## **Supporting Information**

## A highly sensitive fluorescent sensor with aggregation induced emission characteristics for the detection of iodide and mercury ions in aqueous solution

Rui Xue Zhang, Peng Fei Li, Wen Juan Zhang, Nan Li\* and Na Zhao\*

Key Laboratory of Macromolecular Science of Shaanxi Province, School of Chemistry & Chemical Engineering, Shaanxi Normal University, Xi'an 710062, Shaanxi Province, PR

China.

 Table S1 Crystallographic data for TPE-QN.

| Compound                              | TPE-QN              |
|---------------------------------------|---------------------|
| Empirical formula                     | $C_{38}H_{30}NF_6P$ |
| Formula weight                        | 645.60              |
| Crystal system                        | triclinic           |
| Space group                           | P -1                |
| <i>a</i> [Å]                          | 9.4059 (4)          |
| <i>b</i> [Å]                          | 11.4024 (5)         |
| <i>c</i> [Å]                          | 15.4542 (5)         |
| α [ <sup>o</sup> ]                    | 94.338 (3)          |
| β [°]                                 | 105.333 (3)         |
| γ [°]                                 | 92.789 (3)          |
| V [Å <sup>3</sup> ]                   | 1589.81 (11)        |
| Ζ                                     | 2                   |
| <i>T</i> [K]                          | 293                 |
| $D_{\text{calcd}} [\text{g cm}^{-3}]$ | 1.349               |
| $m [{ m mm}^{-1}]$                    | 1.318               |
| <i>q</i> range [ <sup>o</sup> ]       | 7.796-144.394       |
| Total no. reflections                 | 24030               |
| <b>R</b> <sub>1</sub>                 | 0.1202              |
| $wR_2$                                | 0.4019              |
| GOOF                                  | 1.833               |
|                                       |                     |



Fig. S1 ORTEP drawing of TPE-QN omitted with counter anion.



Fig. S2 The UV-vis absorption spectra of (A) TPE-QN (10  $\mu$ M) and (B) TPE-QI (10  $\mu$ M) in DMSO.



**Fig. S3** (A) The emission spectra of TPE-QN (10  $\mu$ M) in aqueous solution (with 1% DMSO) with time in the presence of I<sup>-</sup>(200  $\mu$ M). (B) Plot of *I*/*I*<sub>0</sub> at 610 nm versus the time (0–13 min). Excitation wavelength: 435 nm.



**Fig. S4** (A) Emission spectra of TPE-QN (10  $\mu$ M) in aqueous solution (with 1% DMSO) in the presence of different anions (200  $\mu$ M). (B) Emission spectra obtained by addition of 200  $\mu$ M of I<sup>-</sup> into the solutions in (A). Excitation wavelength: 435 nm.



**Fig. S5** (A) Emission spectra of TPE-QI (10  $\mu$ M) in DMSO and DMSO/water mixtures with different water fractions ( $f_w$ ). (B) Plots of relative emission intensity ( $I/I_0$ ) at 510 nm versus the composition of water in mixtures. Excitation wavelength: 360 nm.



**Fig. S6** (A) Emission spectra of TPEBe-PF<sub>6</sub> (10  $\mu$ M) in aqueous solution (with 1% DMSO) with different concentrations of I<sup>-</sup> (0–4.0 mM). (B) Plot of  $I_0/I$ -1 at 614 nm versus the concentration of I<sup>-</sup> (0–4.0 mM).  $I_0$  = emission intensity of TPE-QN without I<sup>-</sup>. Excitation wavelength: 420 nm.



**Fig. S7** (A) The emission spectra of TPE-QN-I (10  $\mu$ M) in aqueous solution (with 1% DMSO) with time in the presence of Hg<sup>2+</sup> (150  $\mu$ M). (B) Plot of *I*/*I*<sub>0</sub> at 610 nm versus the time (0–13 min). Excitation wavelength: 435 nm.



**Fig. S8** (A) The emission spectra of TPE-QN-I (10  $\mu$ M) in aqueous solution (with 1% DMSO) with different metal ions (150  $\mu$ M). (B) The emission spectra were obtained by addition of 150  $\mu$ M of Hg<sup>2+</sup> into the solutions in (A). Excitation wavelength: 435 nm.



**Fig. S9** (A) Emission spectra of TPE-QN (10  $\mu$ M) in buffer solution (pH 7.2, 20 mm HEPES buffer with 1% DMSO) with different concentrations of I<sup>-</sup> (0–20  $\mu$ M). (B) Plot of emission intensity at 610 nm versus the concentration of Hg<sup>2+</sup> (0.01–6.0  $\mu$ M). Excitation wavelength: 435 nm.



**Fig. S10** (A) Emission spectra of TPE-QN-I (10  $\mu$ M) in buffer solutions (pH 7.2, 20 mM HEPES buffer with 1% DMSO) with different concentrations of Hg<sup>2+</sup> (0–1000  $\mu$ M). (B) Plot of emission intensity at 610 nm versus the concentration of Hg<sup>2+</sup> (0.5–4.0  $\mu$ M). Excitation wavelength: 435 nm.



Fig. S11 Change in the emission intensity of TPE-QN at 610 nm in buffer solution (10  $\mu$ M), following addition of I<sup>-</sup> (20  $\mu$ M) and Hg<sup>2+</sup> (1000  $\mu$ M) with different pH. Excitation wavelength: 435 nm.







