**Supporting Information**

**A Sustainable approach towards the three-component synthesis of unsubstituted 1*H-*imidazoles in the water at ambient conditions**

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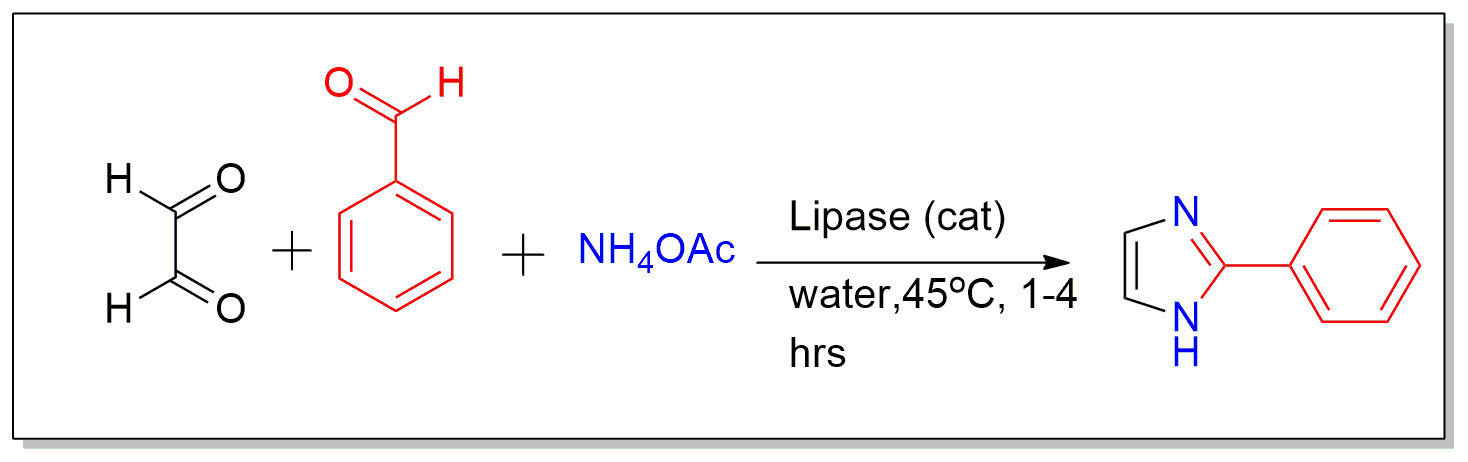
1. **Experimental Section**

**Materials and methods:**

Melting points of all the compounds were recorded by the Analab Thermo Cal melting point apparatus in the open capillary tube and are uncorrected. 1H NMR spectra were recorded on MR400 Agilent Technology NMR spectrometer using tetramethylsilane (TMS) as an internal standard and DMSO-D6/CDCl3 as a solvent. Chemicals and solvents used were of LR grade and purchased from SD fine, Aldrich, Avra Synthesis and Spectrochem and used without purification. The purity determination of the starting materials and reaction monitoring was accomplished by thin-layer chromatography (TLC) on Merck silica gel G F254 plates. All the products are known compounds and were identified by 1H NMR spectroscopy.

**General Procedure for the Synthesis of 2-phenylimidazoles catalyzed by Lipase (**0.05 g**) (3a.-3h.)**

A mixture of glyoxal (0.058 g), benzaldehyde (0.106 g), ammonium acetate (0.154 g), and lipase (0.05 g) were taken in a 50-mL, two-necked, round-bottomed flask. The reaction mixture was stirred for 1 hr under reflux in 10 mL of water. After completion of the reaction as indicated by thin-layer chromatography (TLC; ethyl acetate/n-hexane, 2:1), the reaction mixture was filtered and washed with water (3 × 10 mL), and the solid residue was crystallized from ethyl acetate to give pure product yellowish in colour. All products are known compounds and were identified by their melting point, 1H NMR spectra according to the literature.

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**Scheme 1**

In similar way, tri-substituted imidazoles are synthesized from benzil (0.004 g), benzaldehyde (0.009 g), ammonium acetate (0.026 g), lipase (0.05 g) in 10 ml water, were taken in a 50 ml two-necked round bottomed flask. The reaction mixture was stirred for 4 hrs at 50 °C.



**Scheme 2**

**2. The experimental data of the Products:**

**2-phenyl-1H-imidazole: (**Figure 2, Entry no. 3a) [1]



Mp 145–147°C.yield–67.5%, 13C NMR (100 MHz, CDCl3) δ 125.16, 127.85, 128.33, 128.61, 129.06, 129.10, 131.63; 1H NMR (400 MHz, CDCl3) δ 7.92 (dd, J = 8.0, 2.0 Hz, 1H), 7.38 – 7.31 (m, 3H), 7.15 (s, 2H); HRMS m/z (ESI) calculated for C9H9N2 [M+H]+ 145.0760, found 145.0705.

**2-(p-tolyl)-1H-imidazole:** (Table no. 3, Entry no. 3b) [2]



Mp 219-221°C, yield–57.76%, IR (KBr): νmax (cm−1) 3687, 1578, 1517, 1443, 1104, 822, 731. 13C NMR (100.6 MHz, DMSO-d6): δ 20.8, 124.7, 128.2, 129.2, 137.2, 145.7. 1H NMR (400 MHz, DMSO-d6): δ 2.32 (s, 3H), 7.0 (br s, 1H), 7.2 (br s, 1H), 7.24 (d, J=8.0 Hz, 2H), 7.81 (d, J=8.0 Hz, 2H), 12.39 (s, 1H).  MS m/z: 159.5 (M+). Calculated for C10H10N2: C, 75.92; H, 6.37; N, 17.71. Found: C, 76.03; H, 6.45; N, 17.39.

**2-(4-bromophenyl)-1H-imidazole:** (Table no. 3, Entry no. 3c) [3]



Mp175–176°C, yield–61.5%, 13C NMR (100.6 MHz, DMSO-d6): δ 120.9, 126.7, 130.0, 131.6, 144.5. MS m/z: 225.4 (M+).C, 48.46; H, 3.16; N, 12.56. Found: C, 48.17; H, 3.16; N, 12.75 1H NMR (CDCl3, 300 MHz) δ 12.59 (s, 1H), 7.87 (d, J = 8.1 Hz, 2H), 7.64 (d, J = 8.1 Hz, 2H), 7.27 (s, 1H), 7.04 (s, 1H). MS (ESI) calculated for C9H7BrN2 222.0, found 222.8 [M+H] +.

**4-(1H-imidazol-2-yl) aniline:**(Table no. 3, Entry no. 3d) [4]



**2-(3-nitrophenyl)-1H-imidazole:**(Table no. 3, Entry no. 3e) [5]



Mp193–196°C; yield-­­59.3%; 13C NMR (75 MHz, DMSO-d6) δ 148.7, 143.9, 132.7, 131.1, 130.7, 130.0, 122.6, 119.4, 119.1; 1H NMR (CDCl3): d 7.21–7.26 (d, 2H, CH of C4 and C5 of imidazole), 7.34–7.36 (d, 2H, CH of C3 and C5 of ArH), 7.45–7.47 (d, 2H, CH of C2 and C6 of ArH); IR (KBr pellets) cm1:3489.95 (NH str, imidazole), 1521.73 (C–C str, Ar), 1653.85 (C–H str, Ar), 749.29 (C–Cl str). calculated for C9H7N3O2, Found: 190.0614.

**4-(1H-imidazol-2-yl) benzoic acid:**(Table no. 3, Entry no. 3f) [6]



**2-(1H-imidazol-2-yl) pyridine:**(Table no. 3, Entry no. 3g) [7]



Mp. 132–133 °C, yield–58.56%, IR (KBr):2888 (br C–H str), 1593 (pyridine C=N str), 1567 (imidazole C=N str). 13C NMR (100 MHz, CDCl3) δ 148.8 (*C*7), 148.6 (*C*2), 146.4 (*C*4), 137.5 (*C*6), 130.4 (*C*9-10), 123.3, 1H NMR (400 MHz, CDCl3) δ 8.49 (ddd, *J* = 4.9, 1.7, 1.0 Hz, *H*2, 1H), 8.22 (dt, *J* = 8.0, 1.1 Hz, *H*5, 1H), 7.78 (td, *J* = 7.6, 1.7 Hz, *H*1, 1H), 7.26 (ddd, *J* = 7.5, 4.9, 1.2 Hz, *H*6, 1H), 7.17 (s, *H*9–10, 2H). ESI-MS *m*/*z* 146.0718 (M+H)+,calculated for (C5H4N)(C3H3N2) H, 4.71; N, 28.10.

**2-(thiophen-2-yl)-1H-imidazole:**(Table no. 3, Entry no. 3h) [8]

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Mp 196–197 °C, yield–54.34%, IR (KBr): νmax (cm−1) 3435, 3107, 2913, 1651, 1558, 1520, 1471, 1102. 13C NMR (100.6 MHz, DMSO-d6): δ 123.3, 125.6, 127.8, 134.6, 141.5, 1H NMR (400 MHz, DMSO-d6): δ 6.9 (br s,1H), 7.10 (dd, J=4.8 Hz, J=4.0 Hz, 1H), 7.2 (br s,1H), 7.48 (dd, J=4.8 Hz, J=1.6 Hz,1H), 7.49 (dd, J=4.0 Hz, J=1.6 Hz, 1H), 12.50 (s, 1H).  MS m/z: 151.4 (M+). Calculated for C7H6N2S: C, 55.97; H, 4.03; N, 18.65. Found: C, 55.95; H, 4.21; N, 18.37.

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9. **1HNMR, 13C NMR and Mass spectra of synthesized compounds:**

**2-phenyl 1*H*-imidazole**



**1H NMR spectra of 2-phenyl-1*H*-imidazole**



**13C NMR spectra of 2-phenyl-1*H*-imidazole**



**Mass spectra of 2-phenyl-1*H*-imidazole**