

Course title: Molecular modeling in drug design – selectable / ~~regular course~~

Number of contact hours: 30 hours (30h lectures)

ETCS credits: 2

Course description: The lecture reviews the general strategies of computer-aided rationalization in drug design and introduces the modern computational methods used in drug discovery and drug development. It covers topics such as drug design process, structure and ligand based drug design, molecular mechanics methods, homology model, molecular docking, pharmacophore models, quantitative structure-reactivity relationship (QSAR), de novo ligand design, quantum mechanics techniques, cheminformatics, database search tools, and virtual screening. Hands-on experience in using computational software and visualization tools will be provided. Computer demonstrations and some practical exercises with free available modeling software.

Education effects (P7S_UW, P7S_WG):

- **knowledge:** student knows the most important strategies of computer-aided drug design; knows the methods of computational chemistry used in drug design;
- **skills:** student can search of protein structure database; can use the free available modeling software and visualization tools
- **social:** student is able to work independently and in the group during exercises;

Literature:

- (1) Computational Drug Design: A Guide for Computational and Medicinal Chemists, by David C. Young, John Wiley & Sons, Hoboken, N.J., 2009
- (2) Practical Application of Computer-Aided Drug Design, by Paul S. Charifson, New York, Marcel Dekker, 1997
- (3) Molecular Modeling: Principles and Applications, 2nd Edition, by Andrew R. Leach, Harlow, England, Pearson Education, 2001.
- (4) An Introduction to Medicinal Chemistry, 3rd Ed., Graham L. Patrick, New York, Oxford University Press, 2005
- (5) Computational Techniques and Applications, edited by Lee Banting and Tim Clark, Cambridge, Royal Society of Chemistry, 2012 (electronic resource)
- (6) Computational Drug Discovery and Design, edited by Riccardo Baron, New York, Humana Press, Springer, 2012 (electronic resource)

Assessment method: Final test, presence at lectures

Prerequisites: Basic knowledge in organic chemistry and technology

Primary target group: All specialties students

Lecturer: dr inż. P. Śliwa, Contact person: dr inż. P. Śliwa, e-mail: pśliwa@chemia.pk.edu.pl