BB2280 Molecular Modeling 7.5 credits

Molekylär modellering

This is a translation of the Swedish, legally binding, course syllabus.

Establishment

Course syllabus for BB2280 valid from Autumn 2016

Grading scale

A, B, C, D, E, FX, F

Education cycle

Second cycle

Main field of study

Biotechnology

Specific prerequisites

**Admission requirements for programme students at KTH:
**At least 150 credits from grades 1, 2 and 3 of which at least 100 credits from years 1 and 2, and bachelor's work must be completed. The 150 credits should include a minimum of 20 credits within the fields of Mathematics, Numerical Analysis and Computer Sciences, 5 of these must be within the fields of Numerical Analysis and Computer Sciences, 20 credits of Chemistry, possibly including courses in Chemical Measuring Techniques and 20 credits of Biotechnology or Molecular Biology.

**Admission requirements for independent students:
**A total of 20 university credits (hp) in Biotechnology or Molecular Biology. 20 university

credits (hp) of Chemistry, possibly including courses in Chemical Measuring Techniques , as well as 20 university credits (hp) in Mathematics, Numerical Analysis and Computer Sciences, 5 of these must be within the fields of Numerical Analysis and Computer Sciences. Documented proficiency in English corresponding to English B.

Language of instruction

The language of instruction is specified in the course offering information in the course catalogue.

Intended learning outcomes

Today, computer simulations are an important tool for the study of chemical processes in such different systems as isolated molecules, fluids, polymers, solid state, and biological macromolecules, like proteins and DNA. The enormous development of computer hard drive space means that the molecular modeling field is developing very quickly.

The goal with this course is to provide an overview of the methods and techniques which are used within modern molecular modeling. Basic theory will be covered and applications within chemistry, biochemistry and medicinal chemistry will be discussed.

Course contents

The course consists of both theoretical lectures and practical computer exercises. The following topics will be discussed:

- Basic quantum chemistry: Molecular orbital theory, semi-empirical methods
- Basic density functional theory (DFT)
- Molecular mechanics and molecular dynamics
- Monte Carlo methods
- Energy minimization and potential energy surfaces
- QM/MM methods
- Solvation and surrounding effects
- Theoretical methods in drug discovery: Docking, protein structure prediction, QSAR
- Simulation of chemical reactions in solution
- Modelling of enzymatic catalysis
- Field trip to pharmaceutical company

Course literature

Andrew R. Leach: Molecular Modelling, Principles and Applications, 2ed, samt utdelat material.

Examination

- TEN1 - Written exam, 6.0 credits, grading scale: A, B, C, D, E, FX, F
- LAB1 - Laboratory Work, 1.5 credits, grading scale: A, B, C, D, E, FX, F

Based on recommendation from KTH's coordinator for disabilities, the examiner will decide how to adapt an examination for students with documented disability.

The examiner may apply another examination format when re-examining individual students.

If the course is discontinued, students may request to be examined during the following two academic years.

Other requirements for final grade

Examination (TEN1, 6,0 credits, grading scale A-F) and Lab courses (LAB1, 1,5 credits, grading scale A-F).

Ethical approach

- All members of a group are responsible for the group's work.
- In any assessment, every student shall honestly disclose any help received and sources used.
- In an oral assessment, every student shall be able to present and answer questions about the entire assignment and solution.