A Highly Sensitive and Selective Fluorescent Probe for Hypochlorite in Pure Water with Aggregation Induced Emission Characteristics

Can Wang, Hongyu Ji, Mengshu Li, Likun Cai, Zhipeng Wang, Qianqian Li and Zhen Li*

* Department of Chemistry, Wuhan University, Wuhan 430072, China

* Corresponding authors: Prof. Zhen Li: lizhen@whu.edu.cn or lichemlab@163.com;

Table of Contents

1 Scheme S1. Synthetic route for TPE2B, TPE2OH, TPEB and TPEOH.

2 Figure S1. Fluorescence stability of TPE2B (black) and the fluorescence kinetic response to OCl⁻.

3 Figure S2. Fluorescence responses of TPE2B to OCl⁻ in the presence of other species.

4 Figure S3. Fluorescence changes of TPE2B by mixing TPE2B (0.1 mL, 1 mM) with 9.9 mL different concentrations of NaClO and the plot of fluorescence intensity versus OCl⁻ concentration (0-10 μM).

5 Figure S4. HPLC spectra of TPE2B, TPE2B incubated with NaClO and TPE2OH.

6 Figure S5. ¹H NMR spectra of TPEB, TPEOH and the product from the reaction of TPEB with NaClO.

7 Figure S6. IR spectra of TPEB, TPEOH and the product from the reaction of TPEB with NaClO.
Scheme S1. Synthetic route for TPE2B, TPE2OH, TPEB and TPEOH.

Figure S1. Fluorescence stability of TPE2B (black) and the fluorescence kinetic response to OCT (red) after the addition of NaClO in 100s (ex 323 nm, em 470 nm).
Fig S2 (a) Fluorescence spectra of TPE2B with 50.0 μM different species upon addition of 50.0 μM hypochlorite in an aqueous solution (containing 1% THF). (b) Fluorescence intensity changes of TPE2B with 50.0 μM different species upon addition of 50.0 μM hypochlorite at 470nm. Concentration: 10 μM. (c) The emission photos of TPE2B with 50.0 μM different species under 365 nm UV illumination.

Figure S3. (a) Fluorescence changes of TPE2B by mixing TPE2B (0.1 mL, 1 mM) with 9.9 mL different concentrations of NaClO. The concentration of OCl⁻ was 0, 2.0, 4.0, 6.0, 8.0, and 10.0 μM. (b) Plot of fluorescence intensity versus OCl⁻ concentration (0-10 μM).
Figure S4 HPLC spectra of TPE2B, TPE2B incubated with NaClO and TPE2OH. The mobile phase is methanol.

Figure S5 (a) $^1$H NMR spectra of TPEB. (b) $^1$H NMR spectra of the product after the reaction of TPEB with NaClO. (c) $^1$H NMR spectra of TPEOH. Solvent: CDCl$_3$. 
Figure S6. IR spectra of TPEB (black line), the product separated from TPEB under addition of 5 equiv. NaClO (red line) and TPEOH prepared by synthesis (blue line).