Electronic Supplementary Material

Polyvinylpyrrolidone and 4-mercaptobenzoic acid-

functionalized nickel nanoclusters for selective and sensitive

detection of glutathione-assisted by Fe³⁺

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Instrumentation

Fluorescent intensity measurements were conducted using Shimadzu RF-5301 PC (Tokyo, Japan). UV-Vis absorbance readings were performed using the Shimadzu 1601 PC (Tokyo, Japan). X-ray photoelectron spectroscopy (XPS) spectra were obtained using the Thermo EscalAB 250Xi instrument (Thermoelectric Corporation, USA). Fourier transform infrared (FT-IR) spectra were acquired using the NicoletTM iSTM10 spectrograph (Varian Instrument Co., Ltd, USA). Dynamic light scattering (DLS) and zeta potential measurements were recorded using the ZEN 3600 Nano ZS model (Malvern, UK). Transmission electron microscope (TEM, JEOL, JEM-100CX II-unit, USA) was used to characterize PVP/4-MBA@Ni NCs. The X-ray diffraction spectrometer PW 1710 (XRD, Philips-FEI, Netherlands) was utilized to investigate the peak diffractions of PVP/4-MBA@Ni NCs.

Fluorescence quantum yield measurements of PVP/4-MBA@Ni NCs (X)

The quantum yield (QY) values were calculated using the following equation, with quinine sulfate (QS) as a reference in 0.1 mol/L H₂SO₄ (QY = 54%). The absorbance (kept below 0.05) and emission spectra of a given concentration of PVP/4-MBA@Ni NCs and QS were measured at the same excitation wavelength (360 nm). The absorbance and fluorescence integral areas were then substituted into the formula below:

$$\phi_X = \phi_{QS} \times \frac{F_X}{F_{QS}} \times \frac{A_{QS}}{A_X} \times \frac{\eta_X}{\eta_{QS}}$$

 Φ_X represents the quantum yield of PVP/4-MBA@Ni NCs, ϕ_{QS} represents the quantum yield of QS, F_X is the fluorescence intensity of PVP/4-MBA@Ni NCs, F_{QS} is the fluorescence intensity of QS, A refers to the absorbance value and η refers to the refractive index of the solvent (distilled water). The synthesized PVP/4-MBA@Ni NCs were dissolved in distilled water ($\eta = 1.33$) and QS was dissolved in 0.1 M H₂SO₄ ($\eta = 1.33$).



Fig.S1 Elemental mapping of PVP/4-MBA@Ni NCs showing (A) carbon, (B) oxygen, (C) nitrogen, (D) sulfur, and (E) nickel.



Fig.S2 FTIR spectra of 4-MBA (a), PVP (b), and PVP/4-MBA@Ni NCs (c).



Fig.S3 Stability pattern of PVP/4-MBA@Ni NCs under different NaCl concentrations (A), irradiation times (B), pH values (C), and temperature values (D).



Fig.4 Influence of synthesis conditions for fabrication of PVP/4-MBA@Ni NCs: (A) Fabrication temperature, (B) Fabrication time, (C) dose of PVP (grams), and (D) dose of 4-MBA (mg).



Fig.S5 Influence of (A) PVP/4-MBA@Ni NCs' volumes; (B) metal type (7.5 μ M) on the quenching of fluorescent probe; (C) different amounts of Fe³⁺ on the quenching of the fluorescent probe; (D) effect of pH values; (E) reaction time between PVP/4-MBA@Ni NCs and Fe³⁺ ion; (F) reaction time between PVP/4-MBA@Ni NCs and Fe³⁺ ion; (F) reaction time between PVP/4-MBA@Ni NCs/Fe³⁺ and GSH.



Fig.S6 TEM image (A) and DLS (B) of PVP/4-MBA@Ni NCs after addition of 7.5 μ M Fe³⁺; TEM image (C) and DLS (D) of PVP/4-MBA@Ni NCs / Fe³⁺ after addition of 12.5 μ M GSH.



Fig.S7 (A) UV/VIS absorption spectrum of Fe³⁺ (7.5 μ M) and excitation spectrum of PVP/4-MBA@Ni NCs; (B) Fluorescence lifetimes of PVP/4-MBA@Ni NCs, PVP/4-MBA@Ni NCs / 7.5 μ M Fe³⁺, and PVP/4-MBA@Ni NCs /Fe³⁺/12.5 μ M GSH; (C) Zeta potentials of PVP/4-MBA@Ni NCs, PVP/4-MBA@Ni NCs / 7.5 μ M Fe³⁺, and PVP/4-MBA@Ni NCs /Fe³⁺/12.5 μ M GSH.



Fig.S8 FT-IR spectra of GSH (a) and GSH-Fe³⁺ coordination complex (b).