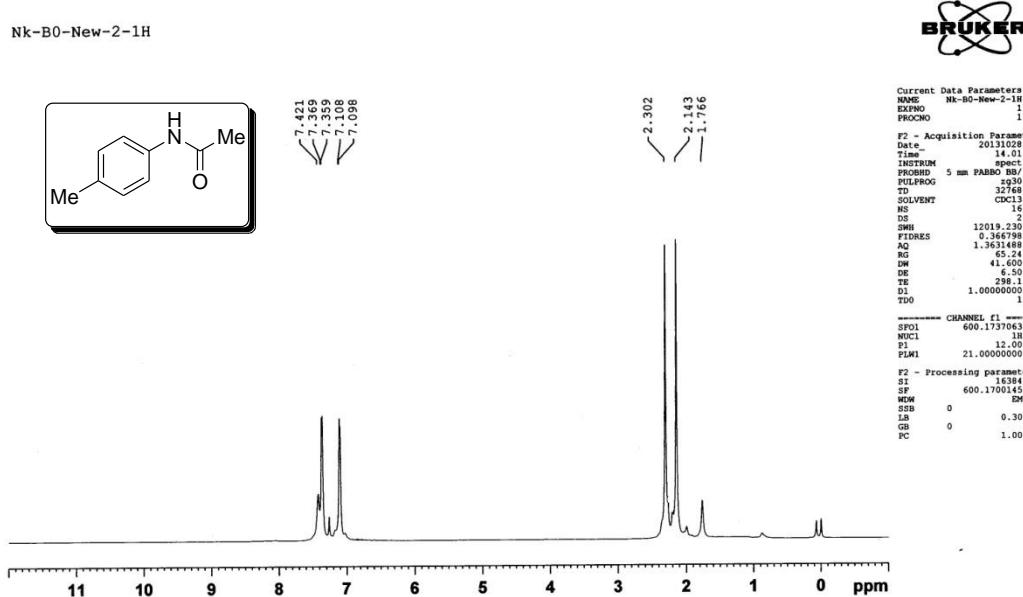
Mixture of *N*-(2-Hydroxyphenyl)acetamide (1a'**) and *N*-phenylacetamide (**1a''**):
¹H NMR (DMSO-*d*₆, 600 MHz)**



Mixture of *N*-(2-Hydroxyphenyl)acetamide (1a'**) and *N*-phenylacetamide (**1a''**):
¹³C NMR (DMSO-*d*₆, 150 MHz)**



N-p-Tolylacetamide (2a''): ^1H NMR (CDCl_3 , 600 MHz)



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

