Design, synthesis and applications of supramolecular Cages: Challenges and Perspectives

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- **Aula: RFP 3er piso DQIAQF/INQUIMAE**
- **Streaming por el canal de YouTube del DQIAyQF**

Resumen

Supramolecular architectures, such as molecular cages, offer synthetic cavities capable of hosting guest molecules through multiple noncovalent interactions. Their monodispersity and their structural versatility enable the development of new systems with novel properties. Through the rational design of cavitands, ligands, and controlled experimental conditions, it is possible to tune cage size, shape, and functionality. In particular, the inclusion of guest species within these systems makes molecular cages promising platforms for new applications like targeted delivery, sensors and decontaminants [1-3].

One of the challenges of my PhD is to engineer organic supramolecular cages that can encapsulate anticancer drug molecules in aqueous solution and release them selectively at the desired biological target, like a tumoral environment. These systems would help to improve therapeutic efficiency while minimizing systemic toxicity. In this presentation I will show the design, synthesis, and functionalization of several calixarene-based molecular cage systems for the encapsulation and controlled release of anticancer drugs [4] and the challenges of that work. I will also report the design, synthesis and computational studies of some metal-organic cages with the formula Pd_2L_4, which involves the reaction of two Pd(II) ions and four ditopic ligands, through metal-pyridine coordination bonds. The application of these cages includes sensors and environment decontaminants [5].

[1] Montà-González, G. *et al. Chem. Rev.* 2022, 122, 13636-13708.
[2] Cox, C. J. *et al. Chem. Soc. Rev.* 2024, 53 (21), 10380–10408.
[3] Martí-Centelles, V. *et al. Tetrahedron Lett.* 2022, 93, 153676.
[4] Montà-González, G. *et al. Chem. Sci.,* 2024, 15, 10010-10017.
[5] Fiorini, G, *et al. CCS Chemistry*. 2025, 7, 3349–3363