Supporting Information

For

Phosphine-Free Hydrazone-Pd-Complex as Catalyst Precursor for Suzuki-Miyaura Reaction under Mild Aerobic Conditions

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General Information

All reactions were performed under air atmosphere unless otherwise indicated.

4-Methylbiphenyl¹ (Table 2, entry 1): 99% as a white solid; m.p. 46 °C; ¹H NMR (CDCl₃) δ: 2.40 (s, 3H), 7.25 (d, *J* = 8.1 Hz, 2H), 7.32 (tt, *J* = 1.9 and 7.2 Hz, 1H), 7.42 (t, *J* = 7.8 Hz, 2H), 7.50 (d, *J* = 8.1 Hz, 2H), 7.58 (td, *J* = 1.4 and 7.2 Hz, 2H); ¹³C NMR (CDCl₃) δ: 21.0, 127.0, 128.7, 129.5, 137.0, 138.3, 141.1; EI-MS *m/z* (rel intensity): 168 (M⁺, 100).

4-Methoxybiphenyl² (Table 2, entry 2): 89% as a white solid; m.p. 85-86 °C; ¹H NMR (CDCl₃) δ: 3.85 (s, 3H), 6.98 (td, *J* = 3.0 and 8.8 Hz, 2H), 7.30 (tt, *J* = 1.8 and 7.4 Hz, 1H), 7.41 (t, *J* = 7.26 Hz, 2H), 7.54 (tt, *J* = 1.4 and 5.8 Hz, 4H); ¹³C NMR (CDCl₃) δ: 55.3, 114.2, 126.7, 126.8, 128.2, 128.7, 133.8, 140.9, 159.2; EI-MS *m/z* (rel intensity): 184 (M⁺, 100).

Biphenyl-4-carbaldehyde³ (Table 2, entry 3): 99% as a white solid; m.p. 58-59 °C; ¹H NMR (CDCl₃) δ: 7.38-7.50 (m, 3H), 7.63 (d, *J* = 7.9 Hz, 2H), 7.74 (d, *J* = 7.9 Hz, 2H), 7.94 (d, *J* = 7.9 Hz, 2H) 10.0 (s, 1H); ¹³C NMR (CDCl₃) δ: 115.3, 127.3, 127.7, 128.5, 129.0, 130.3, 133.7, 135.1, 139.7, 147.2, 192.0; EI-MS *m/z* (rel intensity): 182 (M⁺, 97).

4-Acetylbiphenyl⁴ (Table 2, entry 4): 99% as a white solid; m.p. 116-117 °C; ¹H NMR (CDCl₃) δ: 2.65 (s, 3H), 7.41 (tt, *J* = 2.5 and 7.1 Hz, 1H), 7.48 (tt, *J* = 1.3 and 7.7 Hz 2H), 7.64 (d, *J* = 7.1 Hz, 2H), 7.69 (d, *J* = 8.4 Hz, 2H), 8.04 (d, *J* = 8.4 Hz, 2H); ¹³C NMR (CDCl₃) δ: 27.1, 127.6, 127.7, 128.6, 129.3, 129.4, 136.2, 140.3, 146.2, 198.2; EI-MS *m/z* (rel intensity): 196 (M⁺, 50).

4-*tert*-Butylbiphenyl⁵ (Table 2, entry 5): 94% as a white solid; m.p. 49-50 °C; ¹H NMR (CDCl₃) δ: 1.36 (s, 9H), 7.32 (t, *J* = 7.4 Hz, 1H), 7.40-7.48 (m, 4H), 7.53-7.60 (m, 4H); ¹³C NMR (CDCl₃) δ: 31.4, 34.6, 125.8, 126.8, 127.0, 127.1, 128.7, 138.4, 141.1, 150.3; EI-MS *m/z* (rel intensity): 210 (M⁺, 34).

***p*-Terphenyl**⁴ (Table 2, entry 6): 88% as a white solid; m.p. 212-213 °C; ¹H NMR (CDCl₃) δ: 7.30-7.48 (m, 6H), 7.56-7.68 (m, 8H); ¹³C NMR (CDCl₃) δ: 127.1, 127.4, 127.5, 128.9, 140.1, 140.7; EI-MS *m/z* (rel intensity): 230 (M⁺, 100).

3-Methoxybiphenyl⁶ (Table 2, entry 7): 91% as a colorless liquid; ¹H NMR (CDCl₃) δ: 3.77 (s, 3H), 6.85 (ddd, *J* = 0.9, 2.5 and 8.2 Hz, 1H), 7.06-7.18 (m, 2H), 7.24-7.34 (m, 2H), 7.34-7.44 (m, 2H), 7.51-7.59 (m, 2H); ¹³C NMR (CDCl₃) δ: 55.1, 112.5, 112.8, 119.6, 127.1, 127.3, 128.7, 129.7, 141.0, 142.6, 159.8; EI-MS *m/z* (rel intensity): 184 (M⁺, 100).

2-Methylbiphenyl³ (Table 2, entry 8): 90% as a colorless liquid; ¹H NMR (CDCl₃) δ: 2.27 (s, 3H), 7.20-7.29 (m, 4H), 7.29-7.37 (m, 3H), 7.37-7.43 (m, 2H); ¹³C NMR (CDCl₃) δ: 20.5, 125.7, 126.7, 127.2, 128.0, 129.2, 129.8, 130.3, 135.3, 141.89, 141.91; EI-MS *m/z* (rel intensity): 168 (M⁺, 100).

2-Methoxybiphenyl³ (Table 2, entry 9): 89% as a colorless liquid; ¹H NMR (CDCl₃) δ: 3.77 (s, 3H), 6.94-7.04 (m, 2H), 7.30 (tt, *J* = 1.6 and 7.4 Hz, 3H), 7.39 (tt, *J* = 1.1 and 7.1 Hz, 2H), 7.52 (td, *J* = 1.5 and 7.0 Hz, 2H); ¹³C NMR (CDCl₃) δ: 55.5, 111.1, 120.8, 126.9, 128.0, 128.6, 130.0, 130.6, 130.9, 138.5, 156.4; EI-MS *m/z* (rel intensity): 184 (*M*⁺, 100).

Biphenyl-2-carbaldehyde⁷ (Table 2, entry 10): 87% as a yellow liquid; ¹H NMR (CDCl₃) δ: 7.36-7.40 (m, 2H), 7.43-7.52 (m, 5H), 7.64 (td, *J* = 1.4 and 7.5 Hz, 1H), 8.03 (dd, *J* = 1.1 and 7.7 Hz, 1H), 9.98 (s, 1H); ¹³C NMR (CDCl₃) δ: 127.5, 127.8, 128.1, 128.4, 130.1, 130.8, 133.6, 133.7, 137.7, 146.0, 192.5; EI-MS *m/z* (rel intensity): 182 (*M*⁺, 68).

Biphenyl-2-carbonitrile⁸ (Table 2, entry 11): 88% as a yellow liquid; ¹H NMR (CDCl₃) δ: 7.38-7.52 (m, 5H), 7.53-7.57 (m, *J* = 2H), 7.61 (dt, *J* = 1.2 and 7.7 Hz, 1H), 7.74 (dd, *J* = 0.8 and 7.7 Hz, 1H); ¹³C NMR (CDCl₃) δ: 111.1, 118.6, 127.4, 128.60, 128.63, 129.0, 130.0, 132.7, 133.6, 138.1, 145.4; EI-MS *m/z* (rel intensity): 179 (*M*⁺, 100).

1-Phenylnaphthalene⁹ (Table 2, entry 13): 92% as a colorless liquid; ¹H NMR (CDCl₃) δ: 7.37-7.56 (m, 8H), 7.73 (t, *J* = 7.1 Hz, 1H), 7.84-7.92 (m, 3H); ¹³C NMR (CDCl₃) δ: 125.4, 125.8, 125.9, 126.0, 126.9, 127.2, 127.3, 127.4, 127.6, 128.1, 128.2, 128.4, 128.9, 130.1; EI-MS *m/z* (rel intensity): 204 (*M*⁺, 100).

4,4'-Dimethylbiphenyl⁶ (Table 2, entry 14): 98% as a white solid; m.p. 119 °C; ¹H NMR (CDCl₃) δ: 2.38 (s, 6H), 7.23 (d, *J* = 7.8 Hz, 4H), 7.48 (d, *J* = 8.1 Hz, 4H); ¹³C NMR (CDCl₃) δ: 21.1, 126.8, 129.4, 136.7, 138.3; EI-MS *m/z* (rel intensity): 182 (M⁺, 100).

4-Methoxy-4'-methylbiphenyl¹⁰ (Table 2, entry 15): 68% as a yellow solid; m.p. 106-107 °C; ¹H NMR (CDCl₃) δ: 2.38 (s, 3H), 3.84 (s, 3H), 6.96 (td, *J* = 2.1 and 8.8 Hz, 2H), 7.22 (d, *J* = 7.9 Hz, 2H), 7.45 (td, *J* = 1.8 and 8.1 Hz, 2H), 7.51 (td, *J* = 2.9 Hz and 8.8 Hz 2H); ¹³C NMR (CDCl₃) δ: 21.1, 55.4, 114.2, 126.6, 128.0, 129.5, 133.7, 136.4, 138.0, 158.9; EI-MS *m/z* (rel intensity): 198 (M⁺, 100).

2-Fluoro-4'-methylbiphenyl¹¹ (Table 2, entry 16): 93% as a colorless liquid; ¹H NMR (CDCl₃) δ: 2.32 (s, 3H), 7.11-7.25 (m, 5H), 7.40-7.45 (m, 3H); ¹³C NMR (CDCl₃) δ: 21.2, 116.0 (d, *J* = 22.8 Hz), 124.3 (d, *J* = 3.7 Hz), 128.6, 128.7, 128.8 (d, *J* = 2.9 Hz), 129.1, 130.6 (d, *J* = 3.5 Hz), 132.8, 137.4, 160.0, (d, *J* = 247.3 Hz); EI-MS *m/z* (rel intensity): 186 (M⁺, 100).

4'-Methylbiphenyl-2-carbaldehyde¹² (Table 2, entry 17): 24% as a yellow liquid; ¹H NMR (CDCl₃) δ: 2.35 (s, 3H), 7.17-7.24 (m, 4H), 7.37 (m, 2H), 7.54 (dt, *J* = 1.4 and 7.5 Hz, 1H), 7.94 (dd, *J* = 1.1 and 7.7 Hz, 1H), 9.91 (s, 1H); ¹³C NMR (CDCl₃) δ: 21.2, 127.6, 129.2, 130.0, 130.8, 133.5, 133.7, 134.8, 138.1, 146.0, 192.7; EI-MS *m/z* (rel intensity): 196 (M⁺, 66).

1-(4-Tolyl)-naphthalene¹³ (Table 2, entry 18): 86% as a white solid; m.p. 52-53 °C; ¹H NMR (CDCl₃) δ: 2.46 (s, 3H), 7.30 (d, *J* = 7.8 Hz, 2H), 7.38-7.51 (m, 6H), 7.83-7.91 (m, 3H); ¹³C NMR

(CDCl₃) δ : 21.2, 125.4 125.7 125.9, 126.1, 127.4 128.2 128.9 129.9 131.7, 133.8 136.9 137.8 140.2; EI-MS m/z (rel intensity): 218 (M⁺, 100).

3-Phenylpyridine¹⁴ (Table 2, entry 19): 82% as a colorless liquid; ¹HNMR (CDCl₃) δ : 7.28-7.43 (m, 2H), 7.43-7.52 (m, 2H), 7.53-7.62 (m, 2H), 7.86 (ddd, J = 1.7, 2.3 and 7.9 Hz, 1H), 8.59 (dd, J = 1.6 and 4.8 Hz, 1H), 8.85 (d, J = 1.8 Hz, 1H); ¹³C NMR (CDCl₃) δ : 123.5, 127.1, 128.0, 129.0, 134.3, 136.5, 137.7, 148.3, 148.4; EI-MS m/z (rel intensity): 155 (M⁺, 100).

5-Phenylprimidine¹⁵ (Table 2, entry 20): 94% as a colorless liquid; ¹HNMR (CDCl₃) δ : 7.61-7.45 (m, 5H), 8.96 (s, 2H), 9.21 (s, 1H); ¹³C NMR (CDCl₃) δ : 126.9, 128.9, 129.3, 134.1, 134.2, 154.8, 157.4; EI-MS m/z (rel intensity): 156 (M⁺, 91).

5-Phenyl-furan-2-carboaldehyde¹⁶ (Table 2, entry 21): 83% as a yellow liquid; ¹HNMR (DMSO-*d*₆) δ : 7.32 (d, J = 3.7 Hz, 1H), 7.42-7.58 (m, 3H), 7.68 (d, J = 3.8 Hz, 1H), 7.85-7.93 (m, 2H), 9.64 (s, 1H); ¹³C NMR (DMSO-*d*₆) δ : 109.1, 125.4, 125.8, 129.0, 129.6, 130.1, 152.1, 158.6, 178.2; EI-MS m/z (rel intensity): 172 (M⁺, 73).

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Glyoxal bis(*N*-methyl-*N*-phenylhydrazone) (1)

2,3-Butanedion bis(*N*-methyl-*N*-phenylhydrazone) (2)

2-Pyridinecarboxyaldehyde *N*-methyl-*N*-phenylhydrazone (3)

Benzaldehyde *N*-methyl-*N*-phenylhydrazone (4)

4-Methylbiphenyl

4-Methoxybiphenyl

Biphenyl-4-carbaldehyde

4-Acetylbiphenyl

4-*tert*-Butylbiphenyl

p-Terphenyl

3-Methoxybiphenyl

Current Data Parameters
NAME 12540h
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
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RG 64
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DE 6.00 usec
TE 300.0 K
D1 1.00000000 sec
V1 9.80 usec
SFO1 300.2315011 MHz
NUC1 1H
PL1 2.00 dB

F2 - Processing parameters
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LB 0.30 Hz
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1D NMR plot parameters
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F2 -365.67 Hz
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HZCM 157.07465 Hz/cm

Current Data Parameters
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EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
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d12 0.00002000 sec
PL13 25.00 dB
D1 2.00000000 sec
CPDPRG2 waltz16
PCPD2 100.00 usec
SFO2 300.2312009 MHz
NUC2 13C
PL2 2.00 dB
PL12 25.00 dB
F1 8.00 usec
SFO1 75.5011582 MHz
NUC1 13C
PL1 3.00 dB

F2 - Processing parameters
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LB 1.00 Hz
GB 0
PC 1.40

1D NMR plot parameters
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F1 17311.78 Hz
F2P -10.652 ppm
F2 -804.16 Hz
PPMCM 11.99844 ppm/cm
HZCM 905.79712 Hz/cm

2-Methylbiphenyl

2-Methoxybiphenyl

Current Data Parameters
NAME 10827c
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20020420
Time 17.17
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PULPROG zg30
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SWH 3612.717 Hz
FIDRES 0.110251 Hz
AQ 4.5351410 sec
RG 64
LW 138.400 usec
DE 6.00 usec
TE 300.0 K
D1 1.00000000 sec
P1 9.00 usec
SFO1 300.2315011 MHz
NUC1 1H
PL1 2.00 dB

F2 - Processing parameters
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SF 300.2300387 MHz
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SSB 0
LB 0.30 Hz
GB 0
PC 1.00

1D NMR plot parameters
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F2P -1.146 ppm
F2 -343.93 Hz
PRCM 0.52318 ppm/cm
HZCM 157.07465 Hz/cm

Current Data Parameters
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EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
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PULPROG zgpg30
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SWH 18115.941 Hz
FIDRES 0.276427 Hz
AQ 1.8088436 sec
RG 2896.3
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DE 5.00 usec
TE 300.0 K
d11 0.03000000 sec
d12 0.00000000 sec
PL13 25.00 dB
D1 2.00000000 sec
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PCPD2 100.00 usec
SFO2 300.2312009 MHz
NUC2 13C
PL2 2.00 dB
PL12 25.00 dB
P1 8.00 usec
SFO1 75.5011682 MHz
NUC1 13C
PL1 3.00 dB

F2 - Processing parameters
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LB 1.00 Hz
GB 0
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1D NMR plot parameters
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F2P -10.351 ppm
F2 -784.48 Hz
PRCM 11.99844 ppm/cm
HZCM 905.79712 Hz/cm

Biphenyl-2-carbaldehyde

Biphenyl-2-carbonitrile

1-Phenylnaphthalene

2-Methyl-1-phenylnaphthalene

4,4'-Dimethylbiphenyl

4-Methoxy-4'-methylbiphenyl

2-Fluoro-4'-methylbiphenyl

4'-Methylbiphenyl-2-carbaldehyde

1-(4-Tolyl)-naphthalene

3-Phenylpyridine

5-Phenylprimidine

Current Data Parameters
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EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
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PULPROG zg30
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DS 1
SWH 3612.717 Hz
FIDRES 0.110251 Hz
AQ 4.5351410 sec
RG 256
DW 138.400 usec
DE 6.00 usec
TE 300.0 K
D1 1.00000000 sec
P1 9.00 usec
SFO1 300.2315011 MHz
NUC1 1H
PL1 2.00 dB

P2 - Processing parameters
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SSB 0
LB 0.30 Hz
GB 0
PC 1.00

1D NMR plot parameters
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F1 3306.38 Hz
F2P -1.020 ppm
F2 306.34 Hz
P1MCM 0.52318 ppm/cm
HZCM 157.07465 Hz/cm

Current Data Parameters
NAME 12517c
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
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INSTRUM spect
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PULPROG zgpg30
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SOLVENT CDCl3
NS 256
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SWH 18115.941 Hz
FIDRES 0.276427 Hz
AQ 1.8088436 sec
RG 1625.5
DW 27.600 usec
DE 6.00 usec
TE 300.0 K
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d12 0.00002000 sec
PL13 25.00 dB
D1 2.00000000 sec
CPDPRG2 waltz16
PCPD2 100.00 usec
SFO2 300.2312009 MHz
NUC2 13C
PL2 2.00 dB
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SFO1 75.5011682 MHz
NUC1 13C
PL1 3.00 dB

P2 - Processing parameters
SI 32768
SF 75.4929001 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

1D NMR plot parameters
CX 20.00 cm
F1P 229.492 ppm
F1 17325.05 Hz
F2P -10.476 ppm
F2 -790.90 Hz
P1MCM 11.99844 ppm/cm
HZCM 905.79712 Hz/cm

5-Phenyl-furan-2-carboaldehyde

Palladium Complex 5