Protein structure & structure-based drug design
1,5 ECTS, 15-18 January 2019

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

Venue: "Bioinformatics Dungeon" at the Chemistry Centre

Tuesday Jan 15	
09.15	**Overview of the course** What are the requirements and what we will learn
	Morning lecture Introduction protein structure: amino acids, structure-sequence relationships, folds & classification.
12.00	Lunch
13.15-16.00	**Afternoon tutorial** Sequence & structural databases (UniProt, PDB, PDBsum, CATH, etc.); Introduction to **Chimera** graphics software
18-21	**Get-together including dinner:** Lunch room, Chemistry Centre
Wednesday Jan 16	
9.15	**Lecture:** 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	**Afternoon tutorial**: Internet tools for drug discovery. Chimera graphics software analysis of protein-ligand interactions.
Thursday Jan 17	
09.15-10:00	**Lecture** Introduction to docking
10.30-12.00	**Tutorial** AutoDock Vina; ligand docking and analysis of results.
12.00	Lunch
13.15-16.00	**Continue tutorial** AutoDock Vina; basics of screening.
Friday Jan 18	
09.15	Finish screening tutorial. **Practical project** (2 students in each group): **Docking & real life:** Cure headache and avoid bleeding stomach? Looking into COX1, COX2 and the specificity problem.
12.00	Lunch
13.15-16.00	Finish tutorial, 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/frametut.html.

Additional sites (there is much more on the web):
https://www.youtube.com/watch?v=hQxKYSUdiD8
http://www.ch.embnet.org/CoursEMBnet/Pages3D07/documents/3Dchimera-tutorial07.pdf