Supporting Information

Pd Nanoparticles-Loaded Honeycomb-Structured Bionanocellulose as a Heterogeneous Catalyst for Heteroaryl Cross-Coupling Reaction

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1. GENERAL INFORMATION

The chemicals used in all the experiments were procured commercially and used without further purification. The progress of the reaction was monitored through thin layer chromatography on Merck Kieselgel Silica gel 60 F₂₅₄ plates using short wave UV light (λ =254 nm). The products were purified by column chromatography using Silica gel 60-120 mesh. The identification of the purified products was carried out by NMR (¹H and ¹³C) spectroscopy. The NMR spectrum were recorded on a 400 MHz JEOL NMR spectrophotometer (400 MHz for ¹H and 100 MHz for ¹³C NMR spectroscopy). Chemical shifts for both ¹H (δ_H) and ¹³C (δ_C) NMR are assigned in parts per million (ppm) using TMS (0 ppm) as the internal reference and CDCl₃ and DMSO-*d*₆ as solvent (CDCl₃: δ_H = 7.25 ppm and δ_C = 77.1 ppm; DMSO-*d*₆: δ_H = 2.5 ppm, DMSO-*d*₆ absorbed water = 3.3 ppm and δ_C = 40.0 ppm).



Figure S1: Effect of catalyst recycling on the yield in Suzuki-Miyaura reaction. Reactions were carried out with 4-bromoanisole (0.5 mmol), phenylboronic (0.6 mmol), PdNPs@NCmw (10 wt%), K_2CO_3 (1.5 mmol), EtOH:H₂O (1:1) (4 mL), rt (25 °C), Yields were determined with GC using n-dodecane as internal standard.



Figure S2: Effect of catalyst recycling on the yield in Sonogashira reaction. Reactions were carried out with 4-iodotoluene (0.5 mmol), phenylacetylene (0.75 mmol), PdNPs@NCmw (10 wt%), H₂O:EtOH (1:7, 4 mL) K₂CO₃ (1.5 mmol), reactions were carried out at 70 °C, Yields were determined with GC using benzophenone as internal standard.



Copies of ¹H NMR and ¹³C NMR spectrum of isolated products





Figure S4 (¹³C NMR of 3a)



Figure S5 (¹H NMR of 3b)



Figure S6 (¹³C NMR of 3b)



Figure S7 (¹H NMR of 3c)



Figure S8 (¹³C NMR of 3c)



Figure S9 (¹H NMR of 3d)



Figure S10 (¹³C NMR of 3d)







Figure S12 (¹³C NMR of 3e)







Figure S14 (¹³C NMR of 3f)



Figure S15 (¹H NMR of 3g)



Figure S16 (¹³C NMR of 3g)







Figure S18 (¹³CNMR of 3h)







Figure S20 (¹³C NMR of 3i)





-0.3 --0.2

-0.1 --0.0

90 80 Chemical Shift



Figure S23 (¹H NMR of 3k)



Figure S24 (¹³C NMR of 3k)



Figure S26 (¹³C NMR of 3l)







Figure S28 (¹³C NMR of 3m)



Figure S29 (¹H NMR of 3n)



Figure S30 (¹³C NMR of 3n)



Figure S32 (¹³C NMR of 30)



Figure S34 (¹³C NMR of 6a)



Figure S35 (¹H NMR of 6b)



Figure S36 (¹³C NMR of 6b)



Figure S38 (¹³C NMR of 6c)







Figure S40 (¹³C NMR of 6d)







Figure S42 (¹³C NMR of 6e)







Figure S44 (¹³C NMR of 6f)



Figure S45 (¹H NMR of 6g)



Figure S46 (¹³C NMR of 6g)



Figure S47 (¹H NMR of 6h)



Figure S48 (¹³C NMR of 6h)



Figure S49 (¹H NMR of 9a)



Figure S50 (¹³C NMR of 9a)



Figure S51 (¹H NMR of 9c)



Figure S52 (¹³C NMR of 9c)



Figure S53 (¹H NMR of 9d)



Figure S54 (¹³C NMR of 9d)



Figure S55 (¹H NMR of 9e)



Figure S56 (¹³C NMR of 9e)



Figure S57 (¹H NMR of 9f)



Figure S58 (¹³C NMR of 9f)







Figure S60 (¹³C NMR of 9g)