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Supporting Information

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

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Interactions of LX with various anions

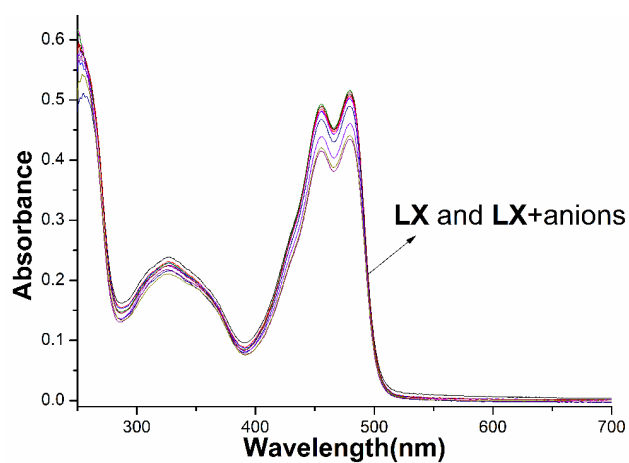


Figure S1. Changes in the UV/Vis spectra of LX ($c=2\times 10^{-5}$ M) after addition of 50 equivalents various anions in DMSO-H₂O (v/v=1:1) HEPES buffer solutions at pH=7.4.

Ratiometric calibration curve

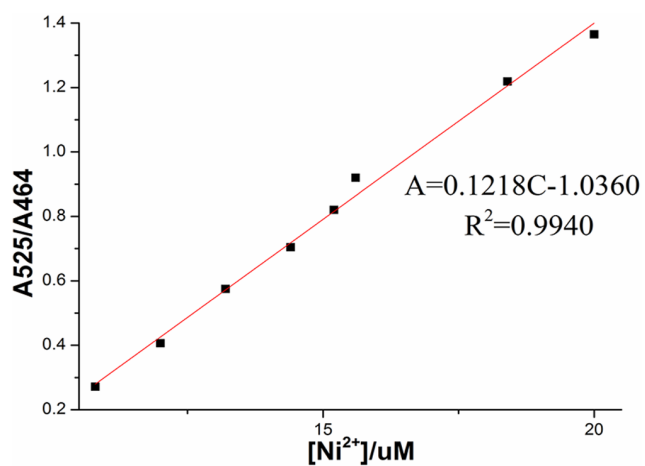


Figure S2. Ratiometric calibration curve A525/A464 as a function of Ni²⁺ concentration.

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_{max} is the saturated absorbance of host in the presence of excess amount of ions; $[G]$ is the concentration of Ni^{2+} added.

$$\frac{1}{A_{\text{max}} - A_0} = \frac{1}{A_1 - A_0} \left[\frac{1}{K_a [G]^2} + 1 \right]$$

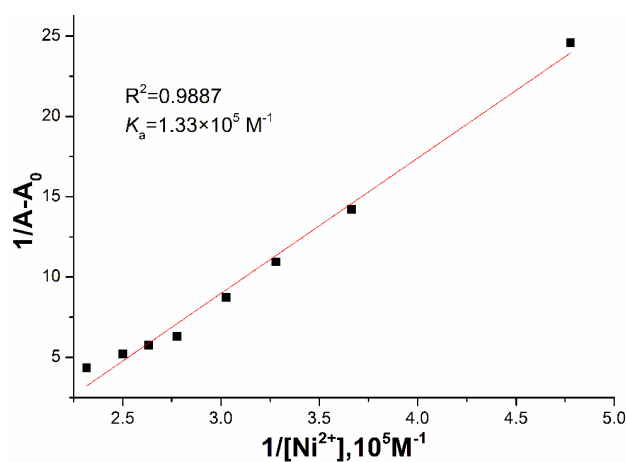


Figure S3. Benesi-Hildebrand plot of **LX** with Ni^{2+} .

The detection limit of LX with Ni²⁺

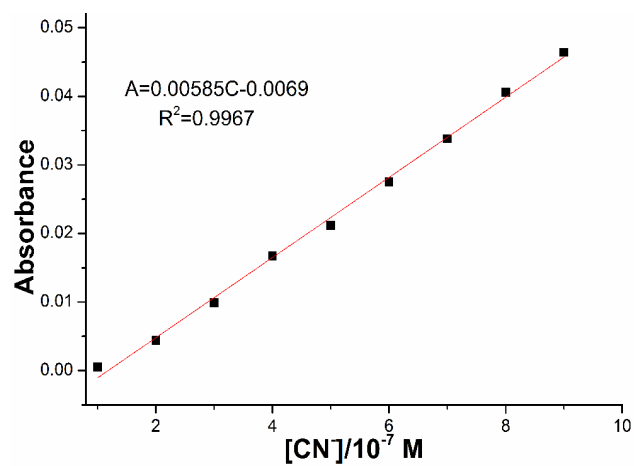


Figure S4. Plot of the absorption at 525 nm for a mixture of LX ($c=2\times 10^{-5}$ M) in DMSO-H₂O ($v/v=1:1$) HEPES buffer solutions at pH=7.4.

^1H NMR experiments

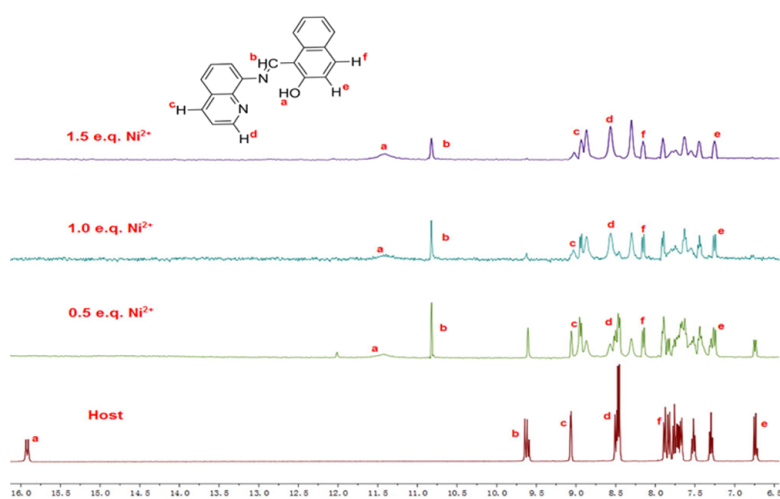


Figure S5. Partial ^1H NMR spectra of LX upon addition of Ni^{2+} in DMSO- d_6

ESI-MS spectra of LX

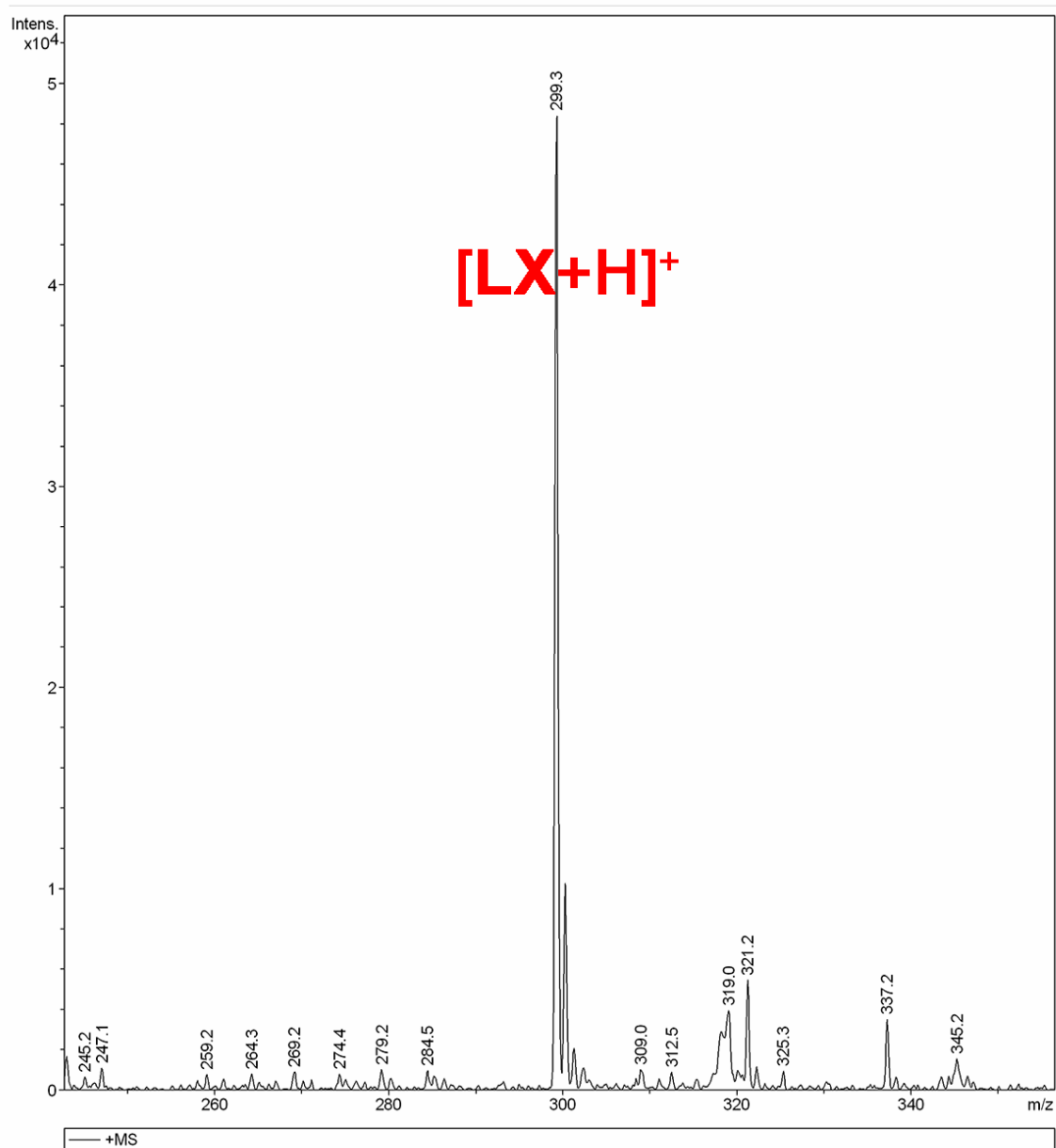


Figure S6. ESI-MS spectra of LX.

ESI-MS spectra of LX-Ni^{2+}

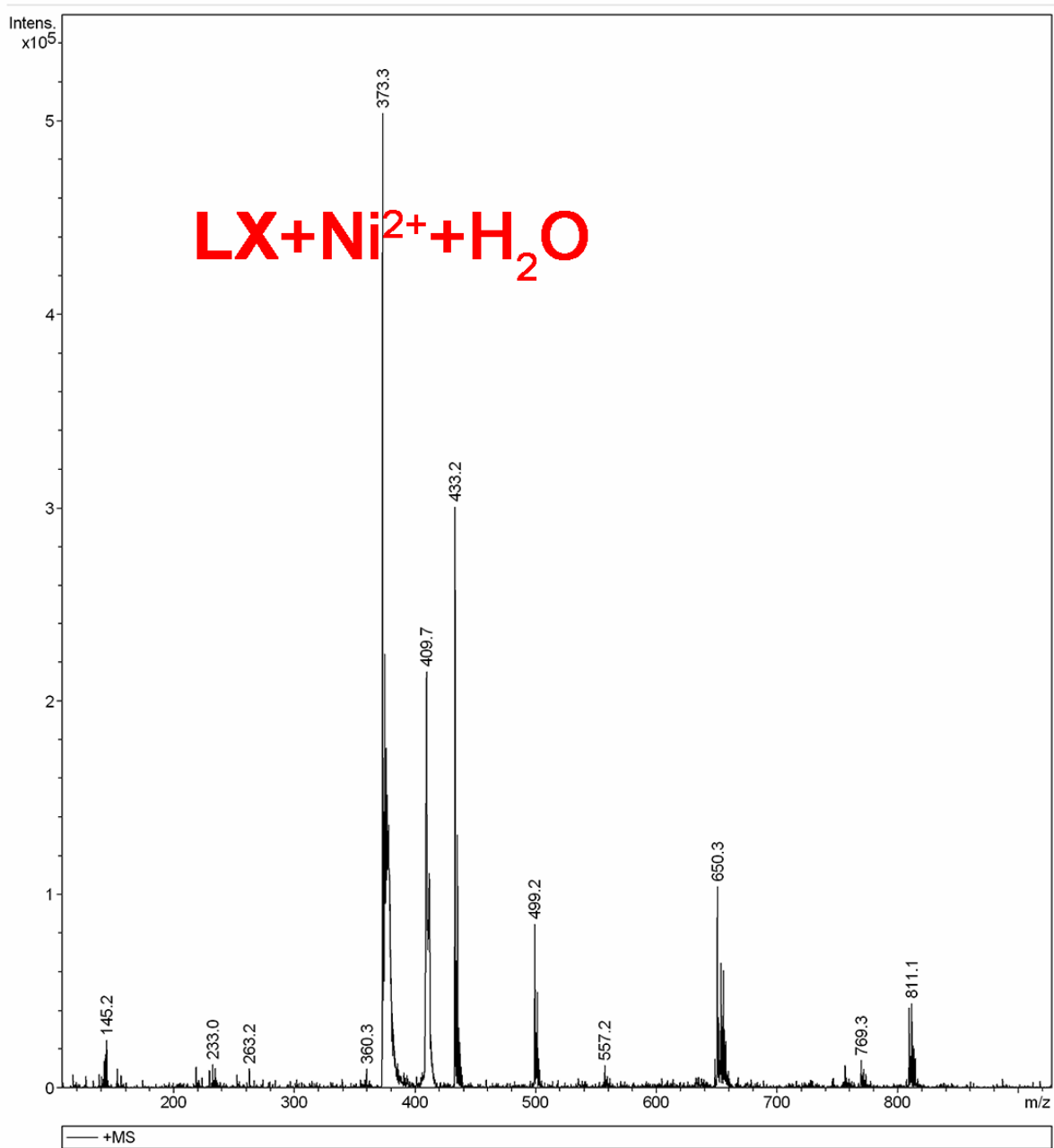


Figure S7. ESI-MS spectra of LX-Ni^{2+} .