Electronic Supplementary Information (ESI)

Sensitively ratiometric detection of Al(III) ions in 100% aqueous buffered solution using fluorescent probe based on the peptide receptor

Gi Won Hwang, Jongyong Jeon, Lok Nath Neupane, and Keun-Hyeung Lee†

†Bioorganic Chemistry Laboratory, Center for Design and Applications of Molecular Catalysts, Department of Chemistry and Chemical Engineering, Inha University, 253 Yonghyun-dong, Nam-gu, Incheon 402-751, Republic of Korea

†Corresponding author. fax: +82 32 867 5604. E-mail address: leekh@inha.ac.kr (K. H. Lee)

Contents:

Figure S1. HPLC chromatograph of 1

Figure S2. ESI-MS spectrum of 1

Figure S3. $^1$H NMR of 1 (20 mM) in 100% DMSO

Figure S4. $^{13}$C NMR of 1 (20 mM) in 100% DMSO

Figure S5. Ratiometric response of 1 with Al(III)

Figure S6. Job’s plot for 1 with Al(III)

Figure S7. Fitting curve of 1

Figure S8. Reversibility study of 1

Figure S9. Determination of detection limits in aqueous solutions

Figure S10. Al(III) titration of 1 under 1% of urine
Figure S1. HPLC chromatograph of 1.
Figure S2. ESI-MS spectrum of 1.

[Mr + H']$^+$

Calculated Mass : 463.14
Observed Mass : 463.1
**Figure S3.** $^1$H NMR of 1 (20 mM) in 100% DMSO.
Figure S4. $^{13}$C NMR of 1 (20 mM) in 100% DMSO.
Figure S5. Ratiometric response of 1 to Al(III) ions in aqueous buffered solution (10 mM Hexamine, pH 5.5).
Figure S6. A Job’s plot for 1 with Al(III) (emission intensity at 395 nm) in aqueous buffered solution (10 mM Hexamine, pH 5.5). ($\lambda_{ex}=342$ nm, slit=15/10 nm, 1% T attenuator).
Figure S7. Titration curve for determination of binding constant of 1 (10 μM) to Al(III) in aqueous buffered solution (10 mM Hexamine, pH 5.5).
Figure S8. Fluorescence emission spectra of 1 (10 μM) with Al(III) (35 μM) in the presence and absence of EDTA (14 equiv.) in aqueous buffered solution (10 mM Hexamine, pH 5.5) ($\lambda_{ex}=342$ nm, slit=15/10 nm, 1% T attenuator).
Figure S9. The emission intensity ratio changes of I (5 μM) with increasing concentrations of Al(III) in aqueous buffered solution (10 mM Hexamine, pH 5.5) prepared by distilled water (100%, v/v) ground water (50%, v/v), and tap water (50%, v/v), respectively.
Figure S10. (a) fluorescence emission spectra and (b) ratiometric response of 1 (50 μM) with increasing concentration of Al(III) in aqueous buffered solutions (10 mM hexamine, pH 5.5) with 1% urine.