

Electronic Supplementary Information

A novel porphyrin-based near-infrared fluorescent probe for hypochlorite detection and its application *in vitro* and *in vivo*

Xiaoyi Wang^a, Jie Min^b, Weijie Wang^a, Yan Wang^a, Gui Yin^{a, c*} and Ruiyong Wang^{b*}

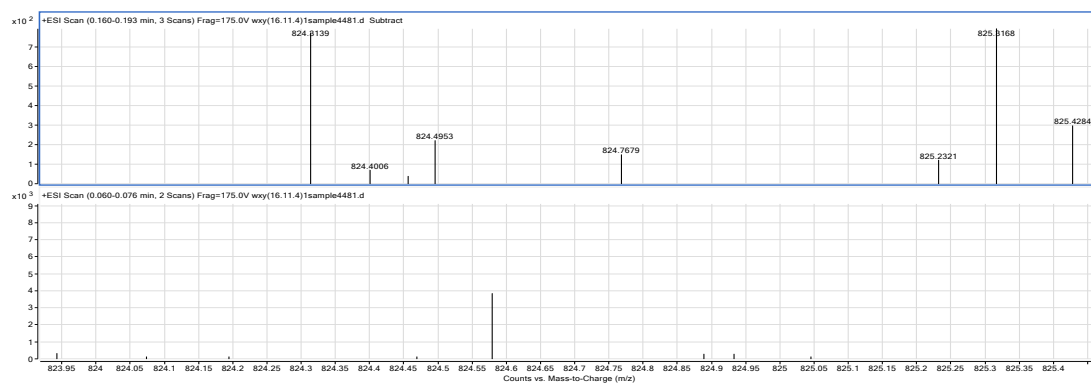
- a. State Key Laboratory of Analytical Chemistry for Life Science, School of Chemistry and Chemical Engineering, Nanjing University, Nanjing 210093, People's Republic of China. E-mail: yingui@nju.edu.cn.
- b. State Key Laboratory of Pharmaceutical Biotechnology, School of Life Science, Nanjing University, Nanjing, 210093, People's Republic of China. E-mail: wangry@nju.edu.cn.
- c. Jiangsu Key Laboratory of Advanced Organic Materials.

Corresponding author: Gui Yin, State Key Laboratory of Analytical Chemistry for Life Science, Jiangsu Key Laboratory of Advanced Organic Materials, School of Chemistry and Chemical Engineering, Nanjing University, Nanjing 210093, People's Republic of China. E-mail: yingui@nju.edu.cn.

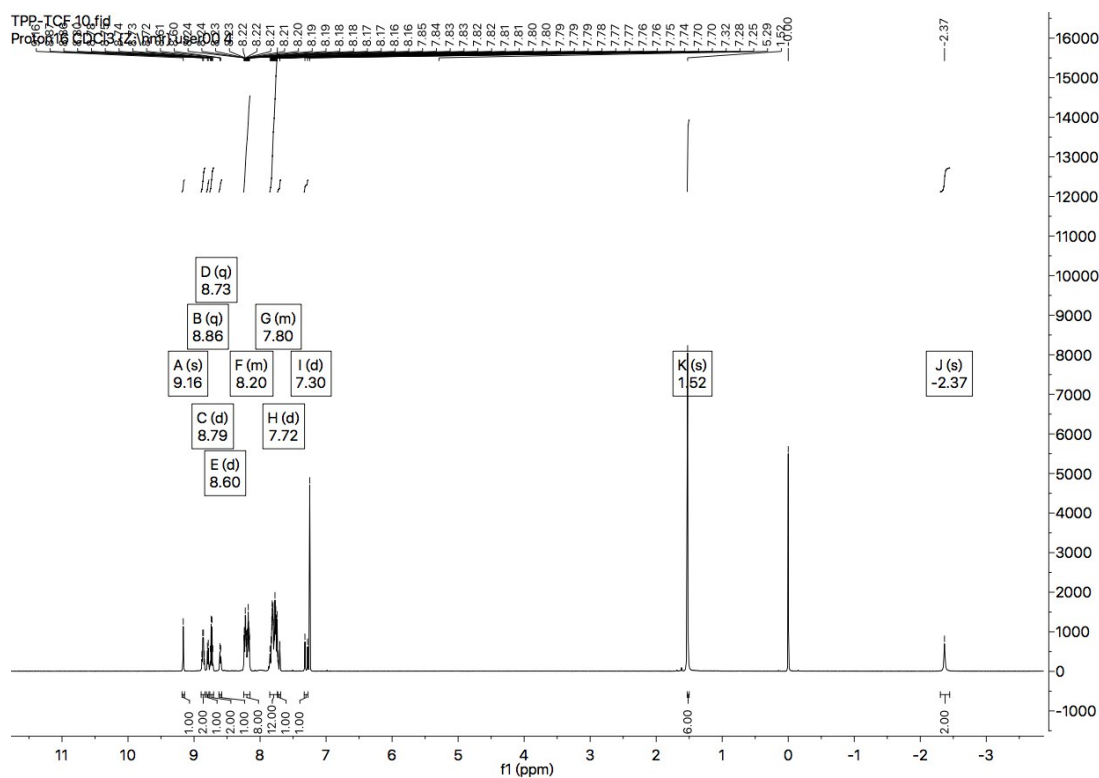
Table of Contents

- 1. NMR and MS spectra of TPP-TCF**
- 2. Anti-interfering ability of TPP-TCF**
- 3. Time-dependent plot of fluorescence intensity**
- 4. The photostability of TPP-TCF**
- 5. Calculation of quantum yield**
- 6. Concentration-dependent plot of fluorescence intensity**
- 7. The response curve of TPP-TCF towards NaClO**
- 8. The cytotoxicity of TPP-TCF**
- 9. HR-MS spectrum of TPP-TCF reacted with NaClO**

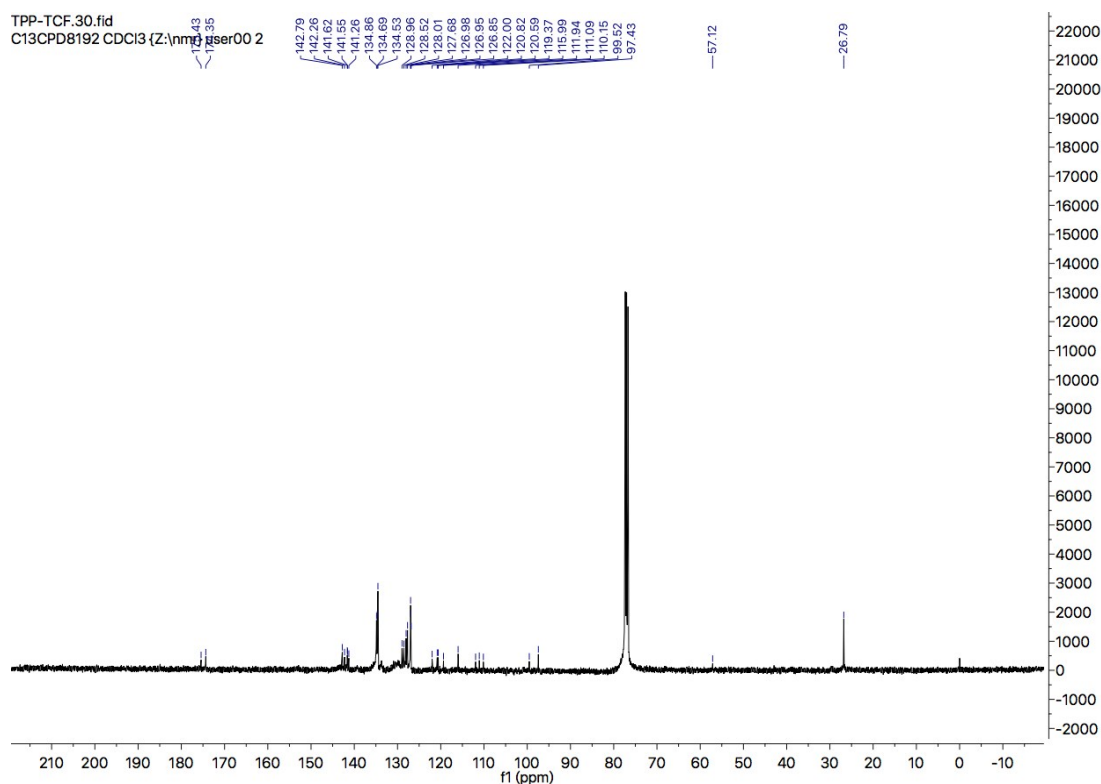
1. NMR and MS spectra of TPP-TCF (S1)



HR-MS spectrum of TPP-TCF



¹H NMR spectrum of TPP-TCF



^{13}C NMR spectrum of **TPP-TCF**

2. Anti-interfering ability of TPP-TCF

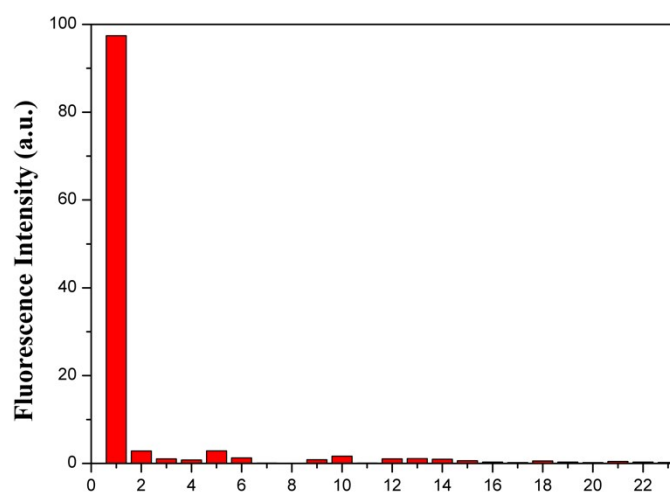


Fig. S2 Fluorescence intensity of **TPP-TCF** (10 μM) at 660 nm before and after addition of various cations and anions in PBS (pH 7.4, 10 mM, containing 20% DMSO). (1: ClO^- , 2: Ag^+ , 3: Fe^{3+} , 4: Fe^{2+} , 5: Cu^{2+} , 6: Zn^{2+} , 7: Co^{2+} , 8: Mn^{2+} , 9: Ni^{2+} , 10: Mg^{2+} , 11: Ca^{2+} , 12: Al^{3+} , 13: Na^+ , 14:

K^+ , 15: Cl^- , 16: Br^- , 17: I^- , 18: F^- , 19: NO_3^- , 20: NO_2^- , 21: SO_4^{2-} , 22: SCN^- , 23: $S_2O_3^{2-}$.
 $[ClO^-]=150\text{ }\mu\text{M}$, $[Ag^+]=[Fe^{3+}]=[Fe^{2+}]=[Cu^{2+}]=[Zn^{2+}]=[Co^{2+}]=[S^{2-}]=[Mn^{2+}]=[Ni^{2+}]=$
 $[Mg^{2+}]=[Ca^{2+}]=[Al^{3+}]=[Na^+]=[K^+]=[Cl^-]=[Br^-]=[I^-]=[F^-]=[NO_3^-]=[NO_2^-]=[SO_4^{2-}]$
 $= [SCN^-]=[S_2O_3^{2-}]=1\text{ mM}$

3. Time-dependent plot of fluorescence intensity

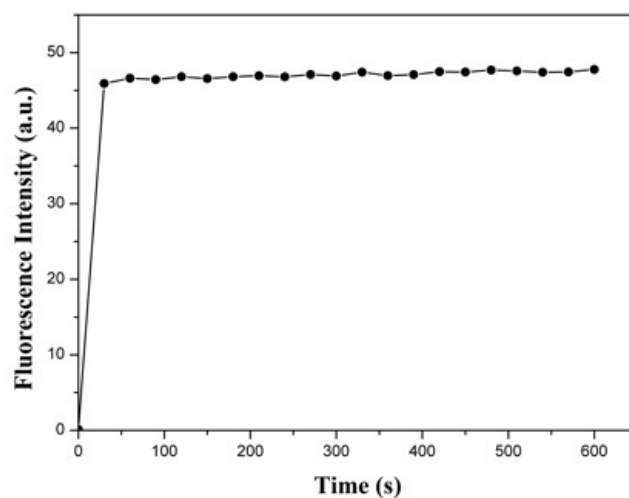


Fig. S3 Time-dependent plot of fluorescence intensity versus time for TPP-TCF (10 μM) upon addition of 100 μM NaClO in PBS (pH 7.4, 10 mM, containing 20% DMSO). $\lambda_{\text{ex}} = 488\text{ nm}$; $\lambda_{\text{em}} = 660\text{ nm}$.

4. The photostability of TPP-TCF

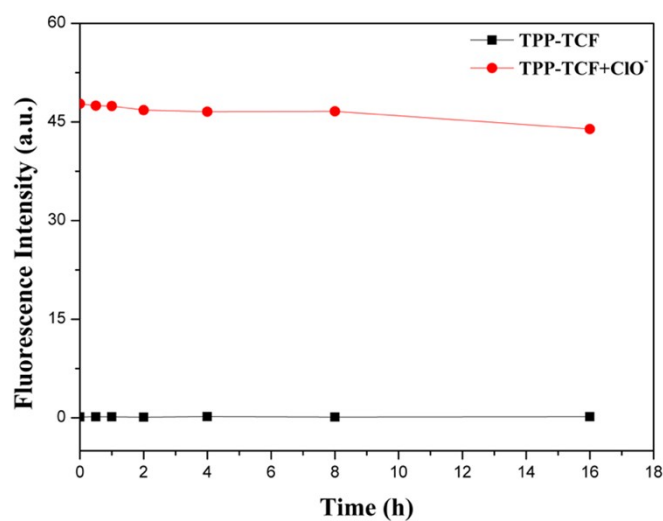


Fig. S4 Change in the fluorescence intensity of TPP-TCF (10 μ M) in the absence or presence of NaClO with light irradiation time at 488 nm. $\lambda_{\text{ex}} = 488$ nm; $\lambda_{\text{em}} = 660$ nm.

5. Calculation of quantum yield

The quantum yields of **TPP-TCF** was determined according to the equation [S1]:

$$\Phi_{\text{un}} = \Phi_{\text{ref}} \cdot \frac{\eta_{\text{un}}^2 \cdot A_{\text{ref}} \cdot OD_{\text{un}}}{\eta_{\text{ref}}^2 \cdot A_{\text{un}} \cdot OD_{\text{ref}}}$$

where A is the area under the fluorescence spectra curve and *OD* is the optical density of the compound at the excitation wavelength, 422 nm, η is the refractive index of the solvent used. The standard used for the measurement of the fluorescence quantum yield was TPP (0.11 in toluene).

6. Concentration-dependent plot of fluorescence intensity

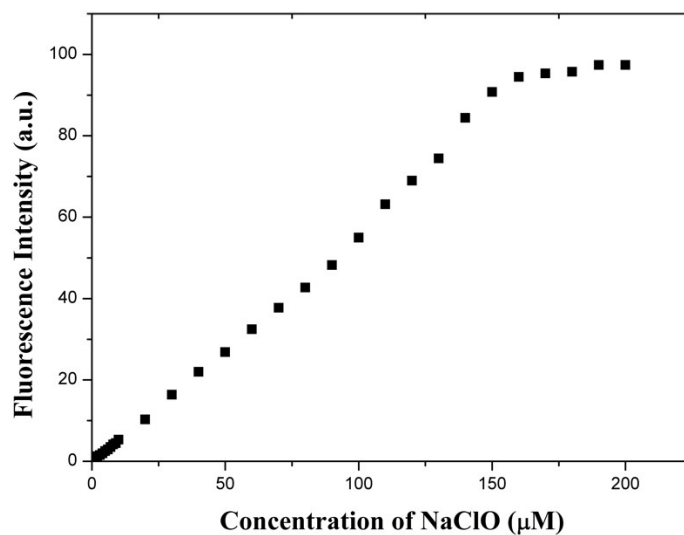


Fig. S6 Concentration-dependent plot of fluorescence intensity versus time for TPP-TCF (10 μM) upon addition of NaClO (0-200 μM) in PBS (pH 7.4, 10 mM, containing 20% DMSO). $\lambda_{\text{ex}} = 488$ nm; $\lambda_{\text{em}} = 660$ nm.

7. The response curve of TPP-TCF towards NaClO

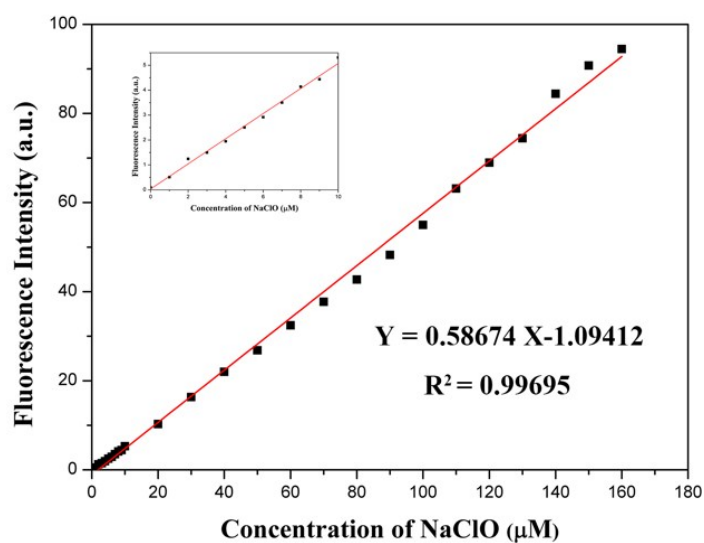


Fig. S7 The linear fitting of fluorescence intensity of TPP-TCF (10 μ M) towards concentrations of NaClO (0-160 μ M) in PBS (pH 7.4, 10 mM, containing 20% DMSO). λ_{ex} = 488 nm; λ_{em} = 660 nm.

8. The cytotoxicity of TPP-TCF

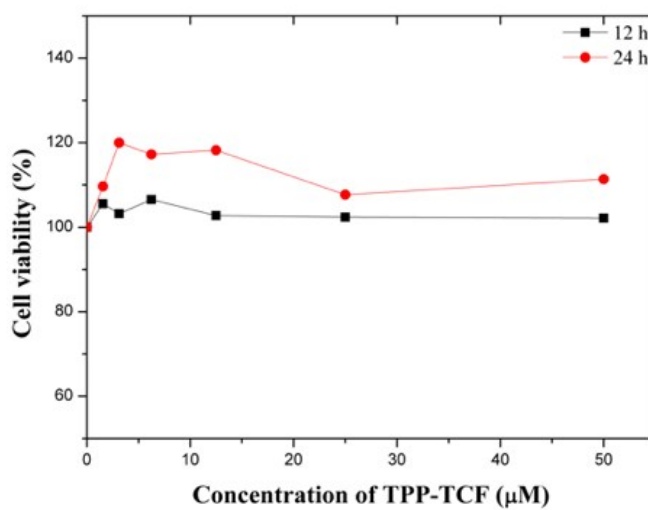


Fig. S8 Changes of cell viability influenced by TPP-TCF at different concentrations for 12 h and 24 h.

9. HR-MS spectrum of TPP-TCF reacted with NaClO

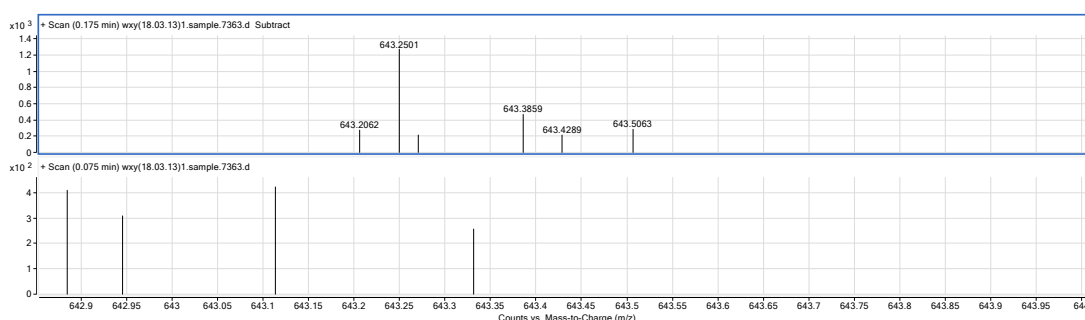


Fig. S9 HR-MS spectrum of the product of TPP-TCF reacted with NaClO.