Supporting Information

Ultra-selective Detection of Fe²⁺ ion by Redox Mechanism Based

on Fluorescent Polymerized Dopamine Derivatives

Taeuk An^{1‡}, Namhun Lee^{1‡}, Hong-Jun Cho², Seongsoo Kim¹, Dong-Sik Shin^{3*}, Sang-Myung Lee^{1*}

¹Department of Chemical Engineering, Kangwon National University, Gangwon-do 24341,

Republic of Korea

²School of Chemical and Biological Engineering, Seoul National University, Seoul 08826,

Republic of Korea

³Department of Chemical and Biological Engineering, Sookmyung Women's University,

Seoul 04310, Republic of Korea

‡ These authors contributed equally to this work.



Figure S1. (a) MALDI-TOF mass spectra of F-ODA (pH 7.4) and (b) the proposed chemical structures of the F-ODA.



Figure S2. The ¹H NMR analysis (D₂O) of (a) pure dopamine and (b) F-ODA.



Figure S3. XPS spectra of polydopamine, (a) C1s, (b) N1s, and (c) O1s.



Figure S4. (a) Fluorescence spectra of F-ODA depending on the final concentration of NaOH and (b) maximum intensity of F-ODA upon the pH of reacting solution.



Figure S5. (a) A concise scheme for the experiment about effect of adding HCl. Normalized fluorescence spectra of (b) 5,6-dihydroxyindole-rich compound before and after centrifugation and (c) F-ODA supernatant and indole-5,6-quinone-rich compound.



Figure S6. Fluorescence spectra of F-ODA depending on the presence or absence of nitrogen purging to eliminate dissolved oxygen before adding HCl.



Figure S7. (a) The F-ODA decay curve measured at room temperature. (b) The plot of absorbance vs. area of fluorescence on anthracene (red dots) and F-ODA (black dots).

$$\begin{array}{c} \stackrel{\circ}{\underset{HN}{\rightarrow}} \stackrel{\circ}{\underset{HN}{\rightarrow}} + 2 \operatorname{H}^{+} + 2e^{-} \longleftrightarrow \qquad \stackrel{H^{\circ}}{\underset{HN}{\rightarrow}} \stackrel{\stackrel{\circ}{\underset{HN}{\rightarrow}} \stackrel{}{\underset{HN}{\rightarrow}} & \operatorname{E} : 0.603 \operatorname{V} (\mathrm{pH 3}) \\ 0.271 \operatorname{V} (\mathrm{pH 7}) \\ 2 \operatorname{Fe}^{2+} & \swarrow & 2 \operatorname{Fe}^{3+} + 2e^{-} \operatorname{E} : - 0.77 \operatorname{V} \\ \end{array}$$

$$\begin{array}{c} \stackrel{\operatorname{net}}{\underset{Reaction}{\overset{\circ}{\underset{HN}{\rightarrow}}} \stackrel{\circ}{\underset{HN}{\rightarrow}} + 2 \operatorname{Fe}^{2+} + 2 \operatorname{H}^{+} & \xleftarrow{\alpha} & \stackrel{H^{\circ}}{\underset{\Lambda}{\rightarrow}} \stackrel{\stackrel{\circ}{\underset{HN}{\rightarrow}} \stackrel{}{\underset{HN}{\rightarrow}} \stackrel{}{\underset{HN}{\rightarrow}} + 2 \operatorname{Fe}^{3+} & \operatorname{E}_{0} : - 0.167 \operatorname{V} (\mathrm{pH3}) \\ & - 0.499 \operatorname{V} (\mathrm{pH7}) \end{array}$$

Figure S8. Redox potentials of half reactions triggered by adding Fe^{2+} ion.



Figure S9. SEM-EDS results of (a) F-ODA (supernatant), (b) PDA (precipitate), and (c) F-ODA chelated with Fe²⁺ ions.

$$aA + bB + n[e^{-}] + h[H^{+}] = cC + dD$$

$$E_{h} = E_{0} + \frac{0.05916}{n} \log \left(\frac{\{A\}^{a} \{B\}^{b}}{\{C\}^{c} \{D\}^{d}} \right) - \frac{0.05916}{n} pH$$

Equation S1. Nernst Equation.