Electronic Supplementary Material (ESI) for Dalton Transactions. This journal is © The Royal Society of Chemistry 2016

Electronic Supporting Information

About the Interaction of Hg²⁺ and Trivalent Ions with Two New Fluorescein Bio-inspired Dual Colorimetric/Fluorimetric Probes

Augusto C. Gonçalves^{†‡}, Viviane Pilla^{ψ ‡}, Elisabete Oliveira^{‡δ}, Sérgio M. Santos^{χ}, José Luis Capelo^{‡δ}, Carlos Lodeiro^{‡δ*}, Alcindo A. Dos Santos^{†*}

- ^x CICECO Aveiro Institute of Materials, Department of Chemistry, University of Aveiro, 3810-193 Aveiro, Portugal.
- $^{\delta}$ Proteomass Scientific Society, Rua dos Inventores, Madan Park, 2829-516 Caparica, Portugal.

[‡] BIOSCOPE Group, UCIBIO-REQUIMTE, Departamento de Química, Faculdade de Ciências e Tecnologia, Universidade Nova de Lisboa, 2829-516 Portugal.

[†] Instituto de Química, Universidade de São Paulo, Av. Prof. Lineu Prestes, 748, CxP. 26077, São Paulo, 05508-00, Brazil.

[♥] Instituto de Física, Universidade Federal de Uberlândia-UFU, Av. João Naves de Ávila 2121, Uberlândia, MG, 38400-902, Brazil,

^{*}Correspondent author: Carlos Lodeiro (cle@fct.unl.pt) / Alcindo Aparecido dos Santos (alcindo@iq.usp.br).

INDEX

¹ H NMR spectrum of 1	S 1
¹³ C NMR spectrum of 1	S2
¹ H NMR spectrum of 2	S 3
¹³ C NMR spectrum of 2	S4
¹ H NMR spectrum of 3	S5
¹³ C NMR spectrum of 3	S 6
Spectrofotometric/spectrofluorimetric titration of 2 and 3 with Al ³⁺	S7
Spectrofotometric/spectrofluorimetric titration of 2 and 3 with Fe ³⁺	S 8
Spectrofotometric/spectrofluorimetric titration of 2 and 3 with Cr ³⁺	S 9
Spectrofotometric/spectrofluorimetric titration of 2 and 3 with Ga ³⁺	S 10
MALDI-TOF-MS spectrum of 1	S11
MALDI-TOF-MS spectrum of 2	S12
HRMS spectrum of 3	S13
Job's plot of $\bf 2$ and $\bf 3$ with Al ³⁺ , Cr ³⁺ , Fe ³⁺ , Ga ³⁺ and Hg ²⁺	S14
Absorption and emission spectra of 1 , 2 and 3 in 1:1 acetonitrile/water	S15

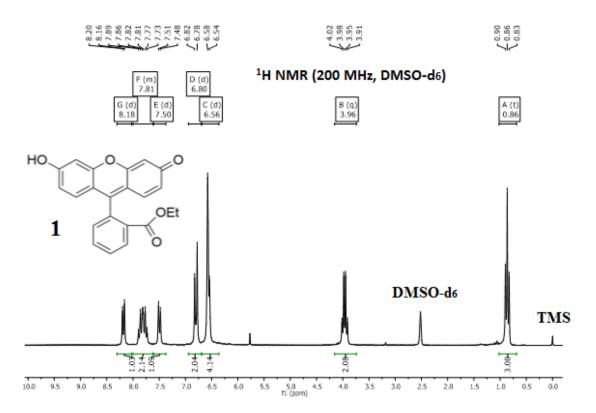


Figure S1. ¹H NMR spectrum of **1**.

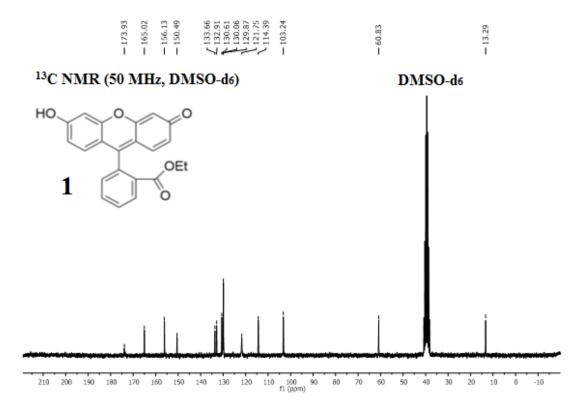


Figure S2. ¹³C NMR spectrum of **1**.

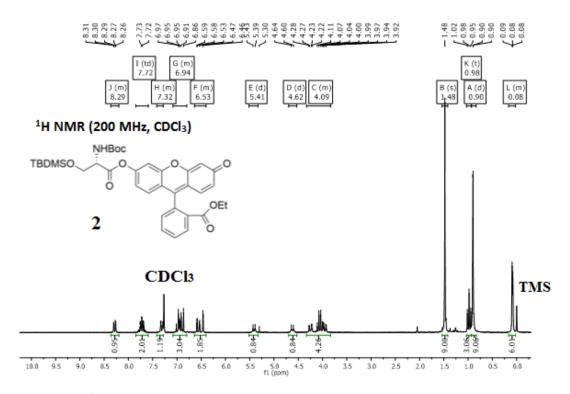


Figure S3. ¹H NMR spectrum of 2.

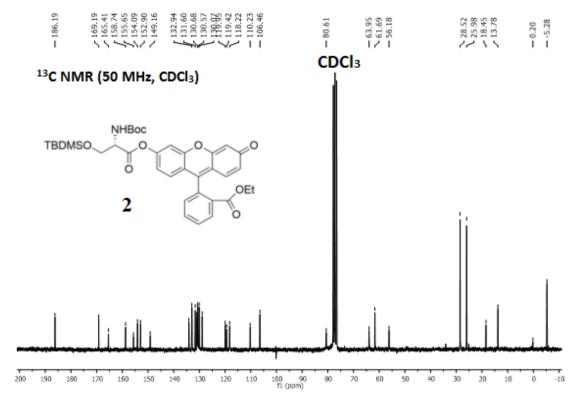


Figure S4. ¹³C NMR spectrum of **2**.

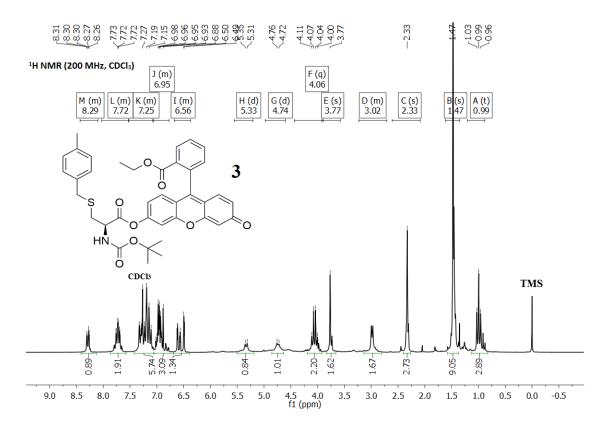


Figure S5. ¹H NMR spectrum of 3.

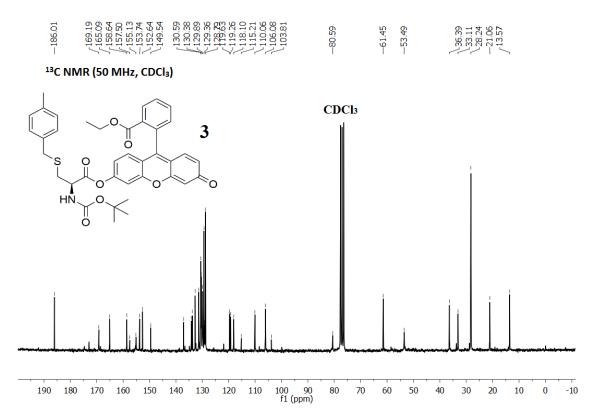


Figure S6. ¹³C NMR spectrum of **3**.

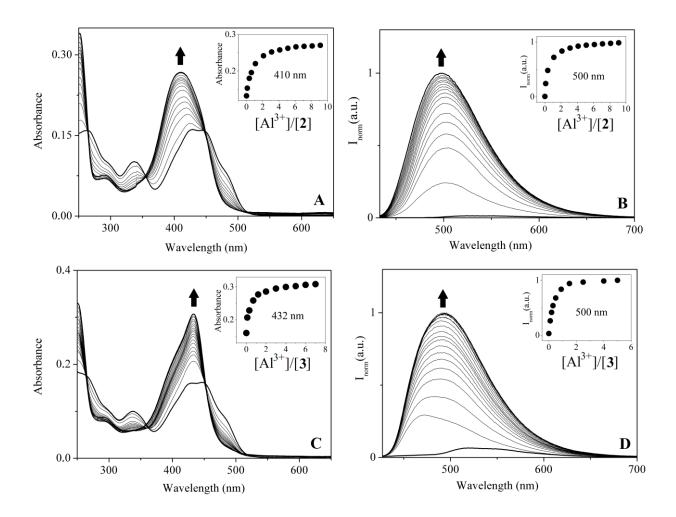


Figure S7. Spectrofotometric titrations of **2** (A) and **3** (C), with increasing amounts of Al³⁺ in acetonitrile solution. Inset: Absorption at 410 nm (A) and 432 nm (C) as a function of $[Al^{3+}]/[2]$ and $[Al^{3+}]/[3]$, respectively (T = 298 K; $[2] = [3] = 1.10^{-5}$ M). Spectrofluorimetric titrations of **2** (B) and **3** (D), with increasing amounts of Al³⁺ in acetonitrile solution. Inset: Emission at 500 nm as a function of $[Al^{3+}]/[2]$ and $[Al^{3+}]/[3]$ (T = 298 K; $[2] = [3] = 1.10^{-5}$ M, $\lambda_{exc} = 362$ nm).

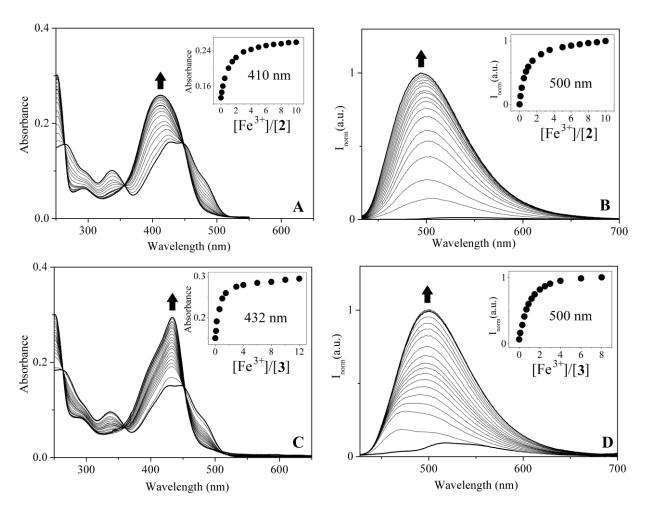


Figure S8. Spectrofotometric titrations of **2** (A) and **3** (C), with increasing amounts of Fe³⁺ in acetonitrile solution. Inset: Absorption at 410 nm (A) and 432 nm (C) as a function of $[Fe^{3+}]/[2]$ and $[Fe^{3+}]/[3]$, respectively (T = 298 K; [2] = [3] = 1.10⁻⁵ M). Spectrofluorimetric titrations of **2** (B) and **3** (D), with increasing amounts of Fe^{3+} in acetonitrile solution. Inset: Emission at 500 nm as a function of $[Fe^{3+}]/[2]$ and $[Fe^{3+}]/[3]$ (T = 298 K; [2] = [3] = 1.10⁻⁵ M, λ_{exc} = 362 nm).

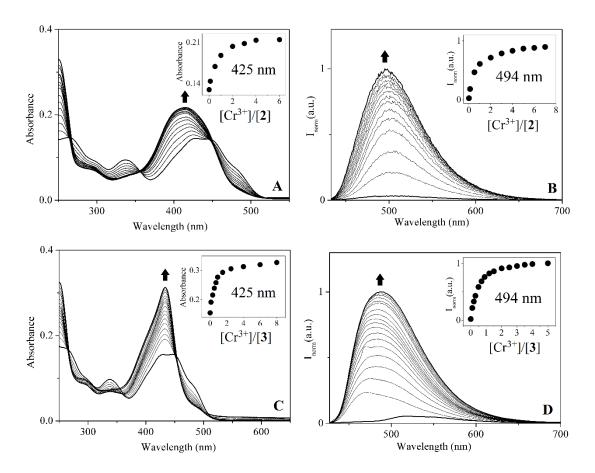


Figure S9. Spectrofotometric titrations of **2** (A) and **3** (C), with increasing amounts of Cr^{3+} in acetonitrile solution. Inset: Absorption at 425 nm as a function of $[Cr^{3+}]/[2]$ and $[Cr^{3+}]/[3]$ (T = 298 K; [2] = [3] = 1.10⁻⁵ M). Spectrofluorimetric titrations of **2** (B) and **3** (D), with increasing amounts of Cr^{3+} in acetonitrile solution. Inset: Emission at 494 nm as a function of $[Cr^{3+}]/[2]$ and $[Cr^{3+}]/[3]$ (T = 298 K; [2] = [3] = 1.10⁻⁵ M, λ_{exc} = 362 nm).

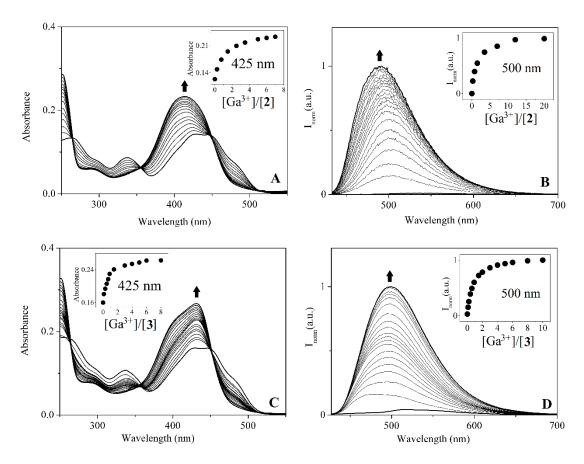


Figure S10. Spectrofotometric titrations of **2** (A) and **3** (C), with increasing amounts of Ga^{3+} in acetonitrile solution. Inset: Absorption at 425 nm as a function of $[Ga^{3+}]/[2]$ and $[Ga^{3+}]/[3]$ (T = 298 K; [2] = [3] = 1.10⁻⁵ M). Spectrofluorimetric titrations of **2** (B) and **3** (D), with increasing amounts of Ga^{3+} in acetonitrile solution. Inset: Emission at 500 nm as a function of $[Ga^{3+}]/[2]$ and $[Ga^{3+}]/[3]$ (T = 298 K; [2] = [3] = 1.10⁻⁵ M, λ_{exc} = 362 nm).

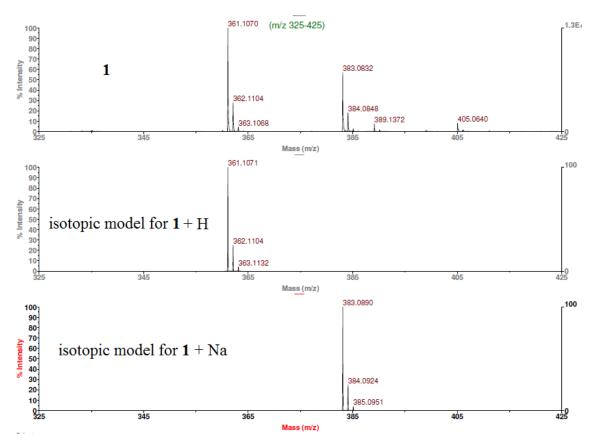


Figure S11. MALDI-TOF-MS spectrum of 1

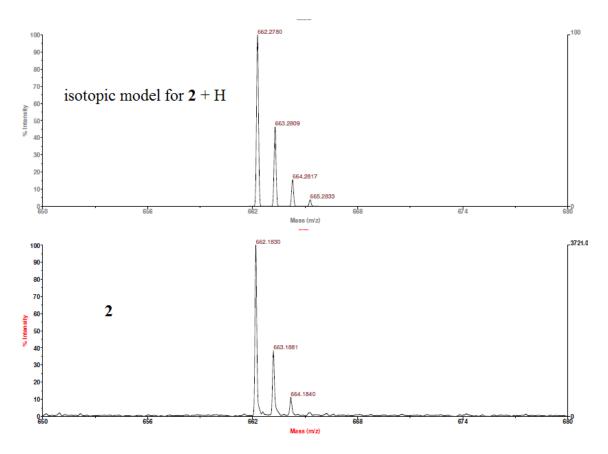


Figure S12. MALDI-TOF-MS spectrum of 2

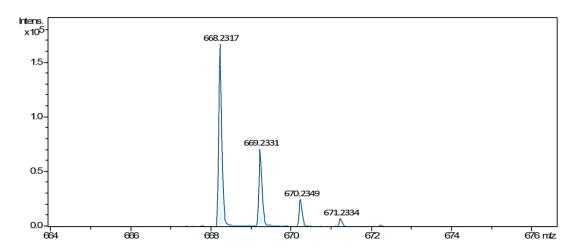


Figure S13. HRMS spectrum of 3

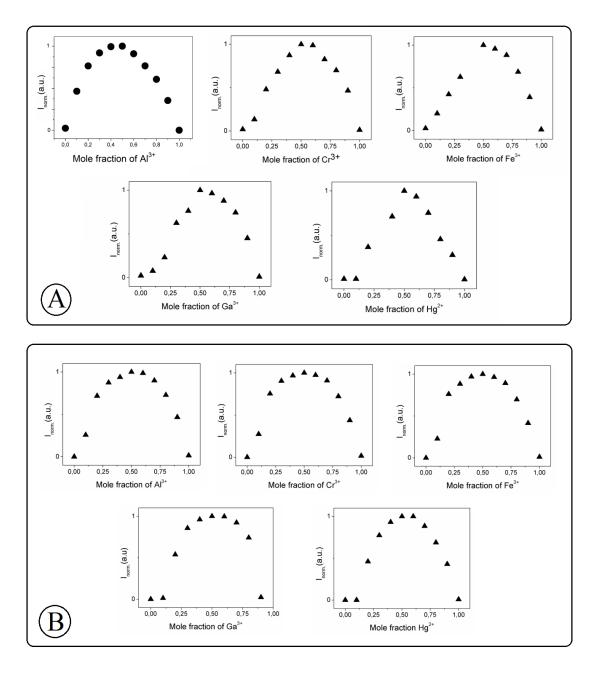


Figure S14. Job's plot of 2 and 3 with Al^{3+} , Cr^{3+} , Fe^{3+} , Ga^{3+} and Hg^{2+} .

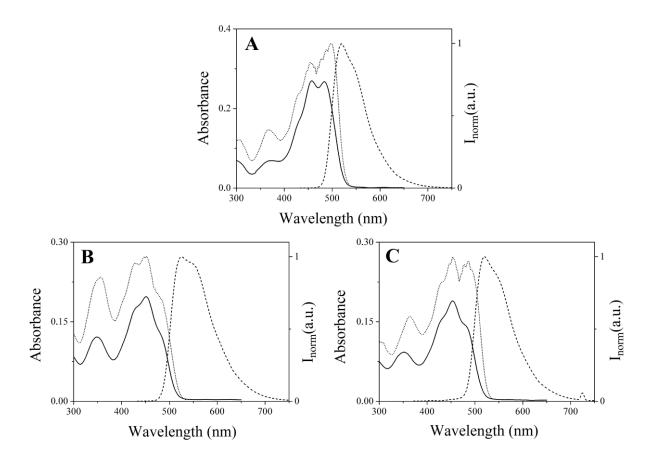


Figure S15. Room temperature absorption (full line), normalized emission (dashed line, $\lambda_{exc} = 423$ nm) and excitation spectra (dotted line, $\lambda_{em} = 545$ nm) of compounds 1 (A), 2 (B) and 3 (C) in 1:1 (v/v) acetonitrile/water solutions (1.10⁻⁵M).