Supporting Information

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

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List of Contents

1. Materials...........................................................................................................................................S2

2. Synthesis of the non-nitro Schiff base (1a, 2a)..................................................................................S2

3. Structural characterization of compounds 1a, 1a’ and 2a . .........................................................S3

4. UV-vis spectra and fluorescence spectrum .. ... ........................................................................... S4
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 °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

(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$_3$O$_3$: 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$_3$O$_3$ (M+H)$^+$ 258.0800, found 258.0872.

IR (KBr, cm$^{-1}$) 3406 and 3314 $\nu$(Ar-NH$_2$), 1611 $\nu$(C=N), 1507, $\nu$(Ar-C), 1339 $\nu$(Ar-NO$_2$), 1169 $\nu$(Ar-OH), 824 $\nu$(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, Ar₂-H), 3.53 (s, 2H, -NH₂); ¹³C NMR (126 MHz, ppm, d₆-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 C₁₃H₁₂N₂O: C, 73.56; H, 5.70; N, 13.20%. Found: C, 73.43; H, 5.26; N, 13.08%. IR (KBr, cm⁻¹) 3236 ν(Ar-NH₂), 1610 ν(C=N), 1448 ν(Ar-C), 1177 ν(Ar-OH), 836 and 743 ν(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).