Differential Tuning of the Electron Transfer Parameters in 1,3,5-Triarylpyrazolines: A Rational Design Approach for Optimizing the Contrast Ratio of Fluorescent Probes

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Supporting Information

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Materials and Reagents. 2-Fluorophenylhydrazine hydrochloride**,** 3-fluorophenylhydrazine hydrochloride, 4-fluorophenylhydrazine hydrochloride**,** 2,4-difluorophenylhydrazine**,** 2,5-difluorophenylhydrazine, 2,3,5,6-tetrafluorophenylhydrazine, pentafluorophenylhydrazine (Oakwood Products); *trans*-chalcone, 3,5-difluorophenylhydrazine hydrochloride **(**Aldrich**)**. The chalcone 3-(4-dimethylamino-phenyl)-1-phenyl-propenone was synthesized according to a published procedure.[1] NMR: δ in ppm vs $SiMe_4$ (0 ppm, ^1H, 400 MHz). MS: selected peaks; m/z. Melting points are uncorrected. Flash chromatography (FC): Merck silica gel (70-230 mesh). TLC: 0.25 mm, Merck silica gel 60 F_{254}, visualizing at 254 nm or with 2% $KMnO_4$ solution.

General Synthetic Procedure.[2] All pyrazoline derivatives **1-4** were synthesized according to the following procedure: A solution of the corresponding phenylhydrazine derivative (1 mmol), chalcone (0.33 mmol), and 98% sulfuric acid (0.5 mmol) in 2.0 mL absolute ethanol was heated at reflux temperature for 8 hours. The reaction mixture was neutralized with saturated aq. $NaHCO_3$ and extracted twice with ethyl acetate. The combined organic phase was dried with anhydrous $MgSO_4$ and concentrated. The crude product was purified by flash chromatography and analytical purity was verified by reversed-phase HPLC (Varian ProStar system with UV detector, acetonitrile-water, gradient 20% –> 2% water).

1,3,5-Triphenyl-4,5-dihydro-1*H*-pyrazole (1a): Yield: 91 %. M.p. 140-141 °C. *Rf* 0.49 (3:1 hexanes:EtOAc). ^1H NMR ($CDCl_3$, 400 MHz) δ 3.14 (dd, *J* = 17.0, 7.1 Hz, 1H), 3.84 (dd, *J* = 17.0, 12.6 Hz, 1H), 5.27 (dd, *J* = 12.6, 7.1 Hz, 1H), 6.78 (tt, *J* = 7.1, 1.1 Hz, 1H), 7.07 (d, *J* = 8.8, 2H), 7.15-7.20 (m, 2H), 7.25-7.40 (m, 8H), 7.71-7.73 (m, 2H). ^{13}C NMR ($CDCl_3$ 100 MHz) δ 43.7, 64.5, 113.3, 119.0, 125.6, 125.7, 127.4, 128.4, 128.5, 128.8, 129.0, 132.6, 142.4, 144.7, 146.5. MS (70 eV) 298 (M^+, 42), 296.1 (100). EI HRMS *m/z* calcd for $[M]^+$ $C_{21}H_{18}N_2$ 298.1470, found 298.1444.

1-(2-Fluoro-phenyl)-3,5-diphenyl-4,5-dihydro-1*H*-pyrazole (1b): Yield: 91%. M.p. 134-136 ºC. *Rf* 0.83 (5:1 hexane:EtOAc). ^1H-NMR ($CDCl_3$, 400 MHz) δ 3.25 (dd, *J* = 16.8, 4.4 Hz, 1H), 3.74 (dd, *J* = 16.8, 11.8 Hz, 1H), 5.63 (ddd, *J* = 11.8, 7.9, 4.0 Hz, 1H), 6.71-6.76 (m, 1H), 6.83 (dd, *J* = 12.9, 7.8 Hz, 1H), 6.98 (t, *J* = 7.6 Hz, 1H), 7.11-7.20 (m, 5H), 7.29-7.39 (m, 3H), 7.61 (t, *J* = 8.4 Hz, 1H), 7.74 (d, *J* = 7.1 Hz, 2H). ^{13}C NMR ($CDCl_3$ 100 MHz) δ 43.0, 66.3 (d, J_{CF} = 7.5 Hz), 116.0 (d, J_{CF} = 20.3 Hz), 119.9 (d, J_{CF} = 3.4 Hz), 121.4 (d, J_{CF} = 7.5 Hz), 124.4 (d, J_{CF} = 3.1 Hz), 126.0, 126.1, 127.6, 128.59, 128.64, 128.8, 132.7, 133.2 (d, J_{CF} = 9.2 Hz), 142.0, 148.2, 151.2 (d, J_{CF} = 243.5 Hz). MS (70 eV) 316.1 (M^+, 100), 239 (50), 109 (65). EI-HRMS *m/e* calculated for $[M]^+$ $C_{21}H_{17}FN_2$ 316.1376, found 316.1375.

1-(3-Fluoro-phenyl)-3,5-diphenyl-4,5-dihydro-1*H*-pyrazole (1c): Yield: 90%. M.p. 123-125 ºC. *Rf* 0.72 (5:1 hexanes:EtOAc). ^1H-NMR ($CDCl_3$, 400 MHz) δ 3.12 (dd, *J* = 17.0, 6.6 Hz, 1H), 3.80 (dd, *J* = 17.0, 12.1 Hz, 1H), 5.20 (dd, *J* = 12.1, 6.6 Hz, 1H), 6.44 (dt, *J* = 8.2, 2.5 Hz, 1H), 6.69 (dd, *J* = 8.2, 2.2 Hz, 1H), 6.87 (td, *J* = 11.9, 2.3 Hz, 1H), 7.05 (dt, *J* = 8.2, 6.7 Hz, 1H), 7.22-7.38 (m, 8H), 7.70 (td, *J* = 7.1, 1.7 Hz, 2H). ^{13}C NMR ($CDCl_3$) δ 43.7, 64.4, 100.7 (d, J_{CF} = 26.9 Hz), 105.5 (d, J_{CF} = 21.9 Hz), 108.7 (d, J_{CF} = 2.3 Hz), 125.8, 125.9, 127.8, 128.6, 128.9, 129.3, 129.9 (d, J_{CF} = 9.9 Hz), 132.4, 142.1, 146.3 (d, J_{CF} = 10.9 Hz), 147.5, 163.7 (d, J_{CF} = 242.6 Hz). MS (70 eV) 316.1 (M^+, 100), 239 (45), 109 (40). EI-HRMS *m/e* calculated for $[M]^+$ $C_{21}H_{17}FN_2$ 316.1376, found 316.1363.

1-(4-Fluoro-phenyl)-3,5-diphenyl-4,5-dihydro-1*H*-pyrazole (1d): Yield: 30%. M.p. 112-114 ºC. *Rf* 0.71 (5:1 hexane:EtOAc). ^1H-NMR ($CDCl_3$, 400 MHz) δ 3.11 (dd, *J* = 17.0, 7.8 Hz, 1H), 3.79 (dd, *J* = 17.0, 12.3 Hz, 1H), 5.16 (dd, *J* = 12.3, 7.8 Hz, 1H), 6.85 (t, *J* = 8.5 Hz, 2H), 6.97-7.00 (m, 2H), 7.25-7.38 (m, 8H), 7.69 (d, *J* = 7.7 Hz, 2H). ^{13}C NMR ($CDCl_3$ 100 MHz) δ 43.7, 65.2, 114.4 (d, J_{CF} = 7.5 Hz), 115.3 (d, J_{CF} = 28.2 Hz), 125.7, 125.9, 127.7, 128.5, 128.6, 129.2,

132.6, 141.6 (d J_{CF} = 2.1 Hz), 142.3, 146.9, 156.7 (d, J_{CF} = 237.3 Hz). MS (70 eV) 316.1 (M^+, 100), 239.1 (45), 109 (60). EI-HRMS *m/e* calculated for $[M]^+$ $C_{21}H_{17}FN_2$ 316.1376, found 316.1359.

1-(2,4-Difluoro-phenyl)-3,5-diphenyl-4,5-dihydro-1*H*-pyrazole (1e): Yield: 96%. M.p. 125-127 ºC. *Rf* 0.66 (5:1 hexanes:EtOAc). ^{1}H-NMR ($CDCl_3$, 400 MHz) δ 3.30 (dd, *J* = 16.9, 4.9 Hz, 1H), 3.75 (dd, *J* = 16.9, 11.5 Hz, 1H), 5.56 (ddd, *J* = 11.5, 4.9, 3.4 Hz, 1H), 6.62 (ddd, *J* = 12.1, 8.5, 2.8 Hz, 1H), 6.72 (ddt, *J* = 7.8, 2.8, 1.3 Hz, 1H), 7.18-7.24 (m, 5H), 7.35-7.44 (m, 3H), 7.50 (dt, *J* = 9.2, 6.0 Hz, 1H), 7.77 (dd, *J* = 8.2 Hz, 1.7 Hz, 2H). ^{13}C NMR ($CDCl_3$ 100 MHz) δ 42.9, 66.7 (d, J_{CF} = 6.5 Hz), 104.2 (dd, J_{CF} = 26.5, 24.3 Hz), 111.0 (dd, J_{CF} = 21.9, 3.6 Hz), 120.9 (dd, J_{CF} = 9.0, 4.6 Hz), 126.0, 126.3, 127.8, 128.6, 128.7, 128.9, 130.0 (dd, J_{CF} = 9.8, 3.2 Hz), 132.6, 141.4, 148.8, 151.5 (dd, J_{CF} = 247.9, 12.0 Hz), 157.5 (dd, J_{CF} = 242.1, 11.0 Hz). MS (70 eV) 334 (M^+, 100), 257 (42), 127 (70). EI-HRMS *m/e* calculated for $[M]^+$ $C_{21}H_{16}F_2N_2$ 334.1282, found 334.1276.

1-(2,5-Difluoro-phenyl)-3,5-diphenyl-4,5-dihydro-1*H*-pyrazole (1f): Yield: 80%. M.p. 179-181 ºC. *Rf* 0.45 (3:1 hexanes:EtOAc). ^{1}H-NMR ($CDCl_3$, 400 MHz) δ 3.27 (dd, *J* = 17.0, 3.8 Hz, 1H), 3.78 (dd, *J* = 17.0, 11.8, 1H), 5.68 (ddd, *J* = 11.8, 3.8, 3.8 Hz, 1H), 6.36-6.42 (m, 1H), 6.75 (ddd, *J* = 13.9, 8.9, 5.1 Hz, 1H), 7.14-7.23 (m, 5H), 7.33-7.43 (m, 4H), 7.35 (dd, *J* = 8.2, 1.7 Hz, 2H). ^{13}C NMR ($CDCl_3$ 100 MHz) δ 43.2, 65.8 (d, J_{CF} = 8.4 Hz), 106.1 (dd, J_{CF} = 28.7, 4.1 Hz), 106.7 (dd, J_{CF} = 24.5, 7.7 Hz), 116.5 (dd, J_{CF} = 23.2, 10.2 Hz), 125.9, 126.1, 127.7, 128.6, 128.7 129.2, 132.2, 134.2 (t, J_{CF} = 11.1 Hz), 141.8, 146.7 (dd, J_{CF} = 238.6, 2.7 Hz), 149.0, 159.2 (dd, J_{CF} = 239.9, 1.8 Hz). MS (70 eV) 334.1 (M^+, 100), 127 (40). EI-HRMS *m/e* calculated for $[M]^+$ $C_{21}H_{16}F_2N_2$ 334.1282, found 334.1287.

1-(3,5-Difluoro-phenyl)-3,5-diphenyl-4,5-dihydro-1*H*-pyrazole (1g): Yield: 79%. M.p. 139-140 ºC. *Rf* 0.68 (5:1 hexanes:EtOAc). ^{1}H-NMR ($CDCl_3$, 400 MHz) δ 3.13 (dd, *J* = 17.3 Hz, 6.6 Hz, 1H), 3.82 (dd, *J* = 17.3 Hz, 12.3 Hz, 1H), 5.17 (dd, *J* = 12.3 Hz, 6.6 Hz, 1H), 6.17 (tt, *J* = 9.1 Hz, 2.3 Hz, 1H), 6.52-6.55 (m, 2H), 7.23-7.28 (m, 3H), 7.31-7.40 (m, 5H), 7.69 (dd, *J* = 8.2 Hz, 1.6 Hz, 2H). ^{13}C NMR ($CDCl_3$ 100 MHz) δ 43.8, 64.2, 93.8 (t, J_{CF} = 26.4 Hz), 96.3 (dd, J_{CF} = 20.9, 9.2 Hz), 125.7, 126.0, 128.0, 128.6, 129.2, 129.4, 132.1, 141.6, 146.6 (t, J_{CF} = 13.7 Hz), 148.4, 163.7 (dd, J_{CF} = 243.5, 15.5 Hz). MS (70 eV) 334.1 (M^+, 100), 257.1 (35). EI-HRMS *m/e* calculated for $[M]^+$ $C_{21}H_{16}F_2N_2$ 334.1282, found 334.1282.

3,5-Diphenyl-1-(2,4,5-trifluoro-phenyl)-4,5-dihydro-1*H*-pyrazole (1h): Yield: 65%. M.p. 134-136 °C. *Rf* 0.35 (10:1 hexanes:EtOAc). ^{1}H NMR ($CDCl_3$, 400 MHz) δ 3.30 (dd, *J* = 17.0, 4.1 Hz, 1H), 3.76 (dd, *J* = 17.0, 11.7 Hz, 1H), 5.57 (ddd, *J* = 11.7, 4.0, 4.0 Hz, 1H), 6.69 (ddd, *J* = 11.6, 10.1, 7.1 Hz, 1H), 7.12-7.23 (m, 5H), 7.34-7.42 (m, 3H), 7.47 (dt, *J* = 12.3, 8.1 Hz, 1H), 7.72-7.75 (m, 2H). ^{13}C NMR ($CDCl_3$ 100 MHz) δ 43.0, 66.0 (d, J_{CF} = 7.4 Hz), 105.6 (ddd, J_{CF} = 25.9, 21.4, 1.1 Hz), 107.7 (dd, J_{CF} = 23.4, 4.8 Hz), 126.0, 127.8, 128.6, 128.7, 129.2, 129.9 (ddd, J_{CF} = 11.3, 7.8, 3.3 Hz), 132.1, 141.2, 143.6 (ddd, J_{CF} = 243.5, 14.5, 11.4 Hz), 145.4 (ddd, J_{CF} = 242.8, 8.6, 2.5 Hz), 146.6 (ddd, J_{CF} = 242.5, 12.9, 3.1 Hz), 149.4. MS (70 eV) 352.1 (M^+, 100), 275 (14), 206 (16), 145 (17). EI HRMS *m/e* calcd for $[M]^+$ $C_{21}H_{15}F_3N_2$ 352.1187, found 352.1184.

3,5-Diphenyl-1-(2,3,5,6-tetrafluoro-phenyl)-4,5-dihydro-1*H*-pyrazole (1i): Yield: 73%. M.p. 150-151 ºC. *Rf* 0.80 (3:1 hexanes:EtOAc). ^{1}H-NMR ($CDCl_3$, 400 MHz) δ 3.30 (dd, *J* = 17.0, 7.3 Hz, 1H), 3.76 (dd, *J* = 17.0, 11.7 Hz, 1H), 5.52 (dd, *J* = 11.7, 7.3 Hz, 1H), 6.62 (tt, *J* = 9.8, 7.0 Hz, 1H), 7.20-7.30 (m, 5H), 7.35-7.42 (m, 3H), 7.70-7.73 (m, 2H). ^{13}C NMR ($CDCl_3$ 100 MHz) δ 42.6, 67.4 (t, J_{CF} = 3.5 Hz), 99.9 (t, J_{CF} = 23.1 Hz), 124.9 (tt, J_{CF} = 10.5, 2.0 Hz), 126.0, 126.5, 128.3, 128.6, 128.9, 129.2, 132.1, 140.6, 141.3 (ddt, J_{CF} = 248.7, 14.7, 4.0 Hz), 146.3 (dtd, J_{CF} = 246.2, 12.9, 3.8 Hz), 149.6. MS (70 eV) 370.1 (M^+, 100), 163 (38). EI-HRMS *m/e* calculated for $[M]^+$ $C_{21}H_{14}F_4N_2$ 370.1093, found 370.1105.

1-Pentafluorophenyl-3,5-diphenyl-4,5-dihydro-1*H*-pyrazole (1j): Yield: 70%. M.p. 164-165 ºC. *Rf* 0.43 (4:1 hexanes:EtOAc). ^{1}H-NMR ($CDCl_3$, 400 MHz) δ 3.29 (dd, *J* = 16.9, 8.4 Hz, 1H), 3.73 (dd, *J* = 16.9.0, 11.5 Hz, 1H), 5.37 (dd, *J* = 11.5, 8.4 Hz, 1H), 7.23-7.31 (m, 5H), 7.35-7.40 (m, 3H), 7.68-7.71 (m, 2H). ^{13}C NMR ($CDCl_3$ 100 MHz) δ 42.8, 68.2 (t, *J* = 2.8 Hz), 120.3 (m, CF), 125.8, 126.5, 128.3, 128.5, 128.8, 129.1, 131.8, 137.8 (ddt, *J* = 244.1, 12.1, 3.1 Hz), 138.0 (ddd, *J* = 238.1, 7.6, 3.1 Hz), 139.9, 142.6 (dtd, *J* = 250.2, 12.1, 3.1 Hz), 150.1. MS (70 eV) 388.1 (M^+, 100), 181 (60). EI-HRMS *m/e* calculated for $[M]^+$ $C_{21}H_{13}F_5N_2$ 388.0999, found 388.1015.

4-(1,5-Diphenyl-4,5-dihydro-1*H*-pyrazol-3-yl)benzonitrile (2a): Yield: 76% M.p. 145-146 °C. *Rf* 0.50 (5:1 hexanes:EtOAc). ^{1}H NMR ($CDCl_3$, 400 MHz) δ 3.13 (dd, *J* = 17.0, 7.1 Hz, 1H), 3.83 (dd, *J* = 17.0, 12.7, 1H), 5.38 (dd, *J* = 12.7, 7.1 Hz, 1H), 6.83 (t, *J* = 7.3 Hz, 1H), 7.08 (dd, *J* = 8.8, 1.0 Hz, 2H), 7.18-7.22 (m, 2H), 7.25-7.36 (m, 5H), 7.64 (d, *J* = 8.6 Hz, 2H), 7.73 (d, *J* = 8.6 Hz, 2H). ^{13}C NMR ($CDCl_3$, 100 MHz) δ 42.8, 64.7, 111.0, 113.6, 118.9, 120.0, 125.67, 125.74, 127.8, 129.0, 129.2, 132.2, 137.0, 141.8, 143.7, 144.2; MS (70 eV) 323 (M^+, 100), 246 (48) 91 (35). EI HRMS *m/e* calcd for $[M]^+$ $C_{22}H_{17}N_3$ 323.1422, found 323.1420.

4-(1-(2-Fluorophenyl)-4,5-dihydro-5-phenyl-1H-pyrazol-3-yl)benzonitrile (2b): Yield: 80%. M.p. 139-141 ºC. *Rf* 0.40 (3:1 hexanes:EtOAc). ^{1}H-NMR ($CDCl_3$, 400 MHz) δ 3.22 (dd, *J* = 16.9 Hz, 4.7 Hz, 1H), 3.73 (dd, *J* = 16.9, 12.1 Hz, 1H), 5.70 (ddd, *J* = 12.1, 4.7, 3.4 Hz, 1H), 6.76-6.89 (m, 2H), 7.00 (dt, *J* = 8.4 Hz, 1.6 Hz, 1H), 7.13-7.23 (m, 5H), 7.58 (dt, *J* = 8.4 Hz, 1.5 Hz, 1H), 7.62 (d, *J* = 8.5 Hz, 2H), 7.76 (d, *J* = 8.5 Hz, 2H). ^{13}C NMR ($CDCl_3$, 100 MHz) δ 42.3, 66.5 (d, J_{CF} = 7.6 Hz), 111.1, 116.0 (d, J_{CF} = 20.5 Hz), 118.7, 119.8 (d, J_{CF} = 3.0 Hz), 122.1 (d, J_{CF} = 7.5 Hz), 124.2 (d, J_{CF} = 3.2 Hz), 125.8, 127.6, 128.5, 131.9 (d, J_{CF} = 9.0 Hz), 132.1, 136.6, 141.1, 145.5, 150.0 (d, J_{CF} = 243.9 Hz). MS (70 eV) 341.1 (M^+, 100), 264.1 (50), 109 (48). EI-HRMS *m/e* calculated for $[M]^+$ $C_{22}H_{16}FN_3$ 341.1328, found 341.1338.

4-[1-(3-Fluoro-phenyl)-5-phenyl-4,5-dihydro-1H-pyrazol-3-yl]-benzonitrile (2c): Yield: 87%. M.p. 189-191 ºC. *Rf* 0.40 (3:1 hexanes:EtOAc). ^{1}H-NMR ($CDCl_3$, 400 MHz) δ 3.15 (dd, *J* = 17.2, 6.8 Hz, 1H), 3.86 (dd, *J* = 17.2, 12.6 Hz, 1H), 5.36 (dd, *J* = 12.6, 6.8 Hz, 1H), 6.51 (dt, *J* = 8.2, 2.2 Hz, 1H), 6.73 (dd, *J* = 8.2, 2.2 Hz, 1H), 6.89 (td, *J* = 11.5, 2.2 Hz, 1H), 7.10 (dd, *J* = 14.9, 8.2 Hz, 1H), 7.28-7.31 (m, 3H), 7.36 (t, *J* = 7.1 Hz, 2H), 7.66 (d, *J* = 8.2 Hz, 2H), 7.78 (d, *J* = 8.2 Hz, 2H). ^{13}C NMR ($CDCl_3$ 100 MHz) δ 43.0, 64.6, 101.0 (d, J_{CF} = 26.9 Hz), 106.3 (d, J_{CF} = 21.5 Hz), 108.9 (d, J_{CF} = 2.3 Hz), 111.3, 118.7, 125.5, 125.8, 127.9, 129.2, 130.0 (d, J_{CF} = 9.9 Hz), 132.1, 136.5, 141.1, 145.0, 145.1 (d, J_{CF} = 10.9 Hz), 163.3 (d, J_{CF} = 242.6 Hz). MS (70 eV) 341 (M^+, 100), 264 (40), 109 (40). EI-HRMS *m/e* calculated for $[M]^+$ $C_{22}H_{16}FN_3$ 341.1328, found 341.1318.

4-[1-(4-Fluoro-phenyl)-5-phenyl-4,5-dihydro-1*H*-pyrazol-3-yl]-benzonitrile (2d). Yield: 80%. M.p. 144-146 ºC. *Rf* 0.40 (3:1 hexanes:EtOAc). ^{1}H-NMR ($CDCl_3$, 400 MHz) δ 3.14 (dd, *J* = 17.0, 7.7 Hz, 1H), 3.84 (dd, *J* = 17.0, 12.1 Hz, 1H), 5.33 (dd, *J* = 12.1, 7.7 Hz, 1H), 6.89 (dd, *J* = 9.2, 8.4 Hz, 2H), 7.01 (dd, *J* = 9.2, 4.7 Hz, 2H), 7.27-7.38 (m, 5H), 7.64 (d, *J* = 8.6 Hz, 2H), 7.76 (d, *J* = 8.6 Hz, 2H). ^{13}C NMR ($CDCl_3$ 100 MHz) δ 43.0, 65.3, 111.0, 114.6 (d, J_{CF} = 7.5 Hz), 115.4 (d, J_{CF} = 22.3 Hz), 118.8, 125.6, 127.8, 129.2, 132.1, 136.7, 140.2 (d, J_{CF} = 2.0 Hz), 141.3, 144.2, 157.0 (d, J_{CF} = 238.1 Hz). MS (70 eV) 341.1 (M^+, 100), 264.1 (50), 109 (48). EI-HRMS *m/e* calculated for $[M]^+$ $C_{22}H_{16}FN_3$ 341.1328, found 341.1338.

4-[1-(2,4-Difluoro-phenyl)-5-phenyl-4,5-dihydro-1*H*-pyrazol-3-yl]-benzonitrile (2e): Yield: 76%. M.p. 179-181 ºC. *Rf* 0.44 (3:1 hexanes:EtOAc). ^{1}H-NMR ($CDCl_3$, 400 MHz) δ 3.29 (dd, *J* = 17.0, 5.5 Hz, 1H), 3.77 (dd, *J* = 17.0, 12.1 Hz, 1H), 5.63 (ddd, *J* = 12.1, 5.5, 3.3 Hz, 1H), 6.67 (ddd, *J* = 12.1, 8.2, 2.7 Hz, 1H), 6.76 (ddt, *J* = 7.7, 2.7, 1.3 Hz, 1H), 7.15-7.24 (m, 5H), 7.48

(dt, J = 9.2, 5.9 Hz, 1H), 7.67 (d, J = 8.6 Hz, 2H), 7.80 (d, J = 8.6 Hz, 2H). ^{13}C NMR ($CDCl_3$ 100 MHz) δ 42.3, 67.1 (d, J_{CF} = 6.3 Hz), 104.3 (dd, J_{CF} = 26.2, 24.4 Hz), 111.1 (dd, J_{CF} = 21.5, 3.1 Hz), 111.4, 118.8, 121.0 (dd, J_{CF} = 8.9, 4.3 Hz), 125.9, 126.1, 128.0, 128.7, 128.8 (dd, J_{CF} = 9.6, 3.5 Hz), 132.2, 136.7, 140.7, 146.2, 151.4 (dd, J_{CF} = 248.5, 11.7 Hz), 157.8 (dd, J_{CF} = 243.6, 11.1Hz). MS (70 eV) 359.1 (M^+, 100), 282 (40), 127 (50). EI-HRMS *m/e* calculated for $[M]^+$ $C_{22}H_{15}F_2N_3$ 359.1234, found 359.1189.

4-[1-(2,5-Difluoro-phenyl)-5-phenyl-4,5-dihydro-1*H*-pyrazol-3-yl]-benzonitrile (2f): Yield: 87%. M.p. 189-191 ºC. *Rf* 0.45 (3:1 hexanes:EtOAc). ^{1}H-NMR ($CDCl_3$, 400 MHz) δ 3.26 (dd, J = 17.0, 3.8 Hz, 1H), 3.80 (dd, J = 17.0, 12.1 Hz, 1H), 5.77 (ddd, J = 12.1, 3.8, 3.8 Hz, 1H), 6.47 (tdd, J = 8.9, 7.4, 3.2 Hz, 1H), 6.80 (ddd, J = 12.1, 9.0, 5.0 Hz, 1H), 7.13-7.16 (m, 2H), 7.21-7.25 (m, 3H), 7.36 (ddd, J = 9.9, 6.6, 3.3 Hz, 1H), 7.68 (d, J = 8.6 Hz, 2H), 7.81 (d, J = 8.6 Hz, 2H). ^{13}C NMR ($CDCl_3$ 100 MHz) δ 42.6, 66.2 (d, J_{CF} = 8.5 Hz), 106.2 (dd, J_{CF} = 28.5, 3.5 Hz), 107.6 (dd, J_{CF} = 24.4, 7.6 Hz), 111.7, 116.7 (dd, J_{CF} = 23.0, 9.9 Hz), 118.7, 125.6, 126.0, 127.8, 128.7, 132.2, 132.9 (t, J_{CF} = 11.1 Hz), 136.3, 140.9, 146.4, 146.5 (dd, J_{CF} = 241.2, 2.3 Hz), 158.8 (dd, J_{CF} = 241.4, 1.9 Hz). MS (70 eV) 359.1 (M^+, 100), 282 (40), 127 (50). EI-HRMS *m/e* calculated for $[M]^+$ $C_{22}H_{15}F_2N_3$ 359.1234, found 359.1189.

4-[1-(3,5-Difluoro-phenyl)-5-phenyl-4,5-dihydro-1*H*-pyrazol-3-yl]-benzonitrile (2g): Yield: 76%. M.p. 224-226 ºC *Rf* 0.45 (3:1 hexanes:EtOAc). ^{1}H-NMR ($CDCl_3$, 400 MHz) δ 3.16 (dd, J = 17.6, 6.6 Hz, 1H), 3.87 (dd, J = 17.6, 12.6 Hz, 1H), 5.32 (dd, J = 12.6, 6.6 Hz, 1H), 6.25 (tt, J = 9.0, 2.3 Hz, 1H), 6.57 (dd, J = 9.9, 2.2 Hz, 2H), 7.24-7.39 (m, 5H), 7.67 (d, J = 8.6 Hz, 2H), 7.79 (d, J = 8.6 Hz, 2H). ^{13}C NMR ($CDCl_3$ 100 MHz) δ 43.2, 64.5, 94.8 (t, J_{CF} = 26.1 Hz), 96.6 (dd, J_{CF} = 20.7, 9.2 Hz), 111.8, 118.6, 125.4, 126.0, 128.1, 129.3, 132.2, 136.1, 140.6, 145.5 (t, J_{CF} = 13.6 Hz), 146.0, 163.4 (dd, J_{CF} = 243.6, 15.3 Hz). MS (70 eV) 359 (M^+, 100), 282 (40), 127 (40). EI-HRMS *m/e* calculated for $[M]^+$ $C_{22}H_{15}F_2N_3$ 359.1234, found 359.1212.

4-[5-Phenyl-1-(2,4,5-trifluoro-phenyl)-4,5-dihydro-1*H*-pyrazol-3-yl]-benzonitrile (2h): Yield: 30%. M.p. 130-132 °C; *Rf* 0.31 (5:1 hexanes:EtOAc); ^{1}H NMR ($CDCl_3$, 400 MHz) δ 3.29 (dd, J = 17.0, 4.4 Hz, 1H), 3.78 (dd, J = 17.0, 12.1 Hz, 1H), 5.67 (dt, J = 12.1, 3.8 Hz, 1H), 6.69-6.77 (m, 1H), 7.12 (dd, J = 8.2, 2.2 Hz, 1H), 7.21-7.21 (m, 3H), 7.42-7.47 (m, 2H), 7.67 (d, J = 8.2 Hz, 2H), 7.80 (d, J = 8.2 Hz, 2H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 42.4, 66.5 (d, J_{CF} = 7.7 Hz), 105.8, (ddd, J_{CF} = 26.9, 22.1, 1.1 Hz), 107.9 (dd, J_{CF} = 23.4, 4.5 Hz), 111.8, 118.7, 125.9, 126.1, 128.1, 128.9, 128.92 (dd, not resolved), 132.2, 136.3, 140.6, 144.1 (ddd, J_{CF} = 244.9, 14.9, 11.3 Hz), 145.6 (ddd, J_{CF} = 243.6, 8.9, 2.6 Hz), 146.7 (ddd, J_{CF} = 242.6, 12.8, 3.1 Hz), 146.9. MS (70 eV) 377.2 (M^+, 100), 300.1 (64), 231.1 (35), 145 (83). EI HRMS *m/e* calcd for $[M]^+$ $C_{22}H_{14}N_3F_3$ 377.1140, found 377.1107.

4-[5-Phenyl-1-(2,3,5,6-tetrafluoro-phenyl)-4,5-dihydro-1*H*-pyrazol-3-yl]-benzonitrile (2i): Yield: 70%. M.p. 192-194 ºC *Rf* 0.53 (3:1 hexane:EtOAc). ^{1}H-NMR ($CDCl_3$, 400 MHz) δ 3.31 (dd, J = 17.0 Hz, J = 7.1 Hz, 1H), 3.78 (dd, J = 17.0 Hz, 12.1 Hz, 1H), 5.60 (dd, J = 12.1 Hz, 7.1 Hz, 1H), 6.69 (tt, J_{HF} = 9.8, 7.1 Hz, 1H), 7.28-7.29 (m, 5H), 7.68 (d, J = 8.2 Hz, 2H), 7.79 (d, J = 8.8 Hz, 2H); ^{13}C NMR ($CDCl_3$ 100 MHz) δ 42.0, 67.7 (t, J_{CF} = 3.5 Hz), 100.6 (t J_{CF} = 23.2 Hz), 111.8, 118.6, 124.0 (tt, J_{CF} = 11.0, 2.6 Hz), 126.0, 126.2, 128.4, 128.9, 132.2, 136.1, 139.8, 141.1 (ddt, J_{CF} = 248.6, 15.0, 3.8 Hz), 146.1 (dtd, J_{CF} = 246.0, 13.1, 4.0 Hz), 147.2. MS (70 eV) 395.1 (M^+, 100), 231 (45), 163 (55). EI-HRMS *m/e* calculated for $[M]^+$ $C_{22}H_{13}N_3F_4$ 395.1046, found 395.1069.

4-(1-Pentafluorophenyl-5-phenyl-4,5-dihydro-1*H*-pyrazol-3-yl)-benzonitrile (2j): Yield: 70%. mp 131-133 ºC *Rf* 0.53 (3:1 hexanes:EtOAc). ^{1}H-NMR ($CDCl_3$, 400 MHz) δ 3.31 (dd, J = 17.0 Hz, 7.1 Hz, 1H), 3.78 (dd, J = 17.0 Hz, 12.1 Hz, 1H), 5.60 (dd, J = 12.1 Hz, 7.1 Hz, 1H), 7.28-

7.29 (m, 5H), 7.68 (d, J = 8.2 Hz, 2H), 7.79 (d, J = 8.2 Hz, 2H); ^{13}C NMR ($CDCl_3$ 100 MHz) δ 42.1, 68.4 (t, J_{CF} = 2.9 Hz), 112.0, 118.6, 119.4 (m), 126.0, 126.4, 128.6, 128.9, 132.2, 136.1, 137.7 (d, J_{CF} = 248 Hz), 138.3 (m, CF), 142.4 (d, J_{CF} = 248 Hz, CF), 147.7. MS (70 eV) 395.1 (M^+, 100), 231 (45), 163 (55). EI-HRMS *m/e* calculated for $[M]^+$ $C_{22}H_{13}N_3F_4$ 395.1046, found 395.1069.

4-(1,3-Diphenyl-4,5-dihydro-1*H*-pyrazol-5-yl)-*N*,*N*-dimethylaniline (3a): M.p. 123-125°C. ^{1}H-NMR ($CDCl_3$, 400 MHz) δ 2.92 (s, 6H), 3.12 (dd, J = 17.1, 7.3 Hz, 1H), 3.78 (dd, J = 17.1, 12.2 Hz, 1H), 5.19 (dd, J = 12.2, 7.3 Hz, 1H), 6.68 (d, J = 8.6 Hz, 2H), 6.78 (t, J = 14.2 Hz, 1H), 7.11 (d, J = 7.6 Hz, 2H), 7.15-7.19 (m, 4H), 7.29-7.39 (m, 3H), 7.72 (d, J = 7.6 Hz, 2H). ^{13}C NMR ($CDCl_3$ 100 MHz) δ 40.6, 43.6, 64.1, 112.9, 113.4, 118.8, 125.7, 126.7, 128.4, 128.5, 128.8, 130.2, 133.0, 145.0, 146.7, 149.9. MS (70 eV) 341 (M^+, 100), 221 (12), 146 (32), 91 (18). EI HRMS *m/e* calcd for $[M]^+$ $C_{23}H_{23}N_3$ 341.1892, found 341.1903.

4-(1-(2-Fluorophenyl)-3-phenyl-4,5-dihydro-1*H*-pyrazol-5-yl)-*N*,*N*-dimethylaniline (3b): M.p. 109-111°C. ^{1}H-NMR ($CDCl_3$, 400 MHz) δ 2.81 (s, 6H), 3.24 (dd, J = 16.8, 4.4 Hz, 1H), 3.68 (dd, J = 16.8, 11.6 Hz, 1H), 5.54 (ddd, J = 11.6, 4.4, 3.8 Hz, 1H), 6.50 (d, J = 8.8 Hz, 2H), 6.70-6.76 (m, 1H), 6.85 (ddd, J = 12.8, 8.1, 1.3, 1H), 6.96 (ddd, J = 9.8, 9.8, 1.3 Hz, 1H), 7.03 (d, J = 8.6 Hz, 2H), 7.29-7.39 (m, 3H), 7.58 (ddd, J = 8.4, 8.4, 1.5 Hz, 1H), 7.74 (dd, J = 8.5, 1.2 Hz, 2H). ^{13}C NMR ($CDCl_3$ 100 MHz) δ 40.4, 42.8, 65.9 (d, J_{CF} = 7.0 Hz), 112.1, 115.7 (d, J_{CF} = 20.3 Hz), 119.8 (d, J_{CF} = 3.4 Hz), 121.1 (d, J_{CF} = 7.2 Hz), 124.1 (d, J_{CF} = 3.0 Hz), 125.7, 126.9, 128.3, 128.4, 129.4, 132.7, 133.2 (d, J_{CF} = 9.2 Hz), 148.2, 149.6, 151.2 (d, J_{CF} = 243.4 Hz). MS (70 eV) 359 (M^+, 100), 257 (19), 249 (16), 147 (70), 109 (24). EI HRMS *m/e* calcd for $[M]^+$ $C_{23}H_{22}FN_3$ 359.1798, found 359.1757.

4-(1-(4-Fluorophenyl)-3-phenyl-4,5-dihydro-1*H*-pyrazol-5-yl)-*N*,*N*-dimethylaniline (3d): M.p. 135-137°C. ^{1}H-NMR ($CDCl_3$, 400 MHz) δ 2.88 (s, 6H), 3.08 (dd, J = 17.0, 7.9 Hz, 1H), 3.71 (dd, J = 17.0, 12.1 Hz, 1H), 5.06 (dd, J = 12.1, 7.9 Hz, 1H), 6.65 (d, J = 8.5 Hz, 2H), 6.84 (t, J = 8.7 Hz, 2H), 7.02 (dd, J = 8.7, 4.4 Hz, 2H), 7.14 (d, J = 8.5 Hz, 2H), 7.26-7.36 (m, 3H), 7.68 (d, J = 7.8 Hz, 2H). ^{13}C NMR ($CDCl_3$ 100 MHz) δ 40.5, 43.8, 64.9, 112.7, 114.4 (d, J_{CF} = 7.2 Hz), 115.1 (d, J_{CF} = 22.2 Hz), 125.5, 126.7, 128.28, 128.33, 129.6, 132.7, 141.6 (d, J_{CF} = 2.0 Hz), 146.7, 149.8, 156.5 (d, J_{CF} = 236.4 Hz). MS (70 eV) 359 (M^+, 100), 239 (12), 147 (48), 109 (26). EI HRMS *m/e* calcd for $[M]^+$ $C_{23}H_{22}FN_3$ 359.1798, found 359.1785.

4-(1-(2,4-Difluorophenyl)-3-phenyl-4,5-dihydro-1*H*-pyrazol-5-yl)-*N*,*N*-dimethylaniline (3e): M.p. 128-130°C. ^{1}H-NMR ($CDCl_3$, 400 MHz) δ 2.85 (s, 6H), 3.29 (dd, J = 16.8, 4.8 Hz, 1H), 3.70 (dd, J = 16.8, 11.5 Hz, 1H), 5.44 (ddd, J = 16.8, 4.8, 3.5 Hz, 1H), 6.52 (d, J = 8.8 Hz, 2H), 6.64 (ddd, J = 12.0, 8.7, 2.8 Hz, 1H), 6.70 (dddd, J = 9.1, 7.8, 2.8, 1.3 Hz, 1H), 7.02 (d, J = 8.6 Hz, 2H), 7.31-7.41 (m, 3H), 7.46 (td, J = 9.2, 6.0 Hz, 1H), 7.74 (dd, J = 8.5, 1.5 Hz, 2H). ^{13}C NMR ($CDCl_3$ 100 MHz) δ 40.4, 42.7, 66.5 (d, J_{CF} = 5.9 Hz), 104.0 (dd, J_{CF} = 25.9, 24.5 Hz), 110.7 (dd, J_{CF} = 21.6, 3.3 Hz), 112.1, 120.8 (dd, J_{CF} = 8.8, 4.6 Hz), 125.7, 127.2, 128.4, 128.5, 128.7 (?), 130.1 (dd, J_{CF} = 9.4, 3.6 Hz), 132.6, 148.8, 149.7, 151.4 (dd, J_{CF} = 258.6, 11.7 Hz), 157.2 (dd, J_{CF} = 252.1, 10.9 Hz). MS (70 eV) 377 (M^+, 100), 249 (18), 146 (44). EI HRMS *m/e* calcd for $[M]^+$ $C_{23}H_{21}F_2N_3$ 377.1704, found 377.1721.

4-(1-(Pentafluorophenyl)-3-phenyl-4,5-dihydro-1*H*-pyrazol-5-yl)-*N*,*N*-dimethylaniline (3j): M.p. 90-92°C. ^{1}H-NMR ($CDCl_3$, 400 MHz) δ 2.89 (s, 6H), 3.29 (dd, J = 16.9, 8.0 Hz, 1H), 3.68 (dd, J = 16.9, 11.4 Hz, 1H), 5.30 (dd, J = 11.4, 8.0 Hz, 1H), 6.58 (d, J = 8.8 Hz, 2H), 7.14 (d, J = 8.7 Hz, 2H), 7.35-7.42 (m, 3H), 7.70 (dd, J = 8.3, 1.6 Hz, 2H). ^{13}C NMR ($CDCl_3$ 100 MHz) δ 40.4, 42.4, 67.9 (t, J_{CF} = 2.8 Hz), 112.2, 120.5 (td, J_{CF} = 11.8, 3.6 Hz, CF), 125.8, 127.1, 127.5, 128.5, 128.9, 132.1, 137.6 (m, CF), 137.7 (m, CF), 142.5 (dm, J_{CF} = 249 Hz, CF), 150.0, 150.2. MS

(70 eV) 431 (M^+, 100), 249 (49), 147 (83). EI HRMS *m/e* calcd for $[M]^+$ $C_{23}H_{19}F_5N_3$ 431.1421, found 431.1455.

4-(5-(4-(dimethylamino)phenyl)-1-phenyl-4,5-dihydro-1*H*-pyrazol-3-yl)benzonitrile (4a) M.p. 162-164°C. ^{1}H-NMR ($CDCl_3$, 400 MHz) δ 2.92 (s, 6H), 3.10 (dd, *J* = 16.9, 6.9 Hz, 1H), 3.76 (dd, *J* = 16.9, 12.2 Hz, 1H), 5.30 (dd, *J* = 12.2, 6.9 Hz, 1H), 6.67 (d, *J* = 8.2 Hz, 2H), 6.82 (t, *J* = 7.1 Hz, 1H), 7.10-7.22 (m, 6H), 7.63 (d, *J* = 8.0 Hz, 2H), 7.76 (d, *J* = 8.0 Hz, 2H). ^{13}C NMR ($CDCl_3$ 100 MHz) δ 40.5, 42.9, 64.4, 110.6, 112.8, 113.6, 118.9, 119.6, 125.5, 126.4, 128.8, 129.1, 132.0, 137.2, 143.7, 144.0, 149.8. MS (70 eV) 366 (M^+, 100), 274 (9), 246 (13), 147 (53). EI HRMS *m/e* calcd for $[M]^+$ $C_{24}H_{22}N_4$ 366.1844, found 366.1835.

4-(5-(4-(Dimethylamino)phenyl)-1-(3-fluorophenyl)-4,5-dihydro-1*H*-pyrazol-3-yl)-benzonitrile (4c): M.p. 149-151°C. ^{1}H-NMR ($CDCl_3$, 400 MHz) δ 2.92 (s, 6H), 3.14 (dd, *J* = 17.2, 6.8 Hz, 1H), 3.79 (dd, *J* = 17.2, 12.5 Hz, 1H), 5.27 (d, *J* = 12.5, 6.8 Hz, 1H), 6.49 (td, *J* = 8.4, 2.3 Hz, 1H), 6.67 (d, *J* = 8.8 Hz, 2H), 6.78 (dd, *J* = 8.3, 2.0 Hz, 1H), 6.90 (dt, *J* = 6.9, 2.2 Hz, 1H), 7.06-7.12 (m, 3H), 7.64 (d, *J* = 8.5 Hz, 2H), 7.77 (d, *J* = 8.5 Hz, 2H). ^{13}C NMR ($CDCl_3$ 100 MHz) δ 40.5, 42.9, 64.3, 100.8 (d, J_{CF} = 26.8 Hz), 106.0 (d, J_{CF} = 21.5 Hz), 109.0 (d, J_{CF} = 2.2 Hz), 111.0, 112.8, 118.7, 125.7, 126.3, 128.7, 129.8 (d, J_{CF} = 9.7 Hz), 132.0, 136.7, 145.0, 145.2 (d, J_{CF} = 10.8 Hz), 149.8, 163.2 (d, J_{CF} = 242.0 Hz). MS (70 eV) 384 (M^+, 100), 274 (13), 174 (69). EI HRMS *m/e* calcd for $[M]^+$ $C_{24}H_{21}FN_4$ 384.1750, found 384.1747.

4-(5-(4-(Dimethylamino)phenyl)-1-(4-fluorophenyl)-4,5-dihydro-1*H*-pyrazol-3-yl)-benzonitrile (4d): M.p. 178-180°C. ^{1}H-NMR ($CDCl_3$, 400 MHz) δ 2.92 (s, 6H), 3.11 (dd, *J* = 17.0, 7.5 Hz, 1H), 3.76 (dd, *J* = 17.0, 12.4 Hz, 1H), 5.24 (dd, *J* = 12.4, 7.5 Hz, 1H), 6.67 (d, *J* = 8.8 Hz, 2H), 6.88 (t, *J* = 8.5 Hz, 2H), 7.04 (dd, *J* = 9.2, 4.6 Hz, 2H), 7.13 (d, *J* = 8.7 Hz, 2H), 7.63 (d, *J* = 8.7 Hz, 2H). ^{13}C NMR ($CDCl_3$ 100 MHz) δ 40.5, 43.0, 65.0, 110.7, 112.7, 114.7 (d, J_{CF} = 7.4 Hz), 115.3 (d, J_{CF} = 22.2 Hz), 118.9, 125.5, 126.5, 128.7, 132.1, 137.0, 140.4 (d, J_{CF} = 2.0 Hz), 144.2, 149.9, 156.9 (d, J_{CF} = 237.6 Hz). MS (70 eV) 384 (M^+, 100), 274 (9), 146 (45). EI HRMS *m/e* calcd for $[M]^+$ $C_{24}H_{21}FN_4$ 384.1750, found 384.1760.

4-(5-(4-(Dimethylamino)phenyl)-1-(2,5-difluorophenyl)-4,5-dihydro-1*H*-pyrazol-3-yl)-benzonitrile (4f): M.p. 198-200°C. ^{1}H-NMR ($CDCl_3$, 400 MHz) δ 2.87 (s, 6H), 3.26 (dd, *J* = 17.0, 4.0 Hz, 1H), 3.72 (dd, *J* = 16.8, 11.9 Hz, 1H), 5.66 (ddd, *J* = 11.9, 3.8, 3.8 Hz, 1H), 6.45-6.48 (m, 1H), 6.54 (d, *J* = 8.7 Hz, 2H), 6.80 (ddd, *J* = 12.1, 9.0, 5.0 Hz, 1H), 6.99 (d, *J* = 8.6 Hz, 2H), 7.32 (ddd, *J* = 9.9, 6.6, 3.1 Hz, 1H), 7.67 (d, *J* = 8.2 Hz, 2H), 7.81 (d, *J* = 8.2 Hz, 2H). ^{13}C NMR ($CDCl_3$ 100 MHz) δ 40.4, 42.4, 66.0 (d, J_{CF} = 8.2 Hz), 106.4 (dd, J_{CF} = 28.3, 3.7 Hz), 107.5 (dd, J_{CF} = 24.9, 8.0 Hz), 111.4, 112.2, 116.5 (dd, J_{CF} = 23.2, 10.1 Hz), 118.7, 126.0, 126.7, 128.4, 132.1, 133.2 (t, J_{CF} = 11.0 Hz), 136.6, 146.6, 146.9 (dd, J_{CF} = 239.1, 2. Hz), 149.8, 158.8 (dd, J_{CF} = 240.2, 1.2 Hz). MS (70 eV) 402 (M^+, 100), 274 (19), 201 (10), 146 (42). EI HRMS *m/e* calcd for $[M]^+$ $C_{24}H_{20}F_2N_4$ 402.1656, found 402.1670.

4-(5-(4-(Dimethylamino)phenyl)-1-(2,3,5,6-tetrafluorophenyl)-4,5-dihydro-1*H*-pyrazol-3-yl)benzonitrile (4i): M.p. 180-181 °C. ^{1}H-NMR ($CDCl_3$, 400 MHz) δ 2.90 (s, 6H), 3.28 (dd, *J* = 17.1, 7.2 Hz, 1H), 3.71 (dd, *J* = 12.0, 17.1 Hz, 1H), 5.52 (dd, *J* = 12.0, 7.2 Hz, 1H), 6.59 (d, *J* = 8.8 Hz, 2H), 6.68 (tt, J_{HF} = 9.8, 7.2 Hz, 1H), 7.11 (d, *J* = 8.8 Hz, 2H), 7.67 (d, *J* = 8.6 Hz, 2H), 7.78 (d, *J* = 8.6 Hz, 2H). ^{13}C NMR ($CDCl_3$ 100 MHz) δ 40.3, 41.6, 67.5 (t, J_{CF} = 3.8 Hz), 100.4 (t, J_{CF} = 22.6 Hz), 111.7, 112.4, 118.8, 124.3, 126.1, 127.2, 127.3, 132.4, 136.7, 141.2 (CF), 146.2 (CF), 147.3, 150.4. MS (70 eV) 438 (M^+, 100), 274 (33), 147 (48). EI HRMS *m/e* calcd for $[M]^+$ $C_{24}H_{18}F_4N_4$ 438.1468, found 438.1449.

4-(5-(4-(Dimethylamino)phenyl)-1-(pentafluorophenyl)-4,5-dihydro-1*H*-pyrazol-3-yl)-benzonitrile (4j): M.p. 59-61°C. ^{1}H-NMR ($CDCl_3$, 400 MHz) δ 2.92 (s, 6H), 3.29 (dd, *J* = 16.9,

8.0 Hz, 1H), 3.69 (dd, J = 16.9, 11.9 Hz, 1H), 5.39 (dd, J = 11.4, 8.4 Hz, 1H), 6.59 (d, J = 8.6 Hz, 2H), 7.11 (d, J = 8.6 Hz, 2H), 7.67 (d, J = 8.2 Hz, 2H), 7.77 (d, J = 8.2 Hz, 2H). $^{13}C\{^{19}F,^{1}H\}$ NMR ($CDCl_3$ 100 MHz) δ 40.3, 41.7, 68.2, 111.7, 112.2, 118.7, 119.7, 126.0, 126.5, 127.4, 132.2, 136.4, 137.7 (CF), 138.0 (CF), 142.4 (CF), 147.6, 150.3. MS (70 eV) 456 (M^+, 100), 274 (38), 147 (51). EI HRMS *m/e* calcd for $[M]^+$ $C_{24}H_{17}F_5N_4$ 456.1373, found 456.1389.

2,4,5-Trifluorophenylhydrazine (**5**): To an ice-cold solution of 2,4,5-trifluoroaniline (1.01 g, 6.87 mmol) in 2.5 M aq. HCl (20 mL) was added dropwise with stirring to a solution of $NaNO_2$ (480 mg) in 20 mL of water. After stirring for 10 min, the resulting mixture was added to an ice-cold solution of $SnCl_2 \bullet H_2O$(6.73 g, 32.4 mmol) in conc. aq. HCl (40 mL). The reaction mixture was allowed to warm to room temperature and stirred for an additional 15 min. The precipitated product was filtered off, washed with diethyl ether, and dried in vacuo affording 1.36 g (6.84 mmol, 99%) of a colorless powder. ^{1}H-NMR (DMSO-d_6, 400 MHz) δ 3.42 (s, br, 1H), 7.41 (ddd, J_{HF} = 12.0, 7.9, 7.9 Hz, 1H), 7.51 (ddd, J_{HF} = 10.6, 10.6, 7.4 Hz, 1H), 10.44 (s, br, 3H). MS (70 eV) 162 (M^+, 100), 146 (68), 119 (74). EI HRMS *m/e* calcd for $[M]^+$ $C_6H_5F_3N_2$ 162.0405, found 162.0413.

(*E*)-4-(3-Phenylprop-2-enoyl)benzonitrile (6): A solution of benzaldehyde (2.0g, 18.8 mmol), 4-acetyl benzonitrile (2.76 g, 19.2 mmol), and piperidine (4.1 mL, 41.5 mmol) in abs. ethanol (20 mL) was heated at reflux temperature for 48 hours. After cooling to room temperature, the reaction mixture was diluted with sat. aqueous NH_4Cl and extracted twice with dichloromethane. The combined organic extracts were dried ($MgSO_4$) and concentrated under reduced pressure. The residue was purified on silicagel (FC, hexanes/EtOAc 10:1 –> 4:1) yielding 1.8 g (7.7 mmol, 41%) of chalcone **6** as yellow solid. M.p. 110-112 °C. ^{1}H-NMR ($CDCl_3$, 400 MHz) δ 7.40-7.43 (m, 3H), 7.46 (d, J = 15. 7 Hz, 1H), 7.62-7.64 (m, 2H), 7.77 (d, J = 8.4 Hz, 2H), 7.81 (d, J = 15.7 Hz, 1H), 8.07 (d, J = 8.3 Hz, 2H). ^{13}C NMR ($CDCl_3$ 100 MHz) δ 115.5, 117.7, 120.7, 128.3, 128.5, 128.7, 130.8, 132.1, 133.9, 140.9, 146.0, 188.5. MS (70 eV) 232 (M^+, 100), 131 (26), 102 (19), 77 (14). EI HRMS *m/e* calcd for $[M]^+$ $C_{16}H_{11}NO$ 233.0841, found 233.0833.

(*E*)-4-(3-(4-(Dimethylamino)phenyl)prop-2-enoyl)benzonitrile (7): Synthesized from 4-dimethylamino benzaldehyde and 4-acetyl benzonitrile following above procedure for chalcone (6). Yield: 71%. ^{1}H-NMR ($CDCl_3$, 400 MHz) δ 6.67 (d, J = 8.9 Hz, 2H), 7.24 (d, J = 15.4 Hz, 1H), 7.53 (d, J = 8.9 Hz, 2H), 7.75 (d, J = 8.2 Hz, 2H), 7.79 (d, J = 15.4 Hz, 1H), 8.04 (d, J = 8.2 Hz, 2H). ^{13}C NMR ($CDCl_3$ 100 MHz) δ 40.1, 111.6, 114.9, 115.4, 118.1, 121.8, 128.4, 130.6, 132.1, 142.3, 147.3, 152.1, 188.5.

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Table S1-1: Cartesian Atomic Coordinates for the Geometry Optimized Structure of Pyrazoline **1a** (B3LYP/6-31+G(d)).

Atom	x/Å	y/Å	z/Å
N	0.819275	-0.936848	-0.066155
N	-0.480063	-0.651985	0.240023
C	1.597589	0.011342	0.347219
C	0.842325	1.110488	1.071480
C	-0.634648	0.631702	0.965489
C	-1.533663	1.630583	0.249828
C	-1.490322	1.767038	-1.144050
C	-2.277324	2.724365	-1.787194
C	-3.119954	3.557337	-1.043895
C	-3.171991	3.424419	0.345724
C	-2.383532	2.464297	0.986968
C	-1.454780	-1.649816	0.149518
C	-2.777778	-1.395823	0.559405
C	-3.749114	-2.393861	0.456651
C	-3.433072	-3.653717	-0.054926
C	-2.117189	-3.904375	-0.460806
C	-1.133113	-2.923928	-0.362384
H	-4.193682	-4.425169	-0.137928
C	3.043533	-0.005434	0.119177
C	3.661186	-1.075874	-0.560902
C	5.036199	-1.082436	-0.772700
C	5.830953	-0.022734	-0.315173
C	5.231823	1.042924	0.358572
C	3.851436	1.052817	0.574588
H	6.904475	-0.030172	-0.484705
H	0.978925	2.087405	0.593912
H	1.173536	1.207921	2.112264
H	-1.050305	0.432102	1.962343
H	-0.849236	1.109208	-1.725823
H	-2.236935	2.816417	-2.869665
H	-3.831545	4.060467	0.931226
H	-2.439326	2.356925	2.069015
H	-3.058159	-0.419427	0.937983
H	-4.764681	-2.172694	0.776258
H	-1.847618	-4.880226	-0.858295
H	-0.115296	-3.129930	-0.670209
H	3.046044	-1.894676	-0.920068
H	5.493812	-1.917675	-1.297045
H	5.836952	1.871680	0.717523
H	3.403704	1.894678	1.095711
H	-3.736534	4.299114	-1.545115

Table S1-2: Cartesian Atomic Coordinates for the Geometry Optimized Structure of Pyrazoline **1b** (B3LYP/6-31+G(d)).

Atom	x/Å	y/Å	z/Å
N	0.921905	0.984284	-0.168533
N	-0.331661	0.678267	-0.628854
C	1.749450	0.033455	-0.461603
C	1.077991	-1.120051	-1.182671
C	-0.424703	-0.735639	-1.109109
C	-1.245758	-1.630993	-0.194143
C	-1.019445	-1.666660	1.190612
C	-1.753158	-2.528403	2.007469
C	-2.724060	-3.368919	1.452242
C	-2.959135	-3.337279	0.076209
C	-2.225454	-2.469780	-0.738808
C	-1.407455	1.457269	-0.186632
C	-2.650918	1.424129	-0.837940
C	-3.735311	2.188499	-0.437782
C	-3.596165	3.060423	0.645154
C	-2.364466	3.139205	1.300853
C	-1.289433	2.347073	0.898958
H	-4.436150	3.670611	0.963671
C	3.179939	0.117685	-0.160413
C	3.726241	1.247703	0.482870
C	5.088898	1.317826	0.755915
C	5.941378	0.266018	0.393772
C	5.412945	-0.857388	-0.244207
C	4.045270	-0.932412	-0.518831
H	7.005764	0.326198	0.605393
H	1.272008	-2.086352	-0.704888
H	1.428796	-1.190195	-2.220280
H	-0.875672	-0.743191	-2.102471
H	-0.272206	-1.012986	1.634097
H	-1.569664	-2.542286	3.078985
H	-3.717598	-3.980004	-0.363662
H	-2.421079	-2.436821	-1.808395
F	-2.805186	0.621727	-1.934345
H	-4.665601	2.101802	-0.990849
H	-2.237299	3.813993	2.143240
H	-0.337141	2.406522	1.412425
H	3.066570	2.064130	0.759245
H	5.492724	2.198096	1.249796
H	6.064321	-1.678857	-0.531661
H	3.651811	-1.815005	-1.015309
H	-3.294514	-4.039626	2.089983

Table S1-3: Cartesian Atomic Coordinates for the Geometry Optimized Structure of Pyrazoline **1c** (B3LYP/6-31+G(d)).

Atom	x/Å	y/Å	z/Å
N	0.994097	0.937503	0.069349
N	-0.280970	0.536175	-0.214546
C	1.844054	0.059506	-0.356718
C	1.174671	-1.108628	-1.058084
C	-0.336094	-0.756699	-0.937105
C	-1.141091	-1.825486	-0.211144
C	-1.085468	-1.948065	1.183609
C	-1.783750	-2.968284	1.832510
C	-2.548495	-3.878421	1.095666
C	-2.611959	-3.760272	-0.294784
C	-1.911862	-2.737714	-0.942196
C	-1.340240	1.429933	-0.072033
C	-2.635190	1.063872	-0.487767
C	-3.670826	1.971904	-0.314534
C	-3.506341	3.227975	0.250035
C	-2.211485	3.576541	0.653475
C	-1.137370	2.704647	0.500219
H	-4.353597	3.894810	0.367374
C	3.286869	0.199015	-0.152302
C	3.824206	1.318839	0.515748
C	5.196658	1.435540	0.710940
C	6.068205	0.441516	0.245798
C	5.548647	-0.670909	-0.418325
C	4.171195	-0.791704	-0.616718
H	7.139526	0.536761	0.401961
H	1.398573	-2.062910	-0.568158
H	1.500368	-1.193074	-2.101398
H	-0.777033	-0.592510	-1.929679
H	-0.506999	-1.232040	1.762056
H	-1.735595	-3.049030	2.915570
H	-3.211911	-4.455857	-0.876263
H	-1.976764	-2.644189	-2.024992
H	-2.855526	0.094335	-0.916370
F	-4.915918	1.592992	-0.720144
H	-2.037741	4.552891	1.098603
H	-0.141879	2.992231	0.812916
H	3.149908	2.087789	0.879035
H	5.592758	2.305766	1.228381
H	6.213549	-1.450175	-0.781941
H	3.784149	-1.667828	-1.129943
H	-3.096412	-4.668284	1.602796

Table S1-4: Cartesian Atomic Coordinates for the Geometry Optimized Structure of Pyrazoline **1d** (B3LYP/6-31+G(d)).

Atom	x/Å	y/Å	z/Å
N	0.866484	0.899794	0.114003
N	-0.356356	0.346744	-0.155797
C	1.813191	0.127221	-0.310390
C	1.287911	-1.114169	-1.005615
C	-0.254572	-0.927725	-0.907394
C	-0.949660	-2.101053	-0.230995
C	-1.041537	-2.187967	1.163969
C	-1.633029	-3.301095	1.765800
C	-2.134855	-4.343544	0.980831
C	-2.045800	-4.264252	-0.411659
C	-1.459338	-3.146899	-1.011955
C	-1.496179	1.161469	-0.125536
C	-2.757714	0.639192	-0.469507
C	-3.897596	1.446013	-0.425405
C	-3.773434	2.770716	-0.035078
C	-2.543101	3.315709	0.311934
C	-1.404380	2.513831	0.263480
F	-4.886875	3.558836	0.011586
C	3.229679	0.432487	-0.099269
C	3.629816	1.585875	0.606702
C	4.978576	1.861687	0.806136
C	5.962118	0.996609	0.307367
C	5.578844	-0.147831	-0.394036
C	4.225588	-0.428705	-0.595838
H	7.014852	1.214302	0.467217
H	1.612350	-2.030027	-0.498967
H	1.632533	-1.177314	-2.044200
H	-0.689699	-0.785453	-1.906559
H	-0.663837	-1.371954	1.774074
H	-1.707261	-3.352122	2.849143
H	-2.438009	-5.066898	-1.031058
H	-1.400469	-3.086109	-2.097446
H	-2.866928	-0.402091	-0.748688
H	-4.872792	1.045889	-0.684818
H	-2.477096	4.358024	0.608418
H	-0.437779	2.926746	0.523232
H	2.867870	2.254046	0.995236
H	5.268283	2.754163	1.355271
H	6.332612	-0.827557	-0.783568
H	3.945308	-1.326037	-1.140783
H	-2.596128	-5.208300	1.450528

Table S1-5: Cartesian Atomic Coordinates for the Geometry Optimized Structure of Pyrazoline **1e** (B3LYP/6-31+G(d)).

Atom	x/Å	y/Å	z/Å
N	-0.998623	-0.961121	-0.265873
N	0.183516	-0.460041	-0.750557
C	-1.961474	-0.127801	-0.497034
C	-1.484055	1.130429	-1.197416
C	0.059827	0.978390	-1.142925
C	0.738323	1.931649	-0.170289
C	0.528806	1.831498	1.213774
C	1.116435	2.745627	2.089458
C	1.922552	3.775928	1.593579
C	2.143680	3.878517	0.218572
C	1.556903	2.958517	-0.655850
C	1.373492	-1.080751	-0.347299
C	2.584375	-0.839800	-1.016663
C	3.782214	-1.443786	-0.663646
C	3.763184	-2.351962	0.387127
C	2.595334	-2.653879	1.074476
C	1.412636	-2.010614	0.708630
F	4.926065	-2.964025	0.740710
C	-3.353804	-0.422041	-0.151444
C	-3.702195	-1.606956	0.529651
C	-5.029787	-1.876478	0.847056
C	-6.042308	-0.975274	0.491580
C	-5.710326	0.200443	-0.184027
C	-4.378286	0.476217	-0.501799
H	-7.078617	-1.191478	0.737585
H	-1.820306	2.045598	-0.700079
H	-1.848443	1.161930	-2.232532
H	0.497080	1.115192	-2.132830
H	-0.090856	1.030962	1.610452
H	0.946565	2.651954	3.159106
H	2.777432	4.669590	-0.174660
H	1.742271	3.036403	-1.725102
F	2.600002	0.014448	-2.078953
H	4.693214	-1.221616	-1.208072
H	2.614258	-3.370230	1.889503
H	0.490420	-2.227752	1.233750
H	-2.918882	-2.308063	0.799731
H	-5.280188	-2.794139	1.373616
H	-6.487182	0.906089	-0.467347
H	-4.137354	1.393367	-1.032301
H	2.378577	4.489282	2.275328

Table S1-6: Cartesian Atomic Coordinates for the Geometry Optimized Structure of Pyrazoline **1f** (B3LYP/6-31+G(d)).

Atom	x/Å	y/Å	z/Å
N	-0.918478	-0.863256	-0.361586
N	0.279826	-0.378135	-0.825097
C	-1.849097	0.017838	-0.540353
C	-1.327464	1.290950	-1.180311
C	0.209358	1.085410	-1.125741
C	0.910088	1.939572	-0.078909
C	0.714646	1.712455	1.291491
C	1.327079	2.531107	2.241670
C	2.144920	3.590293	1.834397
C	2.352344	3.818497	0.472638
C	1.739950	2.994437	-0.477020
C	1.442423	-1.083177	-0.510319
C	2.665635	-0.811870	-1.149941
C	3.832143	-1.501842	-0.864187
C	3.819892	-2.536534	0.075255
C	2.608183	-2.823965	0.690868
C	1.436301	-2.130316	0.431535
H	4.712506	-3.103073	0.316117
C	-3.250114	-0.238920	-0.200250
C	-3.638723	-1.433589	0.440205
C	-4.975237	-1.667582	0.748330
C	-5.955462	-0.720532	0.423214
C	-5.582878	0.465856	-0.211397
C	-4.241844	0.706340	-0.518977
H	-6.998826	-0.909603	0.661681
H	-1.637854	2.194384	-0.646342
H	-1.685761	1.376158	-2.214730
H	0.661845	1.273328	-2.099673
H	0.089567	0.885008	1.617540
H	1.167636	2.340376	3.299901
H	2.996085	4.631835	0.147052
H	1.917100	3.168398	-1.536175
F	2.713556	0.152928	-2.117001
H	4.739744	-1.233693	-1.395734
F	2.565682	-3.827720	1.610245
H	0.520247	-2.391640	0.945311
H	-2.879775	-2.169027	0.687511
H	-5.258145	-2.592800	1.244092
H	-6.334693	1.206894	-0.470517
H	-3.967218	1.632463	-1.016531
H	2.622102	4.227271	2.574897

Table S1-7: Cartesian Atomic Coordinates for the Geometry Optimized Structure of Pyrazoline **1g** (B3LYP/6-31+G(d)).

Atom	x/Å	y/Å	z/Å
N	0.990427	0.813219	0.051422
N	-0.240432	0.272532	-0.218399
C	1.924048	0.016637	-0.355296
C	1.381965	-1.228011	-1.031813
C	-0.158010	-1.035113	-0.913868
C	-0.841735	-2.172501	-0.168998
C	-0.863062	-2.216134	1.231367
C	-1.433955	-3.303859	1.895573
C	-1.987736	-4.362381	1.169188
C	-1.973269	-4.323876	-0.227743
C	-1.405573	-3.232375	-0.890736
C	-1.371337	1.078688	-0.160498
C	-2.634038	0.556057	-0.509888
C	-3.740432	1.390278	-0.430560
C	-3.686600	2.717312	-0.025790
C	-2.419830	3.188306	0.308472
C	-1.267280	2.424324	0.253328
H	-4.569717	3.341839	0.028761
C	3.345606	0.307224	-0.154516
C	3.762443	1.474518	0.517436
C	5.115481	1.736150	0.706844
C	6.084819	0.842738	0.231194
C	5.684380	-0.315614	-0.437042
C	4.326941	-0.582258	-0.628805
H	7.140833	1.049908	0.383025
H	1.709489	-2.142431	-0.525707
H	1.712797	-1.295682	-2.074750
H	-0.611759	-0.934643	-1.908787
H	-0.444271	-1.389567	1.799413
H	-1.450504	-3.322309	2.982339
H	-2.409108	-5.137562	-0.801667
H	-1.406168	-3.202803	-1.979205
H	-2.775275	-0.475381	-0.805517
F	-4.951265	0.872428	-0.768218
F	-2.309730	4.483290	0.705866
H	-0.311285	2.855231	0.517229
H	3.011136	2.165073	0.886982
H	5.419488	2.639750	1.229136
H	6.427601	-1.016616	-0.808374
H	4.032129	-1.490204	-1.147865
H	-2.433360	-5.206986	1.687900

Table S1-8: Cartesian Atomic Coordinates for the Geometry Optimized Structure of Pyrazoline **1h** (B3LYP/6-31+G(d)).

Atom	x/Å	y/Å	z/Å
N	-1.018116	-0.861597	-0.400328
N	0.101811	-0.211361	-0.862228
C	-2.060598	-0.112599	-0.562991
C	-1.720015	1.224257	-1.193471
C	-0.169353	1.233266	-1.136589
C	0.396895	2.166014	-0.074841
C	0.247533	1.889480	1.292556
C	0.722334	2.783561	2.253511
C	1.355733	3.967374	1.861519
C	1.515157	4.247702	0.502982
C	1.039548	3.349686	-0.457730
C	1.349319	-0.755748	-0.549709
C	2.529927	-0.308731	-1.167680
C	3.778326	-0.847748	-0.893840
C	3.871228	-1.897434	0.010352
C	2.719181	-2.380819	0.622990
C	1.478455	-1.821093	0.362205
F	5.070718	-2.457232	0.283000
C	-3.409220	-0.562374	-0.209247
C	-3.621021	-1.806617	0.419945
C	-4.906825	-2.222995	0.750783
C	-6.012356	-1.412024	0.461876
C	-5.815822	-0.178881	-0.162007
C	-4.526227	0.244025	-0.493148
H	-7.015265	-1.741299	0.720196
H	-2.150334	2.072994	-0.653987
H	-2.083867	1.266591	-2.228735
H	0.256335	1.498472	-2.105158
H	-0.236782	0.969403	1.609250
H	0.599317	2.554782	3.309015
H	2.016142	5.159553	0.187954
H	1.178985	3.567694	-1.514416
F	2.464605	0.680693	-2.102721
H	4.660679	-0.467288	-1.396455
F	2.816405	-3.406636	1.498795
H	0.600548	-2.215217	0.857698
H	-2.766143	-2.436794	0.643793
H	-5.050355	-3.184275	1.237900
H	-6.665758	0.457746	-0.394392
H	-4.394093	1.205110	-0.982395
H	1.725962	4.661978	2.611165

Table S1-9: Cartesian Atomic Coordinates for the Geometry Optimized Structure of Pyrazoline **1i** (B3LYP/6-31+G(d)).

Atom	x/Å	y/Å	z/Å
N	-1.126653	-0.807789	-0.371697
N	0.065378	-0.240701	-0.757179
C	-2.091710	0.023730	-0.589965
C	-1.614797	1.335534	-1.187360
C	-0.070880	1.212223	-1.093997
C	0.572178	2.116669	-0.054183
C	0.302517	1.952115	1.313493
C	0.876259	2.805581	2.256661
C	1.728643	3.836593	1.846012
C	2.007767	4.003238	0.488355
C	1.434255	3.144109	-0.455120
C	1.261661	-0.859034	-0.409498
C	2.389716	-0.727238	-1.241986
C	3.601400	-1.331219	-0.933330
C	3.749674	-2.119056	0.200679
C	2.643001	-2.261946	1.027833
C	1.430507	-1.637002	0.753850
H	4.692611	-2.599777	0.433637
C	-3.490555	-0.319398	-0.319524
C	-3.830305	-1.536755	0.305531
C	-5.161554	-1.853452	0.557514
C	-6.183636	-0.967414	0.192098
C	-5.858925	0.241062	-0.426838
C	-4.523566	0.564156	-0.679910
H	-7.222395	-1.218765	0.389478
H	-1.985488	2.208940	-0.641990
H	-1.949251	1.427982	-2.228500
H	0.395797	1.396548	-2.063514
H	-0.348678	1.146158	1.643900
H	0.661320	2.663204	3.312654
H	2.676147	4.795832	0.161521
H	1.660880	3.273939	-1.511437
F	2.287746	-0.018497	-2.389250
F	4.642417	-1.164882	-1.776159
F	2.748876	-2.992028	2.157746
F	0.434215	-1.759852	1.648977
H	-3.037350	-2.221484	0.589189
H	-5.406205	-2.794730	1.043302
H	-6.644016	0.935402	-0.715444
H	-4.288123	1.507228	-1.165879
H	2.174499	4.501322	2.581498

Table S1-10: Cartesian Atomic Coordinates for the Geometry Optimized Structure of Pyrazoline **1j** (B3LYP/6-31+G(d)).

Atom	x/Å	y/Å	z/Å
N	-1.259214	-0.820961	-0.411812
N	-0.127422	-0.140191	-0.799713
C	-2.297793	-0.075386	-0.602143
C	-1.946728	1.284726	-1.180852
C	-0.397798	1.301572	-1.099018
C	0.165071	2.242722	-0.045584
C	-0.070449	2.027397	1.321253
C	0.420538	2.920939	2.274134
C	1.155788	4.042480	1.874931
C	1.400175	4.261262	0.518078
C	0.908346	3.363456	-0.435207
C	1.123730	-0.650132	-0.463383
C	2.225496	-0.425714	-1.309035
C	3.499123	-0.901742	-1.020482
C	3.711788	-1.663826	0.125124
C	2.641066	-1.918637	0.977656
C	1.377646	-1.402675	0.699985
F	4.933910	-2.138418	0.407956
C	-3.657036	-0.541879	-0.314075
C	-3.882137	-1.799838	0.281775
C	-5.177099	-2.229735	0.556089
C	-6.276317	-1.418964	0.243227
C	-6.065365	-0.171877	-0.347321
C	-4.767052	0.264339	-0.622978
H	-7.285941	-1.758537	0.458932
H	-2.390395	2.112752	-0.619586
H	-2.294468	1.362875	-2.218917
H	0.042955	1.550278	-2.066707
H	-0.631534	1.153898	1.644301
H	0.231867	2.739589	3.329125
H	1.977637	5.125104	0.198806
H	1.106619	3.536217	-1.491081
F	2.052390	0.264659	-2.455658
F	4.516153	-0.654045	-1.860765
F	2.839432	-2.627845	2.099508
F	0.409406	-1.617421	1.605502
H	-3.030308	-2.426487	0.526610
H	-5.332559	-3.200959	1.019176
H	-6.910230	0.465599	-0.595193
H	-4.622124	1.236938	-1.085111
H	1.537342	4.737489	2.618388

Table S1-11: Cartesian Atomic Coordinates for the Geometry Optimized Structure of Pyrazoline **2a** (B3LYP/6-31+G(d)).

Atom	x/Å	y/Å	z/Å
N	0.263932	-0.930275	0.023746
N	-1.034672	-0.655013	0.298666
C	1.029799	0.029158	0.443599
C	0.252358	1.130071	1.139873
C	-1.219048	0.642662	0.996338
C	-2.101100	1.623679	0.236887
C	-2.021684	1.736419	-1.157535
C	-2.797173	2.677899	-1.837198
C	-3.662644	3.518491	-1.130008
C	-3.750030	3.409352	0.259855
C	-2.973846	2.464937	0.937889
C	-2.012900	-1.647909	0.157310
C	-3.345892	-1.391817	0.527163
C	-4.317477	-2.383625	0.378073
C	-3.988698	-3.637323	-0.139930
C	-2.661450	-3.889724	-0.505000
C	-1.677615	-2.914945	-0.360714
H	-4.749249	-4.403817	-0.259368
C	2.474913	0.009137	0.245863
C	3.108507	-1.069716	-0.409661
C	4.482022	-1.083238	-0.595308
C	5.272214	-0.011578	-0.130477
C	4.654388	1.067087	0.522887
C	3.274777	1.073383	0.707067
H	0.394817	2.104676	0.659464
H	0.553679	1.236028	2.188945
H	-1.664238	0.454721	1.981999
H	-1.362490	1.073725	-1.713040
H	-2.728964	2.751798	-2.919541
H	-4.427203	4.052191	0.816849
H	-3.057084	2.375832	2.019759
H	-3.634125	-0.419978	0.910922
H	-5.342273	-2.162554	0.665855
H	-2.383285	-4.861238	-0.906473
H	-0.650875	-3.122158	-0.636342
H	2.503308	-1.893437	-0.772810
H	4.957010	-1.919465	-1.099166
H	5.257496	1.895193	0.882289
H	2.817849	1.920210	1.210293
H	-4.269388	4.248483	-1.659557
C	6.691438	-0.021880	-0.325255
N	7.845006	-0.030901	-0.485323

Table S1-12: Cartesian Atomic Coordinates for the Geometry Optimized Structure of Pyrazoline **2b** (B3LYP/6-31+G(d)).

Atom	x/Å	y/Å	z/Å
N	0.395623	-0.925118	0.228637
N	-0.876698	-0.650298	0.622712
C	1.188500	0.047901	0.555100
C	0.459008	1.184661	1.244230
C	-1.029123	0.756718	1.114785
C	-1.847397	1.630523	0.177379
C	-1.559667	1.696827	-1.194758
C	-2.292839	2.538139	-2.032746
C	-3.323913	3.326711	-1.510650
C	-3.618881	3.265105	-0.147203
C	-2.885578	2.417798	0.689233
C	-1.912998	-1.473124	0.158659
C	-3.163769	-1.501972	0.794180
C	-4.205064	-2.314187	0.373257
C	-4.009129	-3.168055	-0.714827
C	-2.767779	-3.181863	-1.357110
C	-1.737859	-2.342825	-0.934321
H	-4.814222	-3.815741	-1.048731
C	2.626045	-0.014476	0.310602
C	3.215061	-1.142861	-0.301257
C	4.581660	-1.199134	-0.526354
C	5.409283	-0.123532	-0.142800
C	4.836024	1.003767	0.467414
C	3.462813	1.053730	0.689519
H	0.641289	2.154342	0.768617
H	0.767314	1.270163	2.294061
H	-1.514692	0.737882	2.091422
H	-0.763940	1.083732	-1.611483
H	-2.063082	2.576627	-3.094565
H	-4.423092	3.868575	0.265706
H	-3.125357	2.361705	1.748761
F	-3.367678	-0.717678	1.893848
H	-5.145396	-2.277990	0.914600
H	-2.598812	-3.841180	-2.204074
H	-0.778088	-2.351035	-1.437394
H	2.581090	-1.973229	-0.593608
H	5.023127	-2.073207	-0.995280
H	5.469064	1.833575	0.766399
H	3.040204	1.934705	1.162960
H	-3.893808	3.981643	-2.164907
C	6.822325	-0.183091	-0.371576
N	7.970671	-0.234874	-0.558727

Table S1-13: Cartesian Atomic Coordinates for the Geometry Optimized Structure of Pyrazoline **2c** (B3LYP/6-31+G(d)).

Atom	x/Å	y/Å	z/Å
N	0.480498	-0.869483	-0.000447
N	-0.806712	-0.522750	0.257142
C	1.288820	0.048137	0.431044
C	0.560884	1.193327	1.109855
C	-0.931657	0.778817	0.960869
C	-1.765800	1.802886	0.204765
C	-1.679759	1.918723	-1.189049
C	-2.412405	2.896900	-1.864214
C	-3.241086	3.771204	-1.153794
C	-3.334175	3.659824	0.235425
C	-2.600415	2.679112	0.909332
C	-1.833589	-1.453116	0.081567
C	-3.149068	-1.128504	0.460717
C	-4.149317	-2.070651	0.262376
C	-3.926209	-3.321289	-0.294093
C	-2.610378	-3.627601	-0.661348
C	-1.570633	-2.719651	-0.481552
H	-4.746302	-4.017461	-0.432320
C	2.734382	-0.045305	0.252805
C	3.321798	-1.156502	-0.390641
C	4.695193	-1.236395	-0.560769
C	5.530490	-0.202197	-0.090460
C	4.958501	0.907845	0.551770
C	3.578718	0.980772	0.719978
H	0.753944	2.153124	0.617414
H	0.860449	1.298055	2.159268
H	-1.387012	0.605719	1.944824
H	-1.051032	1.230131	-1.748279
H	-2.340501	2.972569	-2.946194
H	-3.983805	4.327951	0.795208
H	-2.688758	2.589403	1.990706
H	-3.412703	-0.166084	0.880189
F	-5.414772	-1.732284	0.634203
H	-2.392231	-4.598709	-1.097908
H	-0.557791	-2.975595	-0.764859
H	2.681923	-1.952105	-0.757101
H	5.135613	-2.096212	-1.056230
H	5.596621	1.707742	0.914446
H	3.156290	1.850438	1.214363
H	-3.815725	4.528398	-1.680739
C	6.949897	-0.283956	-0.267898
N	8.103184	-0.353637	-0.413943

Table S1-14: Cartesian Atomic Coordinates for the Geometry Optimized Structure of Pyrazoline **2d** (B3LYP/6-31+G(d)).

Atom	x/Å	y/Å	z/Å
N	0.397538	-0.772582	0.012564
N	-0.862791	-0.340833	0.268184
C	1.267554	0.092773	0.433130
C	0.619386	1.285784	1.110701
C	-0.898113	0.964253	0.975423
C	-1.670400	2.043504	0.230478
C	-1.615407	2.139764	-1.166463
C	-2.279504	3.173308	-1.830241
C	-3.007402	4.123455	-1.106939
C	-3.070587	4.031307	0.285775
C	-2.406051	2.994932	0.948356
C	-1.941031	-1.231966	0.165623
C	-3.245195	-0.813534	0.488611
C	-4.320378	-1.699145	0.381363
C	-4.086655	-2.995703	-0.051146
C	-2.809880	-3.437326	-0.378658
C	-1.736001	-2.556814	-0.268166
F	-5.134880	-3.860316	-0.158391
C	2.701277	-0.092626	0.238630
C	3.208493	-1.230474	-0.426871
C	4.571580	-1.397754	-0.612545
C	5.478086	-0.428123	-0.135828
C	4.986248	0.707404	0.528341
C	3.616227	0.868690	0.711337
H	0.868492	2.228713	0.611271
H	0.933340	1.377125	2.157176
H	-1.354878	0.816276	1.963131
H	-1.064085	1.394927	-1.734707
H	-2.231846	3.234289	-2.914554
H	-3.640136	4.759830	0.857230
H	-2.469306	2.922493	2.032922
H	-3.436737	0.206429	0.800601
H	-5.329591	-1.381788	0.623837
H	-2.659991	-4.460262	-0.709554
H	-0.733871	-2.886740	-0.511927
H	2.513578	-1.976597	-0.797363
H	4.949787	-2.276176	-1.126594
H	5.679314	1.458437	0.894815
H	3.255281	1.756194	1.222715
H	-3.525789	4.925293	-1.625950
C	6.886982	-0.600296	-0.330018
N	8.031680	-0.744311	-0.489729

Table S1-15: Cartesian Atomic Coordinates for the Geometry Optimized Structure of Pyrazoline **2e** (B3LYP/6-31+G(d)).

Atom	x/Å	y/Å	z/Å
N	0.538058	-0.817038	0.355593
N	-0.691199	-0.399207	0.766314
C	1.427293	0.093095	0.605752
C	0.826809	1.329142	1.249131
C	-0.697545	1.049350	1.150058
C	-1.429305	1.926746	0.147012
C	-1.152493	1.849241	-1.226897
C	-1.804360	2.688971	-2.130803
C	-2.741697	3.621977	-1.674083
C	-3.026632	3.703485	-0.309517
C	-2.375916	2.856673	0.593334
C	-1.816269	-1.123259	0.340197
C	-3.051737	-0.990988	0.992219
C	-4.189046	-1.688029	0.611685
C	-4.075534	-2.578223	-0.448490
C	-2.875133	-2.774997	-1.118536
C	-1.756902	-2.039544	-0.725517
F	-5.175835	-3.278548	-0.829695
C	2.845783	-0.106916	0.326548
C	3.316242	-1.296467	-0.271399
C	4.666041	-1.475064	-0.532156
C	5.593609	-0.467144	-0.196713
C	5.138288	0.719007	0.401627
C	3.781617	0.892462	0.657863
H	1.103378	2.254830	0.733779
H	1.153652	1.422064	2.292896
H	-1.175147	1.154772	2.124972
H	-0.429027	1.125201	-1.593919
H	-1.583277	2.613707	-3.192477
H	-3.759051	4.419793	0.053799
H	-2.608512	2.917178	1.654375
F	-3.153432	-0.154262	2.061963
H	-5.124658	-1.549931	1.141674
H	-2.821436	-3.480021	-1.941656
H	-0.812006	-2.170910	-1.239165
H	2.604595	-2.075316	-0.524314
H	5.018213	-2.392522	-0.993722
H	5.848931	1.496820	0.663444
H	3.446873	1.814778	1.122794
H	-3.247563	4.276923	-2.378802
C	6.989282	-0.652781	-0.462347
N	8.123721	-0.805539	-0.677320

Table S1-16: Cartesian Atomic Coordinates for the Geometry Optimized Structure of Pyrazoline **2f** (B3LYP/6-31+G(d)).

Atom	x/Å	y/Å	z/Å
N	0.440288	-0.753083	0.438739
N	-0.799289	-0.344477	0.834465
C	1.305046	0.191485	0.639498
C	0.675192	1.437127	1.234277
C	-0.841476	1.122514	1.130277
C	-1.566975	1.917043	0.054653
C	-1.319467	1.687746	-1.306740
C	-1.959710	2.452084	-2.283311
C	-2.856504	3.459093	-1.911125
C	-3.113529	3.690299	-0.558374
C	-2.474172	2.919519	0.417957
C	-1.902273	-1.135989	0.497466
C	-3.151117	-0.956565	1.116652
C	-4.259680	-1.727147	0.804932
C	-4.153882	-2.750367	-0.140448
C	-2.914252	-2.945322	-0.737036
C	-1.800827	-2.170302	-0.451607
H	-4.997775	-3.379026	-0.401908
C	2.728103	0.015547	0.363196
C	3.225297	-1.183040	-0.192782
C	4.579303	-1.339833	-0.446889
C	5.482760	-0.299603	-0.146687
C	5.000348	0.896360	0.409098
C	3.639730	1.047531	0.658855
H	0.938083	2.351625	0.693213
H	0.990710	1.566549	2.277977
H	-1.338562	1.280318	2.087521
H	-0.633015	0.899412	-1.605424
H	-1.761241	2.259744	-3.334574
H	-3.816646	4.463755	-0.260119
H	-2.688445	3.094882	1.470003
F	-3.283730	-0.003730	2.086591
H	-5.194053	-1.530575	1.320951
F	-2.783717	-3.935532	-1.661180
H	-0.859621	-2.358352	-0.952271
H	2.531878	-1.985898	-0.419812
H	4.952754	-2.264140	-0.876810
H	5.693096	1.698437	0.644206
H	3.283704	1.976955	1.092426
H	-3.355115	4.053350	-2.672557
C	6.882874	-0.462951	-0.404486
N	8.020793	-0.597447	-0.612602

Table S1-17: Cartesian Atomic Coordinates for the Geometry Optimized Structure of Pyrazoline **2g** (B3LYP/6-31+G(d)).

Atom	x/Å	y/Å	z/Å
N	0.527314	-0.687892	0.042840
N	-0.738418	-0.253664	0.290741
C	1.388871	0.191083	0.447497
C	0.734820	1.395611	1.098208
C	-0.781307	1.075123	0.952876
C	-1.541709	2.127925	0.160657
C	-1.457145	2.185739	-1.237156
C	-2.111096	3.197396	-1.943030
C	-2.857974	4.163769	-1.261641
C	-2.951529	4.109178	0.131289
C	-2.296932	3.094768	0.836268
C	-1.809964	-1.137208	0.184619
C	-3.110203	-0.714864	0.526110
C	-4.152527	-1.623838	0.405142
C	-3.995511	-2.930909	-0.035681
C	-2.693431	-3.301182	-0.360774
C	-1.600117	-2.457163	-0.264678
H	-4.830250	-3.615878	-0.120458
C	2.826501	0.006864	0.267702
C	3.341723	-1.142039	-0.370389
C	4.707326	-1.307463	-0.541781
C	5.605130	-0.324525	-0.077010
C	5.104547	0.822198	0.560411
C	3.732256	0.981388	0.728923
H	0.991487	2.329926	0.587121
H	1.038632	1.500875	2.146370
H	-1.251209	0.960386	1.938089
H	-0.890766	1.429417	-1.774867
H	-2.040391	3.228510	-3.027306
H	-3.537944	4.849098	0.669903
H	-2.384659	3.050712	1.920697
H	-3.327793	0.294043	0.851671
F	-5.400608	-1.205314	0.739350
F	-2.482271	-4.571975	-0.789590
H	-0.610807	-2.809303	-0.523401
H	2.652804	-1.898481	-0.730972
H	5.093483	-2.194357	-1.034735
H	5.791895	1.582714	0.917757
H	3.363345	1.876968	1.219954
H	-3.368691	4.948289	-1.813584
C	7.016771	-0.494557	-0.255860
N	8.163357	-0.635741	-0.402763

Table S1-18: Cartesian Atomic Coordinates for the Geometry Optimized Structure of Pyrazoline **2h** (B3LYP/6-31+G(d)).

Atom	x/Å	y/Å	z/Å
N	-0.610193	0.645292	0.475003
N	0.586881	0.130056	0.878393
C	-1.550595	-0.230307	0.646989
C	-1.030201	-1.532836	1.224662
C	0.507793	-1.344905	1.133320
C	1.175759	-2.166332	0.040792
C	0.915688	-1.918770	-1.315587
C	1.509466	-2.701473	-2.306630
C	2.371499	-3.745753	-1.954929
C	2.640115	-3.996385	-0.608114
C	2.047500	-3.206950	0.382906
C	1.754993	0.829793	0.553694
C	2.972373	0.560154	1.199494
C	4.146724	1.238998	0.908826
C	4.114981	2.250718	-0.041632
C	2.918458	2.560796	-0.682522
C	1.754961	1.861188	-0.403464
F	5.237613	2.940292	-0.335200
C	-2.951176	0.069815	0.362039
C	-3.336381	1.309708	-0.192398
C	-4.669133	1.587402	-0.454706
C	-5.663426	0.630902	-0.164502
C	-5.292627	-0.605156	0.389595
C	-3.952511	-0.878232	0.646829
H	-1.366049	-2.413823	0.669010
H	-1.360365	-1.649485	2.265309
H	0.986116	-1.566116	2.087849
H	0.254840	-1.103478	-1.599571
H	1.301974	-2.495169	-3.353474
H	3.315417	-4.800006	-0.325890
H	2.269626	-3.398799	1.430404
F	3.016245	-0.390732	2.173374
H	5.065777	0.996581	1.430899
F	2.899563	3.547899	-1.604391
H	0.840325	2.116667	-0.923810
H	-2.573573	2.049226	-0.411998
H	-4.955120	2.542757	-0.883945
H	-6.055040	-1.343482	0.617826
H	-3.684422	-1.837519	1.079498
H	2.833425	-4.354454	-2.727920
C	-7.042104	0.916282	-0.431729
N	-8.163355	1.145798	-0.647086

Table S1-19: Cartesian Atomic Coordinates for the Geometry Optimized Structure of Pyrazoline **2i** (B3LYP/6-31+G(d)).

Atom	x/Å	y/Å	z/Å
N	-0.686674	-0.659330	-0.445231
N	0.549837	-0.177638	-0.770678
C	-1.580603	0.250900	-0.663832
C	-0.988326	1.540313	-1.204397
C	0.539366	1.288047	-1.084186
C	1.237931	2.113985	-0.016617
C	0.967707	1.911797	1.345252
C	1.595319	2.693922	2.315724
C	2.501878	3.690264	1.937227
C	2.780391	3.894649	0.584528
C	2.153284	3.106671	-0.386406
C	1.687130	-0.902916	-0.419060
C	2.842344	-0.828951	-1.219151
C	3.999410	-1.526756	-0.897384
C	4.058474	-2.354184	0.216221
C	2.922306	-2.441716	1.010206
C	1.765400	-1.723470	0.723551
H	4.958038	-2.907496	0.459312
C	-3.003136	0.007604	-0.433559
C	-3.452881	-1.202347	0.137024
C	-4.803811	-1.421626	0.359465
C	-5.749294	-0.434891	0.012579
C	-5.312963	0.771910	-0.557669
C	-3.955309	0.986228	-0.775851
H	-1.299746	2.422693	-0.636200
H	-1.289605	1.694834	-2.248303
H	1.036448	1.449167	-2.042539
H	0.274594	1.130917	1.649419
H	1.380232	2.523074	3.367394
H	3.489987	4.660480	0.282238
H	2.380643	3.263642	-1.438930
F	2.823825	-0.079173	-2.343550
F	5.072970	-1.410200	-1.704988
F	2.942602	-3.211042	2.117590
F	0.737382	-1.798041	1.587031
H	-2.724722	-1.960506	0.405584
H	-5.141700	-2.352720	0.803915
H	-6.038175	1.533622	-0.826647
H	-3.634138	1.923829	-1.219581
H	2.990723	4.297897	2.694352
C	-7.145986	-0.659587	0.242542
N	-8.281073	-0.841949	0.428481

Table S1-20: Cartesian Atomic Coordinates for the Geometry Optimized Structure of Pyrazoline **2j** (B3LYP/6-31+G(d)).

Atom	x/Å	y/Å	z/Å
N	-0.849602	-0.585617	-0.442186
N	0.349374	-0.024919	-0.784211
C	-1.802297	0.265633	-0.649886
C	-1.300080	1.588904	-1.198256
C	0.241790	1.438483	-1.091066
C	0.894552	2.306508	-0.027950
C	0.606215	2.122504	1.333406
C	1.193849	2.940717	2.298920
C	2.077753	3.956024	1.916666
C	2.373339	4.143399	0.565226
C	1.786492	3.319055	-0.400793
C	1.534534	-0.678083	-0.447698
C	2.654433	-0.580842	-1.291745
C	3.859724	-1.211321	-1.005211
C	3.976828	-1.994524	0.140120
C	2.884852	-2.116963	0.995751
C	1.693574	-1.452002	0.717189
F	5.126795	-2.624846	0.413943
C	-3.204289	-0.074490	-0.413515
C	-3.567048	-1.313762	0.156087
C	-4.898885	-1.629848	0.378006
C	-5.912261	-0.712661	0.032772
C	-5.562702	0.523181	-0.535071
C	-4.223727	0.834813	-0.752741
H	-1.663276	2.450538	-0.629298
H	-1.619678	1.720399	-2.239779
H	0.719864	1.632900	-2.053284
H	-0.071245	1.329493	1.641889
H	0.964966	2.783781	3.349820
H	3.064217	4.925182	0.260410
H	2.024480	3.466119	-1.452388
F	2.561930	0.124190	-2.437904
F	4.897705	-1.093011	-1.846353
F	2.998857	-2.843477	2.117165
F	0.702452	-1.545309	1.617499
H	-2.787497	-2.019535	0.423118
H	-5.168167	-2.583861	0.820728
H	-6.340225	1.231687	-0.803477
H	-3.972709	1.793985	-1.195910
H	2.534379	4.593060	2.669660
C	-7.289931	-1.034930	0.261567
N	-8.410493	-1.292385	0.446209

Table S2-1: Cartesian Atomic Coordinates for the Geometry Optimized Structure of the Pyrazoline **1a** Radical Anion (B3LYP/6-31+G(d)).

Atom	x/Å	y/Å	z/Å
N	0.561718	-1.123970	-0.020652
N	-0.684872	-0.724314	0.472382
C	1.485216	-0.295431	0.507378
C	0.871161	0.673988	1.499339
C	-0.638819	0.572951	1.159301
C	-1.130233	1.728321	0.296619
C	-0.834534	1.775109	-1.075872
C	-1.252414	2.857084	-1.852573
C	-1.971446	3.911069	-1.276018
C	-2.269557	3.872994	0.090367
C	-1.852630	2.786816	0.865531
C	-1.811597	-1.457953	0.226597
C	-3.097275	-1.033097	0.657797
C	-4.222273	-1.821134	0.424278
C	-4.129045	-3.044783	-0.253935
C	-2.863541	-3.460078	-0.695617
C	-1.723156	-2.695936	-0.471800
H	-5.013760	-3.648992	-0.440685
C	2.868453	-0.370706	0.196146
C	3.376970	-1.344352	-0.732499
C	4.728820	-1.423438	-1.027809
C	5.668526	-0.556095	-0.430823
C	5.191655	0.402208	0.486921
C	3.840576	0.495472	0.796616
H	6.728477	-0.631201	-0.663359
H	1.233720	1.703642	1.404585
H	1.046205	0.359078	2.542468
H	-1.246610	0.533626	2.072178
H	-0.285599	0.951322	-1.523393
H	-1.020125	2.876292	-2.915341
H	-2.829619	4.684965	0.550566
H	-2.090223	2.757123	1.928682
H	-3.215113	-0.080745	1.164325
H	-5.191263	-1.463394	0.770036
H	-2.762467	-4.403698	-1.230991
H	-0.748248	-3.022497	-0.811940
H	2.670926	-2.024574	-1.199851
H	5.069758	-2.175648	-1.740200
H	5.892067	1.087733	0.965048
H	3.516153	1.248040	1.512952
H	-2.301329	4.748854	-1.886857

Table S2-2: Cartesian Atomic Coordinates for the Geometry Optimized Structure of the Pyrazoline **1b** Radical Anion (B3LYP/6-31+G(d)).

Atom	x/Å	y/Å	z/Å
N	0.728400	-1.091550	0.052016
N	-0.507628	-0.740584	0.614170
C	1.650467	-0.247643	0.547830
C	1.039343	0.750447	1.510433
C	-0.468571	0.631407	1.187804
C	-0.973310	1.693781	0.224672
C	-0.442955	1.821502	-1.074834
C	-0.900792	2.825367	-1.929995
C	-1.893678	3.720681	-1.514564
C	-2.432603	3.597007	-0.228917
C	-1.975535	2.589987	0.625910
C	-1.633286	-1.391764	0.165889
C	-2.925664	-1.201147	0.706574
C	-4.046540	-1.891976	0.283665
C	-3.930701	-2.866285	-0.720861
C	-2.664602	-3.105298	-1.265464
C	-1.544207	-2.391504	-0.843654
H	-4.804226	-3.420055	-1.054949
C	3.033828	-0.333159	0.228786
C	3.538750	-1.346115	-0.657216
C	4.890955	-1.440677	-0.949629
C	5.830797	-0.549769	-0.391504
C	5.356171	0.451124	0.480429
C	4.004777	0.560814	0.784696
H	6.890950	-0.636951	-0.618589
H	1.403237	1.776512	1.379113
H	1.226204	0.469492	2.560859
H	-1.076525	0.666074	2.092154
H	0.324112	1.129480	-1.409344
H	-0.479482	2.908100	-2.930017
H	-3.214723	4.275939	0.105514
H	-2.411536	2.486218	1.617924
F	-3.103151	-0.302160	1.737856
H	-4.997637	-1.667614	0.759397
H	-2.541280	-3.858535	-2.041888
H	-0.565895	-2.577004	-1.268023
H	2.831148	-2.044016	-1.095175
H	5.229992	-2.224305	-1.628157
H	6.058217	1.154795	0.928452
H	3.681636	1.345981	1.465709
H	-2.247097	4.499586	-2.187279

Table S2-3: Cartesian Atomic Coordinates for the Geometry Optimized Structure of the Pyrazoline **1c** Radical Anion (B3LYP/6-31+G(d)).

Atom	x/Å	y/Å	z/Å
N	0.765566	-1.098116	-0.086583
N	-0.467677	-0.630118	0.376749
C	1.721600	-0.342267	0.491311
C	1.138877	0.646740	1.483153
C	-0.364247	0.645543	1.102722
C	-0.773380	1.845435	0.260608
C	-0.395025	1.935056	-1.089353
C	-0.741679	3.054586	-1.846961
C	-1.470472	4.104047	-1.273733
C	-1.853096	4.021644	0.069197
C	-1.506222	2.898364	0.825806
C	-1.623187	-1.302275	0.115041
C	-2.891456	-0.793561	0.513067
C	-4.025277	-1.537955	0.244304
C	-4.023739	-2.764497	-0.412258
C	-2.766698	-3.250450	-0.812769
C	-1.590689	-2.553872	-0.568801
H	-4.950204	-3.295053	-0.604773
C	3.107148	-0.494754	0.220383
C	3.587107	-1.470619	-0.720485
C	4.941277	-1.620961	-0.976416
C	5.909116	-0.827471	-0.325140
C	5.460005	0.131324	0.605553
C	4.107188	0.296012	0.875584
H	6.970019	-0.957580	-0.526754
H	1.572142	1.651562	1.413037
H	1.267629	0.307951	2.525132
H	-0.997851	0.611219	1.998115
H	0.161026	1.114982	-1.535285
H	-0.446387	3.107445	-2.892756
H	-2.427607	4.826141	0.524503
H	-1.810065	2.834353	1.870218
H	-2.998605	0.167198	1.001937
F	-5.236708	-1.017469	0.643950
H	-2.711425	-4.204700	-1.334229
H	-0.628777	-2.942276	-0.878162
H	2.858175	-2.092902	-1.231510
H	5.260602	-2.370048	-1.701855
H	6.183425	0.759739	1.125767
H	3.803848	1.044518	1.605200
H	-1.743714	4.971914	-1.870169

Table S2-4: Cartesian Atomic Coordinates for the Geometry Optimized Structure of the Pyrazoline **1d** Radical Anion (B3LYP/6-31+G(d)).

Atom	x/Å	y/Å	z/Å
N	0.670511	-1.054100	0.013817
N	-0.481679	-0.458355	0.538102
C	1.726627	-0.367272	0.493160
C	1.302320	0.721634	1.459779
C	-0.218356	0.836359	1.180506
C	-0.576021	2.025209	0.298001
C	-0.249924	2.025835	-1.069771
C	-0.542299	3.133965	-1.865517
C	-1.165873	4.261108	-1.315344
C	-1.497901	4.267535	0.043715
C	-1.205386	3.155414	0.838956
C	-1.718598	-0.995288	0.304910
C	-2.905019	-0.385222	0.788951
C	-4.153678	-0.971836	0.578526
C	-4.235128	-2.164899	-0.129362
C	-3.099370	-2.786112	-0.633536
C	-1.846799	-2.211044	-0.424970
F	-5.474834	-2.736974	-0.345502
C	3.074571	-0.679105	0.171794
C	3.406255	-1.761005	-0.715020
C	4.724230	-2.077320	-1.006006
C	5.799140	-1.354225	-0.446894
C	5.495713	-0.289899	0.425936
C	4.181144	0.041445	0.729596
H	6.830041	-1.616647	-0.673737
H	1.808068	1.681414	1.302434
H	1.478772	0.429153	2.508826
H	-0.787356	0.912043	2.116337
H	0.223598	1.147598	-1.499644
H	-0.286521	3.117365	-2.922941
H	-1.987280	5.135063	0.482584
H	-1.468785	3.161613	1.896519
H	-2.855632	0.554693	1.327817
H	-5.057637	-0.499185	0.952941
H	-3.195108	-3.714774	-1.190527
H	-0.947899	-2.678767	-0.805738
H	2.593717	-2.334424	-1.151653
H	4.930242	-2.906278	-1.684094
H	6.303686	0.289430	0.873561
H	3.992406	0.869488	1.410263
H	-1.396530	5.120509	-1.941310

Table S2-5: Cartesian Atomic Coordinates for the Geometry Optimized Structure of the Pyrazoline **1e** Radical Anion (B3LYP/6-31+G(d)).

Atom	x/Å	y/Å	z/Å
N	-0.839385	-1.053346	-0.163843
N	0.313739	-0.517662	-0.762827
C	-1.881756	-0.305452	-0.563928
C	-1.448075	0.823388	-1.476885
C	0.076249	0.877982	-1.225915
C	0.491095	1.926427	-0.206515
C	-0.015087	1.912820	1.109567
C	0.359785	2.900154	2.022092
C	1.242513	3.920406	1.647782
C	1.757634	3.937227	0.346128
C	1.386324	2.945291	-0.565352
C	1.533479	-1.007699	-0.341173
C	2.766649	-0.633699	-0.916314
C	3.990563	-1.163210	-0.536375
C	3.999406	-2.144001	0.452977
C	2.827324	-2.582695	1.046279
C	1.609973	-2.015590	0.658294
F	5.206607	-2.692236	0.825844
C	-3.229296	-0.584343	-0.202095
C	-3.569100	-1.697548	0.639829
C	-4.887328	-1.976653	0.968364
C	-5.950927	-1.184095	0.489625
C	-5.638956	-0.089003	-0.340549
C	-4.324139	0.206558	-0.678290
H	-6.982291	-1.417791	0.744045
H	-1.924583	1.785607	-1.257219
H	-1.652673	0.590389	-2.535644
H	0.626638	1.052784	-2.151561
H	-0.698111	1.123046	1.408160
H	-0.040183	2.872373	3.033852
H	2.452806	4.718062	0.043126
H	1.802506	2.953878	-1.570936
F	2.790714	0.282353	-1.939225
H	4.903234	-0.826560	-1.015943
H	2.860926	-3.354487	1.810328
H	0.678540	-2.338628	1.104285
H	-2.764757	-2.325678	1.011452
H	-5.101946	-2.831153	1.610973
H	-6.439220	0.541192	-0.728902
H	-4.125706	1.057198	-1.327172
H	1.530457	4.688183	2.362985

Table S2-6: Cartesian Atomic Coordinates for the Geometry Optimized Structure of the Pyrazoline **1f** Radical Anion (B3LYP/6-31+G(d)).

Atom	x/Å	y/Å	z/Å
N	-0.738207	-0.981794	-0.255609
N	0.426531	-0.416448	-0.793767
C	-1.767885	-0.187815	-0.603673
C	-1.312742	0.985999	-1.445592
C	0.212387	0.998849	-1.187665
C	0.634743	1.979012	-0.103463
C	0.312193	1.755608	1.247256
C	0.673647	2.685094	2.224356
C	1.360179	3.854174	1.876470
C	1.691836	4.081128	0.536621
C	1.333572	3.147275	-0.439833
C	1.633112	-0.982845	-0.473369
C	2.879064	-0.558976	-0.998294
C	4.081899	-1.165355	-0.693796
C	4.121845	-2.281623	0.161923
C	2.901913	-2.716927	0.663600
C	1.685723	-2.118310	0.386127
H	5.048109	-2.786270	0.413519
C	-3.120096	-0.460331	-0.259524
C	-3.484079	-1.603677	0.530021
C	-4.808667	-1.871707	0.841648
C	-5.855040	-1.037555	0.396704
C	-5.519164	0.088236	-0.380844
C	-4.197711	0.373459	-0.701080
H	-6.891525	-1.262408	0.637934
H	-1.778482	1.940405	-1.173915
H	-1.515464	0.818108	-2.517413
H	0.767159	1.219748	-2.100224
H	-0.210338	0.843955	1.523791
H	0.420550	2.493101	3.265003
H	2.237146	4.979197	0.252293
H	1.607262	3.322974	-1.478590
F	2.919225	0.490305	-1.890579
H	4.987563	-0.767013	-1.142064
F	2.901635	-3.809091	1.498982
H	0.763779	-2.493914	0.808579
H	-2.692881	-2.260561	0.879583
H	-5.041972	-2.749408	1.445122
H	-6.305727	0.750908	-0.742072
H	-3.980353	1.249736	-1.308614
H	1.638809	4.575944	2.641492

Table S2-7: Cartesian Atomic Coordinates for the Geometry Optimized Structure of the Pyrazoline **1g** Radical Anion (B3LYP/6-31+G(d)).

Atom	x/Å	y/Å	z/Å
N	0.776689	0.984965	-0.008133
N	-0.385923	0.348361	-0.449182
C	1.823205	0.307293	-0.525670
C	1.374401	-0.797319	-1.463045
C	-0.125267	-0.946518	-1.098395
C	-0.403818	-2.137053	-0.191486
C	-0.048839	-2.106187	1.167398
C	-0.267473	-3.220441	1.979287
C	-0.843407	-4.382386	1.451988
C	-1.200774	-4.420887	0.100249
C	-0.982454	-3.303481	-0.710755
C	-1.611646	0.903435	-0.262065
C	-2.806858	0.228091	-0.647994
C	-4.019482	0.861221	-0.458601
C	-4.174883	2.127403	0.103797
C	-2.980751	2.746815	0.478767
C	-1.725360	2.198914	0.326957
H	-5.144244	2.587033	0.249065
C	3.176135	0.640048	-0.251732
C	3.517339	1.726856	0.624671
C	4.838207	2.060213	0.880382
C	5.906015	1.350583	0.291988
C	5.593299	0.283466	-0.573234
C	4.275370	-0.064895	-0.841954
H	6.939201	1.624921	0.492459
H	1.909562	-1.744125	-1.329481
H	1.483280	-0.505699	-2.521341
H	-0.746911	-1.037280	-1.997439
H	0.388791	-1.200734	1.578428
H	0.008448	-3.180493	3.030868
H	-1.653739	-5.316376	-0.320528
H	-1.266399	-3.333123	-1.762341
H	-2.794402	-0.770617	-1.065890
F	-5.158719	0.195031	-0.841752
F	-3.076776	3.996605	1.037894
H	-0.835758	2.733712	0.630639
H	2.709514	2.288529	1.084489
H	5.051447	2.891126	1.553554
H	6.396505	-0.285003	-1.042568
H	4.078953	-0.895177	-1.517767
H	-1.017929	-5.245724	2.090458

Table S2-8: Cartesian Atomic Coordinates for the Geometry Optimized Structure of the Pyrazoline **1h** Radical Anion (B3LYP/6-31+G(d)).

Atom	x/Å	y/Å	z/Å
N	-0.884625	-0.949708	-0.318531
N	0.201024	-0.250922	-0.868619
C	-2.000214	-0.264205	-0.623629
C	-1.694673	0.979939	-1.430901
C	-0.173505	1.149813	-1.207011
C	0.172527	2.136622	-0.103219
C	-0.198853	1.895959	1.233788
C	0.107780	2.822966	2.231320
C	0.783614	4.008754	1.920424
C	1.156919	4.256727	0.594973
C	0.855021	3.324949	-0.402126
C	1.466870	-0.674666	-0.538682
C	2.652739	-0.115819	-1.066310
C	3.921385	-0.584781	-0.768817
C	4.054319	-1.685494	0.078540
C	2.914356	-2.278273	0.600971
C	1.645300	-1.795399	0.320661
F	5.294926	-2.186865	0.359804
C	-3.305944	-0.696011	-0.258347
C	-3.517697	-1.896094	0.500784
C	-4.794280	-2.317957	0.840958
C	-5.938436	-1.591281	0.453558
C	-5.752668	-0.413117	-0.295614
C	-4.480881	0.025342	-0.643482
H	-6.936050	-1.934266	0.717868
H	-2.250181	1.866973	-1.105823
H	-1.907432	0.834517	-2.503785
H	0.332350	1.453676	-2.124799
H	-0.717998	0.975381	1.484255
H	-0.179928	2.615832	3.260035
H	1.691737	5.169204	0.338180
H	1.162671	3.516969	-1.428209
F	2.577845	0.929077	-1.954430
H	4.793121	-0.109644	-1.205031
F	3.052080	-3.361142	1.418909
H	0.769443	-2.267402	0.744984
H	-2.649643	-2.472119	0.807463
H	-4.910464	-3.233538	1.421453
H	-6.618292	0.167503	-0.614815
H	-4.381135	0.936734	-1.229494
H	1.021279	4.727114	2.702184

Table S2-9: Cartesian Atomic Coordinates for the Geometry Optimized Structure of the Pyrazoline **1i** Radical Anion (B3LYP/6-31+G(d)).

Atom	x/Å	y/Å	z/Å
N	-1.024594	-0.921714	-0.375667
N	0.147927	-0.285110	-0.775036
C	-2.053240	-0.110549	-0.661621
C	-1.604676	1.140795	-1.388344
C	-0.078063	1.145496	-1.138515
C	0.363792	2.089601	-0.032139
C	-0.061767	1.900980	1.296038
C	0.328845	2.789630	2.297655
C	1.149592	3.884668	1.997195
C	1.579839	4.078318	0.680976
C	1.191694	3.183675	-0.321157
C	1.374056	-0.778493	-0.400179
C	2.545750	-0.511012	-1.164438
C	3.776249	-1.059423	-0.862789
C	3.957374	-1.947883	0.199095
C	2.820374	-2.225142	0.957547
C	1.579979	-1.663752	0.701599
H	4.919994	-2.389545	0.422818
C	-3.409407	-0.439929	-0.378183
C	-3.760239	-1.640394	0.325380
C	-5.083394	-1.959992	0.587254
C	-6.140155	-1.124548	0.168972
C	-5.816885	0.053660	-0.530231
C	-4.495683	0.390420	-0.800988
H	-7.175698	-1.387561	0.372338
H	-2.076273	2.058004	-1.017520
H	-1.814346	1.080556	-2.469587
H	0.473335	1.387066	-2.048772
H	-0.689283	1.046765	1.536531
H	-0.003580	2.623508	3.320177
H	2.225827	4.918846	0.434762
H	1.539612	3.333541	-1.341608
F	2.454758	0.285463	-2.267554
F	4.842091	-0.745710	-1.653226
F	2.945295	-3.043016	2.039704
F	0.587350	-1.921309	1.581652
H	-2.959021	-2.295531	0.654492
H	-5.307541	-2.878368	1.130321
H	-6.612658	0.716166	-0.870941
H	-4.287452	1.304505	-1.353618
H	1.454089	4.574208	2.781581

Table S2-10: Cartesian Atomic Coordinates for the Geometry Optimized Structure of the Pyrazoline **1j** Radical Anion (B3LYP/6-31+G(d)).

Atom	x/Å	y/Å	z/Å
N	-1.122082	-0.880738	-0.448647
N	-0.041271	-0.131670	-0.811634
C	-2.230417	-0.204247	-0.675031
C	-1.947985	1.125403	-1.352523
C	-0.416906	1.271783	-1.155706
C	-0.038159	2.273036	-0.073403
C	-0.317271	2.022943	1.279382
C	-0.013464	2.973909	2.253644
C	0.575278	4.192825	1.895606
C	0.859587	4.449398	0.552663
C	0.553311	3.494154	-0.422034
C	1.249375	-0.494992	-0.402782
C	2.374723	-0.284483	-1.237959
C	3.613274	-0.816745	-0.966319
C	3.828299	-1.601321	0.180217
C	2.739385	-1.805057	1.035918
C	1.510097	-1.236747	0.781883
F	4.874825	-2.515842	0.182107
C	-3.540690	-0.725048	-0.376458
C	-3.713361	-1.958479	0.312951
C	-4.981205	-2.450058	0.594263
C	-6.136403	-1.747064	0.206277
C	-5.984180	-0.533054	-0.477036
C	-4.716252	-0.030624	-0.765911
H	-7.126262	-2.137770	0.430024
H	-2.499511	1.965685	-0.917005
H	-2.201167	1.086976	-2.423881
H	0.083076	1.556507	-2.083926
H	-0.751005	1.070194	1.568699
H	-0.226656	2.757949	3.298025
H	1.331753	5.385423	0.261633
H	0.789636	3.693580	-1.465482
F	2.244229	0.555521	-2.319607
F	4.678547	-0.490983	-1.766851
F	2.934634	-2.483312	2.209835
F	0.570269	-1.260187	1.773445
H	-2.828474	-2.506027	0.623092
H	-5.077255	-3.393938	1.128913
H	-6.863224	0.028622	-0.789868
H	-4.631054	0.910976	-1.303227
H	0.818865	4.928707	2.658764

Table S2-11: Cartesian Atomic Coordinates for the Geometry Optimized Structure of the Pyrazoline **2a** Radical Anion (B3LYP/6-31+G(d)).

Atom	x/Å	y/Å	z/Å
N	0.227126	-1.012928	-0.048907
N	-1.086016	-0.680628	0.286982
C	1.032464	-0.059731	0.419996
C	0.274835	1.016331	1.182291
C	-1.210030	0.599078	1.000736
C	-2.023508	1.641299	0.241643
C	-1.912049	1.764794	-1.150579
C	-2.624527	2.750770	-1.835724
C	-3.465085	3.627836	-1.140347
C	-3.587496	3.507819	0.246192
C	-2.870871	2.519876	0.928971
C	-2.090901	-1.608577	0.160254
C	-3.422141	-1.320865	0.554900
C	-4.429203	-2.273447	0.403244
C	-4.161327	-3.534159	-0.142952
C	-2.844805	-3.822458	-0.531295
C	-1.821521	-2.891233	-0.388130
H	-4.953193	-4.268966	-0.266896
C	2.439651	-0.058774	0.240809
C	3.110871	-1.113675	-0.473088
C	4.475003	-1.117133	-0.645766
C	5.295651	-0.068568	-0.122393
C	4.642469	0.982913	0.589762
C	3.274339	0.984997	0.763953
H	0.453103	2.020800	0.778330
H	0.558415	1.042755	2.243803
H	-1.690535	0.430814	1.976452
H	-1.271231	1.073376	-1.691791
H	-2.526369	2.832841	-2.915953
H	-4.246525	4.176290	0.796817
H	-2.980031	2.423033	2.008362
H	-3.672365	-0.345680	0.958463
H	-5.441639	-2.016979	0.711210
H	-2.607423	-4.797328	-0.954937
H	-0.805513	-3.123468	-0.682257
H	2.509811	-1.920591	-0.881315
H	4.948594	-1.931624	-1.189944
H	5.240976	1.793762	0.999036
H	2.822403	1.809423	1.311463
H	-4.024312	4.391925	-1.675858
C	6.695858	-0.070287	-0.303505
N	7.861713	-0.068047	-0.455048

Table S2-12: Cartesian Atomic Coordinates for the Geometry Optimized Structure of the Pyrazoline **2b** Radical Anion (B3LYP/6-31+G(d)).

Atom	x/Å	y/Å	z/Å
N	0.257291	-1.031915	0.158733
N	-1.018481	-0.724570	0.653231
C	1.114185	-0.131836	0.644153
C	0.419540	0.882573	1.537311
C	-1.071101	0.659701	1.191678
C	-1.620887	1.674134	0.197964
C	-1.102395	1.783944	-1.104639
C	-1.595191	2.749099	-1.984480
C	-2.613715	3.621934	-1.584676
C	-3.140364	3.516625	-0.294478
C	-2.647155	2.547410	0.584362
C	-2.088633	-1.445424	0.166879
C	-3.409728	-1.304861	0.647714
C	-4.477227	-2.055779	0.189261
C	-4.270560	-3.037735	-0.789311
C	-2.972187	-3.227055	-1.274160
C	-1.907335	-2.453438	-0.816592
H	-5.100960	-3.638649	-1.149840
C	2.509206	-0.164253	0.383642
C	3.098325	-1.201298	-0.423150
C	4.450719	-1.247160	-0.669851
C	5.338889	-0.263244	-0.135511
C	4.767869	0.771378	0.666067
C	3.411742	0.816285	0.913610
H	0.729219	1.917286	1.356209
H	0.606460	0.664238	2.600327
H	-1.694333	0.681120	2.086152
H	-0.313175	1.110187	-1.425750
H	-1.181329	2.819804	-2.988061
H	-3.940862	4.179908	0.026626
H	-3.072624	2.456958	1.582023
F	-3.670176	-0.397884	1.650649
H	-5.457632	-1.870400	0.619718
H	-2.779448	-3.986684	-2.029162
H	-0.903828	-2.602839	-1.193616
H	2.444534	-1.962285	-0.838422
H	4.860759	-2.047128	-1.282978
H	5.420182	1.534276	1.085177
H	3.023288	1.623632	1.530734
H	-2.994852	4.371833	-2.274560
C	6.727783	-0.312029	-0.388397
N	7.883406	-0.349820	-0.598366

Table S2-13: Cartesian Atomic Coordinates for the Geometry Optimized Structure of the Pyrazoline **2c** Radical Anion (B3LYP/6-31+G(d)).

Atom	x/Å	y/Å	z/Å
N	0.330567	-0.996882	-0.022408
N	-0.947601	-0.601475	0.375916
C	1.209688	-0.159651	0.536440
C	0.532347	0.852446	1.448733
C	-0.965046	0.686149	1.083291
C	-1.502935	1.831355	0.233549
C	-1.235836	1.892881	-1.141361
C	-1.688884	2.972078	-1.902129
C	-2.418356	4.005142	-1.302513
C	-2.693969	3.948518	0.066521
C	-2.238034	2.866739	0.825898
C	-2.040058	-1.380681	0.117037
C	-3.348510	-0.957873	0.472157
C	-4.417708	-1.793713	0.200812
C	-4.304748	-3.034653	-0.414343
C	-3.006091	-3.437938	-0.767076
C	-1.892637	-2.646023	-0.517706
H	-5.182400	-3.641765	-0.608939
C	2.609813	-0.234169	0.326250
C	3.192349	-1.234251	-0.530541
C	4.549924	-1.306725	-0.738680
C	5.450418	-0.391908	-0.109321
C	4.886575	0.600873	0.747863
C	3.525406	0.673403	0.956541
H	0.876540	1.880153	1.288893
H	0.705935	0.610833	2.508438
H	-1.581053	0.600667	1.987949
H	-0.677880	1.084828	-1.606935
H	-1.474669	3.005738	-2.967954
H	-3.268742	4.740691	0.541915
H	-2.458926	2.821916	1.891750
H	-3.539564	0.005495	0.929121
F	-5.670558	-1.354862	0.557794
H	-2.865222	-4.402131	-1.251874
H	-0.896863	-2.972495	-0.789035
H	2.529134	-1.941743	-1.019178
H	4.955162	-2.072510	-1.396892
H	5.548147	1.310415	1.239871
H	3.142540	1.445285	1.620831
H	-2.773699	4.842352	-1.899010
C	6.844239	-0.465109	-0.326821
N	8.004019	-0.522400	-0.507322

Table S2-14: Cartesian Atomic Coordinates for the Geometry Optimized Structure of the Pyrazoline **2d** Radical Anion (B3LYP/6-31+G(d)).

Atom	x/Å	y/Å	z/Å
N	0.244072	-0.896371	0.031481
N	-0.996588	-0.390526	0.421032
C	1.190056	-0.110493	0.554405
C	0.600274	0.966471	1.453605
C	-0.911372	0.901592	1.110686
C	-1.374618	2.076073	0.255901
C	-1.127159	2.101094	-1.124054
C	-1.498908	3.207781	-1.889501
C	-2.127172	4.305224	-1.289691
C	-2.383063	4.285911	0.084371
C	-2.008831	3.176369	0.848275
C	-2.142631	-1.121129	0.232273
C	-3.419422	-0.603402	0.567391
C	-4.573528	-1.367719	0.383364
C	-4.466165	-2.646387	-0.146139
C	-3.233658	-3.183811	-0.498780
C	-2.076185	-2.431025	-0.314315
F	-5.608745	-3.395215	-0.334891
C	2.576784	-0.290601	0.320893
C	3.066414	-1.357576	-0.513260
C	4.410023	-1.538471	-0.743764
C	5.389546	-0.673832	-0.163273
C	4.918008	0.387108	0.667925
C	3.570483	0.567122	0.900353
H	1.012724	1.964931	1.271653
H	0.771373	0.731796	2.515346
H	-1.520232	0.873733	2.024627
H	-0.647152	1.243962	-1.588683
H	-1.299103	3.213382	-2.958636
H	-2.875260	5.131292	0.560828
H	-2.212598	3.161291	1.918540
H	-3.517338	0.405926	0.952193
H	-5.550498	-0.966116	0.637587
H	-3.180954	-4.186625	-0.914206
H	-1.104909	-2.831721	-0.575992
H	2.342990	-2.028908	-0.966250
H	4.742642	-2.354262	-1.382440
H	5.639726	1.063587	1.120514
H	3.260584	1.390572	1.540638
H	-2.418601	5.164537	-1.889378
C	6.768856	-0.862422	-0.401165
N	7.916645	-1.019917	-0.598989

Table S2-15: Cartesian Atomic Coordinates for the Geometry Optimized Structure of the Pyrazoline **2e** Radical Anion (B3LYP/6-31+G(d)).

Atom	x/Å	y/Å	z/Å
N	0.405310	-0.921052	0.275297
N	-0.817120	-0.466278	0.795444
C	1.358441	-0.079127	0.681954
C	0.789752	1.047999	1.528175
C	-0.722787	0.953336	1.228150
C	-1.199099	1.942002	0.172895
C	-0.678467	1.929813	-1.134093
C	-1.103945	2.867642	-2.076150
C	-2.055041	3.836259	-1.734668
C	-2.583911	3.852396	-0.441022
C	-2.159763	2.909130	0.499752
C	-1.970531	-1.080445	0.344393
C	-3.250651	-0.797627	0.867125
C	-4.410119	-1.436085	0.455938
C	-4.300848	-2.433307	-0.507858
C	-3.073734	-2.786258	-1.047285
C	-1.924877	-2.111372	-0.628431
F	-5.440879	-3.084199	-0.912889
C	2.736482	-0.246567	0.386735
C	3.215271	-1.364305	-0.383204
C	4.552769	-1.534592	-0.657495
C	5.533523	-0.607305	-0.188602
C	5.072470	0.506674	0.575412
C	3.731684	0.677133	0.849317
H	1.193037	2.035589	1.280200
H	0.984161	0.871833	2.597690
H	-1.316857	1.096968	2.131421
H	0.058933	1.180628	-1.407491
H	-0.689617	2.842459	-3.081718
H	-3.331244	4.593367	-0.164559
H	-2.586232	2.916555	1.500863
F	-3.385609	0.136057	1.863499
H	-5.365014	-1.169699	0.895697
H	-3.013294	-3.574087	-1.792520
H	-0.954623	-2.366392	-1.034525
H	2.490171	-2.085809	-0.747853
H	4.879139	-2.392670	-1.241505
H	5.796487	1.229747	0.944320
H	3.427739	1.541386	1.435794
H	-2.382832	4.566754	-2.471062
C	6.907141	-0.788938	-0.464977
N	8.049792	-0.940112	-0.693112

Table S2-16: Cartesian Atomic Coordinates for the Geometry Optimized Structure of the Pyrazoline **2f** Radical Anion (B3LYP/6-31+G(d)).

Atom	x/Å	y/Å	z/Å
N	0.327406	-0.854309	0.365135
N	-0.910362	-0.388833	0.830268
C	1.255644	0.045028	0.702076
C	0.656991	1.220147	1.456151
C	-0.856659	1.049954	1.185288
C	-1.375994	1.955880	0.076544
C	-1.083194	1.700747	-1.272123
C	-1.534590	2.565426	-2.271492
C	-2.285237	3.699323	-1.942379
C	-2.588320	3.957197	-0.602737
C	-2.138401	3.087860	0.395245
C	-2.038425	-1.089404	0.478878
C	-3.342465	-0.762061	0.924239
C	-4.467986	-1.485284	0.579895
C	-4.360909	-2.625316	-0.232017
C	-3.081613	-2.968266	-0.651610
C	-1.941367	-2.251774	-0.333139
H	-5.223187	-3.219088	-0.514188
C	2.636994	-0.105713	0.416496
C	3.143495	-1.248518	-0.295819
C	4.485194	-1.399339	-0.560838
C	5.441568	-0.425936	-0.137381
C	4.952884	0.713266	0.568994
C	3.607680	0.865221	0.832021
H	1.023736	2.194197	1.114227
H	0.869244	1.148668	2.534404
H	-1.441356	1.229955	2.088288
H	-0.506543	0.817785	-1.533560
H	-1.300315	2.351569	-3.311875
H	-3.181921	4.828617	-0.333824
H	-2.389893	3.284991	1.435701
F	-3.521695	0.308528	1.769547
H	-5.428965	-1.156670	0.964666
F	-2.938190	-4.081402	-1.439661
H	-0.968703	-2.559800	-0.692458
H	2.436516	-2.002559	-0.628431
H	4.833725	-2.276011	-1.102594
H	5.659260	1.469637	0.903624
H	3.280468	1.749526	1.374047
H	-2.635114	4.370569	-2.723624
C	6.819925	-0.586815	-0.404720
N	7.965918	-0.720467	-0.625805

Table S2-17: Cartesian Atomic Coordinates for the Geometry Optimized Structure of the Pyrazoline **2g** Radical Anion (B3LYP/6-31+G(d)).

Atom	x/Å	y/Å	z/Å
N	0.376787	-0.824844	0.068646
N	-0.866536	-0.311055	0.438110
C	1.317888	-0.029833	0.590391
C	0.718205	1.061049	1.465132
C	-0.783865	1.006406	1.085831
C	-1.211754	2.153114	0.178271
C	-0.919088	2.135651	-1.192922
C	-1.263560	3.219509	-2.002675
C	-1.907623	4.335146	-1.455979
C	-2.206438	4.358460	-0.090794
C	-1.859990	3.272094	0.717778
C	-2.008915	-1.028568	0.244941
C	-3.285892	-0.485720	0.560223
C	-4.407560	-1.269551	0.363447
C	-4.386089	-2.567880	-0.138920
C	-3.114662	-3.055524	-0.445375
C	-1.940797	-2.350288	-0.279693
H	-5.286571	-3.150541	-0.286979
C	2.706056	-0.213728	0.370653
C	3.200470	-1.293415	-0.443062
C	4.545718	-1.475190	-0.664713
C	5.519277	-0.598652	-0.094466
C	5.043450	0.473982	0.717254
C	3.694506	0.655257	0.941045
H	1.143555	2.054070	1.284600
H	0.859008	0.832928	2.532664
H	-1.416562	1.013866	1.981990
H	-0.426058	1.264908	-1.616807
H	-1.031167	3.192009	-3.064748
H	-2.712315	5.218128	0.343592
H	-2.096555	3.289944	1.781071
H	-3.407592	0.527608	0.921652
F	-5.628200	-0.730493	0.677876
F	-3.037332	-4.329867	-0.940108
H	-0.982118	-2.785716	-0.527444
H	2.480450	-1.973313	-0.888345
H	4.883042	-2.300803	-1.287844
H	5.762174	1.158736	1.161824
H	3.380153	1.488502	1.566088
H	-2.178484	5.176103	-2.090236
C	6.900940	-0.786975	-0.324449
N	8.049344	-0.943423	-0.515684

Table S2-18: Cartesian Atomic Coordinates for the Geometry Optimized Structure of the Pyrazoline **2h** Radical Anion (B3LYP/6-31+G(d)).

Atom	x/Å	y/Å	z/Å
N	-0.496130	0.750218	0.420818
N	0.688420	0.174948	0.907474
C	-1.501052	-0.078848	0.714633
C	-1.015392	-1.321130	1.441199
C	0.511245	-1.270532	1.198764
C	0.972404	-2.170960	0.060471
C	0.683977	-1.862014	-1.278904
C	1.080664	-2.721076	-2.305507
C	1.770384	-3.903457	-2.015207
C	2.067926	-4.216053	-0.686072
C	1.672942	-3.352420	0.339957
C	1.878501	0.772300	0.556229
C	3.138449	0.351171	1.038531
C	4.330081	0.976884	0.713513
C	4.303333	2.097608	-0.112866
C	3.083289	2.559187	-0.588352
C	1.892854	1.921100	-0.277676
F	5.463297	2.742081	-0.428058
C	-2.860525	0.193419	0.414192
C	-3.259356	1.394536	-0.269789
C	-4.580010	1.664080	-0.546070
C	-5.619542	0.763254	-0.160935
C	-5.238154	-0.431628	0.518704
C	-3.914209	-0.703135	0.792386
H	-1.455423	-2.250175	1.063909
H	-1.239808	-1.264524	2.517938
H	1.062947	-1.535688	2.101806
H	0.153847	-0.942554	-1.511550
H	0.850893	-2.465429	-3.337426
H	2.614358	-5.126080	-0.446917
H	1.919593	-3.593290	1.372376
F	3.216435	-0.710791	1.902418
H	5.266262	0.604962	1.115323
F	3.061542	3.661043	-1.386965
H	0.954315	2.294663	-0.665179
H	-2.487395	2.097019	-0.569172
H	-4.847448	2.580726	-1.067381
H	-6.009738	-1.134184	0.825146
H	-3.668949	-1.623278	1.318070
H	2.077248	-4.569939	-2.818217
C	-6.976525	1.046550	-0.437242
N	-8.105131	1.281083	-0.663298

Table S2-19: Cartesian Atomic Coordinates for the Geometry Optimized Structure of the Pyrazoline **2i** Radical Anion (B3LYP/6-31+G(d)).

Atom	x/Å	y/Å	z/Å
N	-0.624350	0.767614	0.430493
N	0.610792	0.227329	0.795759
C	-1.567000	-0.133170	0.707693
C	-0.994185	-1.386168	1.350116
C	0.525877	-1.227708	1.116971
C	1.071527	-2.093275	-0.008767
C	0.690568	-1.868813	-1.342446
C	1.181471	-2.680565	-2.365521
C	2.060312	-3.731758	-2.075890
C	2.447871	-3.959482	-0.753444
C	1.958920	-3.140599	0.270058
C	1.775247	0.854892	0.426476
C	2.983592	0.636593	1.141914
C	4.166300	1.278337	0.822499
C	4.247477	2.212443	-0.206847
C	3.072224	2.446041	-0.915087
C	1.879653	1.791323	-0.641857
H	5.172006	2.721898	-0.447655
C	-2.950512	0.075738	0.469733
C	-3.439103	1.272069	-0.161227
C	-4.781233	1.471802	-0.387128
C	-5.754858	0.500794	0.002925
C	-5.283587	-0.687676	0.634852
C	-3.937802	-0.889015	0.858888
H	-1.374911	-2.311676	0.904066
H	-1.223371	-1.422876	2.425782
H	1.089289	-1.437614	2.027460
H	0.016283	-1.047522	-1.572624
H	0.880964	-2.489904	-3.393272
H	3.137371	-4.767051	-0.516552
H	2.272779	-3.314344	1.297613
F	2.984061	-0.201482	2.214571
F	5.272741	1.011075	1.566314
F	3.100591	3.318017	-1.956547
F	0.841383	2.026705	-1.469249
H	-2.717240	2.023570	-0.466618
H	-5.117915	2.385178	-0.872659
H	-6.003232	-1.442255	0.944145
H	-3.622564	-1.807424	1.349071
H	2.442217	-4.361911	-2.875958
C	-7.133636	0.711146	-0.225191
N	-8.280069	0.885829	-0.413528

Table S2-20: Cartesian Atomic Coordinates for the Geometry Optimized Structure of the Pyrazoline **2j** Radical Anion (B3LYP/6-31+G(d)).

Atom	x/Å	y/Å	z/Å
N	-0.788757	-0.694822	-0.458319
N	0.407506	-0.076232	-0.842069
C	-1.786862	0.150896	-0.715207
C	-1.297872	1.441121	-1.351563
C	0.230578	1.377697	-1.128688
C	0.726695	2.254455	0.011322
C	0.335380	2.007251	1.338542
C	0.782518	2.828914	2.373653
C	1.627096	3.912985	2.104090
C	2.024572	4.164068	0.788675
C	1.579792	3.335482	-0.247000
C	1.610405	-0.630704	-0.471091
C	2.790880	-0.370804	-1.212809
C	4.017265	-0.944799	-0.917801
C	4.135604	-1.854071	0.131671
C	3.000411	-2.143754	0.883774
C	1.779527	-1.535280	0.613132
F	5.321330	-2.444984	0.404800
C	-3.152331	-0.147678	-0.467153
C	-3.555615	-1.382930	0.149603
C	-4.879461	-1.674321	0.383275
C	-5.918043	-0.764173	0.015732
C	-5.531757	0.461680	-0.602717
C	-4.204326	0.755189	-0.834502
H	-1.733094	2.337784	-0.897901
H	-1.534736	1.469498	-2.425991
H	0.775327	1.641246	-2.037546
H	-0.313417	1.162193	1.554724
H	0.473945	2.620233	3.395493
H	2.687106	4.998121	0.567124
H	1.899980	3.530210	-1.268908
F	2.732370	0.444066	-2.297522
F	5.096549	-0.657275	-1.678386
F	3.106312	-2.984410	1.935109
F	0.775452	-1.794459	1.471166
H	-2.783474	-2.090471	0.436411
H	-5.150246	-2.614758	0.858308
H	-6.302309	1.171021	-0.895958
H	-3.956360	1.698329	-1.316729
H	1.973929	4.551487	2.913390
C	-7.278367	-1.066176	0.251996
N	-8.410364	-1.313463	0.446028

Table S3: Summary of Computational Data for Pyrazolines **1a-j** and **2a-j** (B3LYP/6-31+G(d)//B3LYP/6-31+G(d) level of theory).

Compound	Neutral Species		Radical Anion		AEA [eV][b]
	SCF energy [au]	ZPVE[a] [J/mol]	SCF energy [au]	ZPVE[a] [J/mol]	
1a	-920.5868	211.4	-920.5983	208.1	0.450
1b	-1019.8252	206.2	-1019.8391	203.0	0.514
1c	-1019.8311	206.2	-1019.8472	202.9	0.578
1d	-1019.8290	206.1	-1019.8431	202.6	0.534
1e	-1119.0663	200.9	-1119.0832	197.8	0.594
1f	-1119.0677	201.1	-1119.0863	197.8	0.649
1g	-1119.0742	200.8	-1119.0947	197.8	0.689
1h	-1218.3013	195.8	-1218.3229	192.6	0.723
1i	-1317.5288	190.7	-1317.5470	187.0	0.650
1j	-1416.7546	185.6	-1416.7757	181.9	0.729
2a	-1012.8337	210.5	-1012.8732	207.8	1.189
2b	-1112.0719	205.2	-1112.1137	202.8	1.240
2c	-1112.0775	205.3	-1112.1216	202.9	1.303
2d	-1112.0755	205.1	-1112.1178	202.5	1.264
2e	-1211.3126	199.9	-1211.3571	197.6	1.309
2f	-1211.3138	200.1	-1211.3598	197.6	1.359
2g	-1211.3200	199.9	-1211.3680	197.5	1.408
2h	-1310.5474	195.0	-1310.5957	192.4	1.421
2i	-1409.7747	189.6	-1409.8201	187.1	1.341
2j	-1509.0005	184.5	-1509.0473	181.8	1.388

[a]Unscaled zero point vibrational energy from frequency calculation; [b]Adiabatic electron affinity with ZPVE correction (ZPVE scaled by a factor of 0.9804).

Table S4: Summary of Computational Data for Pyrazolines **1a-j** and **2a-j** (B3LYP/6-311+G(2d,2p)//B3LYP/6-31+G(d) level of theory).

Compound	Neutral SCF energy [au]	Anion SCF energy [au]	AEA [eV][a]	TD-DFT[b]	
				S1 [eV][c]	Oscillator Strength
1a	-920.8198	-920.8328	0.495	3.409	0.649
1b	-1020.0860	-1020.1013	0.552	3.502	0.633
1c	-1020.0917	-1020.1091	0.611	3.463	0.664
1d	-1020.0895	-1020.1049	0.565	3.428	0.613
1e	-1119.3548	-1119.3724	0.614	3.490	0.560
1f	-1119.3563	-1119.3759	0.674	3.519	0.652
1g	-1119.3628	-1119.3842	0.715	3.541	0.688
1h	-1218.6181	-1218.6403	0.739	3.492	0.591
1i	-1317.8741	-1317.8928	0.666	3.766	0.837
1j	-1417.1284	-1417.1485	0.701	3.790	0.768
2a	-1013.0889	-1013.1300	1.234	3.105	0.870
2b	-1112.3550	-1112.3981	1.278	3.228	0.904
2c	-1112.3604	-1112.4059	1.340	3.147	0.846
2d	-1112.3583	-1112.4019	1.297	3.099	0.833
2e	-1211.6234	-1211.6690	1.340	3.232	0.857
2f	-1211.6246	-1211.6721	1.398	3.249	0.890
2g	-1211.6308	-1211.6800	1.441	3.214	0.860
2h	-1310.8865	-1310.9357	1.448	3.246	0.851
2i	-1410.1422	-1410.1887	1.372	3.491	1.036
2j	-1509.3967	-1509.4442	1.409	3.510	0.973

[a]Adiabatic electron affinity with ZPVE correction at B3LYP/6-31+G(d) level (ZPVE scaled by a factor of 0.9804).
[b]Time-dependent density functional theory calculation; [c]Lowest excited singlet state energy.

Table S5: Summary of Computational Data for Pyrazolines **1a-j** and **2a-j**: Estimation of the Reduction Potential Based on Semiempirical Solvent Stabilization Energies (SM5.42R/AM1// B3LYP/6-31+G(d) level of theory).

Compound	AEA [eV][a]	Solvent Stabilization Energy[b]			E_{red} [eV][f]
		Neutral [eV][c]	Anion [eV][d]	$\Delta\Delta G$ [eV][e]	
1a	0.495	-0.673	-2.532	-1.858	-2.79
1b	0.552	-0.681	-2.509	-1.828	-2.76
1c	0.611	-0.651	-2.401	-1.749	-2.78
1d	0.565	-0.642	-2.412	-1.770	-2.81
1e	0.614	-0.625	-2.358	-1.733	-2.80
1f	0.674	-0.645	-2.402	-1.757	-2.71
1g	0.715	-0.602	-2.281	-1.679	-2.75
1h	0.739	-0.596	-2.242	-1.646	-2.76
1i	0.666	-0.607	-2.252	-1.645	-2.83
1j	0.701	-0.529	-2.715		
2a	1.234	-0.724	-2.296	-1.572	-2.34
2b	1.278	-0.740	-2.267	-1.528	-2.34
2c	1.340	-0.715	-2.187	-1.472	-2.33
2d	1.297	-0.709	-2.192	-1.483	-2.36
2e	1.340	-0.690	-2.136	-1.446	-2.36
2f	1.398	-0.704	-2.185	-1.481	-2.26
2g	1.441	-0.675	-2.089	-1.414	-2.29
2h	1.448	-0.667	-2.070	-1.403	-2.29
2i	1.372	-0.665	-2.158	-1.493	-2.28
2j	1.409	-0.599	-1.990	-1.392	-2.34

[a]Adiabatic electron affinity with ZPVE correction at B3LYP/6-311+G(2d,2p)//B3LYP/6-31+G(d) level (ZPVE scaled by a factor of 0.9804); [b]Solvation energy of the corresponding gas-phase species in acetonitrile calculated with the semi-empirical SM5.42R/AM1 solvation model; [c]Based on gas-phase geometry of the neutral compound optimized at B3LYP/6-31+G(d) level; [d]Based on gas-phase geometry of the radical anion optimized at B3LYP/6-31+G(d) level; [e]Differential solvent stabilization energy; [f]Computed reduction potential based on equation (14) with E_{ref} ($Fc^{+/0}$/MeCN) = 5.144 V.