Protein structure & structure-based drug design
1,5 ECTS, 10-13 January 2017

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Venue: "Bioinformatics Dungeon" at the Chemistry Centre

Tuesday Jan 10	
9.15	**Overview of the course** What are the requirements and what we will learn
	Morning lecture Introduction protein structure: amino acids, structure-sequence relationships, protein folds & fold classification.
12.00	Lunch
13.15-16.00	**Afternoon tutorial** Sequence & structural databases (UniProt, PDB, PDBsum, CATH, etc.) tools for 3D structure visualisation and sequence analysis.
18-	**Get-together including dinner:** Cafe Ester, Chemistry Centre
Wednesday Jan 11	
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 for 3D structure visualisation and analysis of protein-ligand interactions.
Thursday Jan 12	
9.15	**Lecture** Introduction to docking
10.30-12.00	**Tutorial** AutoDock Vina. Ligand docking and analysis of results. Basics of screening.
12.00	Lunch
13.15-16.00	**Continue** AutoDock Vina Tutorial.
Friday Jan 13	
9.15	**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	**Afternoon:** 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 are much more on the web):
https://www.youtube.com/watch?v=hQxKYSUdiD8
http://www.ch.embnet.org/CoursEMBnet/Pages3D07/documents/3Dchimera-tutorial07.pdf