

Invitation to the talk

Computational Models for Membrane Proteins and Receptor Mechanisms of Transport, Activation and Inhibition

Dr.

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Seminar room Physiology (HA05 P51)

Vetmeduni, Veterinärplatz 1, 1210 Vienna

ABSTRACT: Tetrameric bundles of transmembrane alpha helical assemblies are a common topology for ion channels in biological membranes. I will present computational studies of two protein types sharing this topology: the ionotropic Glutamate Receptors (iGluRs), which are a class of ligand-gated ion channels in the Central Nervous System (CNS) that initiate transmission of signal in excitatory synapses; and the Transient Receptor Proteins (TRP), ubiquitous ion channels regulated by multiple stimuli, including temperature, pressure and ligands, which are selective to divalent cations. Proteins of both classes are essential for function and present attractive pharmaceutical targets. Detailed understanding of structure-function relationships in such proteins has been a subject of active research, yet it is difficult to connect structural information with physiological measurements. We employed a combination of theoretical and computational approaches, including molecular dynamics (MD) simulations, free energy methods and Machine Learning (ML) techniques to characterize dynamic variability in the structural ensembles of these proteins, to predict ion conductance and selectivity, as well as to analyze their interaction with the drug-like ligands.

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