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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 (ϕ=0.54) for 415 nm or rhodamine (ϕ=0.68) for 598 nm in the water as standard and it calculated by equation (1) as reported. [S1]

$$\Phi_L = \frac{F_L}{F_Q} \times \frac{(1 - 10^{-A_L})}{(1 - 10^{-A_Q})} \times \frac{\eta_L^2}{\eta_Q^2} \times \Phi_Q \qquad (1)$$

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 η is the refractive index of the solvent.

S1. Abeywickrama, C. S.，Wijesinghe, K. J.，Stahelin, R. V.; Pang, Y. *Chem. Commun. (Camb)* **2017**, *53*, 5886-5889

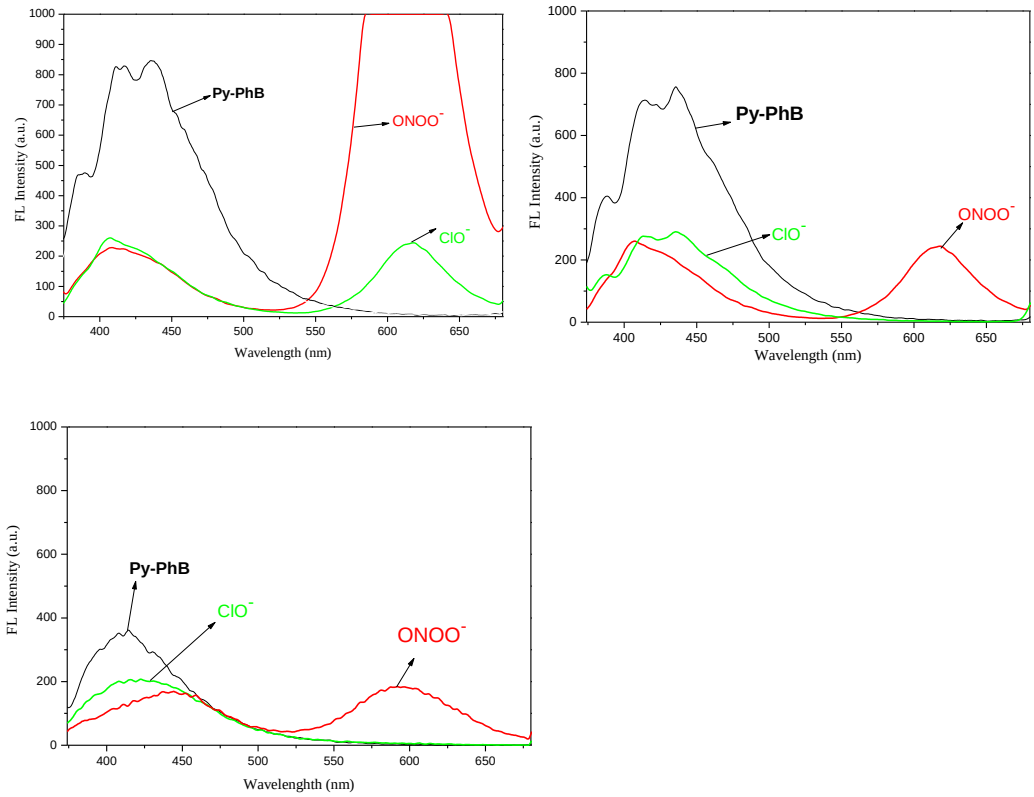

Figure S1**.** Fluorescence spectra of probe **Ph-PyB** (10 μM) with $ONOO^-$ or ClO^- (55 μM) in (a) DMSO, (b) DMSO -PBS (5:5, v/v, pH=7.4) and (c) DMSO-PBS (7:3, v/v, pH=7.4).

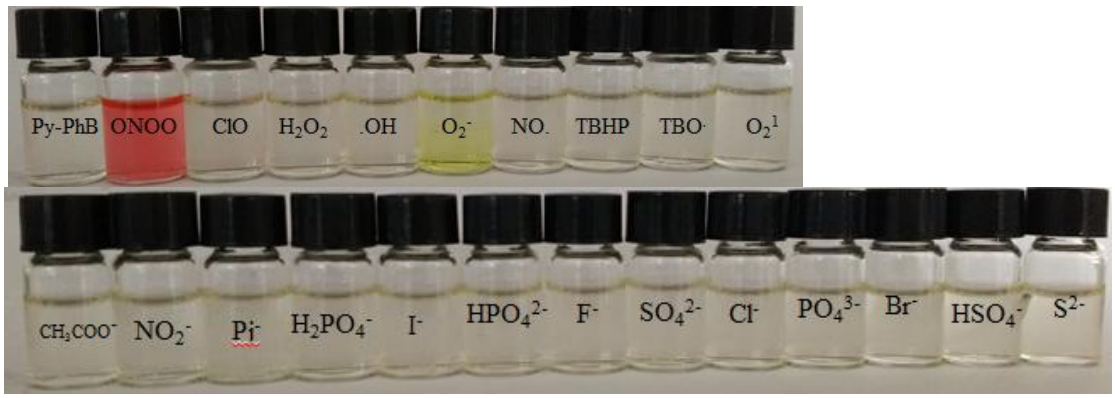

Figure S2. The colour changes of **Py-PhB** (10μM) before and after adding different ions (55 μM for $ONOO^-$ and ClO^-, 250 μM for others).

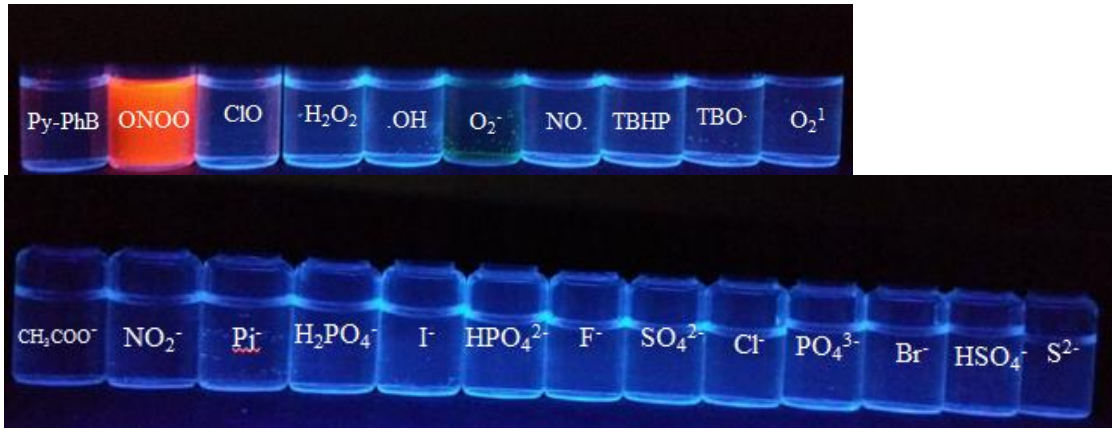

Figure S3. The fluorescent colour changes **Py-PhB** (10μM) before and after adding different ions (55 μM for $ONOO^-$ and ClO^-, 250 μM for others) under 365 nm UV light.

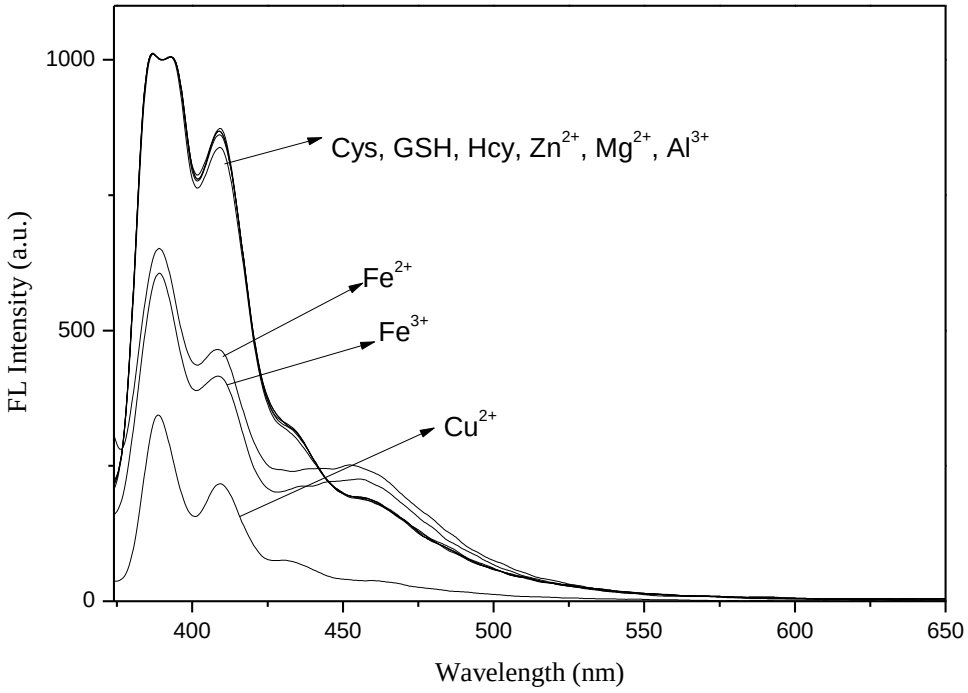

Figure S4. Fluorescence emission spectra of **Py-PhB** (10μM) with some common metal ions in organisms as well as biothiols (250 μM).

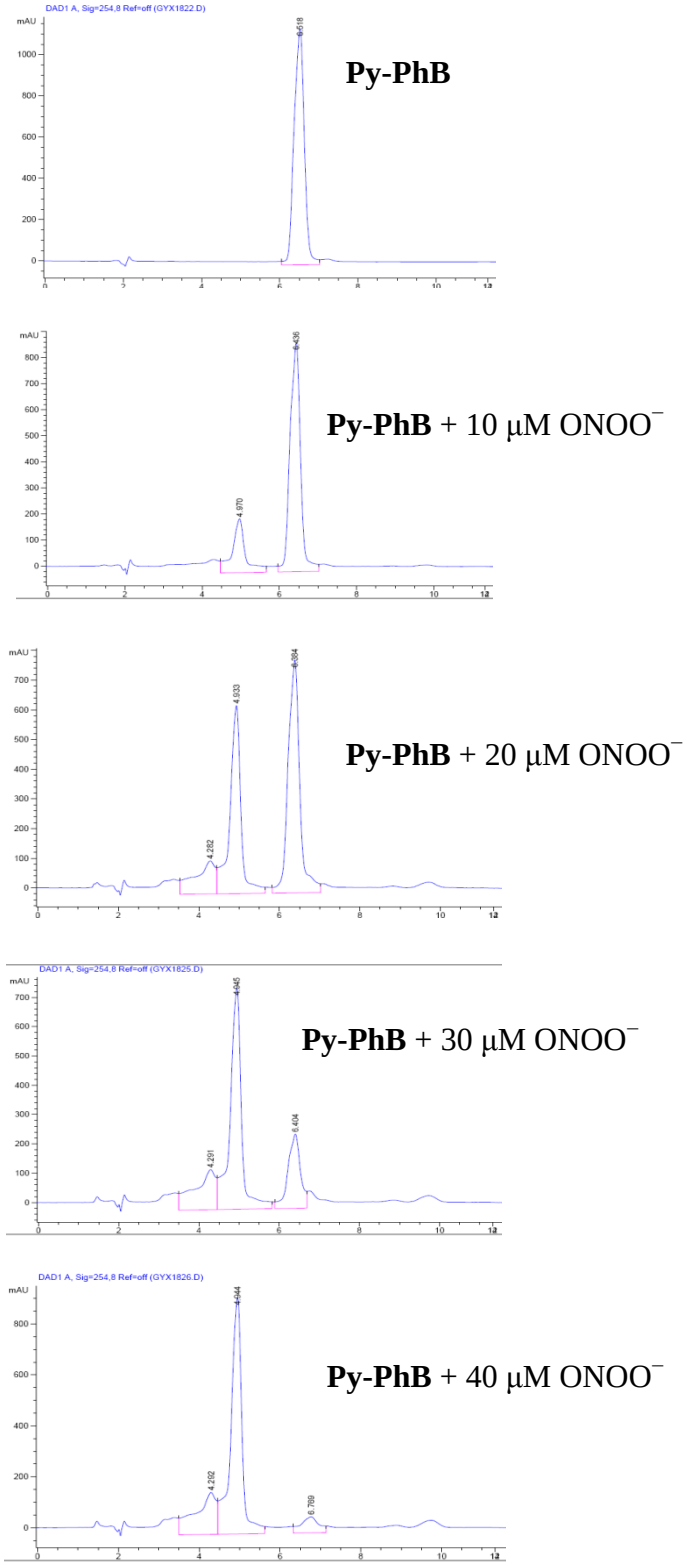

Figure S5. HPLC of probe **Py-PhB** with different concentrations of $ONOO^-$

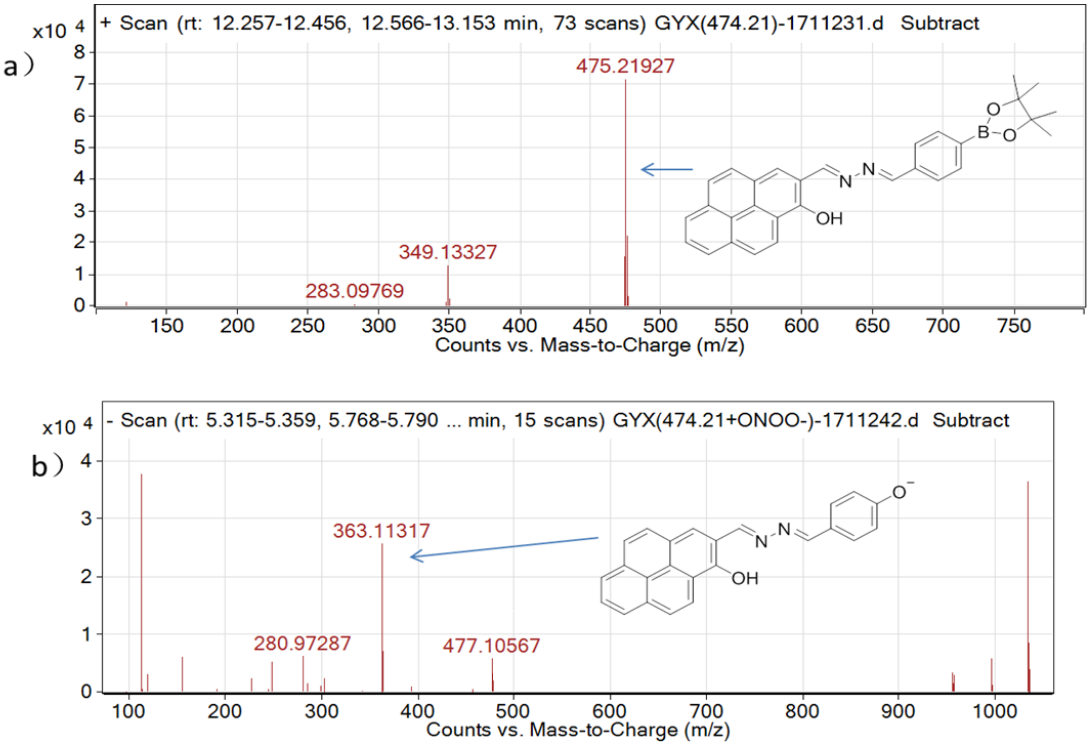

Figure S6. HRMS of probe **Py-PhB** before (a) and after (b) sensing $ONOO^-$

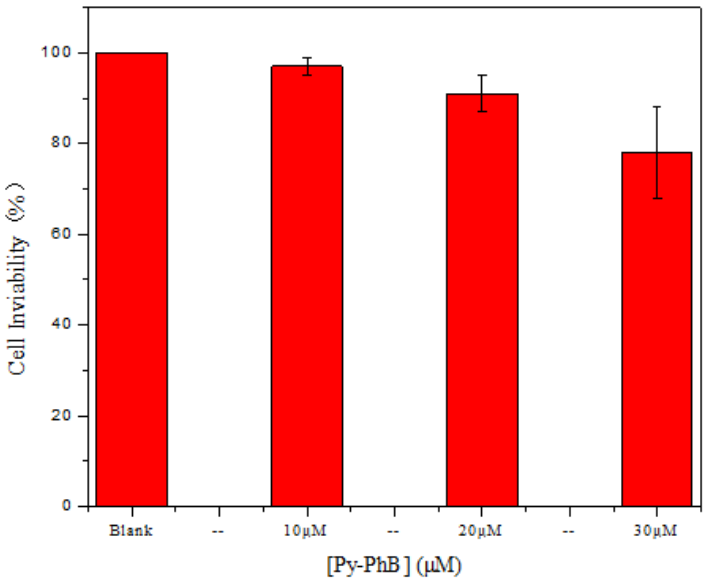

Figure S7. Cell viability incultured with **Py-PhB** in the presence of different concentrations of $ONOO^-$ at 37˚C for 24 h

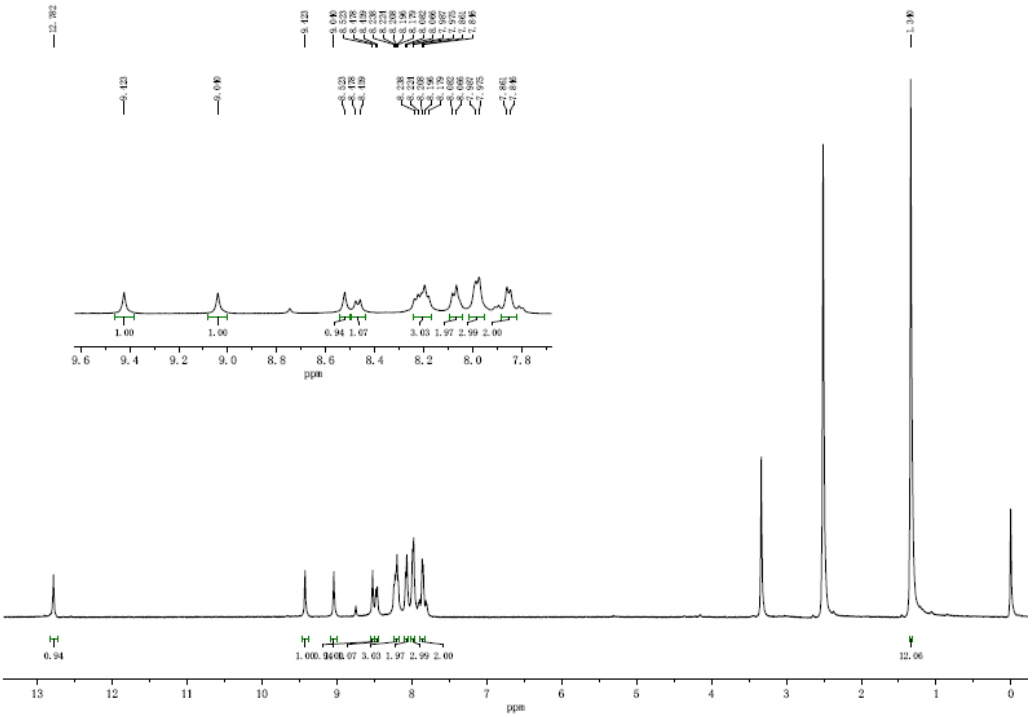

Figure S8. ^{1}H NMR of probe **Py-PhB**

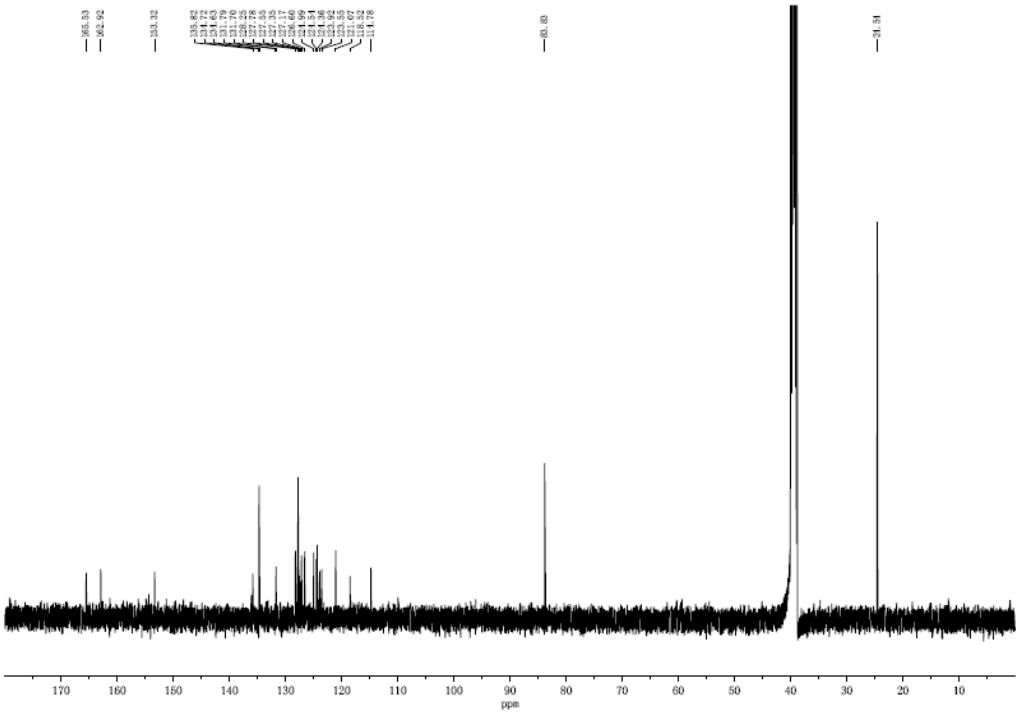

Figure S9. ^{13}C NMR of probe **Py-PhB**