BB2285 Project in Molecular Modelling 5.0 credits

Projekt i molekylär modellering

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

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

Establishment

Course syllabus for BB2285 valid from Autumn 2011

Grading scale

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

Education cycle

Second cycle

Main field of study

Biotechnology

Specific prerequisites

The student must have started or completed the course Molecular Modeling BB2280. The prerequisites for this course are therefore identical to those of BB2280, i.e.

At least 150 credits from grades 1, 2 and 3 of which at least 100 credits from years 1 and 2, and degree project, first level, 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

Language of instruction

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

Intended learning outcomes

This course is an extension of the course Molecular Modeling BB2280, and the aim is that the student should use the theoretical knowledge of BB2280 to solve a real chemical or biochemical problem.

After completion of the course the student is expected to know how to:

- Search for scientific information.

- Perform intermediate level quantum mechanical and molecular mechanical simulations.

- The student should get hands on experience with at least two modern software packages specialized for solving different chemical problems.

- Choose the correct methods for solving chemical and biological problems using modeling

Motivate the choice of method based on the underlying theories

Course contents

The student will need to find and present a chemical or biochemical problem that can be studied using different molecular modeling techniques. The information will be found by searching scientific databases, such as Web of Science. An outline of the performance of the calculations will then be made together with the course responsible. The project should involve using at least two different modern molecular modeling software packages. Finally the project will be presented both as a written report and orally. Each student will also need to function as the opponent of another student's presentation.

Course literature

Suitable scientific papers will be collected by the students and the course responsible.

Examination

• PRO1 - Project, 5.0 credits, grading scale: P, 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.

Other requirements for final grade

Project is reported as a written report and an oral presentation.

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.