Synthesis of a Bis[2-(2’-hydroxyphenyl)benzoxazole]pyridinium Derivative: The Fluoride-Induced Large Spectral Shift for Ratiometric Response

Chathura S. Abeywickrama\textsuperscript{a} and Yi Pang\textsuperscript{a,b} *
\textsuperscript{a}Department of Chemistry & \textsuperscript{b}Maurice Morton Institute of Polymer Science, University of Akron, Akron, Ohio 44325, USA.

Supporting Information

* Corresponding author. E-mail: yp5@uakron.edu
Figure S1.1 $^1$H NMR (500 MHz in DMSO-$d_6$) of 3.
Figure S1.2 $^{13}$C NMR (500 MHz in DMSO-$d_6$) of 3.
Figure S1.3 \(^1\)HNMR (500 MHz in DMSO-\(d_6\)) of \(2\).
Figure S1.4 $^{13}$CNMR (500 MHz in DMSO-$d_6$) of 2.
Figure S2.1 High-resolution mass spectrometric analysis (theoretical vs experimental mass) of probe 3. The error for the ESI mass spectra is 5 ppm.
Figure S2.2 High-resolution mass spectrometric analysis of probe 2.
Figure S3. UV-vis (a) and normalized fluorescence spectra (excited at 390 nm) (b) of 3 ($1 \times 10^{-5}$ M) in different solvents at room temperature.
Figure S4. UV-vis (a) and normalized fluorescence spectra (excited at 390 nm) (b) of 3 (1 x 10^{-5} M) in DMF and ethanol at room temperature.
Figure S5. (a) Represents the normalized fluorescence spectra obtained for 3 (1 x 10^{-5} M) in ethanol in different temperatures. (b) represents the recorded fluorescence intensity as a function of temperature. Probe 3 was excited at 375 nm to obtain the emission spectra.
Figure S6. (a) Represents the normalized fluorescence spectra obtained for 3 (1 x 10⁻⁵ M) in DMF in different temperatures. (b) represents the recorded fluorescence intensity as a function of temperature. Probe 3 was excited at 390 nm to obtain the emission spectra.
Figure S7. Spectrometric titration of the probe 3 (1 x 10^{-5} M in acetonitrile) with the addition of Bu_{4}NF in acetonitrile at room temperature. Figure (a) and (b) represents the absorbance and emission spectra accordingly. Probe 3 was excited at 380 nm to record the emission spectra.
Figure S8. (a) Total emission recorded for the spectrometric titration of the probe 3 (1 x 10^{-5} M in acetonitrile) with the addition of Bu4NF (in acetonitrile) at room temperature. Figure (b) represents emission spectra recorded at 710 nm. Probe 3 was excited at 380 nm to record the emission spectra.
**Figure S9.** (a) The emission spectra recorded for the spectrometric titration of the probe 3 (1 x $10^{-5}$ M in acetonitrile) with the addition of Bu$_4$NF (in acetonitrile) at 710 nm (a) and 450 nm (b). Probe 3 was excited at 390 nm to record the emission spectra.
Figure S10 Spectrometric titration of the probe 3 (1 x 10^{-5} M in acetonitrile) with the addition of Bu$_4$NOH in acetonitrile at room temperature, recorded from (a) the absorbance spectra (b) emission spectra with 380 nm excitation.
Figure S11 The emission spectra recorded for spectrometric titration of the probe 3 (1 x 10^{-5} M in acetonitrile) with the addition of Bu_{4}NF (a) and Bu_{4}NOH (b) in acetonitrile at room temperature. The emission spectra were recorded by exciting the probe at 535 nm.
**Figure S12** Spectrometric titration of the probe 3 (1 x 10^{-5} M in acetonitrile) with the addition of Bu4N+(CH3COO-) in acetonitrile at room temperature, showing the spectral response in the UV-vis absorption (a) and emission spectra with excitation at 380 nm (b).