

## **ELECTRONIC SUPPORTING INFORMATION**

# **Selective and Sensitive Recognition of Zn<sup>2+</sup> by a Dansyl-Derived Peptide Sensor**

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## HPLC: Retention times of D<sub>1</sub>

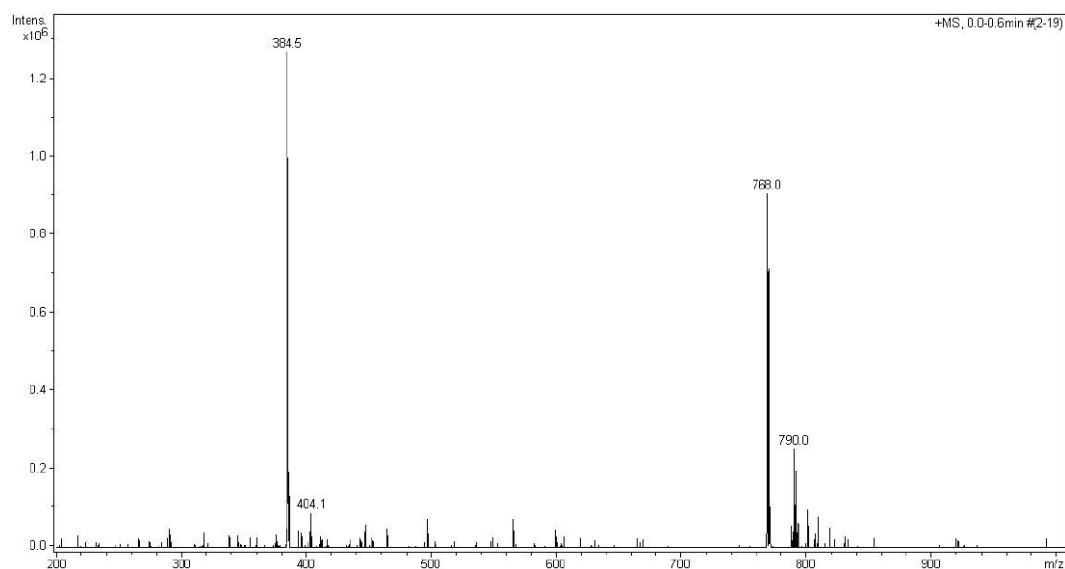
**Table S1** Retention time [min] of D<sub>1</sub> using semi-preparative reverse phase HPLC with a linear gradient from 95% to 70% of A in B, at a flow rate of 5 mL/min for 25 min, where A is a solution of 0.1% TFA in H<sub>2</sub>O, and B is a solution of 0.1% TFA in ACN.

| Model   | Retention time [min] |
|---|----------------------|
| Dansyl-HGHW-NH <sub>2</sub> (D <sub>1</sub> ) | 17.90                |



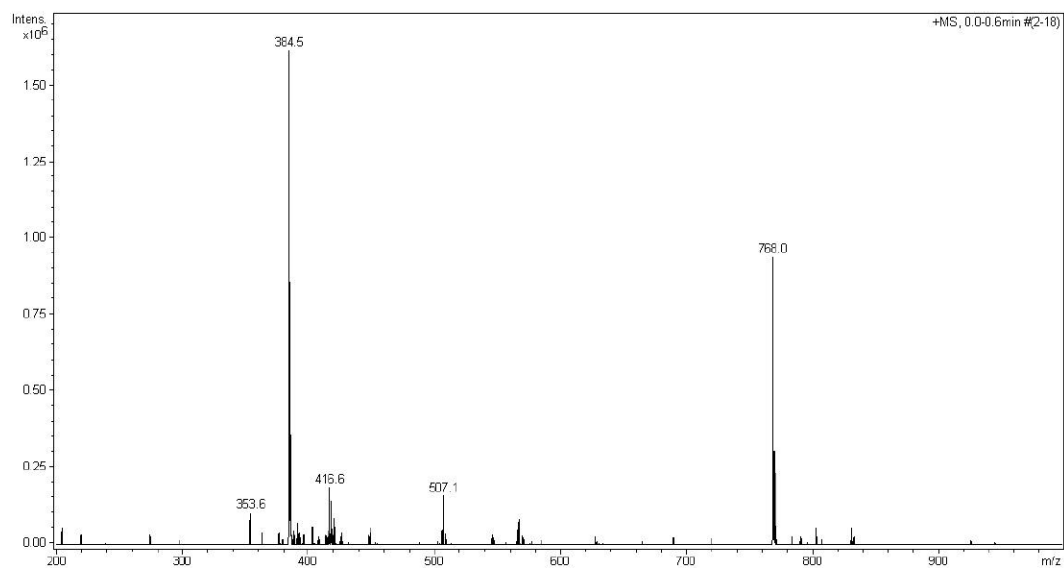
**Fig. S1** HPLC chromatogram of Dansyl-HGHW (D<sub>1</sub>).

## Electrospray ionization mass spectrometry of D<sub>1</sub>



**Fig. S2** ESI-MS spectrum of Dansyl-HGHW (D<sub>1</sub>). [M+H]<sup>+</sup><sub>calc</sub> (m/z) : 767.3 ; [M+H]<sup>+</sup><sub>exp</sub> (m/z) : 768.0 ; [M+Na]<sup>+</sup><sub>exp</sub> (m/z) : 790.0 ; [M+2H]<sup>2+</sup><sub>exp</sub> (m/z) : 384.5.

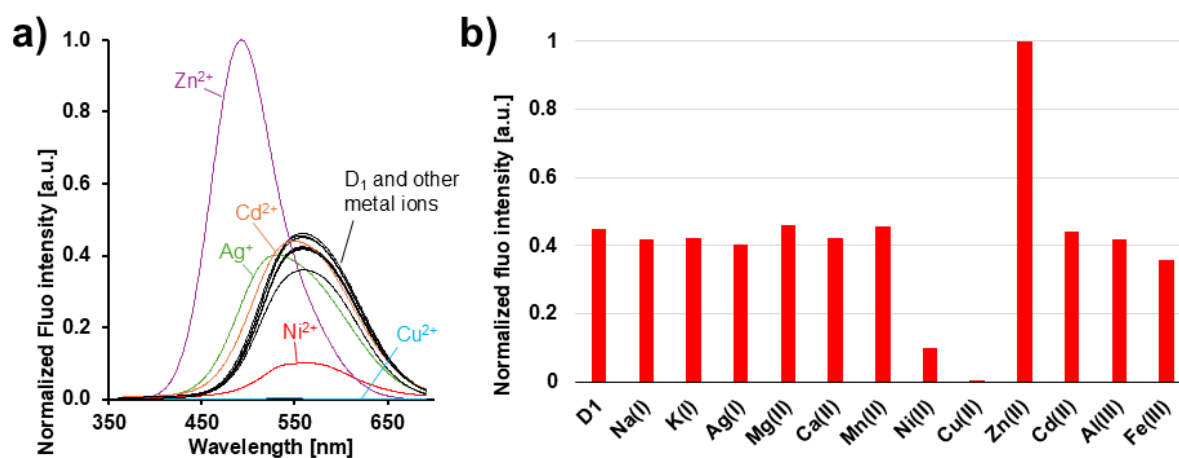
## Electrospray ionization mass spectrometry of D<sub>1</sub>-Zn<sup>2+</sup> complex



**Fig. S3** ESI-MS spectrum of Dansyl-HGHW (D<sub>1</sub>) in the presence of an excess of Zn<sup>2+</sup>. [M+H]<sup>+</sup><sub>calc</sub> (m/z) : 767.3 ; [M+H]<sup>+</sup><sub>exp</sub> (m/z) : 768.0 ; [M+Zn]<sup>2+</sup><sub>exp</sub> (m/z) : 416.6 ; [M+2H]<sup>2+</sup><sub>exp</sub> (m/z) : 384.5.

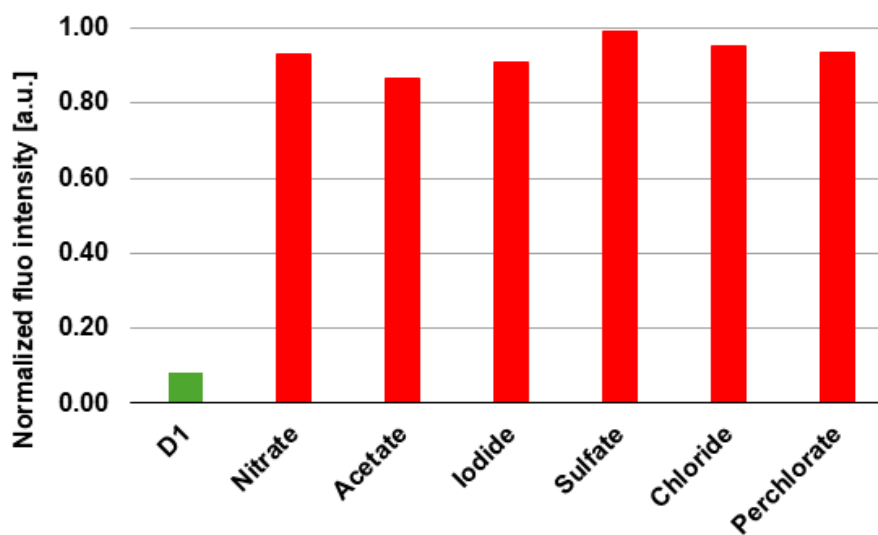
## Various study of D<sub>1</sub> at $\lambda_{\text{ex}} = 340 \text{ nm}$

### Study of selectivity



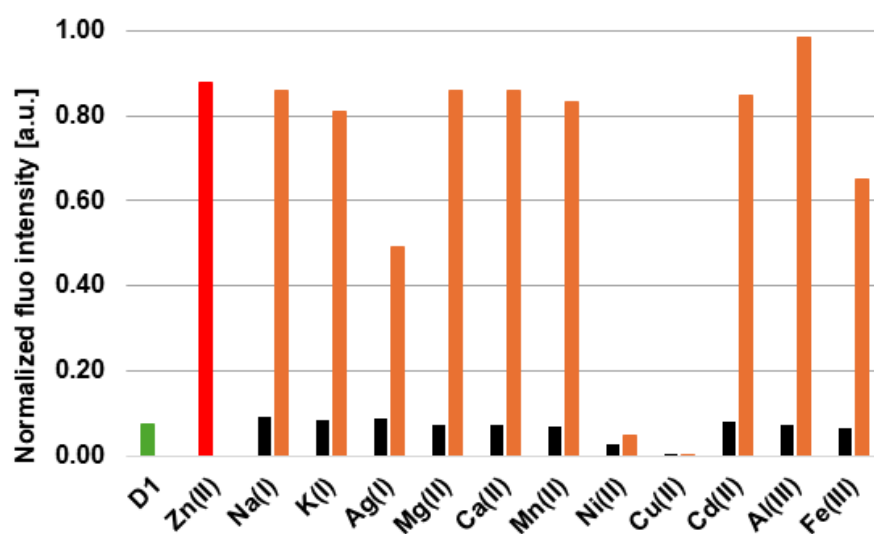
**Fig. S4** a) Voigt-deconvoluted and normalized fluorescence spectra of D<sub>1</sub> ( $1 \times 10^{-5} \text{ M}$ ) in HEPES buffer (20 mM, pH 7.4-7.5) at 25°C,  $\lambda_{\text{ex}} = 340 \text{ nm}$ . D<sub>1</sub> alone (green bar), D<sub>1</sub> + 3 eq. of the indicated metal ions (red bars). b) Corresponding histogram.

### Study of various Zn<sup>2+</sup> counterion salts



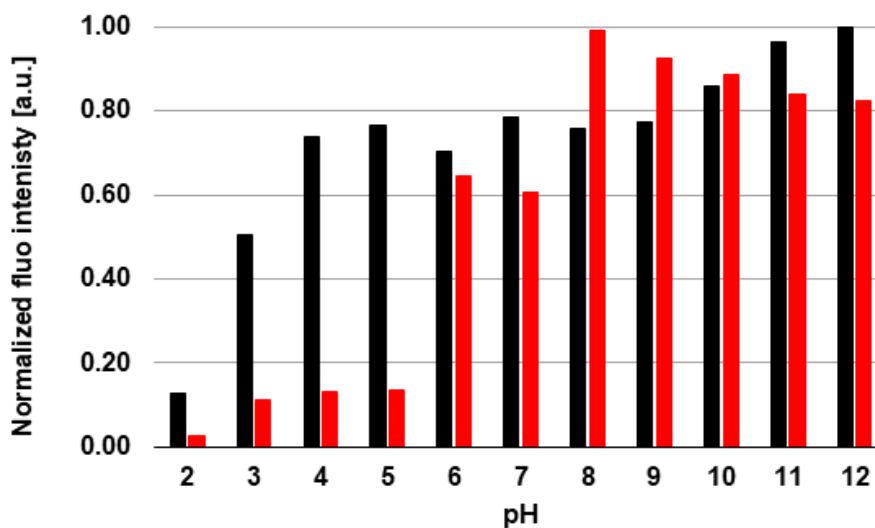
**Fig. S5** Study of various Zn<sup>2+</sup> counterion salts on D<sub>1</sub> ( $1 \times 10^{-5} \text{ M}$ ) in HEPES buffer (20 mM, pH 7.4-7.5) at 25°C,  $\lambda_{\text{ex}} = 340 \text{ nm}$ . D<sub>1</sub> alone (green bar), and D<sub>1</sub> + 3 eq. of the indicated Zn<sup>2+</sup> salts (red bars).

### Study of interference by various metal ions



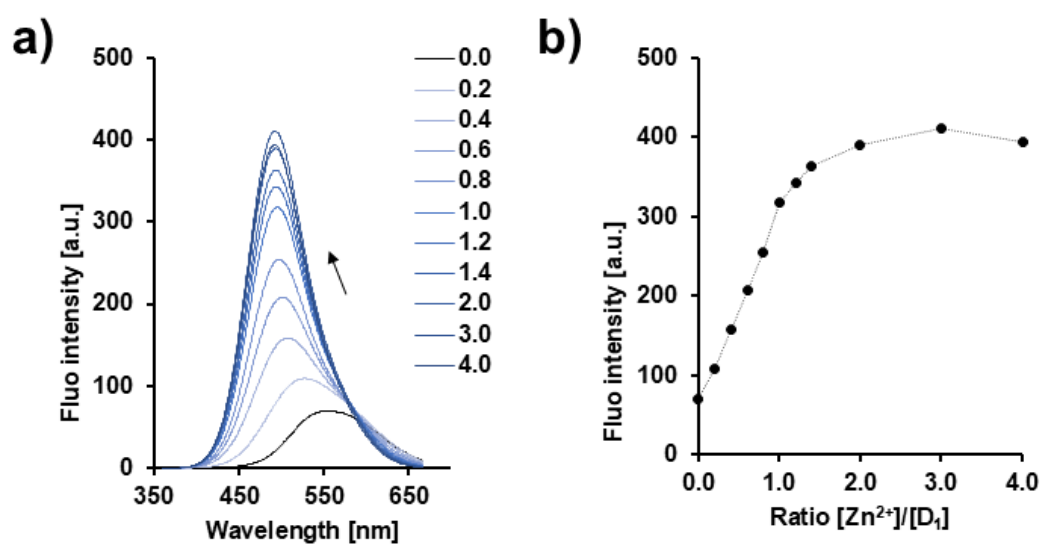
**Fig. S6** Interference study of various metal ions on D<sub>1</sub> ( $1 \times 10^{-5}$  M) in HEPES buffer (20 mM, pH 7.4-7.5) at 25°C,  $\lambda_{\text{ex}} = 340$  nm. D<sub>1</sub> alone (green bar), D<sub>1</sub> + 3 eq. of Zn<sup>2+</sup> (red bar), D<sub>1</sub> + 3 eq. of the indicated metal ions (black bars), then addition of 3 eq. of Zn<sup>2+</sup> (orange bars).

### pH study



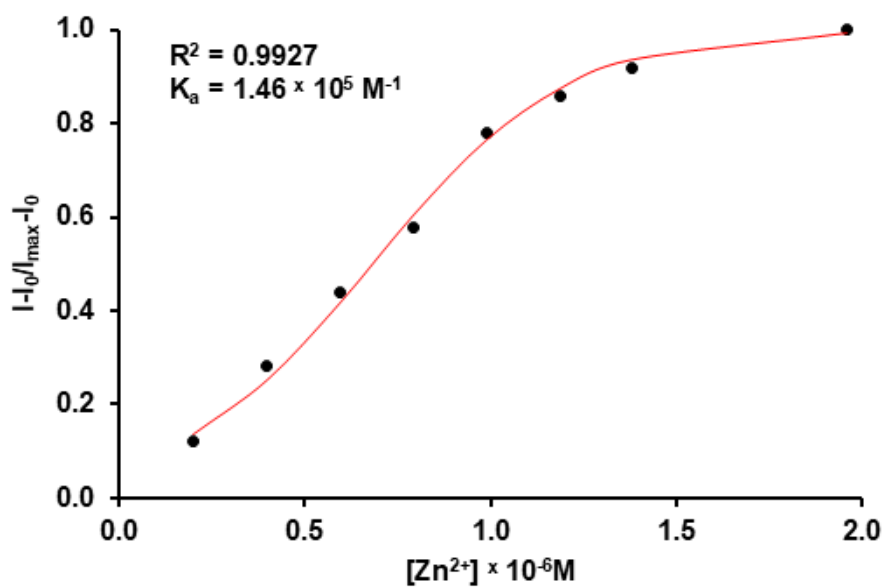
**Fig. S7** pH-dependent fluorescence response of D<sub>1</sub> ( $1 \times 10^{-5}$  M) at 25°C,  $\lambda_{\text{ex}} = 340$  nm. Black bars represent D<sub>1</sub> alone. Red bars represent D<sub>1</sub> + 3 eq. of Zn<sup>2+</sup>. The pH was adjusted using HNO<sub>3</sub> and NaOH solutions, both at 0.1 M.

## Study of the binding interactions between $D_1$ and $Zn^{2+}$



**Fig. S8** a) Voigt-deconvoluted fluorescence titration spectra  $D_1$  (1  $\times$  10<sup>-5</sup> M) in HEPES buffer (20 mM, pH 7.4-7.5) at 25°C,  $\lambda_{ex}$  = 340 nm, recorded with increasing amount of  $Zn^{2+}$  (from 0 to 4.0 eq.). b) Plot of fluo intensity as a function of  $Zn^{2+}$  equivalents.

## Determination of the binding constant between $D_1$ and $Zn^{2+}$



**Fig. S9** Fitting curve of  $I - I_0 / I_{max} - I_0$  versus the amount of  $Zn^{2+}$  to determine the binding constant of the 1:1 complex.

## Lifetime measurements of D<sub>1</sub> and D<sub>1</sub>-Zn<sup>2+</sup> complex

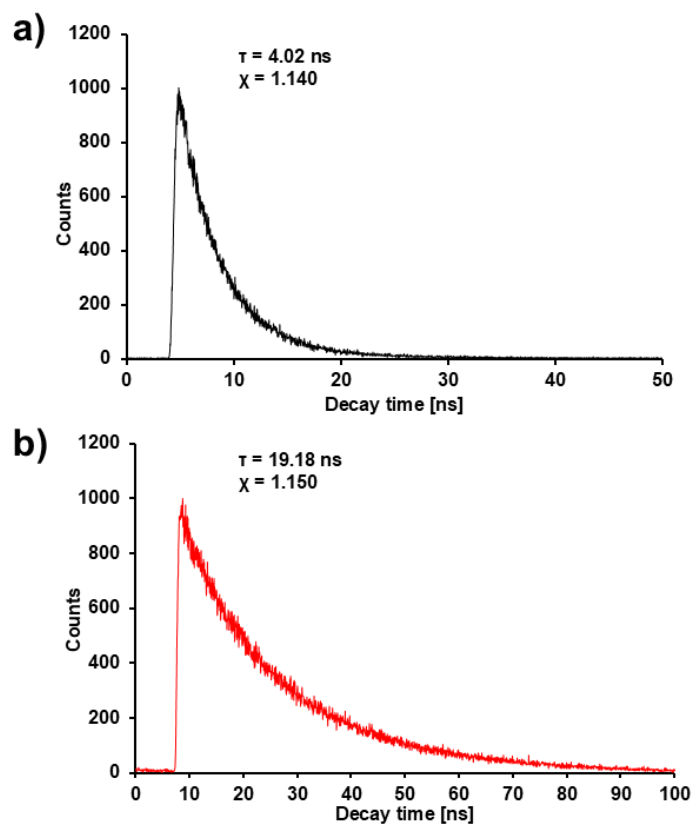


Fig. S10 Fluorescence lifetime measurements at 25°C,  $\lambda_{\text{ex}} = 405$  nm. a) D<sub>1</sub> b) D<sub>1</sub>-Zn<sup>2+</sup> complex.

## Limit of detection

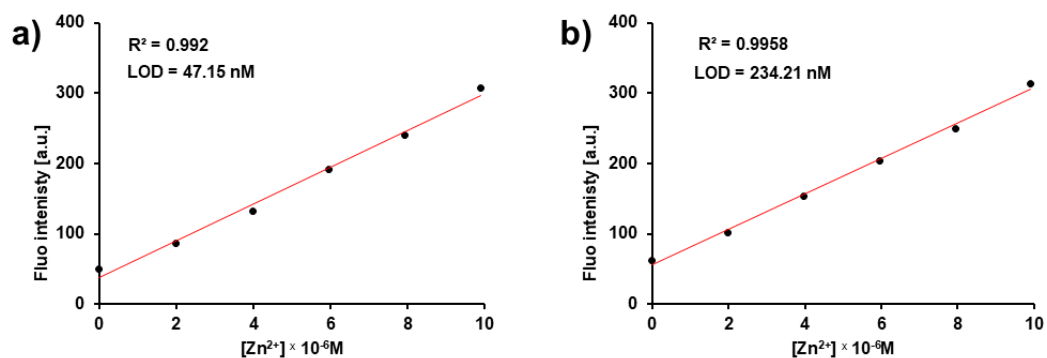
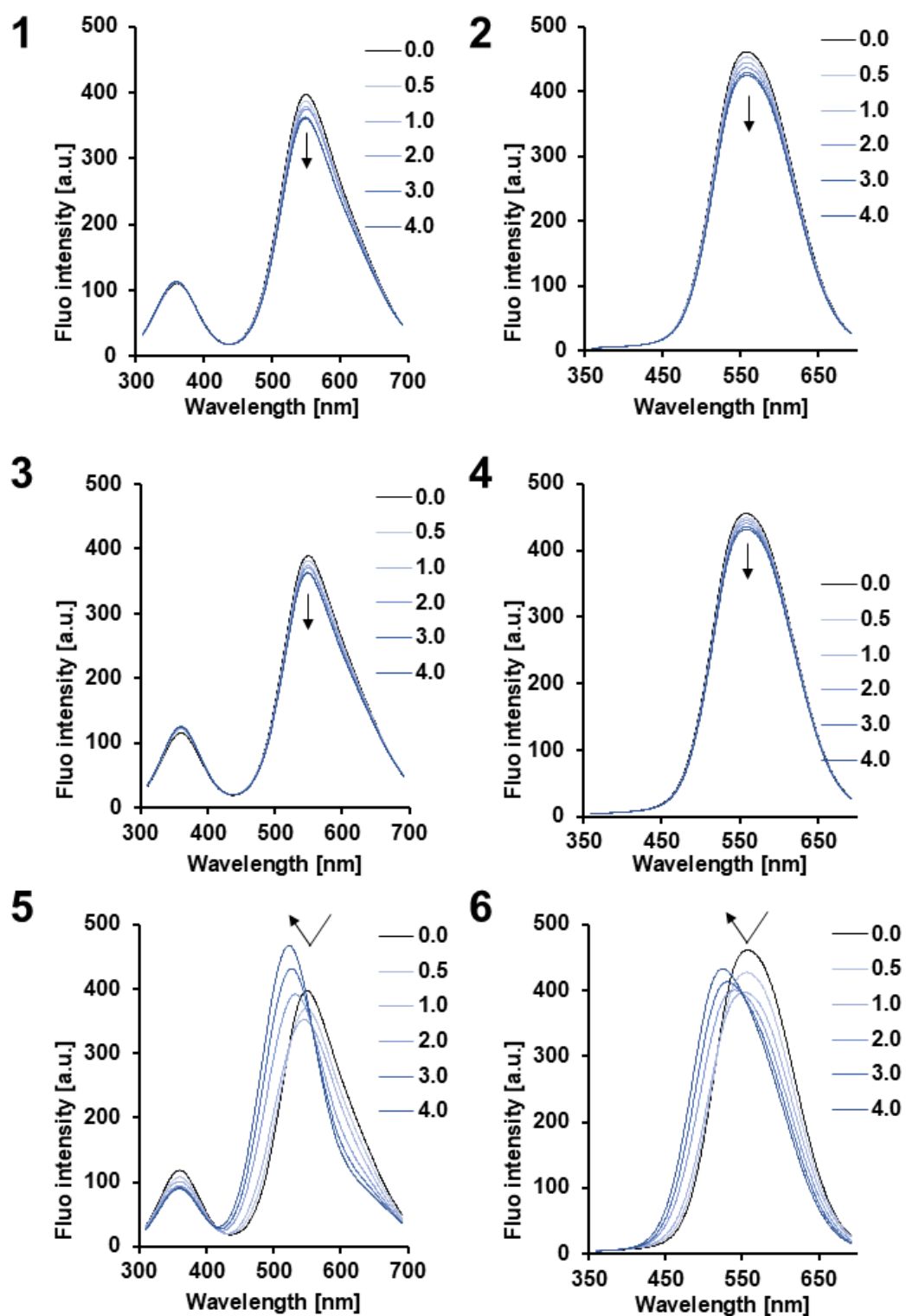
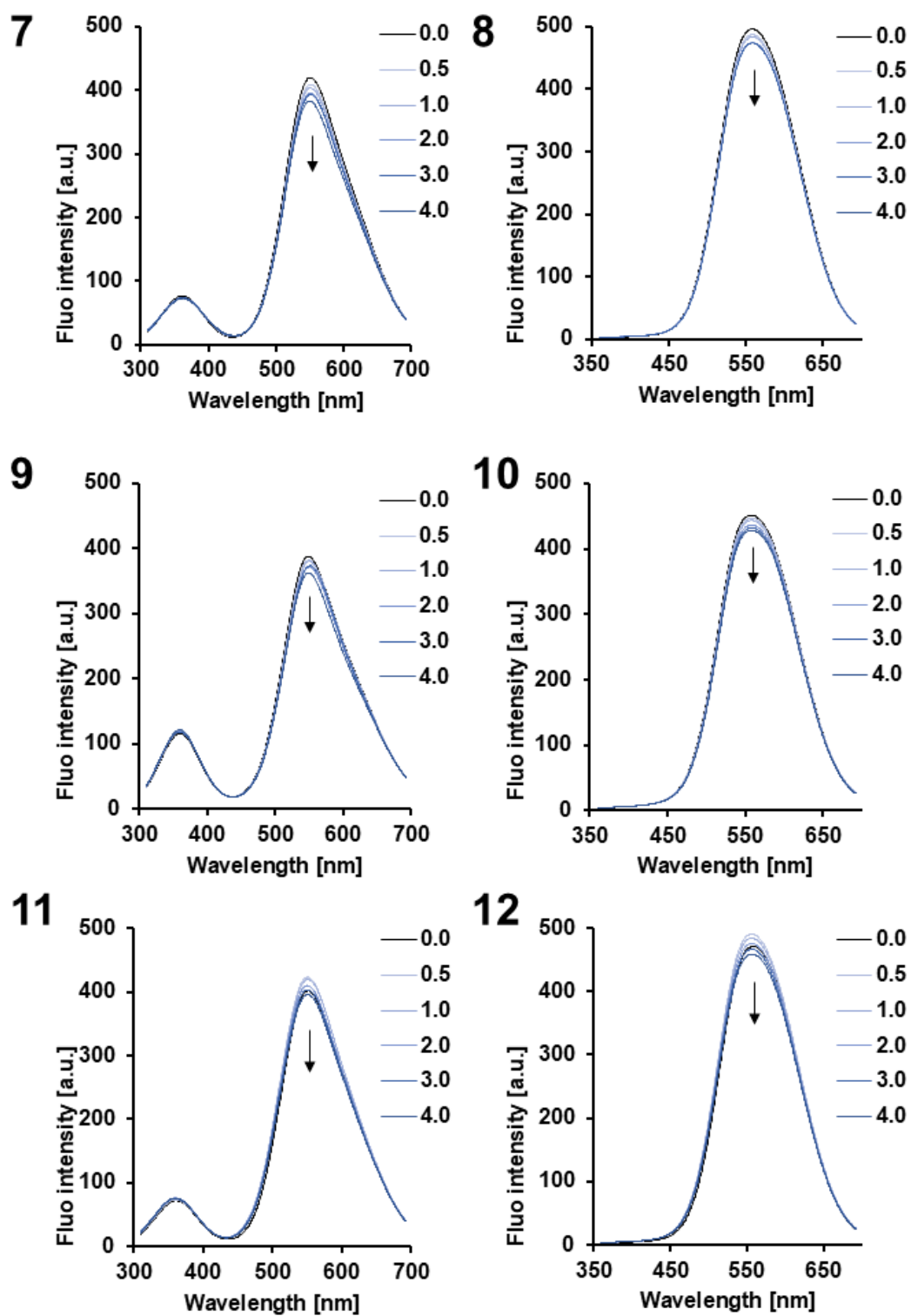


Fig. S11 Standard deviation and linear fitting to determine the limit of detection of D<sub>1</sub> a)  $\lambda_{\text{ex}} = 290$  nm b)  $\lambda_{\text{ex}} = 340$  nm.

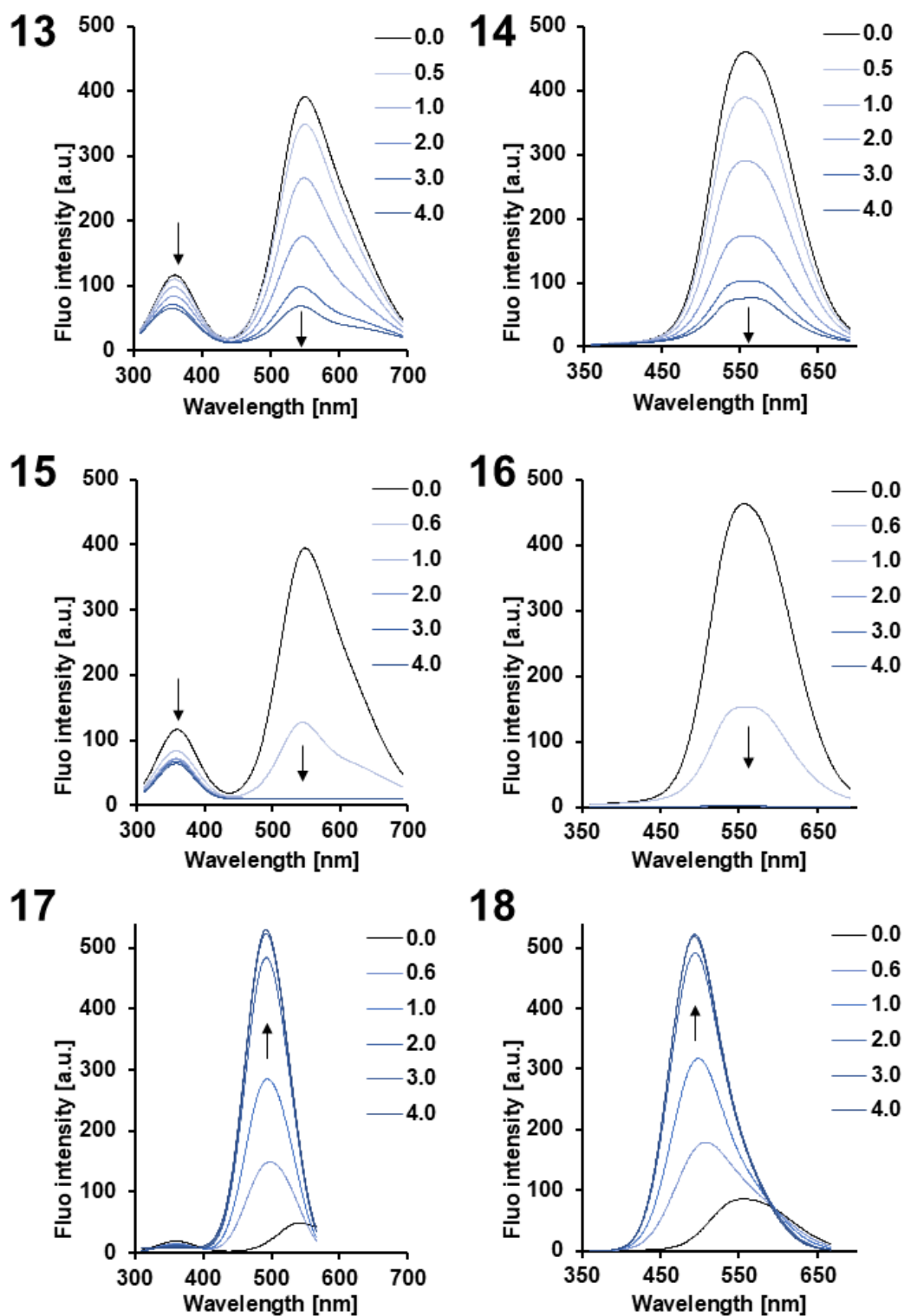
## Fluorescence titrations



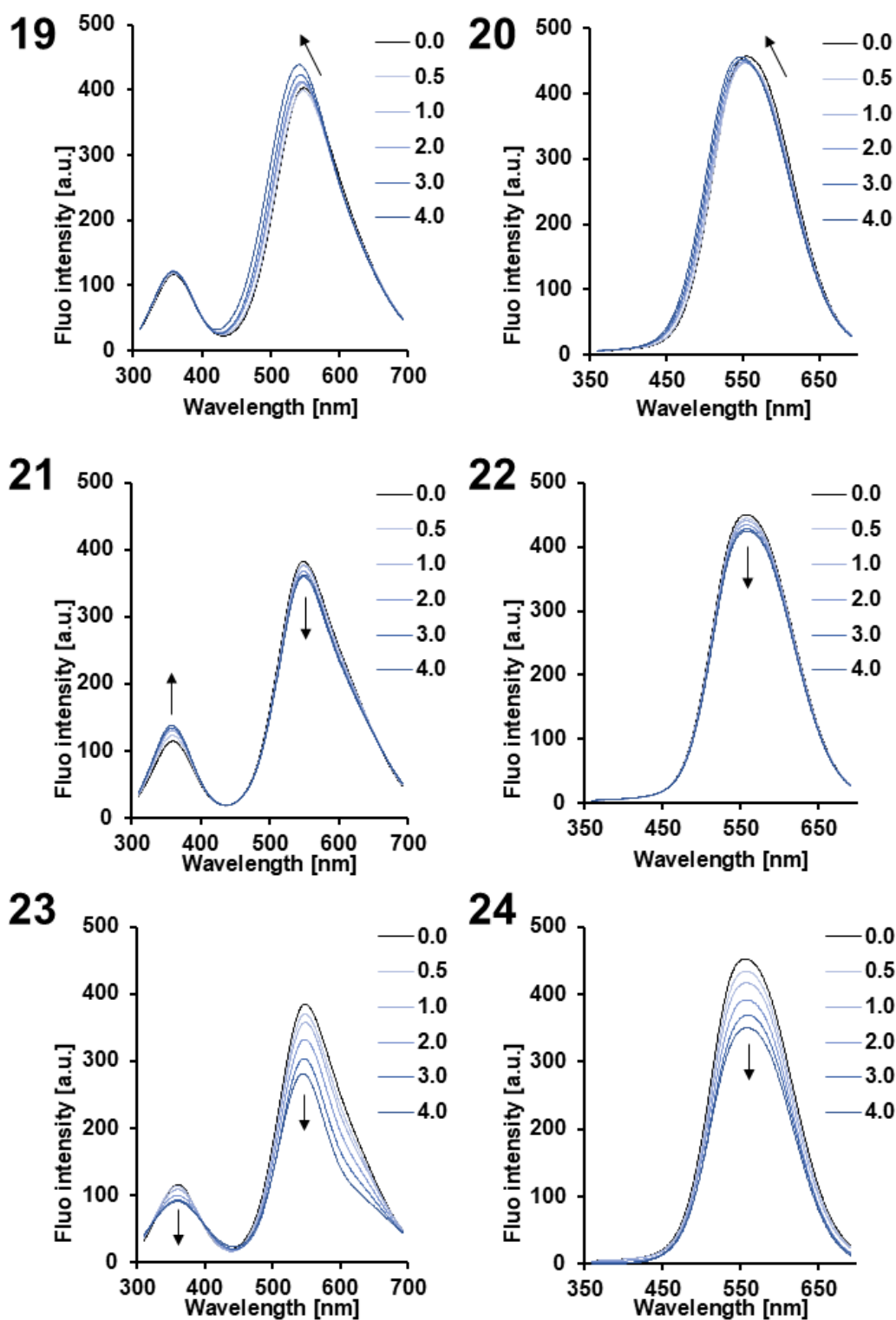
**Fig. S12** Voigt-deconvoluted fluorescence spectra of  $D_1$  ( $1 \times 10^{-5}$  M) in HEPES buffer (20 mM, pH 7.4-7.5) at 25°C upon addition of various nitrate salt solutions. (Odd-numbered spectra)  $\lambda_{ex} = 290$  nm. (Even-numbered spectra)  $\lambda_{ex} = 340$  nm. Spectra 1 & 2:  $Na^+$ ; 3 & 4:  $K^+$ ; 5 & 6:  $Ag^+$ .



**Fig. S13** Voigt-deconvoluted fluorescence spectra of  $D_1$  ( $1 \times 10^{-5}$  M) in HEPES buffer (20 mM, pH 7.4-7.5) at 25°C upon addition of various nitrate salt solutions. (Odd-numbered spectra)  $\lambda_{\text{ex}} = 290$  nm. (Even-numbered spectra)  $\lambda_{\text{ex}} = 340$  nm. Spectra 7 & 8:  $\text{Mg}^{2+}$ ; 9 & 10:  $\text{Ca}^{2+}$ ; 11 & 12:  $\text{Mn}^{2+}$ .



**Fig. S14** Voigt-deconvoluted fluorescence spectra of  $D_1$  ( $1 \times 10^{-5}$  M) in HEPES buffer (20 mM, pH 7.4-7.5) at 25°C upon addition of various nitrate salt solutions. (Odd-numbered spectra)  $\lambda_{\text{ex}} = 290$  nm. (Even-numbered spectra)  $\lambda_{\text{ex}} = 340$  nm. Spectra 13 & 14:  $\text{Ni}^{2+}$ ; 15 & 16:  $\text{Cu}^{2+}$ ; 17 & 18:  $\text{Zn}^{2+}$ .



**Fig. S15** Voigt-deconvoluted fluorescence spectra of  $D_1$  ( $1 \times 10^{-5}$  M) in HEPES buffer (20 mM, pH 7.4-7.5) at 25°C upon addition of various nitrate salt solutions. (Odd-numbered spectra)  $\lambda_{\text{ex}} = 290$  nm. (Even-numbered spectra)  $\lambda_{\text{ex}} = 340$  nm. Spectra 19 & 20:  $\text{Cd}^{2+}$ ; 21 & 22:  $\text{Al}^{3+}$ ; 23 & 24:  $\text{Fe}^{3+}$ .