Supporting Information for

A near infrared fluorescent dye for trivalent ions sensing and working as a molecular keypad lock

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Fig. S1 UV-Vis (a) and fluorescence (b) spectra of probe DNSA-SQ (5 μM) upon addition of AlCl₃ in CH₃CN (λₑₓ = 620 nm).

Fig. S2 The Benesi-Hildebrand plot shows a 2:1 stoichiometry for a complexation between DNSA-SQ (5 μM) and Al³⁺ in CH₃CN solution, where R=I₆₄₅/I₆₈₁.
Fig. S3 IR spectrum of DNSA-SQ and DNSA-SQ+Al(ClO₄)₃. The IR spectrum change of DNSA-SQ before and after addition of Al(ClO₄)₃ indicates that the new species has formed between DNSA-SQ and Al(ClO₄)₃.

Fig. S4 UV-Vis (a) and fluorescence (b) spectra of probe DNSA-SQ (5 μM) upon addition of FeCl₃ in CH₃CN (λₑₓ = 620 nm).

Fig. S5 UV-Vis (a) and fluorescence (b) spectra of probe DNSA-SQ (5 μM) upon addition of CrCl₃ in CH₃CN (λₑₓ = 620 nm).
**Fig. S6** Mass spectra of probe DNSA-SQ upon addition of AlCl$_3$ in CH$_3$CN.

**Fig. S7** Fluorescence spectra of probe DNSA-SQ (5 μM) upon addition of 20 equivalents of Al$^{3+}$, followed by addition of 20 equivalents of EDTA in CH$_3$CN ($\lambda_{ex} = 620$ nm).

**Fig. S8** Fluorescence spectra of probe DNSA-SQ (5 μM) upon addition of different trivalent metal ions (a: Al$^{3+}$; b: Fe$^{3+}$; c: Cr$^{3+}$) in aqueous CH$_3$CN (5/95, V/V) ($\lambda_{ex} = 620$ nm).
Fig. S9 Absorption and fluorescence spectra of DNSA-SQ (5 μM) in aqueous solution upon addition of different concentration of Ag⁺ in the absence of BSA.

Fig. S10 Absorption spectra of DNSA-SQ (5 μM) in aqueous solution to different concentration of Ag⁺ in the presence of 1 eq of BSA.

Fig. S11 The Benesi-Hildebrand plot shows a 1:1 stoichiometry for a complexation between DNSA-SQ+BSA (5 μM) and Ag⁺ in buffer solution (10 mM PBS, pH=7.4).

Fig. S12 Absorption (a) and fluorescence (b) spectra of DNSA-SQ (5 μM) in aqueous solution upon addition of different metal ions in the presence of 1 eq of BSA.
**Fig. S13** Relative fluorescence intensity \((I_{675}/I_0)\) change of DNSA-SQ (5 μM) upon addition of 20 equivalent of various metal ions in the presence of 1 equivalent of BSA and with Ag⁺ or without Ag⁺ in aqueous solution, where \(I_0\) and \(I_{675}\) indicate the fluorescence intensity of DNSA-SQ at 675 nm in the absence and presence of 20 equivalent of various metal ions respectively.

**Fig. S14** The fluorescence spectra response of DNSA-SQ (5 μM) upon addition Ag⁺ (300 μM) or BSA (5 μM) or their mixtures in phosphate buffer solution (10 mM PBS, pH=7.4).