UNIVERSITY OF GOTHENBURG

DEPARTMENT OF CHEMISTRY AND MOLECULAR BIOLOGY

KEM760 Advanced Medicinal Chemistry, 15 credits

Avancerad läkemedelskemi, 15 högskolepoäng

Second Cycle

Confirmation

This course syllabus was confirmed by Department of Chemistry and Molecular Biology on 2016-09-01 and was last revised on 2017-10-06 to be valid from 2017-10-06, autumn semester of 2017.

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

Position in the educational system

The course is classified as a second-cycle course and can be read as a freestanding course.

The course can be part of the following programmes: 1) Master's Programme in Organic and Medicinal Chemistry (N2KEL) and 2) Master's Programme in Chemistry (N2KEM)

Main field of studies	*Specialization*
Chemistry	A1F, Second cycle, has second-cycle course/s as entry requirements

Entry requirements

For admission to the course, passed courses of 90 credits in chemistry are required, including the courses KEM815 Advanced organic chemistry (15 credits) and KEM825 Organic and Medicinal Chemistry (10 credits) or equivalent courses, furthermore English B/English 6 or equivalent competence. Students with equivalent education can after assessment be given admission to the course.

Learning outcomes

On completion of the course the student should be able to:

Knowledge and understanding

- **describe** strategies for design and synthesis of potential lead compounds,
- **explain** important methods and theories of design and synthesis of lead compounds,
- **describe** methods for the biological evaluation of substances.

Competence and skills

- **use** computer-based methods (computational chemistry) to **design** potential lead compounds as well as to study and solve pharmaceutical chemistry problems,
- **carry out** a basic retrosynthetic analysis,
- **suggest** synthesis methods for pharmaceutical substances.

Judgement and approach

- **explain** important methods and theories for the evaluation of lead compounds and **apply** them on specific cases,
- **critically analyse** research publications,
- clearly **describe** and **discuss** their conclusions as well as the knowledge and the arguments that underlie these both oral and written.

Course content

The course is intended to give advanced knowledge in design, synthesis and biological evaluation of small organic substances as potential lead compounds.

A. Theory

Design of substances:

- Conformational analysis and basic cheminformatics; force-field, energy minimisation, 3Ds, pharmacophore identification. Sub-structure search, similarity search, databases
- Physico-chemical properties: drug-likeness, design (diversity, scaffold-hopping)
- Halogenes in biologically active organic substances
- Proteins: structures, protein-ligand interactions, sequence/structure homology, structure-based design, docking

Synthesis of substances

- Retrosynthetic analysis
- Diversity-oriented synthesis
- Scaffold-based synthesis using for example benzodiazepines, piperidinones, indoles, purines, and benzofurans

Biological evaluation of substances

- Cell-free assays
- Whole cell assays
- Animal assays

B. Computer exercises

Computational Chemistry: structure, energies, conformational analysis of small molecules; studies of biomolecules and interactions between drug molecules and receptors, rational design, structure-based design, docking.

Form of teaching

The teaching is given in the form of lectures, group work, project assignments, computer exercises and literature seminars. Group work, project assignments, computer exercises and seminars are compulsory.

Language of instruction: English and Swedish
The course is given as principal rule in English but can be given completely or partly in Swedish if the circumstances admit this.

Assessment

The answers to project assignments, which are presented in writing and orally, will underlie the course grade. A final examination, usually in writing, is arranged at the end of the course.

For students who have not passed the regular examination additional occasions are offered.

A student who has failed twice on the same examining component has the right to change their examiner if this is practically possible.

Grades

The grading scale comprises: Pass with Distinction (VG), Pass (G) and Fail (U).
To pass the laboratory part, approved laboratory results as well as oral and written project presentation with approved result are required.

Concerning application of the ECTS grading scale please see Vice-chancellor's decision 28/05/2007, dnr G 8 197/07

Course evaluation

The course is evaluated and the results become subject to discussion between the teachers in the course and representatives for the students. Notes from this discussion, together with the written course evaluation, will be reported to the student affairs office for chemistry where they are available as public documents.