## TEL AVIV UNIVERSITY GEORGE S. WISE FACULTY OF LIFE SCIENCES The Blavatnik Center for Drug Discovery (BCDD)

SPECIAL GUEST SEMINAR Thursday, October 15<sup>th</sup>, 2015

## Dr. Katalin Phimister

Senior Drug Discovery Support Scientist Schrodinger Inc.

## How can computational tools help in drug design projects?

The lecture will take place at 11:00, Katzir Club, GREEN Bldg., Ground fl.

Host: Prof. Miguel Weil Email: miguelw@tauex.tau.ac.il; Phone 6981

## Abstract

Several case studies will be presented where computational tools can help with design ideas and understanding the key interactions and role of waters in a binding pocket. We will show examples on how tools such as docking and other computation tools can help screening compounds for new leads as well as optimising leads. We will also present tools applicable to protein design projects.