# Electronic Supplemental Information (ESI)

## Palladium salen Complex: An efficient Catalyst for Sonogashira reaction at room temperature

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## 1. General Information:

Unless otherwise noted all the chemicals were used as received. All the room temperature reactions were performed in 50mL oven dried round bottomed flask. Column chromatography was performed with EMerck silica gel (60-120 mesh). Thin-layer chromatography was carried out with EMerck silica gel 60 F254 plates. Visualization of spots on TLC plate was accomplished with UV light. All products are characterized by $^{1}H$ NMR, $^{13}C$ NMR, CHN and EI-MS. $^{1}H$ NMR spectra were recorded at room temperature on Bruker, Avance 400MHz instrument. $^{1}H$ NMR chemical shifts (δ) are reported in parts per million (ppm) downfield of TMS. $^{13}C$ chemical shifts are reported in parts per million downfield of TMS and are referenced to the carbon resonance of the solvent ($CDCl_3$: δ 77.2 ppm) Data are represented as follows: chemical shift, multiplicity (s = singlet, d = doublet, t = triplet, q = quartet) integration, and coupling constants in Hertz (Hz). C, H and N were recorded using a CHN Analyzer, Model PR 2400 Series II Perkin Elmer.

## 2. Experimental Section:

**General procedure for synthesis of Schiff base ligands (*N,N′*-bis(salicylidene)-arylmethanediamines):** A 100 mL round bottomed flask was charged with salicylaldehyde (0.38 g, 3 mmol), benzaldehyde (**L1**) / 4-nitrobenzaldehyde (**L2**) / 4-methoxy-benzaldehyde (**L3**) (1.5 mmol) and $NH_4OAc$ (0.25 g, 3.27 mmol) in the presence of $NEt_3$ (0.12 mL). The mixture was then stirred for 10 min. After completion of the reaction (vide TLC), pale yellow oily substance was obtained. The yellow oily mixture was then dissolved in 1.5 mL MeOH and cooled for one night, a yellow solid was precipitated. This solid product was filtered off and washed with cold MeOH. The crude product was purified by recrystallization from ethanol and the pure Schiff base, *N,N′*-bis(salicylidene)-phenylmethanediamine (**L1**), *N,N′*-bis(salicylidene)-4-nitrophenylmethanediamine (**L2**), *N,N′*-bis-(salicylidene)-4-methoxyphenyl methanediamine (**L3**) were obtained in 80-90% yield. The Schiff base products were identified by comparing the physical and spectroscopic data with the literature report.

**General procedure for synthesis of Pd–*N,N′*-bis(salicylidene)-arylmethanediamine complex**:[1] A solution of Schiff base ligand **L1 / L2 / L3** (1 mmol) and $Pd(OAc)_2$ (224 mg, 1 mmol) was refluxed in methanol (30 mL) for 3 h with stirring. A brown colour precipitate was observed and filtered. The residue was washed with hexane and recrystallized from chloroform to obtained the title compounds **C1 / C2 / C3** (80-86%).

***N,N′*-Bis(salicylidene)-phenylmethanediamine (L1):** pale yellow solid; Anal. Calcd for ($\mathbf{C_{21}H_{18}N_2O_2}$): C. H. N: 76.36 (C), 5.45 (H), 8.48 (N); Found: 76.36 (C), 5.46 (H), 8.49 (N); Mp: 119 °C; MS: m/z = 330 ($M^+$); IR (KBr, υ $cm^{-1}$): 3300-3500 (br, OH), 1628 (C≡N); $^{1}H$ NMR: (DMSO-$d_6$/δ ppm): 12.9 (s, 2 OH), 8.6 (s, 2H, HC=N), 7.37-6.65 (m, 13H, Ph + Ph + Ph); 6.12 (s, 1H, NCHN).

Anal. Calcd for complex **C1** ($\mathbf{C_{21}H_{16}N_2O_2Pd}$), brown solid: 58.01 (C), 3.71 (H), 6.44 (N). Found: 58.18 (C), 3.93 (H), 6.13 (N). MS: m/z: 435 ($M^+$). IR (KBr, υ $cm^{-1}$): 1606 (C≡N); $^{1}H$ NMR: (400 MHz, DMSO-$d_6$, δ ppm): 8.71 (s, 2H, HC=N), 7.09-7.01 (m, 13H, Ph + Ph + Ph); 6.72 (s, 1H, NCHN).

***N,N′*-Bis(salicylidene)-4-nitrophenylmethanediamine (L2)**: pale yellow solid; Anal. Calcd for ($\mathbf{C_{21}H_{17}N_3O_4}$): 67.19 (C), 4.56 (H), 11.19 (N); Found: 67.15 (C), 4.59 (H), 11.21 (N); MS: m/z = 376 ($M^+$+1); IR (KBr), υ $cm^{-1}$) 3400-3600 (br, OH), 1619 (C≡N), 1480, 1570 (Ar), 1350, 1530 (N=O); $^{1}H$ NMR/DMSO-$d_6$/δ ppm: 12.94 (s, 2 OH), 8.9 (s, 2H, HC=N), 7.9-6.8 (m, 12H, Ph + Ph + Ph), 6.2 (s, 1H, NCHN).

Anal. Calcd for complex **C2** ($\mathbf{C_{21}H_{15}N_3O_4Pd}$); brown solid: 52.57 (C); 3.15 (H); 8.67 (N). Found: 52.54 (C), 3.16 (H), 8.65 (N). MS: m/z: 479 ($M^+$). IR (KBr, υ $cm^{-1}$): 1609 (C≡N); $^{1}H$ NMR: (400 MHz, DMSO-$d_6$, δ ppm): 8.56 (s, 2H, HC=N), 7.98-6.92 (m, 12H, Ph + Ph + Ph), 6.27 (s, 1H, NCHN).

***N,N′*-Bis(salicylidene)-4-methoxy-phenylmethanediamine (L3)**: yellow solid; Anal. Calcd. For ($\mathbf{C_{22}H_{20}N_2O_3}$): 73.3 (C), 5.5 (H), 7.7(N); Found: 73.2 (C), 5.4 (H), 7.8 (N); MS: m/z = 361 ($M^+$+1); IR (KBr, υ $cm^{-1}$) 3400-3600 (br, OH), 1629 (C≡N); $^{1}H$ NMR/DMSO-$d_6$/δ ppm: 12.68 (s, 2 OH), 9.0 (s, 2H, HC=N), 7.9-6.7 (m, 12H, Ph + Ph + Ph), 6.41 (s, 1H, NCHN), 3.79 (s, 3H, $OCH_3$).

Anal. Calcd for complex **C3** ($\mathbf{C_{22}H_{20}N_2O_3Pd}$); brown solid: 56.85 (C), 3.90 (H), 6.03 (N). Found: 56.82 (C), 3.93(H), 6.04 (N). MS: m/z: 466 ($M^+$+1). IR (KBr, m $cm^{-1}$): 1614(C≡N) $^{1}H$ NMR: (400 MHz, DMSO-$d_6$/δ ppm): 8.69 (s, 2H, HC=N), 8.01-6.82 (m, 12H, Ph + Ph + Ph), 6.37 (s, 1H, NCHN), 3.79 (s, 3H, $OCH_3$).

**General procedure for the Sonogasira reaction of aryl iodides with aryl/alkyl acetylenes:** A 50 mL oven dried round bottomed flask was charged with aryl iodide (0.5 mmol), alkyne (0.75 mmol), $K_2CO_3$ (1.5 mmol, 207 mg), **C2** complex (2 mol%, 4.79 mg) in 2 mL of isopropanol at room temperature (25 ˚C) under aerobic condition. The reaction mixture was stirred in a magnetic stirrer for appropriate time. The progress of the reaction was monitored by TLC. After the completion of the reaction, the mixture was diluted with 20 mL of water and extracted with diethyl ether (3×20 mL). The combined organic layer were washed with brine and dried over by anhydrous $Na_2SO_4$ and evaporated in a rotary evaporator under reduced pressure. The crude was purified by column chromatography on silica gel (hexane) to afford the desired product. The purity of the compound was confirmed by $^1$H NMR, $^{13}$CNMR and MS data.

## 3. Spectroscopic data for the products:

**Diphenylacetylene (Table 5 entry 1)**[2]: white solid, (m.p. 58-61 °C); $^1$H NMR (400 MHz, $CDCl_3$, δ ppm): 7.54-7.52 (m, 4H, ArH), 7.37-7.32 (m, 6H, ArH). $^{13}$C NMR (100 MHz, $CDCl_3$, δ ppm): 131.9, 128.8, 128.5, 123.6, 89.7. EI-MS: 178 [$M^+$].

**1-Methyl-4-(2-phenylethynyl)benzene (Table 5 entry 2)**[2]: white solid, (m.p. 71-72 °C); $^1$H NMR (400 MHz, $CDCl_3$, δ ppm): 7.53-7.51 (m, 2H, ArH), 7.43 (d, *J* = 8.0 Hz, 2H, ArH), 7.34-7.31 (m, 3H, ArH), 7.16 (d, *J* = 7.6 Hz, 2H, ArH), 2.36 (s, 3H, ArH). $^{13}$C NMR (100 MHz, $CDCl_3$, δ ppm): 138.4, 131.6, 131.5, 129.1, 128.3, 128.1, 123.5, 120.2, 89.6, 88.7, 21.5. EI-MS: 192 [$M^+$].

**1-Methoxy-4-(2-phenylethynyl)benzene (Table 5 entry 3)**[3]: white solid, (m.p. 62-63 °C); $^1$H NMR (400 MHz, $CDCl_3$, δ ppm): 7.49-7.45 (m, 4H, ArH), 7.32-7.30 (m, 3H, ArH), 6.87 (d, *J* = 8.2 Hz, 2H, ArH), 3.81 (s, 3H, ArH). $^{13}$C NMR (100 MHz, $CDCl_3$, δ ppm): 159.7, 133.1, 131.5, 128.3, 128.0, 123.7, 115.4, 114.1, 89.4, 55.3. EI-MS: 208 [$M^+$].

**1-Amino-4-(2-phenylethynyl)benzene (Table 5 entry 4)**[4]: brown solid; , (m.p. 125-126 °C); $^1$H NMR (400 MHz, $CDCl_3$, δ ppm): 7.46-7.42 (m, 2H, ArH), 7.22 (d, *J* = 7.8 Hz, 2H, ArH), 7.17-7.12 (m, 3H, ArH), 6.49- 6.47 (m, 2H, ArH), 4.12 (s, 2H, $NH_2$). $^{13}$C NMR (100 MHz, $CDCl_3$, δ ppm): 147.1, 132.6, 131.8, 129.1, 128.3, 128.1, 123.2, 118.2, 89.9, 88.7, 21.5. EI-MS: 193 [$M^+$].

**1-Nitro-4-(2-phenylethynyl)benzene (Table 5 entry 5)**[3]: light yellow, (m.p. 119-120 °C); $^1$H NMR (400 MHz, $CDCl_3$, δ ppm): 8.17 (d, *J* = 9.0 Hz, 2H, ArH), 7.62 (d, *J* = 9.0 Hz, 2H, ArH), 7.54-7.47 (m, 2H, ArH), 7.36-7.29 (m, 3H, ArH). $^{13}$C NMR (100 MHz, $CDCl_3$, δ ppm): 147.2, 132.4, 132.1, 130.3, 129.6, 128.7, 123.7, 122.2, 94.8, 87.8. EI-MS: 223 [$M^+$].

**1-Acetyl-4-(2-phenylethynyl)benzene (Table 5 entry 6)**[5]: white solid, (m.p. 98-100 °C); $^1$H NMR (400 MHz, $CDCl_3$, δ ppm): 7.94 (d, 2H, *J* = 8.6 Hz, ArH), 7.61 (d, *J* = 8.6 Hz, 2H, ArH), 7.56-7.53 (m, 2H, ArH), 7.37-7.33 (m, 3H, ArH), 2.62 (s, 3H, $COCH_3$). $^{13}$C NMR (100 MHz, $CDCl_3$, δ ppm): 196.2, 136.0, 132.1, 130.3, 129.6, 128.7, 128.4, 128.1, 122.2, 94.8, 87.8, 26.6. EI-MS: 220 [$M^+$].

**1-Methoxy-4-(*p*-tolylethynyl)benzene (Table 5 entry 8)**[3]: white solid, (m.p. 118-120 °C); $^1$H NMR (400 MHz, $CDCl_3$, δ ppm): 7.46 (d, *J* = 8.2 Hz, 2H, ArH), 7.40 (d, *J* = 8.0 Hz, 2H, ArH), 7.14 (d, *J* = 7.6 Hz, 2H, ArH), 6.87 (d, *J* = 8.4 Hz, 2H, ArH), 3.82 (s, 3H, $OCH_3$), 2.36 (s, 3H, $CH_3$). $^{13}$C NMR (100 MHz, $CDCl_3$, δ ppm): 159.5, 138.0, 132.9, 131.3, 129.0, 120.5, 115.6, 113.9, 88.6, 88.2, 55.3, 21.4. EI-MS: 222 [$M^+$].

**1,2-Bis(4-methylphenyl)ethyne (Table 5 entry 9)**[6]**:** white solid, (m.p. 131-133°C); $^1$H-NMR (400 MHz, $CDCl_3$, δ ppm): 7.42 (d, *J* = 7.3 Hz, 4H, ArH), 7.15 (d, *J* = 8.2 Hz, 4H, ArH), 2.36 (s, 6H, $CH_3$). $^{13}$C-NMR (100 MHz, $CDCl_3$, δ ppm): 139.6, 138.2, 132.4, 131.5, 129.3, 129.1, 120.4, 118.8, 89.1, 21.6. EI-MS: 206 [$M^+$].

**1-(4-(*p*-Tolylethynyl)phenyl)ethanone (Table 5 entry 10)**[3]: white solid, (m.p. 125-127 °C); $^1$H NMR (400 MHz, $CDCl_3$, δ ppm): 7.93 (d, *J* = 7.8 Hz, 2H, ArH), 7.60 (d, *J* = 8.2 Hz, 2H, ArH), 7.45 (d, *J* = 7.2 Hz, 2H, ArH), 7.18 (d, *J* = 8.0 Hz, 2H, ArH), 2.61 (s, 3H, $COCH_3$), 2.38 (s, 3H, $CH_3$). $^{13}$C NMR (100 MHz, $CDCl_3$, δ ppm): 197.4, 136.1, 131.6, 131.5, 129.2, 128.5, 128.3, 128.0, 122.4, 92.5, 88.6, 26.4. EI-MS: 234 [$M^+$].

**1-Methyl-4-[2-(4-nitrophenyl)ethynyl]benzene (Table 5 entry 11)**[2]: white solid, (m.p. 149-151 °C); $^1$H NMR (400 MHz, $CDCl_3$, δ ppm): 8.22 (d, *J* = 7.2 Hz, 2H, ArH), 7.66 (d, *J* = 7.2 Hz, 2H, ArH), 7.46 (d, *J* = 6.8 Hz, 2H, ArH), 7.20 (d, *J* = 7.6 Hz,

2H, ArH), 2.39 (s, 3H, $CH_3$). $^{13}C$ NMR (100 MHz, $CDCl_3$, δ ppm): 147.1, 139.6, 132.2, 131.8, 130.6, 129.4, 123.7, 119.2, 95.2, 87.3, 21.6. EI-MS: 237 [$M^+$].

**1-Nitro-2-(2-phenylethynyl)benzene (Table 5 entry 12)[2]:** yellow oil; $^1H$ NMR (400 MHz, $CDCl_3$, δ ppm): 8.25 (d, $J$ = 8.8 Hz, 2H), 7.67 (d, $J$ = 8.2 Hz, 2H), 7.57–7.45 (m, 2H), 7.41–7.32 (m, 3H) ppm, $^{13}C$ NMR (100 MHz, $CDCl_3$, δ ppm): 141.7, 134.8, 132.6, 130.2, 129.4, 128.5, 128.2, 124.9, 122.3, 97.3, 84.7. EI-MS: 223 [$M^+$]. Anal. Calcd for (**$C_{14}H_9NO_2$**): 75.33 (C), 4.07 (H), 6.27 (N); Found: 75.36 (C), 4.02 (H), 6.22 (N).

**1-(Dodec-1-yn-1-yl)-benzene (Table 5 entry 13):** yellow liquid; $^1H$ NMR (400 MHz, $CDCl_3$, δ ppm): 7.37-7.31 (m, 2H, ArH), 7.26-7.18 (m, 3H, ArH), 2.36 (t, $J$ = 6.8 Hz, 2H, $CH_2$), 1.61-1.25 (m, 16H, $C_9H_{16}$), 0.89 (t, $J$ = 6.8 Hz, 3H, $CH_3$). $^{13}C$ NMR (100 MHz, $CDCl_3$, δ ppm): 131.6, 128.3, 127.6, 124.5, 89.1, 80.4, 31.9, 29.6, 29.5, 29.3, 29.2, 29.1, 28.7, 19.5, 14.1. EI-MS: 242 [$M^+$]. Anal. Calcd for (**$C_{18}H_{26}$**): 89.19 (C), 10.81 (H); Found: 89.16 (C), 10.77 (H).

**1-(Dodec-1-yn-1-yl)-4-nitrobenzene (Table 5 entry 14)**: yellow liquid; $^1H$ NMR (400 MHz, $CDCl_3$, δ ppm): 8.15 (d, 2H, $J$ = 8.4 Hz, ArH), 7.51 (d, 2H, $J$ = 8.4 Hz, ArH), 2.45 (t, $J$ = 7.3 Hz, 2H, $CH_2$), 1.64-1.27 (m, 16H, $C_9H_{16}$), 0.88 (t, $J$ = 6.8 Hz, 3H, $CH_3$). $^{13}C$ NMR (100 MHz, $CDCl_3$, δ ppm): 146.6, 132.2, 131.3, 123.53, 96.9, 31.9, 29.6, 29.5, 29.3, 29.1, 29.0, 28.4, 19.6, 14.1. EI-MS: 287 [$M^+$]. Anal. Calcd for (**$C_{18}H_{25}NO_2$**): 75.22 (C), 8.77 (H), 4.87 (N); Found: 75.16 (C), 8.79 (H), 4.82 (N).


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