

Electronic Supplemental Information (ESI)

**Analysis of water extract of waste papaya bark ash and its implications as *in situ*
base in ligandless recyclable Suzuki-Miyaura coupling reaction**

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1. General information

Instrumentation and Chemicals

All the reagents were obtained from commercial source without any further purification. ^1H and ^{13}C NMR spectra were recorded with a JNM ECS 400 MHz NMR spectrophotometer (JEOL) using tetramethylsilane (TMS) as the internal standard. Chemical shift values are expressed in ppm. Coupling constants are expressed in hertz. EDX analyses were carried out with “JEOL, JSM Model 6390 LV” scanning electron microscope, operating at an accelerating voltage of 15 kV. Reactions were monitored by thin-layer chromatography using aluminium sheets with silica gel 60F₂₅₄ (Merck). UV light and Iodine vapour were used to visualize compounds.

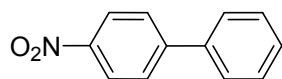
2. Experimental Section:

General experimental procedure for Suzuki reaction:

A mixture of aryl bromide (0.5 mmol), arylboronic acid (0.6 mmol), Pd(OAc)₂ (0.5 mol%), water-extract (2 mL) and EtOH (2 mL) was stirred at room temperature in a 50 mL round bottom flask. After completion (vide TLC); the reaction mixture was extracted with ethyl acetate (3 × 10 mL) and the combined organic layer was washed with brine (2 × 10 mL), dried over Na₂SO₄ and concentrated in vacuo. The residue was purified by column chromatography on silica gel (Eluent: EtOAc-Hexane) to give the corresponding biaryl compound. The desired products are characterized by comparing ^1H and ^{13}C NMR spectral data with authentic samples.

3. Spectroscopic data and copies of ^1H NMR & ^{13}C NMR of isolated compounds:

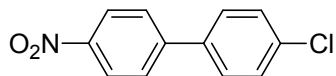
4-Nitrobiphenyl



Pale yellow solid, ^1H NMR (400 MHz, CDCl₃) δ : 8.30-8.28 (d, 2H, $J=8$ Hz), 7.74-7.72 (d, 2H, $J=8$ Hz), 7.61 (d, 2H, $J=8$ Hz), 7.49-7.44 (m, 3H).

^{13}C NMR (CDCl₃, 100 MHz, ppm): δ 147.7, 138.8, 129.2, 127.9, 127.4, 124.2.

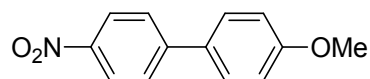
4-Chloro-4'-nitrobiphenyl



Pale yellow solid, ^1H NMR (400 MHz, CDCl₃): δ 8.30-8.28 (d, 2H, $J=8$ Hz), 7.71 (d, 2H, $J=8$ Hz), 7.54-7.45 (m, 4H).

^{13}C NMR (CDCl₃, 100 MHz, ppm): δ 146.4, 137.2, 135.3, 129.4, 128.7, 127.7, 124.3.

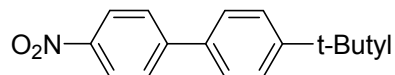
4-Methoxy-4'-nitrobiphenyl



Yellow solid, ^1H NMR (400 MHz, CDCl_3) δ : 8.27-8.25 (d, 2H, $J=8$ Hz), 7.69-7.67 (d, 2H, $J=8$ Hz), 7.56 (d, 2H), 7.02-7.00 (d, 2H, $J=8$ Hz).

^{13}C NMR (CDCl_3 , 100 MHz, ppm) δ : 160.5, 147.3, 146.6, 131.1, 128.6, 127.1, 124.2, 114.6, 55.5.

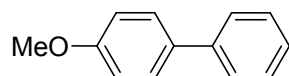
4-Nitro-4'-*t*-butylbiphenyl



Pale Yellow solid, ^1H NMR (CDCl_3 , 100 MHz, ppm) δ : 8.29-8.27 (d, 2H, $J=8$ Hz), 7.73 (d, 2H, $J=8$ Hz), 7.56-7.52 (m, 4H), 1.36 (s, 9H).

^{13}C NMR (CDCl_3 , 100 MHz, ppm) δ : 152.3, 147.5, 146.9, 135.8, 132.5, 127.6, 127.1, 126.2, 124.2, 34.8, 31.3.

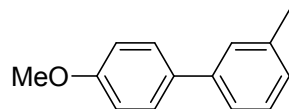
4-Methoxy-biphenyl



White solid, ^1H NMR (400 MHz, CDCl_3) δ : 7.55-7.51 (m, 4H), 7.39-7.29 (m, 3H), 6.98-6.96 (d, 2H, $J=8$ Hz).

^{13}C NMR (CDCl_3 , 100 MHz, ppm) δ : 159.2, 140.9, 133.8, 128.8, 128.2, 126.8, 126.7, 114.2, 55.4.

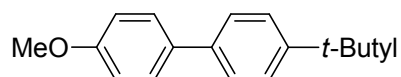
4-Methoxy-3'-methylbiphenyl



White solid, ^1H NMR (CDCl_3 , 400 MHz, ppm) δ : 7.52-7.50 (d, 2H, $J=8$ Hz), 7.35-7.12 (m, 4H), 6.97-6.95 (d, 2H, $J=8$ Hz), 3.84 (s, 3H), 2.40 (s, 3H).

^{13}C NMR (CDCl_3 , 100 MHz, ppm): δ 159.1, 140.9, 138.3, 133.9, 128.7, 128.2, 127.6, 127.5, 123.9, 114.2, 55.4, 21.6.

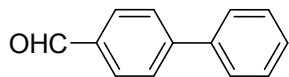
4-Methoxy-4'-*t*-butylbiphenyl



White solid, ^1H NMR (CDCl_3 , 400 MHz, ppm) δ : 7.53-7.48 (m, 4H), 7.45-7.43 (d, 2H, $J=8$ Hz), 6.98-6.95 (m, 2H), 3.84 (s, 3H), 1.36 (s, 9H).

^{13}C NMR (100 MHz, CDCl_3) δ : 159.0, 149.7, 138.0, 133.7, 128.1, 126.4, 125.7, 114.2, 55.4, 34.5, 31.4.

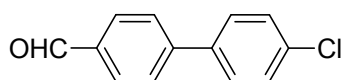
4-Formylbiphenyl



Light brown solid, ^1H NMR (CDCl_3 , 400 MHz, ppm) δ : 10.05 (s, 1H), 7.96-7.94 (d, 2H, $J=8$ Hz), 7.76-7.74 (d, 2H, $J=8$ Hz), 7.63 (d, 2H), 7.48-7.46 (d, 2H, $J=8$ Hz), 7.42 (m, 1H).

^{13}C NMR (CDCl_3 , 100 MHz, ppm) δ : 192.0, 147.3, 139.8, 135.2, 130.3, 129.1, 127.7, 127.4.

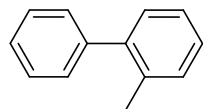
4-Chloro-4'-formylbiphenyl



White solid, ^1H NMR (400 MHz, CDCl_3) δ : 10.05 (s, 1H), 7.96-7.94 (d, 2H, $J=8$ Hz), 7.72 (d, 2H), 7.55-7.45 (m, 4H).

^{13}C NMR (CDCl_3 , 100 MHz, ppm) δ : 191.9, 145.9, 138.2, 135.4, 134.8, 130.4, 128.7, 127.6.

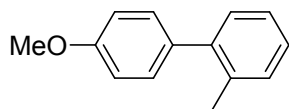
2-Methylbiphenyl



Colourless liquid, ^1H NMR (CDCl_3 , 400 MHz, ppm) δ : 7.63-7.61 (d, 2H, $J=8$ Hz), 7.45-7.43 (m, 3H), 7.35-7.26 (m, 4H), 2.29 (s, 3H).

^{13}C NMR (CDCl_3 , 100 MHz, ppm) δ : 142.0, 135.4, 130.4, 129.9, 129.3, 128.1, 127.3, 126.6, 125.8, 20.5.

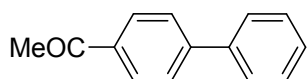
4-Methoxy-2'-methylbiphenyl



Colourless liquid, ^1H NMR (CDCl_3 , 400 MHz, ppm) δ : 7.26-7.21 (m, 6H), 6.96-6.94 (d, 2H, $J=8$ Hz), 3.85 (s, 3H), 2.27 (s, 3H).

^{13}C NMR (CDCl_3 , 100 MHz, ppm) δ : 158.5, 141.6, 135.5, 134.4, 130.3, 129.9, 125.6, 113.5, 55.3, 20.6.

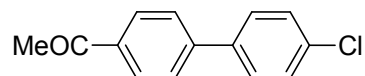
4-Acetylbiphenyl



White solid, ^1H NMR (CDCl_3 , 400 MHz, ppm) δ : 8.04-8.02 (d, 2H, $J=8$ Hz), 7.69-7.67 (d, 2H, $J=8$ Hz), 7.61 (d, 2H), 7.43 (m, 3H), 2.63 (s, 3H).

^{13}C NMR (CDCl_3 , 100 MHz, ppm) δ : 197.9, 145.8, 139.9, 135.9, 129.0, 127.3, 26.7.

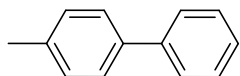
4-Acetyl-4'-chlorobiphenyl



White solid, ^1H NMR (CDCl_3 , 400 MHz, ppm) δ : 8.03-8.01 (d, 2H, $J=8$ Hz), 7.64 (d, 2H), 7.53 (d, 2H), 7.44-7.42 (d, 2H, $J=8\text{Hz}$), 2.63 (s, 3H) ppm.

^{13}C NMR (CDCl_3 , 100 MHz, ppm) δ : 197.7, 144.5, 138.3, 136.1, 134.5, 129.2, 129.1, 127.1, 26.7.

4-Methylbiphenyl



Colourless liquid, ^1H NMR (CDCl_3 , 400 MHz, ppm) δ : 7.60-7.58 (d, 2H, $J=8$ Hz), 7.50 (m, 2H), 7.44 (m, 3H), 7.27-7.25 (d, 2H, $J=8$ Hz), 2.41 (s, 3H).

^{13}C NMR (CDCl_3 , 100 MHz, ppm) δ : 141.2, 138.4, 137.1, 129.5, 128.8, 127.0, 21.2.

