# Supporting Information

## Diaryl Schiff base as a photo- and pH-responsive bifunctional molecule

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## 1. Materials

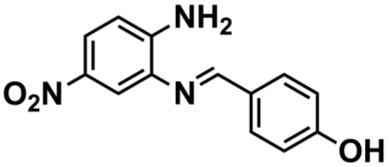
All chemical reagents were purchased from Aldrich Chemical Company and used without further purification. $^1$H and $^{13}$C NMR spectra were recorded using a Bruker AVANCE-500 spectrometer. UV absorption and fluorescence spectra were obtained at room temperature using a double beam UV-visible spectrophotometer (Shimadzu UV-2501 PC) and a Hitachi F-2700 spectrofluorometer, respectively. Elemental analyses (C, H, N) and high resolution mass spectra were performed with a Fison Carlo Erba 1112 and a ESI-Q-TOF mass spectrometry, and IR spectra were obtained using a Bruker Equinox 55 spectrophotometer in the range of 400-4000 cm$^{-1}$.

## 2. Synthesis of the diaryl Schiff bases (1a, 2a)

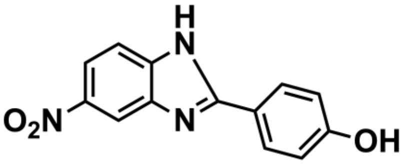
The diaryl Schiff base **1a** was typically prepared as follow: to ethanol (60 mL) was added a mixture of 4-hydroxy benzaldehyde (0.122 g, 1 mmol) and 4-nitro-o-phenylenediamine (0.459 g, 3 mmol), then the mixture was heated to reflux for 48 h under argon atmosphere. After cooling to room temperature, the liquid was poured into the water (1 L), filtered and washed with water and ethanol. Then a 41% yield of the title nitro-substituted Schiff base of 0.105 g was provided.

The non-nitro Schiff base **2a** was synthesized as follow: to ethanol (40 mL) was added a mixture of 4-hydroxy benzaldehyde (0.122 g, 1 mmol) and o-phenylenediamine (0.324 g, 3 mmol), then the mixture was heated to 50 $^{o}$C for 48 h under argon atmosphere. After cooling to room temperature, the liquid was poured into the water (1 L), filtered and washed with water. Then a 87% yield of the title non-nitro Schiff base **2a** was provided.

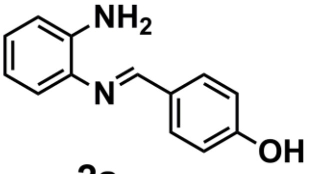
## 3. Structural characterization of compounds 1a, 1a’ and 2a



**1a**



**1a'**



**2a**

**(E)-4-(((2-amino-5-nitrophenyl)imino)methyl)phenol (1a):** $^1$H NMR (500 MHz, ppm, $d_6$-DMSO) δ 10.17 (s, 1H, -OH), 8.67 (s, 1H, -N=CH-), 7.96 – 7.87 (m, 4H, Ar$_1$-H, Ar$_2$-H), 6.88 (d, *J* = 8.5 Hz, 2H, Ar$_2$-H), 6.74 (d, *J* = 8.9 Hz, 1H, Ar$_1$-H), 6.68 (s, 2H, -NH$_2$); $^{13}$C NMR (126 MHz, ppm, $d_6$-DMSO) δ 160.89, 159.34, 150.82, 136.03, 134.74, 131.26, 127.51, 123.73, 115.55, 112.60, 112.38. Anal. Calcd for $C_{13}H_{11}N_3O_3$: C, 60.70; H, 4.31; N, 16.33%. Found: C, 61.02; H, 4.10; N, 16.24%. HRMS (ESI) calculated for $C_{13}H_{11}N_3O_3$ $(M+H)^+$ 258.0800, found 258.0872. IR (KBr, cm$^{-1}$) 3406 and 3314 *v*(Ar-NH$_2$), 1611 *v*(C=N), 1507, *v*(Ar-C), 1339 *v*(Ar-NO$_2$), 1169 *v*(Ar-OH), 824 *v*(Ar-H).

**4-(5-nitro-1H-benzo[d]imidazol-2-yl)phenol (1a’):** $^1$H NMR (500 MHz, ppm, $d_6$-DMSO) δ 10.20 (s, 1H, -OH), 8.40 (d, *J* = 2.0 Hz, 1H, Ar$_1$-H), 8.10 (dd, *J* = 8.8, 2.3 Hz, 1H, Ar$_1$-H), 8.06 (d, *J* = 8.7 Hz, 2H, Ar$_2$-H), 7.70 (d, *J* = 8.8 Hz, 1H, Ar$_1$-H), 6.96 (d, *J* = 8.7 Hz, 2H, Ar$_2$-H).

**(E)-4-(((2-aminophenyl)imino)methyl)phenol (2a):** $^1$H NMR (500 MHz, ppm, $d_6$-DMSO): δ 12.69 (s, 1H, -OH), 10.05 (s, 1H, -N=CH-), 8.06 (d, J = 8.7 Hz, 2H, Ar$_2$-H), 7.57 (m, 2H, Ar$_1$-H), 7.17 (dd, J = 6.0, 3.1 Hz, 2H, Ar$_1$-H), 6.96 (d, J

= 8.7 Hz, 2H, $Ar_2$-H), 3.53 (s, 2H, -$NH_2$); $^{13}$C NMR (126 MHz, ppm, $d_6$-DMSO): δ 159.09, 151.75, 130.57, 128.11, 127.46, 121.57, 121.14, 115.64, 115.51, 115.45. Anal. Calcd for $C_{13}H_{12}N_2O$: C, 73.56; H, 5.70; N, 13.20%. Found: C, 73.43; H, 5.26; N, 13.08%. IR (KBr, cm$^{-1}$) 3236 *v*(Ar-$NH_2$), 1610 *v*(C=N), 1448 *v*(Ar-C), 1177 *v*(Ar-OH), 836 and 743 *v*(Ar-H).

## 4. UV-*vis* spectra and fluorescence spectrum

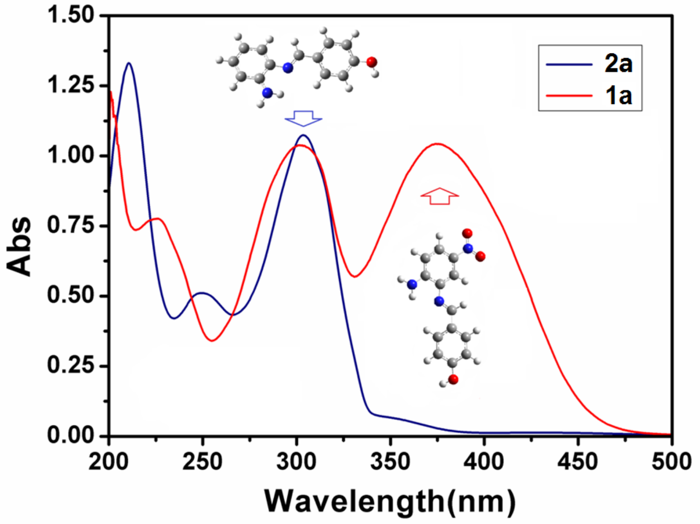


**Fig. S1** UV-*vis* spectra of compounds **1a** (50 μM, in ethanol) and **2a** (100 μM, in ethanol).

As shown in Fig. S1, three red shifts were observed due to the addition of the nitro group. The second absorbing peak of the compound **1a** shared the same absorbing wavelength (307 nm) with the first absorbing peak of the compound **2a**, and the nitro group caused increasing of intensity of UV absorption of the compound **1a**, as well. Besides, the sensitivity to UV light is strengthened because of the nitro group on the compound **1a**.

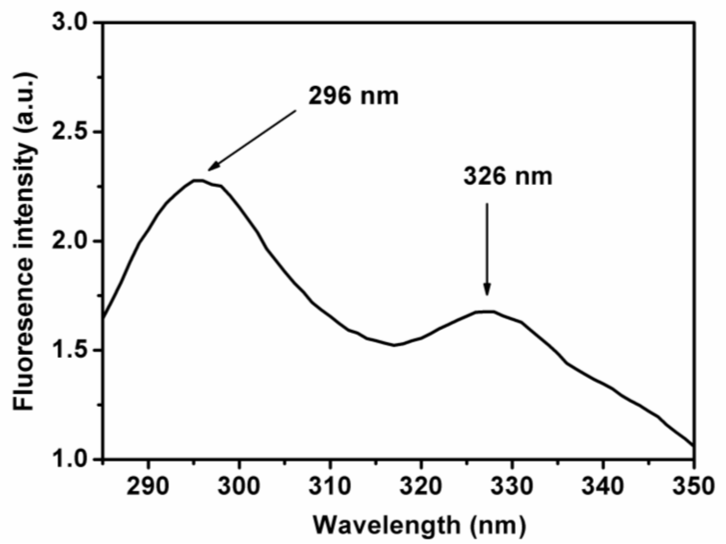


**Fig. S2** Fluorescence spectrum of the compound **1a** in ethanol ($\lambda_{ex}$ = 270 nm).

When the compound **1a** was excited at 270 nm, the weak emission of fluorescence at 296 nm and 326 nm were observed (Fig. S2).