UNIVERSITÀ DEGLI STUDI DI TORINO

ID

VP27_DIP_STF

Visiting Professor Program
Academic year 2019/2020

DEPARTMENT OF DRUG SCIENCE AND TECHNOLOGY

TEACHING COMMITMENT: 16 hours

COURSE TITLE

Thermodynamics of receptor-drug interactions

TEACHING PERIOD

2nd term

SCIENTIFIC AREA

Medicinal Chemistry

LANGUAGE USED TO TEACH

English

COURSE SUMMARY

The course is focused on the analysis of biological interactions with particular attention to drug-receptor systems. The physical-chemical laws regulating molecular interactions will be presented and discussed. Thermodynamic contributions (enthalpy and entropy, Gibbs free energy) will be analysed in detail, along with concepts from kinetics such as transition states, association and dissociation rates, etc. A brief introduction to molecular mechanics and force fields will be provided with emphasis on the structural and energetic factors involved in molecular interactions, especially the roles played by water molecules. Computational methods for the calculation of the free energy will be presented and discussed: Free Energy Perturbation, Thermodynamic Integration, Relative free energy determination.
For illustration, examples of drug-receptor complexes will be provided and analysed.

LEARNING OBJECTIVES

The aim of the course is to provide the chemical and physical fundamentals to understand the thermodynamic and kinetic events driving and characterizing the interaction between molecules in the biological environment. The students will be able to understand the fundamental aspects to

take into account when designing new ligands for a specific receptor or when trying to optimize available lead compounds. Both the basic enthalpic and entropic contributions and aspects related to the kinetics of the interaction. To this aim they will learn about state-of-the-art methodologies used to predict the free energy of binding and related dissociation rate constants. The knowledge acquired during the course will be extremely valuable for the students planning to enroll in the Computer-aided Drug Design course, given by the referent proposer to 4th year students of Pharmacy and Industrial Pharmacy.

TUTORSHIP ACTIVITIES

The visiting professor will tutor one/two research students in the laboratory of the referent proposer in performing their research work and in preparing their experimental thesis in Computational Medicinal Chemistry, as well as other PhD students collaborating with the proposer. The skills and supervision of the visiting professors will be critical to help students in properly performing structure-based drug design campaigns. Moreover, the visiting professor will assist PhD students in writing English language scientific papers and in preparing presentations.

OTHER ACTIVITIES BESIDES THE COURSE

The visiting professor will also give workshops on scientific/technical writing in English for Pharmacy and Industrial Pharmacy students and also for PhD students in Pharmaceutical and Biomolecular Sciences. In particular, the elements of contructing a publishable manuscript will be explored in depth. He will mentor students and fellows individually helping them in writing papers and in preparing presentations.

VISITING PROFESSOR PROFILE

The visiting professor should have significant research experience in the field of computational chemistry, chemical physics and molecular modelling.
Due to the intermediate level background of the students (4th year of five-year courses), 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, and in the theorization of biological interactions will be highly desirable. This high 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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