COMPOFUN

MOLECULAR CONTAINERS WITH POLAR CAVITIES AND VERSATILE FUNCTIONS

Timeline | 09/2021 to 08/2024

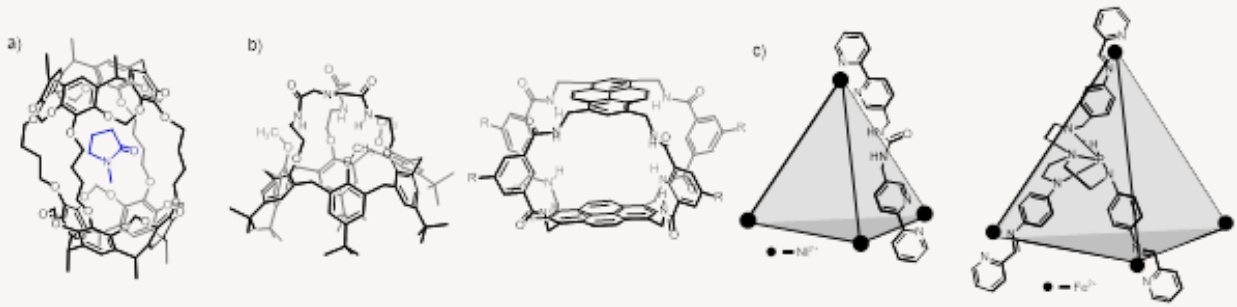
Budget | 217,800 €

ICIQ People | Pau Ballester Research Group

Call | Proyectos I+D - Generación Conocimiento 2020

SUMMARY

The overarching aim of this project is the synthesis of molecular and supramolecular containers / receptors with polar interiors derived from the use of aryl- and super-aryl- extended calix[4]pyrroles, and the evaluation of their applications in different areas ranging from fundamental studies of physical organic chemistry, the development of sensor devices, molecular recognition, supramolecular catalysis and the transport of molecules across lipid membranes. Firstly, we propose the synthesis of new uni- and supra-molecular receptors/containers using different strategies directed to reduce their conformational flexibility. The approaches proposed for this conformational control are based on the use of both irreversible or dynamic covalent bonds and on the formation of coordination bonds and organometallic bonds with transition metals. The use of mechanical bonds is also envisaged in molecular receptors with [2] rotaxane topology. The prepared receptors/containers will have a cavity equipped with convergent functional groups that will be large enough to include or encapsulate polar ions and charged or neutral molecules of low molecular weight and with special relevance for health, environment, or food industry. Secondly, we propose to characterize the complexation and molecular recognition processes of the synthesized receptors/containers from both the kinetic and thermodynamic point of view. These studies will be carried out in organic solution and in water. The results obtained will allow us to advance in the knowledge of the binding properties of the receptors and be able to design modified versions with improved properties. We plan to use some of these receptors/containers as tools for fundamental studies of physical organic chemistry e.g., the quantification of intermolecular interactions in water. Alternative proposals to evaluate the applications of the prepared containers include: a) the development of molecular sensors (e.g. fluorescent receptors) and sensor devices (e.g. ion selective electrodes); b) the transport of polar molecules across lipid membranes (e.g. anions, amino acids); c) the facilitation of chemical reactions and / or the modification of their selectivity with respect to that obtained in the bulk solution; and d) to obtain supramolecular ligands for reactions catalyzed by transition metals.



Line-drawing structures of selected molecular containers: a) carceplex lacking of inner surface functionalization and requiring structure rupturing to release its cargo (guest, N-methyl-Y-lactam); b) calix[6]cryptand and "temple" receptors as examples of synthetically costly uni-molecular containers with multiple portals allowing guest exchange and functionalized inner surfaces producing stable inclusion complexes with polar guest; c) metal-mediated molecular containers with polar cavities.

Reference: PID2020-114020GB-I00