

## UniSysCat - Colloquium

Prof. Antonella Di Pizio

Leibniz Institute for Food Systems Biology Protein Modelling and School of Life Sciences,  
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Start Time: Wednesday, September 6, 2023 05:15 pm

End Time: Wednesday, September 6, 2023 06:30 pm

C 264  
or via Zoom

### Computational Investigations of Understudied GPCRs for Drug Design

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G Protein-Coupled Receptors (GPCRs) constitute the largest and most diverse family of membrane receptors in humans. They play a pivotal role in cellular communication and are involved in a wide range of physiological processes; and are the target of 35% drugs. Despite the high therapeutic potential, a large portion of the human GPCRs is still in the dark and understudied. In this talk, I will focus on olfactory receptors, the largest subfamily of class A GPCRs. I will discuss computational methods and protocols that are being used to model the 3D structure of olfactory receptors and their interaction with odorant molecules, highlighting challenges and opportunities. Additionally, the results of a virtual screening campaign, which led to the discovery of novel olfactory receptor antagonists, are presented as an example of how computational methods can aid in the deorphanization of GPCRs. The second part of the presentation will focus on the Y1 receptor, which is involved in regulating appetite and blood pressure. The structure of the Y1 receptor has been experimentally solved in complex with both small molecule antagonists and neuropeptide Y (NPY). By utilizing structures of NPY, NPY-Y1 complexes, and antagonist-bound Y1 receptors, the conformational dynamics of NPY and its coupling to the Y1 receptor binding event have been explored.

Dr. Ariane Nunes Alves

Organizer