A Highly Selective Colorimetric Chemosensor for Detection of Nickel Ions in Aqueous Solution

Xin Liu, Qi Lin*, Tai-Bao Wei, You-Ming Zhang*

Key Laboratory of Eco-Environment-Related Polymer Materials, Ministry of Education of China; Key Laboratory of Polymer Materials of Gansu Province; College of Chemistry and Chemical Engineering, Northwest Normal University, Lanzhou, Gansu, 730070, P. R. China

Interactions of LX with various anions (Figure S1).................................1

Ratiometric calibration curve (Figure S2)..............................................2

Determination of association constant (Figure S3).................................3

The detection limit of LX with Ni²⁺ (Figure S4).....................................4

¹H NMR experiments (Figure S5)...........................................................5

ESI-MS spectra of LX (Figure S6).........................................................6

ESI-MS spectra of LX-Ni²⁺ (Figure S7)....................................................7

* Corresponding author. E-mail: linqi2004@126.com (Dr. Q. Lin); zhangnwmu@126.com (Prof. Y. M. Zhang)
Tel:+86-931-7973120;
Interactions of LX with various anions

Figure S1. Changes in the UV/Vis spectra of LX (c=2×10⁻⁵ M) after addition of 50 equivalents of various anions in DMSO-H₂O (v/v=1:1) HEPES buffer solutions at pH=7.4.
Ratiometric calibration curve

Figure S2. Ratiometric calibration curve A525/A464 as a function of Ni$^{2+}$ concentration.
Determination of association constant

The association constants ($K_a$) of $LX$ with $Ni^{2+}$ were determined based on the absorbance titration curve using the Benesi-Hildebrand equation as follows: where $A$ and $A_0$ represent the absorbance of host in the presence and absence of ions, respectively, $A_{\text{max}}$ is the saturated absorbance of host in the presence of excess amount of ions; $[G]$ is the concentration of $Ni^{2+}$ added.

$$\frac{1}{A_{\text{max}} - A_0} = \frac{1}{A - A_0} \left[ \frac{1}{K_a[G]^2} + 1 \right]$$

Figure S3. Benesi-Hildebrand plot of $LX$ with $Ni^{2+}$.
The detection limit of LX with Ni$^{2+}$

![Graph with data and equation: A=0.00585C-0.0069, R²=0.9967.](image)

Figure S4. Plot of the absorption at 525 nm for a mixture of LX (c=2×10⁻⁵ M) in DMSO-H₂O (v/v=1:1) HEPES buffer solutions at pH=7.4.
$^1$H NMR experiments

Figure S5. Partial $^1$H NMR spectra of LX upon addition of Ni$^{2+}$ in DMSO-$d_6$
ESI-MS spectra of LX

Figure S6. ESI-MS spectra of LX.
Figure S7. ESI-MS spectra of LX-Ni^{2+}.