UniSysCat -Colloquium

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and via Zoom

Quantitative electrostatic force tomography for proteinaceous capsids in interaction with an approaching nanoscale substrate

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Electrostatic interactions are crucial for the assembly, disassembly and stability of proteinaceous viral capsids. Moreover, at the molecular scale, elucidating the organization and structure of the capsid proteins in response to an approaching nanoprobe/substrate is a major challenge in biomacromolecular research. In this talk, I will present a generalized electrostatic model, based on the Poisson-Boltzmann equation, that quantifies the subnanometric electrostatic interactions between an AFM tip and a proteinaceous capsid from molecular simulations snapshots. This allows us to describe the contributions of specific amino acids and atoms to the interaction force. The validation results are shown in terms of total electrostatic forces with previous semi-empirical generalized models at available length scales (d> 1 nm). Then, the interaction of the Zika capsid with conical, flat and spherical AFM tips is tackled in a tomography-type analysis to identify the most important residues and atoms, showing the localized nature of the interaction. This method can be employed for the interpretation of force microscopy experiments in fundamental virological characterizations and in diverse applications, like trapping proteins with tailor-made substrates. Finally, we will discuss the environment effects in terms of salt concentration and protonation states to the protein-cage functional properties and transcapsid electrostatic interactions with nucleic acids.

Dr. Ariane Ferreira Nunes Alves

Organizer