UNIVERSITÀ DEGLI STUDI DI TORINO

ID
TM21_DIP_FAR

Teach Mob – Visiting Professors
Academic year 2017/2018

2nd Term
COURSE TITLE **Computer-aided Drug Design (module 1 of Advanced Medicinal Chemistry)**
Scientific area **Medicinal Chemistry**
Department of Drug Science and Technology
Language used to teach: English
Teaching Commitment: 16 hours
Course summary The course is focused on the application of molecular modelling techniques in drug design. A short introduction on protein structure and on the experimental, and computational (homology modelling) methodologies used to determine it, will be provided. Particular attention will be paid to protein flexibility as an intrinsic and fundamental property of proteins. The basic of molecular mechanics, force fields and molecular dynamics will be provided. All the elements necessary for a proper modelling of protein-ligand systems will be considered, that is, protonation state of ionizable residues, water molecules. Both ligand-based (QSAR, LBVS) and structure-based techniques (docking, SBVS) will be presented, focusing in particular, on virtual screening (ligand-based, pharmacophore-based and structure-based) and on the screening software FLAP. Scoring functions used to predict protein-ligand interactions will be presented, focusing on the HINT force field.
Learning objectives The aim of the course is to provide an outline of the basic principles of computer-aided drug design. Specific attention will be paid to i) application of homology modelling to model the structure of unknown protein, ii) usage of molecular dynamics to minimize the energy of the protein structure and investigate flexibility, iii) virtual screening techniques to identify new potential pharmacological hits, iv) scoring functions for the prediction of the protein-ligand free energy of binding. At the end of the course the students will be able to correctly apply state of the art computational techniques for the identification, design and optimization of drugs, paying particular attention to the interaction with the biological target. They will be able to understand the rationale for designing and discovering new drugs and to identify the most appropriate techniques to be used according to the available information.
Tutorship activities Two/three students attending the lab to prepare their experimental thesis in Computational Medicinal Chemistry, as well as other PhD students will be tutored by the visiting professor. The skills and supervision of the visiting professors will be critical to help students in properly performing virtual screening experiments and in selecting the most promising candidates possibly active as protein-protein disruptors towards the hemoglobin-S. aureus hemophore interaction.

Moreover, the visiting professor will assist PhD students in writing English language scientific papers and in preparing presentations.

Lab activities

The lab activities provided within the course will be supervised by the reference teacher with the help of the visiting professor. Lab activities include homology modelling, molecular dynamics, virtual screening, docking and scoring simulations.

Other activities besides the course: i.e. seminars and conferences addressed to PhD students and research fellows, dissemination conferences

The visiting professor will hold workshops and mentor students and fellows individually on writing English language scientific manuscripts and in preparing presentations. The visiting professor will present his/her current research in an open seminar.

Visiting Professor Profile

The visiting professor should have significant research experience in the field of computational chemistry, molecular modelling and drug discovery.

Due to the intermediate level background of the students (4th year of a five-year course), the visiting professor should combine a rigorous presentation of the topics with the ability to present basic information, when required. A strong expertise in structure-based drug design, virtual screening approaches, docking, scoring and lead optimization will be highly desirable. This higher scientific level will be especially exploited in the interaction with students involved in computational activities for the preparation of their master theses, as well as in tutoring PhD students.

Contact person at the Department

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