Supporting Information

Ratiometric fluorescence chemosensor based on Tyrosine derivatives for monitoring mercury ions in aqueous solutions

Ponnaboina Thirupathi, Ponnaboina Saritha (née Gudelli) 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, Korea

Email: leekh@inha.ac.kr (K.-H. Lee)

Contents

1. Figures

Fig. S1. HPLC chromatogram of 1
Fig. S2. ESI mass spectrum of 1
Fig. S3. $^1$H NMR spectrum of 1
Fig. S4. $^{13}$C NMR spectrum of 1
Fig. S5. IR spectrum of 1
Fig. S6. HRMS–FAB mass spectrum of 1
Fig. S7. HRMS–FAB elemental composition of 1
Fig. S8. HPLC chromatogram of 2
Fig. S9. ESI mass spectrum of 2
Fig. S10. $^1$H NMR spectrum of 2
Fig. S11. $^{13}$C NMR spectrum of 2
Fig. S12. IR spectrum of 2
Fig. S13. HRMS–FAB mass spectrum of 2
Fig. S14. HRMS–FAB elemental composition of 2
Fig. S15. Uv–visible spectra of 1 and 2
Fig. S16. Uv–visible titration spectra with Hg(II) 1 and 2
Fig. S17. Job’s plot analysis of 1 and 2
Fig. S18. Association constant of 1 and 2
Fig. S19. Determination of detection limit of 1 and 2

Fig. S20. ESI mass spectra of 1–Hg(II)

Fig. S21. ESI mass spectra of 2–Hg(II)

1. Figures

![Fig. S1 HPLC chromatogram of compound 1](image-url)
Fig. S2 ESI mass spectrum of 1
Fig. S3 $^1$H NMR spectrum of compound 1
Fig. S4 $^{13}$C NMR spectrum of compound 1
Fig. S5 IR spectrum of 1
Fig. S6 HRMS-FAB mass spectrum of 1

1) PYSO2-1 with GLY (POS)
Fig. S7 HRMS-FAB elemental composition of 1

m/z 459.1373
Intensity 132772.2
Relative 100.00
Theo. Mass 459.1373
Delta (mnu) -0.01
Composition C26 H23 O4 N2 [32]S1
Fig. S8 HPLC chromatogram of compound 2
Fig. S9 ESI mass spectrum of 2
Fig. S10 $^1$H NMR spectrum of compound 2
Fig. S11 $^{13}$C NMR spectrum of compound 2
Fig. S12 IR spectrum of 2
Fig. S13 HRMS-FAB mass spectrum of 2
Fig. S14 HRMS-FAB elemental composition of 2
**Fig. S15** UV-Visible absorption spectra of (a) 1 (40 μM) and (b) 2 (40 μM) in aqueous solution (H₂O/DMSO = 95:5, v/v, 10 mM HEPES at pH 7.4.
**Fig. S16** UV–Visible absorption spectra of (a) 1 (40 μM) upon gradual addition of Hg(II) (0, 0.125, 0.250, 0.375, 0.500, 0.625, 0.75, 0.875, 1.00 and 1.125 equiv) and (b) 2 (40 μM) upon gradual addition of Hg(II) (0, 0.125, 0.250, 0.375, 0.500, 0.625, 0.75, 0.875, 1.00, 1.125 and 1.25 equiv) in aqueous solution (H₂O/DMSO, 95:5, v/v, 10 mM HEPES at pH 7.4).
Fig. S17 A Job’s plot analysis for (a) 1, and (b) 2 with Hg(II).
Fig. S18 Non-linear fitting of the fluorescence intensity change of (a) 1 at 490 nm vs concentration of Hg(II) (slit 15/5) (b) 2 at 486 nm vs concentration of Hg(II) (slit 15/6) in aqueous solution (H$_2$O/DMSO, 95:5, v/v, 10 mM HEPES at pH 7.4).
Fig. S19 Detection limit for (a) 1 and (b) 2 with Hg(II) (Intensity change at 386 nm) in aqueous solution (H$_2$O/DMSO = 95:5, v/v, 10 mM HEPES at pH 7.4; $\lambda_{ex}$ = 353 nm, slit 15/6).
Fig. S20 ESI mass spectra of 1 (500 μM) in the presence of 1 equiv Hg(II) in aqueous solution (H₂O/ACN, 7:3, v/v).
**Fig. S21** ESI mass spectra of 1 (500 μM) in the presence of 1 equiv Hg(II) in aqueous solution (H$_2$O/ACN, 7:3, v/v).