



# FCB3204 Molecular Modeling

## 7.5 credits

### 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 FCB3204 valid from Autumn 2021

### Grading scale

P, F

### Education cycle

Third cycle

### Language of instruction

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

### Intended learning outcomes

After completion of the course the student shall be able to

- demonstrate in-depth knowledge and analytical ability in molecular modeling adequate for the level of educational level of the course, and critically review others' work in the field [LAB1, PRO1]

- demonstrate good ability to explain and analyze complex concepts in molecular modeling based on relevant research literature, and in a pedagogical way communicate the knowledge in writing and orally [PRO1]
- be able to reflect on and describe how scientific issues in the field's research can contribute to sustainable societal development [PRO1]

## Course contents

The course's theoretical content includes:

- Introduction to 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
- Modeling of enzymatic catalysis

## Specific prerequisites

Eligible for studies at the third-cycle level.

## Examination

- LAB1 - Laboratory work, 1.5 credits, grading scale: P, F
- PRO1 - Project, 6.0 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.

Grading criteria are specified in the course PM.

## Other requirements for final grade

Required for final grade: 90% attendance at lectures, written critical reflection for selected scientific articles, approved written project report and completed oral project presentation (PRO1); and attendance on computer exercises and completed exercise reports (LAB1).

## **Transitional regulations**

If the course is discontinued, the student is given the opportunity to be examined on the course for another two academic years.

## **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.