Electronic Supplementary Material (ESI) for Dalton Transactions.

SUPPORTING INFORMATION

Versatile pyridine-2,6-bis-tetrazolate scaffolds for the formation of highly luminescent lanthanide complexes

Sebastiano Di Pietro,[a] Nicholas Gautier,[a] Jacques Pécaut,[a] Daniel Imbert,*[a] Jacques Pécaut[a] and Marinella Mazzanti.*[b]

a Univ. Grenoble Alpes, INAC-SCIB, RICC, F-38000 Grenoble, France ; CEA, INAC-SCIB, F-38000 Grenoble, France;b Institut des Sciences et Ingénierie Chimique, Ecole Polytechnique Fédérale de Lausanne (EPFL) CH-1015 Lausanne (Switzerland) E-mail: marinella.mazzanti@epfl.ch; daniel.imbert@cea.fr

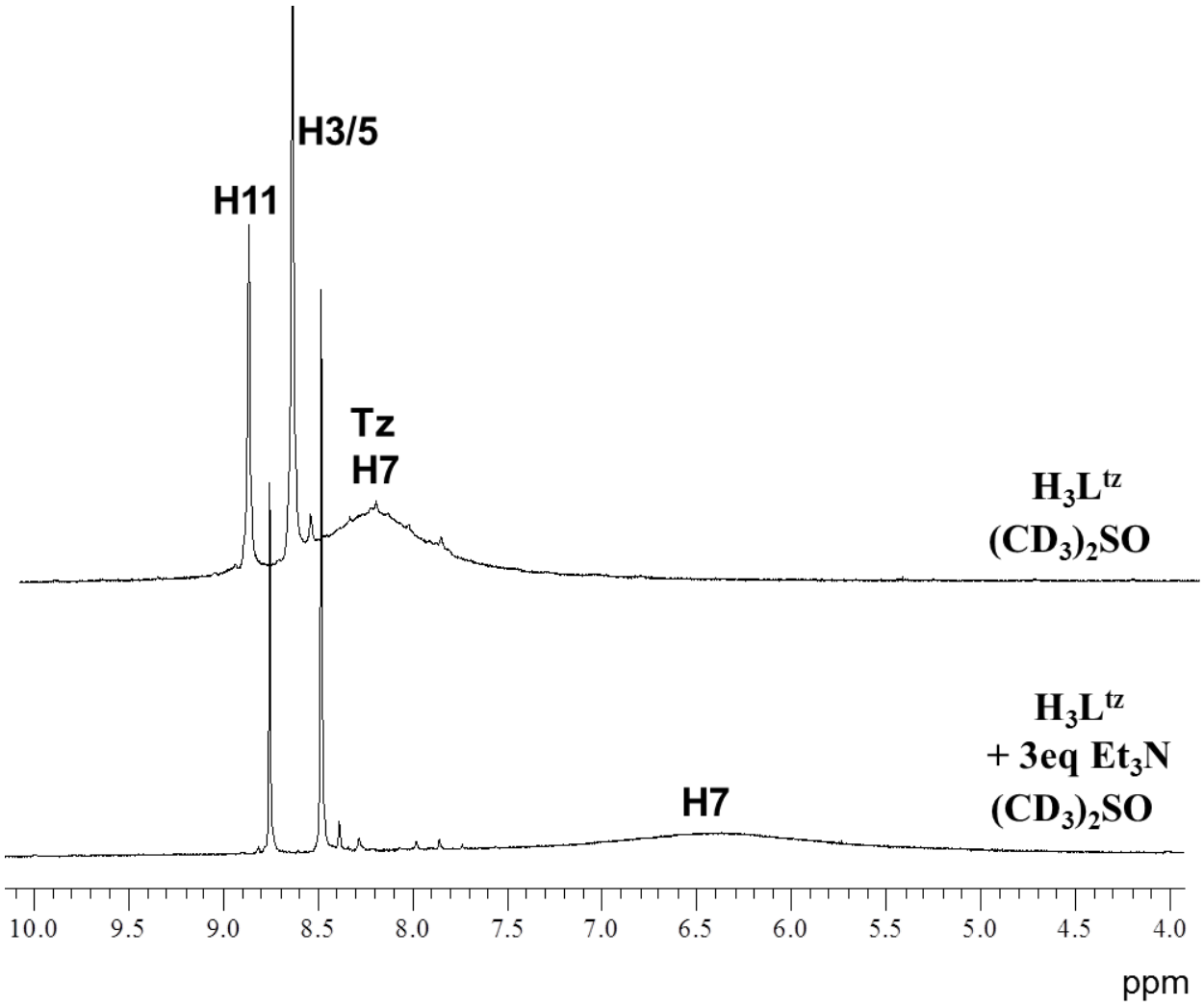

Figure S 1. ^{1}H NMR spectra (200 MHz) of H_3L^{tz} in $DMSOd_6$.

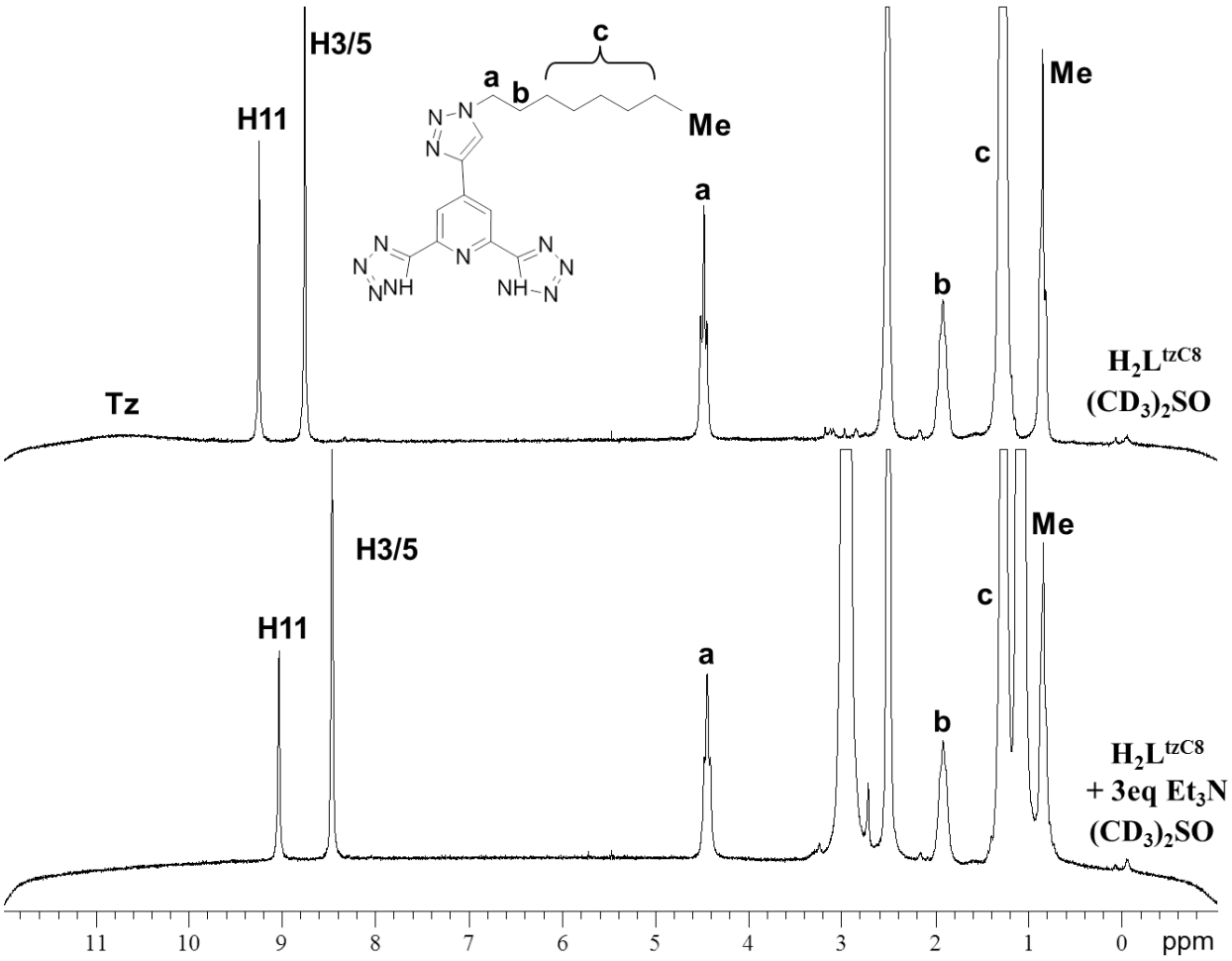

Figure S 2. ^{1}H NMR spectra (200 MHz) H_2L^{tzC8} in $DMSOd_6$.

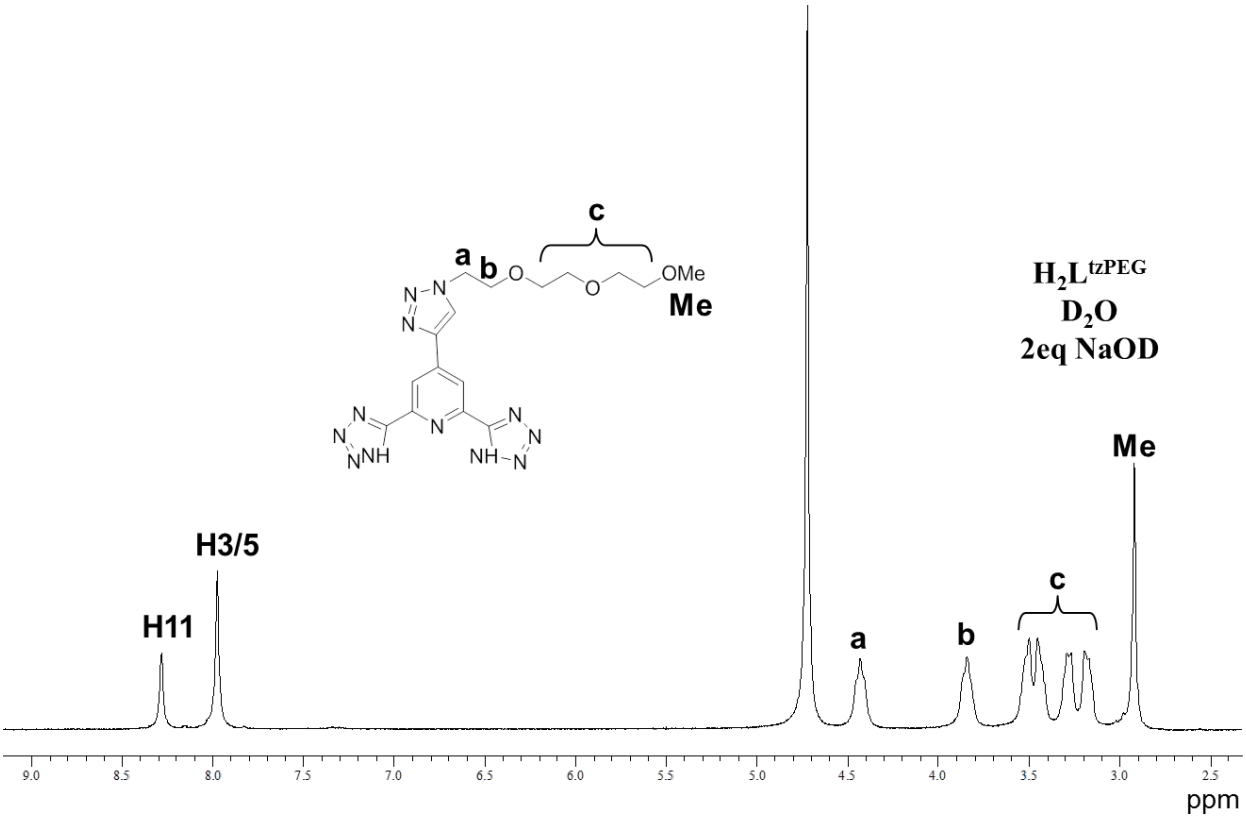

Figure S 3. ^{1}H NMR spectrum (200 MHz) of H_2L^{tzPEG} in D_2O.

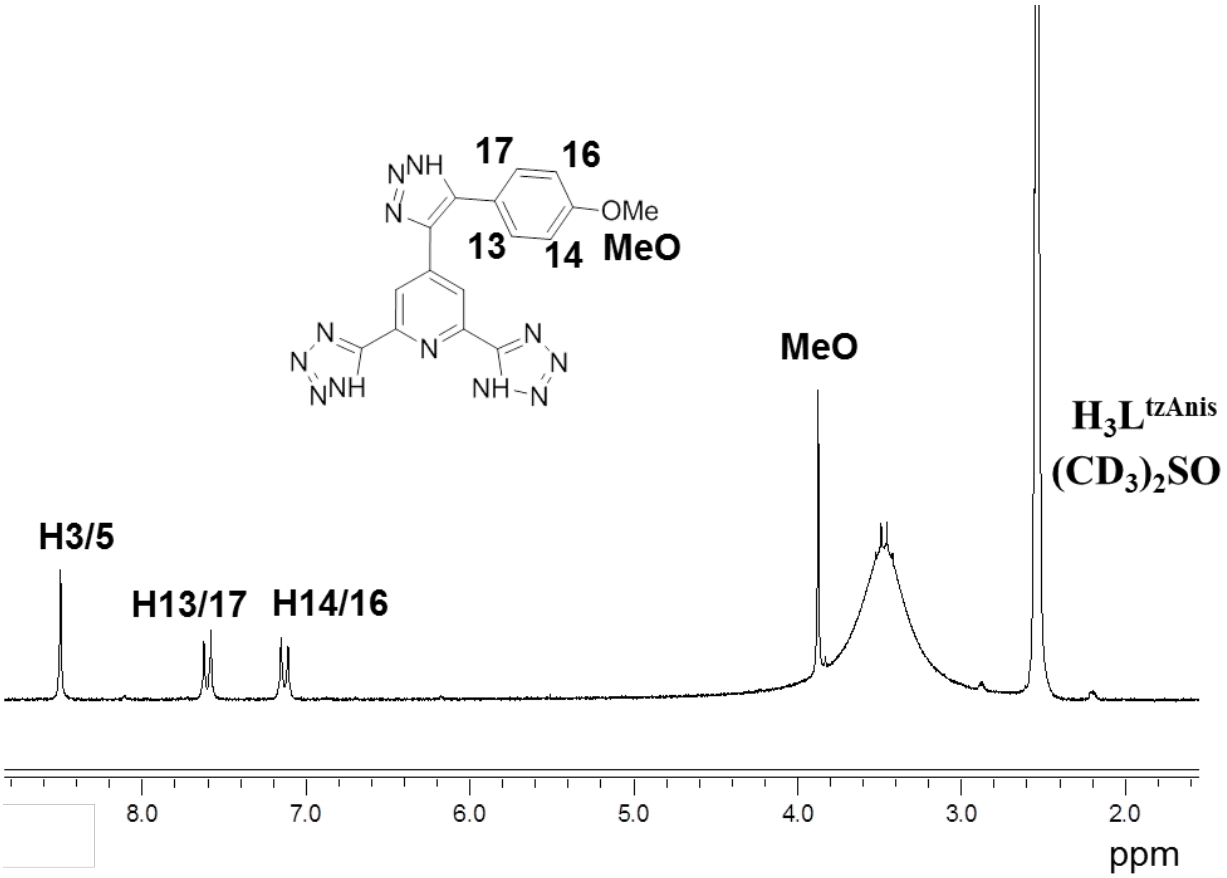

Figure S 4. ^{1}H NMR spectrum (200 MHz) of H_3L^{tzAnis} in $DMSOd_6$

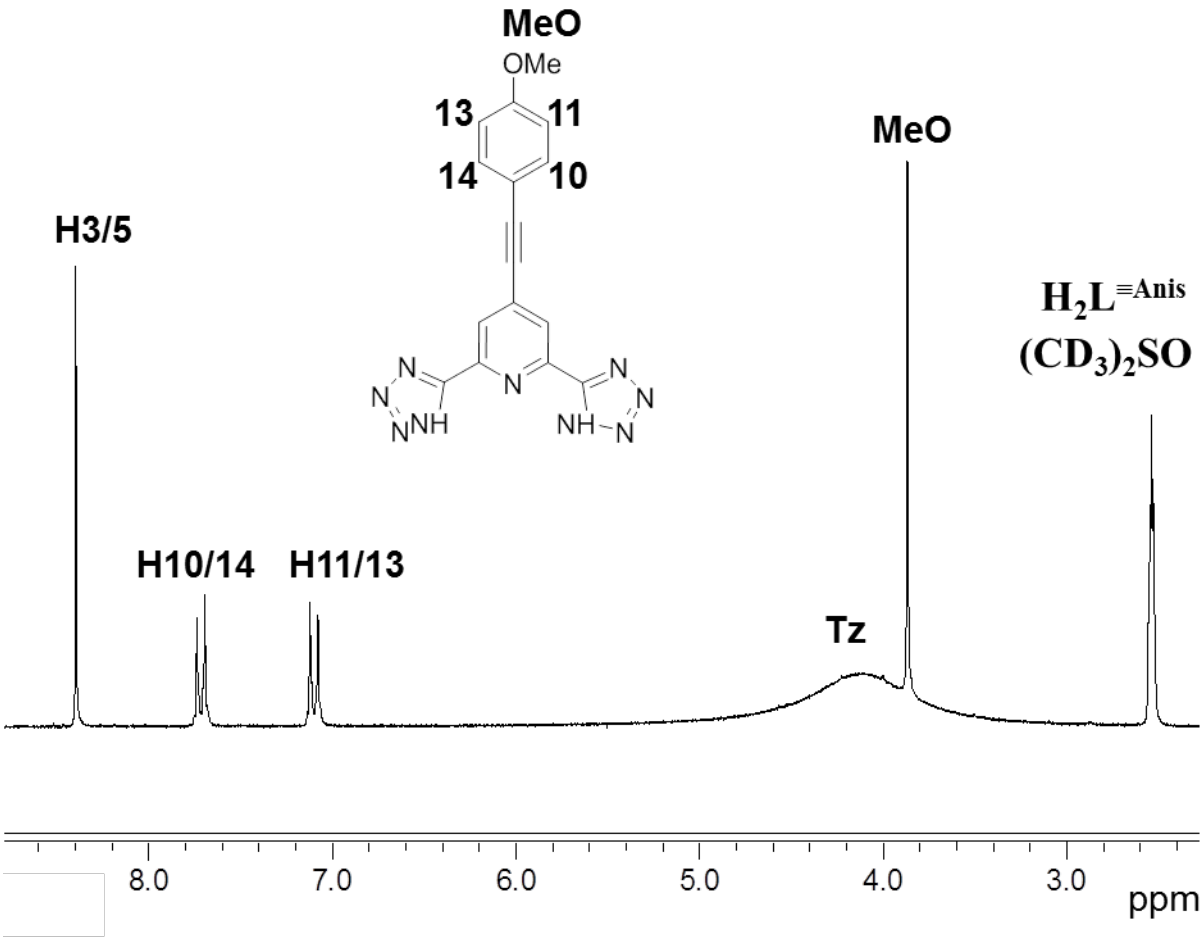

Figure S 5. H_2L_5 ^{1}H NMR spectrum (200 MHz) of $H_2L^{\equiv Anis}$ *in* $DMSOd_6$.

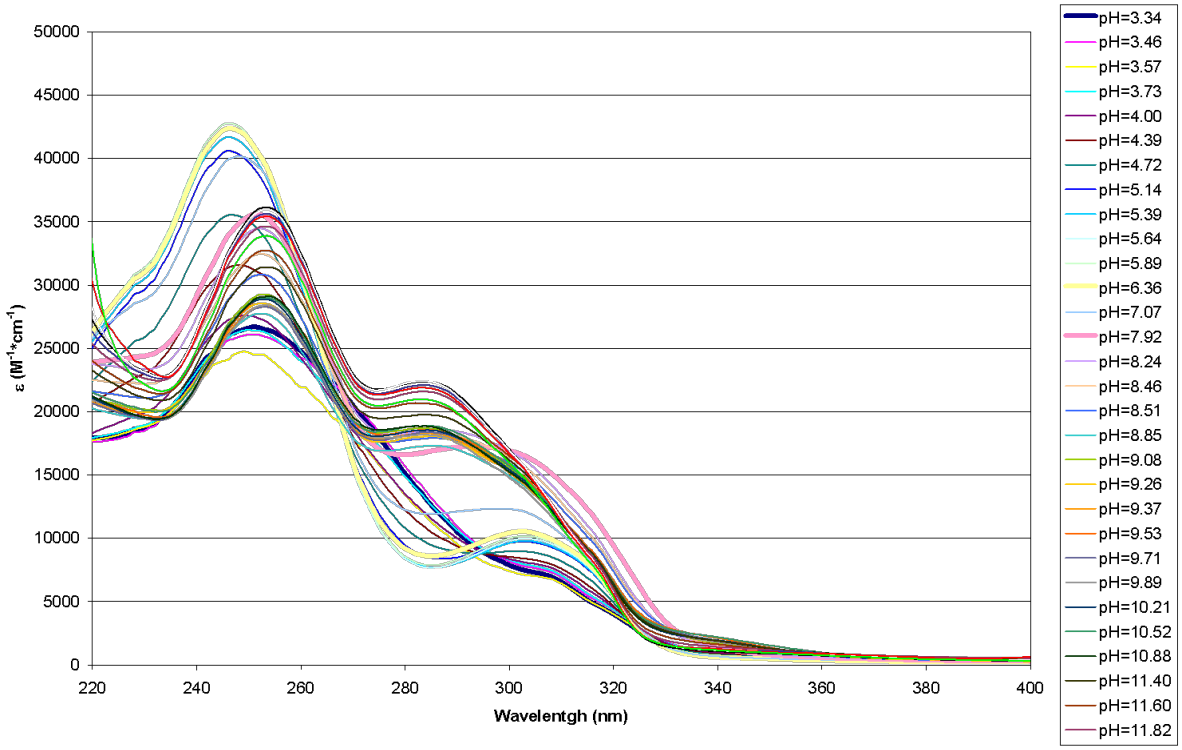

Figure S 6. UV-Vis absorption spectra of L^{tz} ($2.5*10^{-5}$M) as a function of pH, *I* = 1M (KCl) in water.

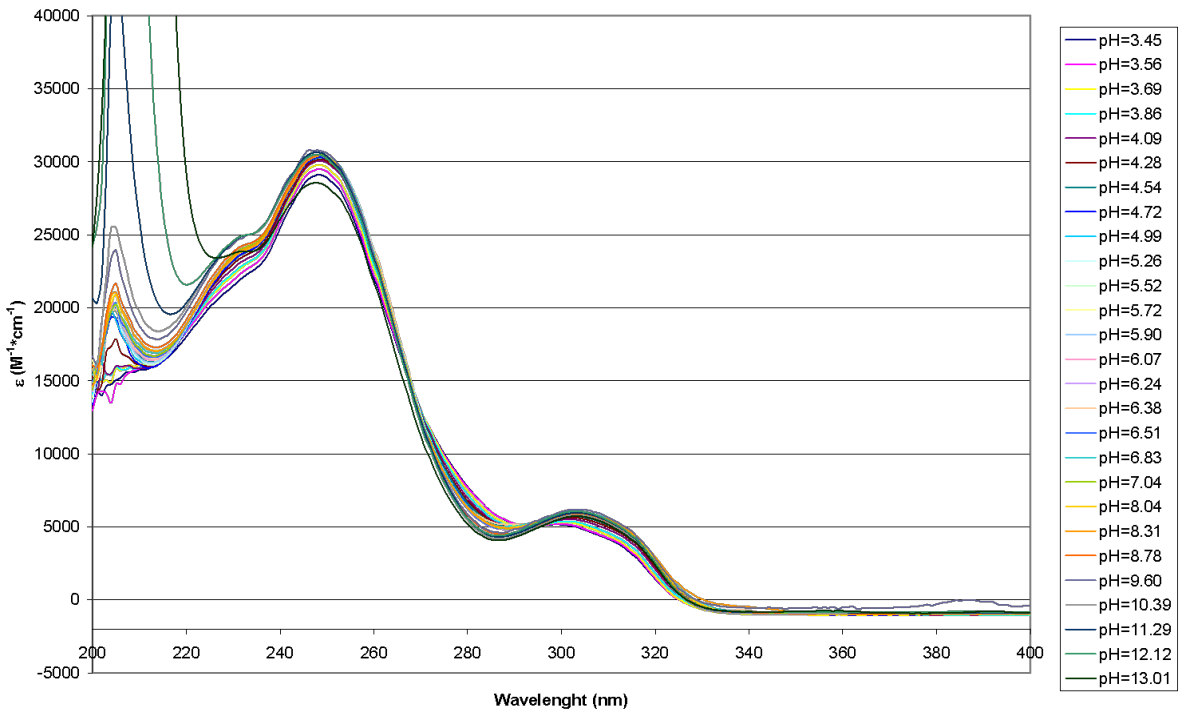

Figure S 7. UV-Vis absorption spectra of L^{tzPEG} ($2.5*10^{-5}$M) as a function of pH, *I* = 1M (KCl) in water.

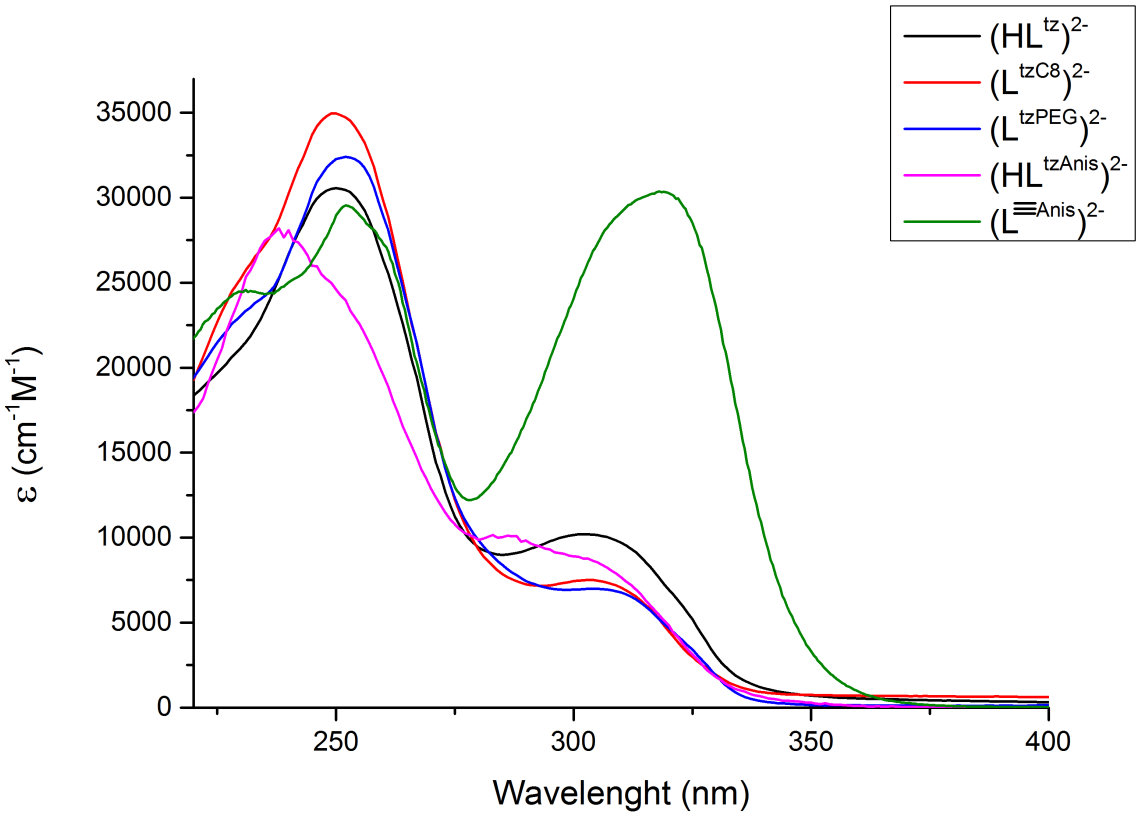

Figure S 8. Calculated extinction coefficient spectra of all the ligands ($2.5*10^{-5}$M), *I* = 1M (TMACl) in MeOH.

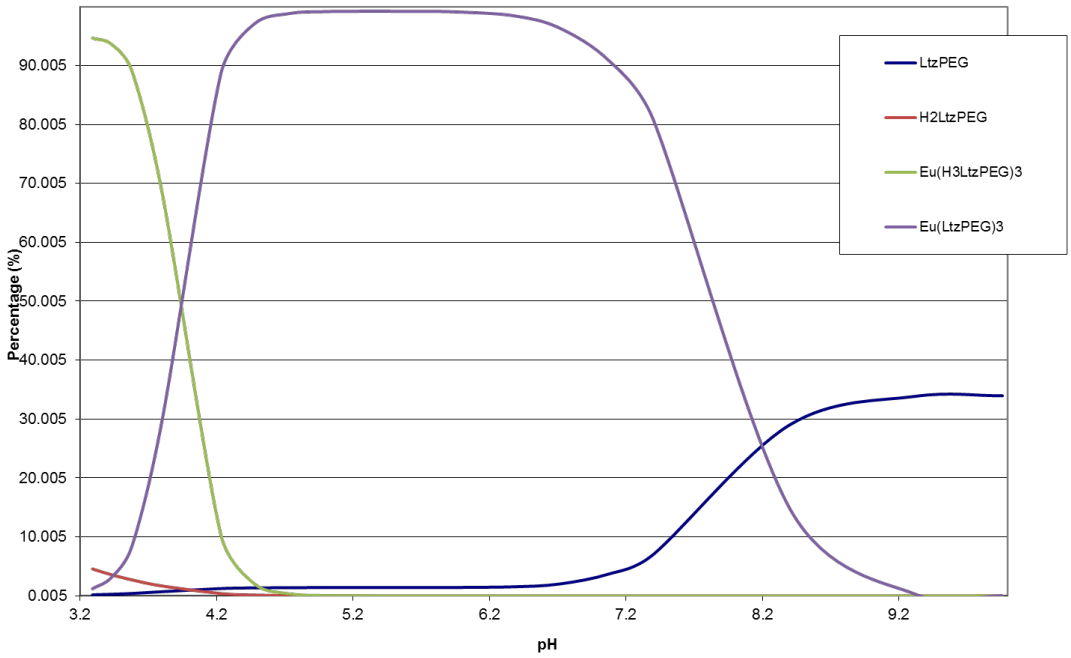

Figure S 9. Species distribution curves for $[Eu(L^{tzPEG})_3][Et_3NH]_3$ as a function of pH.

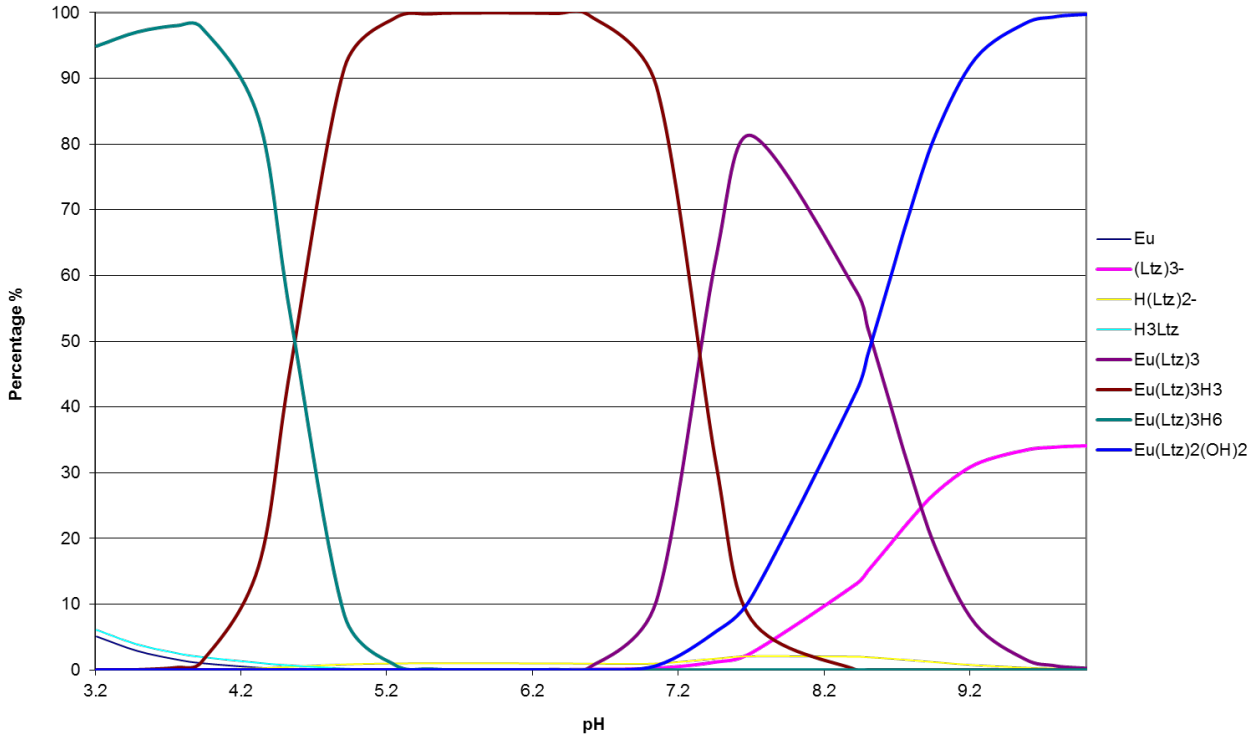

Figure S 10. Species distribution curves for $[Eu(HL^{tz})_3][Et_3NH]_3$ in function of the pH.

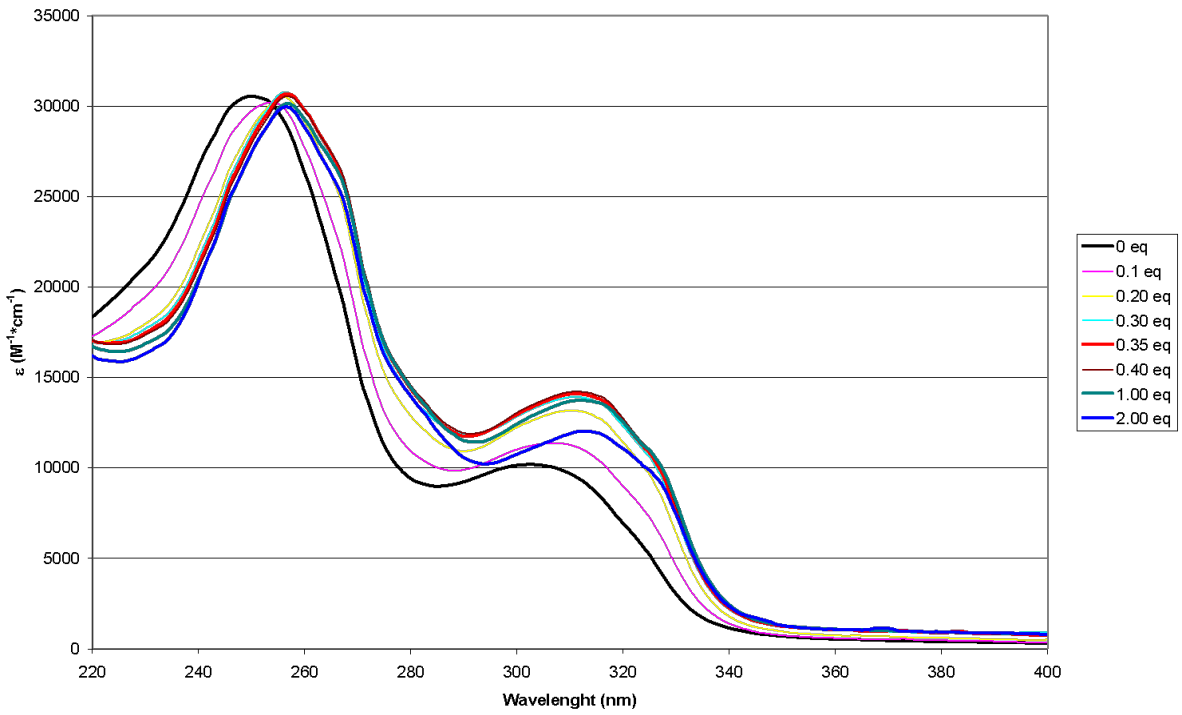

Figure S 11. Titration of L^{tz} ($2.5*10^{-5}$M) with europium triflate, *I* = 1M (TMACl) in MeOH.

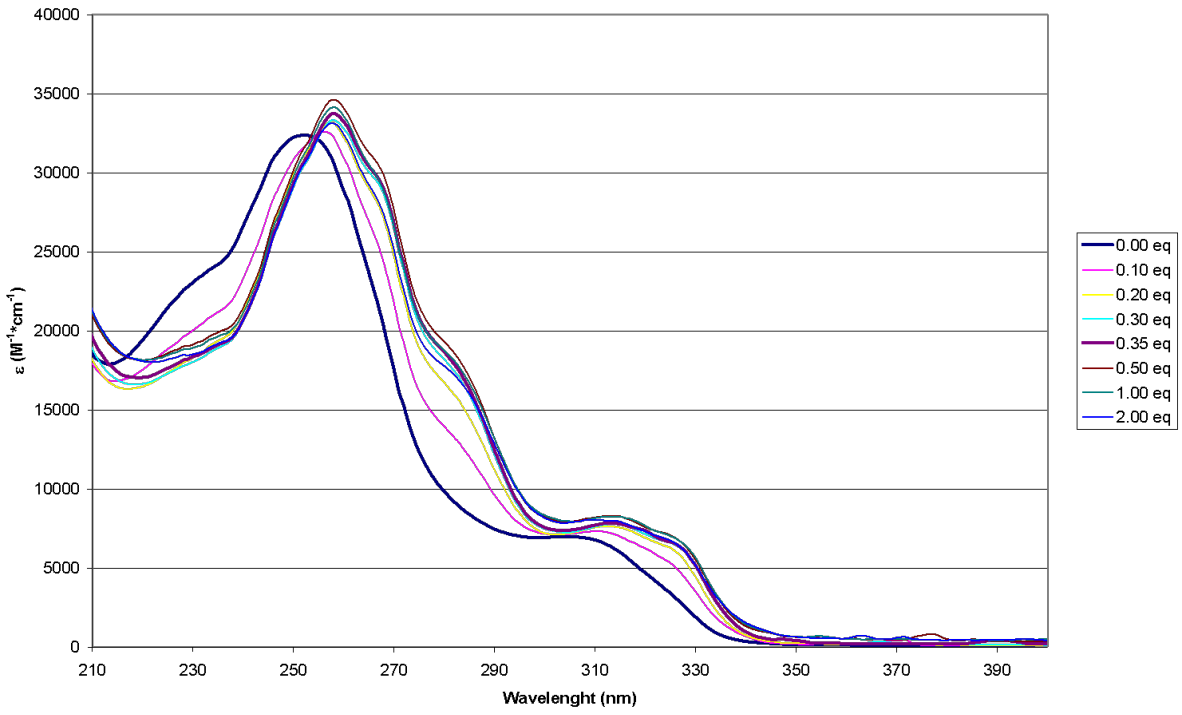

Figure S 12. Titration of L^{tzC8} ($2.5*10^{-5}$M) with europium triflate, *I* = 1M (TMACl) in MeOH.

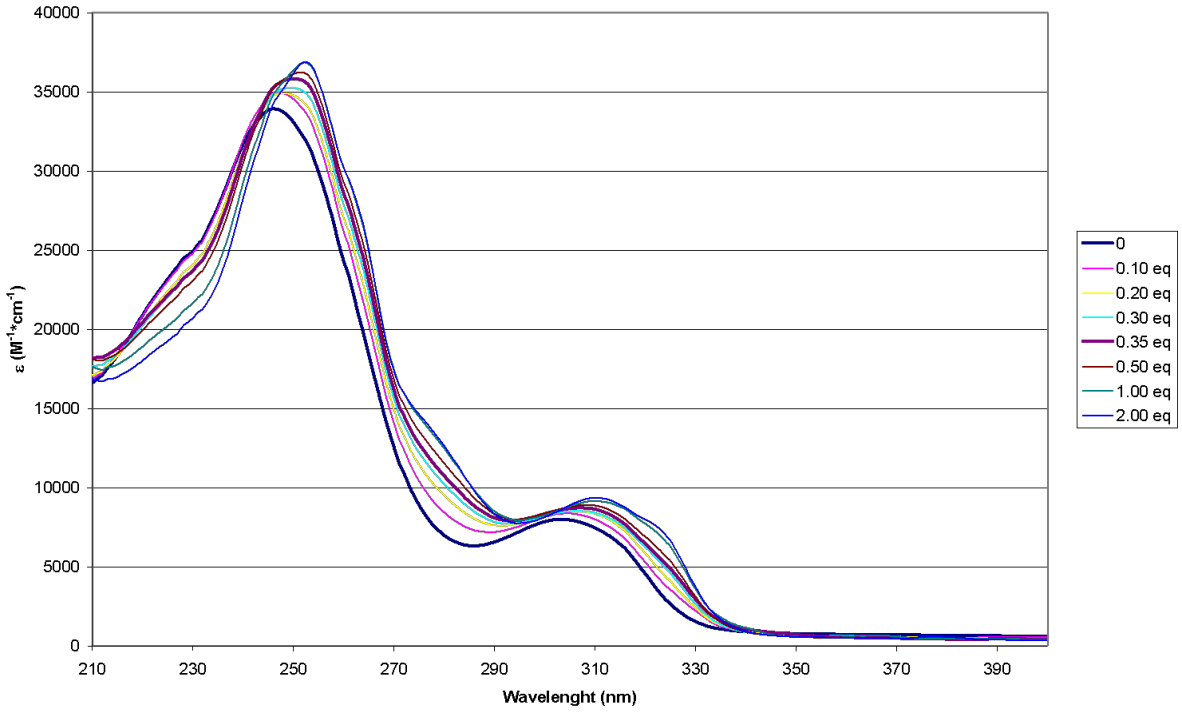

Figure S 13. Titration of L^{tz} ($2.5*10^{-5}$M) with europium triflate in MES buffer.

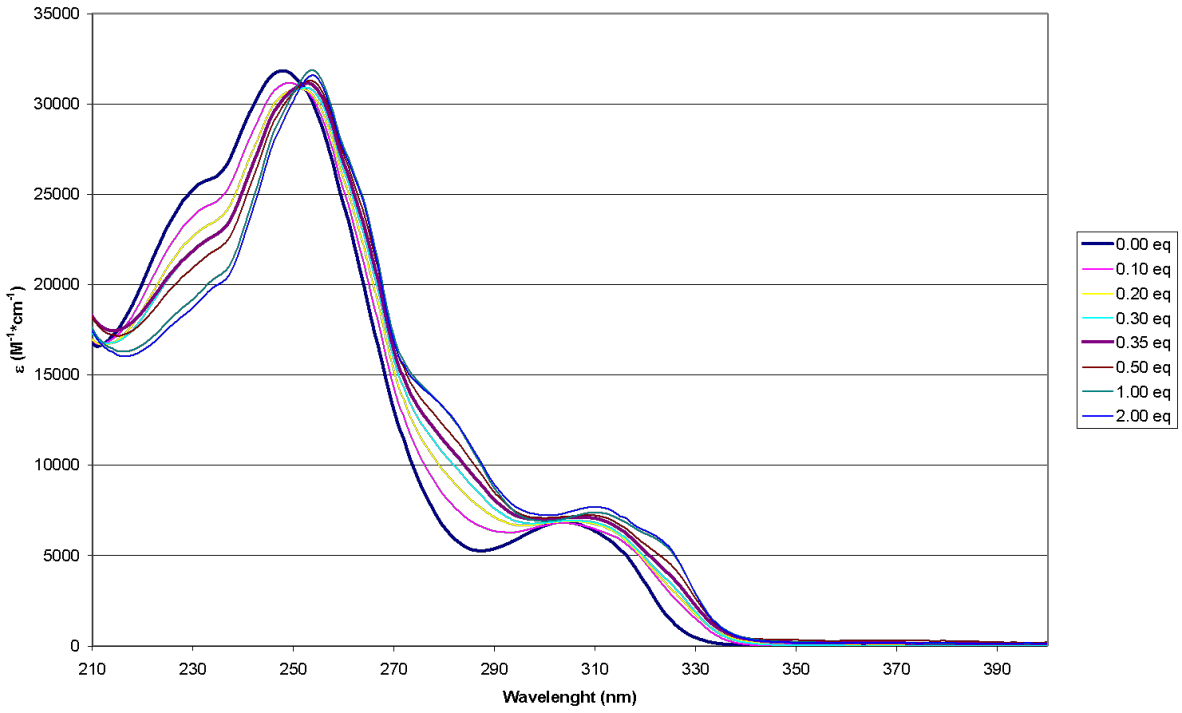

Figure S 14. Titration of L^{tzPEG} ($2.5*10^{-5}$M) with europium triflate in water MES buffer.

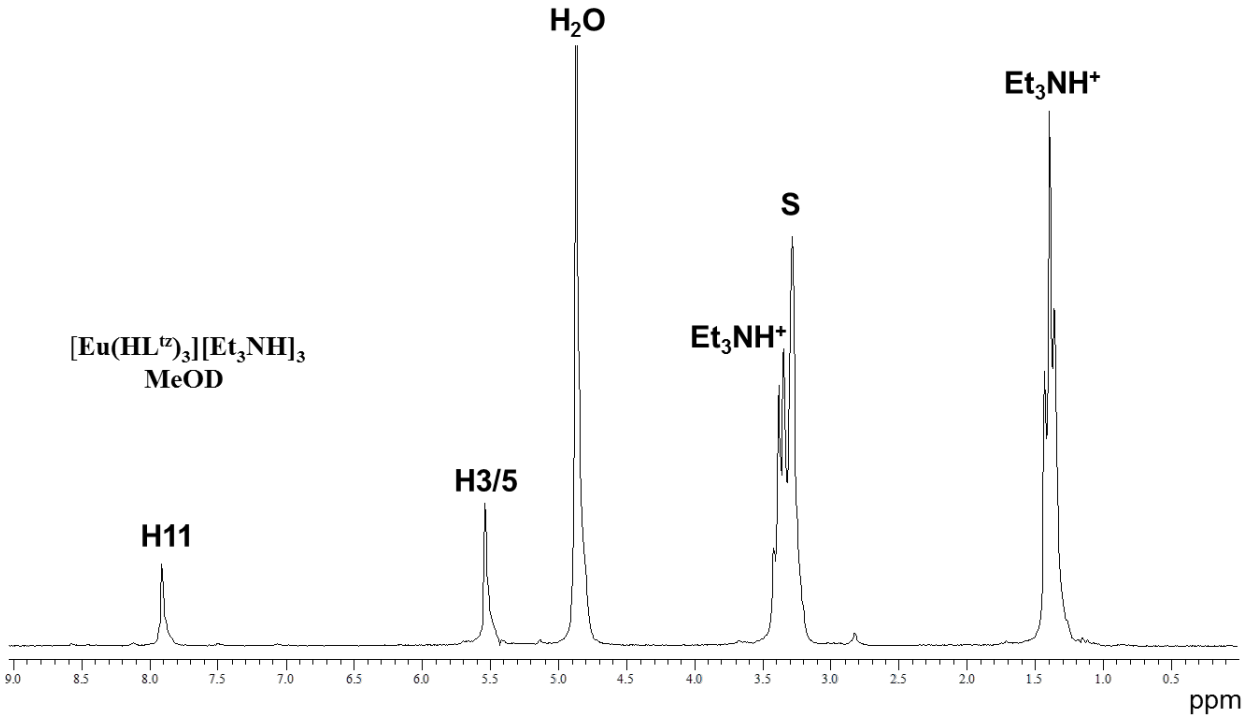

Figure S 15. ^{1}H NMR spectrum of $[Eu(HL^{tz})_3][Et_3NH]_3$ in CD_3OD (200 MHz).

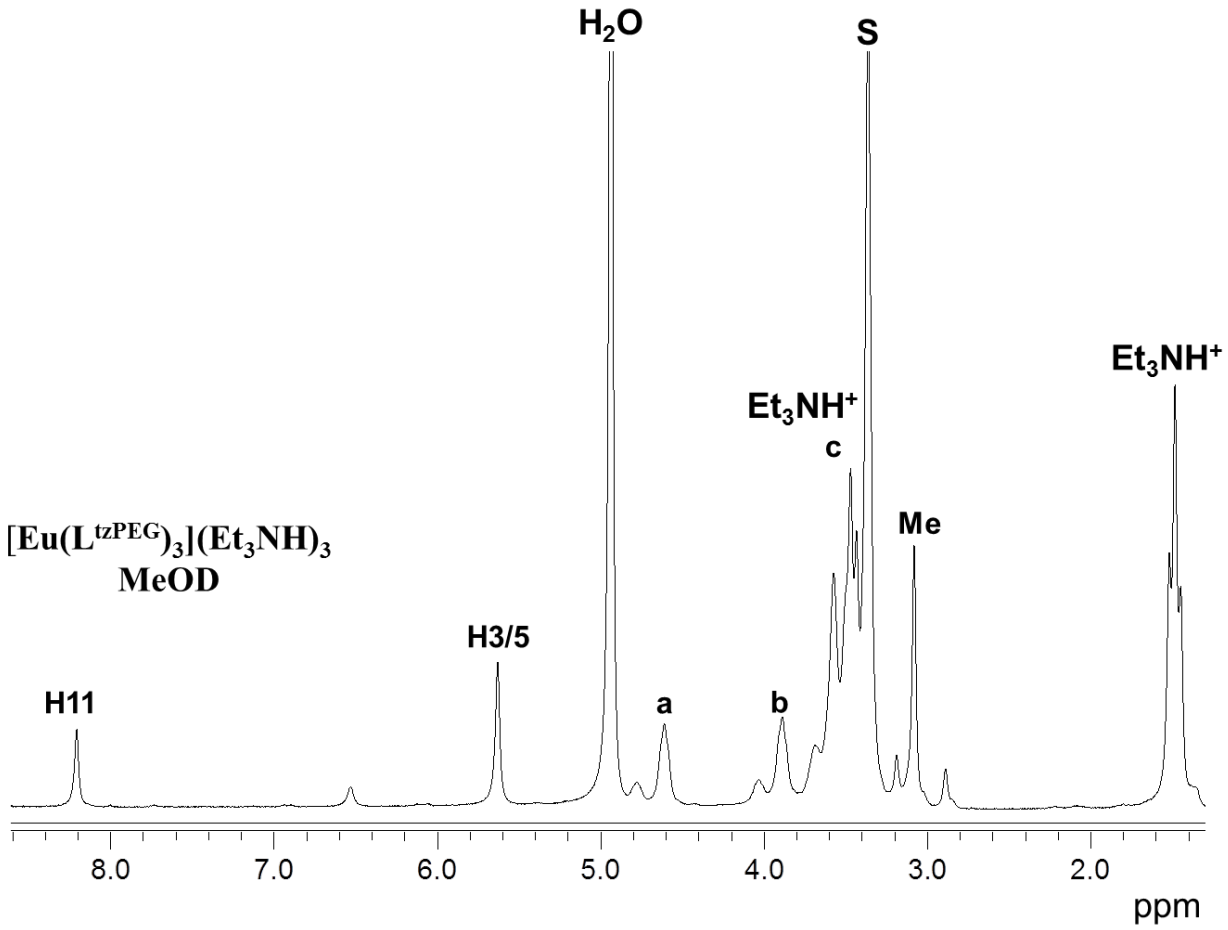

Figure S 16. ^{1}H NMR spectrum of $[Eu(L^{tzPEG})_3][Et_3NH]_3$ ^{1}H NMR spectrum in CD_3OD (200 MHz).

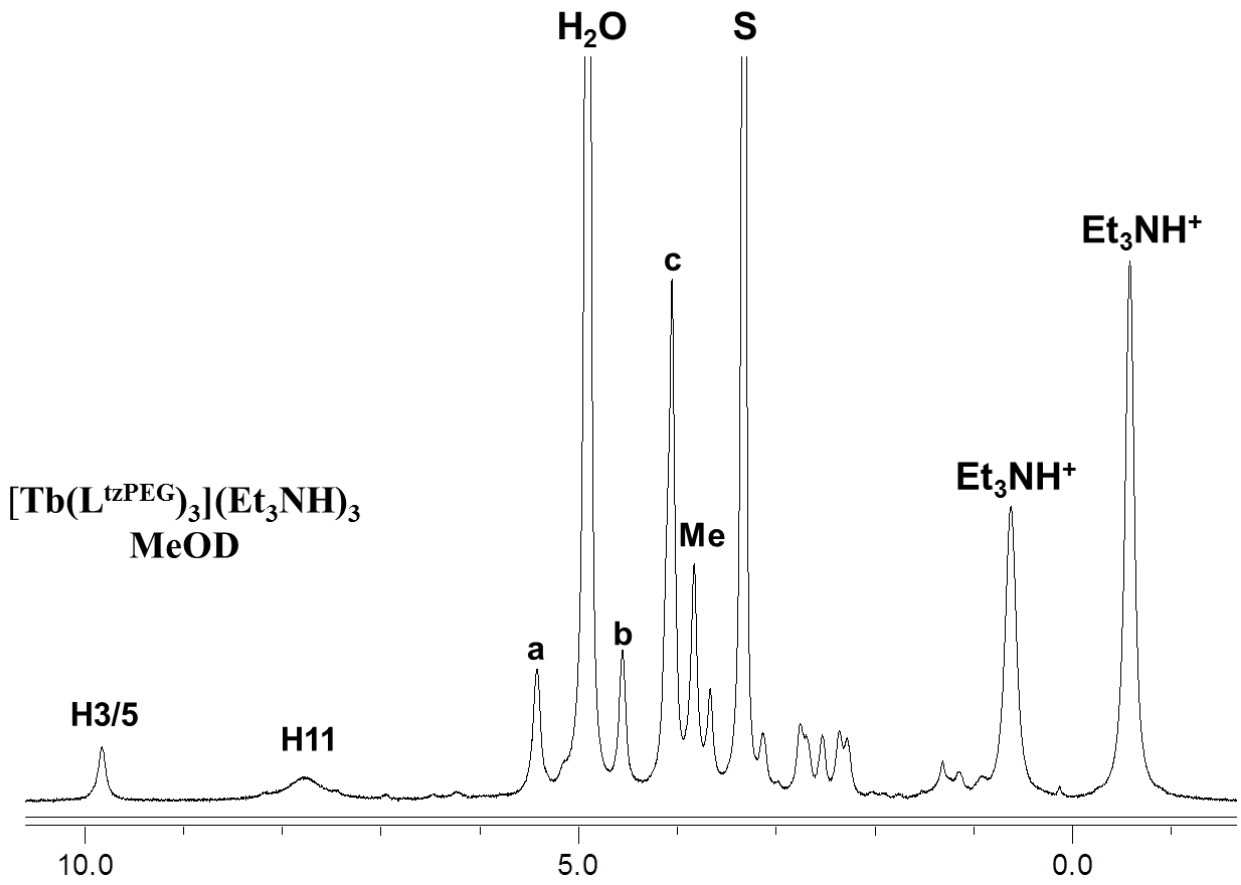

Figure S 17. ^{1}H NMR spectrum of $[Tb(L^{tzPEG})_3][Et_3NH]_3$ in CD_3OD (200 MHz).

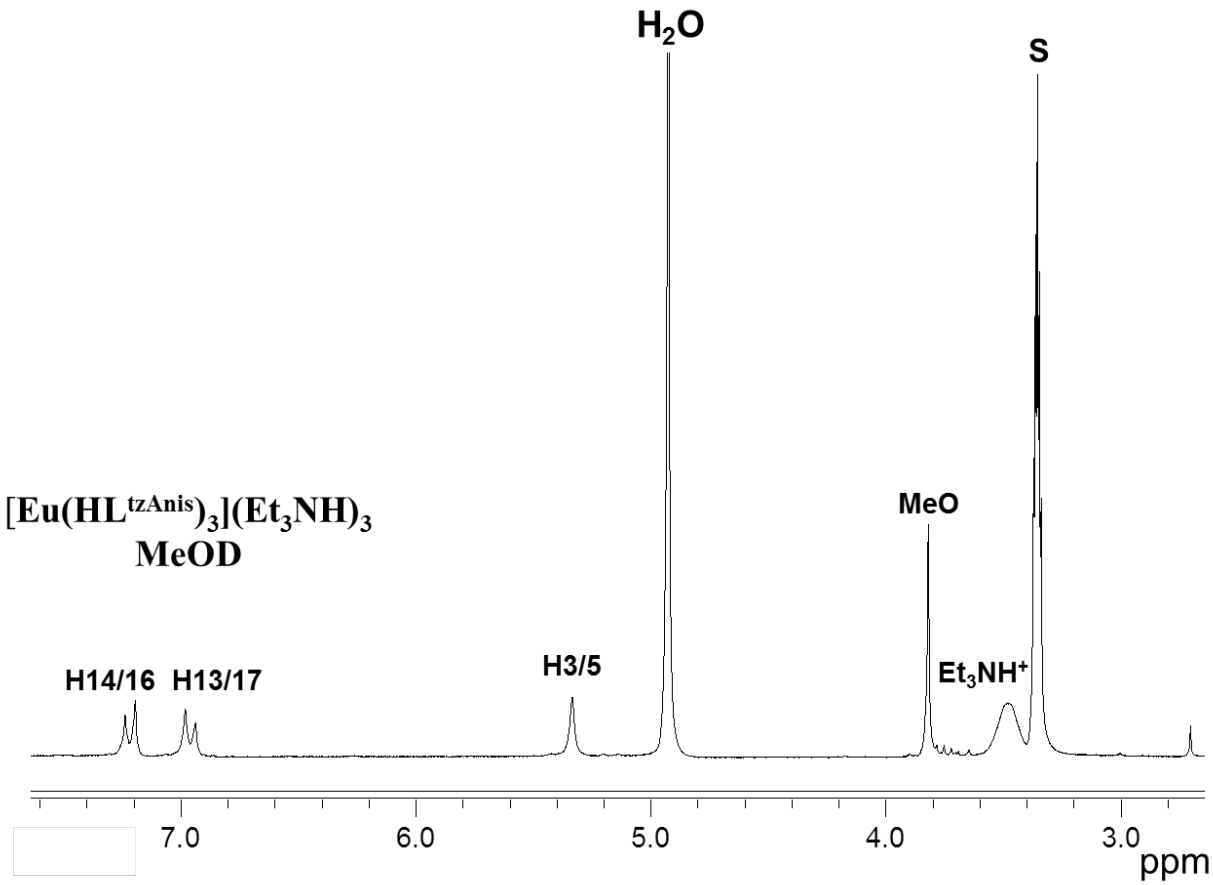

Figure S 18. ^{1}H NMR spectrum of $[Eu(HL^{tzAnis})_3][Et_3NH]_3$ in CD_3OD (200 MHz).

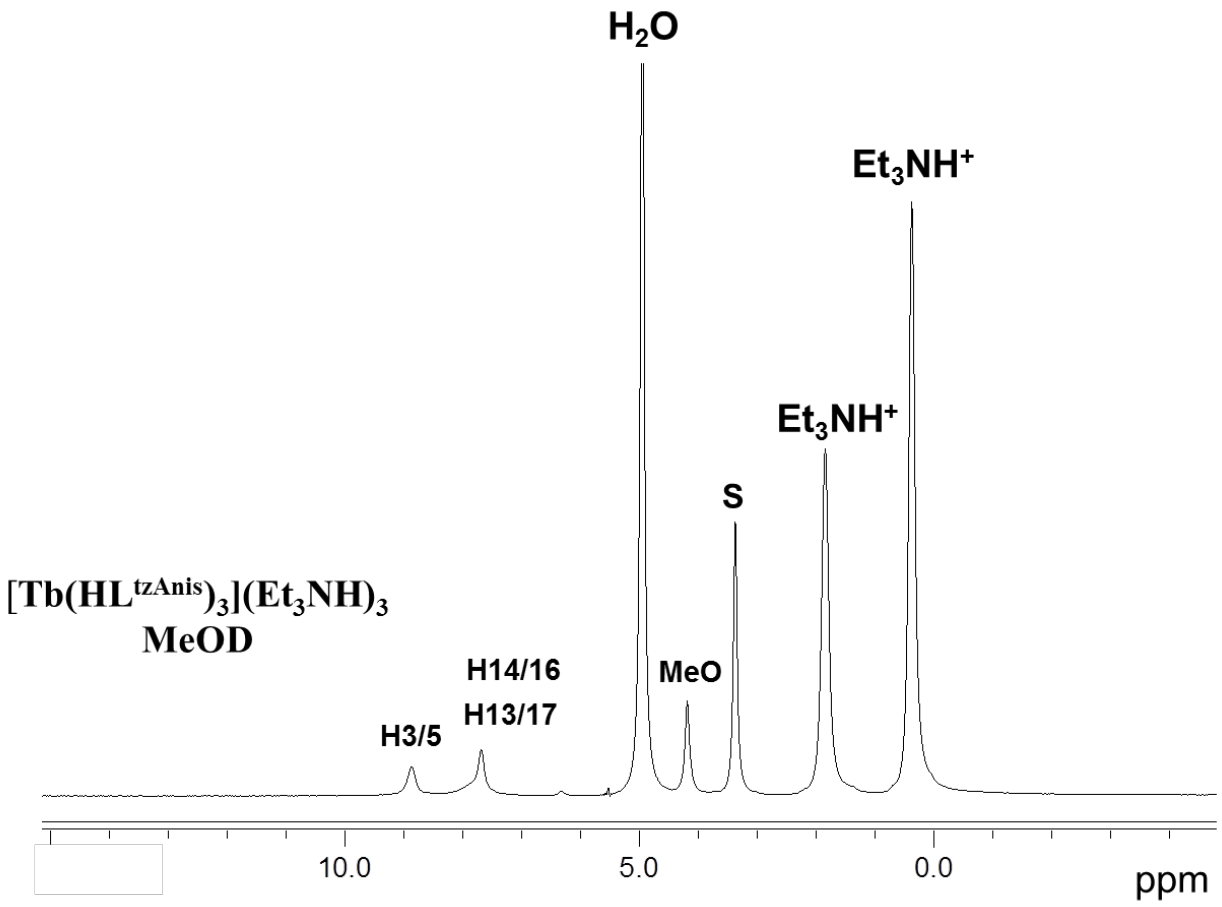

Figure S 19. ^{1}H NMR spectrum of $[Tb(HL^{tzAnis})_3][Et_3NH]_3$ in CD_3OD (200 MHz).

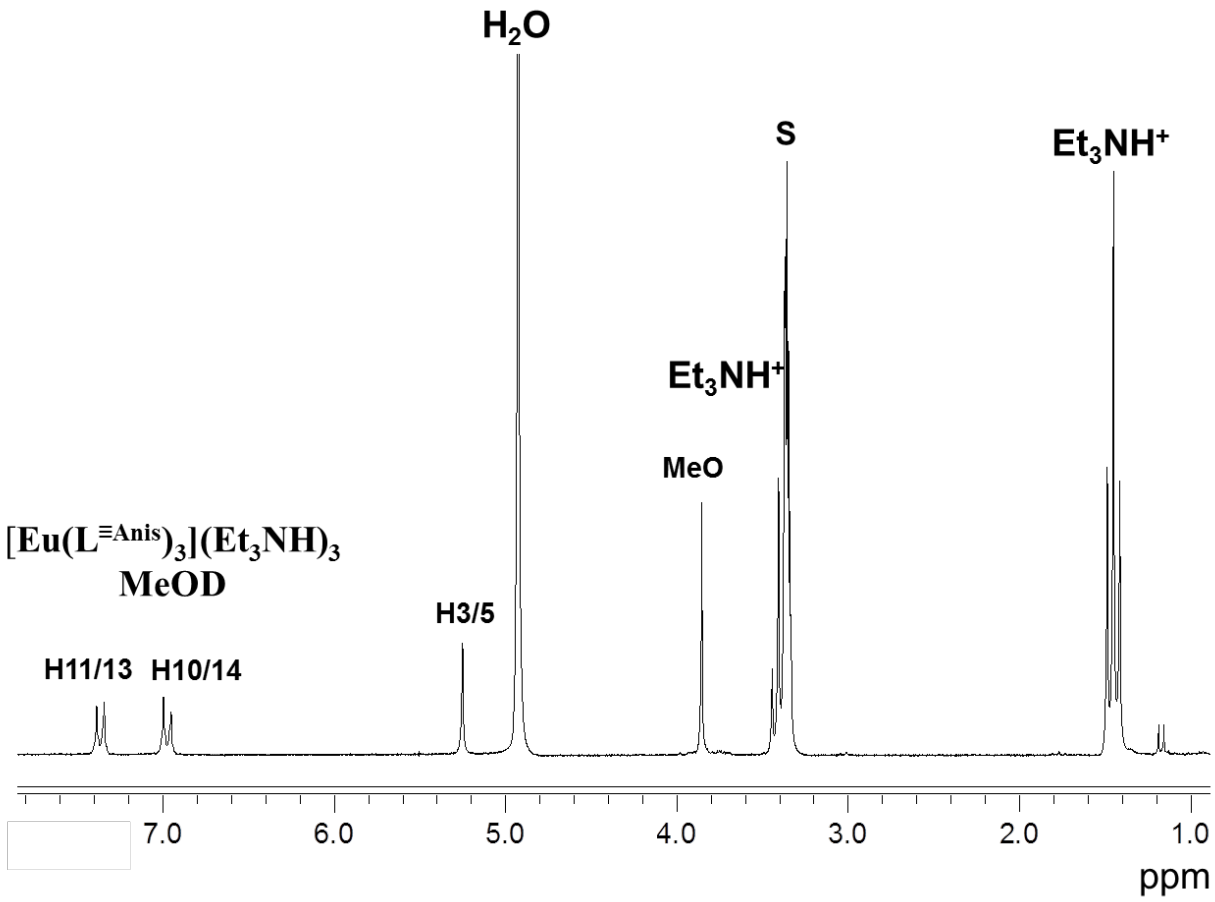

Figure S 20. ^{1}H NMR spectrum of $[Eu(L^{\equiv Anis})_3][Et_3NH]_3$ in CD_3OD (200 MHz).

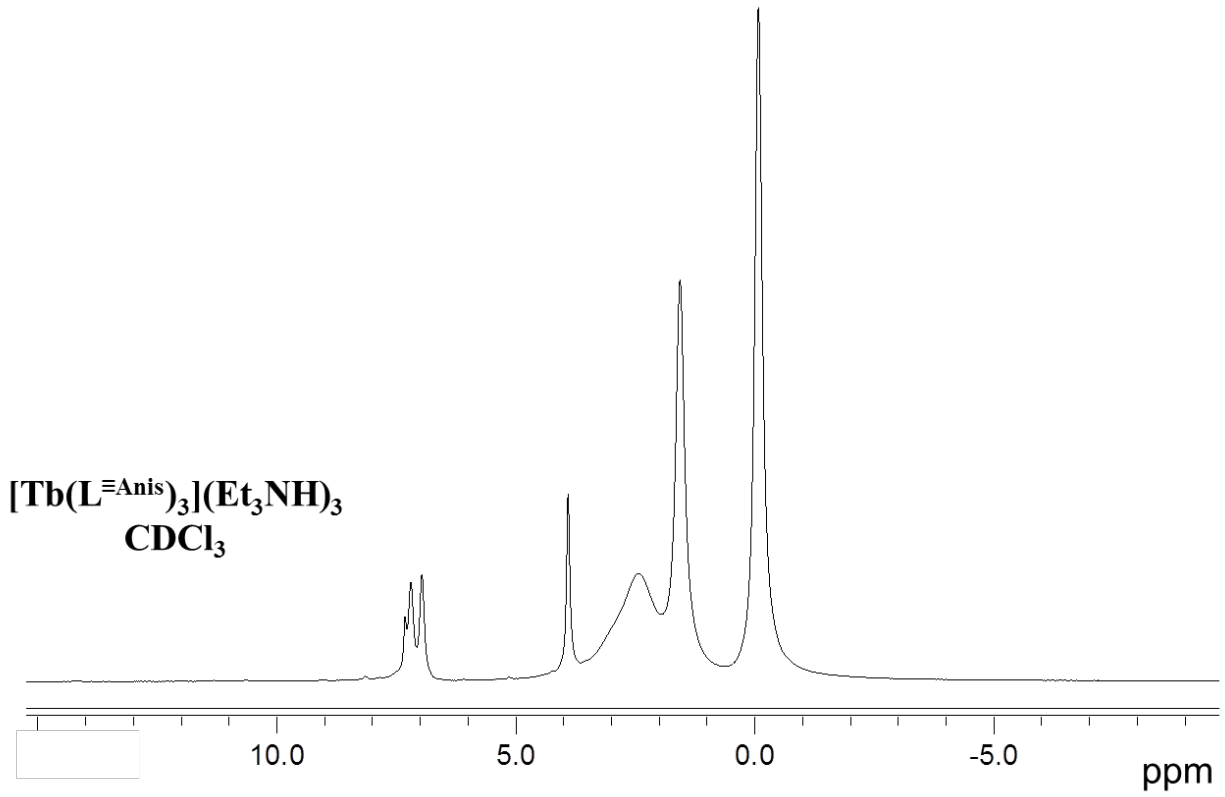

Figure S 21. ^{1}H NMR spectrum of $[Tb(L^{\equiv Anis})_3][Et_3NH]_3$ in CD_3OD (200 MHz).

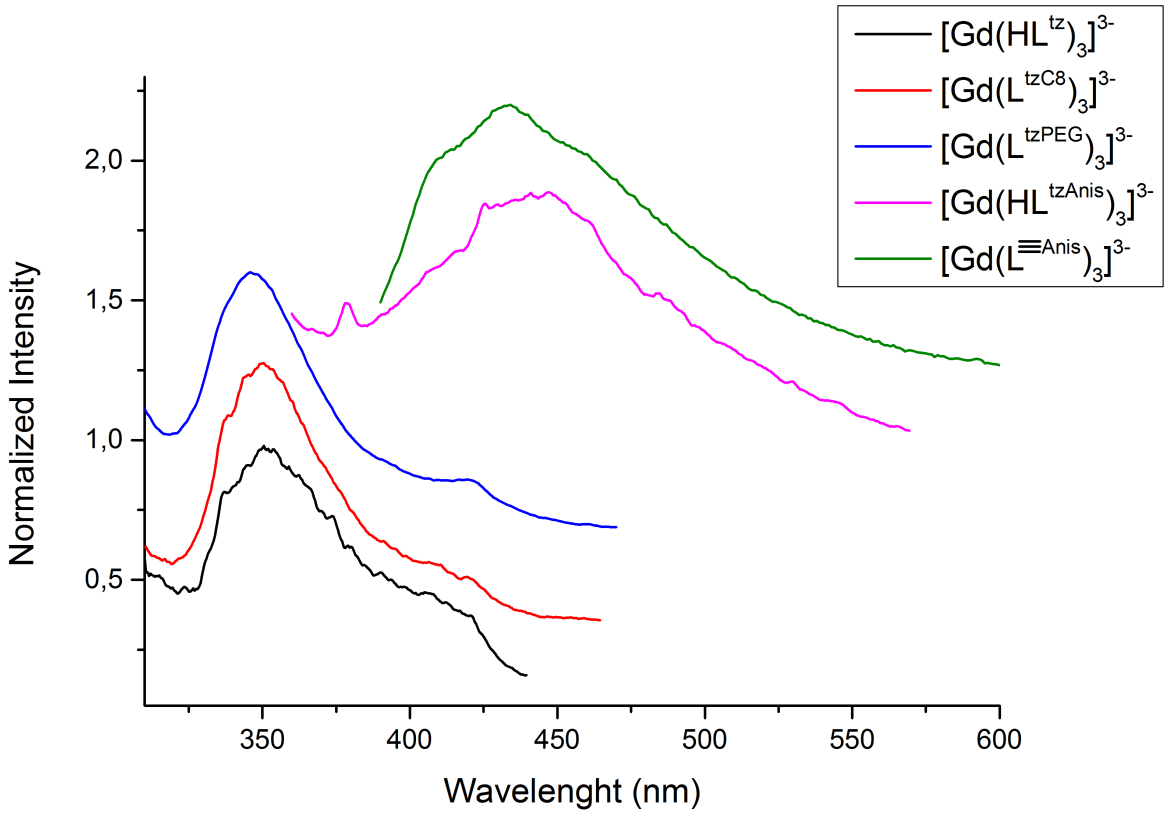

Figure S 22. Normalized emission spectra (singlet state) of the gadolinium complexes of all the ligands in MeOH.

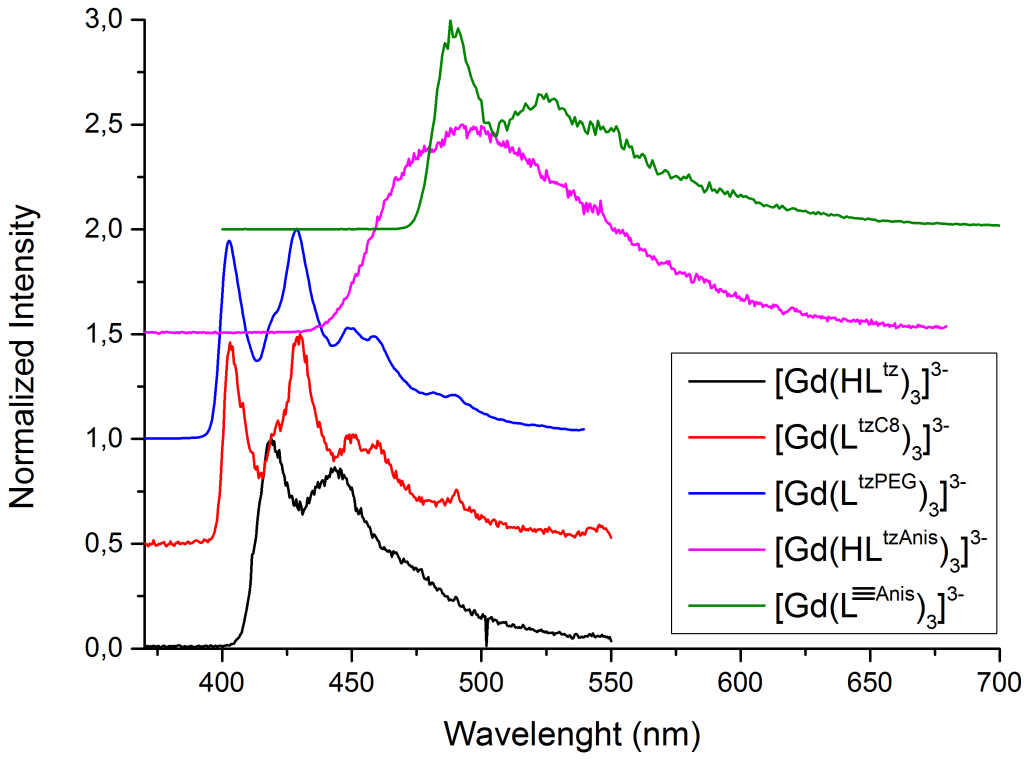

Figure S 23. Normalized emission spectra (triplet state) of the gadolinium complexes of all the ligands upon enforcement of a time delay (0.2 ms), in MeOH at 77 K

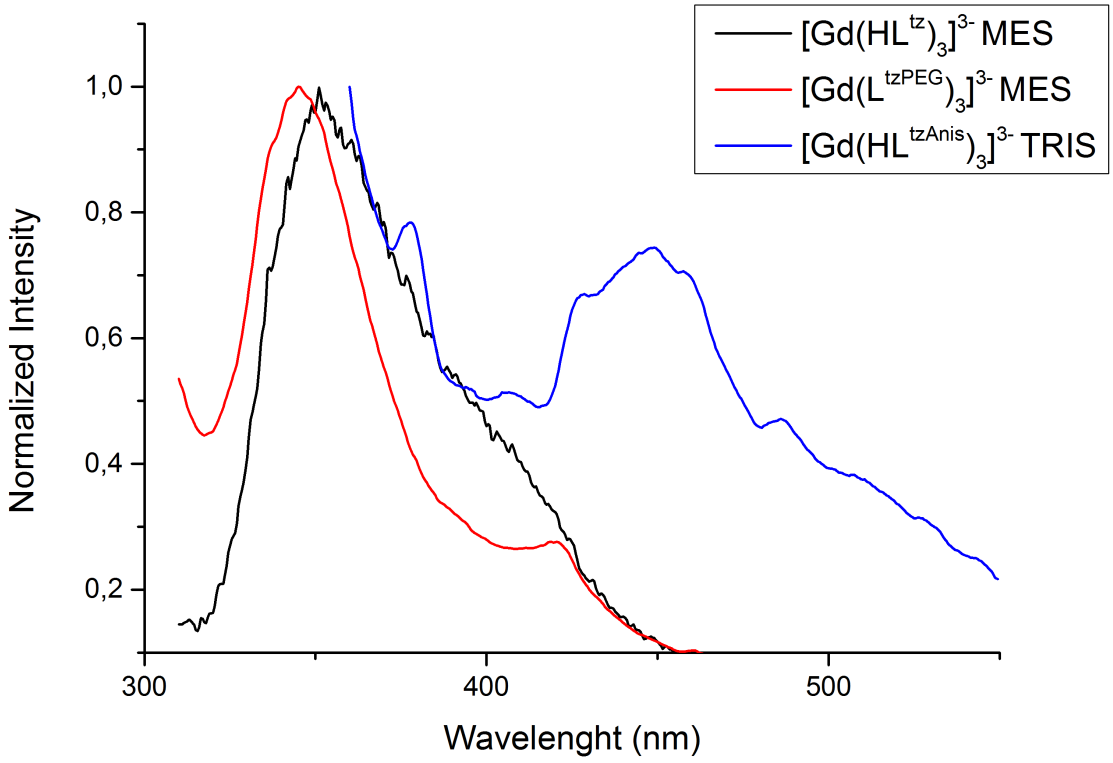

Figure S 24. Normalized emission spectra (singlet state) in water of the gadolinium complexes of L^{tz}, L^{tzPEG} and L^{tzAnis}.

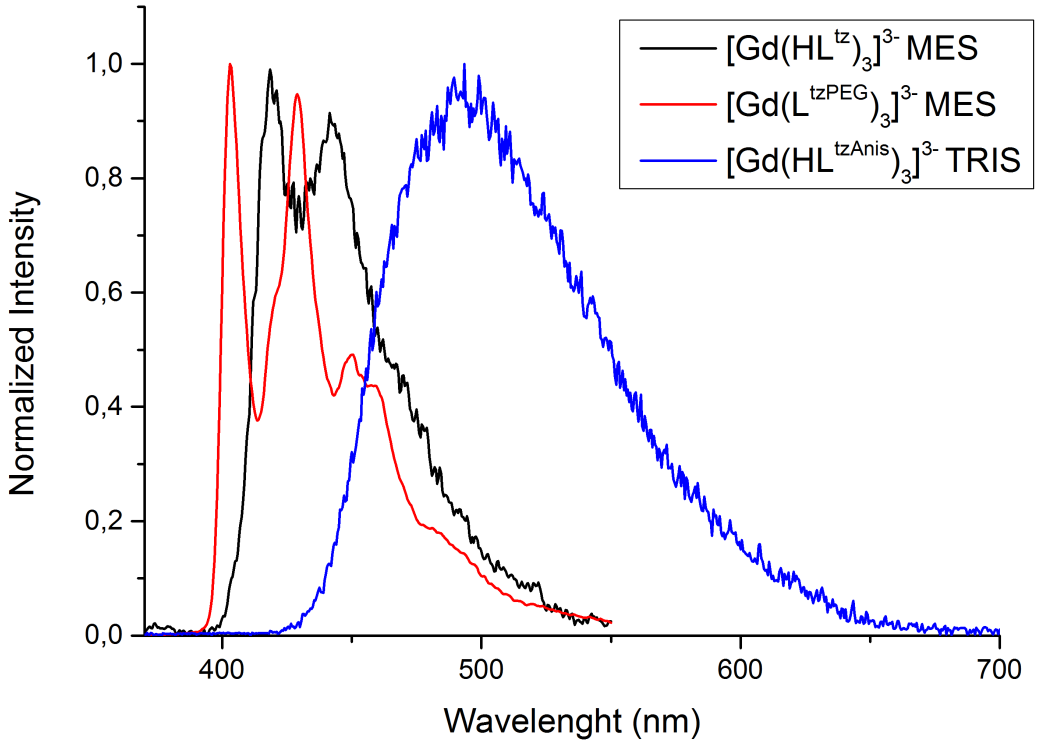

Figure S 25. Normalized emission spectra (triplet state) in water at 77K of the gadolinium complexes of L^{tz}, L^{tzPEG} and L^{tzAnis} upon enforcement of a time delay (0.2 ms).

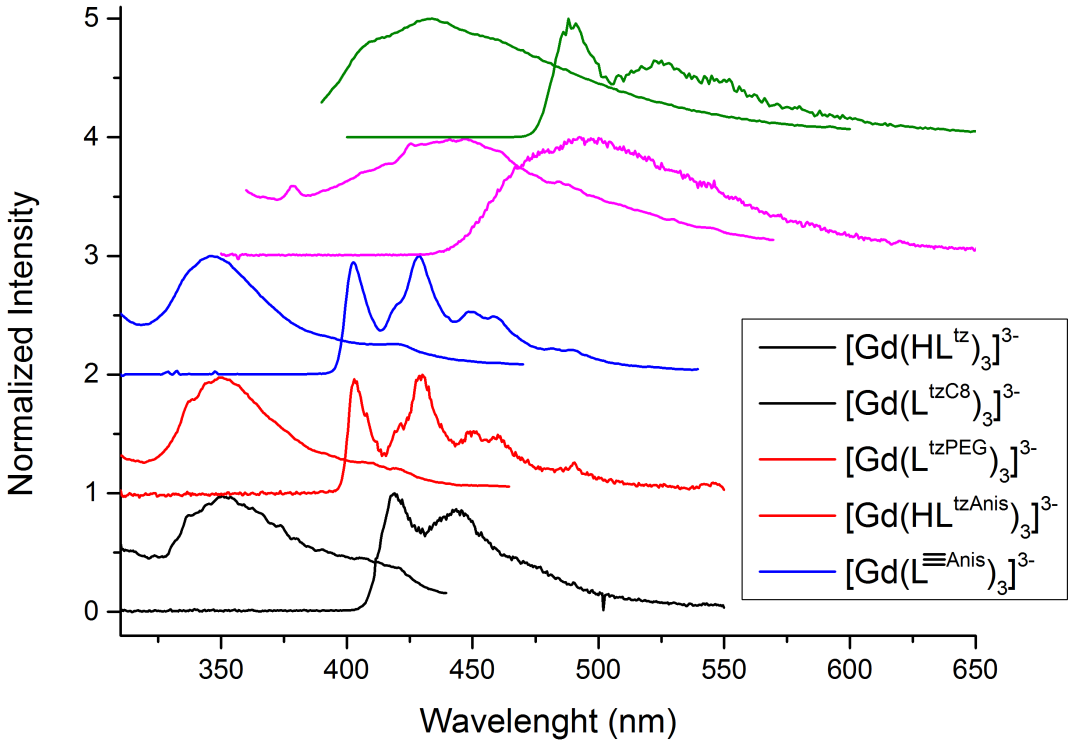

Figure S 26. Overall singlet/triplet state comparison for the gadolinium complexes of all the ligands in methanol.

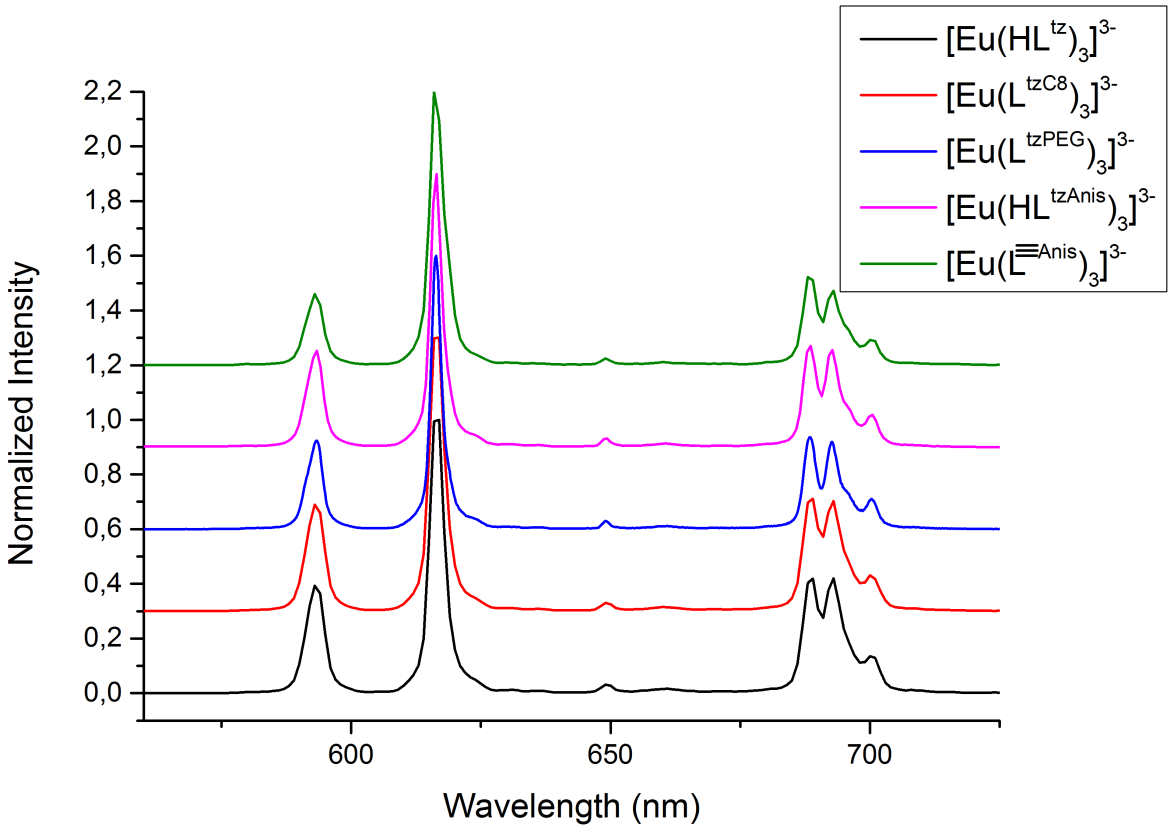

Figure S 27. Normalized emission spectra of the europium complexes of all the ligands in methanol.

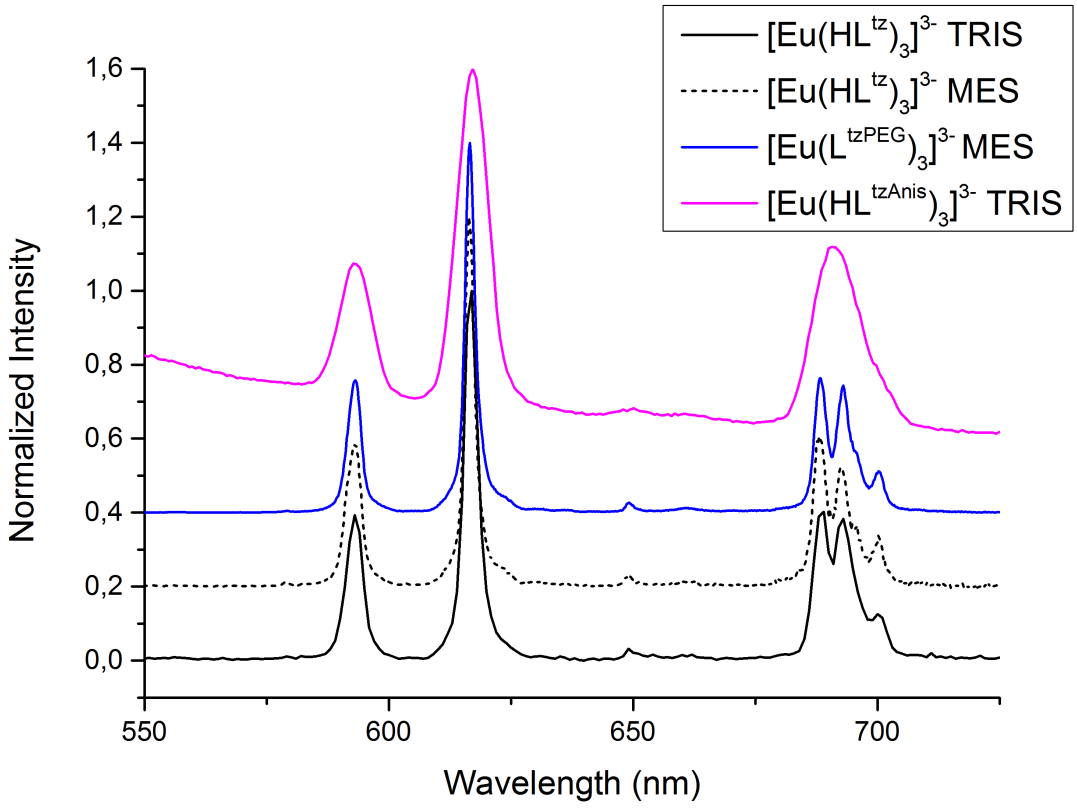

Figure S 28. Normalized emission spectra of europium complexes of L^{tz}, L^{tzPEG} and L^{tzAnis} in MES/TRIS buffer.

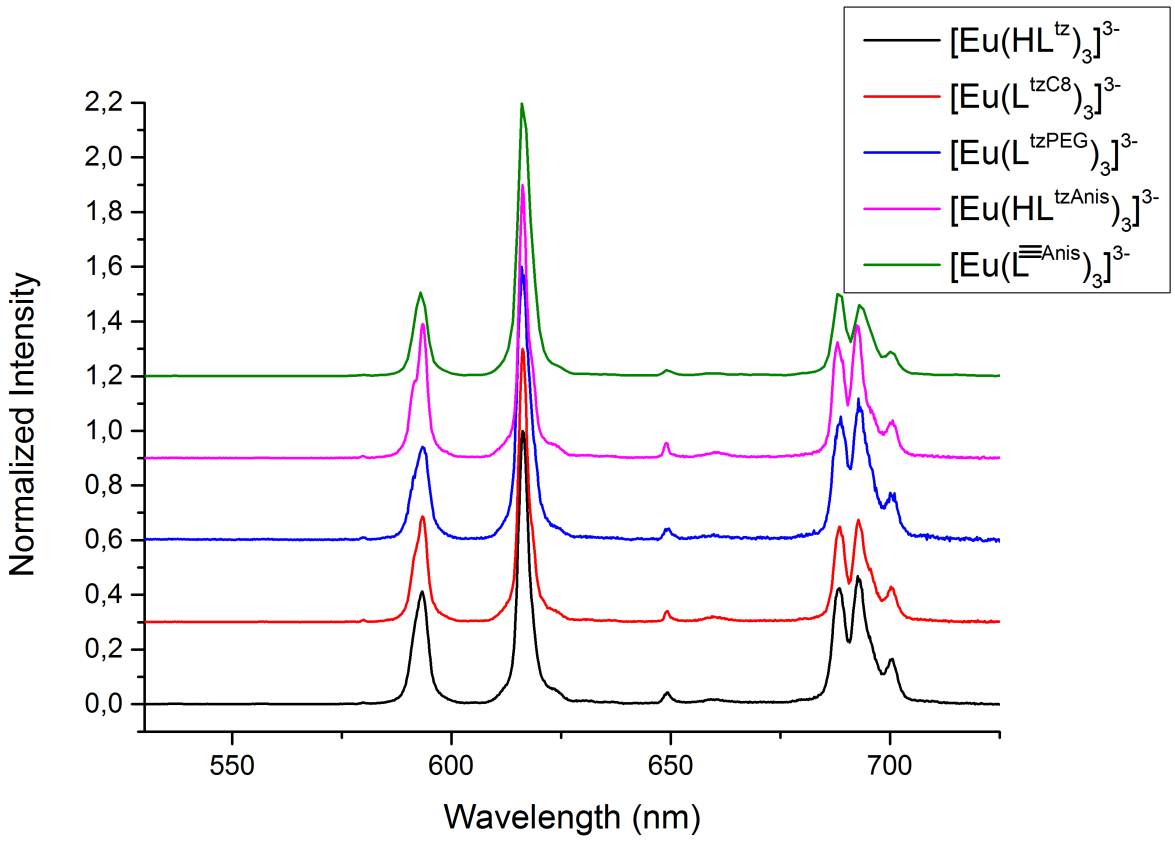

Figure S 29. Normalized emission spectra of the europium complexes of all the ligands in solid state.

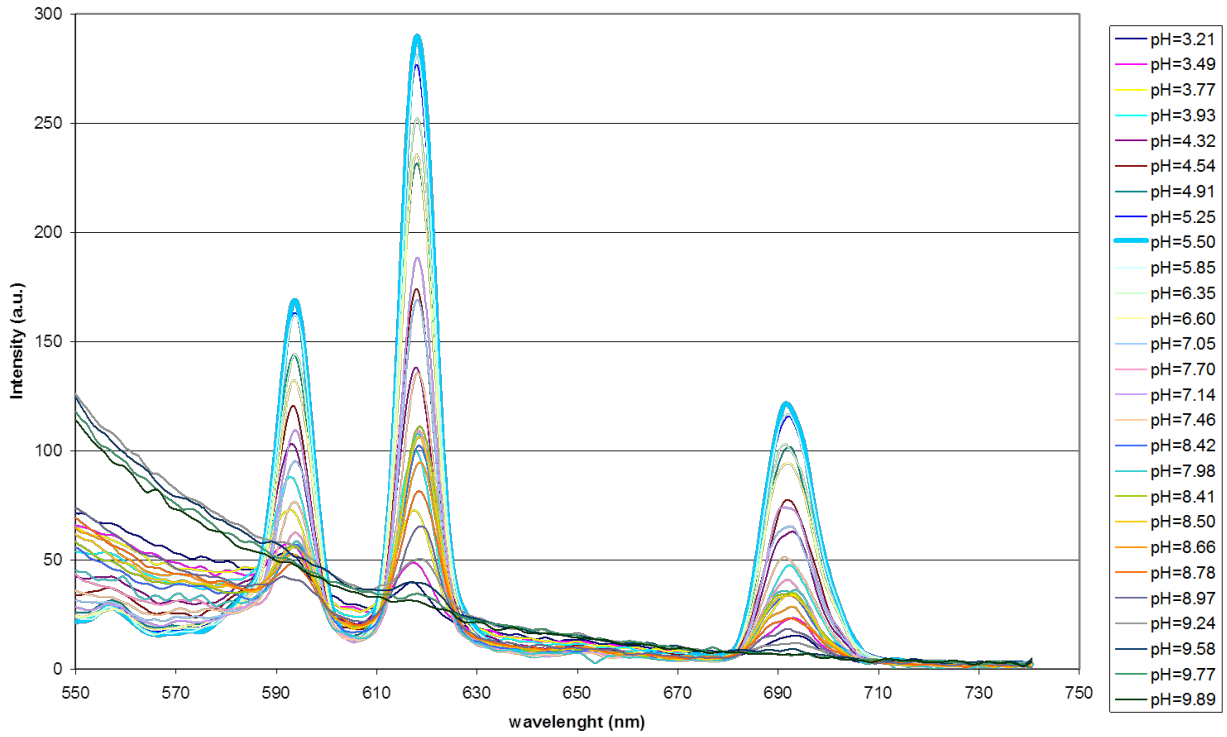

Figure S 30. Emission spectra of $[Eu(HL^{tz})_3][Et_3NH]_3$ in water as a function of pH ($2.5 \cdot 10^{-5}$M, *I* = KCl 1M).