Biochemistry
UNIVERSITY OF TORONTO

Special Guest Seminar

Dr. Ursula Egner

Director/Head of Structural Biology
Global Drug Discovery - Lead Discovery
Bayer Pharma AG

Macromolecular Crystallography in Drug Discovery

At Bayer, Structural Biology together with Protein Technologies is responsible for protein X-ray crystallography and fragment screening. Structural Biology supports projects in lead generation and optimization with a focus on lead discovery. Discovering a new inhibitor binding mode or a new protein conformation may contribute towards the next successful lead compound. Our aim is to support projects with target-ligand complex structures after high-throughput screening is finished and the Hit-2-Lead process is going to start. To meet these time lines, a gene-2-structure platform has been implemented. Parallelization of approaches was a major contributor to the successful and timely delivery of target structures.

For selected targets, fragment screening and high-throughput screening are performed in parallel to effectively use all information during the Hit-2-Lead process. In a case study fragment screening was applied to identify probes for the S1 specificity pocket as well as for other sub sites for several serine proteases using surface plasmon resonance (SPR), high-concentration screening, virtual screening, and thermal shift assays as primary filters. The results of the different screening methods were compared.

Date & Time: Mon, June 2nd, 2014 at 11:00 am
Location: MSB 4279

Hosted by: Emil F. Pai

Everyone Welcome!