**Supporting Information**

Minimizing base-stoichiometry in Pd(0)/g-C$_3$N$_4$O catalyzed Suzuki-Miyaura cross-coupling reaction

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Calculation of green chemistry matrices:

Our work: 1-Bromo-4-nitrobenzene (0.101g, 0.5 mmol) and Phenylboronic acid (0.0609g, 0.5 mmol) reacted in presence of Pd(0)/g-C$_3$N$_4$O (0.005g, 5 wt%), and K$_2$CO$_3$ (0.0345g, 0.25 mmol) in Ethanol medium (2 mL, 0.004g) (excluding water) to form 4-Nitrobiphenyl (0.0978g, 0.49 mmol).

Mass intensity = Total mass used in the process/ Mass of product

\[
= \frac{(0.101+0.0609+0.005+0.0345+0.004)}{0.978}g
\]

= 2.1

Mass productivity = (1/Mass intensity) x 100

\[
= \frac{1}{2.1} \times 100
\]

= 47.6%

E-factor = Mass intensity-1

\[
= 2.1-1
\]

= 1.1

General procedure for synthesis of biaryls:

A mixture of aryl bromide (0.5 mmol), arylboronic acid (0.5 mmol), Pd(0)/g-C$_3$N$_4$O (5wt%), K$_2$CO$_3$ (0.25 mmol), and EtOH:H$_2$O (1:1) (4 mL) were taken in a 50 mL round bottomed flask and stirred at room temperature for 5 hours. After completion of the reaction (monitoring by TLC), the reaction mixture was diluted with water (10 mL) and extracted with ethyl acetate (3 x 20 mL). The combined organic layers were washed with brine solution (20 mL) and the organic layer was dried over anhydrous sodium sulfate. The crude was obtained by evaporating the solvent under reduced pressure in a rotary evaporator. To obtain the desired product, purification of the crude was done by column chromatography using silica gel (60-120 mesh) and hexane:ethyl acetate as solvent system.
1H and 13C NMR analytical data:

4-nitro-1,1’-biphenyl (3a)\textsuperscript{1,2}: Obtained by general procedure, white solid (98% yield), 1H NMR (400 MHz, CDCl\textsubscript{3}) δ 8.30–8.24 (m, 2H), 7.75–7.68 (m, 2H), 7.63–7.59 (m, 2H), 7.52–7.41 (m, 3H); 13C NMR (100 MHz, CDCl\textsubscript{3}) δ 147.7, 147.2, 138.8, 129.3, 127.9, 127.6, 127.5, 124.6.

4-methoxy-1,1’-biphenyl (3b)\textsuperscript{1,2}: Obtained by general procedure, white solid (96% yield), 1H NMR (400 MHz, CDCl\textsubscript{3}) δ 7.58–7.49 (m, 4H), 7.46–7.37 (m, 2H), 7.36–7.26 (m, 1H), 7.01–6.94 (m, 2H), 3.85 (s, 3H); 13C NMR (100 MHz, CDCl\textsubscript{3}) δ 159.2, 141.1, 134.1, 128.9, 128.3, 126.9, 126.7, 114.7, 55.4.

4-methoxy-4'-methyl-1,1’-biphenyl (3c)\textsuperscript{3}: Obtained by general procedure, white solid (90% yield), 1H NMR (400 MHz, CDCl\textsubscript{3}) δ 7.54–7.41 (m, 4H), 7.22 (dd, J = 8.4, 0.6 Hz, 2H), 6.99–6.93 (m, 2H), 3.84 (s, 3H), 2.38 (s, 3H); 13C NMR (100 MHz, CDCl\textsubscript{3}) δ 159.2, 138.0, 136.7, 134.1, 130.2, 128.4, 127.0, 114.7, 55.8, 21.5.

1-(3'-methyl-[1,1'-biphenyl]-4-yl)ethan-1-one (3d)\textsuperscript{3}: Obtained by general procedure, white solid (85% yield), 1H NMR (400 MHz, CDCl\textsubscript{3}) δ 8.04–7.99 (m, 2H), 7.70–7.64 (m, 2H), 7.41 (dd, J = 4.6, 4.1 Hz, 2H), 7.35 (t, J = 7.5 Hz, 1H), 7.21 (dd, J = 4.3, 3.7 Hz, 1H), 2.62 (s, 3H), 2.43 (s, 3H); 13C NMR (100 MHz, CDCl\textsubscript{3}) δ 198.3, 146.1, 140.0, 138.7, 135.8, 129.0, 128.2, 128.1, 127.4, 124.5, 124.4, 26.7, 21.9.
4'-ethyl-[1,1'-biphenyl]-4-carbaldehyde (3e): Obtained by general procedure, white solid (92% yield), \( ^1H \) NMR (400 MHz, CDCl\(_3\)) \( \delta \) 10.03 (s, 1H), 7.95–7.90 (m, 2H), 7.76–7.71 (m, 2H), 7.60–7.53 (m, 2H), 7.34–7.28 (m, 2H), 2.80–2.61 (m, 2H), 1.31–1.21 (m, 3H); \( ^{13}C \) NMR (100 MHz, CDCl\(_3\)) \( \delta \) 192.1, 147.3, 145.0, 137.1, 135.1, 130.4, 128.6, 127.5, 127.4, 28.6, 15.8.

4'-chloro-[1,1'-biphenyl]-4-ol (3f): Obtained by general procedure, white solid (80% yield), \( ^1H \) NMR (400 MHz, CDCl\(_3\)) \( \delta \) 7.49–7.32 (m, 6H), 6.93–6.86 (m, 2H), 4.94 (s, 1H); \( ^{13}C \) NMR (100 MHz, CDCl\(_3\)) \( \delta \) 155.2, 139.4, 132.9, 132.8, 129.0, 128.4, 128.1, 116.0.

2-methoxy-3'-methyl-1,1'-biphenyl (3g): Obtained by general procedure, white solid (65% yield), \( ^1H \) NMR (400 MHz, CDCl\(_3\)) \( \delta \) 7.44–7.33 (m, 5H), 7.24–7.18 (m, 1H), 7.11–7.01 (m, 2H), 3.85 (d, \( J = 1.3 \) Hz, 3H), 2.46 (s, 3H); \( ^{13}C \) NMR (100 MHz, CDCl\(_3\)) \( \delta \) 156.7, 138.7, 137.7, 131.0, 130.4, 130.3, 128.8, 128.0, 120.9, 111.2, 56.3, 21.9.

4'-methyl-3-nitro-1,1'-biphenyl (3h): Obtained by general procedure, white solid (63% yield), \( ^1H \) NMR (400 MHz, CDCl\(_3\)) \( \delta \) 8.44–8.41 (m, 1H), 8.18–8.14 (m, 1H), 7.91–7.86 (m, 1H), 7.61–7.49 (m, 3H), 7.31–7.27 (m, 2H), 2.41 (s, 3H); \( ^{13}C \) NMR (100 MHz, CDCl\(_3\)) \( \delta \) 148.8, 142.9, 138.7, 135.8, 133.0, 130.0, 129.9, 129.7, 127.1, 121.8, 21.3.
2-(3,4-difluorophenyl)naphthalene (3i): Obtained by general procedure, white solid (74% yield), $^1$H NMR (400 MHz, CDCl$_3$) $\delta$ 7.96 (s, 1H), 7.93–7.80 (m, 3H), 7.64 (dd, $J = 8.5, 1.7$ Hz, 1H), 7.56–7.38 (m, 4H), 7.31–7.18 (m, 1H); $^{13}$C NMR (100 MHz, CDCl$_3$) $\delta$ 151.5, 149.5, 138.4, 136.6, 132.8, 128.8, 128.4, 127.9, 126.68 (d, $J_{C-F} = 25.0$ Hz), 126.43, 125.9, 125.1, 123.4; $^{19}$F NMR (376 MHz, CDCl$_3$) $\delta$ -137.34(s), -140.01(s).

5-(4-methoxyphenyl)benzo[1,3]dioxole (3j): Obtained by general procedure, white solid (91% yield), $^1$H NMR (400 MHz, CDCl$_3$) $\delta$ 7.48–7.39 (m, 2H), 7.04–6.91 (m, 4H), 6.88–6.82 (m, 1H), 6.01–5.94 (m, 2H), 3.83 (s, 3H); $^{13}$C NMR (100 MHz, CDCl$_3$) $\delta$ 159.0, 148.2, 146.7, 135.4, 133.8, 127.9, 120.3, 114.3, 108.7, 107.5, 101.1, 55.8.

4'-methyl-3'-nitro-[1,1'-biphenyl]-4-carbonitrile (3k): Obtained by general procedure, white solid (68% yield), $^1$H NMR (600 MHz, CDCl$_3$) $\delta$ 7.92–7.83 (m, 1H), 7.48–7.32 (m, 5H), 7.13 (dd, $J = 9.6, 5.3$ Hz, 1H), 6.98–6.86 (m, 1H), 2.43–2.28 (m, 3H); $^{13}$C NMR (150 MHz, CDCl$_3$) $\delta$ 149.4, 142.6, 137.9, 133.6, 133.4, 132.6, 131.0, 127.3, 122.9, 118.2, 111.7, 19.9.

3,5-dimethyl-4'-(trifluoromethyl)-1,1'-biphenyl (3l): Obtained by general procedure, colourless liquid (70% yield), $^1$H NMR (400 MHz, CDCl$_3$) $\delta$ 7.66 (s, 4H), 7.20 (s, 2H), 7.05 (d, $J = 0.5$ Hz, 1H), 2.42–2.36 (m, 6H); $^{13}$C NMR (100 MHz, CDCl$_3$) $\delta$ 143.2, 138.6, 130.5, 130.1, 129.8, 127.6, 127.4, 125.2, 122.77 ($^1J_{C-F} = 270$ Hz), 120.07, 21.4; $^{19}$F NMR (377 MHz, CDCl$_3$) $\delta$ -62.6.
4'-tert-butyl)-3,5-dimethyl-1,1'-biphenyl (3m): Obtained by general procedure, colourless liquid (68% yield), $^1$H NMR (500 MHz, CDCl$_3$) $\delta$ 7.63–7.59 (m, 2H), 7.55–7.52 (m, 2H), 7.29 (d, $J = 6.8$ Hz, 2H), 7.06 (s, 1H), 2.46 (s, 6H), 1.45 (s, 9H); $^{13}$C NMR (125 MHz, CDCl$_3$) $\delta$ 150.0, 141.1, 138.1, 128.6, 126.8, 126.6, 125.5, 124.9, 34.4, 31.3, 21.4.

4'-nitro-[1,1'-biphenyl]-4-carbaldehyde (3n): Obtained by general procedure, white solid (86% yield), $^1$H NMR (500 MHz, CDCl$_3$) $\delta$ 10.11 (s, 1H), 8.35 (d, $J = 8.9$ Hz, 2H), 8.03 (d, $J = 8.4$ Hz, 2H), 7.83–7.77 (m, 4H); $^{13}$C NMR (125 MHz, CDCl$_3$) $\delta$ 191.5, 147.7, 145.9, 144.4, 136.2, 130.3, 128.1, 128.0, 124.2.

4,4'-dimethyl-3-nitro-1,1'-biphenyl (3o): Obtained by general procedure, white solid (64% yield), $^1$H NMR (500 MHz, CDCl$_3$) $\delta$ 8.21 (d, $J = 1.9$ Hz, 1H), 7.73 (dd, $J = 7.9$, 1.9 Hz, 1H), 7.54–7.49 (m, 2H), 7.39 (dd, $J = 11.7$, 4.6 Hz, 1H), 7.30 (dd, $J = 10.8$, 3.0 Hz, 2H), 2.65 (s, 3H), 2.44 (s, 3H); $^{13}$C NMR (125 MHz, CDCl$_3$) $\delta$ 149.5, 140.1, 138.1, 135.5, 133.1, 131.8, 131.0, 129.7, 126.6, 122.6, 21.0, 20.0.

3',4,5'-trimethyl-3-nitro-1,1'-biphenyl (3p): Obtained by general procedure, colourless liquid (61% yield), $^1$H NMR (500 MHz, CDCl$_3$) $\delta$ 8.22 (d, $J = 1.9$ Hz, 1H), 7.73 (dd, $J = 7.9$, 2.0 Hz, 1H), 7.40 (d, $J = 8.0$ Hz, 1H), 7.24 (s, 2H), 7.08–7.05 (m, 1H), 2.66 (s, 3H), 2.42 (s, 6H); $^{13}$C NMR (125 MHz, CDCl$_3$) $\delta$ 149.4, 140.5, 138.6, 138.4, 133.0, 131.9, 131.2, 129.8, 124.7, 122.8, 21.3, 20.0. Anal. for C$_{15}$H$_{15}$NO$_2$; calcd C, 74.67; H, 6.27; N, 5.81; found C, 74.16; H, 6.37; N, 5.39.
**4,4'-dimethoxy-3-methyl-1,1'-biphenyl (3q)**\(^{14}\): Obtained by general procedure, white solid (68\% yield), \(^1\)H NMR (500 MHz, CDCl\(_3\)) \(\delta\) 7.55–7.48 (m, 2H), 7.38 (dd, \(J = 6.0, 2.2\) Hz, 2H), 7.02–6.97 (m, 2H), 6.94–6.88 (m, 1H), 3.90 (s, 3H), 3.88 (s, 3H), 2.32 (s, 3H); \(^{13}\)C NMR (125 MHz, CDCl\(_3\)) \(\delta\) 158.5, 156.8, 133.6, 133.0, 129.1, 127.6, 126.7, 124.8, 114.0, 110.1, 55.3, 55.2, 16.3.

\[
\text{\begin{center}}
\includegraphics[width=0.2\textwidth]{3q}
\text{\end{center}}
\]

**1-(2'-methoxy-[1,1'-biphenyl]-4-yl)ethan-1-one (3r)**\(^{15}\): Obtained by general procedure, white solid (64\% yield), \(^1\)H NMR (500 MHz, CDCl\(_3\)) \(\delta\) 8.08–7.99 (m, 2H), 7.73–7.62 (m, 2H), 7.46–7.34 (m, 2H), 7.15–6.98 (m, 2H), 3.85 (s, 3H), 2.66 (s, 3H); \(^{13}\)C NMR (125 MHz, CDCl\(_3\)) \(\delta\) 197.8, 156.4, 143.5, 135.4, 130.6, 129.6, 129.4, 129.3, 128.0, 120.9, 111.3, 55.5, 26.5.

\[
\text{\begin{center}}
\includegraphics[width=0.2\textwidth]{3r}
\text{\end{center}}
\]

**4-(tert-butyl)-4'-methyl-1,1'-biphenyl (3s)**\(^{15}\): Obtained by general procedure, white solid (98\% yield), \(^1\)H NMR (500 MHz, CDCl\(_3\)) \(\delta\) 7.60–7.49 (m, 6H), 7.31–7.26 (m, 2H), 2.44 (s, 3H), 1.42 (s, 9H); \(^{13}\)C NMR (125 MHz, CDCl\(_3\)) \(\delta\) 149.8, 138.2, 136.6, 129.3, 126.8, 126.5, 125.6, 125.5, 34.4, 31.3, 21.0.

\[
\text{\begin{center}}
\includegraphics[width=0.2\textwidth]{3s}
\text{\end{center}}
\]

**3,5-dimethyl-1,1'-biphenyl (3t)**\(^{16}\): Obtained by general procedure, colourless liquid (84\% yield), \(^1\)H NMR (500 MHz, CDCl\(_3\)) \(\delta\) 7.73 (d, \(J = 7.1\) Hz, 2H), 7.60–7.46 (m, 4H), 7.37 (s, 2H), 7.14 (s, 1H), 2.53 (s, 6H); \(^{13}\)C NMR (125 MHz, CDCl\(_3\)) \(\delta\) 141.5, 141.3, 138.2, 128.9, 128.7, 127.2, 127.1, 125.1, 21.4.
4-methoxy-3,3',5'-trimethyl-1,1'-biphenyl (3u): Obtained by general procedure, colourless liquid (72% yield), $^1$H NMR (500 MHz, CDCl$_3$) δ 7.49–7.46 (m, 3H), 7.28 (s, 1H), 7.05–6.95 (m, 2H), 3.94 (s, 3H), 2.47 (s, 6H), 2.39 (s, 3H); $^{13}$C NMR (125 MHz, CDCl$_3$) δ 157.2, 138.1, 133.5, 129.5, 129.0, 128.2, 126.7, 125.3, 124.7, 110.0, 55.3, 21.4, 16.3. Anal. for C$_{16}$H$_{18}$O, calcd C, 84.91; H, 8.02; found C, 84.58; H, 8.18.

4-methoxy-3-methyl-4'-nitro-1,1'-biphenyl (3v): Obtained by general procedure, white solid (72% yield), $^1$H NMR (500 MHz, CDCl$_3$) δ 8.31–8.24 (m, 2H), 7.74–7.68 (m, 2H), 7.46 (d, $J$ = 5.9 Hz, 2H), 6.95 (d, $J$ = 8.4 Hz, 1H), 3.92 (s, 3H), 2.32 (s, 3H); $^{13}$C NMR (125 MHz, CDCl$_3$) δ 158.6, 147.4, 146.3, 130.5, 129.5, 127.4, 126.9, 125.8, 124.0, 110.2, 55.4, 16.3.

3-phenylpyridine (3w): Obtained by general procedure, colourless liquid (82% yield), $^1$H NMR (400 MHz, CDCl$_3$) δ 8.87–8.80 (m, 1H), 8.60–8.53 (m, 1H), 7.89–7.82 (m, 1H), 7.59–7.53 (m, 2H), 7.49–7.30 (m, 4H); $^{13}$C NMR (125 MHz, CDCl$_3$) δ 148.5, 148.4, 137.9, 136.8, 134.5, 129.3, 128.2, 127.2, 123.8.

5-phenylpyrimidine (3x): Obtained by general procedure, colourless liquid (74% yield), $^1$H NMR (400 MHz, CDCl$_3$) δ 9.20–9.16 (m, 1H), 8.93 (d, $J$ = 3.3 Hz, 2H), 7.58–7.54 (m, 2H), 7.52–7.42 (m, 3H); $^{13}$C NMR (125 MHz, CDCl$_3$) δ 157.6, 157.5, 155.0, 134.4, 134.3, 129.6, 129.1, 127.1.
4-methyl-1,1'-biphenyl (3y): Obtained by general procedure, white solid (81% yield), $^1$H NMR (500 MHz, CDCl$_3$) $\delta$ 7.66–7.61 (m, 2H), 7.55 (d, $J$ = 8.1 Hz, 2H), 7.48 (dd, $J$ = 10.6, 4.8 Hz, 2H), 7.40–7.35 (m, 1H), 7.32–7.28 (m, 2H), 2.45 (s, 3H); $^{13}$C NMR (125 MHz, CDCl$_3$) $\delta$ 141.1, 138.3, 136.9, 129.4, 128.6, 126.9, 126.8, 21.0.
$^1$H and $^{13}$C NMR spectra

3a.
3b.

Chemical shift

O
C
H₃

Chemical shift

O
C
H₃
Chemical shift

O
C
H
3

Chemical shift

O
C
H
3
31.

Chemical shift (ppm)
3m.
3q.
3r.
Chemical shift (ppm)

1.00  1.98  6.30  1.42  2.44  7.28  7.28  7.30  7.50  7.52  7.54  7.55  7.57  7.57  7.59

Chemical shift (ppm)

21.0  31.3  34.4  76.7  76.9  77.2  125.5  125.6  126.5  126.8  129.3  136.6  138.2  149.8

Chemical shift (ppm)

190  180  170  160  150  140  130  120  110  100  90  80  70  60  50  40  30  20  10  0
3v.
3x.
$^{19}$F NMR spectra

3i.

![Diagram of 3i](image)

Chemical shift (ppm)

-210 -190 -170 -150 -130 -110 -90 -80 -70 -60 -50 -40 -30 -20 -10 0 10 20

-200 -190 -180 -170 -160 -150 -140 -130 -120 -110 -100 -90 -80 -70 -60

3i.

![Diagram of 3i](image)

Chemical shift (ppm)

-140.01 -137.34

-200 -190 -180 -170 -160 -150 -140 -130 -120 -110 -100 -90 -80 -70 -60
Figure S1: XPS survey spectrum of Pd(0)/g-C$_3$N$_4$O
References:


9 Patent number US5612360


