UNIVERSITY OF GOTHENBURG

DEPARTMENT OF CHEMISTRY AND MOLECULAR BIOLOGY

KEM552 Introduction to molecular modelling, 5 credits

Grundläggande molekylmodellering, 5 högskolepoäng

Second Cycle

Confirmation

This course syllabus was confirmed by Department of Chemistry and Molecular Biology on 2013-07-05 and was last revised on 2018-09-04 to be valid from 2018-09-04, autumn semester of 2018.

Field of education: Science 100%
Department: Department of Chemistry and Molecular Biology

Position in the educational system

The course is classified at the level 90-120 credits for Degree of Bachelor. Alternatively, it can be read as a course at second cycle level for Degree of Master (120 credits) or as a freestanding course. The course replaces the earlier courses KEM551 and KEN550 and can not be included together with one of them in the same degree.

The course can be part of the following programmes: 1) Chemistry and learning, Master's Programme (N2KOL), 2) Master's Programme in Organic and Medicinal Chemistry (N2KEL), 3) Master's Programme in Chemistry (N2KEM), 4) Bachelor of Science Programme in Medicinal Chemistry (N1LMK) and 5) Bachelor of Science Programme in Chemistry (N1KEM)

Main field of studies	*Specialization*
Chemistry	A1N, Second cycle, has only first-cycle course/s as entry requirements
Chemistry with Specialization in Medicinal Chemistry	A1N, Second cycle, has only first-cycle course/s as entry requirements

Entry requirements

For admission to the course, completed and approved courses worth 90 credits in the field of science (or 120 credits in pharmaceutics/medicine) are required. Completed

course KEM040, Physical Chemistry (15 credits), or FYP203, Quantum Physics A (7.5 credits) or equivalent knowledge, as well as knowledge equivalent to at least course MMGK11, Mathematics for natural scientists A1 (15 credits) are recommended.

Learning outcomes

After completion of the course the student is expected to be able to:

Knowledge and understanding

- **present** the basic ideas of molecular modelling and its importance to solve chemical problems, **describe** applications of molecular mechanics in different fields of chemistry,
- **explain** the idea behind molecular mechanics and the structure of a force field, **name** the different types of force fields and **explain** the meaning and structure of the terms in a force field,
- **name** some important available force fields, their properties and areas of application,
- **describe** different methods to find the equilibrium geometries of a system,
- **explain** the principle behind the molecular dynamics (MD) and Monte-Carlo (MC) methods as well as areas of application for these methods.

Competence and skills

- **build** molecule models with the program packages Molecular Operating Environment and Chimera,
- **set up** and **carry out** energy minimisations,
- **set up**, **carry out** and **evaluate** simple docking protocols,
- **set up** MC and MD calculations in an appropriate way and analyse result from these calculations,
- **use** visualisation methods efficiently.

Judgement and approach

- **assess** quality and reliability of computational results and **decide** in which cases molecular mechanics is sufficient.

Course content

The course describes the molecular modelling with a focus on molecular mechanics, which is the appropriate method to study large systems (e g proteins or DNA molecules) under realistic conditions (aqueous solution, finite temperature). The following subjects will be treated:

1. Molecular modelling, its aim and problems. Equilibrium structures, potential surfaces, free energies
2. The standard tools of molecular modelling: Molecular mechanics, force fields, types of force fields
3. Finding equilibrium structures: Geometry optimisation
4. Simulations under real conditions: Molecular dynamics (MD) and Monte-Carlo (MC) methods
5. Conformation search
6. Visualisation and molecular properties
7. Applications of molecular modelling: Simulation of large molecules, ligand-receptor docking, pharmacophoric modelling
8. Trends in molecular modelling: Polarisable force fields, force fields for chemical reactions, QM/MM,...

The lectures are accompanied by computer-based laboratory sessions where important topics of the theory are demonstrated and are trained based on modern program packages. The final part of course includes a shorter computational project that the student implements, summarises in a report, and present in class.

The course is divided into two modules. Module 1 (3.0 credits) includes the theory as above, module 2 (2.0 credits) includes the laboratory sessions.

Sub-courses

1. **Theory part** *(Teoridelen),* 3 credits
   Grading scale: Pass with Distinction (VG), Pass (G) and Fail (U)

2. **Computer exercises** *(Datalaborationer),* 2 credits
   Grading scale: Pass (G) and Fail (U)

Form of teaching

Module 1: Teaching is performed in the form of lectures as well as a project work.

Module 2: Teaching is performed in the form of computer-based laboratory sessions including presentations.

Language of instruction: English and Swedish
As a principal rule, the course is given in Swedish but can be given completely or partly in English if the circumstances require it.

Assessment

Module 1: The examination is done by implementation and presentation of project work.

Module 2: The examination is done based on active participation in laboratory sessions and presentations.

If a student who has failed the same examined component twice wishes to change examiner for the next examination, a written application shall be sent to the department responsible for the course and it shall be granted unless there are special reasons against (Chapter 6, Section 22, Higher Education Ordinance).

In case a course has been discontinued or has undergone major changes, the student will normally be guaranteed at least three opportunities to take the examination (including the ordinary examination) during a period of at least one year from the last time the course was given in its original form.

Grades

The grading scale comprises: Pass with Distinction (VG), Pass (G) and Fail (U).
Module 1: Grade Pass with distinction, Pass or Fail will be awarded.

Module 2: Grade Pass or Fail will be awarded.

Final grade: For grade of Pass on the whole course, grades of Pass on module 1 and Pass on module 2 are required. For grade of Pass with distinction on the whole course, grade of Pass with distinction on module 1 and Pass on module 2 are required.

Regarding application of the ECTS grading scale please see the vice chancellor's directive 28/05/2007, diary nr G 8 1976/07.

Course evaluation

Course evaluation is done in relation to the intended learning outcomes and content of the course and is carried out at the end of the course by an individual written questionnaire on University of Gothenburg's virtual learning environment. A student who participates in, or has completed, a course should be given he opportunity to

anonymously express experiences of and views on the course in a course evaluation. A compilation of the course evaluation along with reflections by the responsible teacher should be made available for the students within reasonable time after the end of the course.