

Supporting Information

Chitosan-Proline supported palladium (II) a green nanocatalyst for Suzuki cross-coupling reaction in water

Abdol R. Hajipour^{1,2*}, Elahe Boostani¹, Fatemeh Mohammadsaleh¹

¹*Pharmaceutical Research Laboratory, Department of Chemistry, Isfahan*

University of Technology, Isfahan 84156, IR Iran, E-mail

²*Department of Pharmacology, University of Wisconsin, Medical School, 1300 University*

Avenue, Madison, 53706-1532, WI, USA

*Corresponding author: Tel.: + 98 313 391 3262; fax: + 98 313 391 2350; e-mail:

haji@cc.iut.ac.ir.

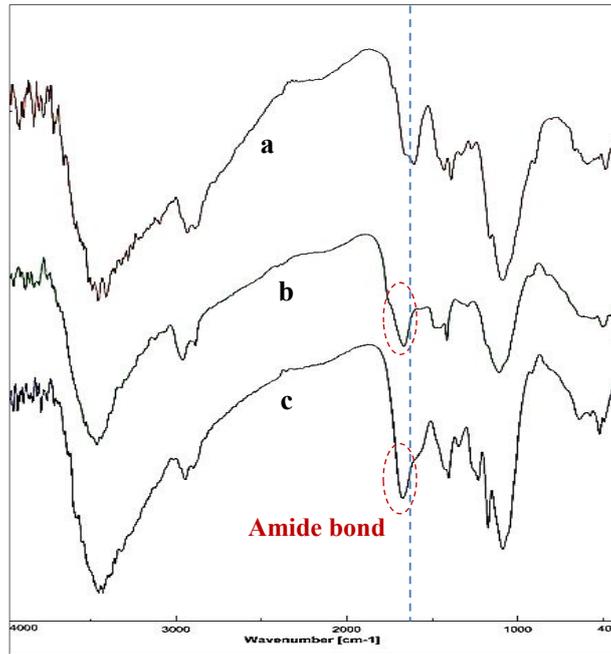


Fig. 1FT-IR Spectra. a) Chitosan, b) Chitosan modified by proline, c) CS-proline-Pd (II) complex

¹H-NMR, ¹³C-NMR, FT-IR and boiling points of some biaryl derivatives

Data section

4-nitro-1,1'-biphenyl

White solid, melting point: 88°C

¹H-NMR (400MHz, CDCl₃, ppm, TMS): δ = 8.3 (d, *J*= 8.7Hz, 2H), 7.7 (d, *J*= 8.7 Hz, 2H), 7.65 (dd, *J*= 1.8, 5.4Hz, 2H), 7.55-7.40 (m, 3H).

¹³C-NMR (100MHz, CDCl₃, ppm): δ = 147.63, 147.09, 138.75, 129.01, 128.92, 127.81, 127.40, 124.23.

FT-IR (KBr, cm⁻¹): ν = 3367, 3242, 1596, 1513, 1345, 853, 739, 699.

9-phenylphenanthrene

White solid, melting point: 60-62°C

¹H-NMR (400MHz, ppm, CDCl₃, TMS) δ = 8.80(d, *J*=8.0 Hz, 1H), 8.74 (d, *J*= 8.4 Hz, 1H), 7.92 (t, *J*= 8.8Hz, 2H), 7.4-7.7 (m, 10H).

¹³C-NMR (100MHz, CDCl₃, ppm): δ = 140.82, 138.76, 131.54, 131.06, 130.66, 130.02, 129.91, 128.67, 128.30, 127.55, 127.32, 126.93, 126.80, 126.62, 126.49, 126.38, 122.92, 122.51.

FT-IR (KBr, cm⁻¹): ν = 3150, 3056, 3021, 1593, 1491, 1450, 893, 746, 700, 588.

4-methoxy-1,1'-biphenyl

White solid, melting point: 116-118°C

¹H-NMR (400MHz, ppm, CDCl₃): δ = 7.44-7.48(t, 2H, *J*= 8.8Hz), 7.31-7.35 (t, 4H, *J*= 8Hz), 7.20-7.24 (t, 1H, *J*= 7.2Hz), 6.89-6.91 (d, 2H, *J*= 8.8 H), 3.77(s, 3H).

¹³C-NMR (100MHz, CDCl₃, ppm): δ = 141.11, 138.32, 137.08, 129.48, 128.71, 127.10, 126.88, 21.15.

4-Acetylbiphenyl

White solid, melting point: 119-121°C

$^1\text{H-NMR}$ (400MHz, CDCl_3 , ppm, TMS): $\delta = 7.95\text{-}7.97$ (d, $J=8.4\text{Hz}$, 2H), $7.60\text{-}7.62$ (dd, $J= 8.1, 1.5$ Hz, 2H), $7.54\text{-}7.56$ (d, $J= 8.8$ Hz, 2H), $7.38\text{-}7.41$ (t, $J= 6$ Hz, 2H), $7.32\text{-}7.34$ (m, 1H), 2.56 (s, 3H).

$^{13}\text{C-NMR}$ (100MHz, CDCl_3 , ppm): $\delta = 198.14, 146.21, 140.31, 136.31, 129.38, 129.34, 128.66, 127.70, 127.65, 27.08$.

FT-IR (KBr, cm^{-1}): $\nu = 2920, 1726, 1670, 1402, 1268, 1120, 764, 690, 593$.

Figure section

2-chloro-1,1'-biphenyl

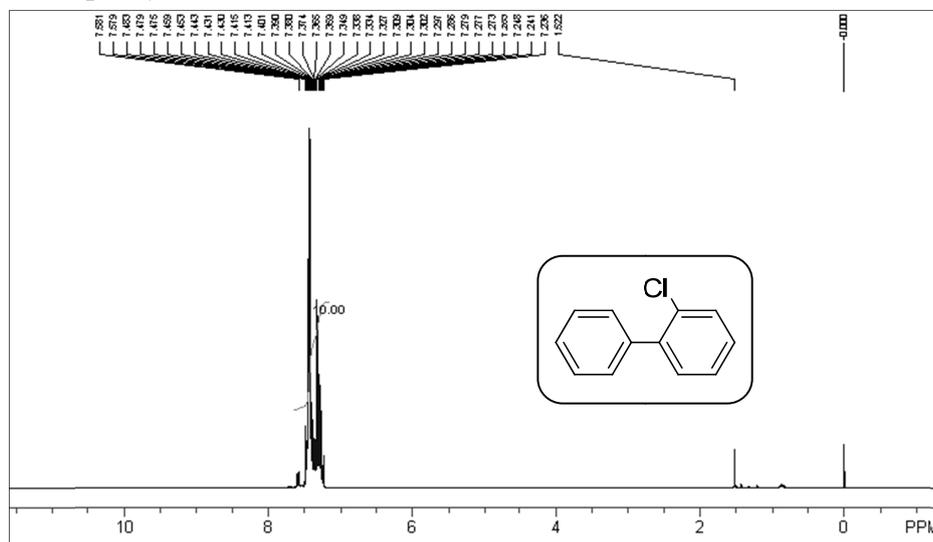


Fig. 2 $^1\text{H-NMR}$ (400MHz, CDCl_3) spectrum of 2-chloro-1,1'-biphenyl

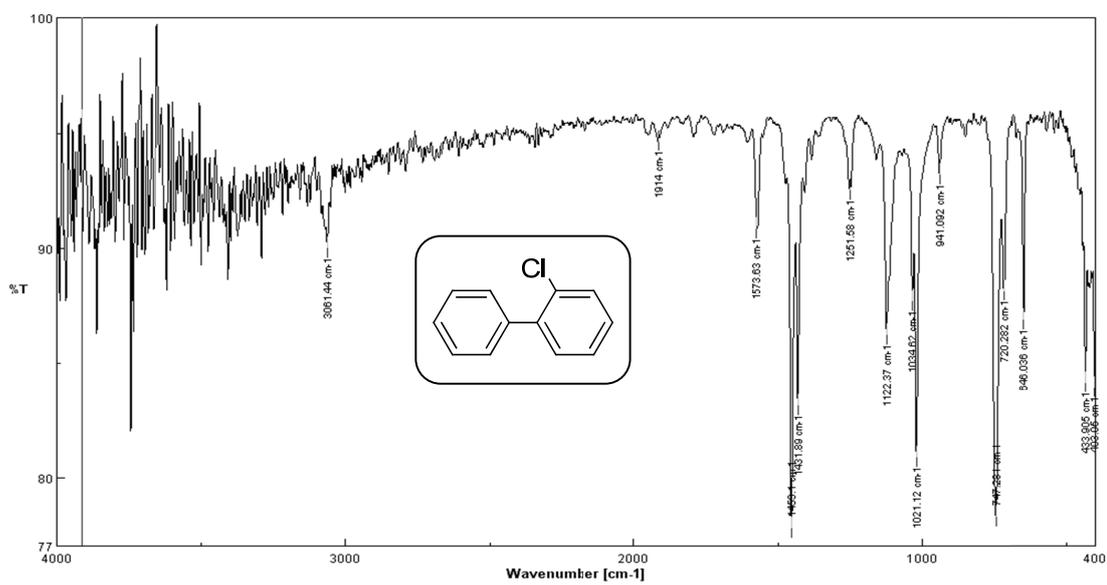
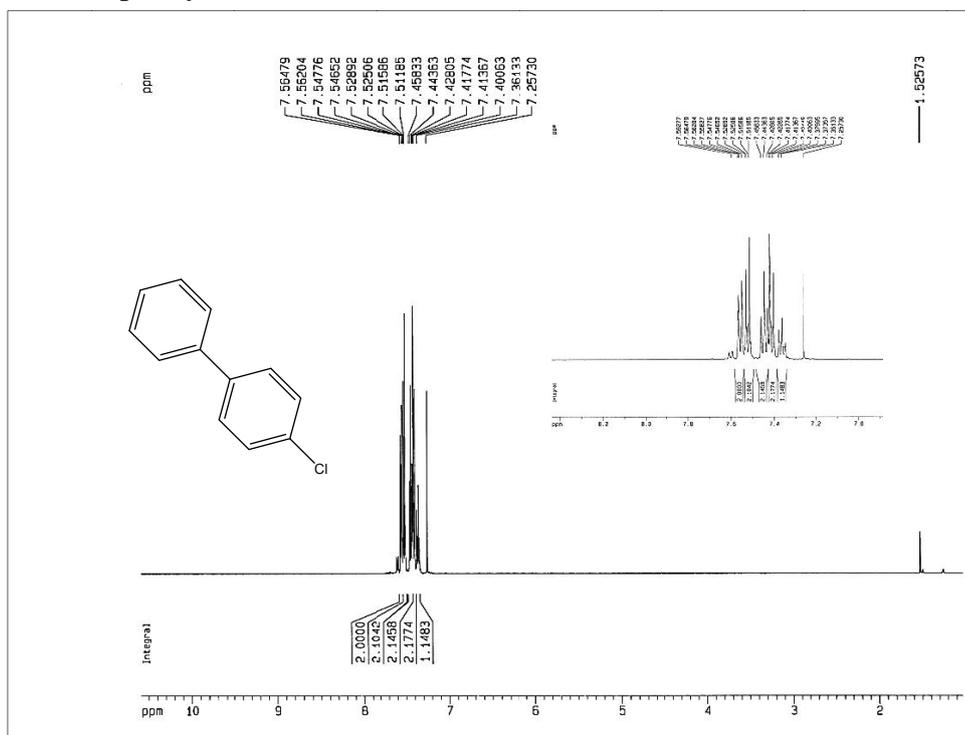


Fig. 3 FT-IR spectrum of 2-chloro-1,1'-biphenyl

4-chloro-1,1'-biphenyl



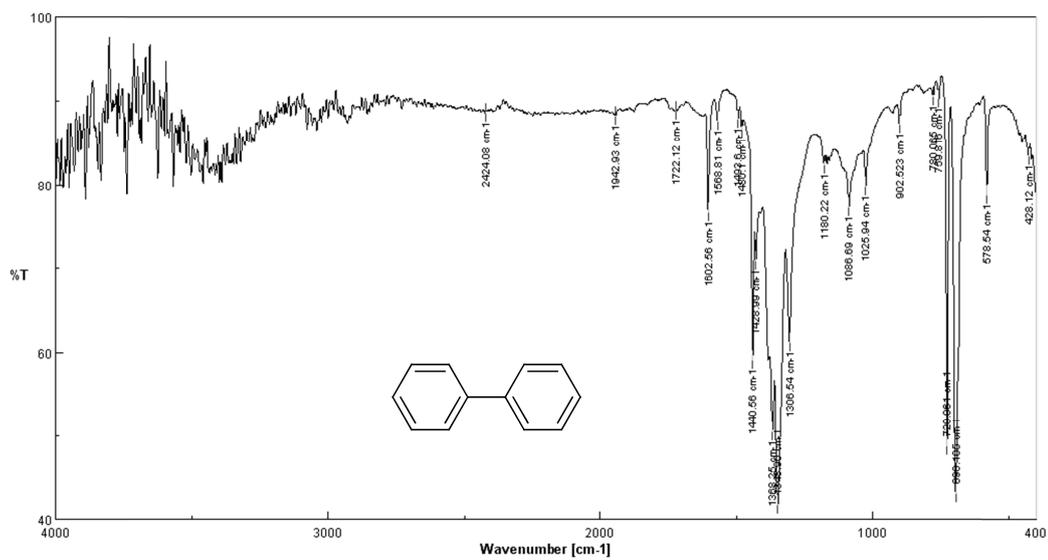


Fig. 6 FT-IR spectrum of 1,1'-biphenyl

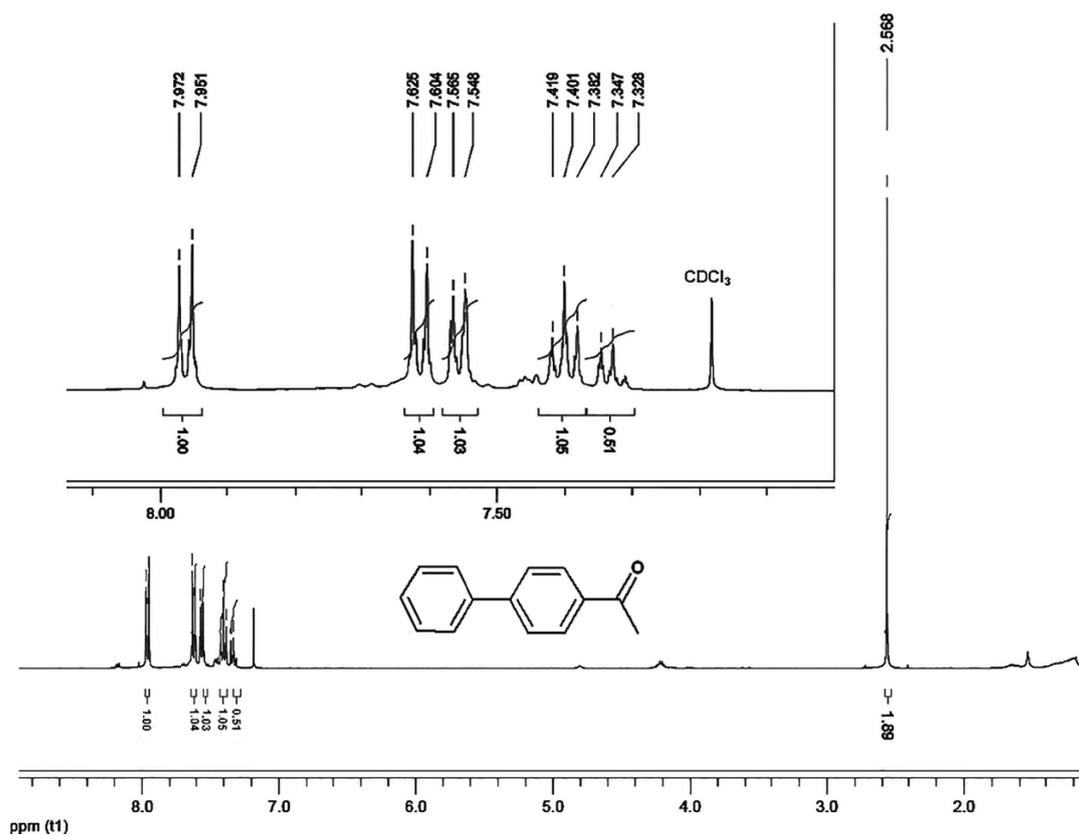


Fig. 7 ¹H-NMR (400MHz, CDCl₃) spectrum of 4-acetylbiphenyl

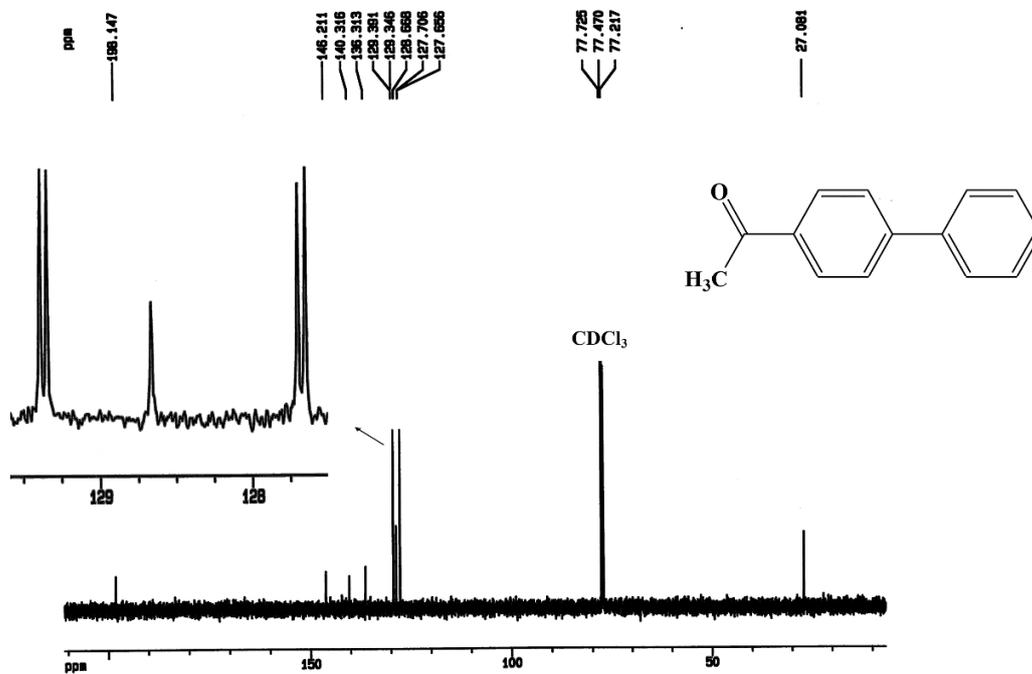


Fig. 8 ^{13}C -NMR (125 MHz, CDCl_3) spectrum of 4-acetylbiphenyl

GC-MS analysis

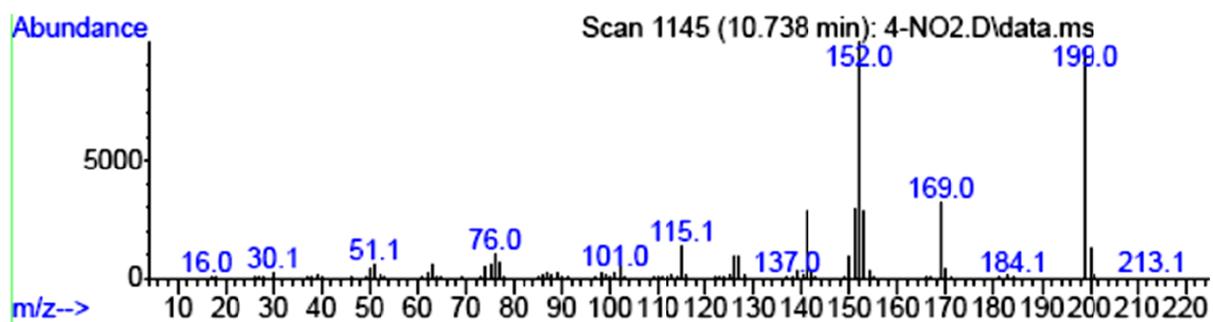


Fig. 9 GC-MS spectrum of 4-nitro-1,1'-biphenyl