Electronic Supplementary Material (ESI) for Dalton Transactions.

Supporting Information

A Bis(PCN) Palladium Pincer Complex with a Remarkably Planar 2,5-Diarylpyrazine Core

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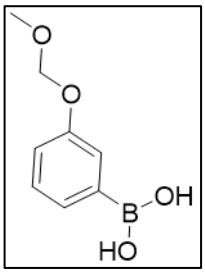
I. General Considerations

Unless otherwise specified, all manipulations were performed under argon atmosphere using standard Schlenk line or glove box techniques. Toluene, THF, diethyl ether, pentane, and isooctane were dried and deoxygenated (by purging) using a solvent purification system and stored over molecular sieves in an Ar-filled glove box. C_6D_6, $CDCl_3$, dichloromethane, fluorobenzene and 1,2-dichlorobenzene were dried with and then distilled from CaH_2 and stored over molecular sieves in Ar-filled glove box. All other chemicals were used as received from commercial vendors. NMR spectra were recorded on a Bruker 400 (^{1}H NMR, 399.535 MHz; ^{11}C NMR, 100.582 MHz; ^{31}P NMR, 161.734 MHz) and Varian Inova 500 (^{1}H NMR, 499.703 MHz; ^{13}C NMR, 125.697 MHz; ^{31}P NMR, 202.265 MHz, ^{19}F NMR, 470.111 MHz) spectrometer. For ^{1}H and ^{13}C NMR spectra, the residual solvent peak was used as an internal reference. (^{1}H NMR: δ 7.16 for C_6D_6, 7.24 for $CDCl_3$, 2.05 for $(CD_3)_2CO$; ^{13}C NMR: δ 128.06 for C_6D_6, 77.16 for $CDCl_3$, 29.84 and 206.26 for $(CD_3)_2CO$). ^{31}P NMR spectra were referenced externally using 85% H_3PO_4 at δ 0 ppm. ^{19}F NMR spectra were referenced externally using CF_3CO_2H at -78.5 ppm. ^{11}B NMR spectra were referenced externally using neat BF_3•Et_2O at 0 ppm. Elemental analysis was performed by Robertson Microlit Laboratories, Ledgewood NJ. Electrochemical studies were conducted using a CH Instruments Model 700 D Series. Electrochemical Analyzer and Workstation in conjunction with a three-electrode cell: the working electrode was a CHI 104 glassy carbon disk with a 3.0 mm diameter, the auxiliary electrode was composed of platinum wire and the reference electrode, was a $Ag/AgNO_3$ electrode, which was prepared as a bulk solution composed of 0.01 M $AgNO_3$ and 0.1 M [*n*-Bu_4N][PF_6] in THF. A fine porosity frit was used for separation from solution. CVs were conducted in THF with 0.1 M supporting electrolyte at a scan rate of 100 mV/s. The concentration of the analyte solutions was approximately 1 mM.

CVs were referenced to ferrocene/ferrocenium redox couple. Fluorescence emission spectra were recorded using a Horiba Fluoromax-4 spectrophotometer equipped with a 150W Xe lamp. Samples were measured in air-free 1 cm^2 quartz optical cells. Ultraviolet-visible (UV-vis) spectra were collected on a UV-2450 UV-Vis spectrophotometer (Shimadzu, Japan).

II. Synthesis and NMR Characterization.



Synthesis of 3-methoxymethoxyphenylboronic acid (12). 1-bromo-3-(methoxymethoxy)benzene **(11)** (200 mg, 0.921 mmol) was dissolved in dry THF (20 mL) and added dropwise using a 20 mL syringe to a stirring mixture of freshly activated magnesium powder (26.9 mg, 1.11 mmol) in dry THF (20 mL) in a 100 mL Schlenk flask connected to Schlenk line. The reaction mixture was heated using a heat gun until a continuous bubbling and a dark reddish brown color was observed. After 30 minutes, the reaction mixture was chilled to -78 °C in a dry ice bath and trimethyl borate (192 mg, 1.84 mmol, 205 µL) was added dropwise using a syringe. The reaction was allowed to stir in the dry ice bath and warm to room temperature overnight. The reaction was quenched with an aqueous solution of saturated NH_4Cl. CH_2Cl_2, 20 mL, was then added to the mixture and the organic product was extracted into the CH_2Cl_2. The aqueous phase was washed with CH_2Cl_2 (3 × 25 mL). The CH_2Cl_2 layer was then dried using Na_2SO_4 and filtered through a pad of celite. The solvent was removed under vacuum to yield as a white solid that was washed with pentane (3 × 10 mL). (83.8 mg, 0.460 mmol, 50%). ^{1}H NMR (400 MHz, C_6D_6): δ 8.00 (d, 7.2 Hz, 1H, Ar-*H*), 7.80 (d, 4 Hz, 1H, Ar*H*), 7.18 (m, 1H, Ar-*H*, overlaps with solvent peak), 7.14 (m, 1H, Ar-*H*, overlaps with solvent peak), 4.84 (s, 2H, OC*H*$_2$O), 3.06 (s, 3H, OC*H*$_3$). ^{13}C{^{1}H}NMR (100 MHz, C_6D_6): 157.7 (s, Ar), 132.7 (br s, Ar C-B), 129.5 (s, Ar), 129.4 (s, Ar), 123.5 (s, Ar), 120.8 (s, Ar), 94.6 (s O*C*H$_2$O), 55.7 (s, O*C*H$_3$). HRMS (ESI) *m/z* calcd. for $C_8H_{11}BO_4$ [M – H]$^-$: 181.0667; Found: 181.0668

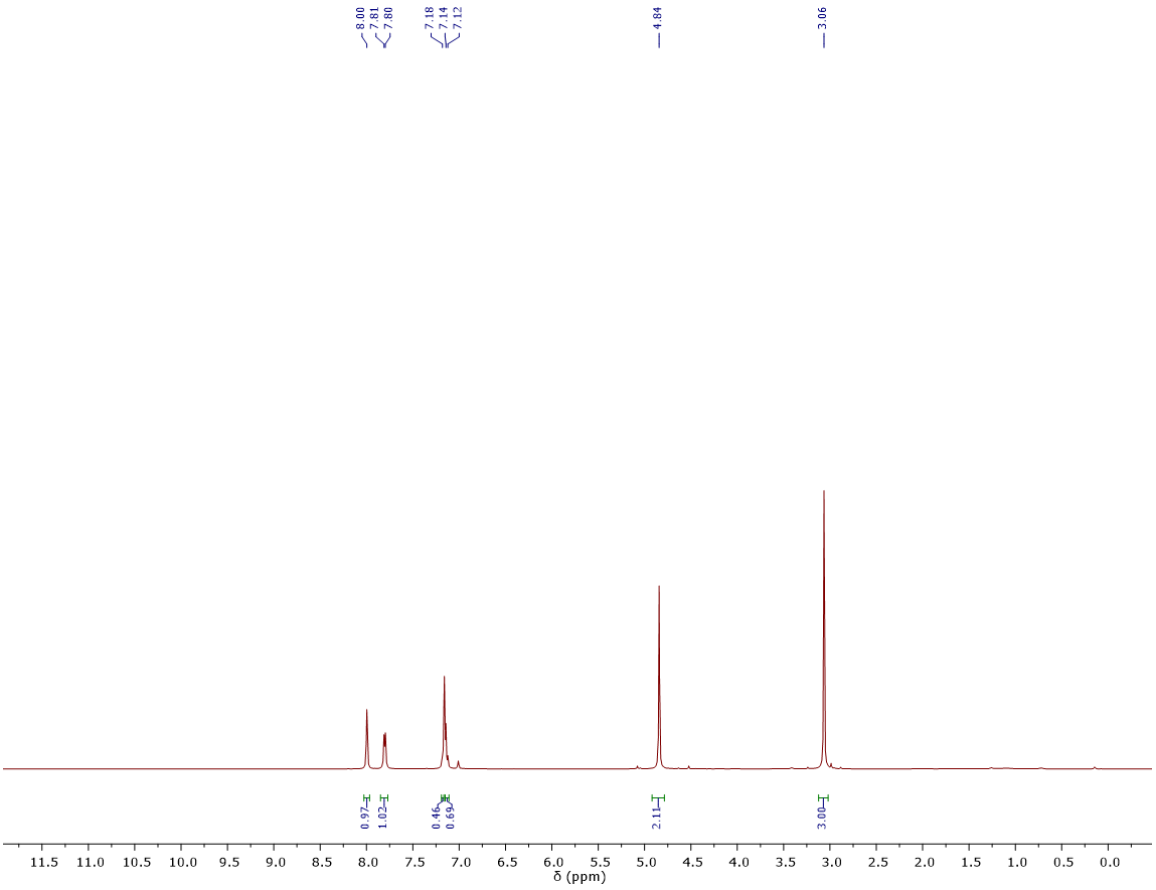
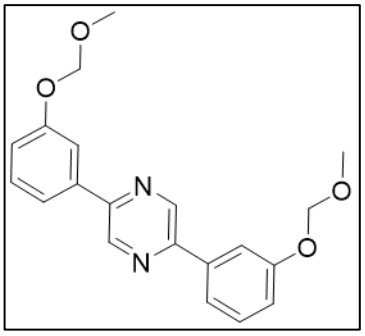


Figure S1. ^{1}H NMR (400 MHz) spectrum of compound **12** in C_6D_6



Synthesis of 2,5-Bis(3-methoxymethoxyphenyl)pyrazine (13). In a 100 mL Schlenk flask, **12** (595 mg, 3.27 mmol), 2,5-dibromopyrazine (370 mg, 1.56 mmol), $Pd(PPh_3)_4$ (36.0 mg, 0.0311 mmol) and Na_2CO_3 (660 mg, 6.22 mmol) were combined in a 22 mL mixture of toluene/EtOH/water (8:2:1) and heated at 110 ˚C over 48 h. After the solvent was removed under vacuum, the remaining solid was extracted using CH_2Cl_2/water. The CH_2Cl_2 fraction was collected and further dried with Na_2SO_4. After passing through a pad of silica gel, the volatiles were removed under vacuum from the filtrate and a subsequent recrystallization in CH_2Cl_2 layered with hexane in 1:1 ratio yielded product as a slightly yellowish solid (332 mg, 0.943 mmol, 61%). ^{1}H NMR (500 MHz, $CDCl_3$): δ 9.06 (s, 2H, pyrazine-*H*), 7.77 (t, 2.1 Hz, 2H, Ar-*H*), 7.69 (dt, 7.7 Hz, 1.2 Hz, 2H, Ar-*H*), 7.45 (t, 8.0 Hz, 2H, Ar-*H*), 7.16 (ddd, 8.2 Hz, 2.5 Hz, 0.8 Hz, 2H, Ar-*H*), 5.28 (s, 2H, OC*H*$_2$O), 3.53 (s, 3H, OC*H*$_3$). ^{13}C{^{1}H}NMR (100 MHz, $CDCl_3$): 158.1 (pyrazine), 150.6 (pyrazine), 141.4 (Ar), 137.9 (Ar), 130.3 (Ar), 120.4 (Ar), 117.9 (Ar), 114.8 (Ar), 94.7 (O*C*H$_2$O), 56.3 (O*C*H$_3$). HRMS (ESI) *m/z* calcd. for $C_{20}H_{20}N_2O_4$ $[M + H]^+$: 353.1496; Found: 353.1487

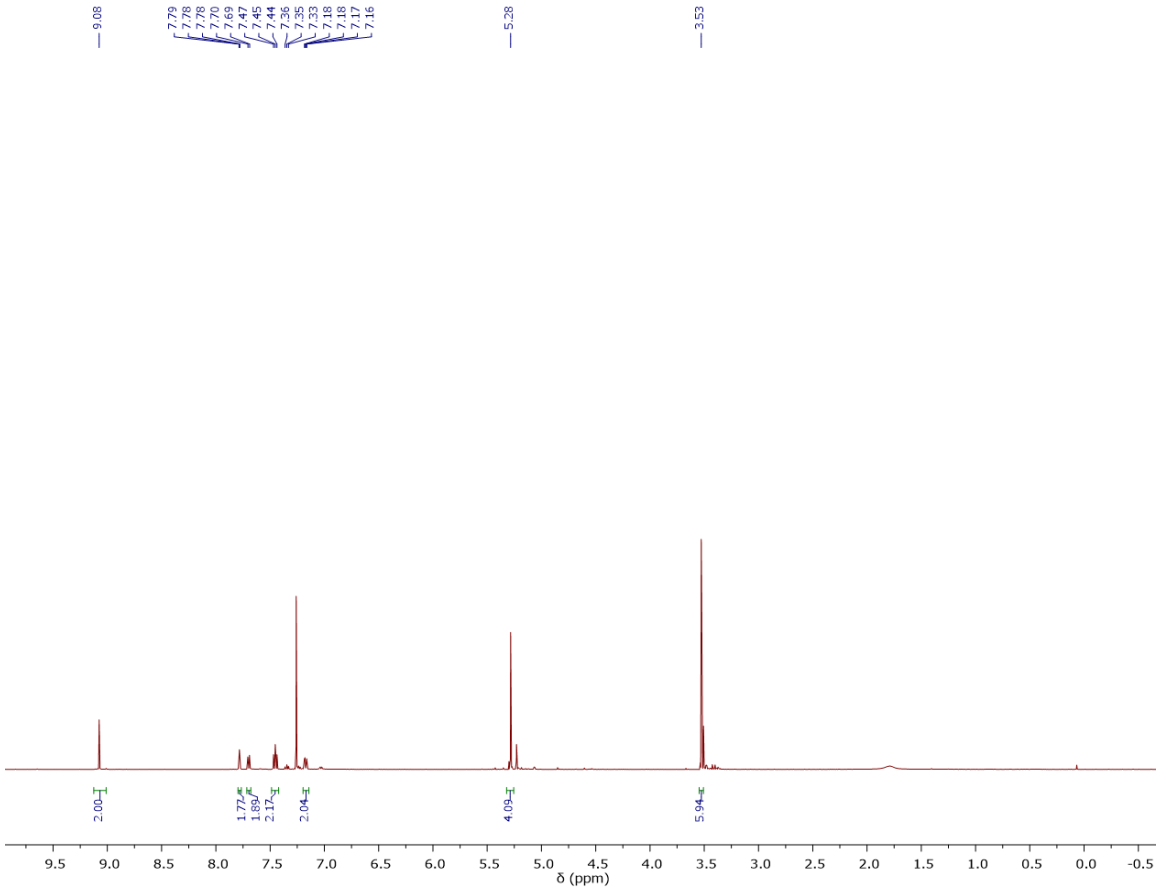
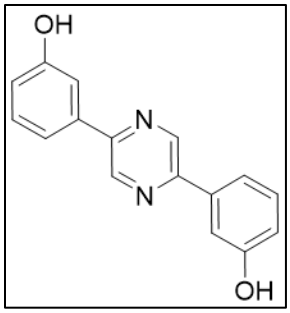


Figure S2. ^{1}H NMR (400 MHz) spectrum of compound **13** in $CDCl_3$. Residual water (1.79 ppm) and grease (0.06 ppm) are observed in the ^{1}H NMR.



Synthesis of 3,3'-(2,5-pyrazinediyl)bisphenol (14). In a 250 mL Schlenk flask, **13** (1.50 g, 4.26 mmol) was dissolved in 50 mL THF and 10% dilute hydrochloric acid was added to acidify the solution to a pH around 1. After stirring for one hour, the volatiles were removed under vacuum and then the yellow solid residue was washed with water followed with CH_2Cl_2. The remaining solids were further dried under vacuum to yield product as a yellow solid (1.10g, 4.16 mmol, 98%): ^{1}H NMR (500 MHz, $(CD_3)_2CO$): δ 9.16 (s, 2H, pyrazine-*H*), 8.60 (bs, O*H*), 7.70 (t, 2.1 Hz, 2H, Ar-*H*), 7.67 (ddd, 7.7 Hz, 1.7 Hz, 1.0 Hz, 2H, Ar-*H*) 7.38 (t, 7.9 Hz 2H, Ar-*H*), 6.98 (ddd, 8.1 Hz, 2.5 Hz, 0.9 Hz, 2H, Ar-*H*). ^{13}C{^{1}H}NMR (100 MHz, $CDCl_3$): 159.1 (pyrazine), 151.2 (pyrazine), 142.0 (Ar), 138.8 (Ar), 131.1 (Ar), 118.8 (Ar), 117.8 (Ar), 114.4 (Ar). HRMS (ESI) *m/z* calcd. for $C_{16}H_{12}N_2O_2$ $[M + H]^+$: 265.0972; Found: 265.0965

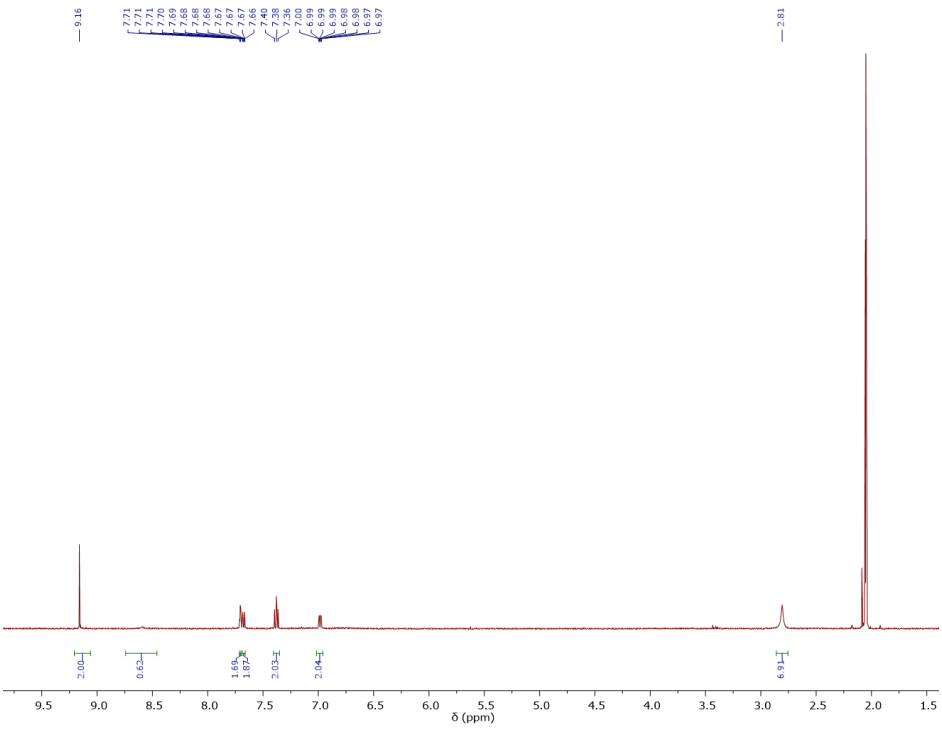
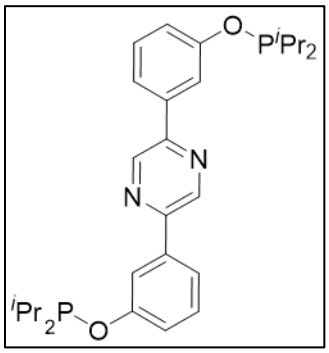


Figure S3. ^{1}H NMR (400 MHz) spectrum of compound **14** in $(CD_3)_2CO$



Synthesis of (15). In a 250 mL Schlenk flask, after **14** (3.85 g, 14.6 mmol) was dissolved in 50 mL THF, Et_3N (3.24 g, 32.0 mmol) was slowly added into the solution. After 30 minutes of stirring, Cl*i*Pr_2 (4.67 g, 30.6 mmol) was added. After stirring overnight at RT, the solution was filtered and the volatiles were removed from the filtrate under vacuum. Recrystallization in 1:2 toluene/pentane at -35 ˚C offered product as a slightly yellow solid (4.50 g, 9.06 mmol, 62%) that was 95% pure by ^{1}H NMR. ^{31}P{^{1}H} NMR (C_6D_6): 148.9 (s); ^{1}H NMR (500 MHz, C_6D_6): δ 8.86 (s, 2H, pyrazine-*H*), 8.28 (q, 2.1 Hz, 2H, Ar-*H*), 7.55 (dt, 7.8 Hz, 2.2 Hz, 2H, Ar-*H*), 7.31 (d, 8.0 Hz, 2H, Ar-*H*), 7.16 (d, 7.9 Hz, 2H, Ar-*H*), 1.79 (heptd, 7.1 Hz, 2.8 Hz, 4H, C*H*Me_2), 1.16 (dd, 10.5 Hz, 7.1 Hz, 12H, CH(CH_3)$_2$), 1.00 (dd, 15.8 Hz, 7.2 Hz, 12H, CH(CH_3)$_2$).). ^{13}C{^{1}H}NMR (100 MHz, C_6D_6): 160.7 (d, $J_{P\text{-}C}$ = 9 Hz, pyrazine), 150.5 (pyrazine), 141.3 (Ar), 138.51 (Ar), 130.2 (Ar), 120.3 (Ar), 120.1 (d, $J_{P\text{-}C}$ = 11 Hz, Ar) 117.6 (Ar), 28.7 (d, $J_{P\text{-}C}$ = 19 Hz, *C*HMe_2), 17.9 (d, $J_{P\text{-}C}$ = 20 Hz, CH*Me*$_2$), 17.2 (d, $J_{P\text{-}C}$ = 8 Hz CH*Me*$_2$).

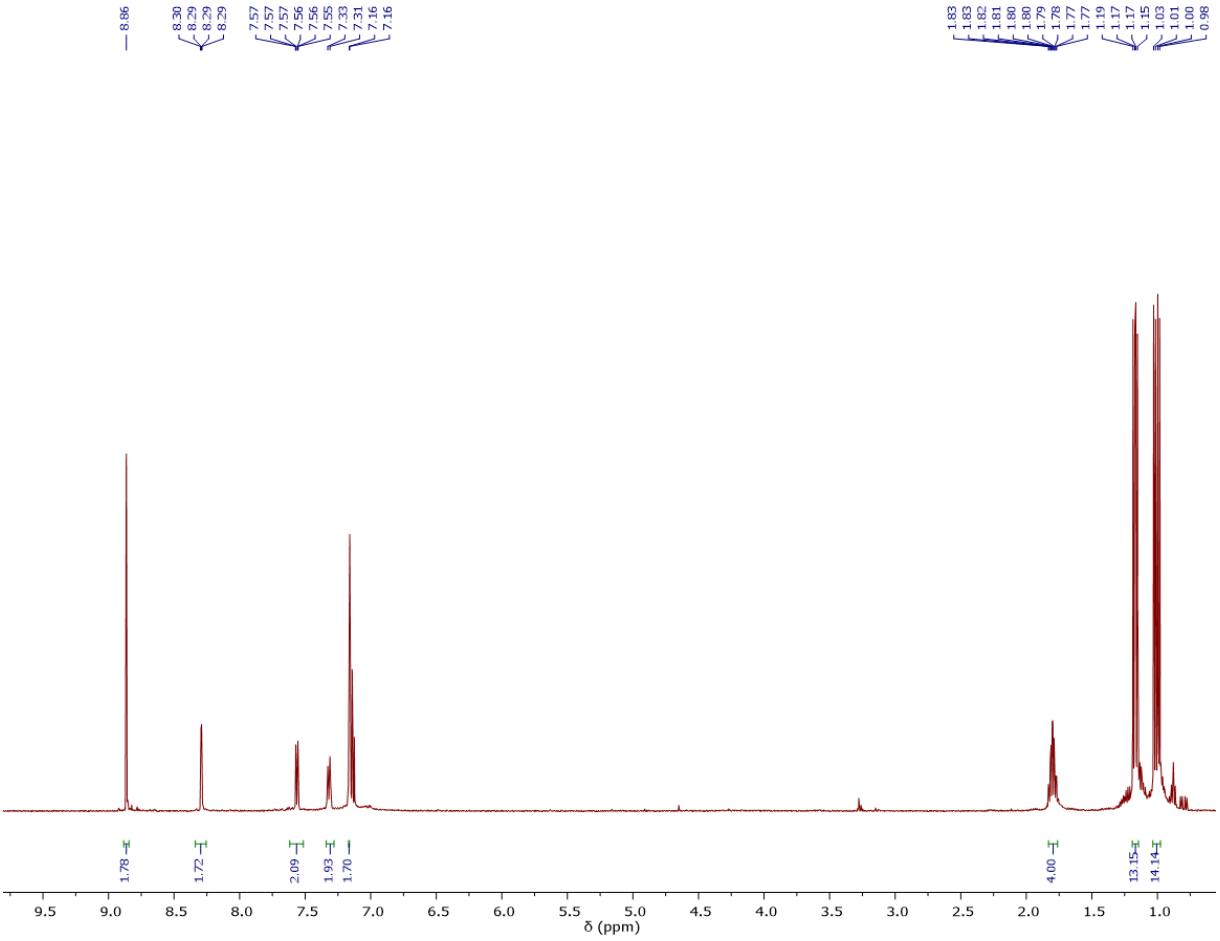
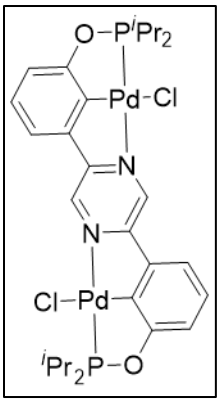


Figure S4. ^{1}H NMR (400 MHz) spectrum of compound **15** in C_6D_6



Synthesis of PCN Bis-pincer Pd-Cl Complex (10). In a 50 mL Schlenk tube, **15** (1.25 g, 2.52 mmol), Pd(COD)Cl_2 (1.44 g, 5.04 mmol) and 2,6-lutidine (0.540 mg, 5.04 mmol) were dissolved in a minimum amount of 1,2-dichlorobenzene under argon. The reaction mixture was stirred overnight at around 180 °C. The yellow mixture was diluted in CH_2Cl_2 and filtered through a pad of Celite. The filtrate was condensed under vacuum and then mixed with pentane in a 1:2 ratio and left in a -35 ˚C freezer overnight. The dark yellow precipitate was dissolved in CH_2Cl_2 and layered with pentane in a 1:1 ratio and left in a -35 ˚C freezer overnight to recrystallize. The residue was washed with pentane and dried under vacuum to yield a yellow solid (1.45 g, 74%). $^{31}P\{^1H\}$ NMR (C_6D_6): δ 205.4 (s); ^1H NMR (C_6D_6, 400 MHz): δ 9.31 (s, 2H, pyrazine-*H*), 6.96 (s, Ar-*H*), 6.70 (s, 4H, Ar-*H*), 2.1 (m, 4H, C*H*Me$_2$), 1.32 (dd, J = 19.3 Hz, 7.1 Hz, 12H, CH(C*H*$_3$)$_2$), 1.09 (dd, J = 16.4 Hz, 7.1 Hz, 12H, CH(C*H*$_3$)$_2$).; $^{13}C\{^1H\}$ NMR (C_6D_6, 100 MHz): δ 164.1 (d, J = 5.7 Hz, pyrazine), 158.5 (t, 2.6 Hz, pyrazine), 151.8 (s, Ar), 143.7 (s, Ar), 139.3 (s, Ar), 122.8 (s, Ar), 119.1 (s, Ar). 113.54 (d, 14.9 Hz, Ar), 29.5 (d, $J_{P\text{-}C}$ = 25.9 Hz, *C*HMe$_2$), 17.3 (d, $J_{P\text{-}C}$ = 6.0 Hz, CH*Me*$_2$), 16.8 (s, CH*Me*$_2$). Anal. Calcd for $C_{28}H_{36}Cl_2N_2O_2P_2Pd_2$: C: 43.21; H: 4.66; N: 3.60. Found: C: 43.36; H: 4.43; N: 3.48.

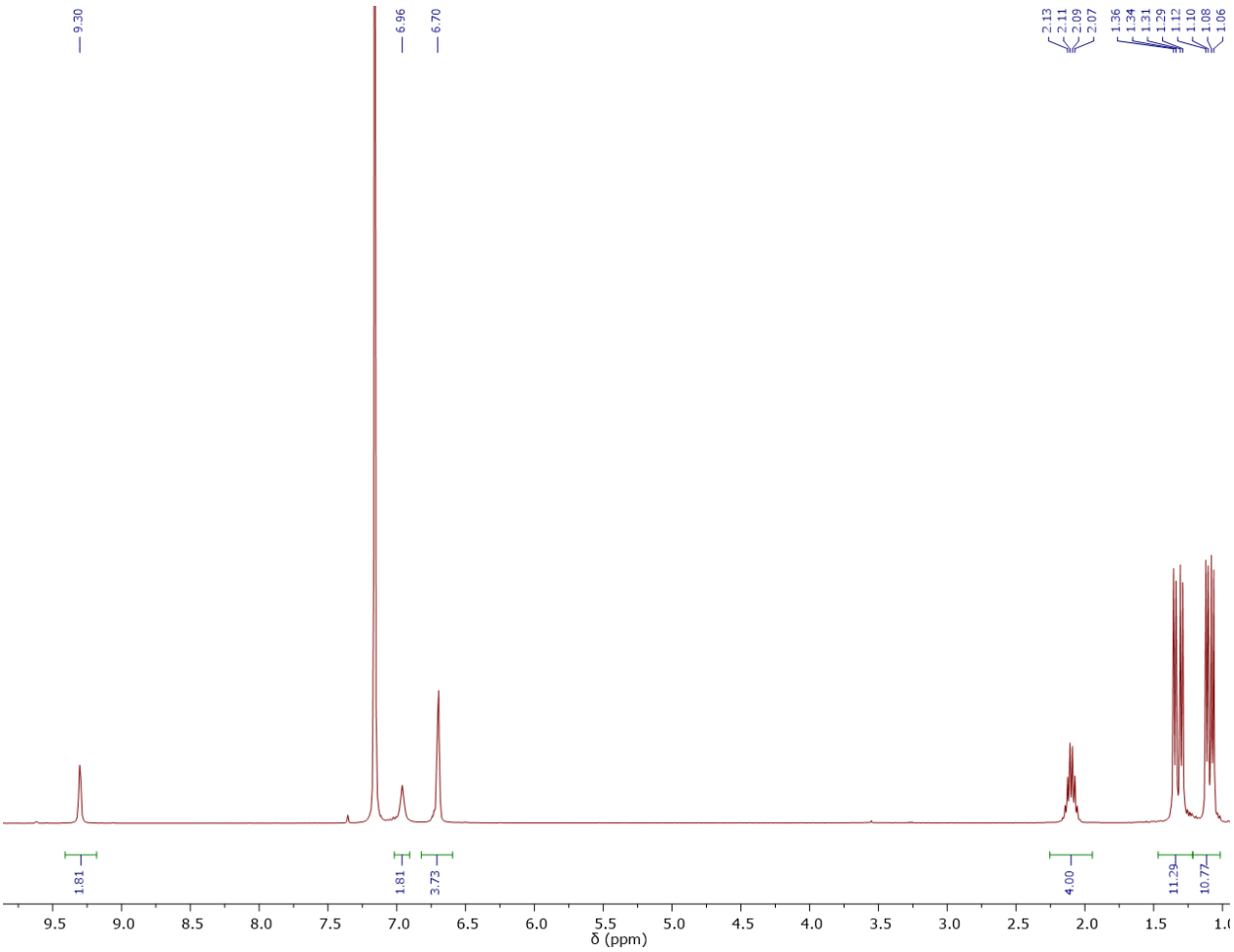


Figure S5. ^{1}H NMR (400 MHz) spectrum in C_6D_6 of PCN Bis-Pincer Pd-Cl complex (**10)**.

Synthesis of PCN Bis-pincer Pd-Br Complex (10-Br). In a J. Young tube, **10** (10 mg, 0.013 mmol) was dissolved into 0.5 mL of $CDCl_3$ then Me_3SiBr (7 µL, 0.051 mmol) was added and the reaction was mixed briefly, which was accompanied by a color change from light yellow to light orange. $^{31}P\{^{1}H\}$ NMR ($CDCl_3$, 202 MHz): δ 208.0 (s); ^{1}H NMR ($CDCl_3$, 400 MHz): δ 9.55 (s, 2H, pyrazine-*H*), 7.45 (d, J = 8 Hz, 2H, Ar-*H*), 7.17 (t, J = 8 Hz, 2H, Ar-*H*), 6.89 (d, J = 8 Hz, 2H, Ar-*H*), 2.51 (m, 4H, C*H*Me_2), 1.46 (dd, J = 20 Hz, 8 Hz, 12H, CH(C*H*$_3$)$_2$), 1.35 (dd, J = 16 Hz, 8 Hz, 12H, CH(C*H*$_3$)$_2$).

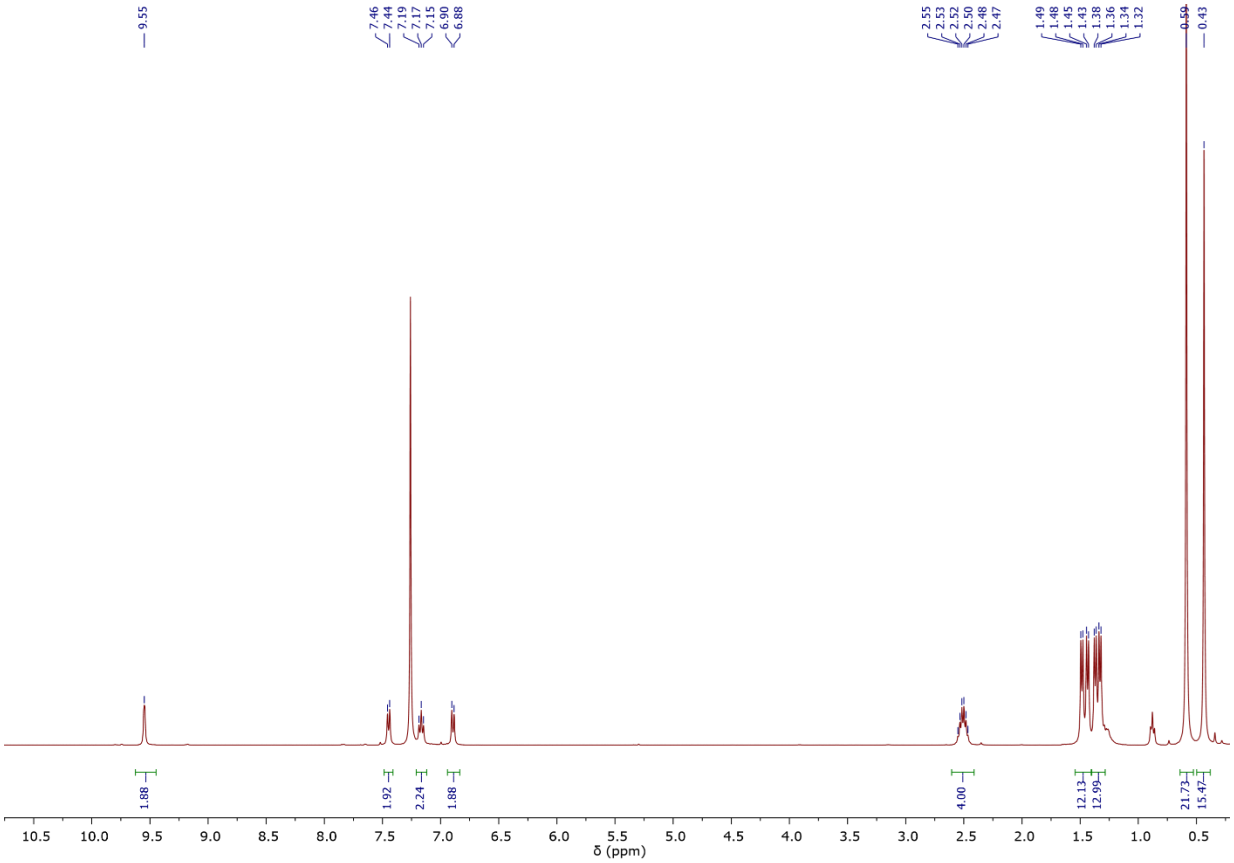


Figure S6. ^{1}H NMR (400 MHz) spectrum in $CDCl_3$ of PCN Bis-Pincer Pd-Br complex (**10-Br)**. Me_3SiBr (0.59 ppm) and Me_3SiCl (0.43 ppm) are present in the spectrum.

Synthesis of PCN Bis-pincer Pd-I Complex (10-I). In a J. Young tube, **10** (10 mg, 0.013 mmol) was dissolved into 0.5 mL of $CDCl_3$ then Me_3SiI (5.5 µL, 0.039 mmol) was added and the reaction was mixed briefly, which was accompanied by a color change from light yellow to dark orange. $^{31}P\{^{1}H\}$ NMR ($CDCl_3$, 202 MHz): δ 212.3 (s); ^{1}H NMR ($CDCl_3$, 400 MHz): δ 9.78 (s, 2H, pyrazine-*H*), 7.45 (d, J = 8 Hz, 2H, Ar-*H*), 7.19 (t, J = 8 Hz, 2H, Ar-*H*), 6.94 (d, J = 8 Hz, 2H, Ar-*H*), 2.51 (m, 4H, C*H*Me_2), 1.47 (dd, J = 20 Hz, 8 Hz, 12H, CH(CH_3)$_2$), 1.33 (dd, J = 16 Hz, 8 Hz, 12H, CH(CH_3)$_2$).

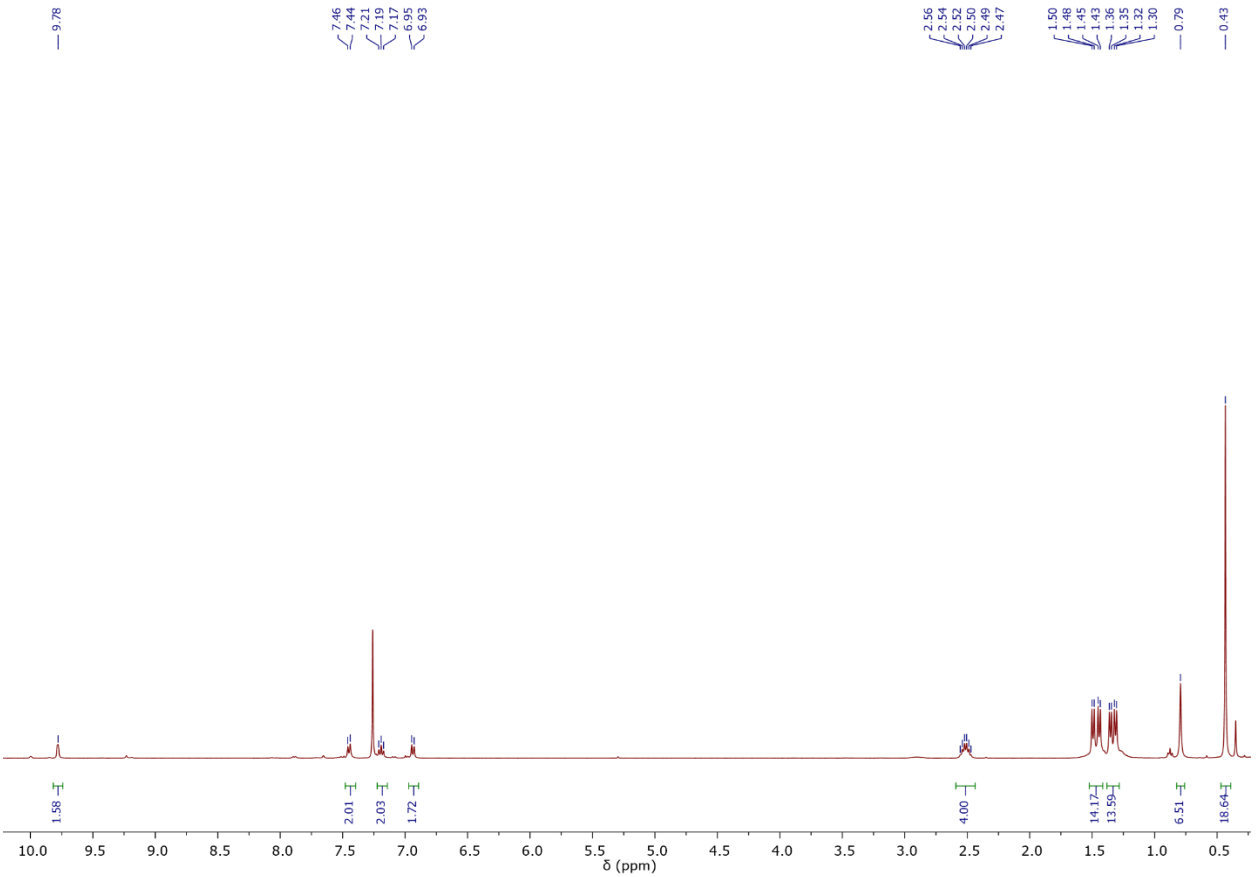


Figure S7. ^{1}H NMR (400 MHz) spectrum in $CDCl_3$ of PCN Bis-Pincer Pd-I complex (**10-I)**.

Me_3SiBr (0. 79 ppm) and Me_3SiCl (0.43 ppm) are present in the spectrum.

III. Electrochemical Analysis.

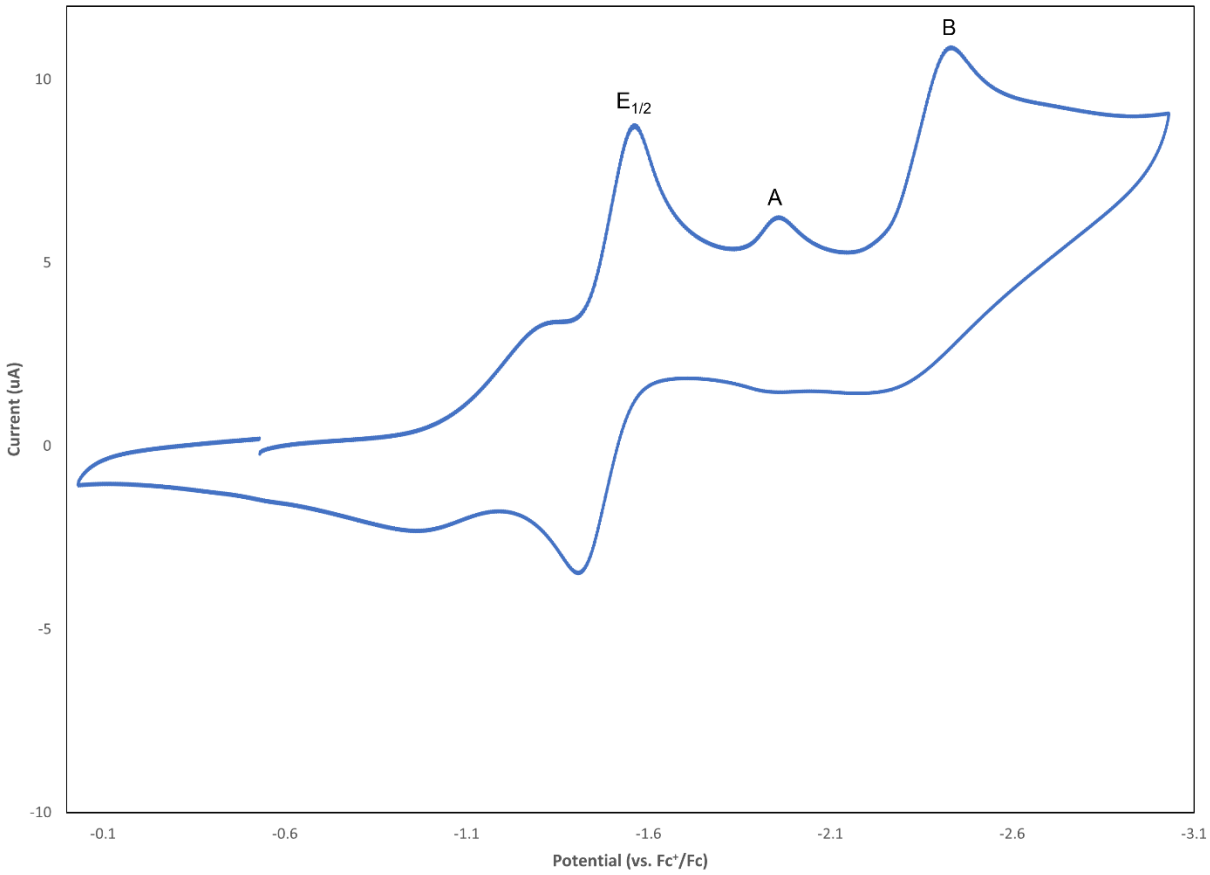


Figure S8. Cyclic Voltammogram of **10** in THF (1 mM) with $[Bu_4N][PF_6]$ (0.1 M) as the supporting electrolyte. $E_{1/2}$ = -1.49 V; Irreversible reduction at -1.98 **(A)** and -2.44 **(B)** V.

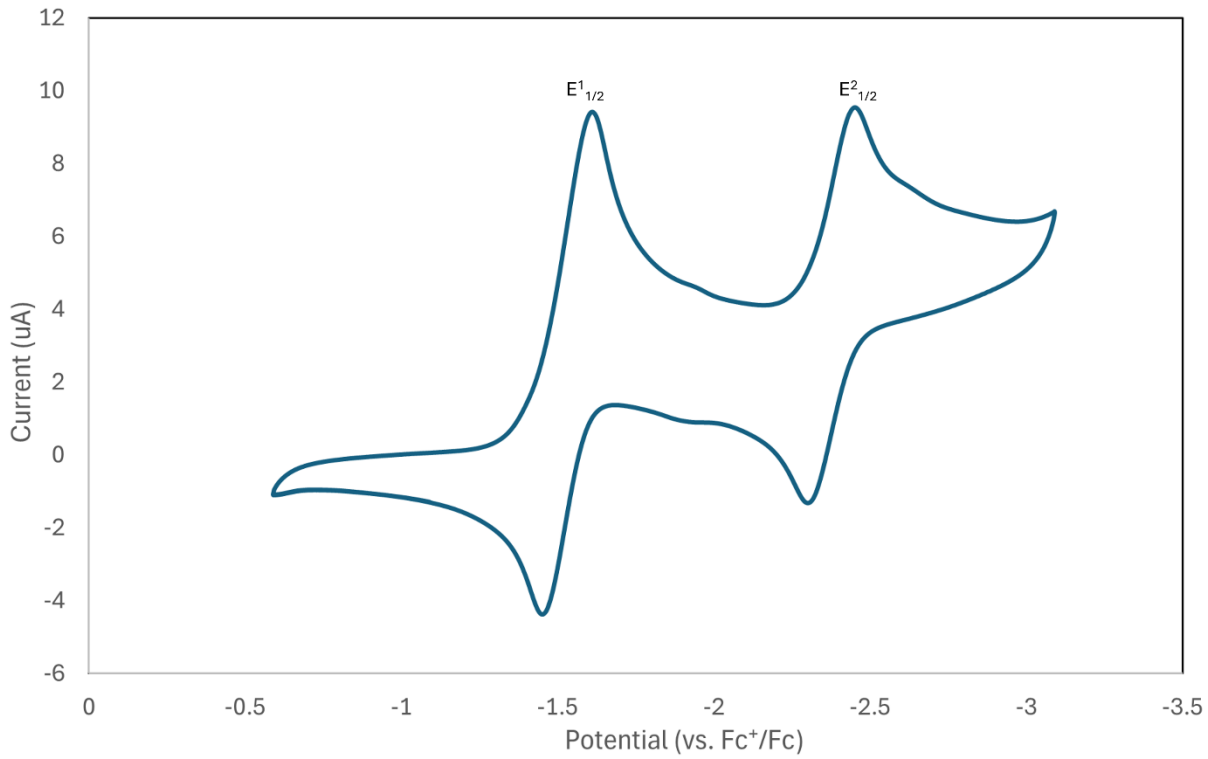


Figure S9. Cyclic Voltammogram of **10** in THF (1 mM) with $[Bu_4N][PF_6]$ (0.1 M) as the supporting electrolyte. Sweep started at -2 V and scanned cathodically. $E^1_{1/2}$ = -1.53 V; $E^1_{1/2}$ = -2.36.

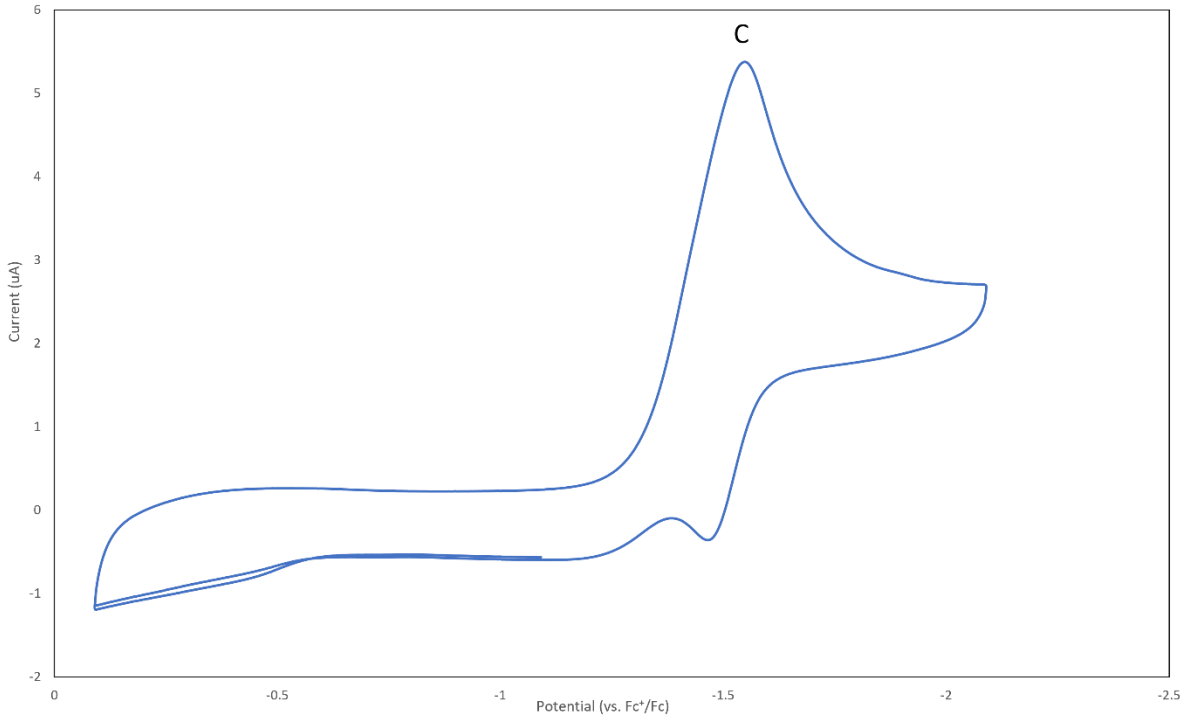


Figure S10. Cyclic Voltammogram of **10** in THF (1 mM) with $[Bu_4N][PF_6]$ (0.1 M) as the supporting electrolyte. Sweep started at -0.1 V and scanned cathodically. Irreversible reduction at -1.56 V **(C).**

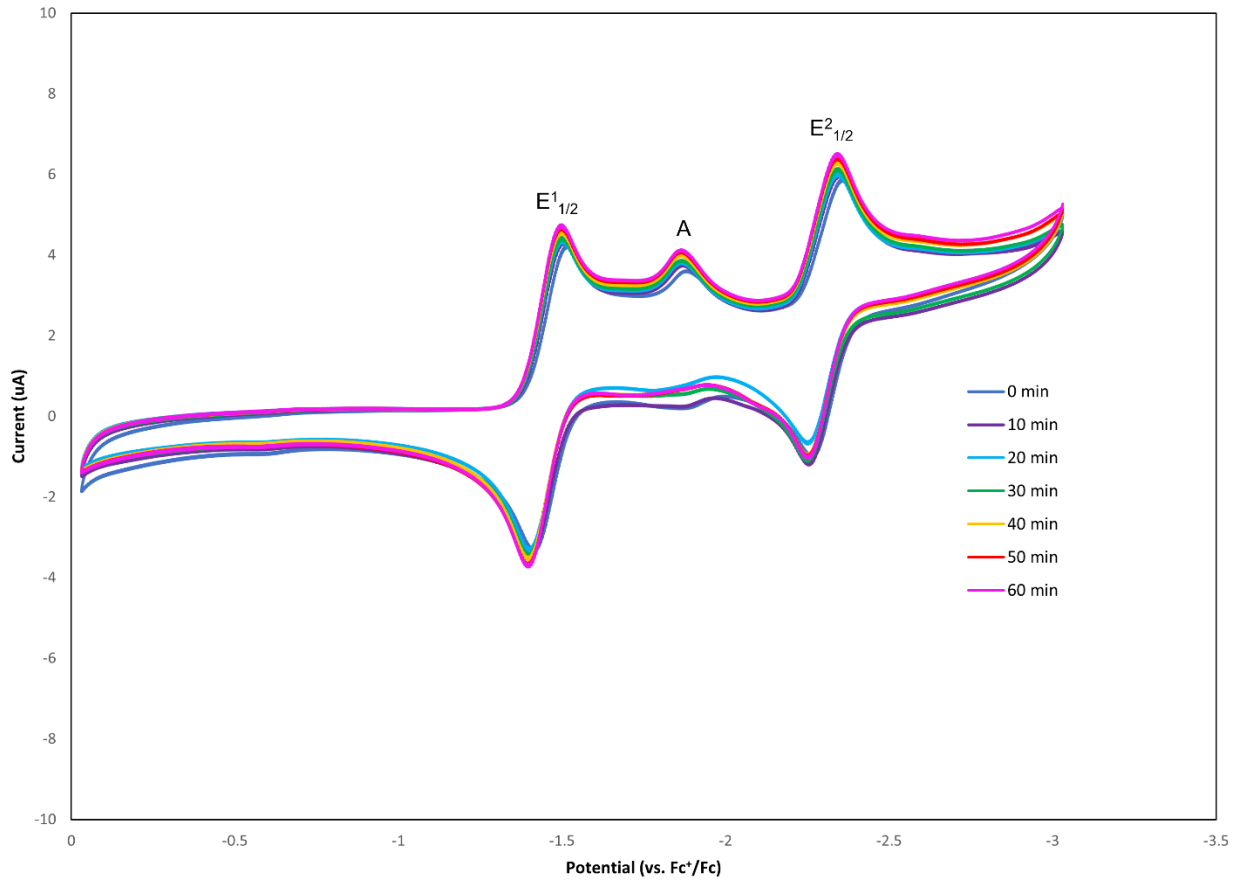


Figure S11. Cyclic voltammograms of **10** in THF (1 mM) with $[Bu_4N][PF_6]$ (0.1 M) as the supporting electrolyte and 20 eq. of $[Bu_4N][Cl]$ (0.02 M) in THF. The CV of the compound was recorded every 10 min. $E^1_{1/2}$ = -1.46 V; $E^2_{1/2}$ = -2.31 V; Irreversible reduction = -1.88 V **(A)**.

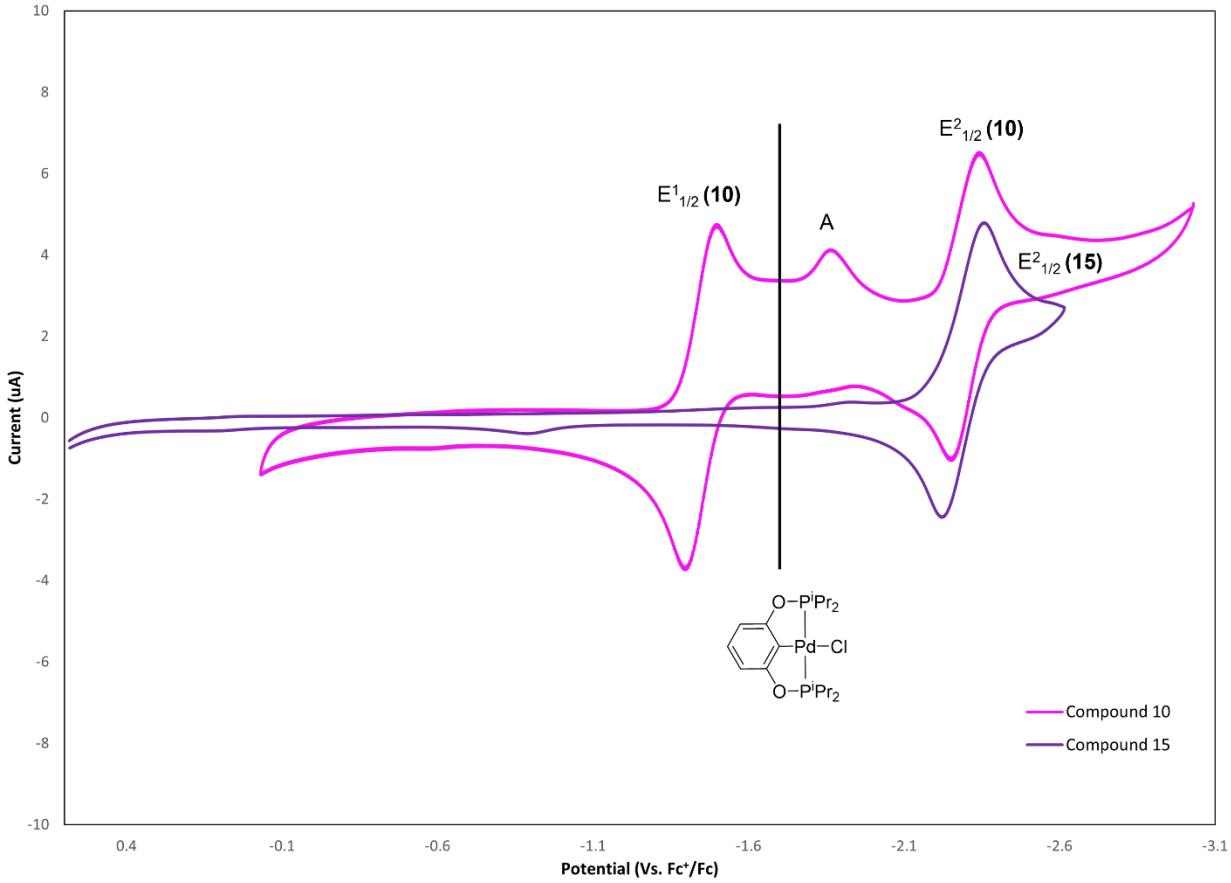


Figure S12. Comparison of cyclic voltammograms of **10** and **15**. Both 1 mM in THF with 0.1 M of $[Bu_4N][PF_6]$ as the supporting electrolyte. The black line is potential at which $P^OC^OP(PdCl)$ is irreversibly reduced. C**ompound 10:** $E^1_{1/2}$ = -1.46 V, $E^2_{1/2}$ = -2.31 V, Irreversible reduction = -1.88 V **(A)**. **Compound 15:** $E_{1/2}$ = -2.29 V.

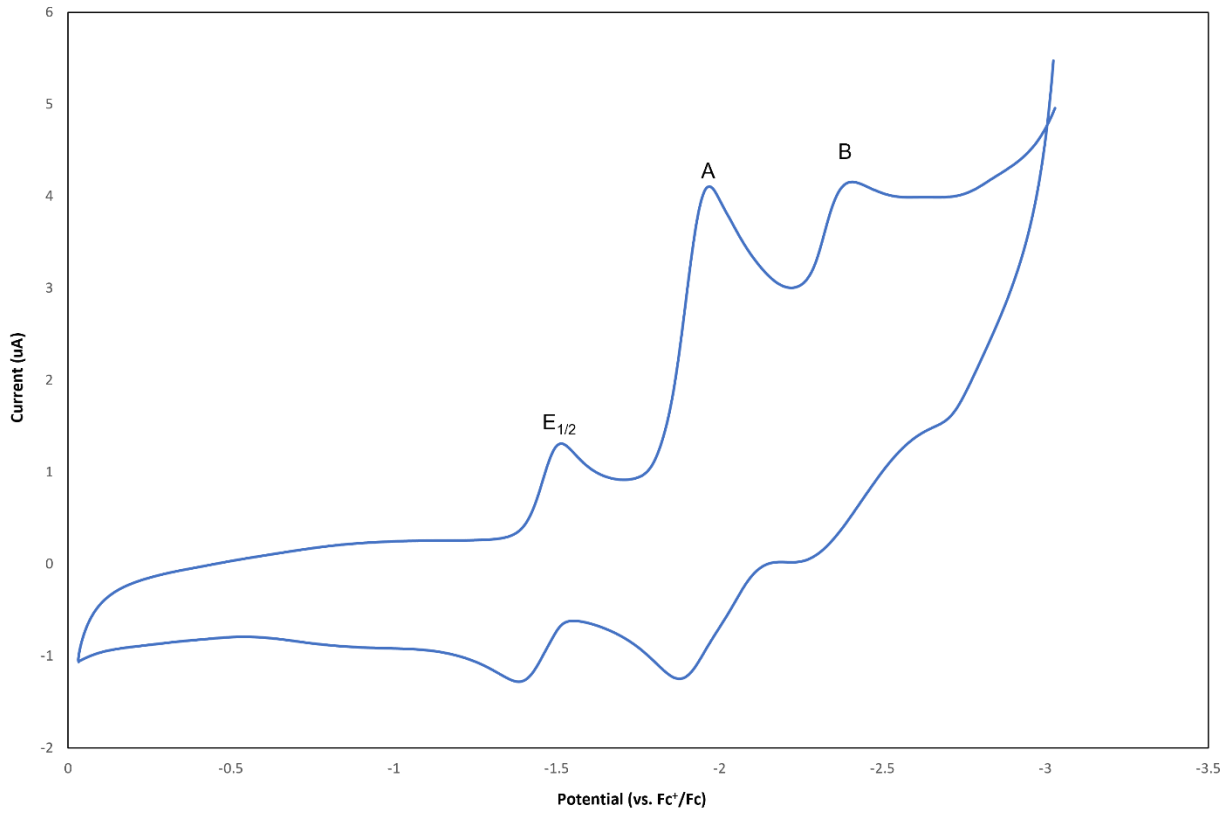


Figure S13. Cyclic Voltammogram of **10-Br** in THF (1 mM) with $[Bu_4N][PF_6]$ (0.1 M) as the supporting electrolyte. $E_{1/2}$ = -1.45 V; Irreversible reduction at = -1.98 **(A)** and -2.41 **(B)** V.

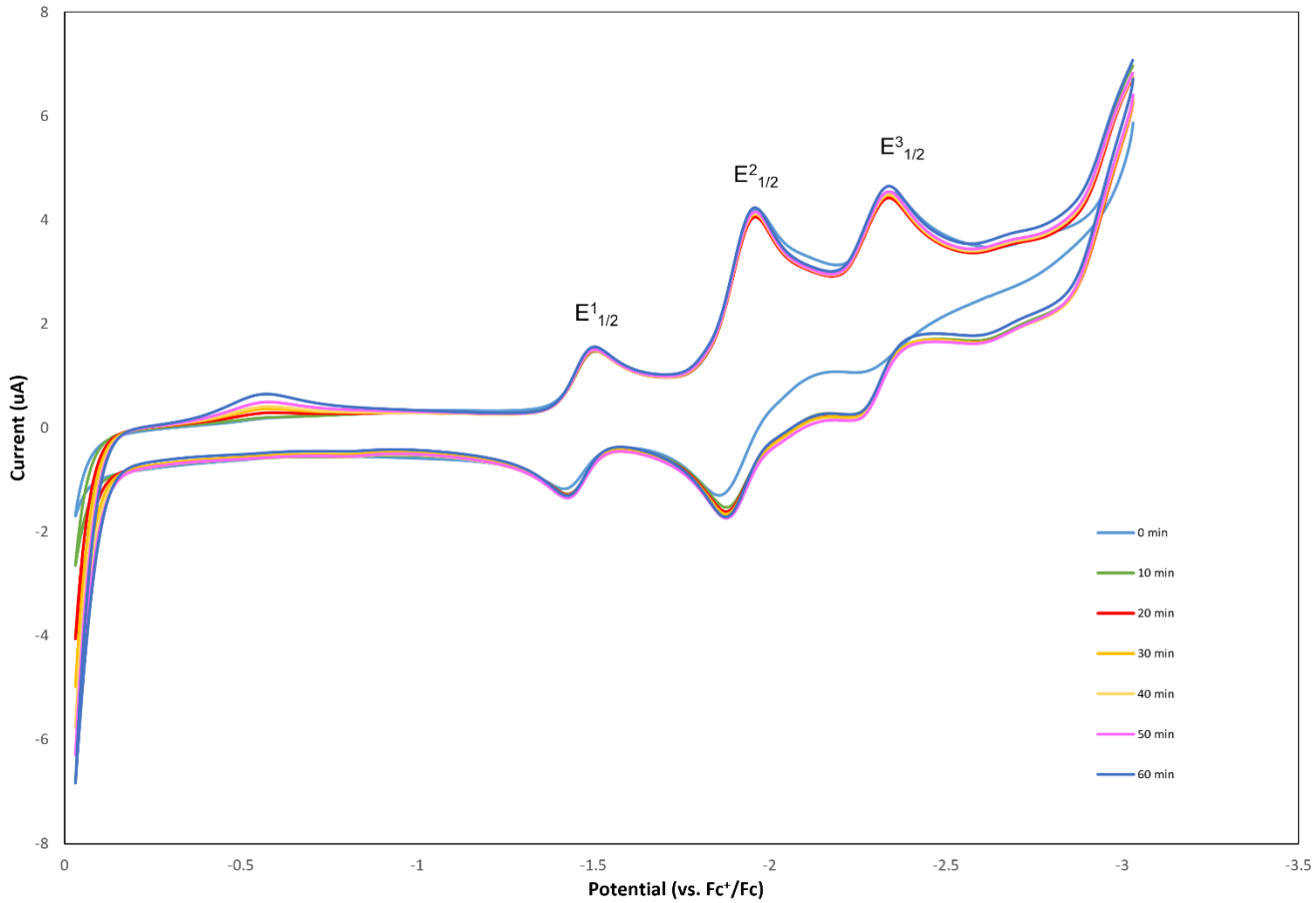


Figure S14. Cyclic voltammograms of **10-Br** in THF (1 mM) with $[Bu_4N][PF_6]$ (0.1 M) as the supporting electrolyte and 20 eq. of $[Bu_4N][Br]$ (0.02 M) in THF. The CV of the compound was recorded every 10 min. $E^1_{1/2}$ = -1.47 V; $E^2_{1/2}$ = -1.91 V; $E^3_{1/2}$ = -2.31 V.

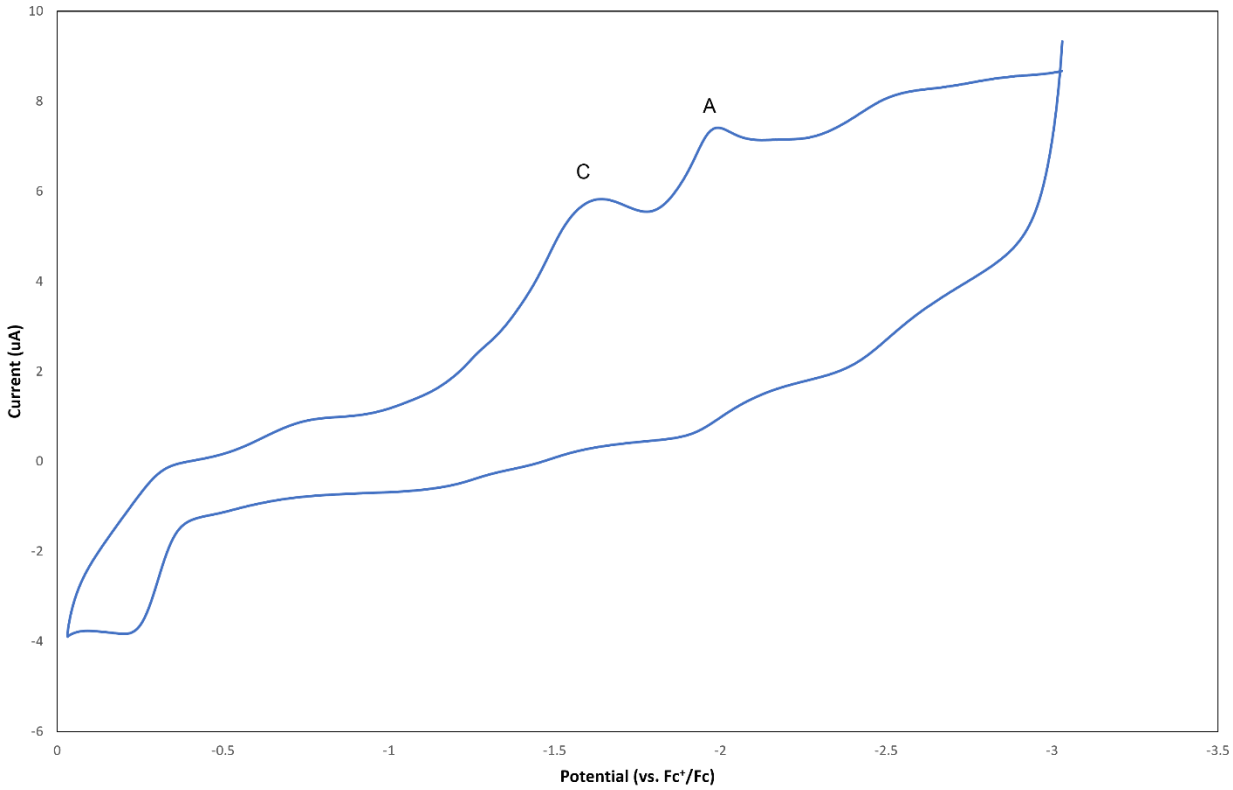


Figure S15. Cyclic Voltammogram of **10-I** in THF (1 mM) with $[Bu_4N][PF_6]$ (0.1 M) as the supporting electrolyte. Irreversible reduction at = -1.62 **(C)** and -2.01 **(A)** V.

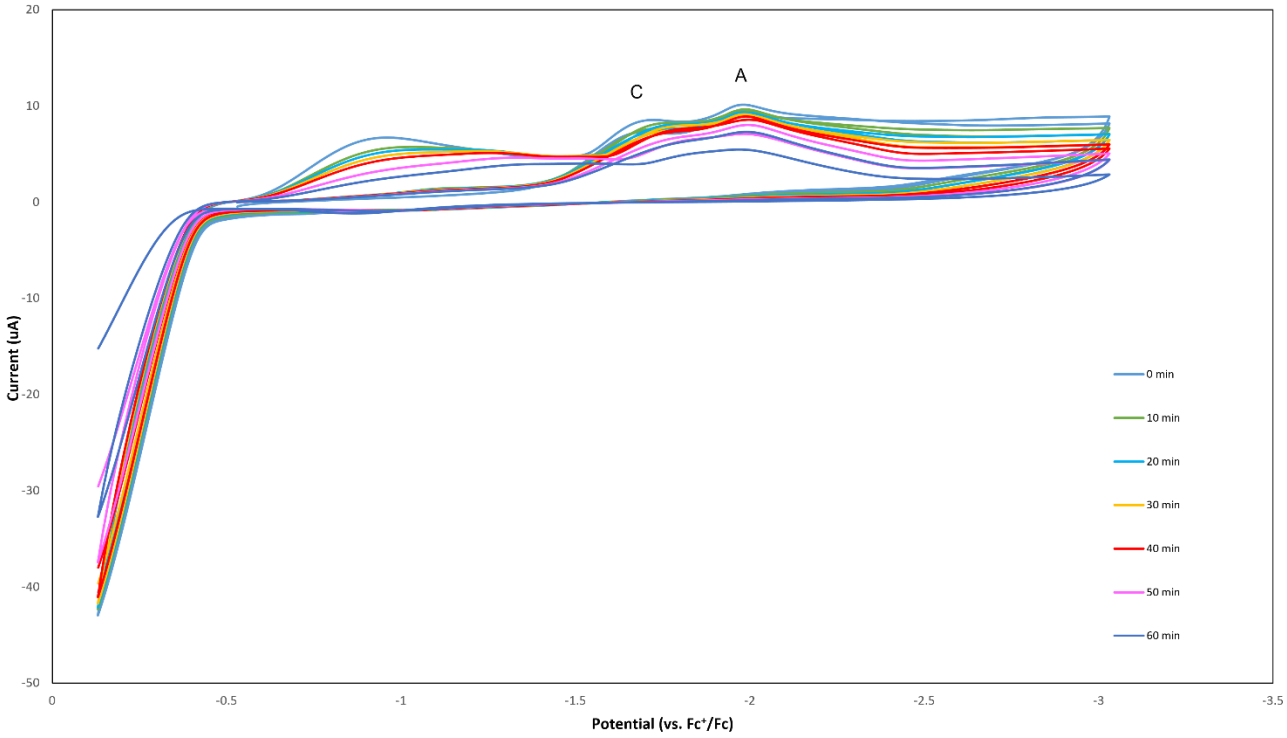


Figure S16. Cyclic voltammograms of **10-I** in THF (1 mM) with $[Bu_4N][PF_6]$ (0.1 M) as the supporting electrolyte and 20 eq. of $[Bu_4N][I]$ (0.02 M) in THF. The CV of the compound was recorded every 10 min. Irreversible reduction at = -1.73 **(C)** and -1.97 **(A)** V.

IV. Fluorescence and UV-Vis Analysis.

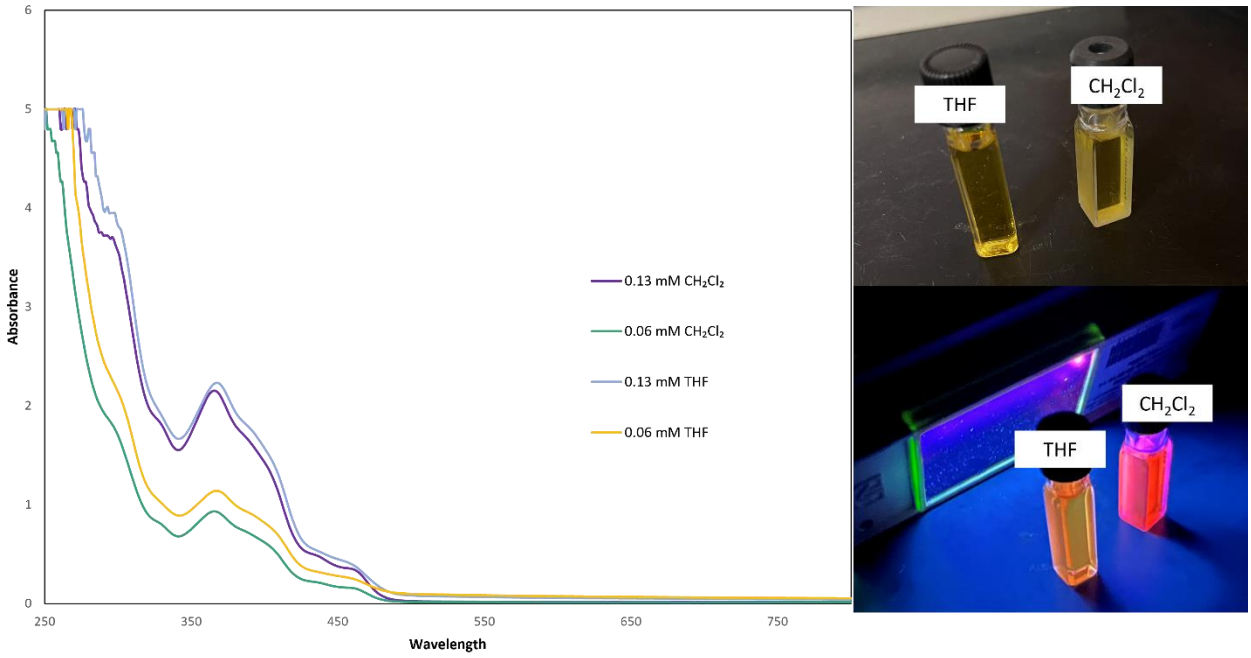


Figure S17. Left: UV-Vis absorbance spectrum of **10** in THF (blue and orange) and CH_2Cl_2 (purple and green) at two different concentrations. Right: Solutions of **10** used for UV-Vis measurements irradiated with a UVG-11 compact UV light at 254 nm with a 4 W bulb. Top picture is ambient room light with no UV irradiation and bottom picture is with only UV irradiation. All solutions for fluorescence at 0.6 mM.

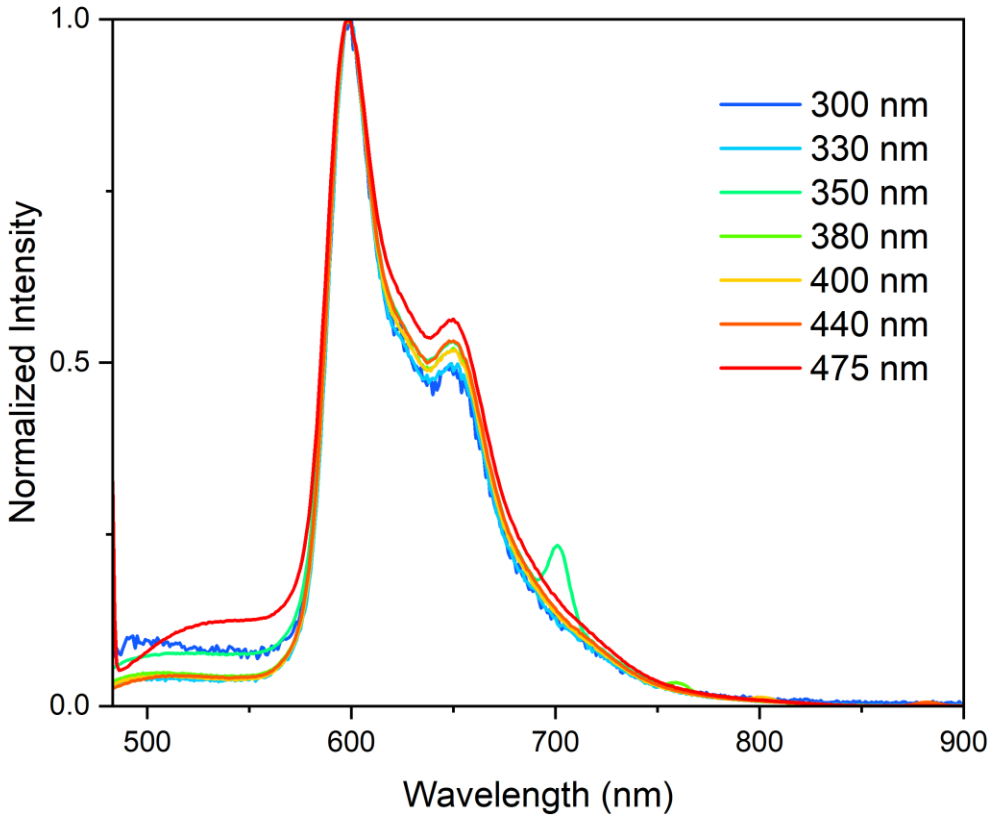


Figure S18. Fluorescence measurements for **10** in CH_2Cl_2 at 0.6 mM.

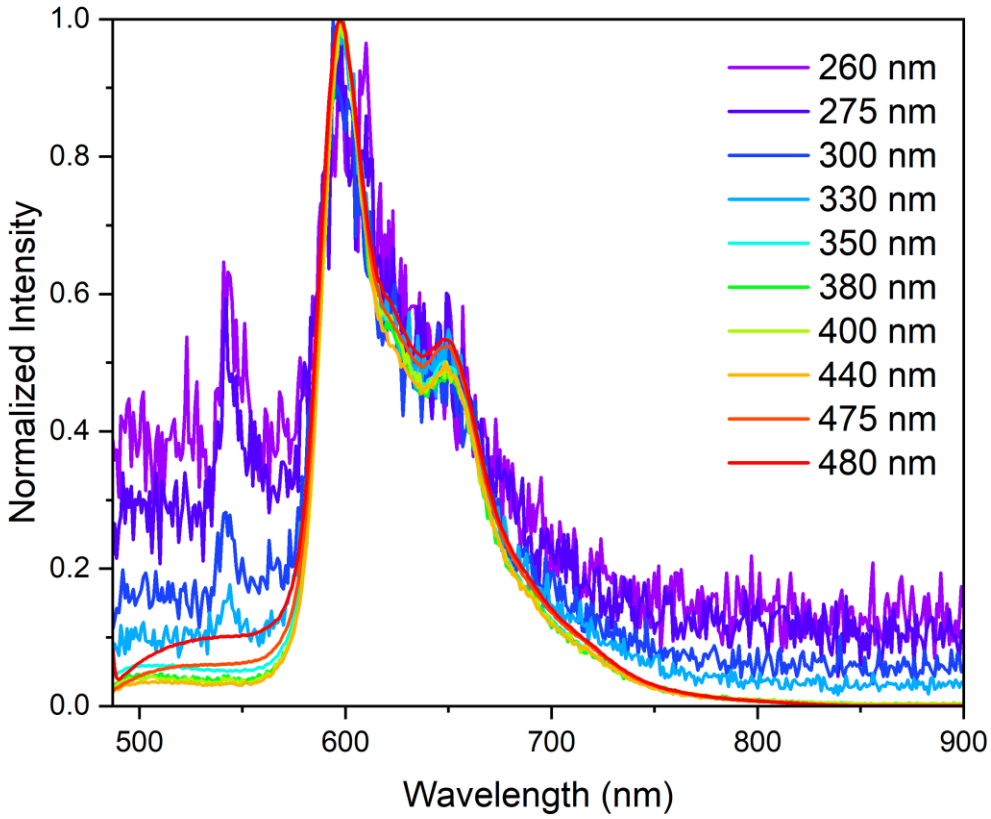
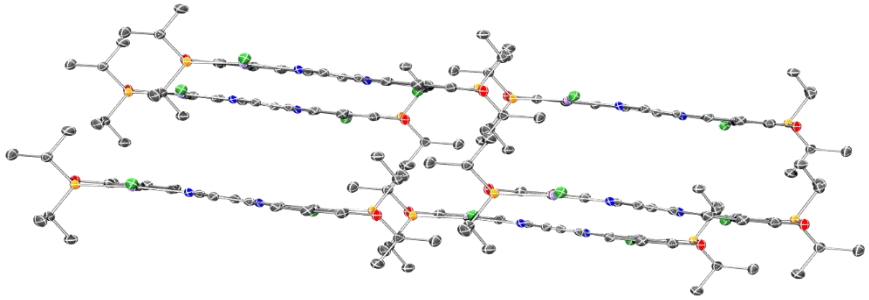


Figure S19. Fluorescence measurements for **10** in THF at 0.6 mM.

V. X-ray Diffractometry Details for PCN Bis-pincer Pd-Cl Complex (10)

A



B

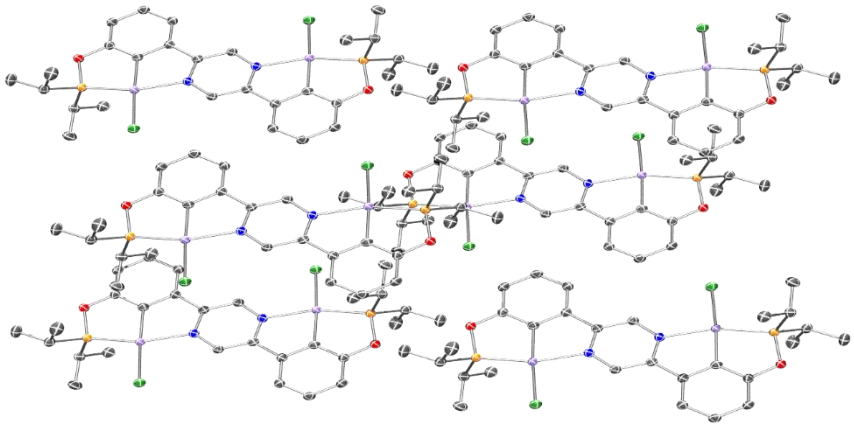


Figure S20. Unit Cell of PCN bis-pincer PdCl complex (**10)** to demonstrate minimal π interactions between molecules, side view (**A**) and top view (**B**) of unit cell. THF and hydrogens are omitted for clarity.

X-Ray data collection, solution, and refinement for PCN bis-pincer Pd-Cl Complex (10) (CCDC 2110893)

A Leica MZ 7$_5$ microscope was used to identify a suitable orange block with very well defined faces with dimensions (max, intermediate, and min) 0.143 x 0.021 x 0.018 mm^3 from a representative sample of crystals of the same habit. The crystal mounted on a nylon loop was then placed in a cold nitrogen stream (Oxford) maintained at 110 K.

A BRUKER Venture X-ray (kappa geometry) diffractometer was employed for crystal screening, unit cell determination, and data collection. The goniometer was controlled using the APEX3 software suite.[1] The sample was optically centered with the aid of a video camera such that no translations were observed as the crystal was rotated through all positions. The X-ray radiation employed was generated from a Cu-Iμs X-ray tube (K_α = 1.5418Å with a potential of 50 kV and a current of 1.0mA).

45 data frames were taken at widths of 1°. These reflections were used to determine the unit cell. The unit cell was verified by examination of the *h k l* overlays on several frames of data. No super-cell or erroneous reflections were observed.

After careful examination of the unit cell, an extended data collection procedure (15 sets) was initiated using omega and phi scans.

Data Reduction, Structure Solution, and Refinement

Integrated intensity information for each reflection was obtained by reduction of the data frames with the program APEX3.[2] The integration method employed a three-dimensional profiling algorithm and all data were corrected for Lorentz and polarization factors, as well as for

crystal decay effects. Finally the data was merged and scaled to produce a suitable data set. The absorption correction program SADABS[3] was employed to correct the data for absorption effects.

Systematic reflection conditions and statistical tests of the data suggested the space group *P*-1. A solution was obtained readily (Z=1; Z'=0.5) using XT/XS in APEX3.[2,3] Two molecules of THF was found solvated per molecule of Pd_2 complex. Hydrogen atoms were placed in idealized positions and were set riding on the respective parent atoms. All non-hydrogen atoms were refined with anisotropic thermal parameters. Unusual thermal ellipsoids on the solvent atoms and the residual electron density peaks around the solvent suggested disorder, which was modeled between two positions. Appropriate restraints and constraints were added to keep the bond distances, angles, and thermal ellipsoids meaningful. Final formula: $C_{28}H_{36}Cl_2N_2O_2P_2Pd_2 \cdot 2(C_4H_8O)$. Absence of additional symmetry or void were confirmed using PLATON (ADDSYM). The structure was refined (weighted least squares refinement on F^2) to convergence.[3, 4]

ORTEP-3 and POV-Ray were employed for the final data presentation and structure plots.[4,5]

VI. ESI References.

[1] APEX3 "*Program for Data Collection on Area Detectors*" BRUKER AXS Inc., 5465 East Cheryl Parkway, Madison, WI 53711-5373 USA.

[2] (a) G. M. Sheldrick, *Acta Cryst*., 2008, **A64,** 112-122. (b) G. M. Sheldrick, *Acta Cryst*., 2015, **A71,** 3-8. (c) G. M. Sheldrick, *Acta Cryst*., 2015, **C71,** 3-8. (d) XT, XS, BRUKER AXS Inc., 5465 East Cheryl Parkway, Madison, WI 53711-5373 USA.

[3] G. M. Sheldrick, SADABS "*Program for Absorption Correction of Area Detector Frames*", BRUKER AXS Inc., 5465 East Cheryl Parkway, Madison, WI 53711-5373 USA.

[4] L. J. Farrugia, *J. Appl. Cryst.* 2012, **45**, 849.

[5] POV-Ray Home Page, http://www.povray.org/, (accessed October, 9 2023).