

*Title:* **Pseudopeptidic molecules for the recognition of biologically interesting ions.**

*Student:* Juan José Herrando Campillos

*Date:* January 2019

*Supervisor/s:* Dr. Laura Radríguez Raurell  
*Departament of Inorganic and Organic Chemistry*  
Dr. Ignacio Alfonso Rodríguez  
IQAC-CSIC

Pseudopeptidic cages are interesting molecules due to the possibility of carrying other species inside and their composition, which resembles to that of the peptides given in living organisms. Due to the different radioisotopes it presents, terbium is a lanthanide with possible MRI, such as PET and SPECT imaging, and radiotherapy applications, the last of which consists on the selective elimination of cancerous cells by emitting radiation toward them. It would be really useful to be able to safely transport terbium to a specific point in the human body safely, so the possibility of making a pseudopeptidic molecular cage transport terbium has awoken interest due to the lack of cytotoxicity of the cage alone.

In this project a specific molecular cage, named TREN-TRP-TMB as an abbreviation of triethylamine-tryptophan-trimethoxybenzene, is synthesized, and all the intermediate products are characterized by using  $^1\text{H-NMR}$ , and  $^{13}\text{C-NMR}$  and 2D NMR when they are found to be pure. Then, the interaction between terbium and the cage has been studied to determine whether a union between them is given and the strength of it by doing a fluorescence titration of the cage with terbium. When excited by an external source, the cage grants part of the energy absorbed to the terbium, which will then emit fluorescence. This phenomenon is known as FRET (Förster Resonance Energy Transfer).

By doing the titration and using a software named Hypspec, a mathematical adjustment has been made to determine the association constant ( $K_{\text{ass}}$ ) between these species. A mass spectrometry has also been made to confirm whether this union is given as the model states.