Supporting Information for

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

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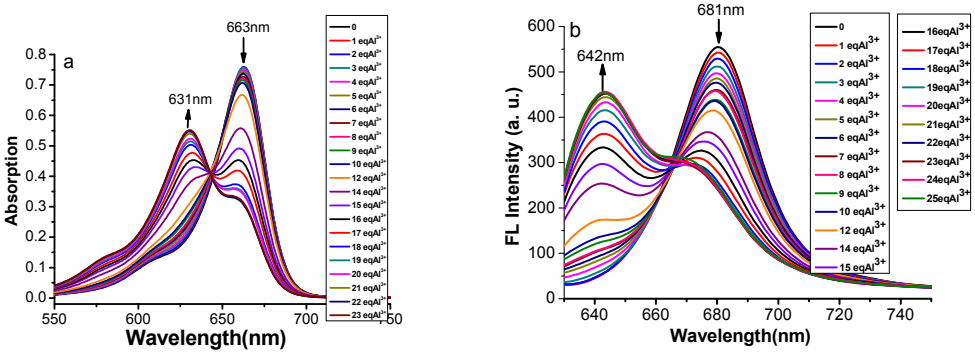

Fig. S1 UV-Vis (a) and fluorescence (b) spectra of probe **DNSA-SQ** (5 μM) upon addition of $AlCl_3$ in CH_3CN (λ_{ex} = 620 nm).

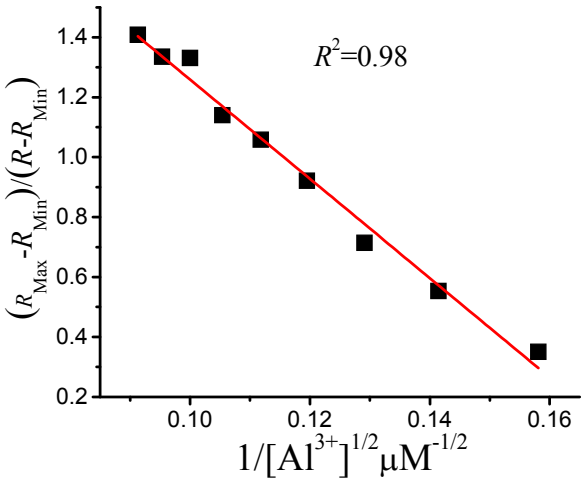

Fig. S2 The Benesi-Hildebrand plot shows a 2:1 stoichiometry for a complexation between **DNSA-SQ** (5 μM) and Al^{3+} in CH_3CN solution, where R=I_{645}/I_{681}.

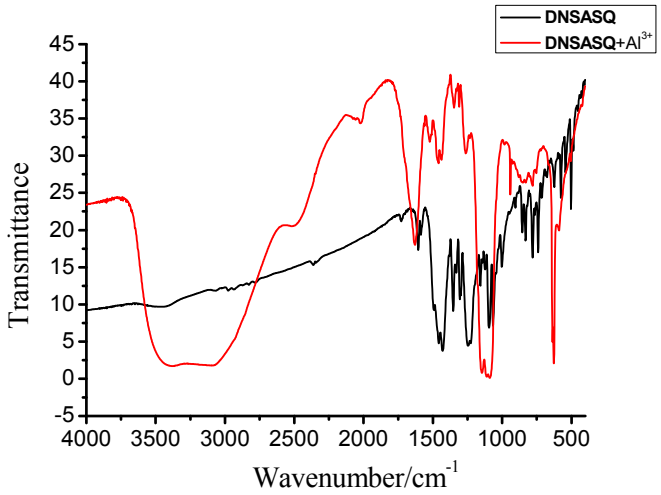

Fig. S3 IR spectrum of **DNSA-SQ** and **DNSA-SQ**+$Al(ClO_4)_3$.

The IR spectrum change of **DNSA-SQ** before and after addition of $Al(ClO_4)_3$ indicates that the new species has formed between **DNSA-SQ** and $Al(ClO_4)_3$.

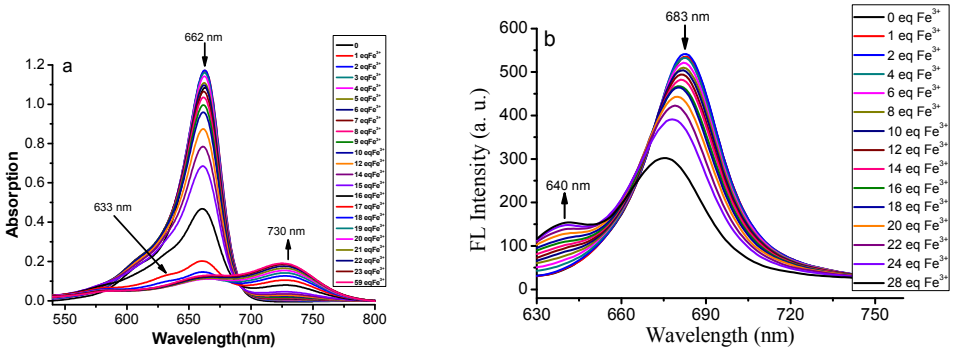

Fig. S4 UV-Vis (a) and fluorescence (b) spectra of probe **DNSA-SQ** (5 μM) upon addition of $FeCl_3$ in CH_3CN (λ_{ex} = 620 nm).

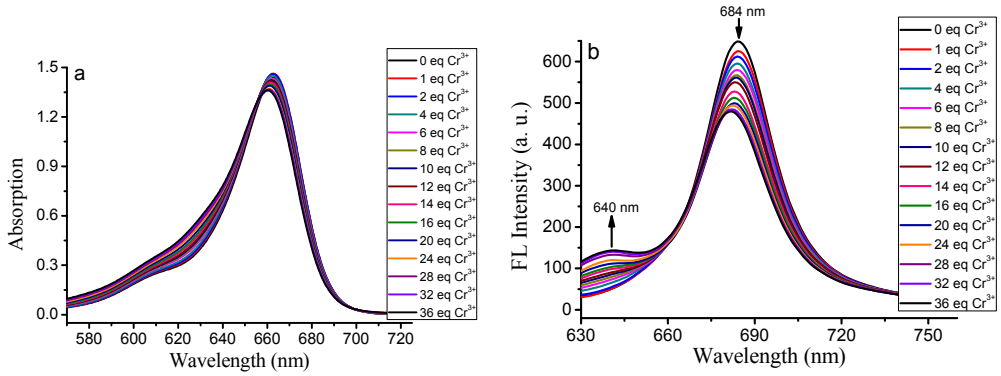

Fig. S5 UV-Vis (a) and fluorescence (b) spectra of probe **DNSA-SQ** (5 μM) upon addition of $CrCl_3$ in CH_3CN (λ_{ex} = 620 nm).

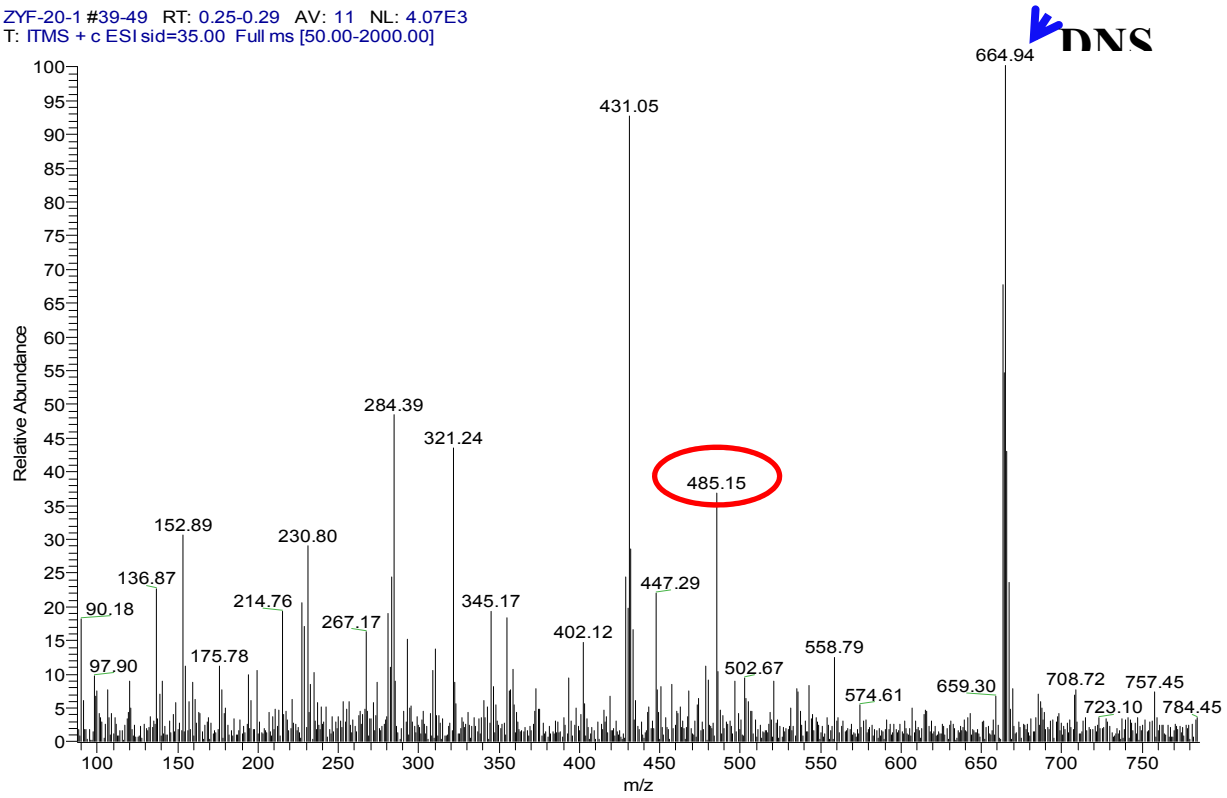

Fig. S6 Mass spectra of probe **DNSA-SQ** upon addition of $AlCl_3$ in CH_3CN.

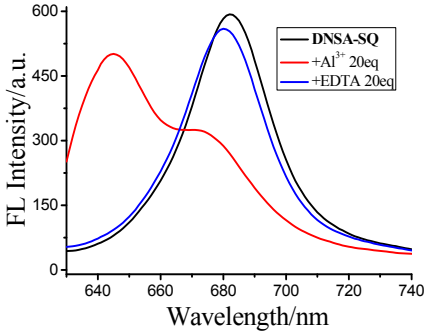

Fig. S7 Fluorescence spectra of probe **DNSA-SQ** (5 μM) upon addition of 20 equivalents of Al^{3+}, followed by addition of 20 equivalents of EDTA in CH_3CN (λ_{ex} = 620 nm).

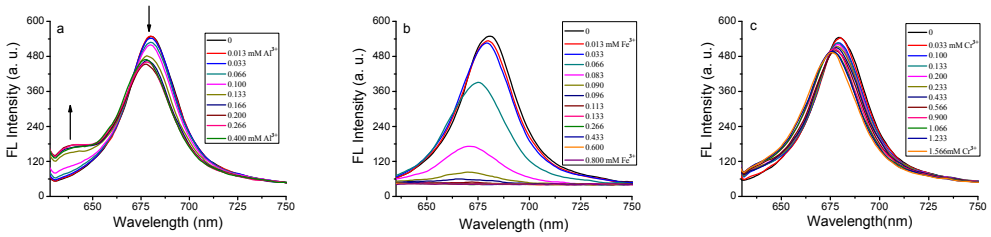

Fig. S8 Fluorescence spectra of probe **DNSA-SQ** (5 μM) upon addition of different trivalent metal ions (a: Al^{3+}; b: Fe^{3+}; c: Cr^{3+}) in aqueous CH_3CN (5/95, V/V) (λ_{ex} = 620 nm).

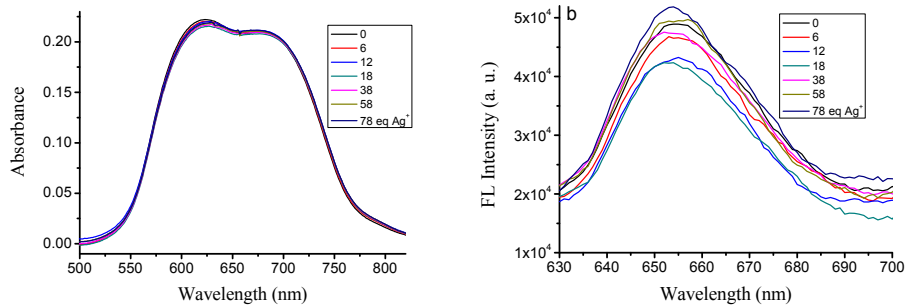

Fig. S9 Absorption and fluorescence spectra of **DNSA-SQ** (5 μM) in aqueous solution upon addition of different concentration of Ag^{+} in the absence of BSA.

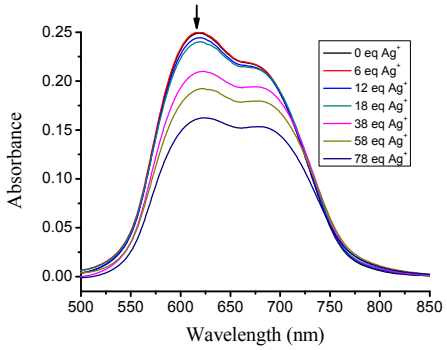

Fig. S10 Absorption spectra of **DNSA-SQ** (5 μM) in aqueous solution to different concentration of Ag^{+} in the presence of 1 eq of BSA.

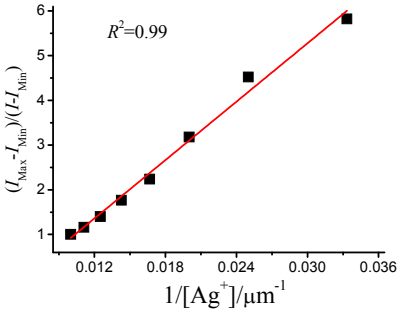

Fig. S11 The Benesi-Hildebrand plot shows a 1:1 stoichiometry for a complexation between **DNSA-SQ**+BSA (5 μM) and Ag^{+} in buffer solution (10 mM PBS, pH=7.4).

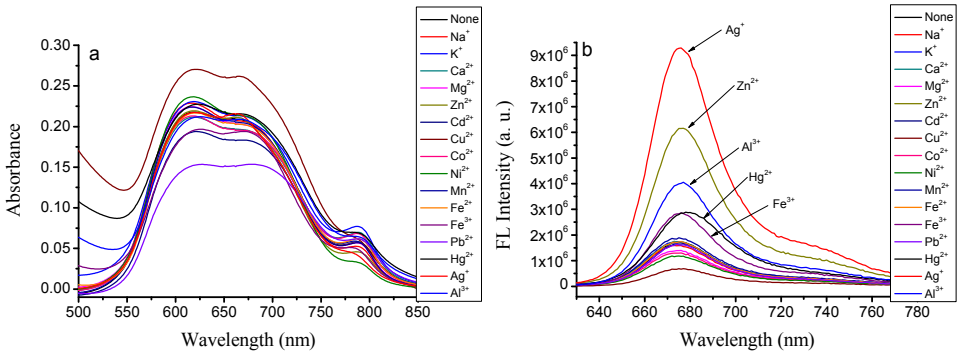

Fig. S12 Absorption (a) and fluorescence (b) spectra of **DNSA-SQ** (5 μM) in aqueous solution upon addition of different metal ions in the presence of 1 eq of BSA.

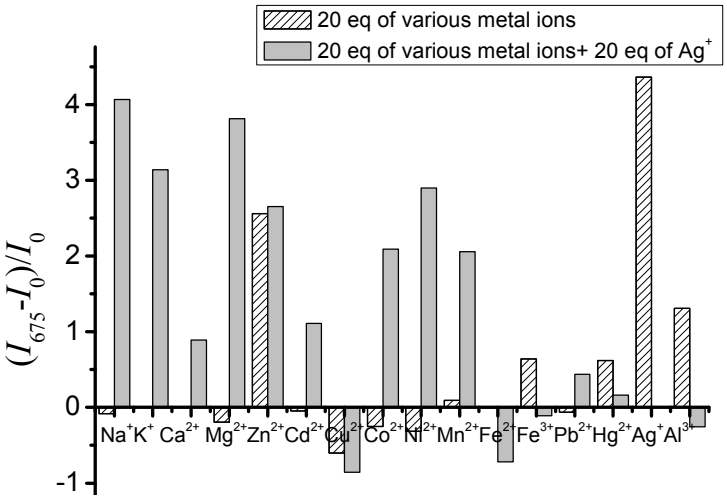

Fig. S13 Relative fluorescence intensity (I_{675}-I_0/I_0) change of **DNSA-SQ** (5 μM) upon addition of 20 equivalent of various metal ions in the presence of 1 equivalent of BSA and with Ag^+ or without Ag^+ in aqueous solution, where I_0 and I_{675} indicate the fluorescence intensity of **DNSA-SQ**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

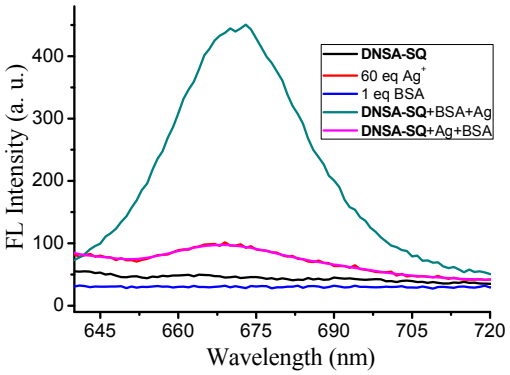

Fig. S14 The fluorescence spectra response of **DNSA-SQ** (5 μM) upon addition Ag^+ (300 μM) or BSA (5 μM) or their mixtures in phosphate buffer solution (10 mM PBS, pH=7.4).