Supplementary Information

Palladium-Catalyzed Coupling of Pyrazole Triflates with Arylboronic Acids

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General Methods. Reagents were purchased from commercial suppliers and used without purification unless noted otherwise. Anhydrous solvents were obtained from a GlassContour Solvent Dispensing System. Anhydrous 1,4-dioxane was purchased from Acros in Acrosealed™ bottles. All reactions were assembled open to air and then placed under nitrogen after the addition of all reagents. Mass spectra were obtained on an Agilent series 1100 MSD using electrospray ionization (ESI) in either positive or negative modes as indicated. Thin-layer chromatography was performed using Merck silica gel 60 F₂₅₄ 2.5 cm × 7.5 cm 250 μm or 5.0 cm × 10.0 cm 250 μm pre-coated silica gel plates. Preparative thin-layer chromatography was performed using EM Science silica gel 60 F₂₅₄ 20 cm × 20 cm 0.5 mm pre-coated plates with a 20 cm × 4 cm concentrating zone. Chromatography was performed using an ISCO SQ16 instrument with prepacked Redisep™ silica gel cartridges utilizing gradient elution. ¹H and ¹³C NMR spectra were recorded on Bruker models DPX400, DPX500 or DRX600 spectrometers at 400, 500 and 600 MHz respectively. Chemical shifts are reported in parts per million downfield from an internal standard (Me₄Si). IR spectra were collected in a Nicolet Avatar 360 FT-IR spectrometer. Melting points were obtained on either a MelTemp or Electrothermal apparatus and are uncorrected. Analytical reverse phase HPLC was performed on a Hewlett Packard Series 1100 instrument with an Agilent ZORBAX® Bonus RP, column utilizing an acetonitrile/water (0.05%TFA) gradient.

Characterization Data.

Trifluoro-methanesulfonic acid 2,5-dimethyl-2H-pyrazol-3-yl ester (5a). Yield:

1.32g, 62%; ¹H NMR (500 MHz, MeOH-d₄) δ 6.10 (s, 1H), 3.74 (s, 3H), 2.22 (s, 3H);

^{13}C NMR (125 MHz, CDCl_3) δ 148.0, 141.6, 118.8 (q, $J = 321.4$ Hz), 94.7, 34.8, 14.5; IR 1433, 1247, 1211, 1131, 866, 787, 636 cm^{-1} ; MS (ESI) exact mass calculated for $\text{C}_6\text{H}_7\text{F}_3\text{N}_2\text{O}_3\text{S}$, 244.01; found, m/z 245.3 $[\text{M}+\text{H}]^+$.

Trifluoro-methanesulfonic acid 5-methyl-2H-pyrazol-3-yl ester (5b). Yield: 0.54 g, 45 %; ^1H NMR (500 MHz, MeOH-d_4) δ 6.00 (s, 1H), 2.31 (s, 3H); ^{13}C NMR (125 MHz, CDCl_3) δ 153.3, 142.3, 118.9 (q, $J = 320.8$ Hz), 95.2, 11.6; IR 1426, 1246, 1208, 1134, 869 cm^{-1} ; MS (ESI) exact mass calculated for $\text{C}_5\text{H}_5\text{F}_3\text{N}_2\text{O}_3\text{S}$, 230.00; found, m/z 231.3 $[\text{M}+\text{H}]^+$.

Trifluoro-methanesulfonic acid 2-methyl-5-trifluoromethyl-2H-pyrazol-3-yl ester (5c). Yield: 0.62 g, 62%; ^1H NMR (500 MHz, MeOH-d_4) δ 6.72 (s, 1H), 3.92 (s, 3H); ^{13}C NMR (125 MHz, CDCl_3) δ 141.7, 141.2 (q, $J = 39.3$ Hz), 120.1 (q, $J = 268.7$ Hz), 118.5 (q, $J = 321.5$ Hz), 94.1, 35.8; IR 1216, 1128, 1097, 856, 602 cm^{-1} ; MS (ESI) exact mass calculated for $\text{C}_6\text{H}_4\text{F}_6\text{N}_2\text{O}_3\text{S}$, 297.98; found, m/z 299.3 $[\text{M}+\text{H}]^+$.

Trifluoro-methanesulfonic acid 5-methyl-2-phenyl-2H-pyrazol-3-yl ester (5d).¹ Yield: 1.83 g, 92 %; ^1H NMR (500 MHz, MeOH-d_4) δ 7.58-7.48 (m, 5H), 6.35 (s, 1H), 2.33 (s, 3H); ^{13}C NMR (125 MHz, CDCl_3) δ 149.3, 140.9, 136.9, 129.4, 128.4, 123.7, 118.5 (q, $J = 321.5$ Hz), 96.5, 14.5; IR 1434, 1212, 1130, 853, 758, 665 cm^{-1} ; MS (ESI) exact mass calculated for $\text{C}_{11}\text{H}_9\text{F}_3\text{N}_2\text{O}_3\text{S}$, 306.03; found, m/z 307.3 $[\text{M}+\text{H}]^+$.

Trifluoro-methanesulfonic acid 2-phenyl-5-trifluoromethyl-2H-pyrazol-3-yl ester (5e). Yield: 0.60 g, 60 %; ^1H NMR (500 MHz, MeOH-d_4) δ 7.63-7.57 (m, 5H), 6.98 (s, 1H); ^{13}C NMR (125 MHz, CDCl_3) δ 142.4 (q, $J = 40.3$ Hz), 141.3, 135.8, 129.8, 129.6, 124.2, 120.4 (q, $J = 269.4$ Hz), 118.6 (q, $J = 321.7$ Hz), 95.4; IR 1214, 1128, 845,

764, 647 cm^{-1} ; MS (ESI) exact mass calculated for $\text{C}_{11}\text{H}_6\text{F}_6\text{N}_2\text{O}_3\text{S}$, 360.00; found, m/z 361.3 $[\text{M}+\text{H}]^+$.

Trifluoro-methanesulfonic acid 2-methyl-4,5,6,7-tetrahydro-2H-indazol-3-yl ester

(5f). Yield: 0.88 g, 88%; ^1H NMR (400 MHz, MeOH-d_4) δ 3.71 (s, 3H), 2.57 (t, $J = 6.1\text{Hz}$, 2H), 2.47 (t, $J = 6.1\text{Hz}$, 2H), 1.83-1.70 (m, 4H); ^{13}C NMR (125 MHz, CDCl_3) δ 148.7, 137.0, 118.4 (q, $J = 320.5\text{ Hz}$), 105.2, 34.8, 23.6, 22.7, 22.5, 19.1; IR 1211, 1134, 887, 843, 814, cm^{-1} ; MS (ESI) exact mass calculated for $\text{C}_9\text{H}_{11}\text{F}_3\text{N}_2\text{O}_3\text{S}$, 284.04; found, m/z 285.3 $[\text{M}+\text{H}]^+$.

Trifluoro-methanesulfonic acid 2-phenyl-4,5,6,7-tetrahydro-2H-indazol-3-yl ester

(5g). Yield: 0.94g, 94%; ^1H NMR (500 MHz, MeOH-d_4) δ 7.57-7.52 (m, 2H), 7.51-7.45 (m, 3H), 2.71 (t, $J=6.3\text{ Hz}$, 2H), 2.61 (t, $J = 6.3\text{Hz}$, 2H), 1.92-1.86 (m, 2H), 1.85-1.80 (m, 2H); ^{13}C NMR (125 MHz, CDCl_3) δ 150.2, 137.1, 136.6, 129.2, 127.9, 123.6, 118.1 (q, $J= 321.7\text{ Hz}$), 107.2, 23.8, 22.7, 22.5, 19.4; IR 1428, 1238, 1211, 1134, 867, 839, 758, 603 cm^{-1} ; MS (ESI) exact mass calculated for $\text{C}_{14}\text{H}_{13}\text{F}_3\text{N}_2\text{O}_3\text{S}$, 346.06; found, m/z 347.3 $[\text{M}+\text{H}]^+$.

1,3-Dimethyl-5-phenyl-1H-pyrazole (6a).² Yield: 0.143g, 83%; ^1H NMR (500 MHz, MeOH-d_4) δ 7.50-7.41 (m, 5H), 6.14 (s, 1H), 3.78 (s, 3H), 2.25 (s, 3H); ^{13}C NMR (125 MHz, CDCl_3) δ 147.5, 144.3, 130.9, 128.6, 128.5, 128.2, 105.5, 37.0, 13.4; IR 1469, 775, 755, 698 cm^{-1} ; MS (ESI) exact mass calculated for $\text{C}_{11}\text{H}_{12}\text{N}_2$, 172.10; found, m/z 173.4 $[\text{M}+\text{H}]^+$.

3-Methyl-5-phenyl-1H-pyrazole (6b).³ Yield: 0.127 g, 81%; ^1H NMR (500 MHz, MeOH-d_4) δ 7.71 (bs, 2H), 7.38 (t, $J = 7.4\text{ Hz}$, 2H), 7.32-7.27 (m, 1H), 6.40 (s, 1H), 2.32 (s, 3H); ^{13}C NMR (125 MHz, CDCl_3) δ 133.8, 131.4, 128.8, 128.3, 127.6, 125.8, 102.6,

11.8; IR 1334, 1306, 762, 689 cm^{-1} ; MS (ESI) exact mass calculated for $\text{C}_{10}\text{H}_{10}\text{N}_2$, 158.08; found, m/z 159.4 $[\text{M}+\text{H}]^+$.

1-Methyl-5-phenyl-3-trifluoromethyl-1H-pyrazole (6c). Yield: 0.179 g, 79 %; ^1H NMR (400 MHz, CDCl_3) δ 7.52-7.46 (m, 3H), 7.43-7.40 (m, 2H), 6.56 (s, 1H), 3.92 (s, 3H); ^{13}C NMR (125 MHz, CDCl_3) δ 145.3, 141.7 (q, $J = 37.9$ Hz), 129.5, 129.5, 129.1, 129.0, 121.6 (q, $J = 268.5$ Hz), 104.5, 38.2; IR 1173, 1142, 1111, 974, 701 cm^{-1} ; MS (ESI) exact mass calculated for $\text{C}_{11}\text{H}_9\text{F}_3\text{N}_2$, 226.07; found, m/z 227.4 $[\text{M}+\text{H}]^+$.

3-Methyl-1,5-diphenyl-1H-pyrazole (6d).⁴⁵ Yield: 0.189 g, 81%; ^1H NMR (500 MHz, MeOH-d_4) δ 7.40-7.34 (m, 3H), 7.31-7.27 (m, 3H), 7.26-7.19 (m, 4H), 6.41 (s, 1H); 2.35 (s, 3H); ^{13}C NMR (125 MHz, CDCl_3) δ 149.6, 143.9, 140.4, 130.9, 129.0, 128.8, 128.6, 128.2, 127.3, 125.3, 107.9, 13.8; IR 1504, 759, 693 cm^{-1} ; MS (ESI) exact mass calculated for $\text{C}_{16}\text{H}_{14}\text{N}_2$, 234.12; found, m/z 235.4 $[\text{M}+\text{H}]^+$.

1,5-Diphenyl-3-trifluoromethyl-1H-pyrazole (6e).⁶ Yield: 0.212 g, 74%; ^1H NMR (500 MHz, MeOH-d_4) δ 7.46-7.42 (m, 3H), 7.39-7.31 (m, 5H), 7.29-7.26 (m, 2H), 6.93 (s, 1H); ^{13}C NMR (125 MHz, CDCl_3) δ 144.9, 143.6 (t, $J = 38.5$ Hz), 139.5, 129.4, 129.3, 129.2, 129.0, 128.9, 128.6, 125.7, 121.5 (q, $J = 269.4$ Hz), 105.8; IR 1234, 1168, 1120, 1099, 977, 762, 694 cm^{-1} ; MS (ESI) exact mass calculated for $\text{C}_{16}\text{H}_{11}\text{F}_3\text{N}_2$, 288.09; found, m/z 289.4 $[\text{M}+\text{H}]^+$.

2-Methyl-3-phenyl-4,5,6,7-tetrahydro-2H-indazole (6f). Yield: 0.150 g, 71%; ^1H NMR (500 MHz, MeOH-d_4) δ 7.50 (t, $J = 8.2$ Hz, 2H), 7.43 (t, $J = 7.4$ Hz, 2H), 7.38 (d, $J = 8.2$ Hz, 1H), 3.73 (s, 3H), 2.65 (t, $J = 6.3$ Hz, 2H), 2.47 (t, $J = 6.3$ Hz, 2H), 1.88-1.83 (m, 2H), 1.78-1.72 (m, 2H); ^{13}C NMR (CDCl_3 , 100 MHz) δ 148.4, 139.6, 130.9, 129.3,

128.8, 128.2, 114.9, 37.2, 23.8, 23.6, 23.6, 21.4; IR 1489, 1372, 766, 702 cm^{-1} ; MS (ESI) exact mass calculated for $\text{C}_{14}\text{H}_{16}\text{N}_2$, 212.13; found, m/z 213.4 $[\text{M}+\text{H}]^+$.

2,3-Diphenyl-4,5,6,7-tetrahydro-2H-indazole (6g).⁷ Yield: 0.202g, 74%; ^1H NMR (500 MHz, MeOH-d_4) δ 7.35-7.28 (m, 5H), 7.22-7.14 (m, 4H), 6.81-6.74 (m, 1H), 2.76 (t, $J = 6.3$ Hz, 2H), 2.60 (t, $J = 6.3$ Hz, 2H), 1.95-1.90 (m, 2H), 1.84-1.80 (m, 2H); ^{13}C NMR (125 MHz, CDCl_3) δ 150.5, 140.6, 138.6, 131.0, 129.4, 128.9, 128.5, 127.9, 126.7, 124.9, 117.0, 23.7, 23.7, 23.5, 21.7; IR 1592, 1503, 1363, 762, 754, 692 cm^{-1} ; MS (ESI) exact mass calculated for $\text{C}_{19}\text{H}_{18}\text{N}_2$, 274.15; found, m/z 275.4 $[\text{M}+\text{H}]^+$.

5-(4-Fluoro-phenyl)-1,3-dimethyl-1H-pyrazole (6h). Yield: 0.1085 g, 85%; ^1H NMR (600 MHz, CDCl_3) δ 7.37-7.33 (m, 2H), 7.15-7.10 (m, 2H), 6.05 (s, 1H), 3.78 (s, 3H), 2.28 (s, 3H); ^{13}C NMR (150 MHz, CDCl_3) δ 162.6 (d, $J = 248.9$ Hz), 147.6, 144.3, 130.4, (d, $J = 8.0$ Hz), 126.9 (d, $J = 3.4$ Hz), 115.5, (d, $J = 21$ Hz), 105.6, 36.9, 13.4; IR 1503, 1219, 1157, 1002, 838, 821, 636 cm^{-1} ; MS (ESI) exact mass calculated for $\text{C}_{11}\text{H}_{11}\text{FN}_2$, 190.22; found, m/z 191.4 $[\text{M}+\text{H}]^+$.

5-(4-Methoxy-phenyl)-1,3-dimethyl-1H-pyrazole (6i).⁸ Yield: 0.181 g, 90 %; ^1H NMR (500 MHz, CDCl_3) δ 7.33 (d, $J = 8.8$ Hz, 2H), 6.98 (d, $J = 8.8$ Hz, 2H), 6.04 (s, 1H), 3.86 (s, 3H), 3.78 (s, 3H), 2.30 (s, 3H); ^{13}C NMR (125 MHz, CDCl_3) δ 159.8, 147.7, 144.4, 130.1, 123.6, 114.2, 105.4, 55.5, 37.1, 13.6; IR 1504, 1245, 1172, 1035, 835, 822, 795 cm^{-1} ; MS (ESI) exact mass calculated for $\text{C}_{12}\text{H}_{14}\text{N}_2\text{O}$, 202.11; found, m/z 203.4 $[\text{M}+\text{H}]^+$.

1,3-Dimethyl-5-o-tolyl-1H-pyrazole (6j). Yield: 0.147 g, 79 %; ^1H NMR (500 MHz, CDCl_3) δ 7.33-7.26 (m, 2H), 7.24-7.21 (m, 1H), 7.19-7.16 (m, 1H), 5.96 (s, 1H), 3.57 (s, 3H), 2.30 (s, 3H), 2.17 (s, 3H); ^{13}C NMR (125 MHz, CDCl_3) δ 147.6, 143.4, 137.6,

130.9, 130.3, 129.0, 125.8, 106.1, 36.3, 19.9, 13.6; IR 1493, 770, 750, 725 cm^{-1} ; MS (ESI) exact mass calculated for $\text{C}_{12}\text{H}_{14}\text{N}_2$ 186.12, found, m/z 187.4 $[\text{M}+\text{H}]^+$.

1-[4-(2,5-Dimethyl-2H-pyrazol-3-yl)-phenyl]-ethanone (6k). Yield: 0.151g, 71%; ^1H NMR (500 MHz, CDCl_3) δ 8.04 (d, $J = 8.5$ Hz, 2H), 7.52 (d, $J = 8.5$ Hz, 2H), 6.17 (s, 1H), 3.86 (s, 3H), 2.65 (s, 3H), 2.31 (s, 3H); ^{13}C NMR (125 MHz, CDCl_3) δ 197.6, 148.1, 143.4, 136.8, 135.6, 128.9, 128.8, 106.4, 37.6, 26.8, 13.6; IR 1687, 1607, 1355, 1264, 1001, 839, 816 cm^{-1} ; MS (ESI) exact mass calculated for $\text{C}_{13}\text{H}_{14}\text{N}_2\text{O}$, 214.11; found, m/z 215.4 $[\text{M}+\text{H}]^+$.

5-(4-Methoxy-phenyl)-3-methyl-1-phenyl-1H-pyrazole (6l).² Yield: 0.101 g, 76%; ^1H NMR (500 MHz, CDCl_3) δ 7.34-7.25 (m, 5H), 7.14 (d, $J = 9.0$ Hz, 2H), 6.81 (d, $J = 9.0$ Hz, 2H), 6.25 (s, 1H), 3.80 (s, 3H), 2.38 (s, 3H); ^{13}C NMR (125 MHz, CDCl_3) δ 159.6, 149.6, 143.8, 140.5, 130.1, 129.0, 127.2, 125.4, 114.1, 107.4, 55.4, 13.8; IR 1509, 1499, 1247, 1177, 1032, 834, 792, 762, 694 cm^{-1} ; MS (ESI) exact mass calculated for $\text{C}_{17}\text{H}_{16}\text{N}_2\text{O}$ 264.13, found, m/z 265.5 $[\text{M}+\text{H}]^+$.

3-Methyl-1-phenyl-5-o-tolyl-1H-pyrazole (6m). Yield: 0.229g, 92%; ^1H NMR (500 MHz, CDCl_3) δ 7.29-7.16 (m, 9H), 6.21 (s, 1H), 2.42 (s, 3H), 2.01 (s, 3H); ^{13}C NMR (125 MHz, CDCl_3) δ 149.4, 143.1, 140.5, 137.2, 131.3, 130.7, 130.5, 128.9, 128.9, 126.6, 125.9, 123.7, 108.9, 20.1, 13.9; IR 1503, 1493, 1361, 782, 766, 755, 687 cm^{-1} ; MS (ESI) exact mass calculated for $\text{C}_{17}\text{H}_{16}\text{N}_2$, 248.13, found, m/z 249.4 $[\text{M}+\text{H}]^+$.

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19601-102 Solvent: CDCl3
Purified, colorless liquid
proton.prd CDCl3 d: DRudolph 64

19601-102 Solvent: CDCl3
Purified, colorless oil
c13cpd.prd CDCl3 d: DRudolph 2

Current Data Parameters
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PROCNO 1

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***** CHANNEL f2 *****
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F2P -20.021 ppm
F2 -2517.99 Hz
PPMCM 12.50213 ppm/cm
HZCM 1572.33069 Hz/cm

S10 1112
after chrom 3.3

1.0

S10

570-27a
after chrom,
colorless oil.

570-90a
after chrom

after chrom

after chrom
C13CPD CDC13 d: SMe 5

570-21b

→ referenced
as
T1.23
& peaks shifted
accordingly

Current Data Parameters
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PROCNO 1

F2 - Acquisition Parameters
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***** CHANNEL f1 *****
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PL1 0.00 dB
SFO1 125.7773176 MHz

***** CHANNEL f2 *****
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PL2 0.00 dB
PL12 16.23 dB
PL13 120.00 dB
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F3 - Processing parameters
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F2P 1532.00 Hz
F2 1532.00 Hz
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570-40-2c
after
chrom

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570-119b

570-10212
after chrom

570-101
after chrom

570-106 a
after chrom

570-106 b
after chrom

570-104a
after chrom