

## Supporting information for

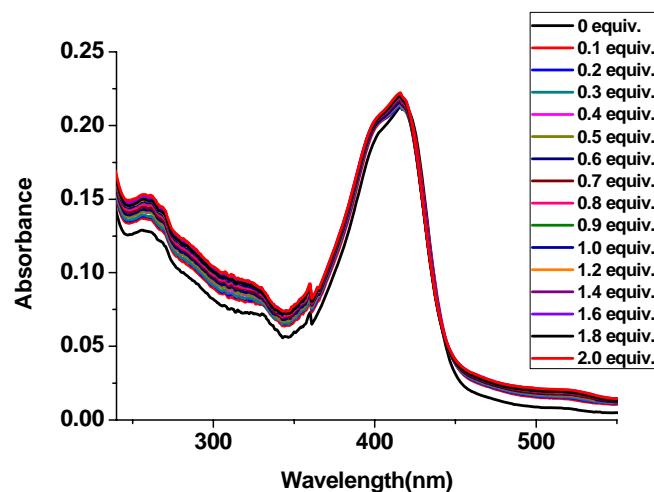
# **A selective turn-on fluorescent probe for Cd<sup>2+</sup> based on boron difluoride β-dibenzoyl dye and its application in living cells**

**Li Xin, Yu-Zhe Chen\*, Li-Ya Niu, Li-Zhu Wu, Chen-Ho Tung, Qing-Xiao Tong\*  
and Qing-Zheng Yang**

### **Contents:**

- 1. Absorption changes upon addition of cadmium ion**
- 2. Binding constant**
- 3. Detection limit**
- 4. pH effect on fluorescence**
- 5. Solvent effect on fluorescence**
- 6. <sup>1</sup>H NMR, MS, ESI-MS, ESI-HRMS**
- 7. References**

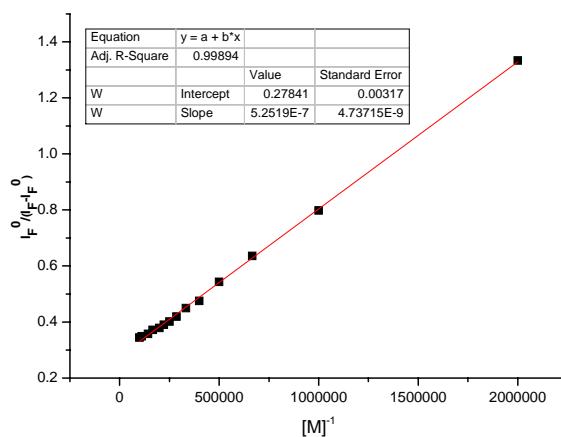
## 1. Absorption changes upon addition of cadmium ion.



**Figure 1S.** Changes in the absorption spectra of **1** (5 μM) upon titration of Cd<sup>2+</sup>, [Cd<sup>2+</sup>] = 0-10 μM. All data were obtained in HEPES buffer (1:1, CH<sub>3</sub>CN/Water, V/V; 20 mM; pH 7.4).

## 2. Association constant

$$I_F^0/(I_F - I_F^0) = [a/(b-a)] \{ (1/K_s[M]) + 1 \}$$

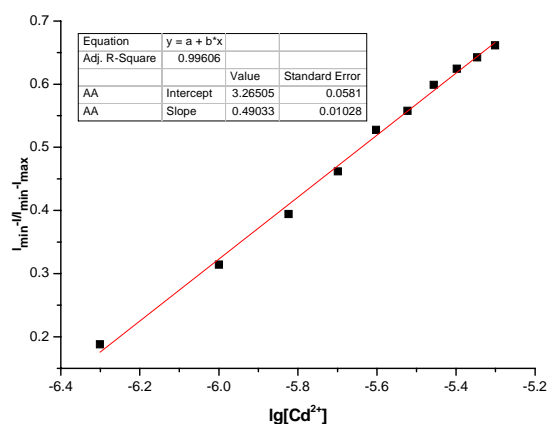


**Figure 2S.** Fitting of fluorescence titration curve of Cd-1 in HEPES buffer (1:1, CH<sub>3</sub>CN/Water, V/V; 20 mM; pH 7.4).

## 3. Detection limit

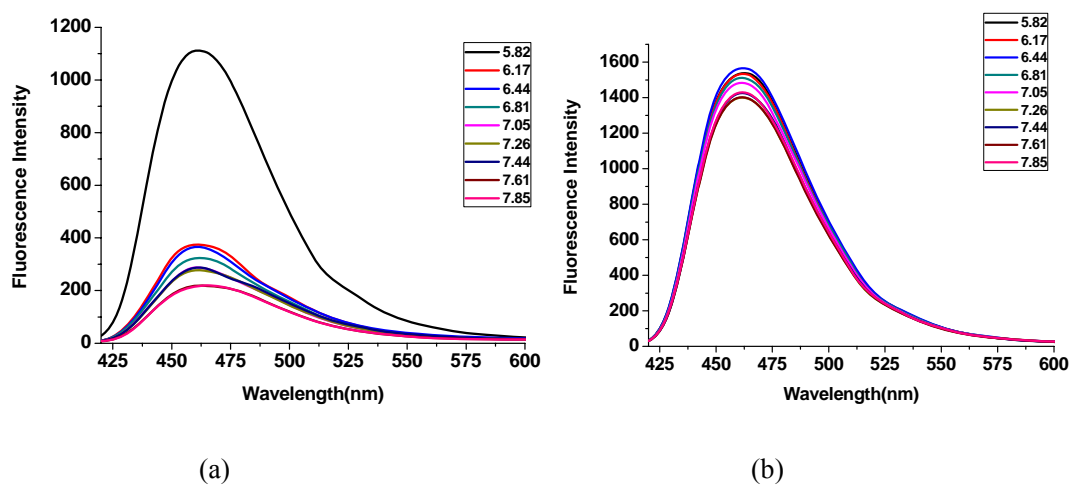
The titrating data were processed according to the reported methods. A linear regression curve was then fitted to these normalized data, and the point at which the

line crossed the ordinate axis was considered as the lowest detection concentration ( $2.19 \times 10^{-7}$  M).



**Figure 3S.** Fitting of fluorescence titration curve of Cd-1 in HEPES buffer (1:1, CH<sub>3</sub>CN/Water, V/V; 20 mM; pH 7.4).

#### 4. pH effect on fluorescence

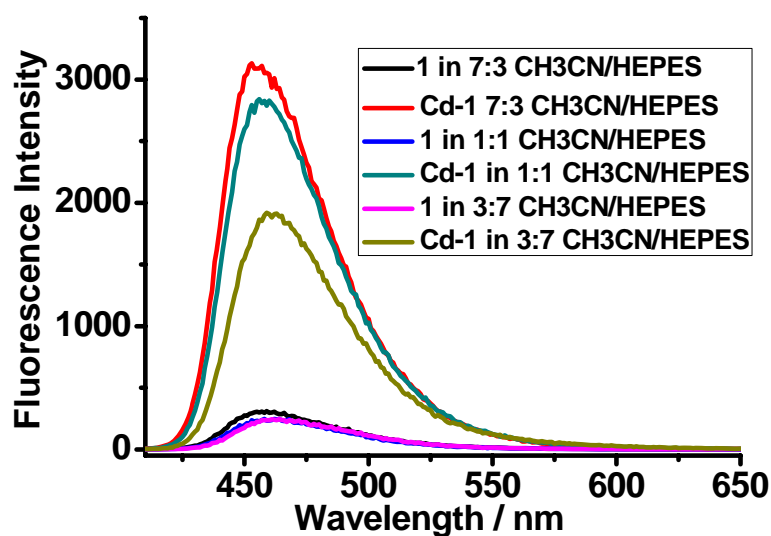


**Figure 4S.** The effect of pH on **1** (5  $\mu$ M) (a) and on **1** (5  $\mu$ M) with Cd<sup>2+</sup> ion (25  $\mu$ M) (b) at room temperature in HEPES buffer (1:1, CH<sub>3</sub>CN/Water, V/V; 20 mM).

#### 5. Solvent effect on fluorescence

The solvent effects on the fluorescence of **1** and Cd-**1** in different ratios of CH<sub>3</sub>CN/HEPES buffer were shown in Figure 5S. Obviously, fluorescence enhancement upon adding Cd<sup>2+</sup> to **1** were quite similar in CH<sub>3</sub>CN/HEPES buffer at

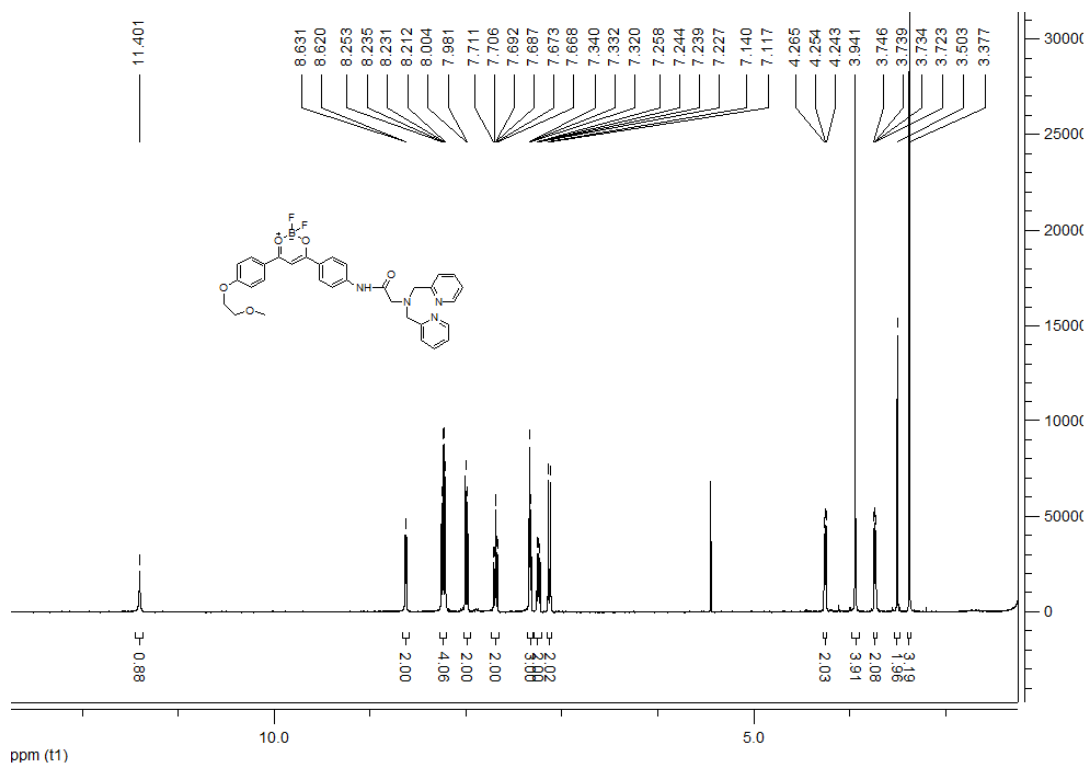
the ratio of 7:3 v/v and 1:1 v/v, much higher than in 3:7 v/v. For best performance and less organic solvent for application, CH<sub>3</sub>CN/HEPES buffer (1:1, v/v) was chosen for all the experiments.



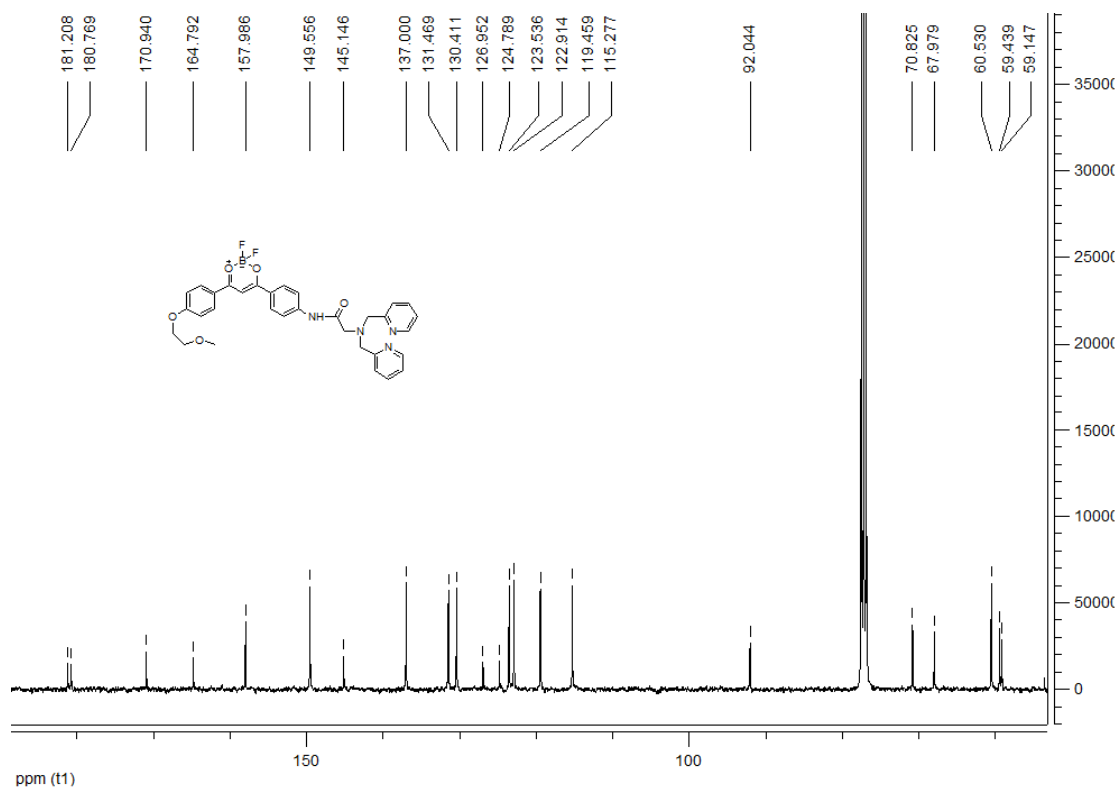
**Figure 5S.** The fluorescence response of **1** (5  $\mu$ M) towards Cd<sup>2+</sup> (10  $\mu$ M) in different ratios of CH<sub>3</sub>CN/HEPES buffer (20 mM, pH = 7.4) at room temperature,  $\lambda_{\text{ex}} = 400$  nm. The black bar: **1** in CH<sub>3</sub>CN/HEPES buffer (7:3 v/v); The red bar: Cd-**1** in CH<sub>3</sub>CN/HEPES buffer (7:3 v/v); The blue bar: **1** in CH<sub>3</sub>CN/HEPES buffer (1:1 v/v); The green bar: Cd-**1** in CH<sub>3</sub>CN/HEPES buffer (1:1 v/v); The pink bar: **1** in CH<sub>3</sub>CN/HEPES buffer (3:7 v/v); The dark yellow bar: Cd-**1** in CH<sub>3</sub>CN/HEPES buffer (3:7 v/v).

## 6. $^1\text{H}$ NMR, $^{13}\text{C}$ NMR, HRMS (ESI), ESI-MS

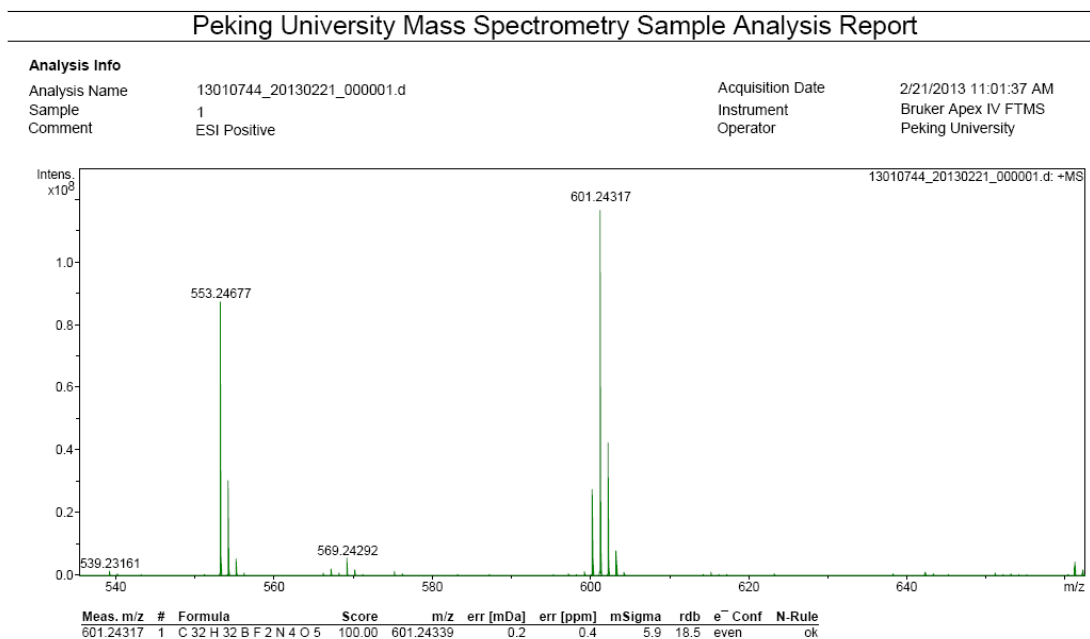
$^1\text{H}$  NMR of **1** in  $\text{CDCl}_3$



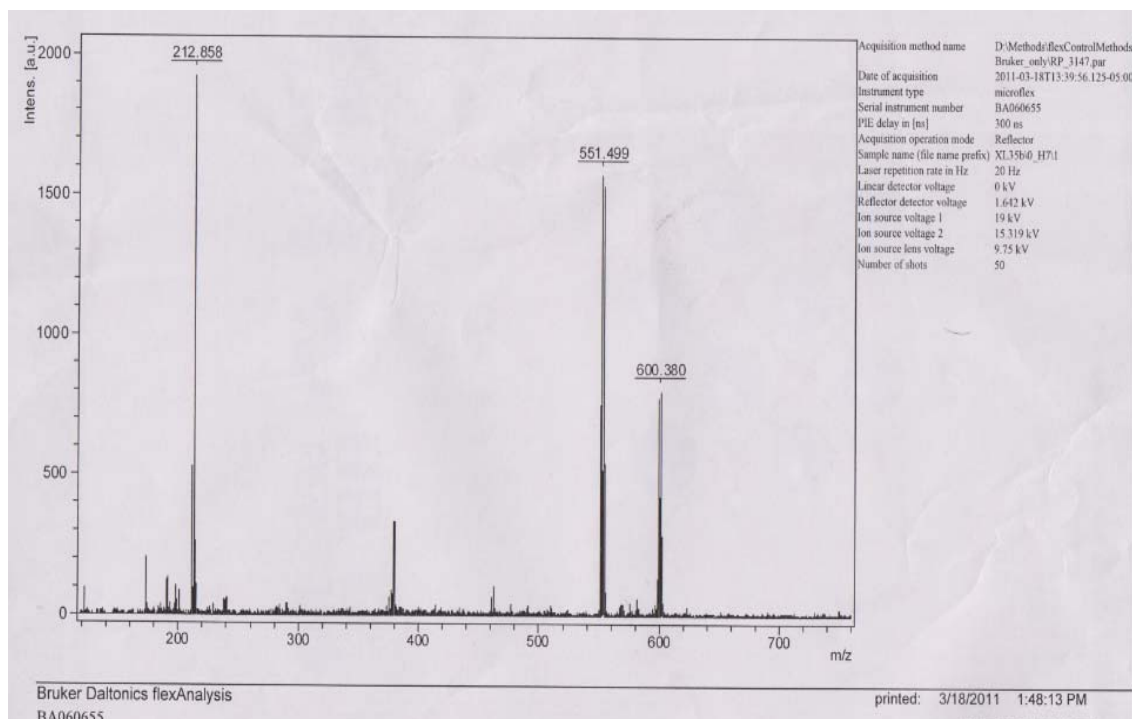
$^{13}\text{C}$  NMR of **1** in  $\text{CDCl}_3$



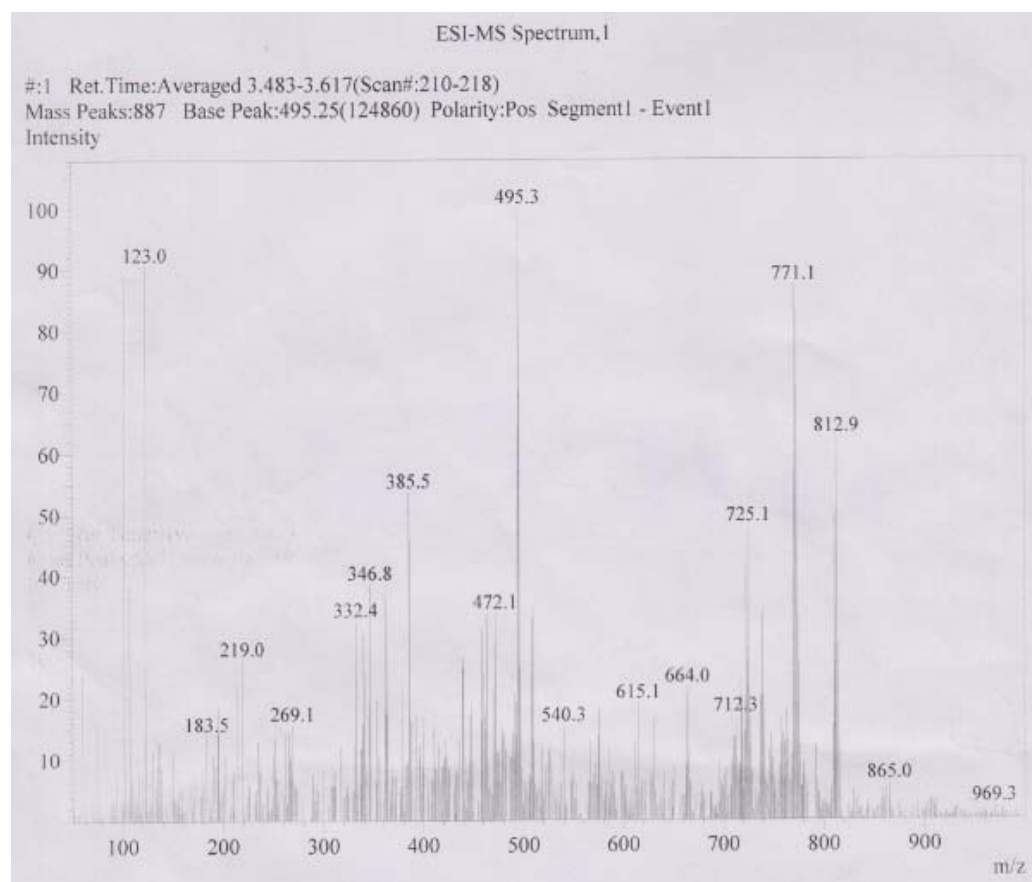
## HRMS (ESI) of 1.



## ESI-MS of 1.



## ESI-MS of Cd-1.



## References

- (1) Cogne-Laage, E.; Allemand, J. F.; Ruel, O.; Baudin, J. B.; Croquette, V.; Blanchard-Desce, M.; Jullien, L. *Chemistry-a European Journal* **2004**, *10*, 1445.
- (2) Demas, J. N.; Crosby, G. A. *Journal of Physical Chemistry* **1971**, *75*, 991.