



PHYSICAL CHEMISTRY SEMINAR

Ligand-driven allostery and interdomain communication in nuclear receptors



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ZOOM

<https://udel.zoom.us/j/92777070899>

Nuclear receptors are ligand-regulated transcription factors that controls genes important for metabolism, development and reproduction. Allostery is a critical aspect of nuclear receptor function. Ligands of diverse shapes and sizes selectively modulate the transcriptional output of FXR by influencing the distantly located DNA binding domain. Our laboratory aims to understand how the structure of ligands allow them to achieve specific transcriptional outcomes. We also seek to understand how ligand binding (LBD) and DNA binding domains (DBD) of nuclear receptors ‘talk to one another’ to permit ligand-specific transcriptional outcomes. We combine molecular dynamics simulations with biochemical experiments to elucidate mechanisms of ligand-specificity and interdomain communication. In this talk, I will discuss our work using the farnesoid X receptor (FXR) as a model to study these fundamental mechanisms in nuclear receptors.

Denise Okafor is an assistant professor in the Departments of Biochemistry and Molecular Biology (BMB) and Chemistry at Pennsylvania State University. She earned her Ph.D. in Chemistry from the Georgia Institute of Technology. As an NIH-IRACDA postdoctoral fellow at Emory University School of Medicine, she used molecular dynamics simulations to study ligand regulation and functional evolution in nuclear receptors. She began her independent career in 2020. Her lab combines MD simulations with biochemical experiments to understand mechanisms of transcriptional activation in nuclear receptors.



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