

# Protein structure & structure-based drug design

## 1,5 ECTS, 20-23 March 2018

Salam Al-Karadaghi, Dept of Biochemistry and Structural Biology, Lund University,  
Venue: "Bioinformatics Dungeon" at the Chemistry Centre

<b>Tuesday March 20</b>	
09.15	<b>Overview of the course</b> What are the requirements and what we will learn
	<b>Morning lecture</b> Introduction protein structure: amino acids, structure-sequence relationships, folds & classification.
12.00	Lunch
13.15-16.00	<b>Afternoon tutorial</b> Sequence & structural databases (UniProt, PDB, PDBsum, CATH, etc.); the <b>Chimera</b> graphics software
18-21	<b>Get-together including dinner:</b> Cafe Ester, Chemistry Centre
<b>Wednesday March 21</b>	
9.15	<b>Lecture:</b> Structure in drug discovery – using structural information in drug discovery – screening, hit identification, lead generation and optimization; examples.
12.00	Lunch
13.15-16.00	<b>Afternoon tutorial:</b> Internet tools for drug discovery. Chimera graphics software analysis of protein-ligand interactions.
<b>Thursday March 22</b>	
09.15-10:00	<b>Lecture</b> Introduction to docking
10.30-12.00	<b>Tutorial</b> AutoDock Vina; ligand docking and analysis of results.
12.00	Lunch
13.15-16.00	<b>Continue tutorial</b> AutoDock Vina; basics of screening.
<b>Friday March 23</b>	
09.15	<b>Practical project</b> (2 students in each group): <b>Docking &amp; real life:</b> Cure headache and avoid bleeding stomach? Looking into COX1, COX2 and the specificity problem.
12.00	Lunch
13.15-16.00	<b>Afternoon:</b> Discussion of results, course evaluation

### Prior to course start:

Students are strongly recommended before the start of the course to acquire basic knowledge in protein structure and function (see for example <http://www.proteinstructures.com>).

Students are also urged to go through the basic tutorial on the use of Chimera - **the official Chimera site tutorials:**

<https://www.cgl.ucsf.edu/chimera/current/docs/UsersGuide/frameset.html>.

Additional sites (there are much more on the web):

<https://www.youtube.com/watch?v=hQxKYSUdiD8>

<http://www.ch.embnet.org/CourseEMBnet/Pages3D07/documents/3Dchimera-tutorial07.pdf>