BB2285 Projekt i molekylär modellering 5,0 hp

Project in Molecular Modelling

När kurs inte längre ges har student möjlighet att examineras under ytterligare två läsår.

Fastställande

Kursplan för BB2285 gäller från och med HT11

Betygsskala

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

Utbildningsnivå

Avancerad nivå

Huvudområden

Bioteknik

Särskild behörighet

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

Undervisningsspråk

Undervisningsspråk anges i kurstillfällesinformationen i kurs- och programkatalogen.

Lärandemål

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

Kursinnehåll

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.

Kurslitteratur

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

Examination

- PRO1 - Projekt, 5,0 hp, betygsskala: P, F

Examinator beslutar, baserat på rekommendation från KTH:s handläggare av stöd till studenter med funktionsnedsättning, om eventuell anpassad examination för studenter med dokumenterad, varaktig funktionsnedsättning.

Examinator får medge annan examinationsform vid omexamination av enstaka studenter.

Övriga krav för slutbetyg

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

Etiskt förhållningssätt

- Vid grupparbete har alla i gruppen ansvar för gruppens arbete.
- Vid examination ska varje student ärligt redovisa hjälp som erhållits och källor som använts.
- Vid muntlig examination ska varje student kunna redogöra för hela uppgiften och hela lösningen.