UC RIVERSIDE

BCH 252 Seminar Series

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Seminar Title: "Structures and Dynamics Beyond the Traditional Drug Space"

Abstract: The discovery of novel therapeutics has undergone a notable transformation over the recent decades driven by the emergence of new chemical modalities which are able to modulate previously "undruggable" targets such as protein surfaces. These new modalities include large and complex macrocycles, peptides and natural products, typically referred to as beyond rule of 5 compounds. Their ability to act as molecular chameleons and adapt to different environments is essential for their success. However, their design and development is slow and inefficient as methods for their evaluation are still not established.

By using a combination of the cryo-EM method MicroED and NMR, the biologically relevant conformational ensembles and structures can be derived, including the conformations adopted in aqueous solution, when crossing a cell membrane and when bound to the protein target, and the gained knowledge can be used in precision design. MicroED is a new tool in drug discovery in which challenging ligand structures can be determined directly from powder formulations. Target structures can be obtained from nanocrystals in solution giving access to new opportunities of ligand soaking and studying dynamics. These developments gives access to a world of ligand and protein structures beyond the traditional drug space, which were previously unattainable.

Tuesday, October 1st, 2024 12:00 p.m. - 12:50 p.m. PST

In-Person: Genomics Auditorium 1102A

Host: Dr. Chia-en Chang