

Molecular Clefts, CavitanDs and Cages derived from Calix[4]pyrroles: Synthesis and Studies of their applications



Timeline | 09/2024 to 08/2028



ICIQ People | [Pau Ballester Research Group](#)



Budget | 306.250 €



Call | Proyectos I+D
Generación Conocimiento 2023

SUMMARY

MOCACUBE - This project aims to synthesizing unprecedented covalent molecular clefts and cavitanDs, as well as self-assembling large molecular cages based on dynamically covalent imine bonds. The transformation of post-synthesized imine cages into covalent derivatives will also be pursued. We will prepare different versions of the container compounds to be soluble in organic solvents and in water. All compounds share in common having large aromatic cavities equipped with convergent functional groups deriving from aryl-extended calix[4]pyrrole units. In this way, they act as molecular containers for polar substrates. The cavities volumes are adequate for the inclusion of one or two sizable molecules or ions. On the one hand, cavitanDs possess cavities open only at one end that define their upper rims. On the other hand, cages display cavities with two closed hemispheres that are connected by spacers providing portals allowing the in-out passage of substrates (reversible inclusion). We will address the control of the cages volume, portals sizes and functionalization. We propose the study and characterization (kinetically and thermodynamically) of the complexes formed by clefts, cavitanDs and cages with polar, neutral and ionic compounds both in organic solvents and in water. In addition, calix[4]pyrrole clefts and cavitanDs will be applied for the quantification of relevant intermolecular interactions. Au(I) and Pt(II) organometallic complexes of calix[4]pyrrole clefts will be used as scaffolds for the development of molecular receptors and sensors. Finally, we will include chemical reactions in the prepared cages to evaluate the acceleration levels achieved by their enzyme-like properties in converting bimolecular reactions into unimolecular counterparts upon substrates binding.

