Supporting Information for

Nickel-Catalyzed sp² C-H Bonds Arylation of N-Aromatic Heterocycles with Grignard Reagents at Room Temperature

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General:

Melting points were recorded with a micro melting point apparatus and uncorrected. NMR spectra were recorded with a 400 NMR spectrometer for $^1$H-NMR, 100 MHz for $^{13}$C-NMR. Proton chemical shifts $\delta$ were given in ppm relative to tetramethylsilane (0.00 ppm) in CDCl$_3$ or to the residual proton signals of the deuterated solvent CD$_3$OD (3.31 ppm). High resolution mass spectra were taken with a 3000 mass spectrometer, using Waters Q-TofMS/MS system. For column chromatography 200-300 mesh silica gel (GF254) was used as the stationary phase. All reactions were monitored by thin layer chromatography (TLC). All reactions were set up in air (with no use of a glove box) and carried out under nitrogen atmosphere. Ni(dppp)Cl$_2$ was purchased from commercial source and used as received. 1,2-Dichloroethane and THF were purified using standard methods before used. All other reagents were purchased from commercial sources and used as received.

**General procedure for the Ni-catalyzed direct sp$^2$ C-H bond arylation of purine with Grignard reagents.** An oven-dried Schlenk tube containing a stirbar was charged with purine derivatives (0.125 mmol) and Ni(dppp)Cl$_2$ (20 mg, 30 mol %). The Schlenk tube was fitted with a rubber cap, evacuated and back-filled with nitrogen (this sequence was repeated an additional two times). Then the 1,2-dichloroethane (0.03 mL, 3 equiv) was added to the tube along with THF (1 mL). The mixture was then stirred at room temperature. The Grignard reagent (5 equiv) was then added drop by drop via syringe and stirred for the corresponding reaction time at room temperature. After completion of the reaction, the mixture was then diluted with brine (3 mL) and extracted with ethyl acetate (3×3 mL). The organic layer was collected and dried over anhydrous Na$_2$SO$_4$, filtered and concentrated under reduced pressure. The crude material was purified by column chromatography on silica gel (eluting with petroleum ether/ethyl acetate mixtures) to give the desired products.
Characterization of compounds

9-Benzyl-6-methoxy-8-phenyl-9H-purine (3a)

![Chemical structure of 9-Benzyl-6-methoxy-8-phenyl-9H-purine (3a)](image)

White solid. M.p. 98-100 °C. $^1$H NMR (400 MHz, CDCl$_3$) $\delta$ 8.58 (s, 1H), 7.68 (d, $J = 7.2$ Hz, 2H), 7.50-7.42 (m, 3H), 7.28 (d, $J = 4.8$ Hz, 3H), 7.07 (d, $J = 7.6$ Hz, 2H), 5.56 (s, 2H), 4.23 (s, 3H). $^{13}$C NMR (100 MHz, CDCl$_3$) $\delta$ 160.8, 154.0, 153.3, 152.0, 136.2, 130.4, 129.3, 128.9, 128.7, 127.9, 126.5, 121.3, 54.3, 47.3. HRMS: calcd for C$_{19}$H$_{17}$N$_4$O [M+H]$^+$ 317.1402, found 317.1404.

6-Methoxy-9-phenethyl-8-phenyl-9H-purine (3b)

![Chemical structure of 6-Methoxy-9-phenethyl-8-phenyl-9H-purine (3b)](image)

White solid. M.p. 110-112 °C. $^1$H NMR (400 MHz, CDCl$_3$) $\delta$ 8.56 (s, 1H), 7.50-7.40 (m, 5H), 7.14 (t, $J = 2.4$ Hz, 3H), 6.89 (s, 2H), 4.55 (t, $J = 7.4$ Hz, 2H), 4.19 (s, 3H), 3.08 (t, $J = 7.4$ Hz, 2H). $^{13}$C NMR (100 MHz, CDCl$_3$) $\delta$ 160.7, 153.6, 153.1, 151.6, 137.1, 130.1, 129.5, 129.1, 128.6, 126.8, 121.2, 54.1, 45.5, 35.5. HRMS: calcd for C$_{20}$H$_{19}$N$_4$O [M+H]$^+$ 331.1559, found 331.1554.

9-Benzyl-2-chloro-6-methoxy-8-phenyl-9H-purine (3c)

![Chemical structure of 9-Benzyl-2-chloro-6-methoxy-8-phenyl-9H-purine (3c)](image)

White solid. M.p. 133-135 °C. $^1$H NMR (400 MHz, CDCl$_3$) $\delta$ 7.63 (d, $J = 7.2$ Hz, 2H), 7.51-7.41 (m, 3H), 7.27 (s, 3H), 7.03 (t, $J = 3.8$ Hz, 2H), 5.51 (s, 2H), 4.24 (s, 3H). $^{13}$C NMR (100 MHz, CDCl$_3$) $\delta$ 161.3, 155.4, 154.0, 152.9, 136.0, 130.8, 129.5, 129.2, 129.1, 129.0, 128.2, 126.9, 120.4, 55.3, 47.6. HRMS: calcd for C$_{19}$H$_{16}$ClN$_4$O [M+H]$^+$ 351.1013, found 351.1010.
6-Methoxy-9-methyl-8-phenyl-9H-purine (3d)

Yellow solid. M.p. 118-119 °C. $^1$H NMR (400 MHz, CDCl$_3$) $\delta$ 8.56 (s, 1H), 7.83 (q, $J$ = 3 Hz, 2H), 7.53 (t, $J$ = 3.2 Hz, 3H), 4.30 (s, 3H), 3.95 (s, 3H). $^{13}$C NMR (100 MHz, CDCl$_3$) $\delta$ 160.7, 154.0, 152.9, 151.6, 130.3, 129.3, 129.2, 128.7, 121.3, 54.2, 31.0. HRMS: calcd for C$_{13}$H$_{13}$N$_4$O [M+H]$^+$ 241.1089, found 241.1084.

9-Ethyl-6-methoxy-8-phenyl-9H-purine (3e)

Yellow solid. M.p. 62-64 °C. $^1$H NMR (400 MHz, CDCl$_3$) $\delta$ 8.48 (s, 1H), 7.71-7.69 (m, 2H), 7.44 (t, $J$ = 3.2 Hz, 3H), 4.32 (q, $J$ = 7.2 Hz, 2H), 4.13 (s, 3H), 1.38 (t, $J$ = 7.2 Hz, 3H). $^{13}$C NMR (100 MHz, CDCl$_3$) $\delta$ 160.6, 153.5, 152.6, 151.5, 130.2, 129.6, 129.0, 128.7, 121.3, 54.0, 39.2, 15.2. HRMS: calcd for C$_{14}$H$_{15}$N$_4$O [M+H]$^+$ 255.1246, found 255.1241.

6-Methoxy-8-phenyl-9-propyl-9H-purine (3f)

White solid. M.p. 76-77 °C. $^1$H NMR (400 MHz, CDCl$_3$) $\delta$ 8.53 (s, 1H), 7.73 (q, $J$ = 3 Hz, 2H), 7.49 (t, $J$ = 3.2 Hz, 3H), 4.29 (t, $J$ = 7.6 Hz, 2H), 4.18 (s, 3H), 1.85-1.76 (m, 2H), 0.82 (t, $J$ = 7.4 Hz, 3H). $^{13}$C NMR (100 MHz, CDCl$_3$) $\delta$ 160.7, 153.7, 152.9, 151.5, 130.2, 129.8, 129.1, 128.7, 121.2, 107.0, 54.1, 45.7, 23.1, 11.0. HRMS: calcd for C$_{15}$H$_{17}$N$_4$O [M+H]$^+$ 269.1402, found 269.1404.

9-Cyclopentyl-6-methoxy-8-phenyl-9H-purine (3g)

Yellow solid. M.p. 103-105 °C. $^1$H NMR (400 MHz, CDCl$_3$) $\delta$ 8.52 (s, 1H), 7.68 (t, $J$
$= 3.6 \text{ Hz, } 2H), 7.52 (t, J = 2.8 \text{ Hz, } 3H), 4.85 \text{-} 4.76 (m, 1H), 4.18 (s, 3H), 2.57 (q, J = 6.6 \text{ Hz, } 2H), 2.12 (t, J = 7 \text{ Hz, } 2H), 2.03 (q, J = 3.6 \text{ Hz, } 2H), 1.65 (d, J = 5.6 \text{ Hz, } 2H).

$^{13}$C NMR (100 MHz, CDCl$_3$) δ 160.8, 153.5, 153.1, 150.8, 130.1, 129.6, 128.6, 122.0, 58.1, 53.9, 31.0, 24.8. HRMS: calcd for C$_{17}$H$_{19}$N$_4$O [M+H]$^+$ 295.1559, found 295.1554.

9-Methyl-6,8-diphenyl-9H-purine (3h)

White solid. M.p. 138-140 °C. $^1$H NMR (400 MHz, CDCl$_3$) δ 8.99 (s, 1H), 8.89 (d, $J$ = 7.2 Hz, 2H), 7.86-7.84 (m, 2H), 7.53-7.45 (m, 6H), 3.90 (s, 3H). $^1$C NMR (100 MHz, CDCl$_3$) δ 154.9, 154.6, 153.6, 151.8, 135.9, 131.0, 130.7, 130.6, 129.8, 129.4, 129.3, 128.9, 128.5, 30.7. HRMS: calcd for C$_{18}$H$_{15}$N$_4$ [M+H]$^+$ 287.1297, found 287.1295.

9-Benzyl-6,8-diphenyl-9H-purine (3i)

White solid. M.p. 130-132 °C. $^1$H NMR (400 MHz, CDCl$_3$) δ 9.03 (s, 1H), 8.92 (d, $J$ = 7.6 Hz, 2H), 7.70 (d, $J$ = 8 Hz, 2H), 7.56-7.42 (m, 6H), 7.25 (d, $J$ = 6.4 Hz, 3H), 7.07 (d, $J$ = 6.8 Hz, 2H), 5.55 (s, 2H). $^{13}$C NMR (100 MHz, CDCl$_3$) δ 155.3, 154.6, 153.9, 152.3, 136.2, 135.9, 131.0, 130.8, 130.7, 129.9, 129.4, 128.9, 128.9, 128.6, 127.9, 126.6, 47.1. HRMS: calcd for C$_{24}$H$_{19}$N$_4$ [M+H]$^+$ 363.1610, found 363.1607.

9-Benzyl-2,6,8-triphenyl-9H-purine (3j)

Light yellow solid. M.p. 200-202 °C. $^1$H NMR (400 MHz, CDCl$_3$) δ 9.11 (d, $J$ = 7.6
Hz, 2H), 8.73 (d, J = 7.2 Hz, 2H), 7.76 (d, J = 7.2 Hz, 2H), 7.62 (t, J = 7.6 Hz, 2H), 7.56-7.48 (m, 7H), 7.29 (t, J = 8.4 Hz, 3H), 7.20 (d, J = 7.2 Hz, 2H), 5.64 (s, 2H). \(^{13}\)C NMR (100 MHz, CDCl\(_3\)) \(\delta\) 158.3, 155.6, 155.3, 153.4, 138.6, 136.6, 136.4, 130.7, 130.5, 129.9, 129.8, 129.7, 129.5, 128.9, 128.8, 128.6, 128.4, 128.3, 127.9, 127.1, 47.1. HRMS: calcd for C\(_{30}\)H\(_{23}\)N\(_4\) [M+H]\(^+\) 439.1923, found 439.1917.

6,9-Dibenzyl-8-phenyl-9\(H\)-purine (3k)

\[
\text{White solid. M.p. 102-104 °C. } ^{1}\text{H NMR (400 MHz, CDCl}_3\text{) } \delta \text{ 8.91 (s, 1H), 7.67 (d, } J = 7.2 \text{ Hz, 2H), 7.55-7.49 (m, 5H), 7.29 (q, } J = 7.6 \text{ Hz, 5H), 7.22 (d, } J = 7.2 \text{ Hz, 1H), 7.08 (d, } J = 4.8 \text{ Hz, 2H), 5.52 (s, 2H), 4.60 (s, 2H). } ^{13}\text{C NMR (100 MHz, CDCl}_3\text{) } \delta \text{ 165.0, 153.9, 152.5, 152.5, 144.5, 141.9, 138.4, 136.0, 133.6, 132.7, 131.7, 131.2, 130.4, 130.1, 128.8, 128.2, 127.8, 124.3, 61.8, 14.3. HRMS: calcd for C}_{25}\text{H}_{21}\text{N}_4\text{ [M+H]}^+ \text{ 377.1766, found 377.1760.}
\]

6-Benzyl-9-butyl-8-phenyl-9\(H\)-purine (3l)

\[
\text{Colorless oil. } ^{1}\text{H NMR (400 MHz, CDCl}_3\text{) } \delta \text{ 8.92 (s, 1H), 7.77 (t, } J = 3.6 \text{ Hz, 2H), 7.58 (t, } J = 3 \text{ Hz, 3H), 7.51 (d, } J = 7.2 \text{ Hz, 2H), 7.29 (t, } J = 7.4 \text{ Hz, 2H), 7.20 (t, } J = 7.2 \text{ Hz, 1H), 4.57 (s, 2H), 4.33 (t, } J = 7.8 \text{ Hz, 2H), 1.79 (t, } J = 7.6 \text{ Hz, 2H), 1.28 (q, } J = 7.6 \text{ Hz, 2H), 0.86 (t, } J = 7.4 \text{ Hz, 3H). } ^{13}\text{C NMR (100 MHz, CDCl}_3\text{) } \delta \text{ 160.0, 155.1, 153.1, 152.4, 138.3, 132.6, 130.8, 130.1, 129.7, 129.5, 129.2, 128.7, 126.7, 43.9, 39.4, 31.9, 20.0, 13.7. HRMS: calcd for C}_{22}\text{H}_{23}\text{N}_4\text{ [M+H]}^+ \text{ 343.1927, found 343.1918.}
\]
9-Benzyl-6-methoxy-8-(p-tolyl)-9H-purine (3m)

Yellow solid. M.p. 109-111 °C. $^1$H NMR (400 MHz, CDCl$_3$) δ 8.58 (s, 1H), 7.59 (d, $J$ = 8 Hz, 2H), 7.27 (q, $J$ = 7.6 Hz, 5H), 7.09 (d, $J$ = 6.4 Hz, 2H), 5.56 (s, 2H), 4.24 (s, 3H), 2.41 (s, 3H). $^{13}$C NMR (100 MHz, CDCl$_3$) δ 160.7, 154.0, 153.5, 151.9, 140.7, 136.3, 129.4, 129.2, 128.9, 127.8, 126.5, 126.4, 121.2, 54.2, 47.3, 21.4. HRMS: calcd for C$_{20}$H$_{19}$N$_4$O [M+H]$^+$ 331.1559, found 331.1556.

9-Benzyl-6-methoxy-8-(m-tolyl)-9H-purine (3n)

Yellow solid. M.p. 74-76 °C. $^1$H NMR (400 MHz, CDCl$_3$) δ 8.57 (s, 1H), 7.52 (s, 1H), 7.42 (d, $J$ = 6 Hz, 1H), 7.28 (q, $J$ = 5.2 Hz, 5H), 7.07 (d, $J$ = 6.4 Hz, 2H), 5.53 (s, 2H), 4.22 (s, 3H), 2.34 (s, 3H). $^{13}$C NMR (100 MHz, CDCl$_3$) δ 160.8, 154.0, 153.5, 151.9, 138.6, 136.3, 131.1, 130.2, 129.1, 128.9, 128.5, 127.9, 126.6, 126.1, 121.2, 54.2, 47.4, 21.3. HRMS: calcd for C$_{20}$H$_{19}$N$_4$O [M+H]$^+$ 331.1559, found 331.1554.

9-Benzyl-8-(4-ethylphenyl)-6-methoxy-9H-purine (3o)

Light yellow oil. $^1$H NMR (400 MHz, CDCl$_3$) δ 8.56 (s, 1H), 7.61 (d, $J$ = 8 Hz, 2H), 7.27 (t, $J$ = 7.2 Hz, 5H), 7.08 (d, $J$ = 6.4 Hz, 2H), 5.55 (s, 2H), 4.23 (s, 3H), 2.70 (q, $J$ = 7.2 Hz, 2H), 1.26 (t, $J$ = 7.6 Hz, 3H). $^{13}$C NMR (100 MHz, CDCl$_3$) δ 160.7, 154.0, 153.5, 151.8, 146.9, 136.3, 129.3, 128.9, 128.2, 127.8, 126.6, 126.4, 121.3, 54.2, 47.3, 28.7, 15.2. HRMS: calcd for C$_{21}$H$_{21}$N$_4$O [M+H]$^+$ 345.1715, found 345.1714.
9-Benzyl-6-methoxy-8-(4-methoxyphenyl)-9H-purine (3p)

Yellow solid. M.p. 114-116 °C. $^1$H NMR (400 MHz, CDCl$_3$) $\delta$ 8.55 (s, 1H), 7.63 (d, $J$ = 8.8 Hz, 2H), 7.28 (q, $J$ = 7.6 Hz, 3H), 7.08 (d, $J$ = 6.8 Hz, 2H), 6.94 (d, $J$ = 8.4 Hz, 2H), 5.54 (s, 2H), 4.23 (s, 3H), 3.84 (s, 3H). $^{13}$C NMR (100 MHz, CDCl$_3$) $\delta$ 161.3, 160.6, 154.1, 153.3, 151.7, 136.3, 130.8, 128.9, 127.8, 126.4, 121.6, 121.2, 114.1, 55.3, 54.2, 47.3. HRMS: calcd for C$_{20}$H$_{19}$N$_4$O$_2$ [M+H]$^+$ 347.1508, found 347.1505.

9-Benzyl-8-(3,5-dimethylphenyl)-6-methoxy-9H-purine (3q)

Light yellow oil. $^1$H NMR (400 MHz, CDCl$_3$) $\delta$ 8.58 (s, 1H), 7.29 (d, $J$ = 10 Hz, 5H), 7.11 (d, $J$ = 6 Hz, 3H), 5.53 (s, 2H), 4.23 (s, 3H), 2.29 (s, 6H). $^{13}$C NMR (100 MHz, CDCl$_3$) $\delta$ 160.7, 154.1, 153.7, 151.9, 138.3, 136.5, 132.0, 129.0, 128.8, 127.8, 127.1, 126.7, 121.2, 107.0, 54.2, 47.4, 21.1. HRMS: calcd for C$_{21}$H$_{21}$N$_4$O [M+H]$^+$ 345.1715, found 345.1716.

9-Benzyl-6-methoxy-8-(o-tolyl)-9H-purine (3r)

White solid. M.p. 112-114 °C. $^1$H NMR (400 MHz, CDCl$_3$) $\delta$ 8.62 (s, 1H), 7.43-7.39 (m, 1H), 7.29 (s, 1H), 7.25-7.14 (m, 5H), 6.89 (d, $J$ = 6.4 Hz, 2H), 5.27 (s, 2H), 4.22 (s, 3H), 2.00 (s, 3H). $^{13}$C NMR (100 MHz, CDCl$_3$) $\delta$ 161.0, 153.2, 153.1, 152.1, 138.6, 136.0, 130.7, 130.5, 130.2, 129.4, 128.8, 128.2, 127.9, 125.9, 121.3, 54.4, 47.1, 19.7. HRMS: calcd for C$_{20}$H$_{19}$N$_4$O [M+H]$^+$ 331.1559, found 331.1554.
**8-((1,1′-Biphenyl)-4-yl)-9-benzyl-6-methoxy-9H-purine (3s)**

![Structure Image]

Light yellow solid. M.p. 134-136 °C. \(^1\)H NMR (400 MHz, CDCl\(_3\)) \(\delta\) 8.58 (s, 1H), 7.77 (d, \(J = 8.4\) Hz, 2H), 7.66 (d, \(J = 8.4\) Hz, 2H), 7.61 (d, \(J = 7.6\) Hz, 2H), 7.44 (t, \(J = 7.4\) Hz, 2H), 7.36 (t, \(J = 7.2\) Hz, 1H), 7.28 (t, \(J = 7.6\) Hz, 3H), 7.11 (dt, \(J = 6.4\) Hz, 2H), 5.59 (s, 2H), 4.24 (s, 3H). \(^{13}\)C NMR (100 MHz, CDCl\(_3\)) \(\delta\) 160.8, 154.1, 153.0, 152.0, 143.15, 139.8, 136.2, 129.7, 129.0, 128.9, 128.1, 128.0, 127.9, 127.3, 127.1, 126.4, 121.4, 54.3, 47.4. HRMS: calcd for C\(_{25}\)H\(_{21}\)N\(_4\)O \([\text{M+H}]^+\) 393.1715, found 393.1713.

**9-Benzyl-8-(4-fluorophenyl)-6-methoxy-9H-purine (3t)**

![Structure Image]

Light yellow oil. \(^1\)H NMR (400 MHz, CDCl\(_3\)) \(\delta\) 8.58 (s, 1H), 7.68-7.64 (m, 2H), 7.49-7.42 (m, 1H), 7.28 (t, \(J = 5.6\) Hz, 2H), 7.13 (t, \(J = 8.6\) Hz, 2H), 7.06 (t, \(J = 3.4\) Hz, 2H), 5.54 (d, \(J = 8\) Hz, 2H), 4.24 (d, \(J = 4.8\) Hz, 3H). \(^{13}\)C NMR (100 MHz, CDCl\(_3\)) \(\delta\) 161.0, 154.2, 152.5, 152.4, 136.2, 131.6, 131.6, 129.5, 129.2, 129.1, 128.9, 128.2, 126.6, 121.4, 116.3, 116.1, 54.5, 47.5. HRMS: calcd for C\(_{19}\)H\(_{16}\)FN\(_4\)O \([\text{M+H}]^+\) 335.1308, found 335.1310.

**9-Benzyl-8-(4′-fluoro-[1,1′-biphenyl]-4-yl)-6-methoxy-9H-purine (3u)**

![Structure Image]

Yellow solid. M.p. 154-156 °C. \(^1\)H NMR (400 MHz, CDCl\(_3\)) \(\delta\) 8.58 (s, 1H), 7.76 (d, \(J = 8.4\) Hz, 2H), 7.62-7.56 (m, 4H), 7.29 (t, \(J = 6.8\) Hz, 3H), 7.13 (q, \(J = 8.6\) Hz, 4H), 5.60 (d, \(J = 6\) Hz, 2H), 4.24 (s, 3H). \(^{13}\)C NMR (100 MHz, CDCl\(_3\)) \(\delta\) 161.0, 154.3, 153.1, 152.3, 142.3, 136.4, 136.2, 130.0, 129.2, 129.0, 128.9, 128.3, 128.2, 127.4, 126.6, 121.6, 116.2, 116.0, 54.5, 47.6. HRMS: calcd for C\(_{25}\)H\(_{20}\)FN\(_4\)O \([\text{M+H}]^+\) 411.1621, found 411.1624.
Copies of $^1$H and $^{13}$C NMR spectra
Electronic Supplementary Material (ESI) for Chemical Communications
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