SEPTEMBER 20, 2023

APEX LECTURE SERIES

IVET BAHAR

Stony Brook University

"Merging Machine Learning Methods and Elastic Network Models for Modeling Protein Dynamics and Function"

4:00 p.m., 214 Light Hall

Co-sponsored by the Department of Pharmacology and the Center for Applied Artificial Intelligence in Protein Dynamics

Machine learning (ML)-based approaches have recently shown remarkable success in predicting protein structures. Progress made in physics-based computational evaluation of structural dynamics, not only structure, can also be leveraged if used in conjunction with ML methods. One bottleneck has been the computing time cost of molecular simulations. However, in recent years, with the introduction of elastic network models, it is possible to efficiently evaluate biomolecular properties dependent on dynamics.

We will present recent applications to evaluating the pathogenicity of single amino acid variants, as well as the impact of deletions on stability.

VANDERBILT
School *of* Medicine Basic Sciences