

Electronic supplementary information to

Acid-base and coordination properties of 2-phenyl-3-hydroxy-4-quinolones in aqueous media

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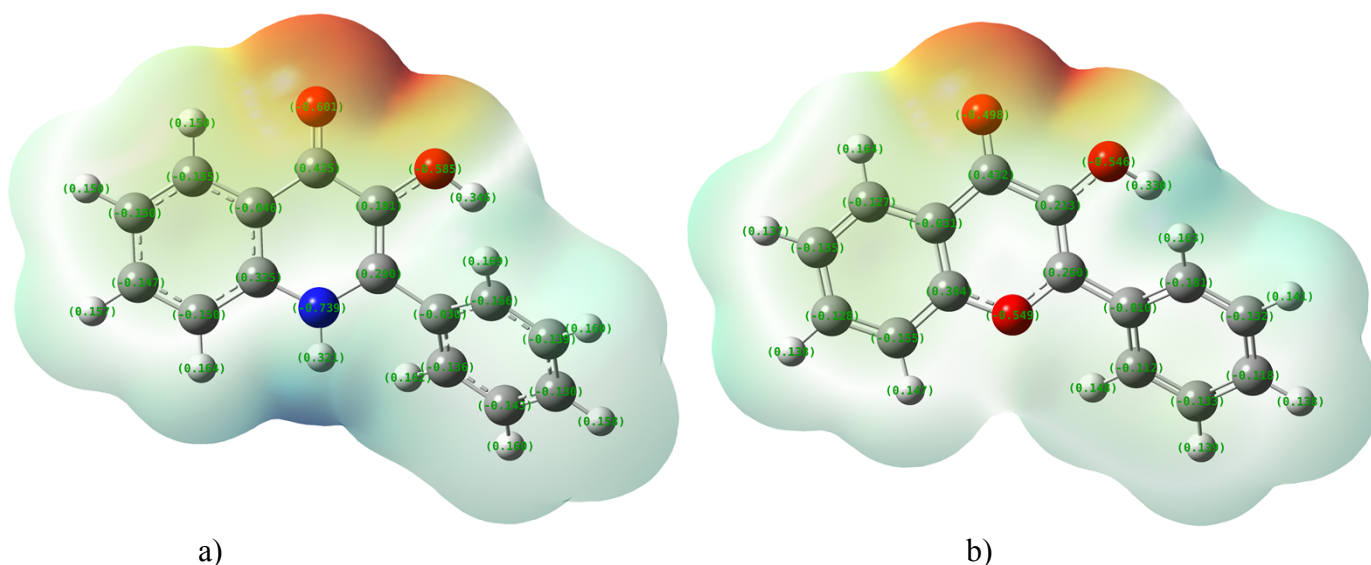
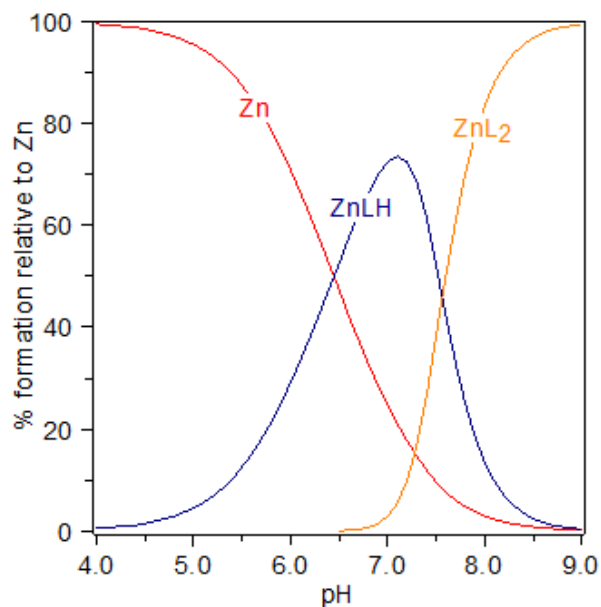


Figure S1. Electrostatic potential mapped onto total electron density for the ground state of a) **1** and b) **3**, using DFT at the PBE0/G-31+G(d,p) level of theory. Areas marked in red and yellow gain electric charge, while cyan and blue are depleted of electron density in the ground state. Clear color depicts neutral regions. Mulliken charges of individual atoms are tagged in green.

Table S1. Crystal data and structure refinement for **2**.

Crystal color	Pale yellow
Empirical formula	C ₁₆ H ₁₃ N ₁ O ₂
Mol wt.	251.28
Crystal System	Triclinic
Space group	<i>P</i> -1
a (Å)	9.0099(12)
b (Å)	9.0949(15)
c (Å)	9.5264(14)
α (°)	115.448(19)
β (°)	114.236(18)
γ (°)	96.055(13)
V (Å ³)	603.931(12)
Z	2
$\rho_{\text{calcd.}}$ (g/cm ³)	1.381
F(000)	264.0
Abs. Coeff. (mm ⁻¹)	0.092
No. of reflections:	
Measured	10199
Unique	3015
Observed	2353
R [<i>I</i> > 2 σ (<i>I</i>)]	0.0569
Rw (all data)	0.0711
Parameters	174
ρ_{min} (e/Å ³)	-0.358
ρ_{max} (e/Å ³)	0.445
GOOF	1.080
CCDC Ref. No	1401533

**Figure S2.** Species distribution diagram for 1 mM Zn(II) in the presence of 2 mM **1**.

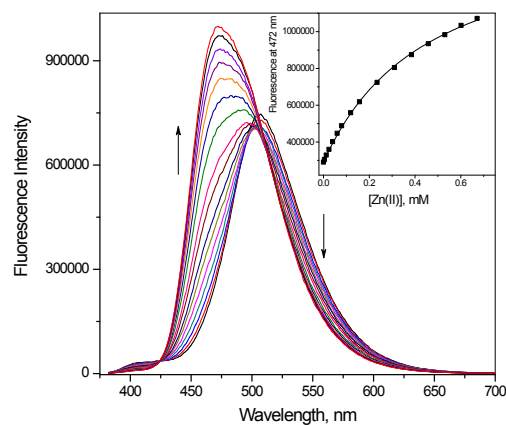
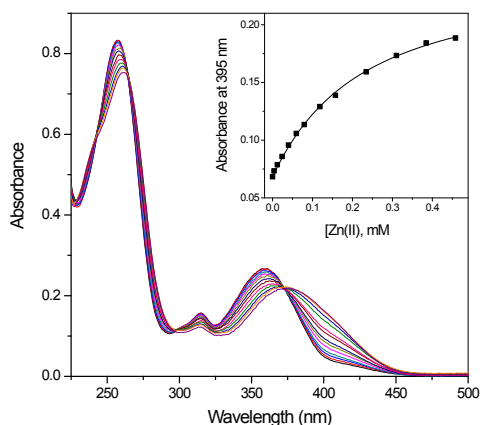


Figure S3. Left: UV-Vis spectra of **1** [3.2×10^{-5}] M upon Zn(II) additions HTAB 5 mM at pH 7.0, $K = 5000 \pm 200 \text{ M}^{-1}$. Right: Fluorescence spectra of **1** [4×10^{-5}] M upon Zn(II) additions HTAB 5 mM at pH 7.0, $K = 2400 \pm 100 \text{ M}^{-1}$.

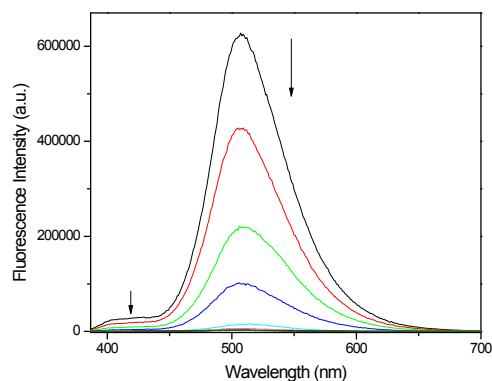
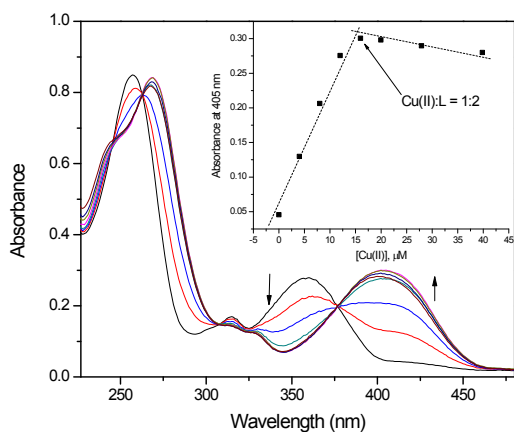
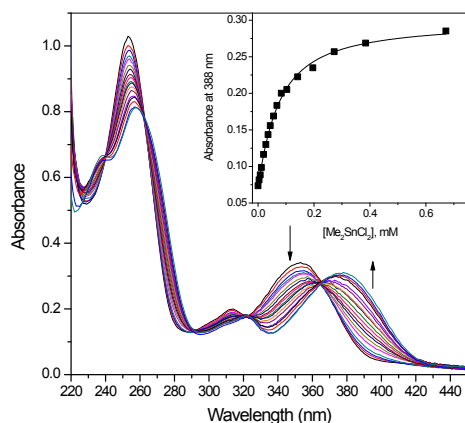
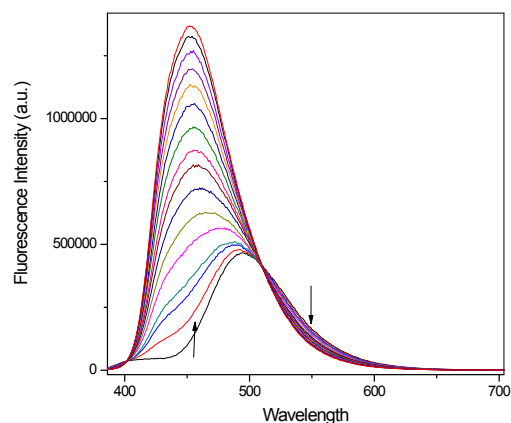


Figure S4. UV-Vis (left) and fluorescence (right) spectra of **1** [3.2×10^{-5}] M upon Cu(II) additions in HTAB 5 mM at pH 7.0



A



B

Figure S5. UV-Visible (A) and fluorescence (excitation at 376 nm) (B) spectra of 32 μM **1** in 5% MeCN at pH 7 and variable concentration of Me_2SnCl_2 . Insets show absorbance or fluorescence vs. Me_2SnCl_2 concentration profiles at selected wavelengths. Arrows show directions of the spectral changes on increase in Me_2SnCl_2 concentration.

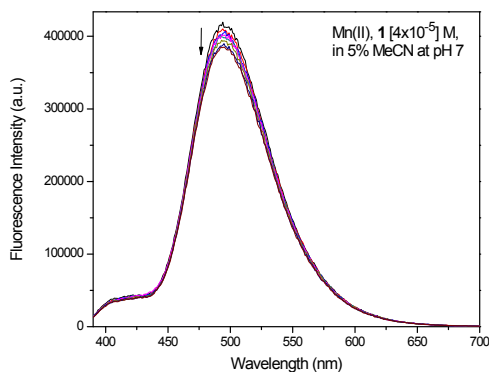
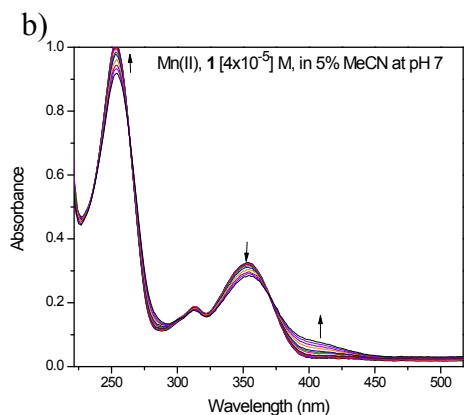
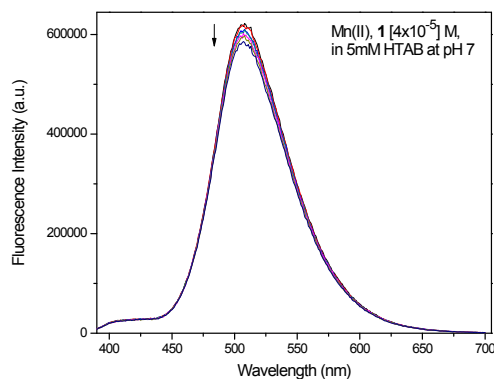
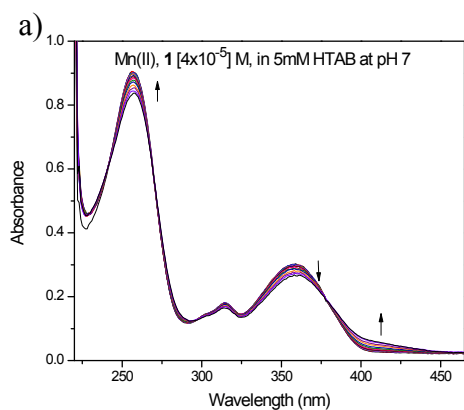


Figure S6. UV-Visible (left) and fluorescence (right) spectra of 40 μM **1** in a): 5 mM HTAB ($\lambda_{\text{exc}} = 376$ nm) and b): 5% MeCN ($\lambda_{\text{exc}} = 370$ nm) at pH 7 and variable concentration of Mn(II) .

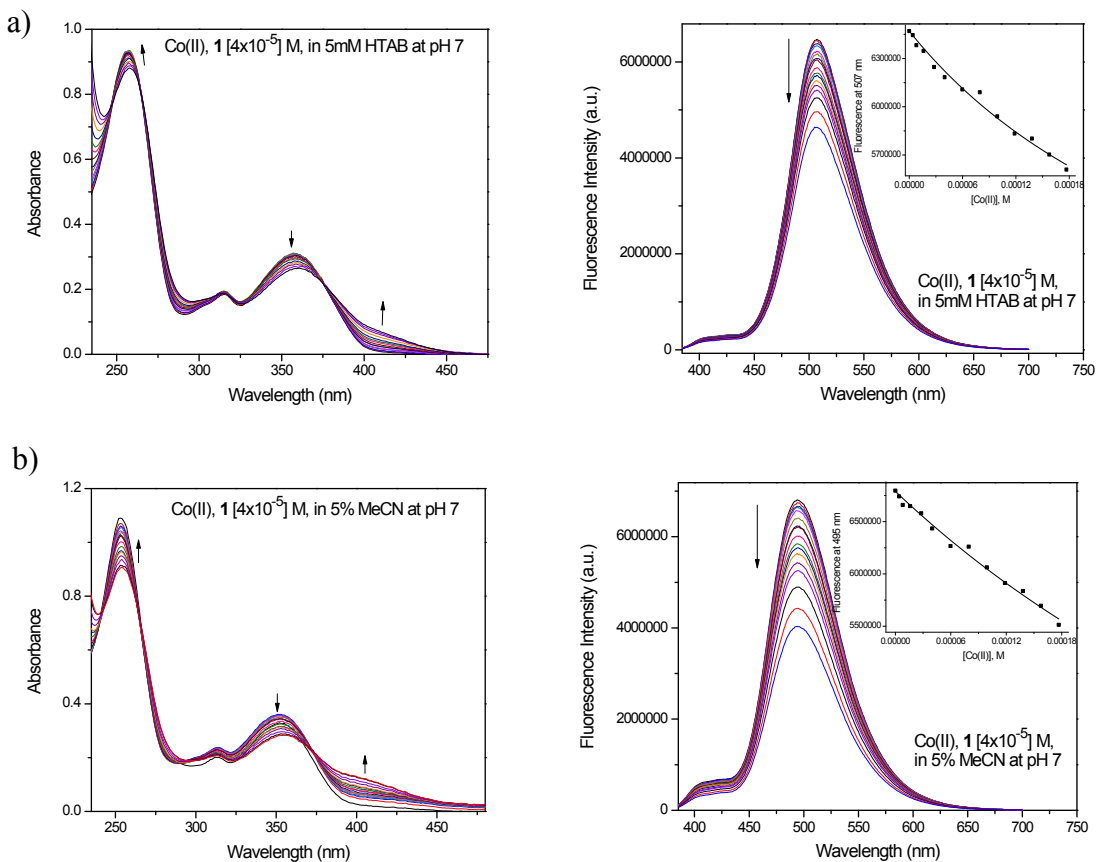


Figure S7. UV-Visible (left) and fluorescence (right) spectra of $40 \mu\text{M}$ **1** in a): 5 mM HTAB ($\lambda_{\text{exc}} = 373 \text{ nm}$) and b): 5% MeCN ($\lambda_{\text{exc}} = 368 \text{ nm}$) at pH 7 and a variable concentration of Co(II) .

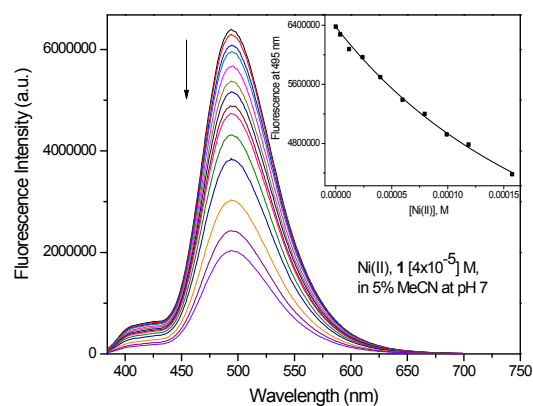
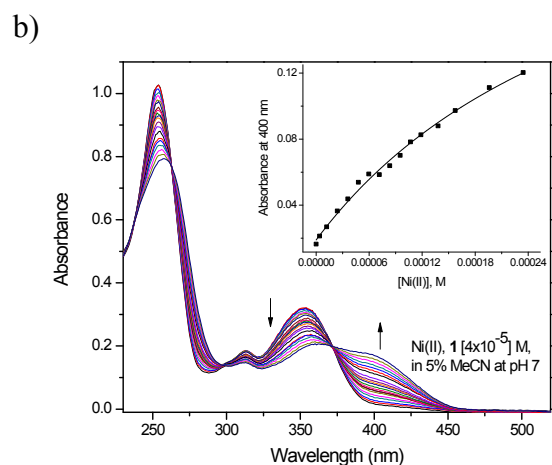
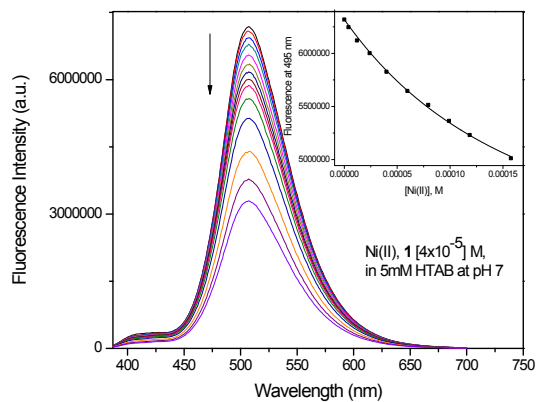
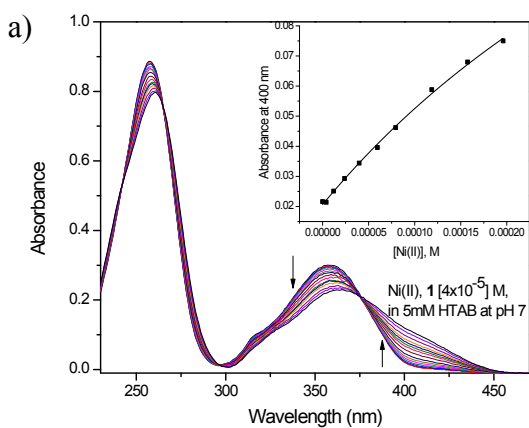
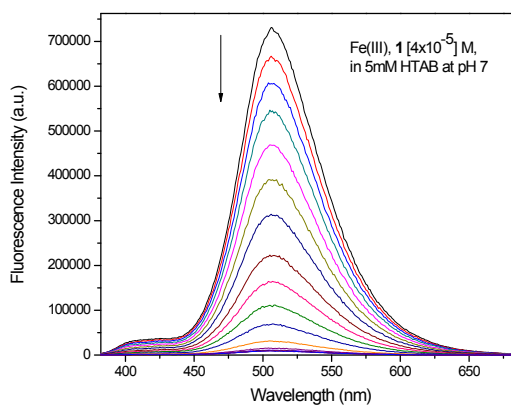
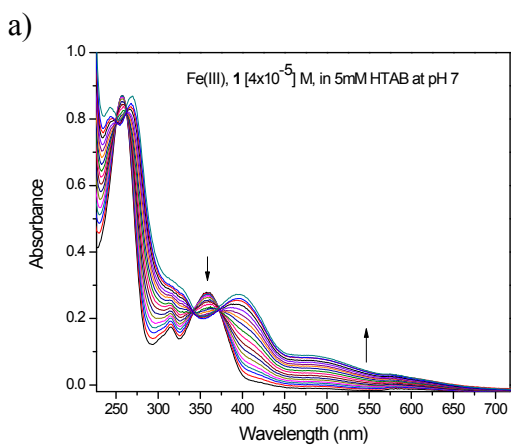


Figure S8. UV-Visible (left) and fluorescence (right) spectra of 40 μM **1** in a): 5 mM HTAB ($\lambda_{\text{exc}} = 375$ nm) and b): 5% MeCN ($\lambda_{\text{exc}} = 370$ nm) at pH 7 and variable concentration of Ni(II).



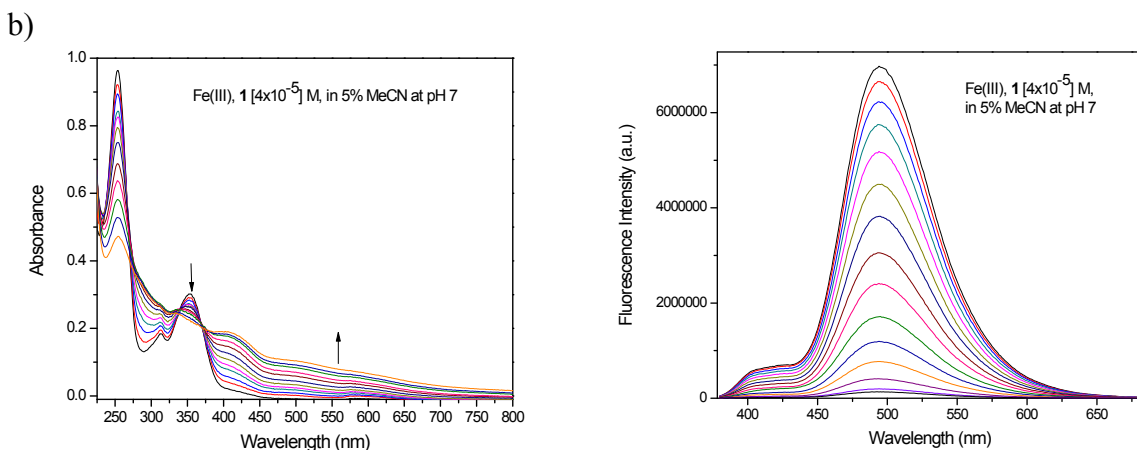


Figure S9. UV-Visible (left) and fluorescence (right) spectra of 40 μM **1** in a): 5 mM HTAB ($\lambda_{\text{exc}} = 370$ nm) and b): 5% MeCN ($\lambda_{\text{exc}} = 368$ nm) at pH 7 and variable concentration of Fe(III).

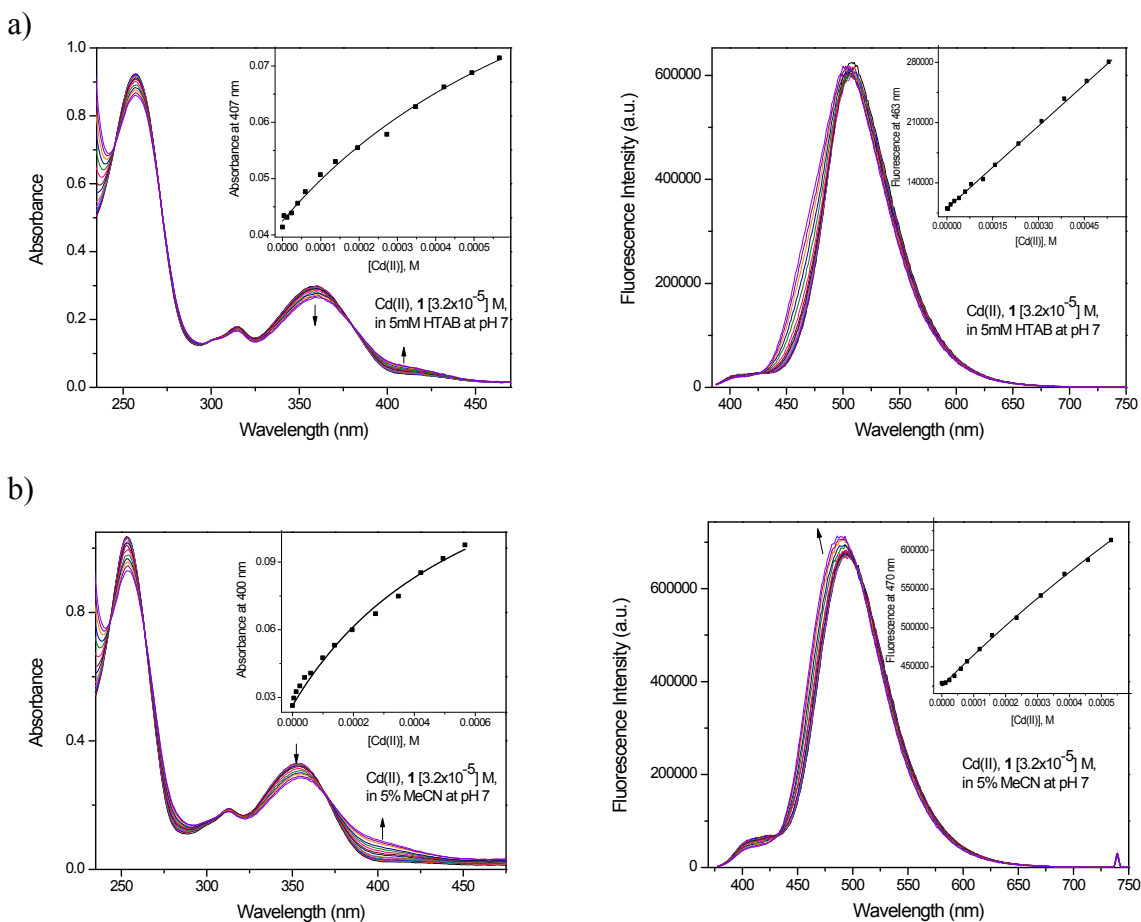


Figure S10. UV-Visible (left) and fluorescence (right) spectra of 40 μM **1** in a): 5 mM HTAB ($\lambda_{\text{exc}} = 380$ nm) and b): 5% MeCN ($\lambda_{\text{exc}} = 368$ nm) at pH 7 and variable concentration of Cd(II).

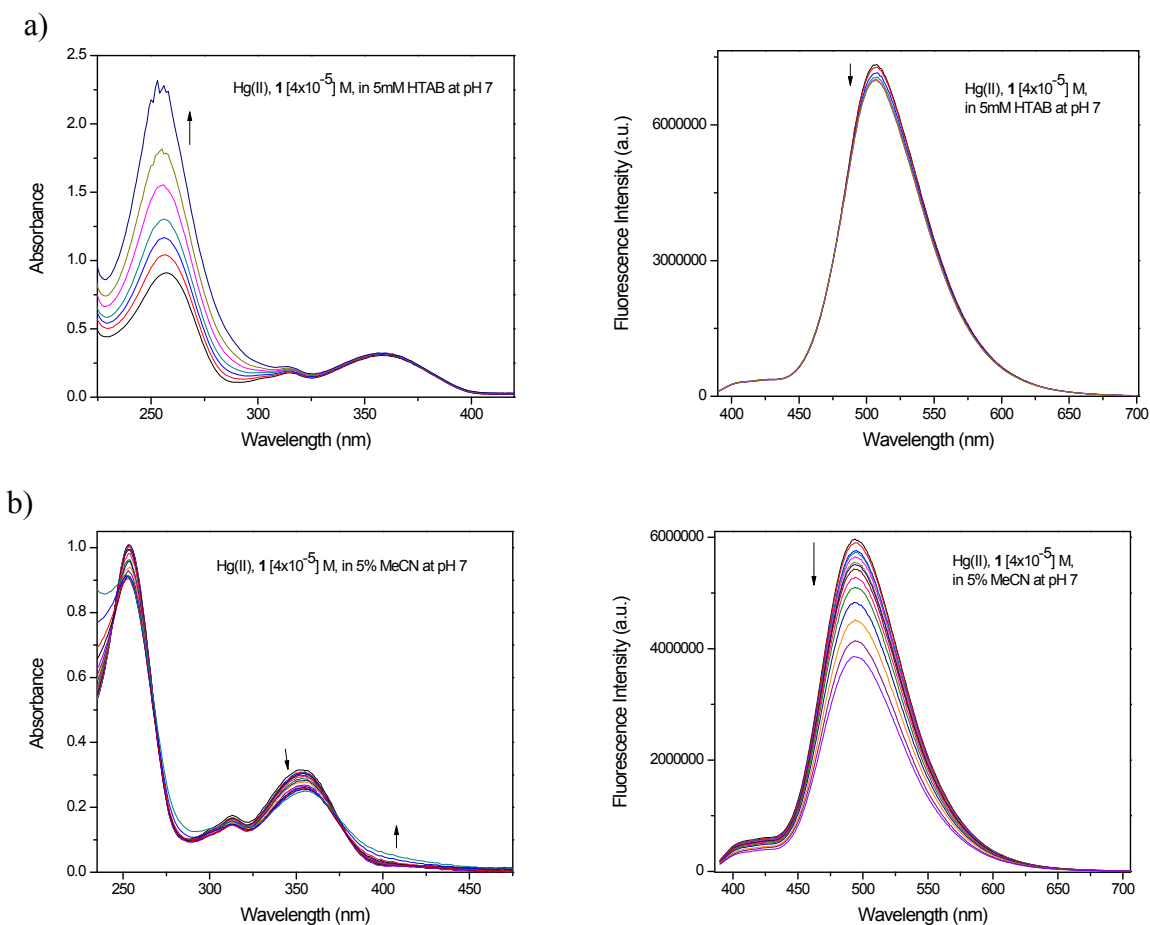
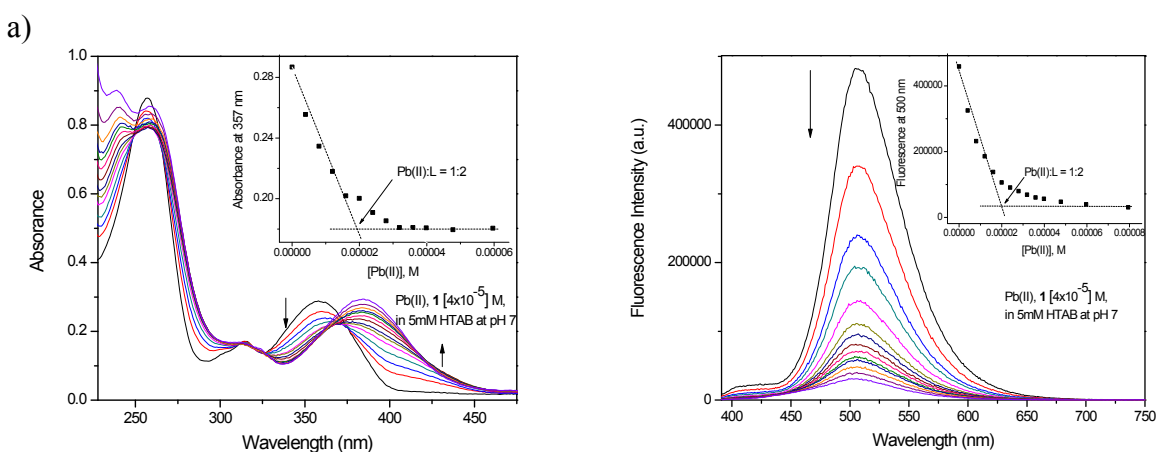


Figure S11. UV-Visible (left) and fluorescence (right) spectra of 40 μ M **1** in a): 5 mM HTAB ($\lambda_{\text{exc}} = 360$ nm) and b): 5% MeCN ($\lambda_{\text{exc}} = 375$ nm) at pH 7 and variable concentration of Hg(II).



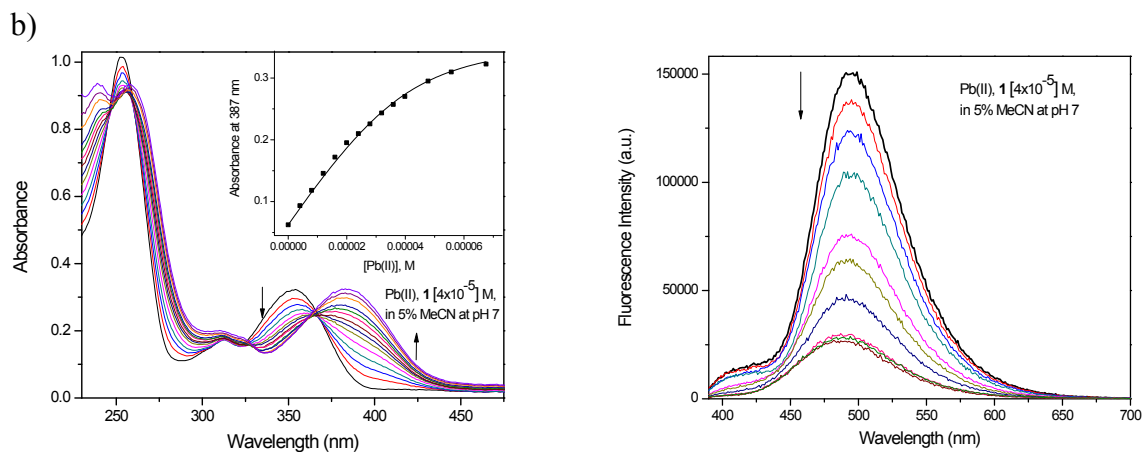


Figure S12. UV-Visible (left) and fluorescence (right) spectra of 40 μM **1** in a): 5 mM HTAB ($\lambda_{\text{exc}} = 370$ nm) and b): 5% MeCN ($\lambda_{\text{exc}} = 365$ nm) at pH 7 and variable concentration of Pb(II).

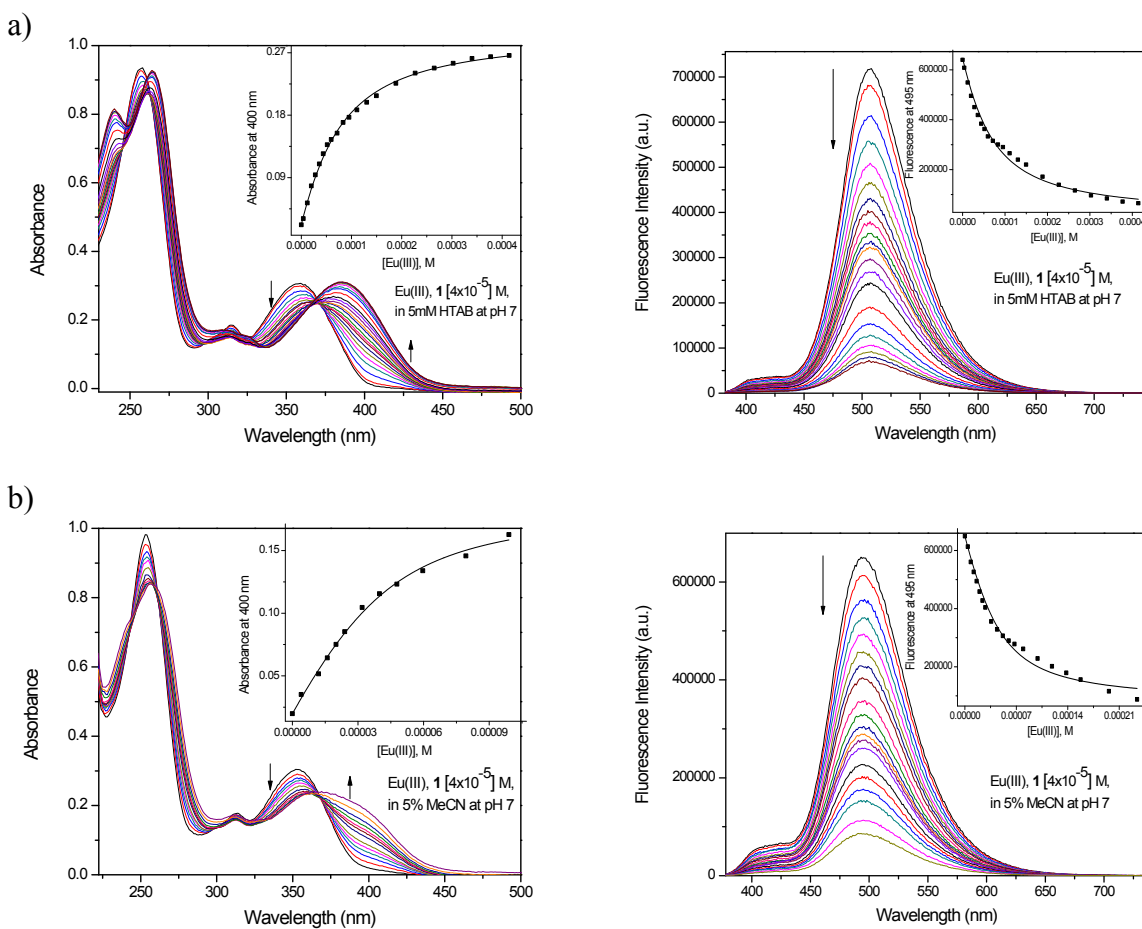
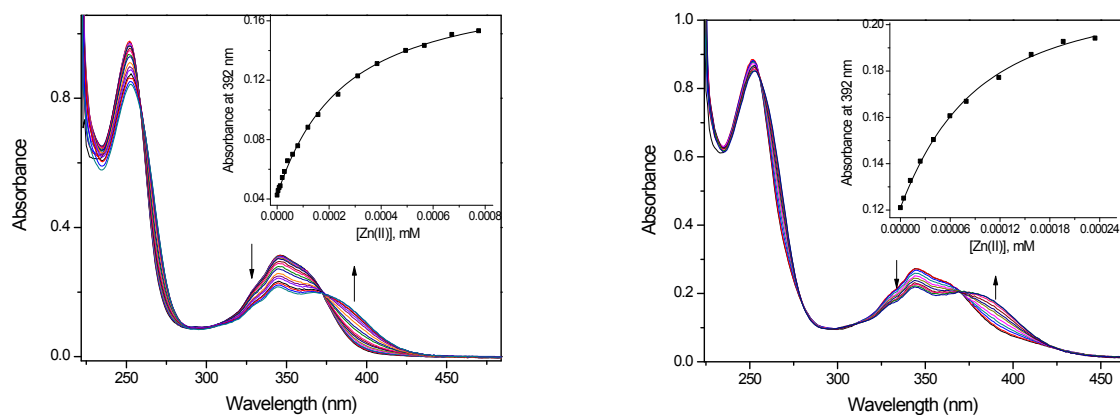
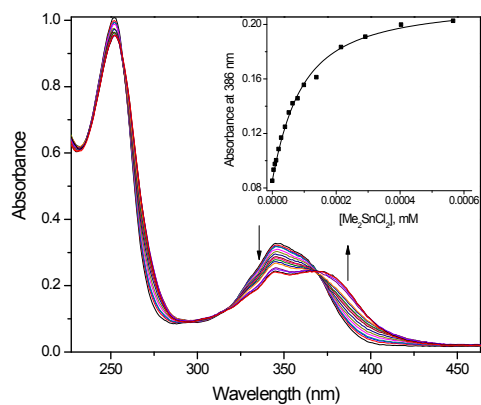


Figure S13. UV-Visible (left) and fluorescence (right) spectra of 40 μM **1** in a): 5 mM HTAB ($\lambda_{\text{exc}} = 370$ nm) and b): 5% MeCN ($\lambda_{\text{exc}} = 367$ nm) at pH 7 and variable concentration of Eu(III).



(a) Zn(II) at pH 7 (left) and pH 8 (right)



(b) pH 7; Me_2Sn

Figure S14. UV-Visible spectra of 40 μM 2 in 5 mM HTAB at pH 7 and variable concentration of (a): Zn(II) at pH 7– 8; and (b): Me_2SnCl_2 .