Adam Mickiewicz University in Poznań

Faculty of Chemistry

INNChem - *rozwój kompetencji doktorantów kluczowych w pracy o charakterze badawczo-rozwojowym*

Introduction to computational drug design

Prof. Jacek A. Tuszynski

Foreign lecture

Field of science	Chemistry
Teaching method	lecture
Language	ENGLISH
ECTS credits	1
Numbers of hours	14
Aims of the course	The course offers a description of the state of the art of computer-aided drug design and biomedical modelling within both academic research and pharmaceutical/biotech industry applications starting from a historical perspective providing a solid theoretical basis of the presented computational approaches. The student will gain competence in specific computational techniques at the level of molecular target modeling, ligand-protein interactions and pharmacokinetic simulations. To better understand the practical use of these methods, examples will illustrate drug development from oncology, virology and immunology
Course contents	Rational drug design to treat a variety of diseases is a dream, which is fast becoming a practically achievable goal of computer-aided drug discovery research. This course will expose the student to methods and application of computational drug discovery providing a historical overview followed by an in-depth introduction to present-day methods. Today, quantitative structure–activity relationships are found for targeted structure-based and computer-aided design of drugs. Discoveries of new targets and the validation of their therapeutic value is achieved through genomic, transcriptomic, metabolomic and proteomic analysis, knock-in and knockout animal models, and gene silencing with siRNA. Main focus will be placed on both ligand-based and structure-based computer-aided design of an active substance, which is validated by in vitro and in vivo tests to determine the activity of new investigational compounds. At the organ and whole body level pharmacokinetics is a field that uses sophisticated modeling tachniques that will be discussed in this course.
Prerequisites and co-requisites	Good knowledge of the basic principles of physics, mathematics, chemistry, biology, mechanics at an undergraduate level is expected. The lecturer may

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	consider to fill specific background gaps by giving ad hoc explanations when needed.

Learning outcomes	
On completion of the course PhD candidates will be able to:	**Assessment mode**
The graduate knows and understands methodology of research work used in the area of chemistry and selected related disciplines.	exam
The graduate knows the issues concerning the transfer of knowledge and commercialisation of research results.	
The graduate knows the principles of functioning of open science.	

Literature	
Additional information	Schedule (suggested dates): 16.04.2019, 09:30-11:30 and 13:30-15:00 17.04.2019, 09:30-11:30 and 13:30-15:00 18.04.2019, 09:30-11:30 and 13:30-15:00 Contact: jackt@ualberta.ca

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