

Supporting Information

Nanocontainer of Fluorescence Sensor of Cadmium Ion in Water and Biological Applications

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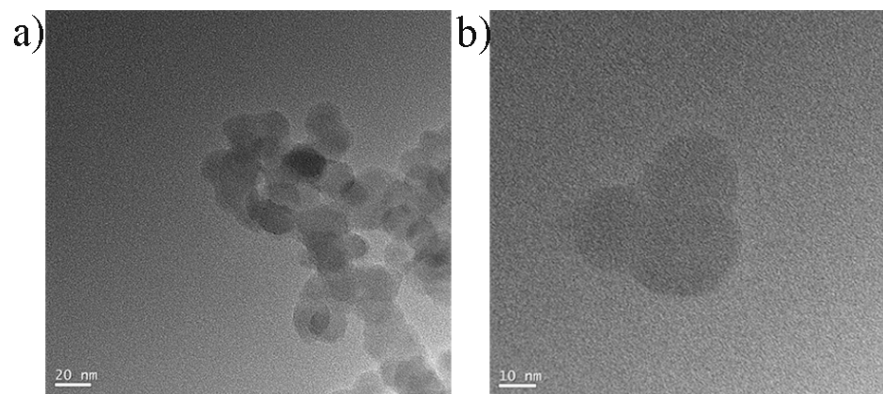


Figure S1. TEM images of NC-FQDIPA.

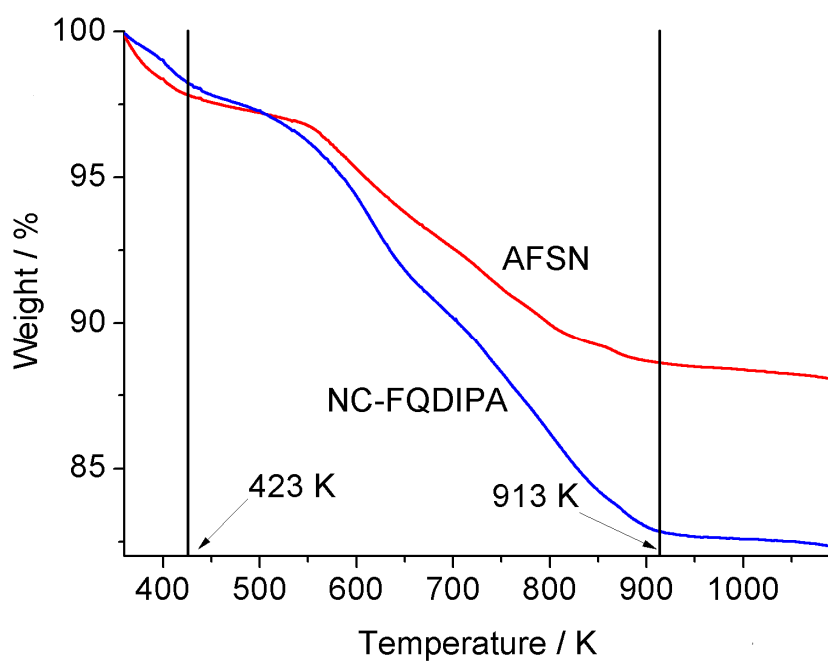


Figure S2. TGA plots of materials AFSN and NC-FQDIPA (loss of physisorbed water completes at 423 K, constant weight after 913 K).

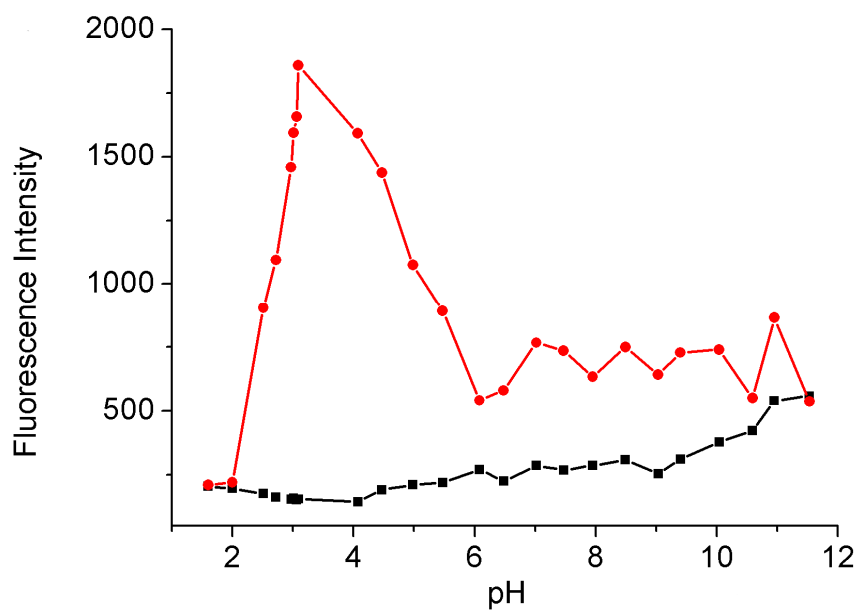


Figure S3. Fluorescence intensities of NC-FQDIPA and Cd-NC-FQDIPA in water at various pH values at room temperature ($\lambda_{\text{ex}} = 315 \text{ nm}$). Red line, the fluorescence intensities at 419 nm of Cd-NC-FQDIPA at various pH ($[\text{NC-FQDIPA}] = 0.4 \text{ gL}^{-1}$, $[\text{Cd}^{2+}] = 0.10 \text{ mM}$); black line, the fluorescence intensities at 500 nm of NC-FQDIPA at various pH ($[\text{NC-FQDIPA}] = 0.4 \text{ gL}^{-1}$).

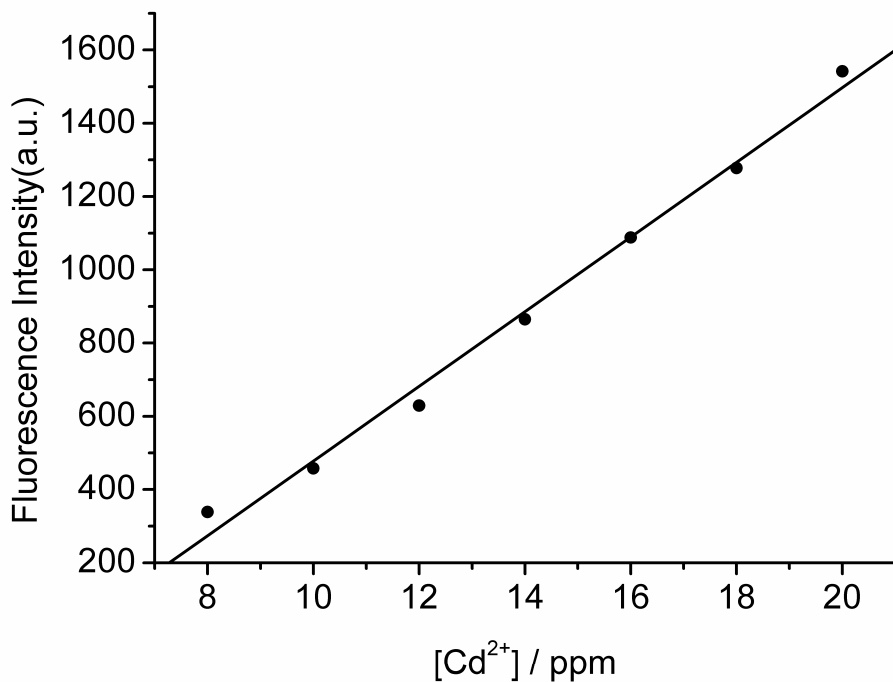


Figure S4. Cd^{2+} concentration (at the parts per million level) dependent fluorescence intensity change at 419 nm.

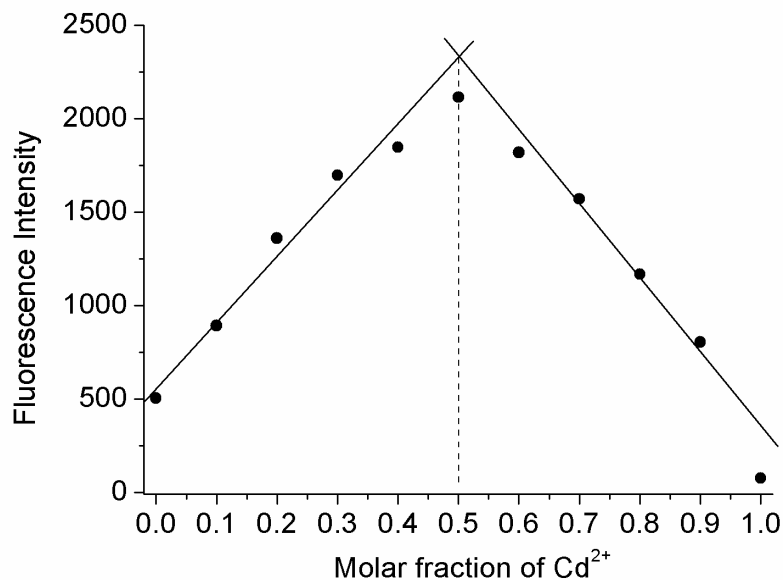


Figure S5. Job's plot shows the 1:1 binding of NC-FQDIPA to Cd²⁺.

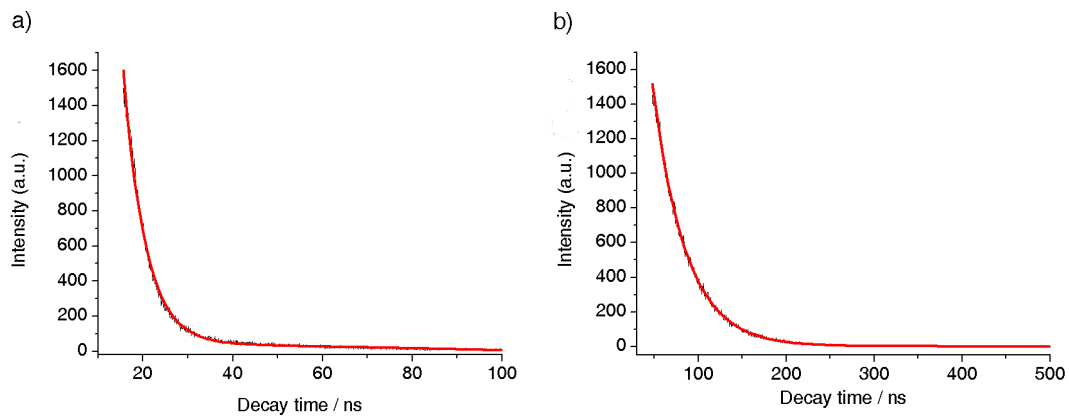


Figure S6. Time-resolved fluorescence decay of NC-FQDIPA (0.4 gL⁻¹, suspended in water, pH = 3) in the absence (S6a) and presence (S6b) of Cd²⁺ (0.1 mM) ($\lambda_{\text{ex}} = 315$ nm). The red solid lines indicate the fitting of the data.

Table S1. Radiative and total nonradiative rate data, where χ^2 represents the fitting parameter.

Sample	τ_f [ns]	Φ_f	$k_f (10^8 \text{ s}^{-1})$	$k_{nr} (10^8 \text{ s}^{-1})$	χ^2
NC-FQDIPA ^[a]	16.72	0.0472	0.02823	0.5699	1.129
NC-FQDIPA ^[a] + Cd ²⁺ (1.0×10 ⁻⁴ M)	37.33	0.4903	0.1313	0.1366	0.917

^[a] 0.4 gL⁻¹, suspended in water, pH = 3

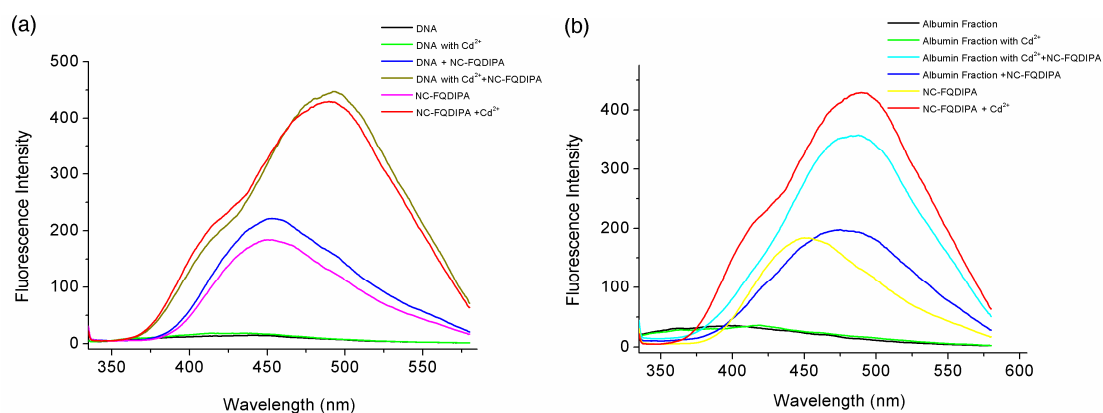


Figure S7. a) Fluorescence response of NC-FQDIPA (0.4 gL^{-1}) upon addition of DNA (0.1 mM) with Cd^{2+} and the control experiments in Tris—HCl (pH 7.3) (excitation at 315 nm). Slit: excitation/emission = 10.0:2.5. b) Fluorescence response of NC-FQDIPA (0.4 gL^{-1}) upon addition of Albumin Fraction (0.1 mM) with Cd^{2+} and the control experiments in Tris—HCl (pH 7.3) (excitation at 315 nm). Slit: excitation/emission = 10.0:2.5.

Crystal Violet staining

HeLa cell line was cultured in DMEM (Hyccone), containing 10% FBS (Gibco), in 6-well plate (Costar) and treated with $10 \mu\text{M}$, $160 \mu\text{M}$, $320 \mu\text{M}$, $640 \mu\text{M}$, $1280 \mu\text{M}$ NC-FQDIPA for 4 hours. After the culture medium was pumped out by a vacuum pump, cells were washed twice with PBS and then discarded the PBS. Add appropriate amount of 95% ethanol to fixate the cells for 30 minutes at room temperature. Discard the ethanol and add appropriate amount of 0.5% crystal violet solution and keep it for 30 min at room temperature. Recycle the crystal violet solution and wash the cells with DI water for 4 times to decolor the background. Then, pump the water by a vacuum pump. The cells morphological features were examined by Nikon *Ti-U* Fluorescent Inverted Microscope and the photos were taken with a digital camera (COOPLIX P5100, Nikon).

Cell incubation and imaging

HeLa cells were cultured in DMEM (Hyclone) supplemented with 10% FBS (Gibco). One day before imaging, cells were seeded in 6-well flat-bottomed plates (Costar). The next day, the HeLa cells were incubated with $100 \mu\text{M}$ NC-FQDIPA for 1.5 h at 37°C under 5% CO_2 and then washed with phosphate-buffered saline (PBS) three times before incubating with $100 \mu\text{M}$ $\text{Cd}(\text{NO}_3)_2$ for another 1 h, cells rinsed with PBS three times again, then the fluorescence imaging of cell membrane was observed under 340-380 nm by Zeiss Leica DM 4000B microscope.

The HeLa cells only incubated with Cd^{2+} , without and with $100 \mu\text{M}$ 1.5 for hour at 37°C under 5% CO_2 was as a control. For all images, the microscope settings, such as brightness, contrast, and exposure time were consistent with the control group.

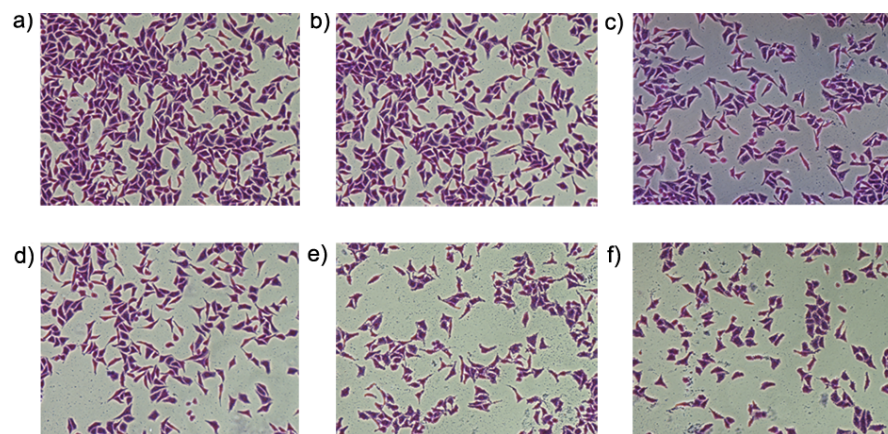


Figure S8. Crystal Violet stain. Bright-field measurements after treatment with NC-FQDIPA (a), b), c), d), e), f): control, 10 μM , 160 μM , 320 μM , 640 μM , 1280 μM) (Nikon *Ti-U* Fluorescent Inverted Microscope, 20 \times objective lens).

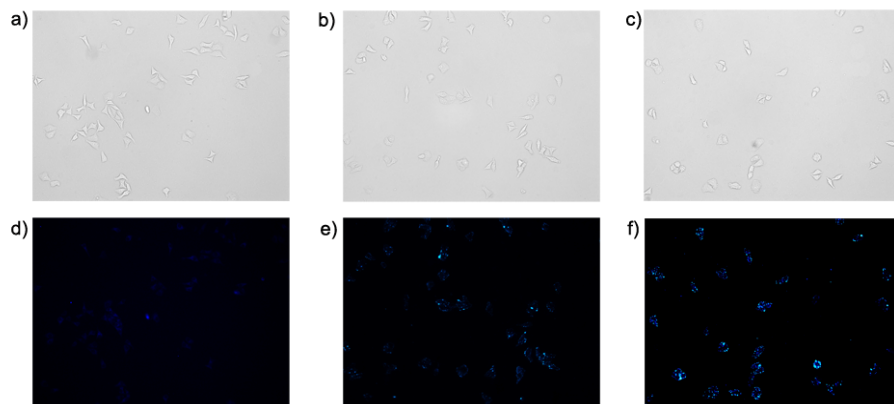


Figure S9. Fluorescence images of Cd^{2+} in HeLa cells incubated with NC-FQDIPA (100 μM). (a), b), c) Bright-field transmission images of HeLa cells. d), e), f) Fluorescence images of HeLa cells in a), b), c). a), d) Only HeLa Cells. b), e) HeLa cells incubated with 100 μM NC-FQDIPA for 1.5 h, washed three times. c), f) HeLa cells incubated with 100 μM NC-FQDIPA for 1.5 h, wash three times, then added DMEM (containing 10% FBS), incubated with 100 μM Cd^{2+} for 1.5 h, washed three times again. (Zeiss Leica DM 4000B microscope, 10 \times objective lens).

Full authors list for reference [20]

[20] M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, Jr., J. A. Montgomery, J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, N. J. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, Ö. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, D. J. Fox, Gaussian, Inc., Wallingford CT, 2009.