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## Supporting Information

### **High selectivity and sensitivity chemosensor based on 2,3-Diaminophenazine hydrochloride for detection of cyanide in pure water and its application in plant seeds sample**

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## 1. Experimental

### 1.1 Materials and instruments

All solvents were used with fresh distilled water in this experiment, unless otherwise noted. Fresh distilled water was used throughout the experiment. All other reagents and solvents were commercially available at analytical grade and were used without further purification.  $^1\text{H}$ -NMR was recorded on a Mercury-600BB spectrometer at 600 MHz and  $^{13}\text{C}$  NMR spectra were recorded on a Mercury-600BB spectrometer at 150 MHz.  $^1\text{H}$  chemical shifts are reported in ppm downfield from tetramethylsilane (TMS,  $\delta$  scale with the solvent resonances as internal standards). Electrospray ionization mass spectra (ESI-MS) were recorded on an esquire 6000 MS instrument and version 3.4 of Bruker Daltonics Data Analysis as the data collection system. The infrared spectra were performed on a Digilab FTS-3000 Fourier transform-infrared spectrophotometer. UV-vis spectra were recorded on a Shimadzu UV-2550 spectrometer. Fluorescence spectra were performed on a Shimadzu RF-5301 fluorescence spectrophotometer.

### 1.2 General procedure for UV-vis experiments

The UV-vis experiments were carried out in fresh distilled water on a Shimadzu UV-2550 spectrometer. Any changes in the UV-vis spectra of the synthesized compounds were recorded on addition of tetrabutylammonium salts while keeping the **Q1** concentration constant ( $2.0 \times 10^{-5}$  M) in this experiment. Tetrabutylammonium salt of anions ( $\text{F}^-$ ,  $\text{Cl}^-$ ,  $\text{Br}^-$ ,  $\text{I}^-$ ,  $\text{AcO}^-$ ,  $\text{H}_2\text{PO}_4^-$ ,  $\text{HSO}_4^-$  and  $\text{ClO}_4^-$ ) and sodium salt of anions ( $\text{CN}^-$ ,  $\text{SCN}^-$  and  $\text{S}^{2-}$ ) were used ( $1.0 \times 10^{-3}$  M) for all the UV-vis experiments.

### 1.3 General procedure for fluorescence spectra experiments

All the fluorescence spectroscopy was carried out in fresh distilled water on a Shimadzu RF-5301 spectrometer. Any changes in the fluorescence spectra of the synthesized compounds were recorded on addition of tetrabutylammonium salts while keeping the **Q1** concentration constant ( $2.0 \times 10^{-5}$  M) in this experiment. Tetrabutylammonium salt of anions ( $\text{F}^-$ ,  $\text{Cl}^-$ ,  $\text{Br}^-$ ,  $\text{I}^-$ ,  $\text{AcO}^-$ ,  $\text{H}_2\text{PO}_4^-$ ,  $\text{HSO}_4^-$  and  $\text{ClO}_4^-$ ) and sodium salt of anions ( $\text{CN}^-$  and  $\text{SCN}^-$ ) were used ( $1.0 \times 10^{-3}$  M) for the

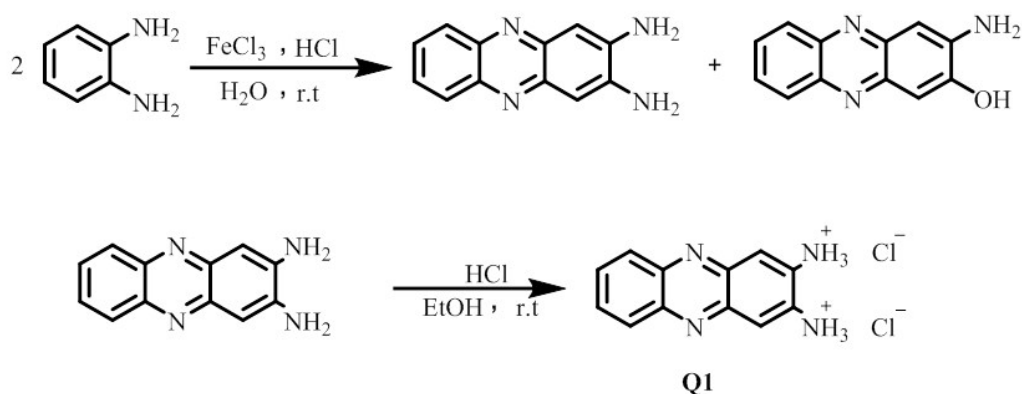
fluorescence experiments.

#### 1.4 General procedure for $^1\text{H}$ NMR experiments

For  $^1\text{H}$  NMR titrations, the solution of **Q1** and  $\text{CN}^-$  were prepared in deuterium water. Aliquots of the two solutions were mixed directly in NMR tubes.

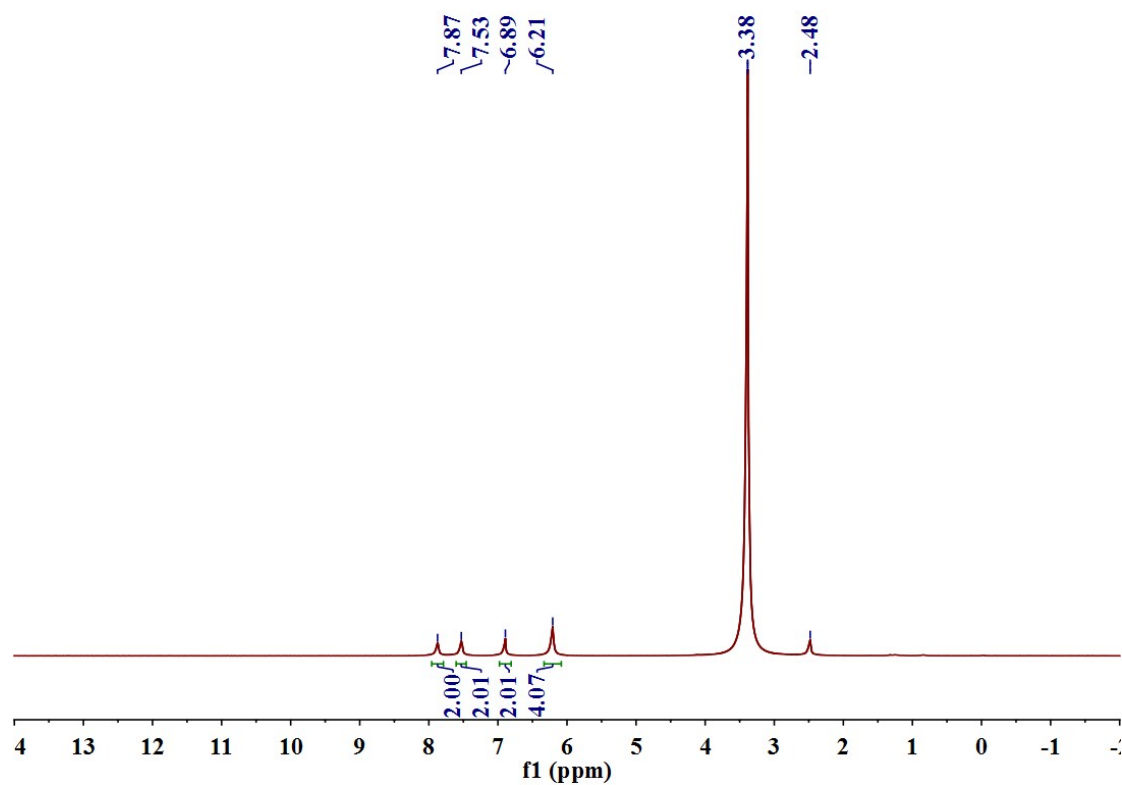
#### 1.5 Synthesis and characterization of 2, 3-diaminophenazine and **Q1**

2, 3-diaminophenazine was prepared according to the literature procedures<sup>[10]</sup>. To dissolve 2, 3-diaminophenazine (0.4205 g, 2 mmol) in 20 mL of EtOH, and take 3 mL concentrated hydrochloric acid, diluted with EtOH to 10 mL. The diluted hydrochloric acid was added dropwise to the dissolved 2, 3-diaminophenazine solution and stirred the above solution fully at room temperature. By filtration and drying, the reserved solids are end-product **Q1**. **Q1** as dark brown solid and has a good solubility in fresh distilled water.  $^1\text{H}$  NMR ( $\text{D}_2\text{O}$ , 600 MHz)  $\delta$ : 7.61 (s, 4H); 7.51 (s, 2H); 6.51 (s, 6H).  $^{13}\text{C}$  NMR ( $\text{DMSO-d}_6$ , 150 MHz)  $\delta$ /ppm 149.53, 132.57, 129.11, 127.75, 123.02, 96.88. ESI-MS calcd for  $\text{C}_{12}\text{H}_{12}\text{N}_4^{2+}$  212.1051, found 212.1010.



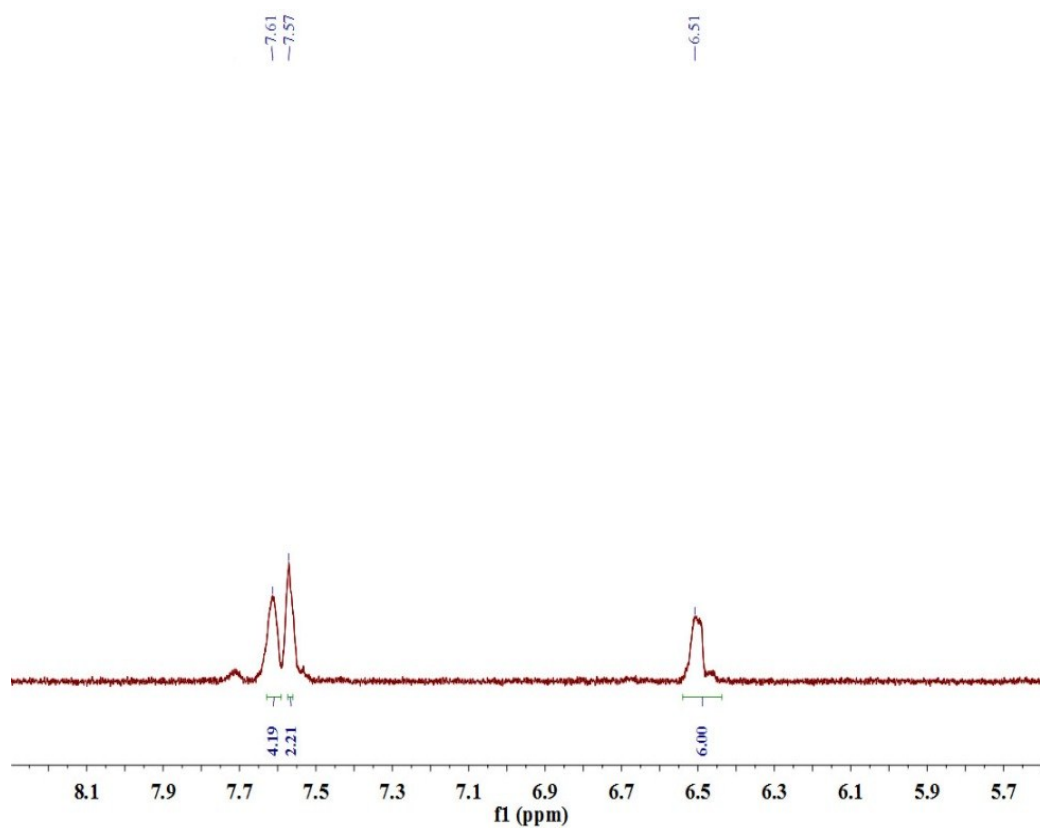
**Scheme S1.** Synthesis of **Q1**

## 2. $^1\text{H}$ -NMR spectrum of 2, 3-diaminophenazine



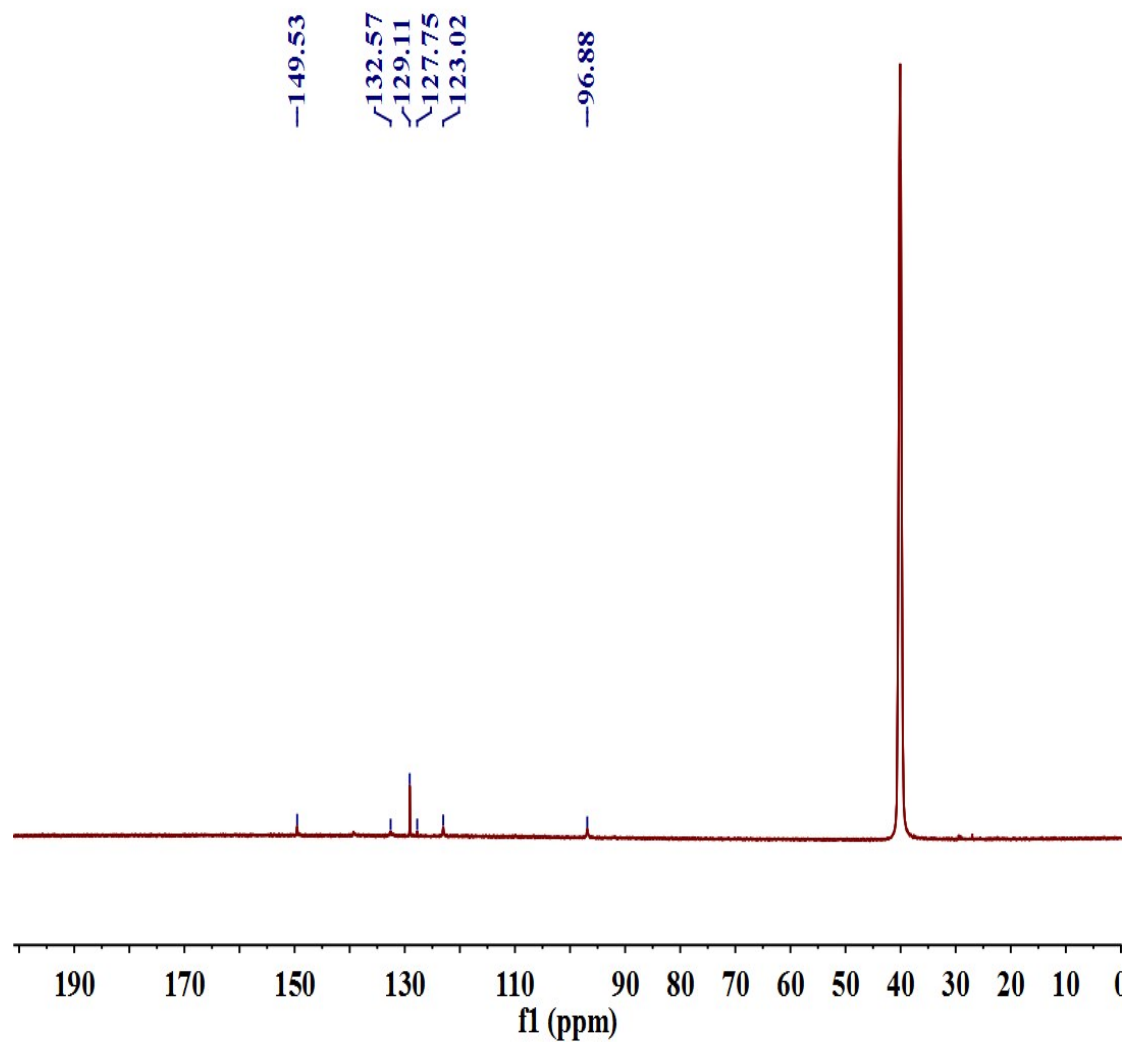
**Fig. S1:**  $^1\text{H}$ -NMR spectrum of 2, 3-diaminophenazine in  $\text{DMSO-}d_6$ .

### 3. $^1\text{H}$ -NMR spectrum of Q1



**Fig. S2:**  $^1\text{H}$ -NMR spectrum of Q1 in  $\text{D}_2\text{O}$ .

#### 4. $^{13}\text{C}$ -NMR spectrum of Q1



**Fig. S3:**  $^{13}\text{C}$ -NMR spectrum of Q1 in  $\text{DMSO}-d_6$ .

## 5. ESI/MS of Q1

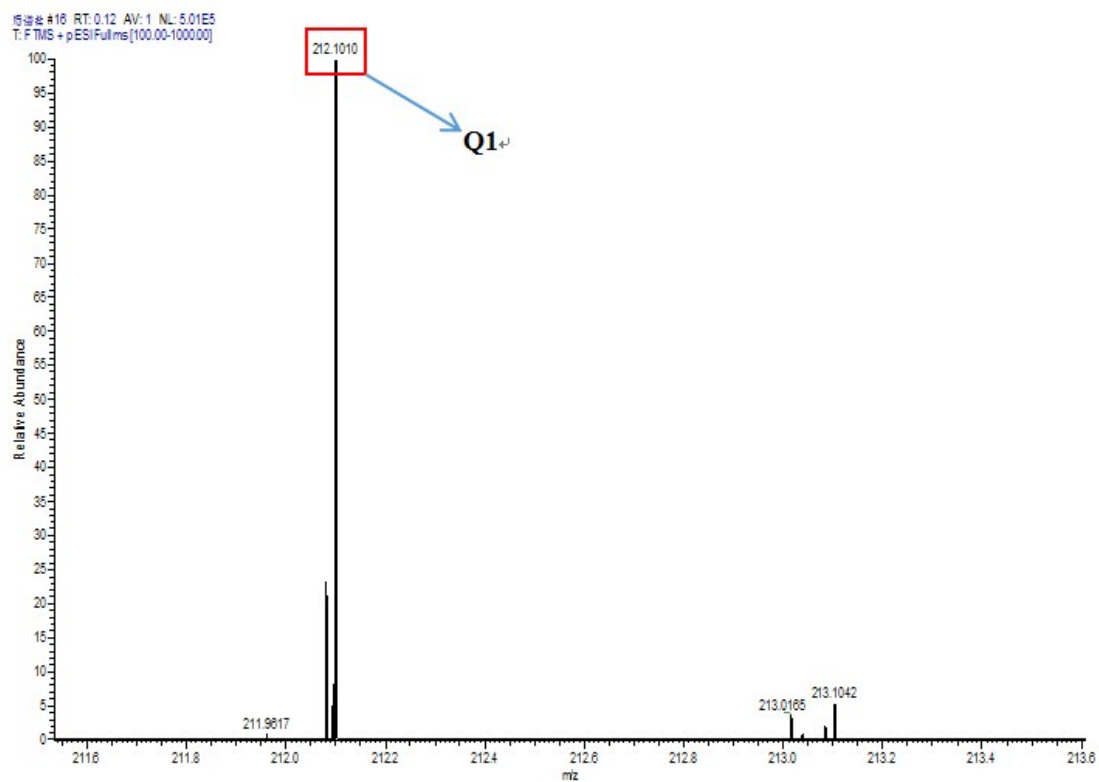
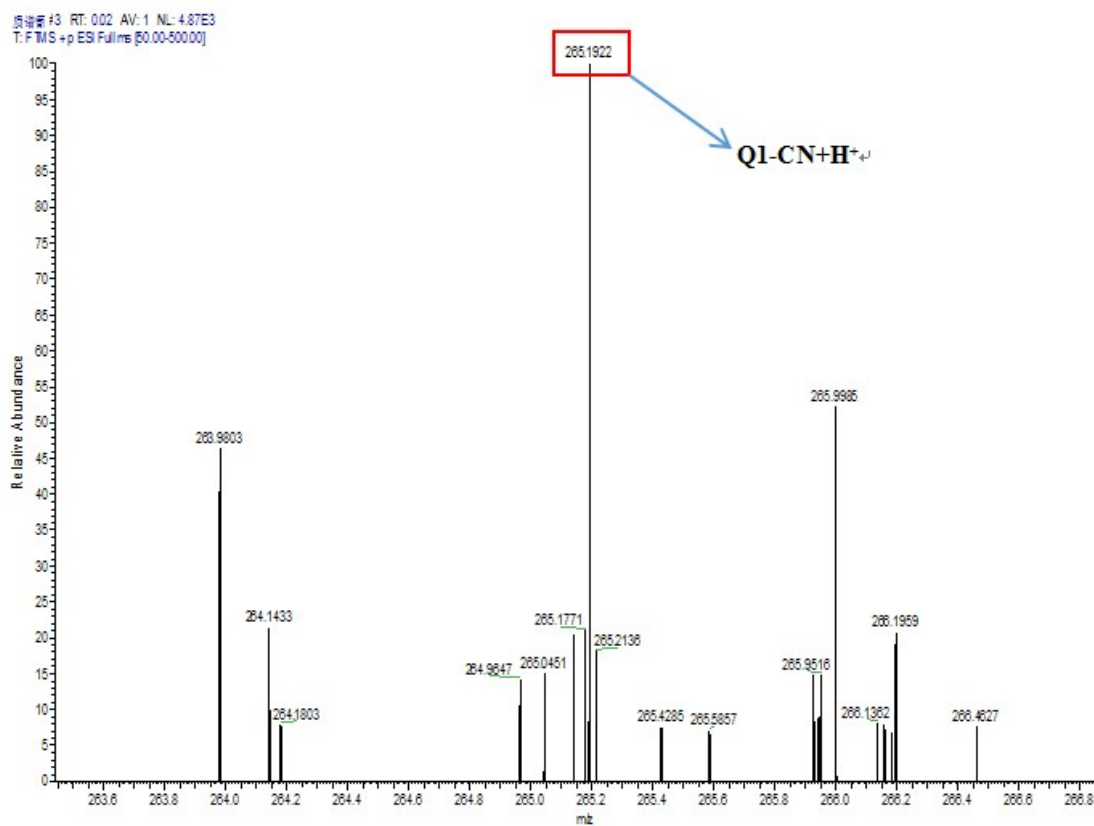


Fig. S4: The ESI/MS of Q1.

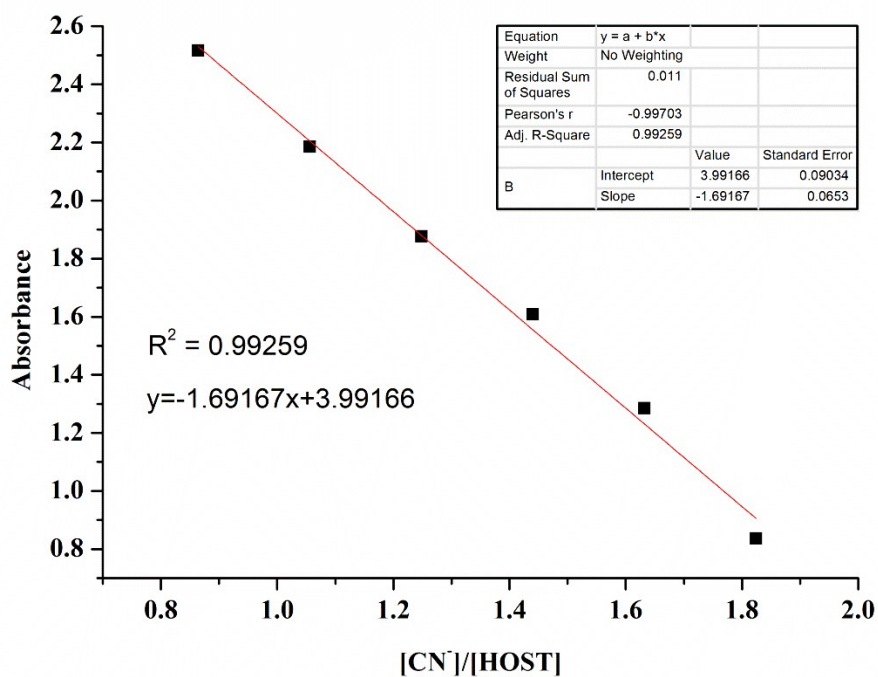
## 6. The ESI/MS examined between NaCN and Q1 [Q1+CN+H]<sup>+</sup>



**Fig. S5:** The ESI/MS examined between **Q1** and NaCN in fresh distilled water, indicating the 1:2 stoichiometry for **Q1** and NaCN.



## 7. Determine of the UV-vis detection limit for cyanide



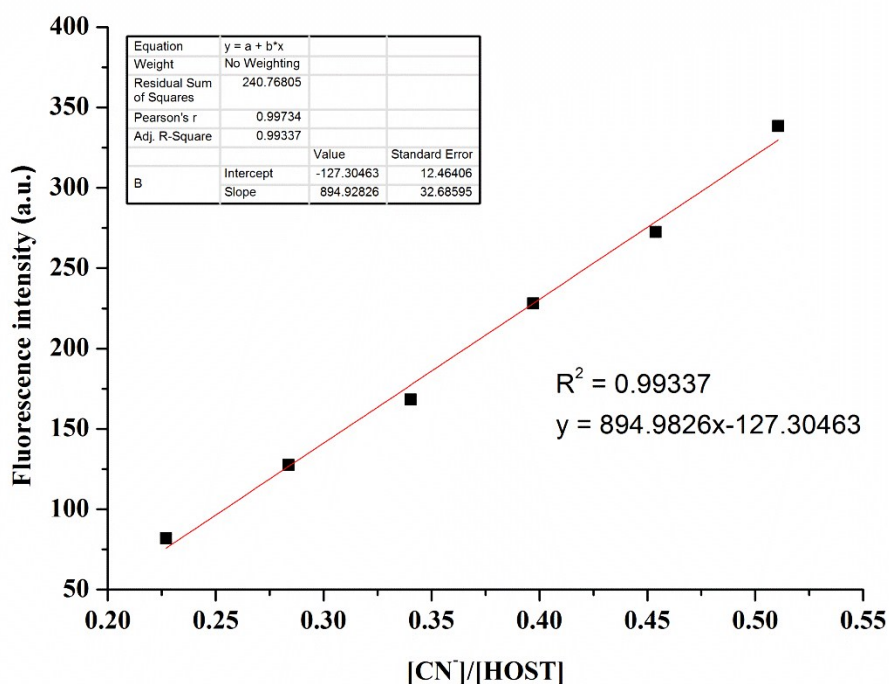
Linear Equation:  $Y = -1.69167 \times X + 3.99166$      $R^2 = 0.99259$

$$S = 1.69167 \times 10^6 \quad \delta = \sqrt{\frac{\sum(A - \bar{A})^2}{(N - 1)}} = 0.32969 \quad (N = 20) \quad K = 3$$

$$\text{LOD} = K \times \delta / S = 1.94890 \times 10^{-7} \text{ M}$$

**Fig. S6:** The photograph of the UV-vis spectrum linear range for cyanide.

## 8. Determine of the fluorescent detection limit for cyanide



Linear Equation:  $Y = 894.9826 \times X - 127.30463$   $R^2 = 0.99337$

$$S = 894.9826 \times 10^6 \quad \delta = \sqrt{\frac{\sum(A - \bar{A})^2}{(N - 1)}} = 0.33826 \quad (N = 20) \quad K =$$

3

$$\text{LOD} = K \times \delta/S = 1.13385 \times 10^{-9} \text{ M}$$

**Fig. S7:** The photograph of the fluorescent spectrum linear range for cyanide.