A Receptor Incorporating OH, NH and CH Binding Motifs: Dual-Modal Sensing Fluoride

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S1. Materials

All reagents were obtained from commercial suppliers and used as received unless otherwise noted.

S2. Instruments

Column chromatography was performed on silica gel (160 - 200 mesh), and thin-layer chromatography (TLC) was performed on precoated silica gel plates and observed under UV light. Nuclear magnetic resonance (NMR) spectra were recorded on Bruker Avance DPS-400 and Bruker Avance DPS-600 spectrometers at room temperature (298 K). Chemical shifts were referenced to the residual solvent peaks. Electrospray ionization (EI) mass spectrometry was performed on a Waters QP-2010 gas chromatography mass spectrometer. UV/Vis spectra were measured on a Hitachi U-3010 spectrometer. Fluorescence excitation and emission spectra were recorded using a Hitachi F-4500.

S3. Synthesis of Compound 7

Compound 7 ((5-Bromo-3-hydroxymethyl-2-methoxy-phenyl)-methanol) was synthesized in
accordance with literature procedures.23

S4. ¹H NMR and ¹³C NMR of compound 1, 2, 3, 4, 5, and 6.

¹H NMR spectrum (400 MHz, 298 K, CDCl₃) of compound 6

![NMR spectrum of compound 6](image)

¹³C NMR (CDCl₃, 298 K, 100 MHz) of compound 6
1H NMR spectrum (400 MHz, 298 K, CDCl₃) of compound 5

13C NMR (CDCl₃, 298 K, 100 MHz) of compound 5
$^1$H NMR spectrum (400 MHz, 298 K, CDCl$_3$) of compound 4
$^{13}$C NMR (CDCl$_3$, 298 K, 100 MHz) of compound 4
$^1$H NMR spectrum (400 MHz, 298 K, CDCl$_3$) of compound 3
$^{13}$C NMR (CDCl$_3$, 298 K, 100 MHz) of compound 3
$^1$H NMR spectrum (400 MHz, 298 K, CDCl$_3$) of compound 2
$^{13}$C NMR (CDCl$_3$, 298 K, 100 MHz) of compound 2

100 MHz, CDCl$_3$, 298 K
$^{13}$C NMR (CDCl$_3$, 298 K, 100 MHz) of compound I

400 MHz, CDCl$_3$, 298 K
$^{13}$C NMR (CDCl$_3$, 298 K, 100 MHz) of compound 1

S5. Emission spectra of compound 1 (1 × 10$^{-5}$ M) upon addition of 60 equivalents of various anions.

Fig S5 Emission spectra of compound 1 (1 × 10$^{-5}$ M) upon addition of 60 equivalents of tetrabutylammonium fluoride, chloride, bromide, iodide, hexafluorophosphate, acetate, dihydrogen phosphate, and sulfate in CH$_2$Cl$_2$. Excitation wavelength was 320 nm with 10.0 nm slit widths.