UC RIVERSIDE

BCH 252 Seminar Series

Dr. Giulia Palermo, Associate Professor, Department of Bioengineering, UC Riverside

Seminar Title: "Dynamics and mechanisms of CRISPR-Cas9 through the lens of computational methods"

Abstract: The clustered regularly interspaced short palindromic repeat (CRISPR) genome-editing revolution established the beginning of a new era in life sciences. I will review the role of state-of-the-art computations in the CRISPR-Cas9 revolution, from the early refinement of cryo-EM data to enhanced simulations of large-scale conformational transitions. Molecular simulations reported a mechanism for RNA binding and the formation of a catalytically competent Cas9 enzyme, in agreement with subsequent structural studies. Inspired by single-molecule experiments, molecular dynamics offered a rationale for the onset of off-target effects, while graph theory unveiled the allosteric regulation. Finally, the use of a mixed quantum-classical approach established the catalytic mecha- nism of DNA cleavage. Overall, molecular simulations have been instrumental in understanding the dynamics and mech- anism of CRISPR-Cas9, contributing to understanding func- tion, catalysis, allostery, and specificity.

ZOOM Link: https://ucr.zoom.us/j/92569273073
Meeting ID: 925 6927 3073
Passcode: 689525

Tuesday, February 14th, 2023
12:00 p.m. - 12:50 p.m. PST

Hosts: Dr. Richard Debus & Dr. Russ Hille