A visible-near-infrared fluorescent probe for peroxynitrite with large Pseudo-Stokes and emission shift via through-bond energy and charge transfers controlled by energy matching

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Calculation of fluorescence quantum yield

Fluorescence quantum yields of probe Py-PhB and its sensing product were determined using quinine ($\phi=0.54$) for 415 nm or rhodamine ($\phi=0.68$) for 598 nm in the water as standard and it calculated by equation (1) as reported. \[^{[S1]}\]

$$\phi_L = \frac{F_L}{F_Q} \times \frac{(1 - 10^{-A_L})}{(1 - 10^{-A_Q})} \times \frac{\eta_Q^2}{\eta_Q^2} \times \phi_Q \quad (1)$$

where the subscripts L and Q respectively refer to the sample and the reference, F is the integrated fluorescence intensity under fluorescence emission spectrum, A is the absorbance at the excitation wavelength and $\eta$ is the refractive index of the solvent.

Figure S1. Fluorescence spectra of probe **Ph-PyB** (10 μM) with ONOO\(^-\) or ClO\(^-\) (55 μM) in (a) DMSO, (b) DMSO - PBS (5:5, v/v, pH=7.4) and (c) DMSO-PBS (7:3, v/v, pH=7.4).

Figure S2. The colour changes of **Py-PhB** (10μM) before and after adding different ions (55 μM for ONOO\(^-\) and ClO\(^-\), 250 μM for others).
Figure S3. The fluorescent colour changes Py-PhB (10μM) before and after adding different ions (55 μM for ONOO⁻ and ClO⁻, 250 μM for others) under 365 nm UV light.

Figure S4. Fluorescence emission spectra of Py-PhB (10μM) with some common metal ions in organisms as well as biothiols (250 μM).
Figure S5. HPLC of probe **Py-PhB** with different concentrations of ONOO$^-$. 
Figure S6. HRMS of probe Py-PhB before (a) and after (b) sensing ONOO$^-$

Figure S7. Cell viability incultured with Py-PhB in the presence of different concentrations of ONOO$^-$ at 37°C for 24 h
Figure S8. $^1$H NMR of probe Py-PhB

Figure S9. $^{13}$C NMR of probe Py-PhB