ЦЕНТЪР ЗА ОБУЧЕНИЕ – БАН

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Basic Information:
Course Title: **Computer-Aided Drug Design (CADD)**
Lecturer: Acad. Ilza Pajeva
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Total Teaching Hours: 30

Annotation (up to 150 words)

The course aims to introduce PhD students to the fundamental principles and methods of drug development using computational approaches (also known as *in silico* drug design). The subject matter is interdisciplinary, utilizing knowledge from pharmacology, molecular biology, organic and quantum chemistry, molecular mechanics, and mathematical modeling. The curriculum covers both ligand- and structure-based methods. The objective is to characterize the relationship between the chemical structures of compounds and their effects, expressed through molecular models (2D or 3D)—where the effect can be therapeutic, toxic, etc. The goal is, on one hand, to achieve a better understanding and insight into the molecular mechanisms leading to the effect, and on the other, to predict the effect using these models.In practical terms, PhD students will become familiar with software programs for molecular modeling, structure generation, optimization, calculation of structural descriptors, derivation of QSAR models, docking, analysis of ligand-protein interactions, among others.

Course content (brief description by topics or modules)
Topic / Module 1: Basic theoretical propositions
Topic / Module 2: Ligand-based methods
Topic / Module 3: Structure-based methods

Teaching and assessment methods

- Ongoing assessment: Seminars with presentations on a topic chosen by the doctoral student based on the taught material
- Final assessment: a/ Multiple choice test; b/ Interview on the test

Competencies acquired as a result of training (3–5 points):

- Acquisition of theoretical knowledge in the field of CADD
- Mastery of some basic CADD methods
- Acquisition of certain practical skills

Literature:
http://onlinelibrary.wiley.com/bookseries/10.1002/SERIES6138
QSAR: Hansch Analysis and Related Approaches
Chemometric Methods in Molecular Design
Advanced Computer-Assisted Techniques in Drug Discovery, Second Edition
Molecular Modeling: Basic Principles and Applications

Molecular Descriptors for Chemoinformatics: Volume I: Alphabetical Listing / Volume II: Appendices, References

Virtual Screening: Principles, Challenges, and Practical Guidelines

Additional information

- It is desirable that the student has an interdisciplinary focus.
- The course can be conducted on-line