Supporting Information

for

A SELF-SUPPORTED PALLADIUM–BIPYRIDYL CATALYST FOR THE SUZUKI–MIYaura COUPLING IN WATER

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¹H NMR spectrum of PdCl₂BPy
GC and GC-MS analyses for the Suzuki-Miyaura Coupling of phenyl iodide with 4-methylphenyboronic acid (Table 1, entry 1).

Product: 4-phenyltoluene [CAS: 644-08-6]
Comparison with NIST Mass Database Library

Library Searched: C:\Database\Nist98.l
Quality : 93
ID : 1,1'-Biphenyl, 4-methyl-

\[\text{MS result}\]

93% similarity with authentic data.

\[\text{Authentic data from database}\]
GC and GC-MS analyses for the Suzuki-Miyaura Coupling of phenyl iodide with phenylboronic acid (Table 1, entry 3).

Comparison with NIST Mass Database Library

Library Searched: C:\Database\Nist98.l
Quality: 91
ID: Biphenyl

91% similarity with authentic data.

Authentic data from database
GC and GC-MS analyses for the Suzuki-Miyaura Coupling of phenyl iodide with 4-methoxyphenylboronic acid (Table 1, entry 5).

Product: 4-methoxybiphenyl [CAS: 613-37-6]
Comparison with NIST Mass Database Library

Library Searched: C:\Database\Nist98.l
Quality ID: 91
: 1,1'-Biphenyl, 4-methoxy-

91% similarity with authentic data.

Authentic data from database

\[\text{OMe}\]
GC and GC-MS analyses for the Suzuki-Miyaura Coupling of phenyl iodide with 4-biphenylboronic acid (Table 1, entry 7).

Product: \( p \)-terphenyl [CAS: 92-94-4]
Comparison with NIST Mass Database Library

Library Searched: C:\Database\Nist98.1
Quality: 90
ID: p-Terphenyl

90% similarity with authentic data.

Authentic data from database
GC and GC-MS analyses for the Suzuki-Miyaura Coupling of phenyl iodide with 4-tert-butyldiphenylboronic acid (Table 1, entry 9).

Product: 4-tert-butyldiphenyl [CAS: 1625-92-9]
Authentic MS data of this product was not available in NIST data. Instead, $^1$H and $^{13}$C NMR analyses were performed. After the workup, the resulting solid was purified by silica gel column chromatography on silica gel (eluent: hexane). Isolated yield: 190 mg, 90%.

$^1$H NMR (500 MHz, CDCl$_3$): $\delta$ 7.59 (d, $J = 8.0$ Hz, 2H), 7.54 (d, $J = 8.5$ Hz, 2H), 7.47 (d, $J = 8.5$ Hz, 2H), 7.42 (t, $J = 7.5$ Hz, 2H), 7.32 (t, $J = 7.5$ Hz, 1H), 1.36 (s, 9H); $^{13}$C NMR (126 MHz, CDCl$_3$): $\delta$ 150.2, 141.0, 138.2, 128.6, 126.9, 126.9, 126.7, 34.5, 31.3.

$^1$H NMR spectrum of 4-tert-butylbiphenyl
$^{13}\text{C}^1\text{H}$ NMR spectrum of 4-tert-butylbiphenyl
GC and GC-MS analyses for the Suzuki-Miyaura Coupling of phenyl iodide with 4-(trifluoromethyl)phenylboronic acid (Table 1, entry 11).

Product: 4-(trifluoromethyl)biphenyl [CAS: 398-36-7]
Authentic MS data of this product was not available in NIST data. Instead, $^1$H and $^{13}$C NMR analyses were performed. After the workup, the resulting solid was purified by silica gel column chromatography on silica gel (eluents: hexane:ethyl acetate = 9:1). Isolated yield: 184 mg, 85%.

$^1$H NMR (500 MHz, CDCl$_3$): $\delta$ 7.70 (s, 4H), 7.60 (d, $J = 7.5$ Hz, 2H), 7.48 (t, $J = 7.5$ Hz, 2H), 7.41 (t, $J = 7.5$ Hz, 1H); $^{13}$C NMR (126 MHz, CDCl$_3$): $\delta$ 144.7, 139.8, 129.3 (q, $J = 33.2$ Hz), 129.0, 128.2, 127.4, 127.3, 125.7 (q, $J = 4.1$ Hz), 124.3 (q, $J = 271.9$ Hz).

$^1$H NMR spectrum of 4-(trifluoromethyl)biphenyl.
$^{13}$C\{$^1$H\} NMR of 4-(trifluoromethyl)biphenyl.
GC and GC-MS analyses for the Suzuki-Miyaura Coupling of phenyl iodide with 4-cyanophenylboronic acid (Table 1, entry 13).

Product: 4-phenylbenzonitrile [CAS: 2920-38-9]

**GC Analysis**

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<th>RT / min</th>
<th>Peak width</th>
<th>Area</th>
<th>Area%</th>
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<td>28.32202</td>
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**GC-MS Analysis**

[Diagram showing GC-MS analysis]
Comparison with NIST Mass Database Library

Library Searched: C:\Database\Nist98.1
Quality: 95
ID: p-Phenylbenzonitrile

95% similarity with authentic data.

Authentic data from database

\[
\begin{align*}
\text{Ar} & \quad \text{CN}
\end{align*}
\]
GC and GC-MS analyses for the Suzuki-Miyaura Coupling of phenyl iodide with 3-methylphenylboronic acid (Table 1, entry 15).

Product: 3-methyltoluene [CAS: 643-93-6]

**GC Analysis**

<table>
<thead>
<tr>
<th>RT / min</th>
<th>Peak width</th>
<th>Area</th>
<th>Area%</th>
</tr>
</thead>
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</table>

**GC-MS Analysis**

Product: 3-methyltoluene [CAS: 643-93-6]
Comparison with NIST Mass Database Library

Library Searched: C:\Database\Nist98.l
Quality: 87
ID: 1,1'-Biphenyl, 3-methyl-

87% similarity with authentic data.
GC and GC-MS analyses for the Suzuki-Miyaura Coupling of phenyl iodide with 2-methylphenylboronic acid (Table 1, entry 17).

Product: 2-methyltoluene [CAS: 643-58-3]
Comparison with NIST Mass Database Library

Library Searched: C:Database\Nist98.1
Quality: 93
ID: 1,1'-Biphenyl, 2-methyl-

Scan 258 (5.280 min): TO3075-4.D

MS result

93% similarity with authentic data.

Authentic data from database

\[\text{\includegraphics[width=0.2\textwidth]{biphenyl-methyl.png}}\]
GC and GC-MS analyses for the Suzuki-Miyaura Coupling of phenyl iodide with 1-naphtylboronic acid (Table 1, entry 19).

Product: 1-phenylnaphthalene [CAS: 605-02-7]
Comparison with NIST Mass Database Library

Library Searched: C:\Database\Nist98.1
Quality: 89
ID: Naphthalene, 1-phenyl-

89% similarity with authentic data.

Authentic data from database