Novel binuclear lanthanide luminescent peptide conjugates: Structural analysis in aqueous solution of potential metallo enzymatic mimics

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Electronic Supplementary Information

Figure 1. ES MS spectrum of **1**

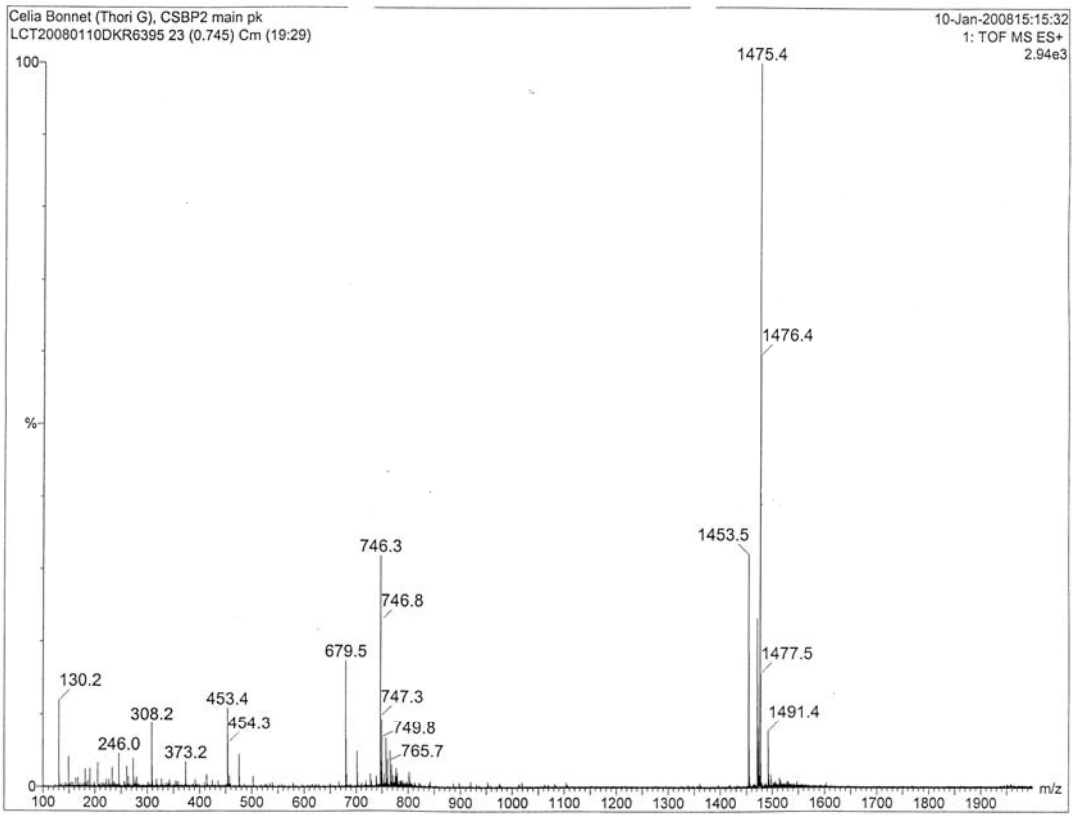

Figure 2. Maldi-Tof spectrum of **2**

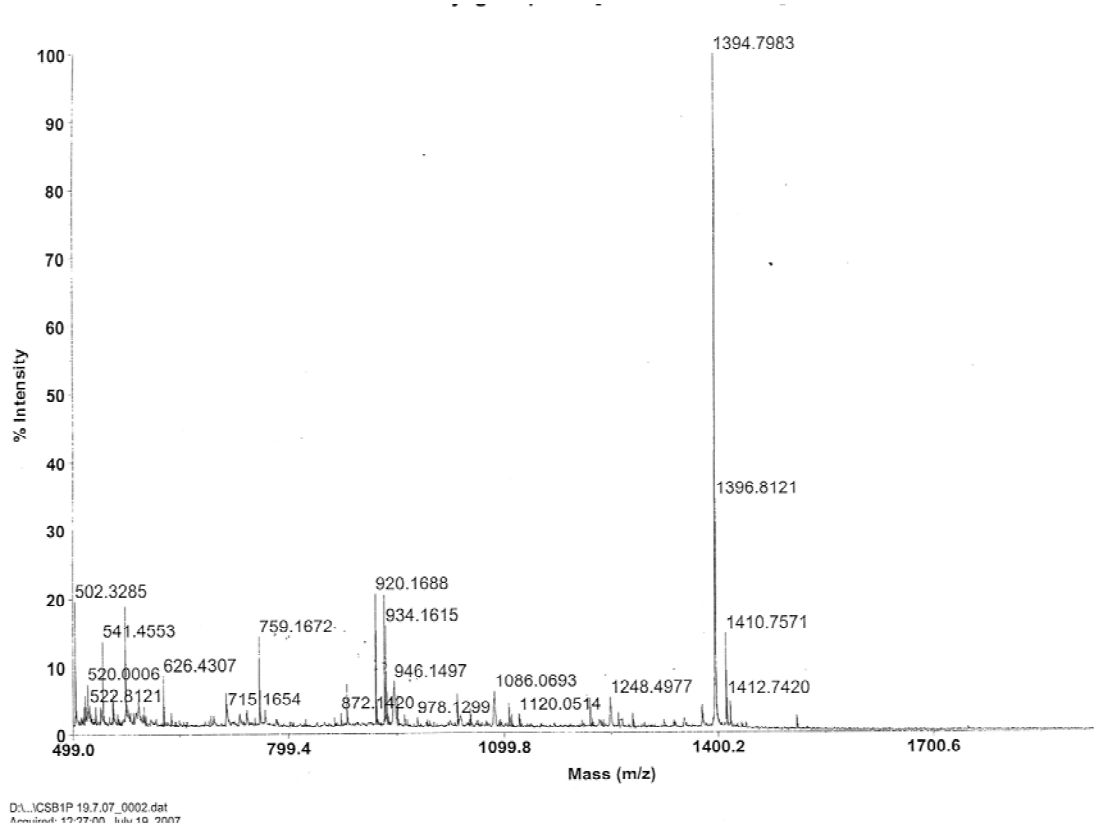

Figure 3. ^{1}H NMR spectrum (600 MHz) of **1** in a mixture 9:1 H_2O:D_2O

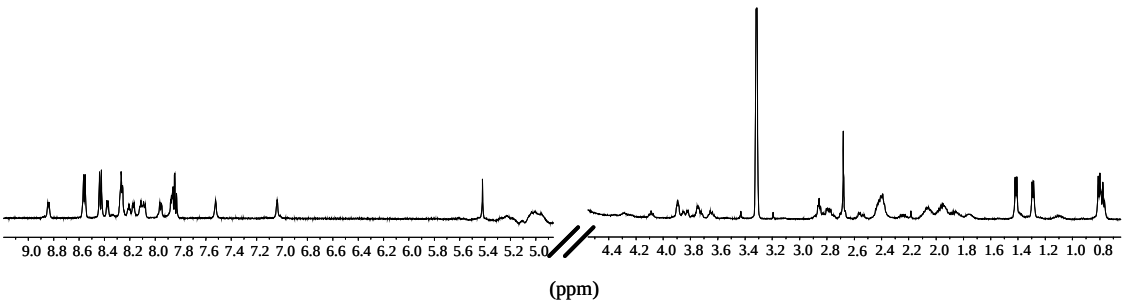

Figure 4. Speciation distribution obtained at pH 7, with [**2**] = 35 µM and with the following conditional stability constant : log β_{11} = 6.8, log β_{21} = 11.9. It should be noted that when [M] = 0.8*[**2**] (conditions used for the measurements of q-value), no free metal is present and less than 5% of binuclear complex is in solution.

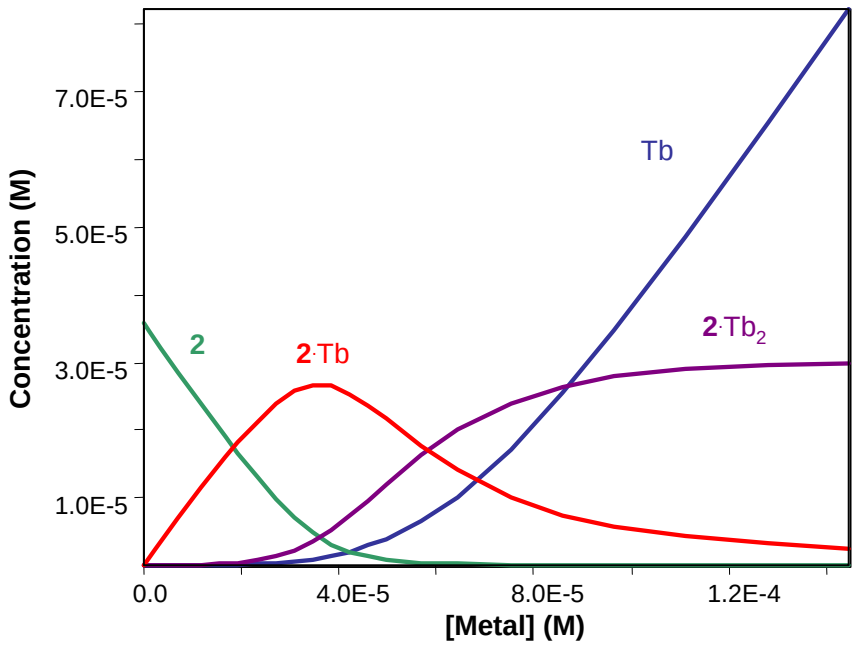

Figure 5. Luminescent decay rates of a Tb^{3+} bound to **2** with increasing H_2O concentration. [Tb^{3+}] = 0.8*[P] = 13.5 mM, pH = 7.0, [HEPES] = 10 mM, [NaCl] = 0.1 M. The excitation wavelength was 280 nm, and Tb^{3+} sensitized emission was recorded at 545 nm. Same results are obtained by direct excitation on the metal at 368 nm. Extrapolation to an H_2O-free solution provides the rate constant in D_2O.

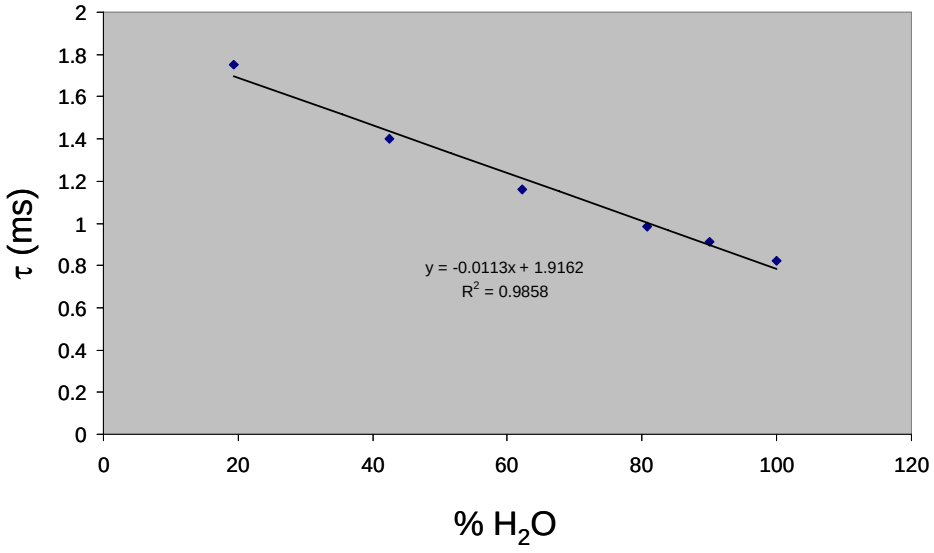

Figure 6. Luminescent decay rates of a Eu^{3+} bound to **2** with increasing H_2O concentration. [Eu^{3+}] = 0.8*[P] = 15.5 mM, pH = 7.0, [HEPES] = 10 mM, [NaCl] = 0.1 M. The excitation wavelength was 344 nm, and Eu^{3+} sensitized emission was recorded at 616 nm. Extrapolation to an H_2O-free solution provides the rate constant in D_2O.

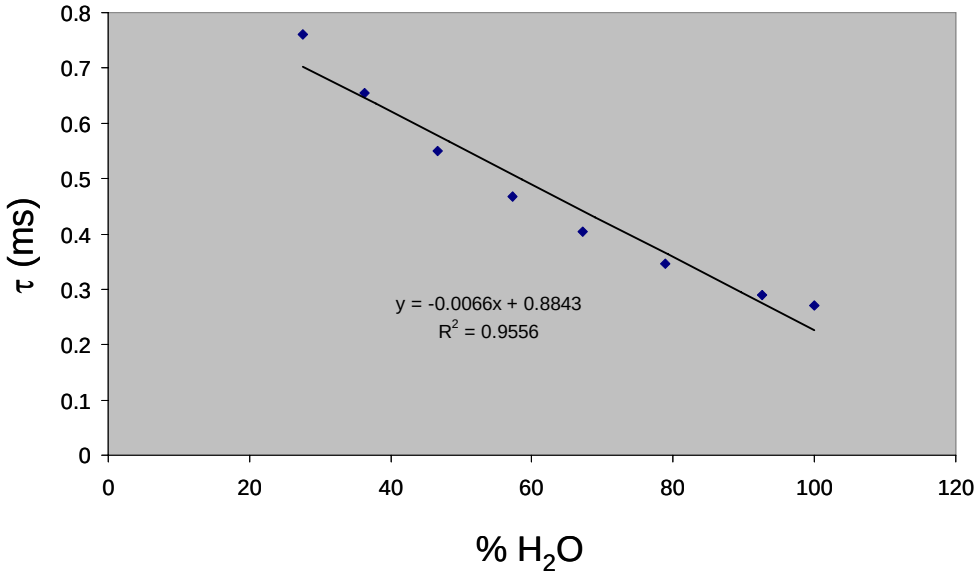

Figure 7. ^{1}H NMR spectra (600 MHz) of **2**, **2** basified by NaOH and the corresponding Eu(III) complexes in a mixture 9:1 H_2O:D_2O

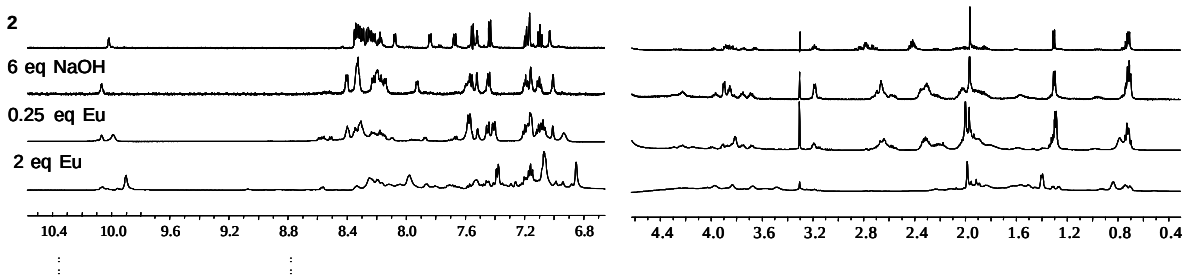

Figure 8. CD-Spectra of **2** (shown as P1) and the changes observed upon addition of one and two equivalents of Tb(III).

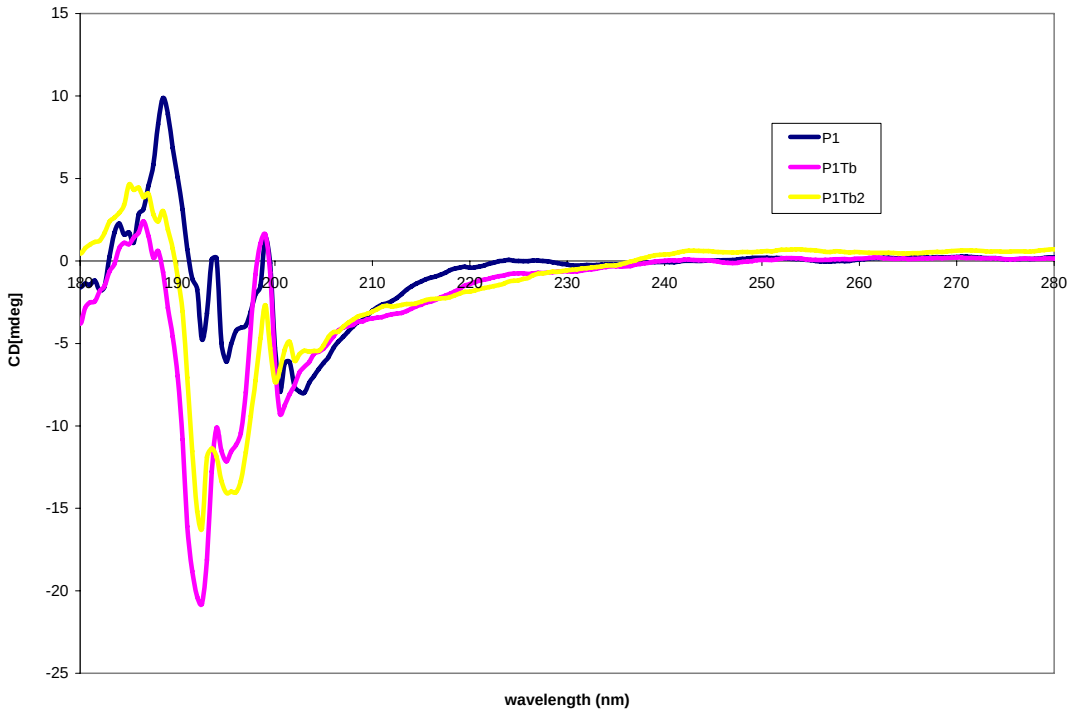

Figure 9. Schematic representation of the mono and di-nuclear complexes of **2**.