# **Supplementary material**

# Sapindus mukorossi seed shell extract mediated green synthesis of CuO

## nanostructures: An efficient catalyst for C-N bond-forming reactions

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#### **Characterization of the catalyst**

The synthesized CuO was characterized by different spectroscopic, microscopic and diffractometric techniques. X-ray diffraction (XRD) study of the dried powder samples was carried out on an X'Pert Pro (Panalytical) powder X-ray diffractometer using Cu  $k_a$  radiation with a wavelength of 0.154 nm at an accelerating voltage of 40 kV with 35 mA current. For the scanning electron microscopic (SEM) study, a small amount of the dry powder samples was spread on carbon tape pasted on an aluminium stub and then sputter-coated with platinum to minimize the charging effect. The micrographs were then recorded in a field emission scanning electron microscope (FESEM) (Carl ZEISS Sigma 300VP) at an accelerating voltage of 5 kV. An energy-dispersive X-ray (EDX) spectroscopy study was performed on Oxford Instrument attached to the electron microscope. For transmission electron microscopic (TEM) studies, a drop of an aqueous suspension of an individual powder sample was cast on a carbon-coated copper grid. The excess solutions were soaked with tissue paper followed by drying in the air. The micrographs were then recorded in a high-resolution JEOL electron microscope (JEM

2100EM) at an accelerating voltage of 200 kV. X-ray photoelectron spectroscopy (XPS) analyses of the dried powder samples were performed in JEOL makes X-ray photoelectron spectrometer (JPS 9030) using Mg  $k_{\alpha}$  radiations with an incident energy of 1253.6 eV under ultrahigh vacuum. The charging effect on the sample was corrected by setting the binding energy of the carbon (C-1s) at 284.6 eV and this carbon peak was used as a reference position for scaling all the other peaks. The nitrogen (N<sub>2</sub>) gas adsorption-desorption isotherms of the CuO NPs were recorded at 77 K (Quantachrome Nova 1000 Instrument) after degassing the powder samples at 120 °C for 2 h in an inert atmosphere. Brunauer-Emmett-Teller (BET) specific surface areas and pore diameters of the samples were determined from the adsorption-desorption isotherms following the well-known Barrett-Joyner-Halenda (BJH) method. <sup>1</sup>*H* and <sup>13</sup>*C* NMR spectra were recorded in a JNM ECS 400 MHz NMR spectrophotometer (JEOL) using tetramethylsilane (TMS) as the internal standard. Chemical shift values and coupling constants are expressed in ppm and Hz.



Figure S1. N<sub>2</sub> gas adsorption-desorption curve for samples CuO-2 and CuO-4.

### Characterization of the catalytic products:

Entry 1: 3-Phenylamino-propionitrile



Physical appearance: Brown coloured solid

<sup>1</sup>**H** NMR (CDCl<sub>3</sub>, 400 MHz): δ 7.18 (*t*, 2H, *J*=7.2Hz), 6.72 (*t*, 1H, *J*=7.6Hz), 6.57 (*d*, 2H, *J*=8Hz), 3.46 (*t*, 2H, *J*=6.40Hz), 2.57(*t*, 2H, *J*=6.4Hz) ppm.

<sup>13</sup>C NMR (CDCl<sub>3</sub>, 125 MHz): 146.25, 129.89, 119.32, 118.48, 113.62, 40.12, 19.724 ppm.

Entry 4: 3-p-Tolylamino-propionitrile



Physical appearance: Brown coloured solid

<sup>1</sup>**H** NMR (CDCl<sub>3</sub>, 400 MHz): δ 7.0125 (*d*, *J*=8.4Hz, 2H), 6.540 (*d*, *J*=8.4Hz, 2H) 3.491 (*t*, *J*=6.4Hz, 2H), 2.613 (*t*, *J*=6.4Hz, 2H), 2.224 (*s*, 3H) ppm.

<sup>13</sup>C NMR (CDCl<sub>3</sub>, 125 MHz): 143.74, 130.14, 128.22, 118.59, 113.48, 40.06, 20.41, 18.07 ppm.

Entry 5: 3-((4-hydroxyphenyl)amino) propanenitrile



Physical appearance: Black coloured crystal

**1H NMR (CDCl<sub>3</sub>, 400 MHz):** δ 2.66 (t, 2H), 3.22 (d, 2H), 5.21 (1H, s), 6.46-6.48 (d, J= 8Hz, 2H), 6.56-6.58 (d, J= 8Hz, 2H), 8.48 (s, 1H)

Entry 8: 3-(diethylamino)propanenitrile



Physical appearance: Lightbrown colored semisolid

<sup>1</sup>**H NMR (CDCl<sub>3</sub>, 400 MHz):** δ 2.764 (*t*, *J*=6.8, 2H), 2.510 (*q*, *J*=7.2Hz, 4H), 2.404 (*t*, *J*=7.2Hz, 2H), 1.001 (*t*, *J*= 7.2Hz, 6H) ppm.

<sup>13</sup>C NMR (CDCl<sub>3</sub>, 125 MHz): 119.176, 48.409, 46.49, 15.97, 11.928 ppm.



# <sup>1</sup>H and <sup>13</sup>C NMR spectra of some isolated products

<sup>1</sup>H NMR spectra of 3-phenylamino-propionitrile (Entry 1)



<sup>13</sup>C NMR spectra of 3-phenylamino-propionitrile (Entry 1)



<sup>1</sup>H NMR spectra of 3-p-tolylamino-propionitrile (Entry 4)



<sup>13</sup>C NMR spectra of 3-p-tolylamino-propionitrile (Entry 4)



<sup>1</sup>H NMR spectra of the product 3-((4-hydroxyphenyl)amino) propanenitrile (Entry 5)



<sup>1</sup>H NMR spectra of the product 3-(diethylamino)propanenitrile (Entry 8)



<sup>13</sup>C NMR spectra of the product 3-(diethylamino)propanenitrile (Entry 8)