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Supporting Information

A multisite-complexation-regulating solvent-dependent

monomolecular chemosensor for quantifying Fe³⁺/ClO⁻ and fast

detecting Al³⁺/Cr³⁺/Cu²⁺

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Fig. S1 The ¹H NMR and ¹³C NMR spectra of DHSF in DMSO-d₆.



Fig. S2 The ESI-MS spectra of DHSF.



Fig. S3 The fluorescence linear change of DHSF (20 μ M) with the increase of Fe³⁺ amounts being 0-3 and 3-20 equiv. in a 5% H₂O-DMF mixed solvent, respectively.



Fig. S4 ESI-MS spectra of DHSF upon addition of Fe^{3+} with the different concentration being 3 (A) and 10 equiv. (B), respectively.



Fig. S5 The absorption spectra of DHSF (20 $\mu M)$ upon increasing amount of Al^{3+} from 0 to 20 equiv.



Fig. S6 ESI-MS spectra of DHSF upon addition of Al^{3+.}



Fig. S7 The IR spectra for DHSF upon respective addition of $A1^{3+}$ and Fe^{3+} (10 eqiuv.), respectively.



Fig. S8. The maps of the highest occupied molecular orbital (HOMO, top) and lowest unoccupied molecular orbital (LUMO, middle) as well as the charge transfer difference map for the lowest energy electronic absorption band (407.54 nm) (bottom) of DHSF1.



Fig. S9 The fluorescence emission spectra of DHSF-Al³⁺ upon addition of other tested metal ions (1:10:10), respectively.



Fig. S10 The fluorescence titration experiment of DHSF-Al³⁺ complex with Cu^{2+} , the inset in B showing the fluorescence linear change of DHSF-Al³⁺ complex along with increasing Cu^{2+} amounts on the basis of Benesi-Hildebrand in a 5% H₂O-DMF mixed solvent.



Fig. S11 The fluorescence emission spectra of DHSF-Fe³⁺ upon addition of other tested metal ions (1:10:10), respectively.



Fig. S12 The fluorescence titration experiment of DHSF-Fe³⁺ complex with Cu²⁺, the inset in B showing the fluorescence linear change of DHSF- Fe³⁺ complex along with increasing Cu²⁺ amounts on the basis of Benesi-Hildebrand in a 5% H₂O-DMF mixed solvent.



Fig. S13 The fluorescence emission (A, B, C) and electronic absorption (D) of DHSF in DMF-H₂O mixture with H₂O fractions (f_w) changing from 0 to 95%.



Fig. S14 Fluorescence emission of DHSF after adding different metal ions in a 50% H₂O-DMF mixed solvent.



Fig. S15 The fluorescence linear change of DHSF with the increasing Cr^{3+} amounts in a 50% H₂O-DMF mixed solvent.



Fig. S16 The electronic absorption of DHSF after sodium salts with different anion were studied in 50% H₂O-DMF mixed solvent.



Fig. S17 The electronic absorption of DHSF along with the increasing amount of ClO⁻ in 50% H_2O -DMF mixed solvent.



Fig. S18 The fluorescence linear change of DHSF with the increasing amount of ClOin 50% H_2O -DMF.



Fig. S19 The ¹H of DHSF upon addition of different ClO⁻ amount.



Fig. S20 The fluorescence emission (A) and electronic absorption spectra (B) of the reference DAF and DHSF; The fluorescence emission of DAF upon addition of Al^{3+}/Fe^{3+} in 5% DMF-H₂O (C) and Cr^{3+}/ClO^{-} in 50% H₂O-DMF solvent (D), respectively; The fluorescence emission (E) and electronic absorption spectra (F) of DAF upon addition of different Fe³⁺ amounts; The fluorescence emission (G) and electronic absorption spectra (H) of DAF upon addition of different ClO⁻ amounts.



Fig. S21 The responsive times of DHSF towards Fe^{3+} , Al^{3+} , Cr^{3+} , ClO^{-} and Cu^{2+} , respectively.

Structures of different isomers	Relative energy (eV)
DHFS1	0. 000
	1. 230
	1. 042
	0. 880
Planar, C2V, -imaginary frequency of 37.5568 cm ⁻¹	0. 063
DHSF2	0. 113
	0. 829

Table S1. Isomers of DHFS and relative electronic energy (in eV).