



ACS Local Section
New York
Long Island Subsection

It's in the Perturbation: Conformational Dynamics of Proteins from Molecular Simulations.

Arlind Kacirani

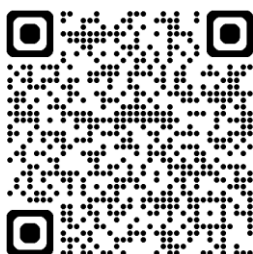
PhD Candidate, Yale University

Thursday, March 6th, 2025, 6:45 PM

St. John's University, D'Angelo Center

Room 407 and online (Zoom)

Registration required
prior to the event.
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Abstract: Human γ D-crystallin belongs to a crucial family of proteins known as crystallins located in the fiber cells of the human lens. Since crystallins do not undergo any turnover after birth, they need to possess remarkable thermodynamic stability. However, their sporadic misfolding and aggregation, triggered by environmental perturbations or genetic mutations, constitute the molecular basis of cataracts, which is the primary cause of blindness in the globe according to the World Health Organization. In this talk I will present our work on the impact of high pressure on the conformational landscape of wild-type HyD-crystallin using replica exchange molecular dynamics simulations augmented with principal component analysis. This exploration sheds light on the intricate responses of HyD-crystallin to elevated pressures, offering insights into potential mechanisms underlying its stability and susceptibility to environmental perturbations, crucial for understanding cataract formation.

Biography: Arlind is a 4th year PhD candidate in Chemical Engineering at Yale University. He is also a fellow in the Integrated Graduate Program in Physical & Engineering Biology (PEB). Previously, he graduated summa cum laude with a B.E. in Chemical Engineering and double minors in Chemistry and Mathematics from The City College of New York. There he researched the structure and dynamics of fungal melanins using ^{13}C solid-state NMR spectroscopy in Prof. Ruth E. Stark's Lab. Before that Arlind earned an A.S. in Chemistry (with Honors) from Queensborough Community College. At Yale, his current research interests focus on protein aggregation, statistical mechanics, and liquid phase transitions

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