Green Progression for Synthesis of Regioselective β–Aminoalcohols and Chemoselective Alkylated Indoles

Boningari Thirupathi, Rapelli Srinivas, Avvari N. Prasad, J. K. Prashanth Kumar, and Benjaram M. Reddy*

Inorganic and Physical Chemistry Division, Indian Institute of Chemical Technology, Uppal Road, Hyderabad – 500 607, India

Supplementary Information

INDEX

1. Characterization of Catalyst

1a. Spectroscopic Techniques for Characterization. X-ray powder diffraction patterns have been recorded on a Siemens D-5000 instrument by using CuKα radiation source and scintillation counter detector. The XRD phases present in the samples were identified with the help of JCPDS data files.

Raman spectrum was recorded at ambient temperature on a Nicolet FT-Raman 960 spectrometer with a range of 4000–100 cm^{-1} and a spectral resolution of 2 cm^{-1} using the 1064 nm exciting line (~600 mV) of a Nd:YAG laser (Spectra Physics, USA). Finely powdered sample was placed in a 5mm (outer diameter) NMR tube. Before measurements, sample was dried in a vacuum oven for several hours.

The XPS measurements were made on a Shimadzu (ESCA 3400) spectrometer by using MgKα (1253.6 eV) radiation as the excitation source. The spectra were recorded after argon-ion etching for 1 min (2 kV, 30 mA). Charging of catalyst samples was corrected by setting the binding energy of adventitious carbon (C 1s) at 284.6 eV. The finely ground oven dried sample was dusted on a double stick graphite sheet and mounted on the standard sample holder. The sample holder was then transferred to the analysis chamber, through a rod attached to it. The XPS analysis was done at room temperature and pressure typically in the order of less than 10^{-6} Pa. The samples were out gassed in a vacuum oven overnight before XPS measurements.

1b. Observations from Spectral Techniques. The X–ray powder diffraction patterns of TiO_2–ZrO_2 mixed oxide is shown in Figure 1. The formation of $ZrTiO_4$ compound can be clearly evident (JCPDS file no. 7-290) in the case of TiO_2–ZrO_2. FT–Raman spectrum of

the catalyst exhibited (Figure 2) bands at around 135, 168, 280, 338, 412, 640 and 803 cm^{-1}, which are characteristic lines for $ZrTiO_4$.

The TiO_2–ZrO_2 mixed oxide calcined at 923 K has been investigated by XPS technique. The photoelectron peaks of O 1s, Ti 2p, and Zr 3d are shown in Figures 3–5, respectively. The binding energies (E_b) of all the elements in TiO_2–ZrO_2 are shown in Table 1. As shown in Figure 3, the O 1s profile is, in general, more complicated due to the overlapping contribution of oxygen from titania and zirconia. Figure 4 shows the binding energy of Ti photoelectron peak at 459.3 for Ti 2p. Normally, the Ti $2p_{3/2}$ line in the case of pure TiO_2 samples can be observed at 458.5 eV.[3] An increase in the binding energy of the same in the present study may be due to the formation of $ZrTiO_4$ compound. Figure 5 shows the binding energy of the Zr 3d photoelectron peaks at 182.9 and 185.3 eV for Zr $3d_{5/2}$ and Zr $3d_{3/2}$ lines, respectively. The Zr 3d lines are well resolved with high intensity.

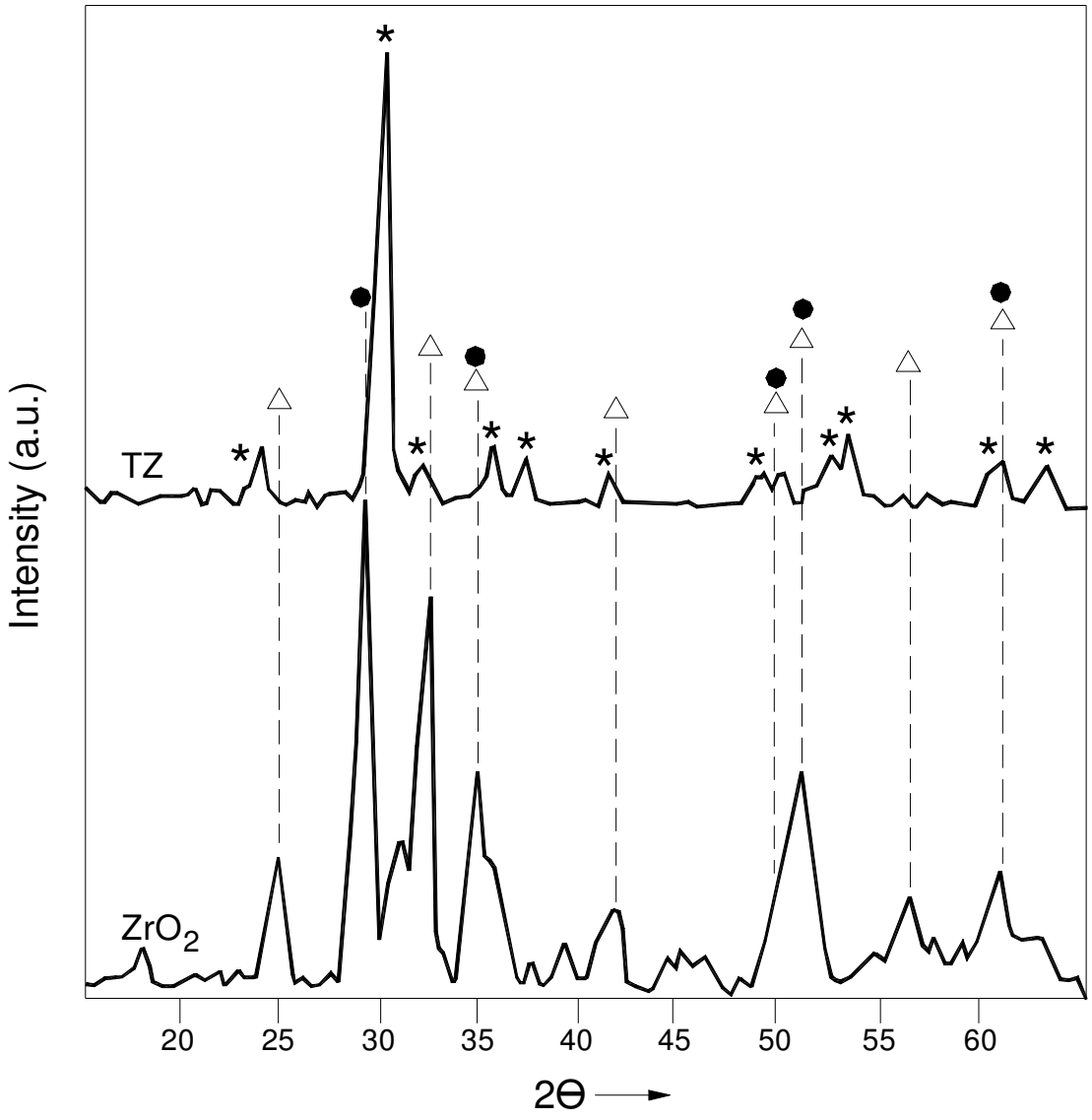


Figure 1: X-ray powder diffraction patterns of TiO_2–ZrO_2 and ZrO_2 samples calcined at 923 K (●) lines due to tetragonal ZrO_2; (Δ) lines due to monoclinic ZrO_2; (*) lines due to $ZrTiO_4$; TZ: TiO_2–ZrO_2)

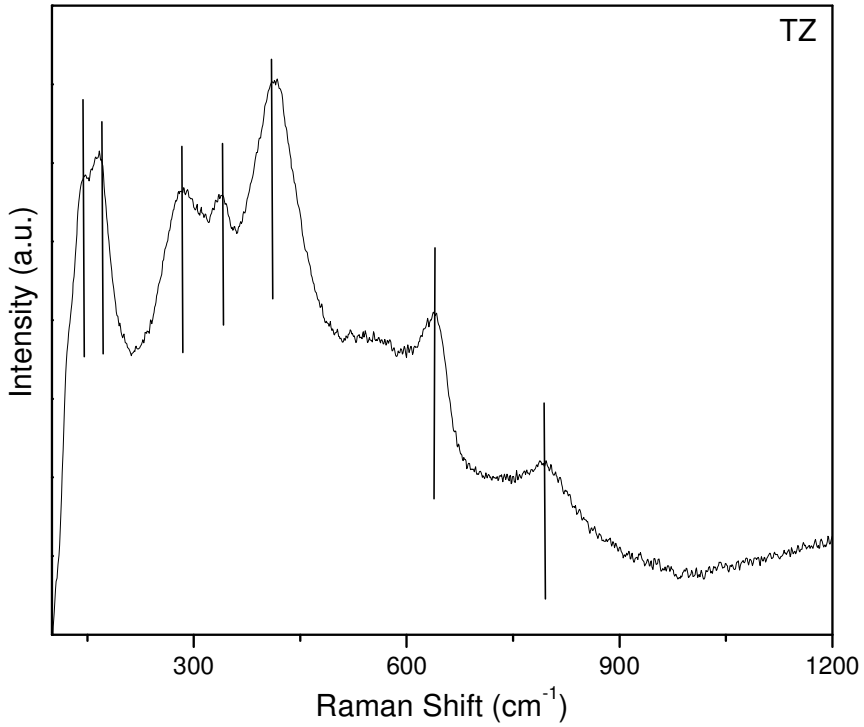


Figure 2: FT–Raman spectrum of TiO_2–ZrO_2 (1:1 mole ratio according to oxides) mixed oxide calcined at 923 K; (TZ) **—** TiO_2–ZrO_2

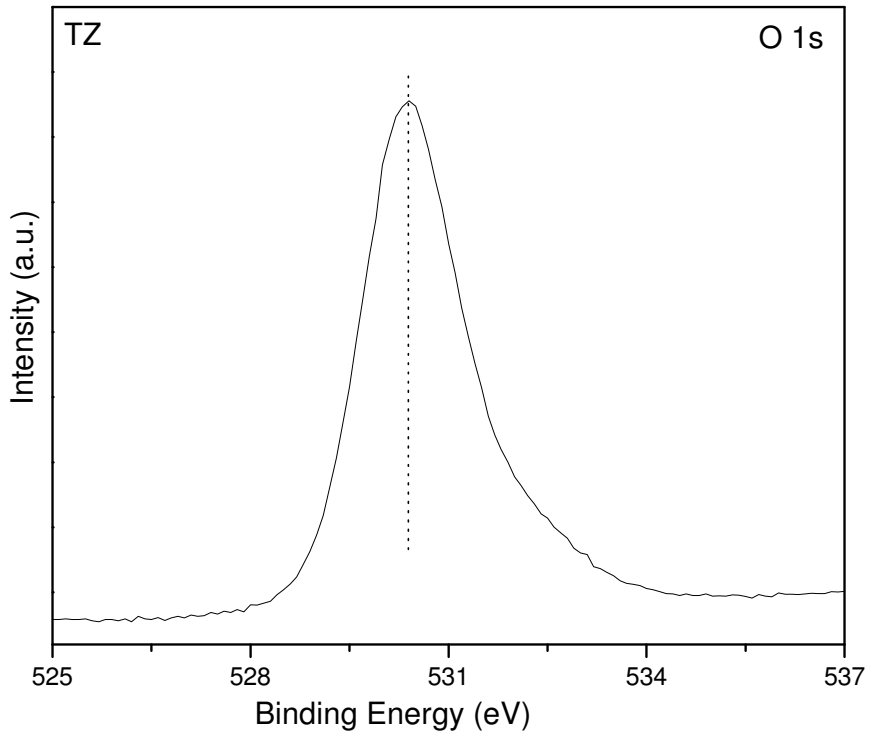


Figure 3: The O 1s XPS spectrum of TiO_2–ZrO_2 (1:1 mole ratio) mixed oxide calcined at 923 K; (TZ) **—** TiO_2–ZrO_2

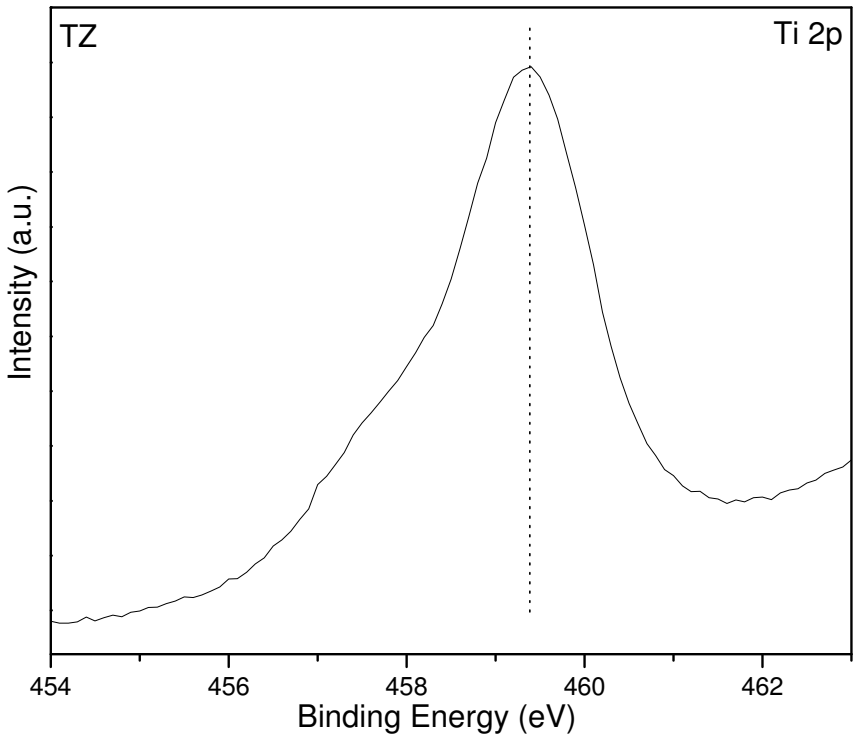


Figure 4: The Ti 2p XPS spectrum profile of TiO_2–ZrO_2 (1:1 mole ratio) mixed oxide calcined at 923 K; (TZ) **—** TiO_2–ZrO_2

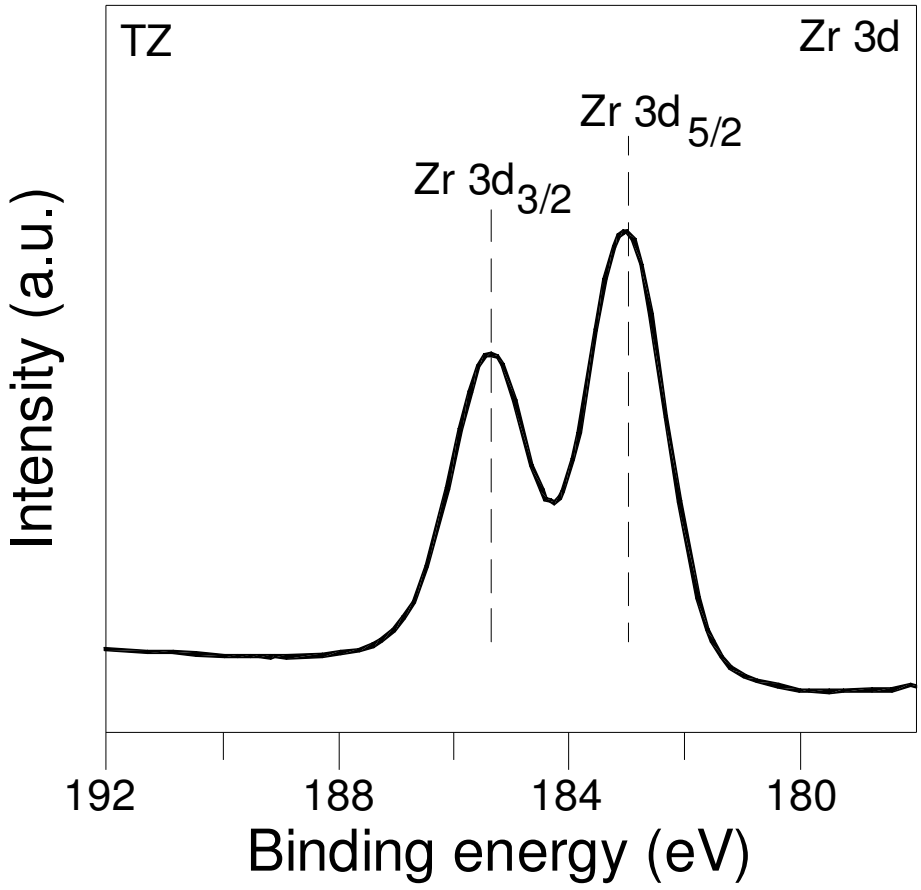


Figure 5: The Zr 3d XPS spectrum profile of TiO_2–ZrO_2 (1:1 mole ratio) mixed oxide calcined at 923 K; (TZ) — TiO_2–ZrO_2

***Table 1*:** Electron binding energies (eV), BET surface area and total acidity of TiO_2–ZrO_2

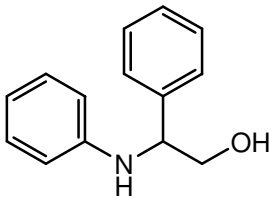
Catalyst	O 1s	Ti $2p_{3/2}$	Zr $3d_{3/2}$	Zr $3d_{5/2}$	BET surface area (m^2/g)	Total acidity (ml/g)
TiO_2–ZrO_2	530.4	459.3	185.3	182.9	30	6.03

2. ^{1}H NMR, FTIR, MS Data of all Isolated Products

2a. Experimental Techniques. NMR spectra were recorded on a Varian VXR-Unity 200 MHz, Bruker UXNMR/XWIN-NMR Avance-300 MHz, and GEMINI spectrometers. Chemical shifts are reported downfield from TMS (δ=0) for ^{1}H NMR. Data for ^{1}H NMR are reported as follows:

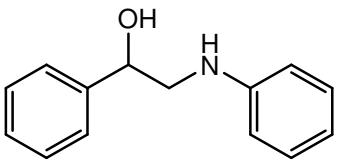
2b. Spectral data of products.

Table 3, Entry 1; 2-phenyl-2-(phenylamino)ethanol:



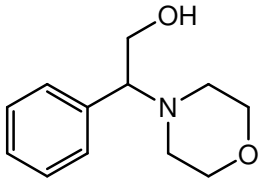
^{1}H NMR ($CDCl_3$) δ 3.69 (dd, *J*=4.15, 6.98 Hz, 1H), 3.89 (dd, *J*=4.15, 6.98 Hz, 1H), 4.43 (dd, *J*=2.83, 4.15 Hz, 1H), 6.46-6.51 (m, 2H), 6.59-6.64 (m, 1H), 6.99-7.07 (m, 2H), 7.19-7.34 (m, 5H); IR (KBr): *v* 3394, 3025, 2926, 2856, 1601, 1502, 1316, 1266, 1067, 1027, 752, 697 cm^{-1}; ESI-MS: *m*/*z* 214 [M$^+$+1]

Table 3, Entry 1; 1-phenyl-2-(phenylamino)ethanol:



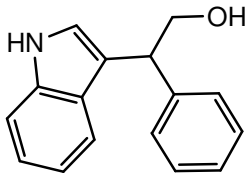
^{1}H NMR ($CDCl_3$) δ 3.24 (dd, *J*=4.53, 9.06 Hz,1H), 3.38 (dd, *J*=4.53, 9.06 Hz,1H), 4.88 (dd, *J*=3.77, 5.28 Hz, 1H), 6.60-6.70 (m, 3H), 7.00-7.15 (m, 2H), 7.25-7.39 (m, 5H); IR (KBr): *v* 3397, 2924, 1739, 1602, 1503, 1317, 1259, 1061, 752 696 cm^{-1}; ESI-MS: *m*/*z* 214 [M^++1]

Table 3, Entry 2; 2-morpholino-2-phenylethanol:



^{1}H NMR ($CDCl_3$) δ 1.25-1.49 (m, 4H), 2.10-2.37 (m, 4H), 3.64 (dd, *J*=3.91, 8.80 Hz, 1H), 3.74 (dd, *J* =3.91, 8.80 Hz, 1H), 4.81(dd, *J*=3.91, 5.86 Hz, 1H), 7.28-7.36 (m, 5H); IR (KBr): *v* 3442, 2924, 1734, 1377, 1242, 1038, 758, 701, 534 cm^{-1}; ESI-MS: *m*/*z* 208 [M^++1]

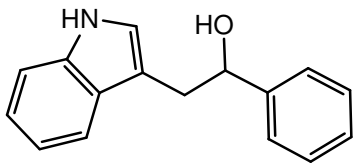
Table 3, Entry 3; 2-(1H-Indol-3-yl)-2-phenylethanol:



^{1}H NMR ($CDCl_3$) δ 1.43 (br s, 1H), 4.08-4.22 (m, 2H), 4.43 (t, *J*=6.79 Hz, 1H), 6.96-7.21 (m, 4H), 7.24-7.31 (m, 5H), 7.37 (d, *J*=8.31 Hz, 1H), 7.99 (br s, 1H); IR (KBr):

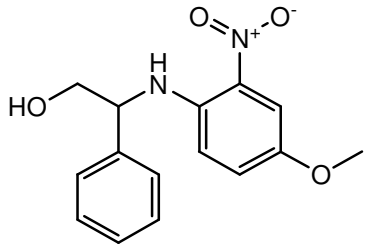
v 3411, 3376, 2875, 1614, 1452, 1048, 1006, 742, 696, 495 cm^{-1}; ESI-MS: *m*/*z* 238 $[M^+ +1]$, 220 $[M^+ - OH]$

Table 3, Entry 3; 2-(1H-Indol-3-yl)-1-phenylethanol:



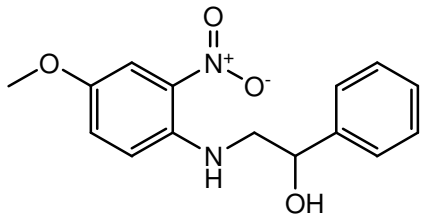
^{1}H NMR ($CDCl_3$) δ 1.71 (br s, 1H), 4.04-4.13 (m, 1H), 4.16-4.32 (m, 2H), 6.25 (s, 1H), 6.98-7.09 (m, 3H), 7.20-7.33 (m, 5H), 7.48 (d, *J*=7.55 Hz, 1H); IR (KBr): *v* 3396, 3057, 1716, 1453, 1296, 1032, 751 cm^{-1}; ESI-MS: *m*/*z* 238 $[M^+ +1]$

Table 3, Entry 4; 2-(4-methoxy-2-nitrophenylamino)-2-phenylethanol:



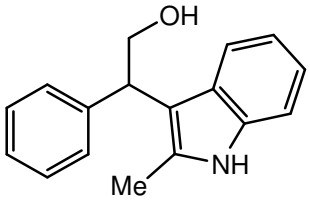
^{1}H NMR ($CDCl_3$) δ 3.76 (s, 3H), 3.84-3.93 (m, 1H), 3.95-4.02 (m, 1H), 4.64 (dd, *J*=4.53, 6.04 Hz, 1H), 6.56 (d, *J*=9.44 Hz, 1H), 6.92 (dd *J*=3.02, 6.42 Hz, 1H), 7.30-7.36 (m, 5H), 7.59 (d, *J*=3.02 Hz, 1H); IR (KBr): *v* 3369, 2926, 1571, 1517, 1411, 1228, 1143, 1035, 759, 702, 548 cm^{-1}; ESI-MS: *m*/*z* 289 $[M^+ +1]$

Table 3, Entry 4; 2-(4-methoxy-2-nitrophenylamino)-1-phenylethanol:



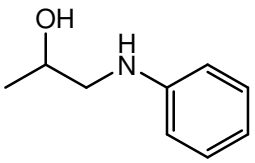
^{1}H NMR ($CDCl_3$) δ 3.48-3.55 (m, 2H), 3.79 (s, 3H), 4.98 (m, 1H), 6.81-6.84 (m, 1H), 7.05-7.09 (m, 1H), 7.30-7.41 (m, 5H), 7.57-7.62 (m, 1H); IR (KBr): *v* 3379, 2924, 1663, 1518, 1455, 1226, 1144, 1035, 761, 702, 540 cm^{-1}; ESI-MS: *m*/*z* 289 [M^++1]

Table 3, Entry 5; 2-(2-methyl-1H-indol-3-yl)-2-phenylethanol:



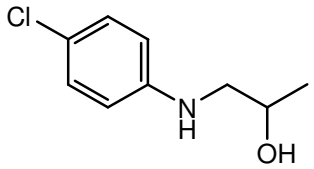
^{1}H NMR ($CDCl_3$) δ 1.53 (br s, 1H), 2.30 (s, 3H), 4.21-4.27 (m, 2H), 4.40 (t, *J*=6.78 Hz, 1H), 6.92-6.97 (m, 1H), 7.00-7.06 (m, 1H), 7.10-7.13 (m, 1H), 7.18-7.28 (m, 5H), 7.38 (d, *J*=8.30 Hz, 1H), 7.87 (br s, 1H); IR (KBr): *v* 3540, 3404, 2927, 1613, 1258, 1302, 1028, 748, 701, 584 cm^{-1}; ESI-MS: *m*/*z* 252 [M^++1]

Table 3, Entry 6; 1-(phenylamino)propan-2-ol:



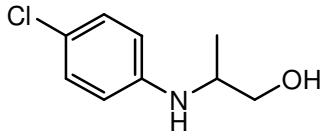
^{1}H NMR ($CDCl_3$) δ 1.25 (d, *J*=6.55 Hz, 3H), 2.89 (br s, 1H), 2.96 (dd, *J*=3.62, 9.05 Hz, 1H), 3.20 (dd, *J*=3.62, 9.05 Hz, 1H), 3.98 (m, 1H), 6.57-6.68 (m, 3H), 7.11 (t, *J*=8.14 Hz, 2H); IR (KBr): *v* 3395, 2924, 1710, 1602, 1504, 1318, 1259, 1074, 751, 693 cm^{-1}; EI-MS: *m*/*z* 152 [M^++1]

Table 3, Entry 7; 1-(4-chlorophenylamino)propan-2-ol:



^{1}H NMR ($CDCl_3$) δ 1.23 (d, *J*=5.85 Hz, 3H), 2.88 (dd, *J*=2.92, 9.75 Hz, 1H), 3.15 (dd, *J*=2.92, 9.75 Hz,1H), 3.92-3.97 (m, 1H), 6.48-6.50 (m, 2H), 7.05-7.07 (m, 2H); IR (KBr): *v* 3396, 2925, 1599, 1500, 1317, 1256, 1092, 929, 816, 666 504 cm^{-1}; EI-MS: *m*/*z* 186 [M^++1]

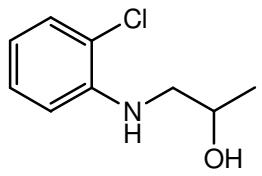
Table 3, Entry 7; 2-(4-chlorophenylamino)propan-1-ol:



^{1}H NMR ($CDCl_3$) δ 1.15 (d, *J*=3.39 Hz, 3H), 2.94 (dd, *J*=5.28,9.82 Hz, 1H), 3.07 (dd, *J*=5.28, 9.82 Hz, 1H), 3.47-3.59 (m, 1H), 6.39 (d, *J*=8.87 Hz, 1H), 6.62-6.85 (m,

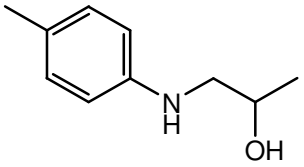
1H), 7.06-7.11 (m, 2H); IR (KBr): *v* 3357, 2969, 1595, 1499, 1372, 1234, 1127, 1067, 809, 640,503 cm^{-1}; EI-MS: *m*/*z* 186 [M^++1]

Table 3, Entry 8; 1-(2-chlorophenylamino)propan-2-ol:



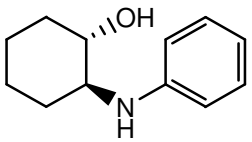
^{1}H NMR ($CDCl_3$) δ 1.18 (d, *J*=6.04 Hz, 3H), 2.97 (dd, *J*=4.53, 8.30 Hz, 1H), 3.15 (dd, *J*=3.02, 9.82 Hz, 1H), 3.44-3.62 (m, 1H), 3.89-3.99 (m, 1H), 4.46 (br s, 1H), 6.49-6.63 (m, 2H), 6.99 (ddd, *J*=1.51, 8.30, 9.82 Hz, 1H), 7.15 (dd, *J*=1.51, 6.79 Hz, 1H); IR (KBr): *v* 3406, 2969, 1598, 1509, 1322, 1034, 928, 742, 690 cm^{-1}; EI-MS: *m*/*z* 185 [M^+]

Table 3, Entry 9; 1-(p-tolylamino)propan-2-ol:



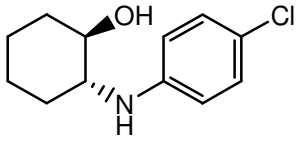
^{1}H NMR ($CDCl_3$) δ 1.21 (d, *J*=5.85 Hz, 3H), 2.22 (s, 3H), 2.82 (br s, 1H), 2.89 (dd, *J*=4.87, 7.80 Hz, 1H), 3.14 (dd, *J*=2.92, 9.75 Hz, 1H), 3.90-3.97 (m, 1H), 6.48-6.51 (m, 2H), 6.90-6.92 (m, 2H); IR (KBr): *v* 3382, 2923, 1730, 1616, 1519, 1304, 1257, 1092, 809, 508 cm^{-1}; EI-MS: *m*/*z* 166 [M^++1]

Table 3, Entry 10; (1S,2S)-2-(phenylamino)cyclohexanol:



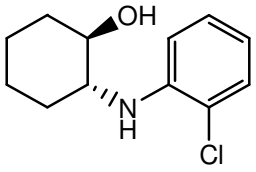
^{1}H NMR ($CDCl_3$) δ 0.91-1.07 (m, 1H), 1.17-1.41 (m, 3H), 1.62-2.81 (m, 2H), 2.03-2.09 (m, 2H), 2.86 (br s, 1H), 3.07 (ddd, *J*=3.90, 9.75, 13.66 Hz, 1H), 3.26 (ddd, *J*=3.90, 9.75, 13.66 Hz, 1H), 6.60-6.70 (m, 3H), 7.05-7.13 (m, 2H); IR (KBr): *v* 3390, 3051, 2929, 2856, 1601, 1502, 1258, 1068, 749, 693 cm^{-1}; EI-MS: *m*/*z* 191 [M^+]

Table 3, Entry 12; 2-(4-chlorophenylamino)cyclohexanol:



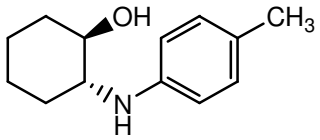
^{1}H NMR ($CDCl_3$) δ 0.96-1.09 (m, 1H), 1.28-1.43 (m, 3H), 1.71-1.80 (m, 2H), 2.07-2.11 (m, 2H), 2.81 (br s, 1H), 3.03 (ddd, *J*=3.96, 9.44, 13.40 Hz, 1H), 3.29 (ddd, *J*=3.96, 9.44, 13.40 Hz, 1H), 6.58 (d, *J*=8.68 Hz, 2H), 7.07 (d, *J*=8.68 Hz, 2H); IR (KBr): *v* 3401, 2923, 2853, 1597, 1503, 1322, 1257, 1049, 810, 670, 501 cm^{-1}; ESI-MS: *m*/*z* 226 [M^++1]

Table 3, Entry 13; 2-(2-chlorophenylamino)cyclohexanol:



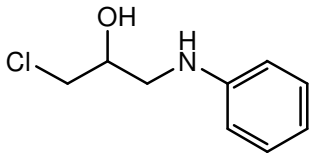
^{1}H NMR ($CDCl_3$) δ 1.03-1.17 (m, 1H), 1.21-1.43 (m, 3H), 1.67-1.78 (m, 2H), 2.01-2.11 (m, 2H), 2.56 (br s, 1H), 3.12 (ddd, *J*=4.15, 9.63, 13.40 Hz, 1H), 3.37 (ddd, *J*=4.15, 9.63, 13.40 Hz, 1H), 3.98 (br s, 1H), 6.58 (ddd, *J*=1.51, 7.36, 9.25 Hz, 1H) 6.78 (dd, *J*=1.51, 6.98 Hz, 1H), 7.05 (m, 1H), 7.18 (dd, *J*=1.51, 6.42 Hz, 1H); IR (KBr): *v* 3401, 2932, 2858, 1596, 1509, 1457, 1323, 1067, 741, 693, 590 cm^{-1}; ESI-MS: *m/z* 226 [M^++1]

Table 3, Entry 14; 2-(p-tolylamino)cyclohexanol:



^{1}H NMR ($CDCl_3$) δ 0.86-1.04 (m, 1H), 1.26-1.41 (m, 3H), 1.64-1.78 (m, 2H), 2.04-2.13 (m, 2H), 2.23 (s, 3H), 3.01 (ddd, *J*=3.77, 9.82, 13.59 Hz, 1H), 3.25 (ddd, *J*=3.77, 9.82, 13.59 Hz, 1H), 6.56 (d, *J*=8.30 Hz, 2H), 6.92 (d, *J*=8.30 Hz, 2H); IR (KBr): *v* 3387, 2928, 2857, 1616, 1518, 1450, 1298, 1066, 809, 500 cm^{-1}; ESI-MS: *m/z* 206 [M^++1]

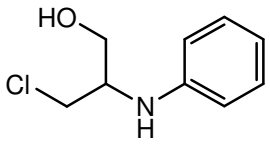
Table 3, Entry 15; 1-chloro-3(phenylamino)propan-2-ol:



^{1}H NMR ($CDCl_3$) δ 3.08 (br s, 1H), 3.17 (dd, *J*=6.04, 6.79 Hz, 1H), 3.34 (dd, *J*= 4.53, 9.06 Hz, 1H), 3.58 (dd, *J*=5.28, 6.04 Hz, 1H), 3.62 (dd, *J*=4.53, 6.79 Hz, 1H),

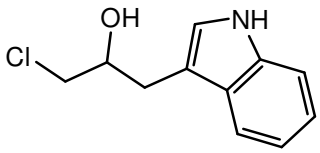
3.97-4.05 (m, 1H), 6.56-6.60 (m, 2H) 6.67-6.72 (m, 1H), 7.09-7.15 (m, 2H); IR (KBr): *v* 3391, 2922, 1603, 1506, 1318, 1260, 1090, 752, 694 cm^{-1}; EI-MS: *m*/*z* 186 [M^++1]

Table 3, Entry 15; 3-chloro-2-(phenylamino)propan-1-ol:



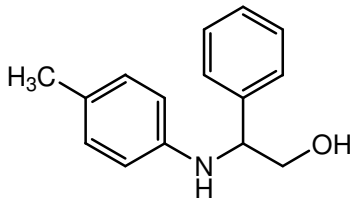
^{1}H NMR ($CDCl_3$) δ 3.15 (m, 1H), 3.41(dd, *J*=6.79, 8.30 Hz, 1H), 3.51-3.57 (m, 2H), 3.90 (dd, *J*=3.02, 12.08 Hz, 1H), 4.06-4.13 (m, 1H), 4.14-4.22 (m, 1H), 6.63-6.80 (m, 3H), 7.16-7.24 (m, 2H); IR (KBr): *v* 3334, 2923, 1598, 1503, 1362, 1225, 1101, 752, 696 cm^{-1}; EI-MS: *m*/*z* 186 [M^++1]

Table 3, Entry 16; 1-chloro-3-(1H-indol-3-yl)propan-2-ol:



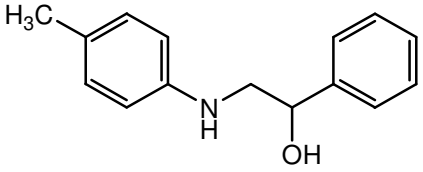
^{1}H NMR ($CDCl_3$) δ 2.12 (br s, 1H), 3.02 (dd, *J*=6.04, 8.30 Hz, 1H), 3.08 (dd, *J*=6.04, 8.30 Hz, 1H), 3.46-3.61 (m, 2H), 4.11 (quintet, *J*=5.28 Hz, 1H), 7.06-7.19 (m, 3H), 7.31 (d, *J*=7.55 Hz, 1H), 7.59 (d, *J*=8.30 Hz, 1H), 7.98 (br s, 1H); IR (KBr): *v* 3411, 3055, 2923, 2853, 1710, 1620, 1456, 1427, 1339, 1257, 1087, 1044, 746, 586, 425 cm^{-1}; ESI-MS: *m*/*z* 210 [M^++1]

Table 3, Entry 18; 2-phenyl-2-(p-tolylamino)ethanol:



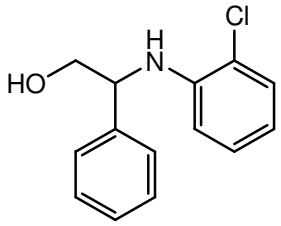
^{1}H NMR ($CDCl_3$) δ 2.11(s, 3H), 3.02 (br s, 1H), 3.60 (dd, *J*=4.16, 7.28 Hz, 1H), 3.80 (dd, *J*=4.16, 7.28 Hz, 1H), 4.33 (dd, *J*=4.16, 7.28 Hz, 1H), 6.34 (d, *J*=8.32 Hz, 2H), 6.77 (d, *J*=8.32 Hz, 2H), 7.12-7.24 (m, 5H); IR (KBr): *v* 3390, 2923, 1616, 1518, 1305, 1262, 1069, 808, 701, 513 cm^{-1}; ESI-MS: *m/z* 228 [M^++1], 210 [M^+–OH]

Table 3, Entry 18; 1-phenyl-2-(p-tolylamino)ethanol:



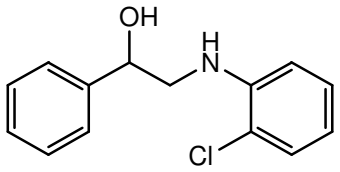
^{1}H NMR ($CDCl_3$) δ 2.17 (s, 3H), 3.20 (br s, 1H), 3.62 (dd, *J*=4.16, 7.28 Hz, 1H), 3.81 (dd, *J*=4.16, 7.28 Hz, 1H), 4.36 (dd, *J*=3.12, 4.16 Hz, 1H), 6.39 (d, *J*=8.32 Hz, 2H), 6.83 (d, *J*=8.32 Hz, 2H), 7.23-7.31 (m, 5H); IR (KBr): *v* 3390, 2924, 1615, 1518, 1261, 1092, 1022, 802, 701 cm^{-1}; ESI-MS: *m/z* 228 [M^++1]

Table 3, Entry 19; 2-(2-chlorophenylamino)-2-phenylethanol:



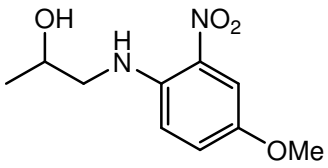
^{1}H NMR ($CDCl_3$) δ 1.83 (br s, 1H), 3.75 (dd, *J*=4.34, 7.17 Hz, 1H), 3.92 (dd, *J*=4.34, 7.17 Hz, 1H), 4.47 (dd, *J*=3.77, 4.34 Hz,1H), 5.12 (br s, 1H), 6.34 (d, *J*=8.12 Hz, 1H), 6.55 (ddd, *J*=1.13, 7.93, 8.87 Hz, 1H), 6.90 (ddd, *J*=1.13, 7.93, 8.87 Hz, 1H), 7.19-7.25. (m, 2H), 7.27-7.35 (m, 4H); IR (KBr): *v* 3405, 2929, 1597, 1506, 1320, 1033, 745, 701 cm^{-1}; ESI-MS: *m*/*z* 248 [M^++1]

Table 3, Entry 19; 2-(2-chlorophenylamino)-1-phenylethanol:



^{1}H NMR ($CDCl_3$) δ 3.51 (dd, *J*=3.02, 4.53 Hz, 1H), 3.92 (dd, *J*=4.53, 6.79 Hz, 1H), 4.09 (dd, *J*=4.53, 6.79 Hz, 1H), 4.83 (br s, 1H), 5.28 (br s, 1H), 6.48 (dd, *J*=1.51, 6.79 Hz, 1H), 6.66-6.84 (m, 2H), 7.04 (ddd, *J*=1.51, 8.30, 9.06 Hz, 1H), 7.21 (ddd, *J*=1.51, 8.30, 9.06 Hz, 1H), 7.41-7.54 (m, 4H); IR (KBr): *v* 3403, 2923, 1596, 1506, 1261, 1069, 1031, 799, 748 cm^{-1}; ESI-MS: *m*/*z* 248 [M^++1]

Table 3, Entry 20; 1-(4-methoxy-2-nitrophenylamino)propan-2-ol:



^{1}H NMR ($CDCl_3$) δ 1.32 (d, J=6.04 Hz, 3H), 3.19-3.28 (m, 1H), 3.32-3.39 (m, 1H), 3.65-3.72 (m, 1H), 3.79 (s, 3H), 6.82-6.90 (m, 1H), 7.07-7.11 (dd, J=3.02, 6.04 Hz, 1H), 7.59 (d, J=3.02 Hz, 1H); IR (KBr): v 3370, 2924, 2854, 1742, 1571, 1519, 1283, 1222, 1146, 1035, 804 cm^{-1}; ESI-MS: m/z 227 [M^++1]