

Electronic Supplementary Information

**Investigation of the Colorimetric Characteristics of VX in Squaraine-Based
Solutions**

Bin Du, Shu Geng, Wei Cao, Lei Guo, Jianjie Xu, Feng Huang and Lina Chen*

State Key Laboratory of NBC Protection for Civilian, Beijing 102205, China.

Corresponding Author:mail: nana19870105@163.com

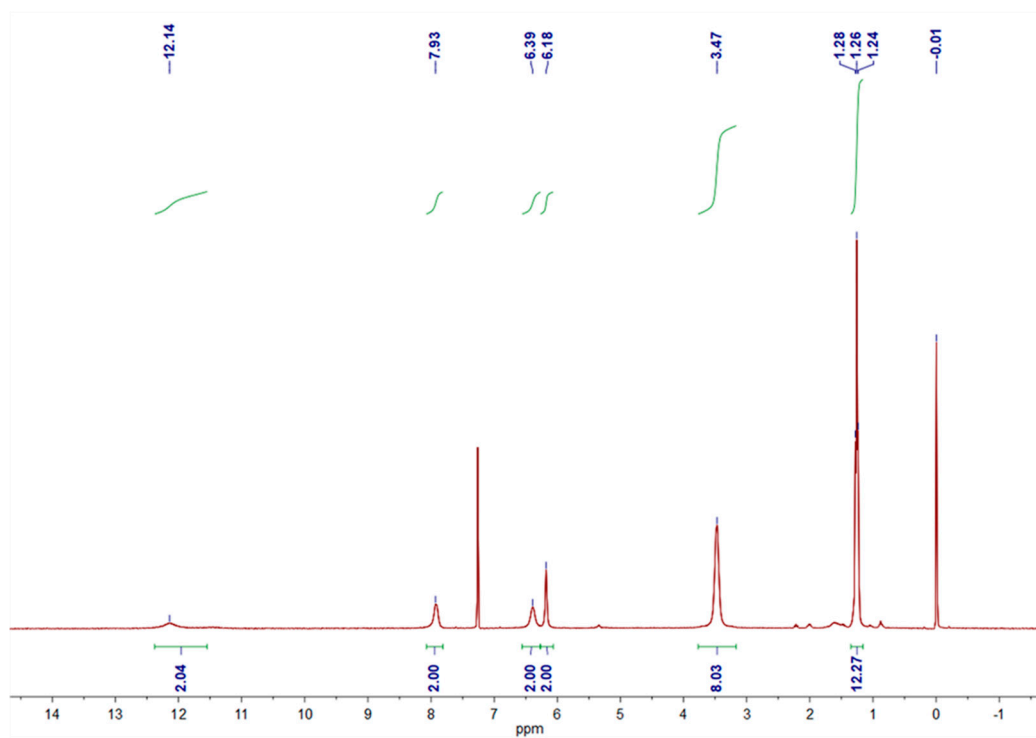


Figure S1 ^1H NMR spectrum of SP in CDCl_3 .

Optimization of TABF concentration:

A series of 2 $\mu\text{g/mL}$ SP solutions (solvent CH_2Cl_2) containing different concentrations of TABF (100 $\mu\text{g/mL}$, 250 $\mu\text{g/mL}$, 500 $\mu\text{g/mL}$, 750 $\mu\text{g/mL}$, 1000 $\mu\text{g/mL}$) were prepared. Sequentially, the UV-Vis absorption spectra of these solutions were determined by Mettler Toledo UV5Nano Spectrophotometer. Then, solutions mixed with 50 $\mu\text{g/mL}$ VX and 2 $\mu\text{g/mL}$ SP containing the above five concentrations of TABF were prepared respectively, and UV-Vis absorption spectra of each solution were measured. The UV-Vis absorption spectrum changes of mixed SP solution before and after adding VX caused by different concentrations of TABF were plotted respectively.

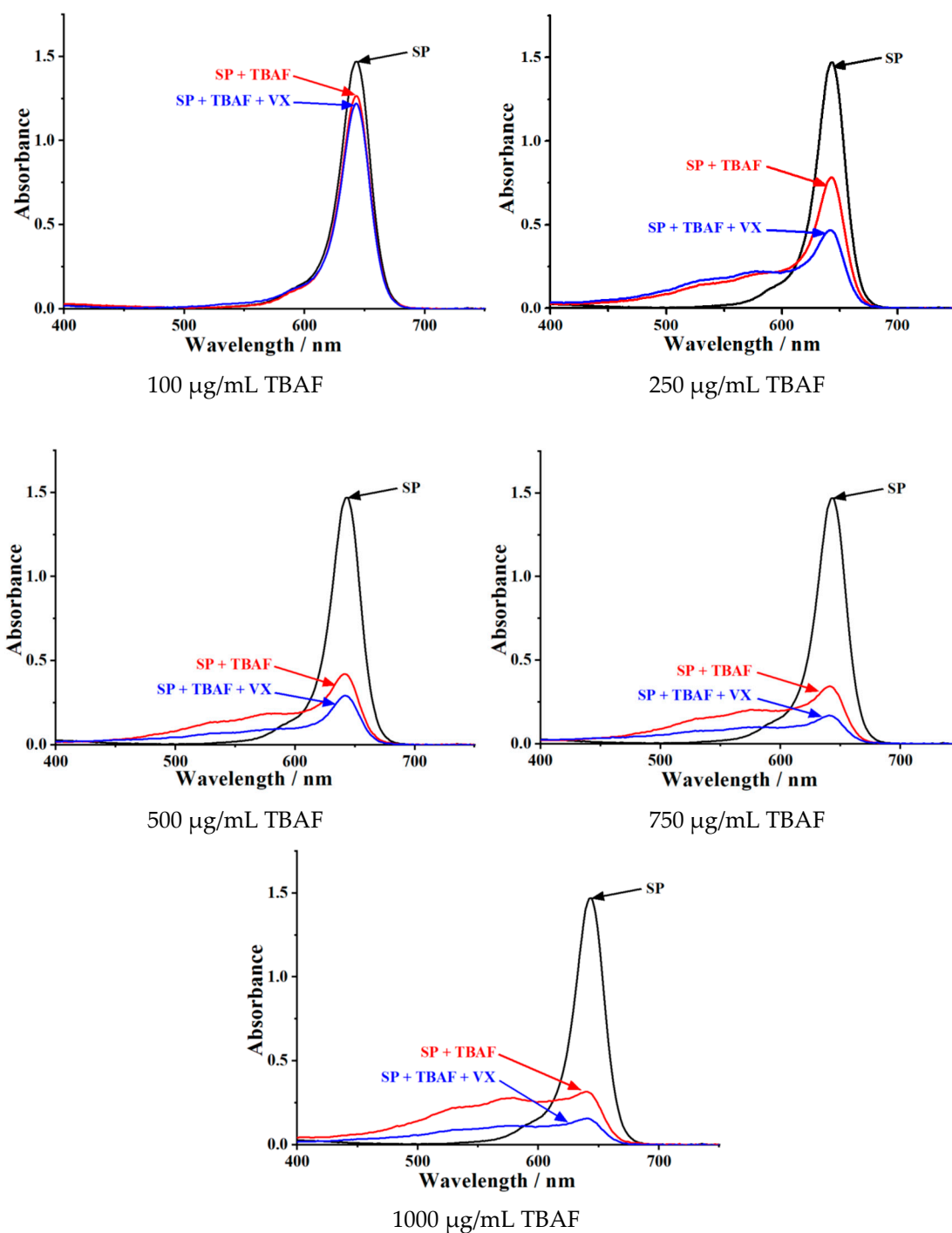


Figure S2. UV-Vis spectra changes of colorimetric solutions contained TABF of different concentrations.

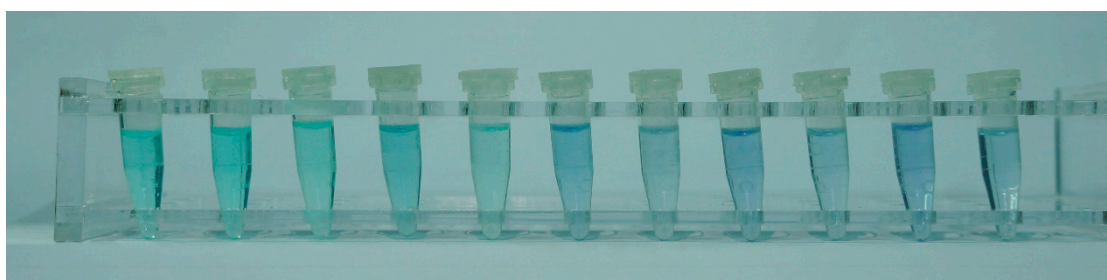


Figure S3. Color changes of colorimetric solutions. From left to right: 2 $\mu\text{g/mL}$ SP; 2 $\mu\text{g/mL}$ SP + 100 $\mu\text{g/mL}$ TBAF, 2 $\mu\text{g/mL}$ SP + 100 $\mu\text{g/mL}$ TBAF + 50 $\mu\text{g/mL}$ VX; 2 $\mu\text{g/mL}$ SP + 250 $\mu\text{g/mL}$ TBAF, 2 $\mu\text{g/mL}$ SP + 250 $\mu\text{g/mL}$ TBAF + 50 $\mu\text{g/mL}$ VX; 2 $\mu\text{g/mL}$ SP + 500 $\mu\text{g/mL}$ TBAF, 2 $\mu\text{g/mL}$ SP + 500 $\mu\text{g/mL}$ TBAF + 50 $\mu\text{g/mL}$ VX; 2 $\mu\text{g/mL}$ SP + 750 $\mu\text{g/mL}$ TBAF, 2 $\mu\text{g/mL}$ SP + 750 $\mu\text{g/mL}$ TBAF + 50 $\mu\text{g/mL}$ VX; 2 $\mu\text{g/mL}$ SP + 1000 $\mu\text{g/mL}$ TBAF, 2 $\mu\text{g/mL}$ SP + 1000 $\mu\text{g/mL}$ TBAF + 50 $\mu\text{g/mL}$ VX.

As can be seen from Fig. S2 above, after adding TBAF into CH_2Cl_2 solution of 2 $\mu\text{g/mL}$ SP, the absorption peak decreased significantly, and the absorbance value at 655nm gradually decreased with the increase of TBAF concentration, and the color of the solution changed from light green to light gray-blue and gradually to light purple. Meanwhile, the absorbance of the solution was further decreased by adding 50 $\mu\text{g/mL}$ VX in the presence of TBAF. The absorbance changes of the above 5 solutions containing different concentrations of TBAF at 655 nm were plotted as a table.

Table S1. Absorbance change of colorimetric solutions.

Concentration of TBAF	100 $\mu\text{g/mL}$	250 $\mu\text{g/mL}$	500 $\mu\text{g/mL}$	750 $\mu\text{g/mL}$	1000 $\mu\text{g/mL}$
Absorbance of SP solution mixed with TBAF	1.265	0.784	0.421	0.343	0.316
Absorbance of solutions mixed with VX and SP containing TBAF	1.221	0.385	0.292	0.169	0.157
Reduction rate of absorbance	3.48%	50.89%	30.64%	50.73%	50.32%

It can be seen from Table S1 that when the TBAF concentration in the colorimetric solution system was 250 $\mu\text{g/mL}$ 、500 $\mu\text{g/mL}$ 、750 $\mu\text{g/mL}$ 、1000 $\mu\text{g/mL}$, the absorbance of value solutions mixed with VX and SP containing TBAF could be reduced by more than 30%. But when the TBAF concentration was 750 $\mu\text{g/mL}$, it is difficult to distinguish the peak of the solution absorption spectra before and after adding VX. And it also can be found from Figure S3 that, it is difficult to distinguish the solution before and after adding VX when the TBAF concentration reached 500 $\mu\text{g/mL}$. What is more important, the absorbance of the colorimetric solution significantly reduced than that without TBAF, and the absorbance variation range was small, which was not conducive to highly sensitive colorimetric detection. Therefore, the concentration of TBAF in the colorimetric solution was determined to be 250 $\mu\text{g/mL}$. At this concentration of TBAF, the colorimetry not only has a large range of absorbance change, but also has a good rate of change in absorbance at the same target concentration.

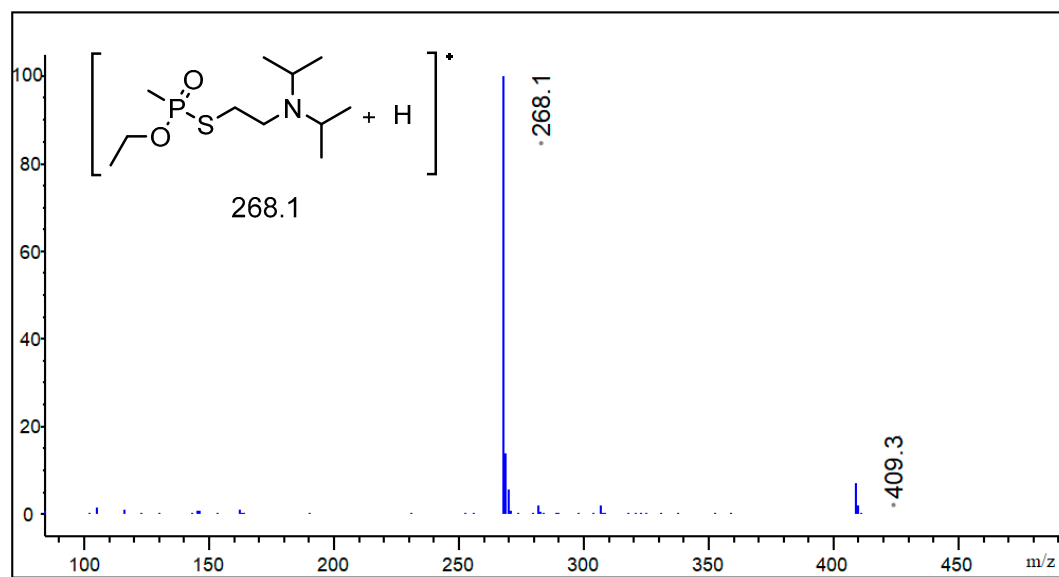


Figure S4. MS of the SP with VX, where the two positive ion peaks located at 268.1 and 409.3 are attributed to VX and SP respectively.