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Supporting information for

Sensing and Imaging of PPi *in vivo* using Lanthanide-based Second Near-infrared Luminescent Probes

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Fig. S1 The TEM images of (a) NaGdF₄:Nd and (b) NaGdF₄:Nd@NaGdF₄. (c) The size distribution of NaGdF₄:Nd and NaGdF₄:Nd@NaGdF₄ measured by the DLS method.



Fig. S2 Dynamic light scattering measurements of DCNPs, TA-DCNPs and TA/Fe³⁺-DCNPs.



Fig. S3 The ξ -potentials of DCNP, TA-DCNPs, TA/ Fe³⁺-DCNPs.



Fig. S4 The FI-IR spectra of DCNPs, TA, TA-DCNPs and TA/Fe³⁺-DCNPs.



Fig. S5 (a) Plot of luminescence intensity at 1058 nm against the different mass ratio of TA:DCNPs (b) Plot of luminescence intensity at 1058 nm against the Fe^{3+} concentration (n = 5). The line joining the data points are the guide to the eye only.



Fig. S6 The UV–vis spectra of TA-DCNPs at different concentration of Fe³⁺.



Fig. S7 The luminescence spectra of TA-DCNPs ($0.2 \text{ mg} \cdot \text{mL}^{-1}$) with different ions in PBS buffer (pH=7.2).



Fig. S8 The (a) pictures and (b) NIR-II spectra of TA-DCNPs+ Cu^{2+} in PBS buffer with different pH values. The concentration of Cu^{2+} was 2 mM.



Fig. S9 The luminescence spectra of DCNPs, TA-DCNPs, TA/ Fe³⁺-DCNPs and TA/ Fe³⁺-DCNPs + PPi (2 mM). Excitation wavelength: 808 nm.



Fig. S10 The variation of the luminescence intensity of the TA/Fe³⁺-DCNPs and TA/Fe³⁺-DCNPs + PPi after 1-7 h.



Fig. S11 The luminescence intensity of TA/Fe³⁺-DCNPs and luminescence TA/Fe³⁺-DCNPs response to PPi in different pH environments (HEPES).



Fig. S12 The luminescence responses of TA/Fe³⁺-DCNPs (0.2 mg \cdot mL⁻¹) in the presence of AMP, ADP and ATP (1 mM).



Fig. S13 (a) The luminescence responses of TA/Fe³⁺-DCNPs ($0.2 \text{ mg} \cdot \text{mL}^{-1}$) in the presence of several amino acids (1 mM). (b) The interference assay of the luminescence of TA/Fe³⁺-DCNPs with PPi in the presence of several amino acids.



Fig. S14 (a) The DLS measurements of TA/ Fe³⁺-DCNPs and TA/Fe³⁺- DCNPs + PPi. The TEM images of TA/ Fe³⁺-DCNPs (b) and TA/Fe³⁺- DCNPs + PPi (c).



Fig. S15 Z-potential of TA/ Fe³⁺-DCNPs and TA/ Fe³⁺-DCNPs + PPi.



Fig. S16 (a) The UV–vis spectra of TA/ Fe^{3+} -DCNPs at different concentration of PPi. (b) The photos of TA/ Fe^{3+} -DCNPs before and after added PPi.



Fig. S17 (a) *In vivo* luminescence images of the mice at different times after gastric lavage of TA/ Fe³⁺-DCNPs and PPi. (b) H&E images of organs from mice treated with PBS or TA/Fe³⁺-DCNPs + PPi (0.25 mg·kg⁻¹), scale bars are 20 μ m.