Electronic Supporting Information for:
Efficient Cross-Coupling of Secondary Amines/Azoles and Activated (Hetero)Aryl Chlorides Using an Air-Stable DPEPhos/Nickel Pre-Catalyst

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1. General Considerations

Unless stated, all reactions were set up inside a nitrogen atmosphere and products were isolated using standard benchtop conditions. Toluene used in the glove box was purified by sparging with nitrogen followed by passage through a double column purification system equipped with one alumina packed column and one copper-Q5 packed column. THF was purified by distillation under nitrogen atmosphere over sodium and benzophenone. Solvents used in the glovebox were stored over 4 Å molecular sieves. Ligand L6 was prepared using literature protocols. All other reagents, solvents and materials were used as received from commercial sources. Unless stated, product purification was performed via column chromatography on Silicycle Siliaflash 60 silica (particle size 40 - 63 µm; 230-400 mesh), or by using a Biotage Isolera One automated column using 25 g Snap KP-Sil cartridges (silica particle size 15 - 40 µm). All $^1$H NMR and $^{13}$C NMR spectra were recorded using a Bruker AV-500 or AV-300 spectrometer at 300 K. Chemical shifts are expressed in parts per million (ppm) using the residual solvent peak ($^1$H 7.26 ppm of CHCl$_3$ and $^{13}$C 77.1 ppm for CDCl$_3$; and $^1$H 5.32 ppm of CHDCl$_2$ and $^{13}$C 53.8 ppm for CD$_2$Cl$_2$) as an internal reference. Coupling constants are ($J$) are reported in Hertz (Hz). Splitting patterns are described as follows: br, broad; s, singlet; d, doublet; t, triplet; q, quartet; m, multiplet. Mass spectra were obtained using ion trap instruments using electrospray ionization, in positive ion mode. Calibrated GC data were obtained using an instrument equipped with a SGE BP-5, 30 m, 0.25 mm internal diameter column.

2. Crystallographic Solution and Refinement Details.

Crystallographic data for C1 were obtained at -100 °C on a Bruker D8/APEX II CCD diffractometer equipped with a CCD area detector using Cu Kα ($\lambda = 1.54178$ Å) (microfocus source) radiation employing a sample that was mounted in inert oil and transferred to a cold gas stream on the diffractometer. Data reduction, correction for Lorentz polarization, and absorption correction (Gaussian integration; face-indexed) were each performed. Structure solution by using intrinsic phasing was carried out, followed by least-squares refinement on $F^2$. All non-hydrogen atoms were refined with anisotropic displacement parameters, while all hydrogen atoms were added at calculated positions and refined by use of a riding model employing isotropic displacement parameters based on the isotropic displacement parameter of the attached atom. Crystallographic data have been deposited with the Cambridge Crystallographic Data Centre (1534212).
Table S1. Crystallographic Experimental Details for C1.

A. Crystal Data

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B. Data Collection and Refinement Conditions

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\textsuperscript{a}Obtained from least-squares refinement of 9924 reflections with 6.56° < 2θ < 146.80°.

\textsuperscript{b}Programs for diffractometer operation, data collection, data reduction and absorption correction were those supplied by Bruker.
3. Characterization Data for Isolated Cross-Coupling Products

4-morpholinobenzonitrile, 2a

Following GP (aryl halide 137.6 mg, amine 96.2 µL), the title product was obtained via flash chromatography using 30% EtOAc in hexanes. The product was isolated as light yellow solid (81%). \(^1\)H NMR (500 MHz, CDCl\(_3\)): \(\delta\) 7.54 (d, \(J = 9.1\) Hz, 2H), 6.89 (d, \(J = 9.1\) Hz, 2H), 3.88 (t, \(J = 4.9\) Hz, 4H), 3.31 (t, \(J = 4.9\) Hz, 4H); \(^{13}\)C\({^1}\)H NMR (125.8 MHz, CDCl\(_3\)): \(\delta\) 153.7, 133.7, 120.0, 114.2, 101.2, 66.6, 47.5; this is in agreement with previously reported spectra.\(^2\)

4-(benzo[d]thiazol-2-yl)morpholine, 2b

Following GP (aryl halide 134.6 uL, amine 96.2 µL), the title product was isolated via flash chromatography using 20% EtOAc in hexanes. The product was isolated as a beige solid (66%). \(^1\)H NMR (500 MHz, CDCl\(_3\)): \(\delta\) 7.65 (d, \(J = 7.8\) Hz, 1H), 7.61 (d, \(J = 7.9\) Hz, 1H), 7.37-7.32 (m, 1H), 7.16-7.14 (m, 1H), 3.87 (t, \(J = 4.7\) Hz, 4H), 3.66 (t, \(J = 5.0\) Hz, 4H); \(^{13}\)C\({^1}\)H NMR (125.8 MHz, CDCl\(_3\)): \(\delta\) 169.2, 125.7, 130.8, 126.3, 121.9, 120.9, 119.5, 66.4, 48.7; this is in agreement with previously reported spectra.\(^3\)

N-(2-methoxyethyl)-N-methylbenzo[d]thiazol-2-amine, 2c

Following GP (aryl halide 130.2 uL, amine 119.6 µL), the title product was isolated via automated column using a 0-20% EtOAc in hexanes gradient. The product was isolated as a yellow oil (45%). \(^1\)H NMR (500 MHz, CDCl\(_3\)): \(\delta\) 7.62 (d, \(J = 7.8\) Hz, 1H), 7.58 (d, \(J = 8.0\) Hz, 1H), 7.33-7.28 (m, 1H), 7.10-7.05 (m, 1H), 7.39 (t, \(J = 5.4\) Hz, 2H), 7.31 (t, \(J = 5.2\) Hz, 2H), 3.40 (s, 3H), 3.27 (s, 3H); \(^{13}\)C\({^1}\)H NMR (125.8 MHz, CDCl\(_3\)): \(\delta\) 168.5, 153.3, 131.0, 126.1, 121.1, 120.7, 118.9, 70.7, 59.2, 52.9, 39.8; \(m/z\) ESI\(^+\) found 245.0719 [M+Na]\(^+\) calculated for C\(_{11}\)H\(_{14}\)N\(_2\)NaOS 245.0725.

3-methyl-2-(pyrrolidin-1-yl)quinoline, 2d

Following GP (aryl halide 177.6 mg, amine 91.8 µL), the title product was isolated via flash chromatography using 5% EtOAc in hexanes. The product was isolated as a yellow oil (50%). \(^1\)H NMR (500 MHz, CDCl\(_3\)): \(\delta\) 7.75 (d, \(J = 8.4\) Hz, 1H), 7.67 (s, 1H), 7.57 (d, \(J = 7.9\) Hz, 1H), 7.53-7.48 (m, 1H), 7.25-7.20 (m, 1H), 3.76-3.71 (m, 4H), 2.52 (s, 3H), 2.03-1.97 (m, 4H); \(^{13}\)C\({^1}\)H NMR (125.8 MHz, CDCl\(_3\)): \(\delta\) 158.7, 146.6, 138.1, 128.5, 126.5, 126.4, 124.3, 122.3, 50.0, 25.9, 21.5; \(m/z\) ESI\(^+\) found 213.1386 [M+Na]\(^+\) calculated for C\(_{14}\)H\(_{17}\)N\(_2\) 213.1386.
6,7-dimethoxy-4-(piperidin-1-yl)quinazoline, 2e

Follow GP (aryl halide 224.6 mg, amine 108.7 μL), the title product was isolated via flash chromatography using 80-100% EtOAc in hexanes. The product was isolated as a yellow solid (90%). $^1$H NMR (500 MHz, CDCl$_3$): $\delta$ 8.67 (s, 1H), 7.24 (s, 1H), 7.14 (s, 1H), 4.04 (s, 3H), 4.01 (s, 3H), 3.63-3.59 (m, 4H), 1.86-1.75 (m, 6H); $^{13}$C {$^1$H} NMR (125.8 MHz, CDCl$_3$): $\delta$ 164.6, 154.5, 153.4, 149.2, 149.2, 111.8, 107.6, 103.6, 56.3, 56.1, 21.2, 26.1, 24.9; m/z ESI$^+$ found 274.1550 [M+H]$^+$ calculated for C$_{15}$H$_{20}$N$_3$O$_2$ 274.1556.

4-(4-(pyridin-2-yl)piperazin-1-yl)benzonitrile 2f

Following GP (aryl halide 137.6 mg, amine 175.5 μL), the title product was obtained via automated column using a 0-20% EtOAc in hexanes gradient. The product was isolated as light yellow solid (85%). $^1$H NMR (500 MHz, CDCl$_3$): $\delta$ 8.26-8.21 (m, 1H), 7.58-7.49 (m, 3H), 6.94-6.87 (m, 2H), 6.73-6.69 (m, 2H), 3.77-3.71 (m, 4H), 3.53-3.47 (m, 4H); $^{13}$C {$^1$H} im?z NMR (125.8 MHz, CDCl$_3$): $\delta$ 159.1, 153.3, 148.2, 137.8, 133.7, 120.1, 114.3, 114.0, 107.2, 100.6, 47.0, 44.8; m/z ESI$^+$ found 265.1448 [M+H]$^+$ calculated for C$_{16}$H$_{17}$N$_4$ 265.1454.

2-methyl-4-(4-(pyridin-2-yl)piperazin-1-yl)quinolone, 2g

Following GP (aryl halide 201.6 μL, amine 267.5 μL), the title product was obtained via automated column using a 20-50% EtOAc in hexanes gradient. The product was isolated as a light yellow solid (78%). $^1$H NMR (500 MHz, CDCl$_3$): $\delta$ 8.29-8.24 (m, 1H), 8.08-7.98 (m, 2H), 7.69-7.61 (m, 1H), 7.59-7.51 (m, 1H), 7.50-7.43 (m, 1H), 6.81-6.67 (m, 3H), 3.86-3.80 (m, 4H), 3.38-3.31 (m, 4H), 2.70 (s, 3H); $^{13}$C {$^1$H} NMR (125.8 MHz, CDCl$_3$): $\delta$ 159.5, 159.4, 156.7, 149.3, 148.0, 137.6, 129.3, 129.1, 124.6, 123.3, 121.8, 113.8, 109.5, 107.2, 52.0, 45.4, 25.6; m/z ESI$^+$ found 305.1761 [M+H]$^+$ calculated for C$_{19}$H$_{21}$N$_4$ 305.1760.

(4-(4-benzoylphenyl)piperazin-1-yl)(furan-2-yl)methanone, 2h

Following GP (aryl halide 217.0 mg, amine 198.2 mg), the title product was isolated via flash chromatography using 80% EtOAc in hexanes. The product was isolated as a thick yellow oil
(63%). $^1$H NMR (500 MHz, CDCl$_3$): δ 7.87-7.82 (m, 2H), 7.79-7.75 (m, 2H), 7.61-7.56 (m, 1H), 7.55-7.54 (m, 1H), 7.51-7.47 (m, 2H), 7.12-7.10 (m, 1H), 6.96-6.92 (m, 2H), 6.56-6.53 (m, 1H), 4.03 (br s, 4H), 3.53-3.47 (m, 4H); $^{13}$C{ $^1$H} NMR (125.8 MHz, CDCl$_3$): δ 195.3, 159.3, 153.6, 148.0, 144.1, 138.8, 132.7, 131.7, 129.7, 128.3, 128.1, 117.1, 113.8, 111.6, 47.7, 44.0 (br); m/z ESI$^+$ found 383.1366 [M+Na]$^+$ calculated for C$_{22}$H$_{20}$N$_2$NaO$_3$ 383.1372.

N-(diphenylmethene)-2-methylquinolin-4-amine, 2i

Follow GP (aryl halide 201.6 uL, amine 199.4 mg), the title product was isolated via flash chromatography using 40% EtOAc in hexanes. The product was isolated as a light yellow solid (91%). $^1$H NMR (300 MHz, CDCl$_3$, at 340 K): δ 7.93 (t, $J$ = 7.9 Hz, 2H), 7.72-7.22 (br m, 12H), 6.32 (s, 1H), 2.52 (s, 3H); $^{13}$C{ $^1$H} NMR (125.8 MHz, CDCl$_3$): δ 169.5, 159.3, 155.9, 148.4, 131.4 (br), 129.6, 129.5 (br), 128.7, 128.3, 125.2, 123.7, 121.3, 109.5, 25.6; m/z ESI$^+$ found 323.1543 [M+H]$^+$ calculated for C$_{23}$H$_{19}$N$_2$ 323.1549.

4-(1H-pyrrol-1-yl)benzonitrile, 2j

Following GP (aryl halide 137.6 mg, amine 128.9 mg), the title product was obtained via flash chromatography using 10% EtOAc in hexanes. The product was isolated as beige solid (72%). $^1$H NMR (500 MHz, CDCl$_3$): δ 7.75 (d, $J$ = 8.8 Hz, 2H), 7.52 (d, $J$ = 8.8 Hz, 2H), 7.17 (t, $J$ = 2.2 Hz, 2H), 6.44 (t, $J$ = 2.2 Hz, 2H); $^{13}$C{ $^1$H} NMR (125.8 MHz, CDCl$_3$): δ 143.9, 134.0, 120.2, 119.1, 118.6, 112.3, 108.8; m/z ESI$^+$ found 191.0580 [M+Na]$^+$ calculated for C$_{11}$H$_8$N$_2$Na 191.0585.

4-(1H-indol-1-yl)benzonitrile, 2k

Following GP (aryl halide 137.6 mg, amine 76.3 µL), the title product was obtained via flash chromatography on basic alumina using 5% EtOAc in hexanes. The product was isolated as beige solid (99%). $^1$H NMR (500 MHz, CDCl$_3$): δ 7.84 (d, $J$ = 8.5 Hz, 2H), 7.74 (d, $J$ = 7.7 Hz, 1H), 7.69-7.63 (m, 3H), 7.38 (d, $J$ = 3.3 Hz, 1H), 7.30 (t, $J$ = 7.3, 1H), 7.26 (t, $J$ = 7.7, 1H) 6.79 (d, $J$ = 3.3 Hz, 1H); $^{13}$C{ $^1$H} NMR (125.8 MHz, CDCl$_3$): δ 143.7, 135.4, 133.9, 130.1, 127.2, 124.0, 123.4, 121.8, 121.5, 118.6, 110.5, 109.5, 105.9; this is in agreement with previously reported spectra.\(^4\)
1-(4,6-dimethoxypyrimidin-2-yl)-1H-indole, 2I

Following GP (aryl halide 174.5 mg, amine 128.7 mg), the title product was isolated via automated column using a 0-20% EtOAc in hexanes gradient. The product was isolated as a white solid (87%). $^1$H NMR (500 MHz, CDCl$_3$): $\delta$ 8.80 (d, $J = 8.4$ Hz, 1H), 8.29 (d, $J = 3.6$ Hz, 1H), 7.66 (d, $J = 7.7$ Hz, 1H), 7.39-7.34 (m, 1H), 7.30-7.25 (m, 1H), 6.70 (d, $J = 3.6$ Hz, 1H), 4.11 (s, 6 H); $^{13}$C{$^1$H} NMR (125.8 MHz, CDCl$_3$): $\delta$ 172.1, 156.4, 135.5, 131.5, 126.2, 123.7, 122.1, 121.0, 116.2, 106.7, 85.1, 54.5; m/z ESI$^+$ found 278.0900 [M+Na]$^+$ calculated for C$_{14}$H$_{13}$N$_3$NaO$_2$ 278.0906.

2-(2-methyl-1H-indol-1-yl)quinolone, 2m

Following GP (aryl halide 133.0 uL, amine 144.3 mg), the title product was isolated via flash chromatography on basic alumina using 5% EtOAc in hexanes. The product was isolated as a thick yellow oil (88%). $^1$H NMR (500 MHz, CDCl$_3$): $\delta$ 8.36 (d, $J = 8.6$ Hz, 1H), 8.16 (d, $J = 8.4$ Hz, 1H), 7.94 (d, $J = 8.0$ Hz, 1H), 7.85-7.79 (m, 1H), 7.66-7.60 (m, 3H), 7.58-7.53 (m, 1H), 7.23-7.16 (m, 2H), 6.52 (s, 1H), 2.61 (s, 3H); $^{13}$C{$^1$H} NMR (125.8 MHz, CDCl$_3$): $\delta$ 150.7, 147.8, 138.6, 137.3, 137.2, 130.4, 129.2, 129.1, 127.7, 126.9, 126.8, 121.9, 121.1, 120.0, 119.3, 110.7, 104.1, 14.5; this is in agreement with previously reported spectra.5

9-(pyrimidin-2-yl)-9H-carbazole, 2n

Following GP (aryl halide 114.5 mg, amine 183.9 mg), the title product was isolated via automated column using a 0-5% EtOAc in hexanes gradient. The product was isolated as a white solid (70%). $^1$H NMR (500 MHz, CDCl$_3$): $\delta$ 8.92-8.86 (m, 4H), 8.12 (d, $J = 7.7$ Hz, 2H), 7.57-7.53 (m, 2H), 7.41 (t, $J = 7.6$ Hz, 2H), 7.15 (t, $J = 4.7$ Hz, 1H); $^{13}$C{$^1$H} NMR (125.8 MHz, CDCl$_3$): $\delta$ 159.4, 158.0, 139.3, 126.8, 126.0, 122.5, 119.7, 116.4, 116.1; this is in agreement with previously reported spectra.6
4. SI References


Supplementary Figure 1. $^1$H NMR of C1 (CD$_2$Cl$_2$, 300.1 MHz)
Supplementary Figure 2. $^{31}\text{P}^{[\text{H}]}$ NMR of C1 (CD$_2$Cl$_2$, 121.5 MHz)
Supplementary Figure 3. $^1$H NMR 4-morpholinobenzonitrile, 2a (CDCl$_3$, 500.1 MHz)
Supplementary Figure 4. $^{13}\text{C}(1\text{H})$ NMR of 4-morpholinobenzonitrile, 2a (CDCl$_3$, 125.7 MHz)
Supplementary Figure 5. $^1$H NMR 4-(benzo[d]thiazol-2-yl)morpholine, 2b (CDCl$_3$, 500.1 MHz)
Supplementary Figure 6. $^{13}$C($^1$H) 4-(benzo[d]thiazol-2-yl)morpholine, 2b (CDCl$_3$, 125.7 MHz)
Supplementary Figure 7. $^1$H NMR N-(2-methoxyethyl)-N-methylbenzo[d]thiazol-2-amine, 2c (CDCl$_3$, 500.1 MHz)
Supplementary Figure 8. $^{13}$C($^1$H) N-(2-methoxyethyl)-N-methylbenzo[d]thiazol-2-amine, 2c (CDCl$_3$, 125.7 MHz)
Supplementary Figure 9. $^1$H NMR 3-methyl-2-(pyrrolidin-1-yl)quinoline, 2d (CDCl$_3$, 500.1 MHz)
Supplementary Figure 10. $^{13}\text{C}^{$(1\text{H})$} 3$-methyl-2-(pyrrolidin-1-yl)quinoline, 2d (CDCl$_3$, 125.7 MHz)
Supplementary Figure 11. $^1$H NMR 6,7-dimethoxy-4-(piperidin-1-yl)quinazoline, 2e (CDCl$_3$, 500.1 MHz)
Supplementary Figure 12. $^{13}$C($^1$H) 6,7-dimethoxy-4-(piperidin-1-yl)quinazoline, 2e (CDCl₃, 125.7 MHz)
Supplementary Figure 13. $^1$H NMR 4-(4-(pyridin-2-yl)piperaizin-1-yl)benzonitrile, 2f (CDCl$_3$, 500.1 MHz)
Supplementary Figure 14. $^{13}$C($^1$H) NMR 4-(4-(pyridin-2-yl)piperazin-1-yl)benzonitrile, 2f (CDCl$_3$, 125.7 MHz)
Supplementary Figure 15. $^1$H NMR 2-methyl-4-(4-(pyridin-2-yl)piperazin-1-yl)quinolone, 2g (CDCl$_3$, 500.1 MHz)
Supplementary Figure 16. $^{13}$C($^1$H) NMR 2-methyl-4-(4-(pyridin-2-yl)piperazin-1-yl)quinolone, 2g (CDCl$_3$, 125.7 MHz)
Supplementary Figure 17. $^1$H NMR \((4\text{-}(4\text{-benzoylphenyl})\text{piperazin-1-yl})(\text{furan-2-yl})\text{methanone, 2h} (\text{CDCl}_3, 500.1 \text{ MHz})$
Supplementary Figure 18. $^{13}$C\textsuperscript{1}H\textsuperscript{1} (4-(4-benzoylphenyl)piperazin-1-yl)(furan-2-yl)methanone, 2h (CDCl\textsubscript{3}, 125.7 MHz)
Supplementary Figure 19. $^1$H NMR N-(diphenylmethylene)-2-methylquinolin-4-amine, 2i (CDCl$_3$, 300.1 MHz at 340 K)
Supplementary Figure 20. $^{13}$C($^1$H) N-(diphenylmethylene)-2-methylquinolin-4-amine, 2i (CDCl$_3$, 125.7 MHz)
Supplementary Figure 21. $^1$H NMR 4-(1H-pyrrol-1-yl)benzonitrile, 2j (CDCl$_3$, 500.1 MHz)
Supplementary Figure 22. $^{13}$C($^1$H) NMR 4-(1H-pyrrol-1-yl)benzonitrile, 2j (CDCl$_3$, 125.7 MHz)
Supplementary Figure 23. $^1$H NMR 4-(1H-indol-1-yl)benzonitrile, 2k (CDCl$_3$, 500.1 MHz)
Supplementary Figure 24. $^{13}$C($^1$H) NMR 4-(1H-indol-1-yl)benzonitrile, 2k (CDCl$_3$, 125.7 MHz)
Supplementary Figure 25. $^1$H NMR 1-(4,6-dimethoxypyrimidin-2-yl)-1H-indole, 2l (CDCl$_3$, 500.1 MHz)
Supplementary Figure 26. $^{13}$C($^1$H) 1-(4,6-dimethoxypyrimidin-2-yl)-1H-indole, 2I (CDCl$_3$, 125.7 MHz)
Supplementary Figure 27. $^1$H NMR 2-(2-methyl-1H-indol-1-yl)quinolone, 2m (CDCl$_3$, 500.1 MHz)
Supplementary Figure 28. $^{13}$C($^1$H) 2-(2-methyl-1H-indol-1-yl)quinolone, 2m (CDCl$_3$, 125.7 MHz)
Supplementary Figure 29. $^1$H NMR 9-(pyrimidin-2-yl)-9H-carbazole, 2n (CDCl$_3$, 500.1 MHz)
Supplementary Figure 30. $^{13}$C($^1$H) 9-(pyrimidin-2-yl)-9H-carbazole, 2n (CDCl$_3$, 125.7 MHz)