Eu(III) Complexes of Functionalised Octadentate 1-Hydroxypyridin-2-ones: Stability, Bioconjugation and LRET Studies

*Evan G. Moore, Jide Xu, Christoph J. Jocher, Todd M. Corneillie and Kenneth N. Raymond**

Department of Chemistry, University of California, Berkeley, CA, 94720-1460.

E-mail: raymond@socrates.berkeley.edu

Supporting Information

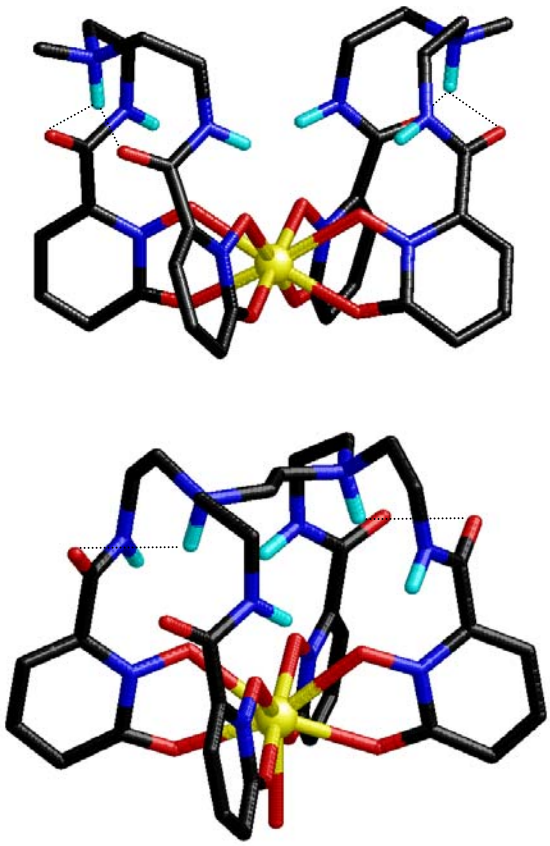

Figure S1. MM2 optimized molecular models of [Eu(5LIN^{Me}-1,2-HOPO)$_2$] (top) and [Eu(H(2,2)-1,2-HOPO)(H$_2$O)] complexes (bottom) illustrating feasible rotation of -C(O)-NH-CH$_2$-CH$_2$- groups to form H-bonds between protonated tertiary amine backbones and amide carbonyl group(s) that can influence the electronic structure of the 1,2-HOPO chromophore and may be responsible for quenching of Eu(III) metal centered luminescence (see text).

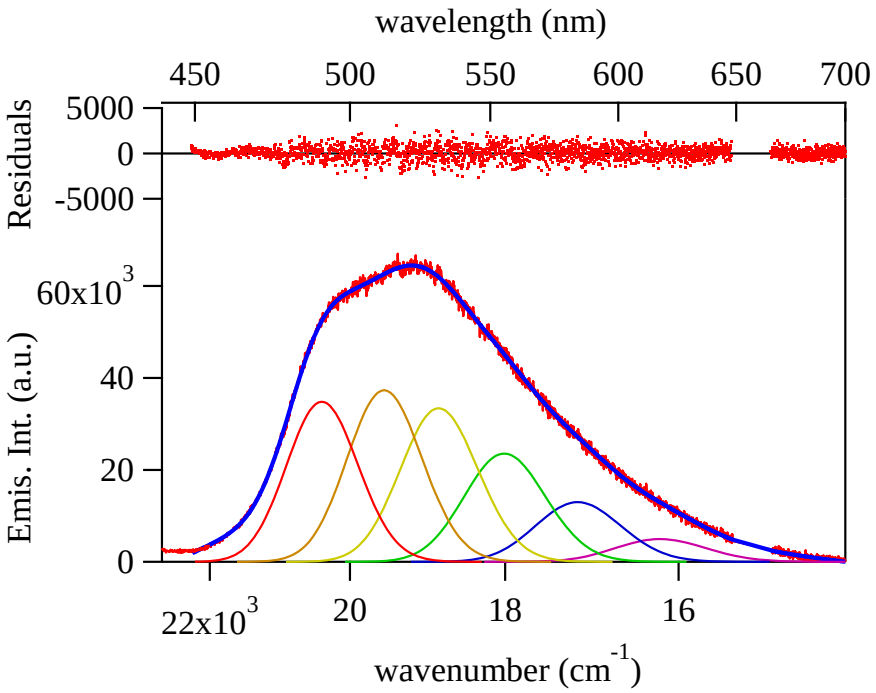

Figure S2. Low temperature (77 K) emission spectrum (red) of [Gd(H(2,2)-1,2-HOPO)] complex in 95 % 1:1 (v/v) EtOH:MeOH with 5 % (v/v) aqueous 1.0 M TRIS buffer at pH 7.4, and corresponding fit (blue line) to observed phosphorescence to a series of overlapping Gaussian functions to estimate the zero phonon ($\nu_{0\text{-}0}$) energy of the lowest energy T_1 triplet state.

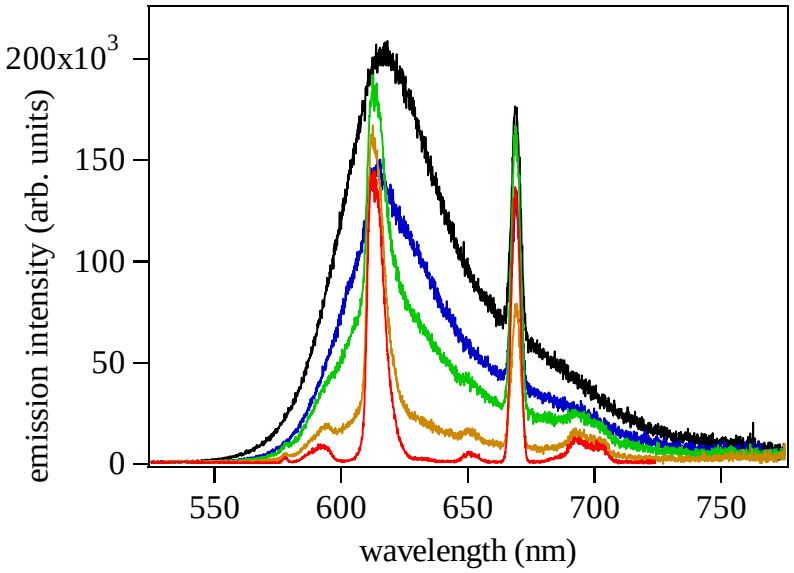

Figure S3. Observed emission spectra (λ_{ex} = 335 nm) from a 500 nM solution of SAv-[Eu(Lys-GlutA-H(2,2)-1,2-HOPO)] in 0.1 M TRIS buffered aqueous solution at pH 7.4 in the presence of *ca*. 0, 0.5, 2.0, 3.75 and 7.5 molar equivalents (red to black respectively) of biotinylated Alexa Fluor® 594. The sharp peak at 670 nm is due to second order excitation.