Electronic Supplementary Information for

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

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I. Photophysical and sensing properties of four probes

Table S1. Photophysical and sensing properties of four probes

<table>
<thead>
<tr>
<th>probe</th>
<th>( \lambda_{\text{abs}}^{c} )/nm</th>
<th>((\epsilon)/(\text{L} \cdot \text{mol}^{-1} \cdot \text{cm}^{-1})^{c} )</th>
<th>( \lambda_{\text{em}}^{b} )/nm</th>
<th>LOD</th>
</tr>
</thead>
<tbody>
<tr>
<td>PI-CN</td>
<td>518</td>
<td>30320</td>
<td>499</td>
<td>22 nM</td>
</tr>
<tr>
<td>PI-Br</td>
<td>537</td>
<td>28320</td>
<td>452</td>
<td>28 nM</td>
</tr>
<tr>
<td>PI-H</td>
<td>545</td>
<td>29180</td>
<td>455</td>
<td>27 nM</td>
</tr>
<tr>
<td>PI-OH</td>
<td>568</td>
<td>25846</td>
<td>470</td>
<td>37 nM</td>
</tr>
</tbody>
</table>

\(^{c}\) absorption maxima (nm) and molar absorption coefficients

\(^{b}\) 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 \(\mu\)M) 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 NaHSO₃

![Mass spectra image](image1)

$m/z$ calcd for $C_{31}H_{32}N_3S$: 478.2317 ([M]⁺)

![Mass spectra image](image2)

$m/z$ calcd for $C_{31}H_{32}N_3NaO_3S_2$: 582.1861 ([M+NaHSO₃]⁺)

**Fig. S2** High-resolution MS of probe PI-CN (upper) and the mixture of PI-CN+NaHSO₃ (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/v:1:3, 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$_3^-$/$\text{SO}_3^{2-}$

**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$_3^-$.
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.

(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