

Protein structure and drug design (1 ECTS)

18-19 of January 2016, Chemistry Centre, Lund

Deadline for registration: 1/12/2015

Course leader

Salam Al-Karadaghi, Dept. of Biochemistry and Structural Biology, Lund University

Course content

Day 1 - 18 January (start 9 a.m.)

1- Morning lecture by Salam Al-Karadaghi

Protein-ligand interactions and drug design. Structure-based drug design (SBDD): Hit identification, hit optimisation and lead generation.

The lecture will describe forces in protein-ligand interactions, the use of structural information in drug design and will provide examples of structure-based drug design.

2- Tutorial

***In silico* screening and compound docking**

Here we will talk about the basics of *in silico* screening and the use of docking to assess protein-ligand interactions.

Day 2 - 19 January (end 4 p.m.)

3- Morning lecture by Andres Liljas

Structural aspect of protein synthesis inhibition by antibiotics

The lecture will provide an overview of ribosome structure, the mechanism of protein synthesis and the way antibiotics interfere with protein synthesis.

4- Tutorial

Assessment and analysis of docking results

Requirements for participants

Basic understanding of protein structure and knowledge of a graphics programmes such as SwissPDB viewer. See for example www.proteinstructures.com for general information on protein structures. Software for download of SwissPDB viewer and tutorial can be found at <http://spdbv.vital-it.ch/>.

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