

Supplementary material

Alizarin Red-Tb³⁺ complex as ratiometric colorimetric and fluorescent dual probe for the smartphone-based detection of anthrax biomarker

Miao Xu,^{a, b, c} Wei Huang,^{b, c} Dingkun Lu,^{b, c} Chunyu Huang,^{a, b, c} Jingjing Deng,^{*a, b, c}
and Tianshu Zhou^{b, c}

^a Shanghai Key Laboratory of Forensic Medicine, Academy of Forensic Science, 1347
West Guangfu Road, Shanghai 200063, China

^b School of Ecological and Environmental Sciences, Shanghai Key Lab for Urban
Ecological Process and Eco-Restoration, East China Normal University, 500 Dongchuan
Road, Shanghai 200241, China.

^c Institute of Eco-Chongming (IEC), 3663 North Zhongshan Road, Shanghai 20062.

*Corresponding author email: jjdeng@des.ecnu.edu.cn

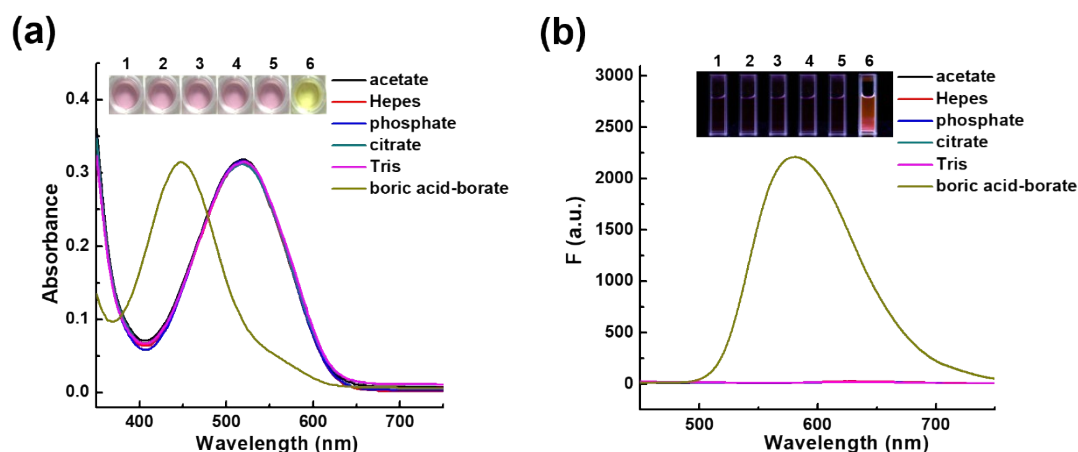


Fig. S1. (a) UV-vis spectra and photographs (inset) of AR (100 μM) dispersed in different kinds of buffer solutions (20 mM, pH = 7.4), from left to right: acetate (vial 1), Hepes (vial 2), phosphate (vial 3), citrate (vial 4), Tris (vial 5), boric acid-borate (vial 6). (b) Fluorescence spectra and photographs (inset) of AR (100 μM) dispersed in different kinds of buffer solutions (20 mM, pH = 7.4), from left to right: acetate (vial 1), Hepes (vial 2), phosphate (vial 3), citrate (vial 4), Tris (vial 5), boric acid-borate (vial 6).

The effect of different kinds of buffer solutions on AR has been studied. Firstly, for the detection of DPA released from bacterial spores, the pH value was settled as 7.4 according to the literature reported before.¹ AR (100 μM) was then dispersed into different kinds of buffer solutions, including acetate, Hepes, phosphate, citrate, Tris and boric acid-borate (20 mM, pH = 7.4) and its optical property was next characterized by UV-vis spectrophotometer and fluorescent spectrophotometer (Fig. S1). As displayed in Fig. S1, when AR was dispersed in acetate, Hepes, phosphate, citrate and Tris buffer solutions, AR shows a purple-red color and the characteristic peak of AR appears at 528 nm. Meanwhile, there is no fluorescence emission. However, when AR was added into the boric acid-borate buffer solution, the dispersion clearly turns into a yellow color accompanying with

a new absorption peak at 448 nm. At the same time, the orange fluorescence of AR turns on, which showed great consistency with the previous report,² and the unique optical property of AR in boric acid-borate buffer solution could then be explored for DPA detection, as will be demonstrated.

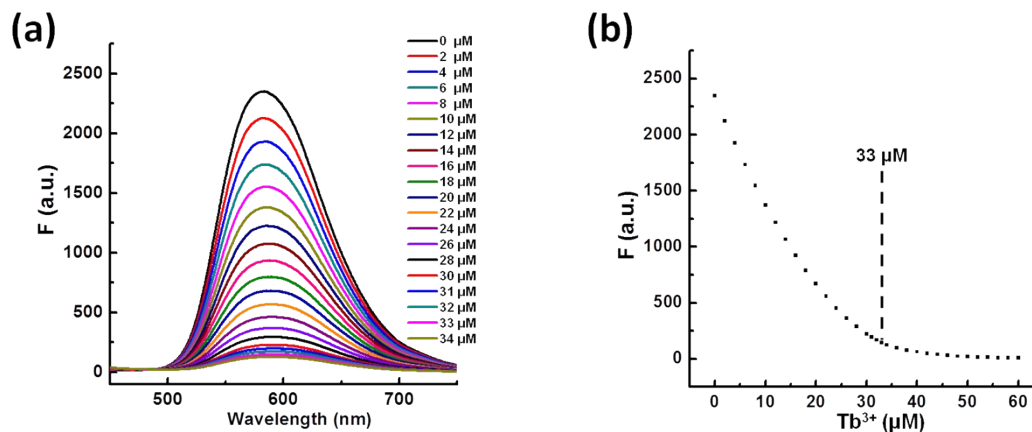


Fig. S2. (a) Fluorescence spectra of AR (100 μM) with consecutive addition of Tb^{3+} ions. (d) Plot of change in the fluorescent intensity (I_{580}) against the concentration of Tb^{3+} ions.

To obtain the AR- Tb^{3+} probe with good analytical performance, different concentrations of Tb^{3+} were added into boric acid-borate buffer solution containing 100 μM AR. As shown in Fig. 1 and Fig. S2, when the concentration of Tb^{3+} is higher than 33 μM , the ratio of A_{448}/A_{528} and fluorescent intensity I_{580} decreased almost to minimum and are no longer changed, while high concentration of Tb^{3+} may bring a negative influence on sensitive DPA detection, the concentration of Tb^{3+} was rationally optimized at 33 μM for 100 μM AR.

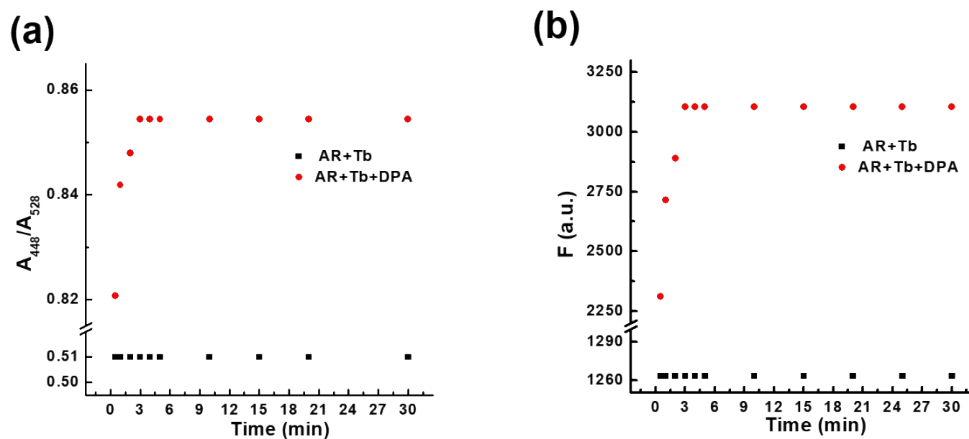


Fig. S3. Effect of reaction time on the ratio A_{448}/A_{528} (a) and the fluorescent intensity I_{545} (b) of AR/Tb³⁺ complex without (black) and with (red) the addition of 10 μM DPA as a function of time course.

The time courses of UV-vis spectra and fluorescent emission spectra of AR-Tb³⁺ complex without and with the addition of 10 μM DPA were investigated and the results were shown in Fig. S3. The DPA-induced the increase of the ratio A_{448}/A_{528} and the fluorescent intensity I_{545} reaches to maximum and becomes stable after 3 min, indicating the coordination interaction was completed. Hence, 3 min was chosen as the adequate reaction time. Moreover, as could be seen from Fig. S3, even after 30 min, the dual-channel probe shows same response as it does at 3 min, demonstrating the good stability of the developed AR-Tb³⁺ probe.

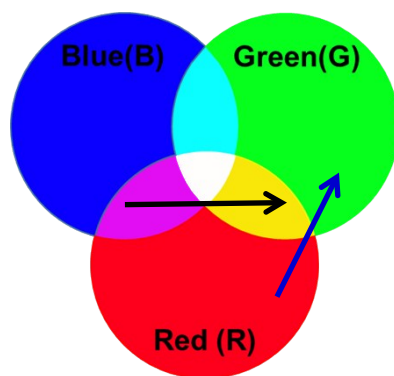


Fig. S4. Illustration of color change by using RGB color model.

References:

1. N. Gao, Y. Zhang, P. Huang, Z. Xiang, F. Wu, L. Mao, *Anal. Chem.*, 2018, 90, 7004-

7011.

2. G. Springsteen, B. Wang, Chem. Commun., 2001, 1608-1609.