Electronic Supplementary Information for

Phenothiazine and semi-cyanine based colorimetric and fluorescent probes for detection of sulfites in solutions and in living cells

Hong-Wei Chen, Hong-Cheng Xia*, O. A. Hakeim, Qin-Hua Song*

Department of Chemistry, University of Science and Technology of China, Hefei 230026, China.

Table of Contents

Table of Contents

I. Photophysical and sensing properties of four probes .................................................................S2
II. Spectral response of probes to HSO$_3^-$/SO$_3^{2-}$ ..................................................................S2
III Mass spectra of PI-CN without and with NaHSO$_3$ ...............................................................S3
IV. Measurement of detection limits ......................................................................................... S4
V. pH effects on optical response of PI-CN to HSO$_3^-$/SO$_3^{2-}$ ..................................................S5
VI. NMR spectra of related compounds .......................................................................................S6-S11

* Corresponding author. E-mail address: qhsong@ustc.edu (Q.-H. Song)
* Corresponding author. E-mail address: xiahc@mail.ustc.edu.cn (H.-C. Xia)
I. Photophysical and sensing properties of four probes

Table S1. Photophysical and sensing properties of four probes

| probe | $\lambda_{\text{abs}}$ /nm | $\varepsilon$ (L·mol$^{-1}$·cm$^{-1}$) | $\lambda_{\text{em}}$ /nm | LOD |
|-------|----------------|----------------|----------------|-----|
| PI-CN | 518           | 30320          | 499            | 22 nM |
| PI-Br | 537           | 28320          | 452            | 28 nM |
| PI-H  | 545           | 29180          | 455            | 27 nM |
| PI-OH | 568           | 25846          | 470            | 37 nM |

* absorption maxima (nm) and molar absorption coefficients

* emission maxima (nm)

II. Spectral response of probes to HSO$_3^-$/SO$_3^{2-}$

Fig. S1 Time-dependent UV/vis absorption (left) and fluorescence spectra (right) of probes (15 μM) in EtOH/PBS (v/v1:3, pH 7.4) in the presence of HSO$_3^-$ (1.0 equiv.) recorded at 0-30 min, excitation at 320 nm. Inset of PI-OH: plots of absorption maxima of probes vs time in the presence of HSO$_3^-$ incubation for 15 min
III. Mass spectra of PI-CN without and with NaHSO$_3$

**Fig. S2** High-resolution MS of probe PI-CN (upper) and the mixture of PI-CN+NaHSO$_3$ (bottom).
IV. Measurements of detection limits

**Figure S3.** UV/vis absorption PI-CN (a), PI-Br (b), PI-H (c) and PI-OH (d) in EtOH/PBS (v/v1:3, pH 7.4) with titration of various amounts of HSO$_3^-$ (0–15 μM), and the corresponding linear correlation between the absorbance toward concentrations of HSO$_3^-$. 
V. pH effects on optical response of PI-CN to HSO$_3^-$/$SO_3^{2-}$

![Figure S4a. Plots of absorbance at 520 nm to pH values for 15μM PI-CN solutions (EtOH/PBS v/v 1:3) before (black) and after (red) the addition of 15 μM HSO$_3^-$.

![Figure S4b. Plots of fluorescence intensity at 499 nm to pH values for 15μM PI-CN solutions (EtOH/PBS v/v 1:3) before and after the addition of 15 μM HSO$_3^-$.

55
IV. NMR spectra of related compounds

$^1$H NMR of compound 3.

$^{13}$C NMR of compound 3.
$^1$H NMR of compound 4.

$^{13}$C NMR of compound 4.
\(^1\)H NMR of compound 5.

\(^{13}\)C NMR of compound 5.
$^1$H NMR of PI-CN.

$^{13}$C NMR of PI-CN.
$^1$H NMR of PI-Br.

$^{13}$C NMR of PI-Br.
$^1$H NMR of PI-H.

$^{13}$C NMR of PI-H.
$^1$H NMR of PI-OH.

$^{13}$C NMR of PI-OH