Azo Schiff bases as colorimetric, fluorescent and electrochemical sensing for selective recognition of fluoride ion and

Supporting information Sheet

Fig. 1: The absorption spectra of $\text{H}_2\text{L}^2$ in solvents with different polarities

Fig. 2: The absorption spectra of $\text{H}_2\text{L}^3$ in solvents with different polarities
Fig. 3: The visible color changes observed for $\text{H}_2\text{L}^1$ - $\text{H}_2\text{L}^3$ in DMSO solution upon addition of 2 equiv. of anions as TBA salts.
Fig. 4: Absorption spectra of the receptors $\text{H}_2\text{L}^1$ - $\text{H}_2\text{L}^3$ (a, b and c, respectively) recorded in DMSO after addition of 0–2 equiv. of TBAOH.
Fig. 5: UV–Vis absorption spectra of $\text{H}_2\text{L}_2^2$ - $\text{H}_2\text{L}_3^3$ (a and b, respectively) upon addition of a particular anion salt in DMSO.
Fig. 6: Plot of $1/\Delta A$ against $1/[F]$ for (a) $H_2L^1$, (b) $H_2L^2$, (c) $H_2L^3$. 

(a)
Fig. 7: Job’s plots determined by UV-Vis method of receptors $\text{H}_2\text{L}^1 - \text{H}_2\text{L}^3$ (a, b and c, respectively) with tertiarybutylammonium fluoride.
Fig. 8: Changes in the absorption spectra of $\text{H}_2\text{L}^1 \ (2 \times 10^{-5} \text{ M})$ in DMSO upon addition from 0 to 2 equiv of (a). Hg$^{2+}$ and (b). Cd$^{2+}$ ions.
Fig. 9: Changes in the absorption spectra of $\text{H}_2\text{L}^3$ ($2 \times 10^{-5}$ M) in DMSO upon addition from 0 to 2 equiv of (a). Hg$^{2+}$ and (b). Cd$^{2+}$ ions.
Fig. 10: Plot of $1/\Delta A$ against $1/[\text{Hg}]$ for (a). $\text{H}_2\text{L}^1\cdot \text{Hg}^{2+}$, (b). $\text{H}_2\text{L}^2\cdot \text{Hg}^{2+}$, (c). $\text{H}_2\text{L}^3\cdot \text{Hg}^{2+}$. 
Fig. 11: Plot of $1/\Delta A$ against $1/[\text{Cd}]$ for (a). $\text{H}_2\text{L}_1^- \cdot \text{Cd}^{2+}$, (b). $\text{H}_2\text{L}_2^- \cdot \text{Cd}^{2+}$, (c). $\text{H}_2\text{L}_3^- \cdot \text{Cd}^{2+}$. 
Fig. 12: Absorption spectral change of mixture between (a) H$_2$L$_1$, (b) H$_2$L$_3$ and Hg$^{2+}$ and Cd$^{2+}$ upon addition of F$^-$ in DMSO.
Fig. 13: Absorption spectral change of mixture between (a) \( \text{H}_2\text{L}_1 \), (b) \( \text{H}_2\text{L}_3 \) and \( \text{F}^- \) upon addition of \( \text{Hg}^{2+} \) and \( \text{Cd}^{2+} \) in DMSO.

**UV-Vis Absorption Studies**

The binding constant of the receptor (1a-1d) were calculated from the fluoride-induced absorption changes using the following Eq. (1)
\[ \frac{b}{\Delta A} = \frac{1}{S_i K_a \Delta \varepsilon} \times \frac{1}{[L]} + \frac{1}{S_i \Delta \varepsilon} \]  

(1)

\[ \Delta A = A_{\text{substrate+anion}} - A_{\text{substrate}}, \ b = \text{path length, } S_i = \text{total concentration of substrate, } K_a = \]

association constant, \( \Delta \varepsilon = \varepsilon_{\text{substrate+anion}} - \varepsilon_{\text{substrate}} - \varepsilon_{\text{anion}}. \)

Plotting \( 1/\Delta A \) against \( 1/[L] \) gives:

\[ \text{Slope} = \frac{1}{S_i K_a \Delta \varepsilon} \]  

(2) \hspace{1cm} \text{Intercept} = \frac{1}{S_i \Delta \varepsilon} \]  

(3)

Thus, \( K_a = \frac{\text{Intercept}}{\text{Slope}} \)