
Seminar 2016

Ligand discovery for challenging targets from homology modeling and virtual screening.



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Friday March 25, 2016

2:30 PM

Laufer Center Lecture Hall 101

Host: Markus Seeliger

Research Topics: Cancer, Computational Biology

Drug Design and Discovery, Membrane Proteins/Channels

Protein Structure/Function, Transporters, Training Areas

Biophysics and Systems Pharmacology [BSP],

Cancer Biology [CAB]

Our lab focuses on the development and application of computational tools to annotate the functions of proteins. The two major research areas of our group include:

1. Structure-based drug design for membrane transporters. Our group characterizes cancer-related membrane transporter proteins, using a structure-based discovery approach, including homology modeling and virtual ligand screening, in collaboration with experimental labs. We rationally design novel chemical tools to study transporters' role in cancer metabolism pathways, with a long-term goal of developing drugs against these potential cancer drug targets.

2. Structural bioinformatics. The lab works on developing and applying sequence-based and structure-based methods to predict different features of proteins using various machine-learning techniques. We analyze the predicted features of proteins in the context of networks and proteomes, to characterize protein functions.

Refreshments following seminar

Laufer Hub 110

