

## Supporting Information

# A quinolinyl antipyrine based fluorescence sensor for Zn<sup>2+</sup> and its application in bioimaging

Qi-Hua You,<sup>a</sup> Pui-Shan Chan,<sup>b</sup> Wing-Hong Chan,<sup>\*a</sup> Sam C. K. Hau,<sup>c</sup> Albert W. M. Lee,<sup>a</sup>  
N. K. Mak,<sup>b</sup> Thomas C. W. Mak<sup>c</sup> and Ricky N. S. Wong<sup>b</sup>

<sup>a</sup>Department of Chemistry, Hong Kong Baptist University, Hong Kong, China

<sup>b</sup>Department of Biology, Hong Kong Baptist University, Hong Kong

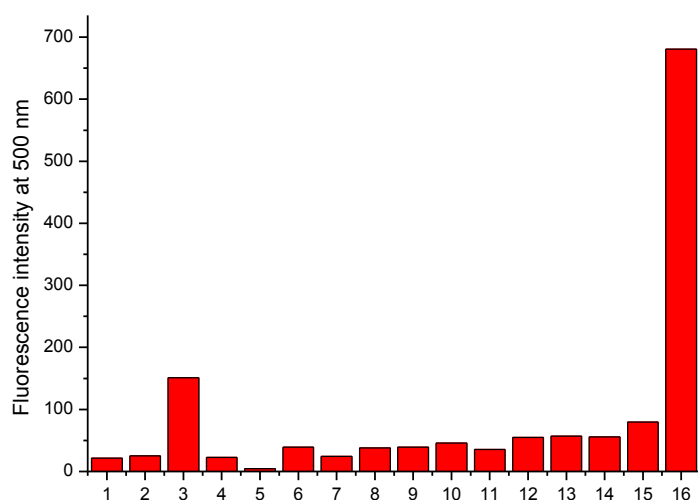
<sup>c</sup>Department of Chemistry, The Chinese University of Hong Kong, Shatin, Hong Kong, China

Tel.: +852-3411-7076; fax: +852-3411-7348

E-mail: whchan@hkbu.edu.hk

### Content:

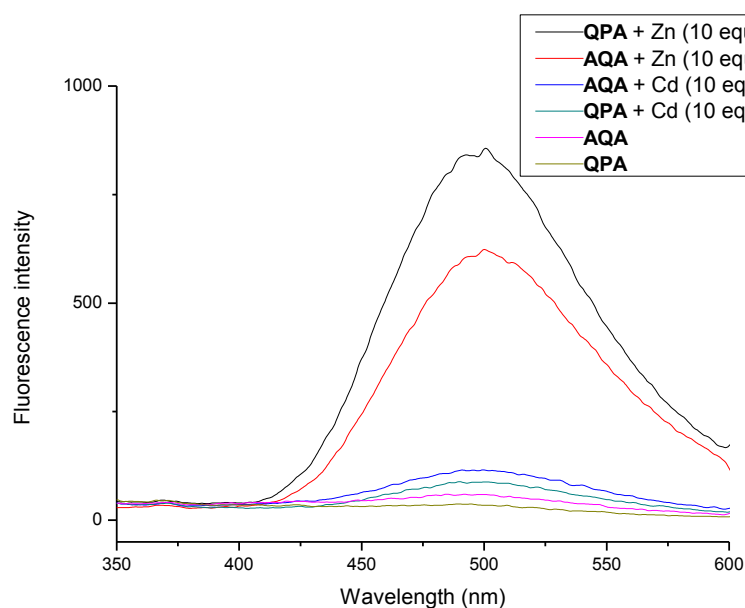
<b>Fig. S1</b>	Fluorescence intensity at 500 nm of <b>AQA</b> (10 μM) in 25% ACN-HEPES buffer (100 mM, pH = 7.0) upon addition of different metal ions (10 equiv).	2
<b>Fig. S2</b>	Fluorescence spectra of <b>QPA</b> and <b>AQA</b> (10 μM) in 25% ACN-HEPES buffer (100 mM, pH = 7.0) upon addition of Zn <sup>2+</sup> and Cd <sup>2+</sup> respectively.	2
<b>Fig. S3</b>	Fluorescence intensity at 500 nm of <b>QPA</b> (1 μM) in 25% ACN-HEPES buffer (100 mM, pH = 7.0) as a function of concentration of free Zn <sup>2+</sup> (0 ~ 10 μM). Slit = 10 nm.	3
<b>Fig. S4</b>	Time-dependent fluorescence enhancement of <b>QPA</b> (10 μM) in 25% ACN-HEPES buffer (100 mM, pH = 7.0) upon addition of different concentrations of Zn <sup>2+</sup> .	3
<b>Fig. S5</b>	Fluorescence intensity at 500 nm of <b>QPA</b> (10 μM) in 25% ACN-HEPES (100 mM, pH = 7.0) upon alternate addition of Zn <sup>2+</sup> (100 μM) and EDTA (100 μM).	4
<b>Fig. S6</b>	MALDI-TOF HRMS spectrum of <b>QPA</b> .	4
<b>Fig. S7</b>	MALDI-TOF HRMS spectrum of <b>QPA</b> + Zn(ClO <sub>4</sub> ) <sub>2</sub> .	5
<b>Fig. S8</b>	<sup>1</sup> H NMR spectrum of <b>QPA</b> .	5
<b>Fig. S9</b>	<sup>13</sup> C NMR spectrum of <b>QPA</b> .	6



**Fig. S1** Fluorescence intensity at 500 nm of **AQA** (10  $\mu$ M) in 25% ACN-HEPES buffer (100 mM, pH = 7.0) upon addition of different metal ions (10 equiv.).

Ex = 330 nm, slit = 5 nm.

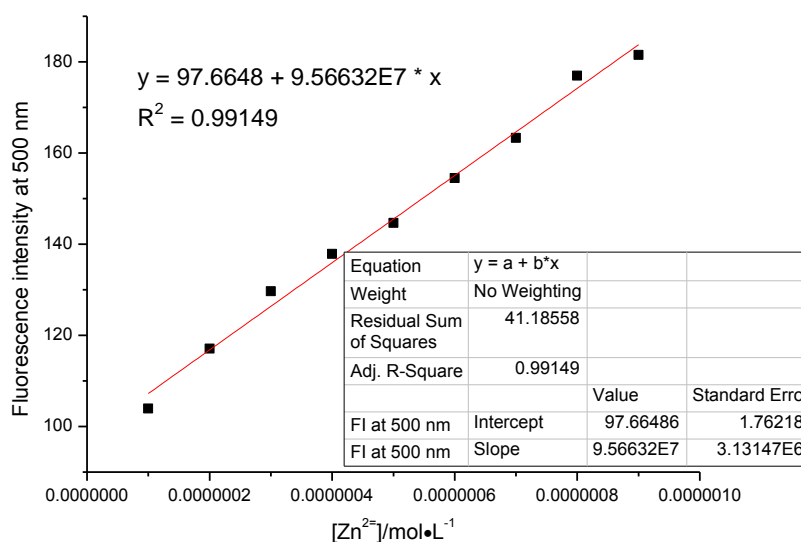
(1) Free, (2) Ca<sup>2+</sup>, (3) Cd<sup>2+</sup>, (4) Co<sup>2+</sup>, (5) Cu<sup>2+</sup>, (6) Fe<sup>2+</sup>, (7) Fe<sup>3+</sup>, (8) Hg<sup>2+</sup>, (9) K<sup>+</sup>, (10) Li<sup>+</sup>, (11) Mg<sup>2+</sup>, (12) Na<sup>+</sup>, (13) Ni<sup>2+</sup>, (14) Ag<sup>+</sup>, (15) Pb<sup>2+</sup>, (16) Zn<sup>2+</sup>



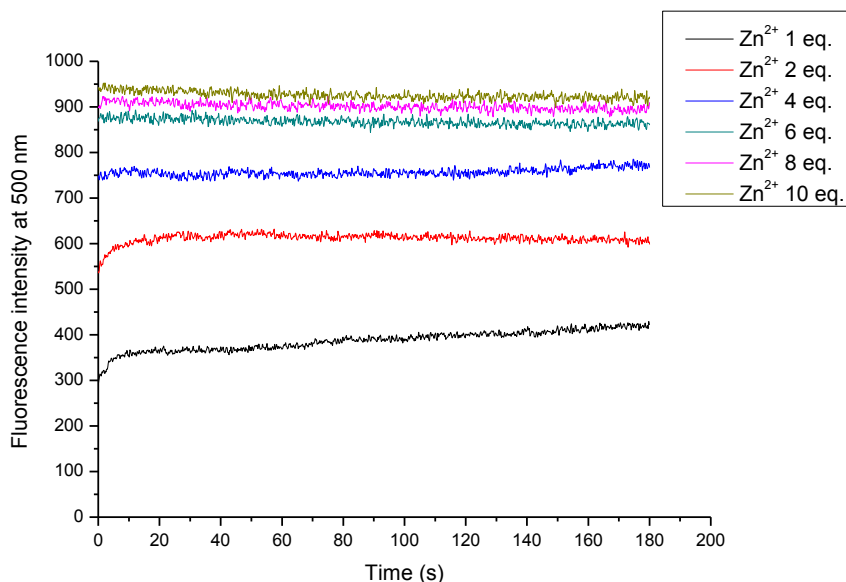
**Fig. S2** Fluorescence spectra of **QPA** and **AQA** (10  $\mu$ M) in 25% ACN-HEPES buffer (100 mM, pH = 7.0) upon addition of Zn<sup>2+</sup> and Cd<sup>2+</sup> respectively.

### Detection of limit

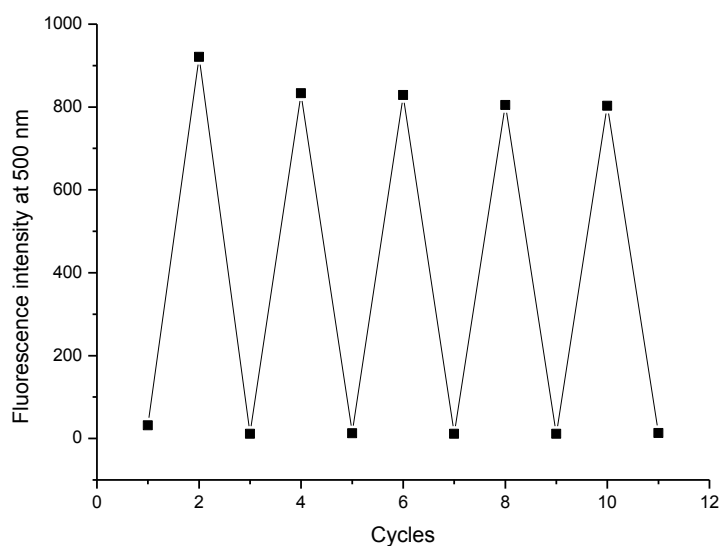
The detection limit was calculated based on the fluorescence titration. To improve the sensitivity, probe **QPA** was employed at 1  $\mu\text{M}$  and the slit was adjusted to 15 nm/15 nm. To determine the S/N ratio, the emission intensity of **QPA** without any cation was measured by 10 times and the standard deviation of blank measurements was determined. Under the present conditions, a good linear relationship between the fluorescence intensity and  $\text{Zn}^{2+}$  concentration could be obtained in the 0 – 0.9  $\mu\text{M}$  ( $R^2 = 0.9915$ ), as shown in Fig. S13. The detection limit is then calculated with the equation: detection limit =  $3\sigma_{\text{bi}}/m$ , where  $\sigma_{\text{bi}}$  is the standard deviation of blank measurements,  $m$  is the slope between intensity versus sample concentration. The detection limit was measured to be  $1.3 \times 10^{-7}$  M at S/N = 3 (signal-to-noise ratio of 3:1).



**Fig. S3** Fluorescence intensity at 500 nm of **QPA** (1  $\mu\text{M}$ ) in 25% ACN-HEPES buffer (100 mM, pH = 7.0) as a function of concentration of free  $\text{Zn}^{2+}$  (0 ~ 10  $\mu\text{M}$ ). Slit = 10 nm.

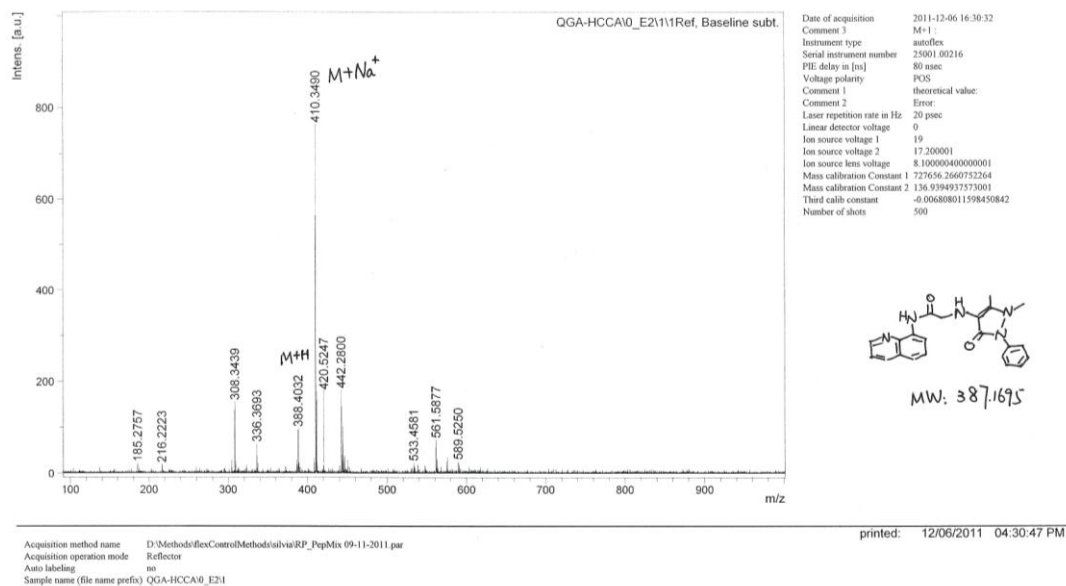


**Figure S4** Time-dependent fluorescence enhancement of **QPA** (10  $\mu\text{M}$ ) in 25% ACN-HEPES buffer (100 mM, pH = 7.0) upon addition of different concentrations of  $\text{Zn}^{2+}$ . Fluorescence intensity was recorded at 500 nm.  $\lambda_{\text{ex}} = 330$  nm.

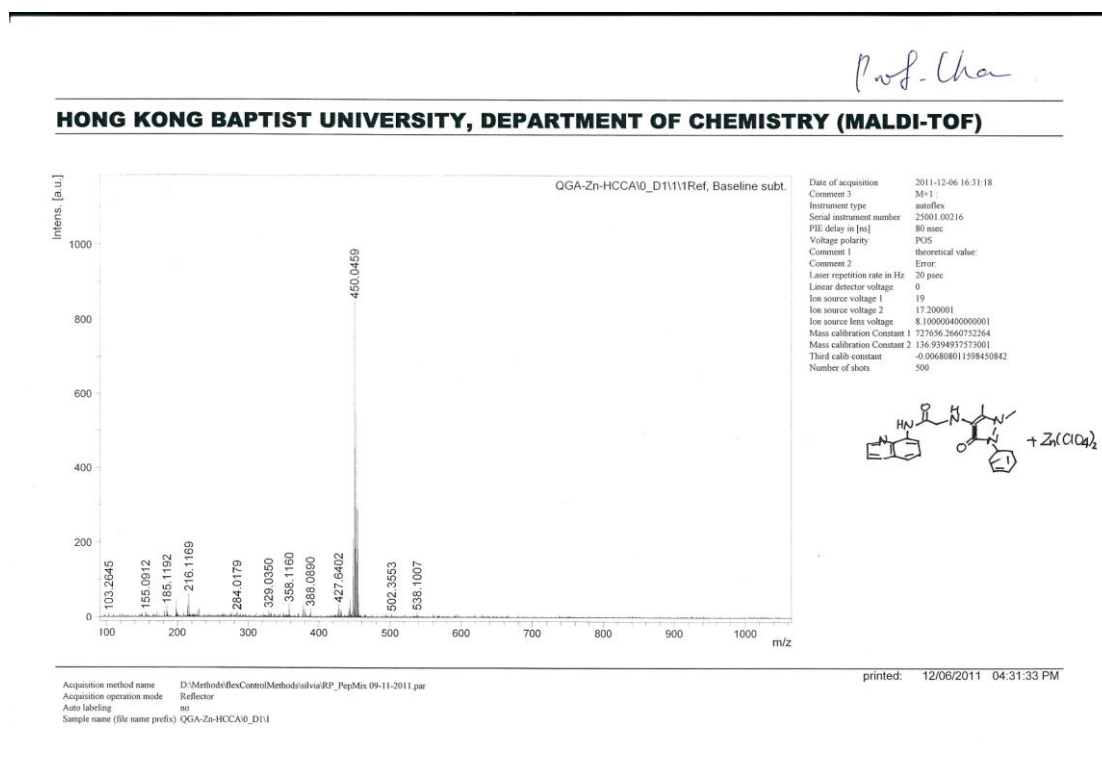


**Fig. S5** Fluorescence intensity at 500 nm of **QPA** (10  $\mu$ M) in 25% ACN-HEPES (100 mM, pH = 7.0) upon the alternate addition of  $\text{Zn}^{2+}$ /EDTA with several concentrations (0:0, 100:0, 100:100, 200:100, 200:200, 300:200, 300:300, 400:300, 400:400, 500:400 and 500:500  $\mu$ M, respectively).  $\lambda_{\text{ex}}$  = 330 nm.

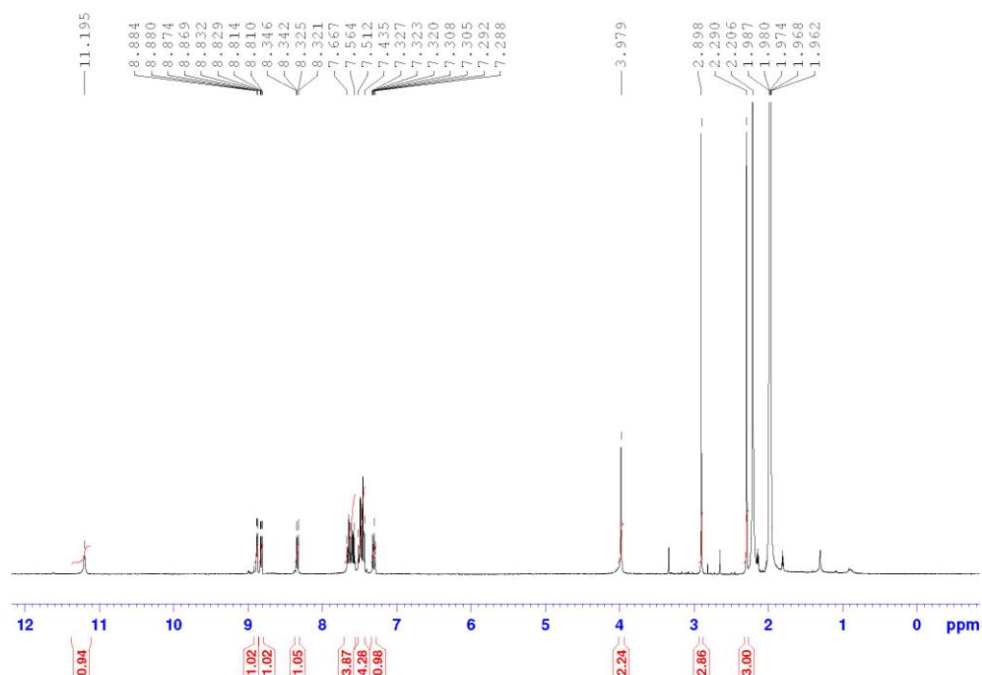
**HONG KONG BAPTIST UNIVERSITY, DEPARTMENT OF CHEMISTRY (MALDI-TOF)**



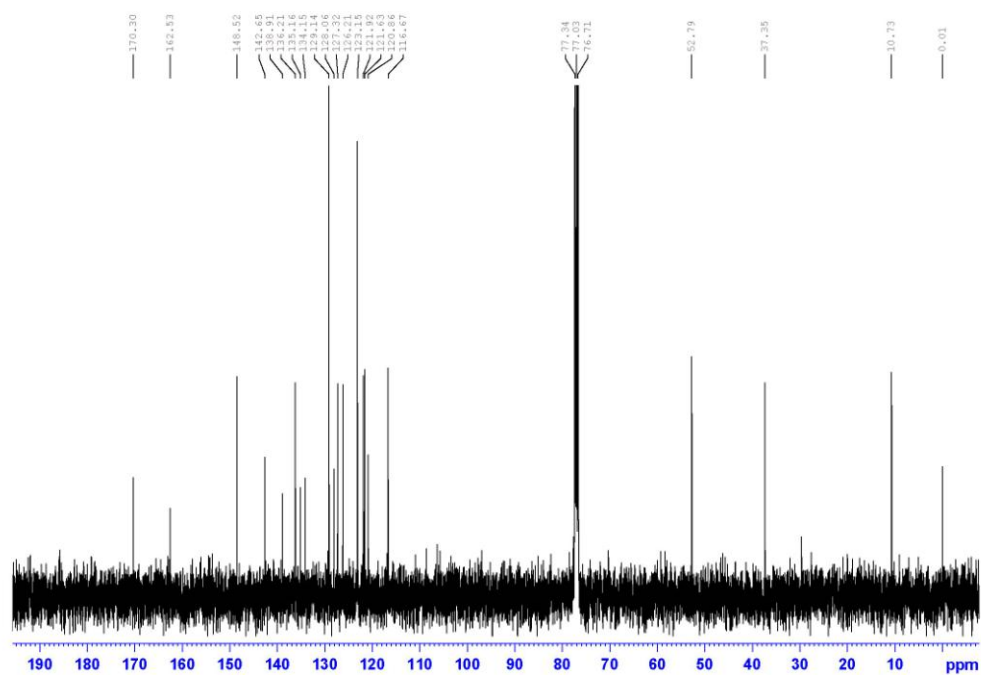
**Fig. S6** MALDI-TOF HRMS spectrum of **QPA**.



**Fig. S7** MALDI-TOF HRMS spectrum of **QPA** +  $\text{Zn}(\text{ClO}_4)_2$ .



**Fig. S8**  $^1\text{H}$  NMR spectrum of **QPA**.



**Fig. S9**  $^{13}\text{C}$  NMR spectrum of **QPA**.