Electronic Supporting Information for:

# A potential fluorescence detection approach to trace hexachlorobenzene via disaggregating with ethanol

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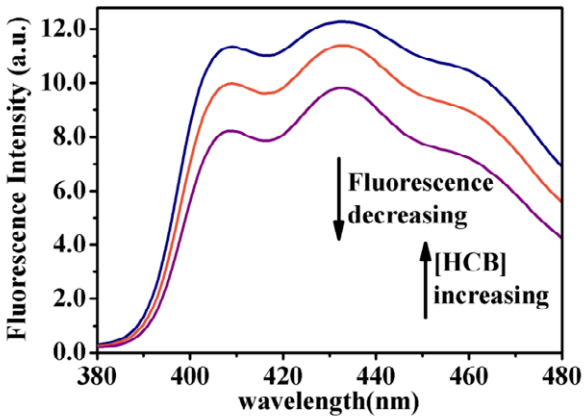


**Fig. S1.** Fluorescence emission spectra of HCB in ethanol solution with HCB concentrations of $10^{-7}$, $10^{-6}$, $10^{-5}$ M (showing arrowhead), respectively.

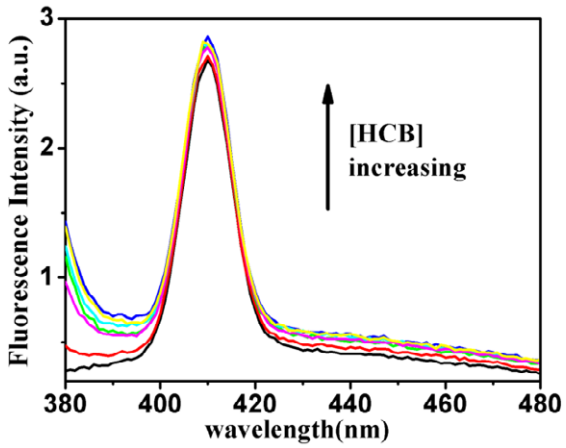


**Fig. S2.** Fluorescence emission spectra of HCB in water solution with HCB concentrations of $1\times10^{-9}$ to $6\times10^{-9}$ M, respectively.

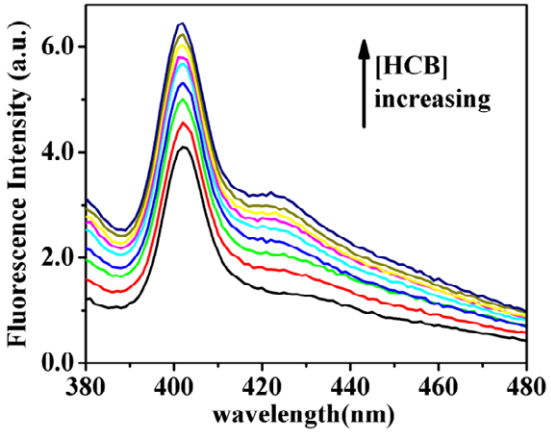


**Fig. S3.** Fluorescence emission spectra of HCB in 1-butanol solution with HCB concentrations of 0, $10^{-14}$, $10^{-13}$, $10^{-12}$, $10^{-11}$, $10^{-10}$, $10^{-9}$, $10^{-8}$, $10^{-7}$ M (showing arrowhead), respectively.

**Fluorescence quantum yield of HCB in ethanol:**

An easy way to estimate the quantum yield of a fluorophore is by comparison with the quantum yield of a known standard fluorophore, which is usually called the relative method.

The quantum yield of the unknown, $Q_X$, is calculated according to the following equation[1]:

$$Q_X = Q_R \cdot \frac{A_R}{A_X} \cdot \frac{E_X}{E_R} \cdot \frac{I_R}{I_X} \cdot \frac{n_X^2}{n_R^2} \qquad \text{(S-1)}$$

where, $Q_R$ is the quantum yield of the standard, $A$ is the absorbance of the solution, $E$ is the corrected emission intensity, $I$ is the relative intensity of the exciting light and $n$ is the average refractive index of the solution. Subscripts $R$ and $X$ refer to the reference and unknown compound, respectively. Eq. (S-1) can be simplified given that the intensity of the excitation light for different samples (i.e., the tested and the reference fluorophore) keeps the same, so we have:

$$Q_X = Q_R \cdot \frac{A_R}{A_X} \cdot \frac{E_X}{E_R} \cdot \frac{n_X^2}{n_R^2} \qquad \text{(S-2)}$$

In our experiment, the ultraviolet absorption spectra of $10^{-5}$ M HCB, $10^{-6}$ M rhodamine 6G (R6G) and $10^{-6}$ M rhodamine B (RB) in ethanol were taken on the Shimadzu UV-vis UV-1750 spectrophotometer (Kyoto, Japan). And fluorescence measurements were performed on a FluoroMax-4 spectrometer (Horiba Jobin Yvon Inc., France) with the slits for both excitation and emission of 2 nm.

We have known that the quantum yield of R6G is 0.94 in ethanol.[2] In order to check the accuracy of the relative method and these equipments, RB in ethanol was

used as the testable fluorophore. The ultraviolet absorption spectra of R6G and RB in ethanol are shown in Fig. S4. The fluorescence emission spectra of R6G and RB in ethanol with excitation of 360 nm are shown in Fig. S5. According to Eq. (S-2), the quantum yield of RB is 0.50 in ethanol, which is close to the known value 0.49,[3] justifying the reliability of the relative method for the estimation of HCB's quantum yield.

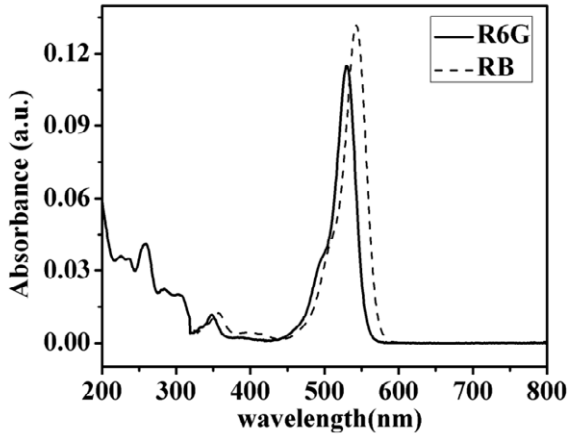


**Fig. S4.** Ultraviolet absorption spectra of R6G and RB in ethanol.

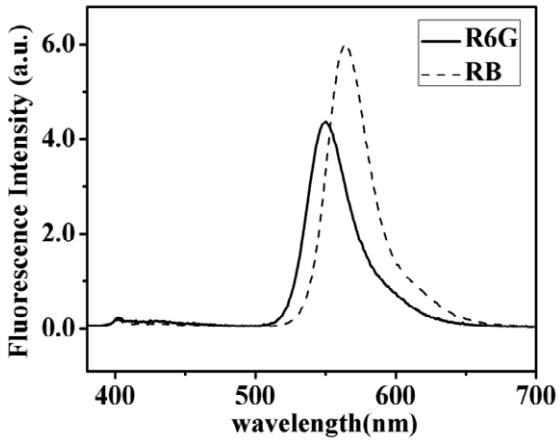


**Fig. S5.** Fluorescence emission spectra of R6G and RB in ethanol ($\lambda_{ex}$=360 nm).

Similarly, to estimate the quantum yield of HCB, the ultraviolet absorption and fluorescence emission spectra of R6G and HCB in ethanol were obtained (Fig. S6 and Fig. S7), and according to Eq. (S-2), the quantum yield of HCB is calculated as 0.78 in ethanol.

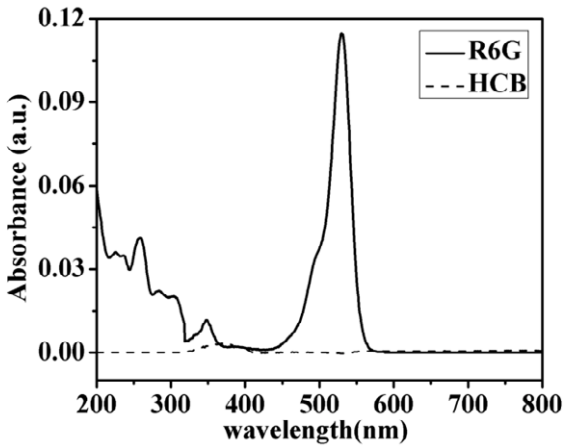


**Fig. S6.** Ultraviolet absorption spectra of R6G and HCB in ethanol.

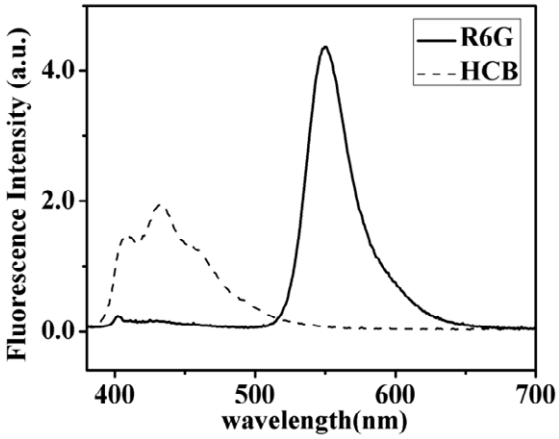


**Fig. S7.** Fluorescence emission spectra of R6G and HCB in ethanol ($\lambda_{ex}$=360 nm).

1 A. T. R. Williams and S. A. Winfield, *Analyst*, 1983, **108**, 1067-1071.

2 M. Fischer and J. Georges, *Chemical Physics Letters*, 1996, **260**, 115-118.

3 K. G. Casey and E. L. Quitevis, 1988, **92**, 6590-6594.