



## Course syllabus

Faculty of Health and Life Sciences

Department of Chemistry and Biomedical Sciences

4KE503 Modern kemi och dess tillämpningar, 15 högskolepoäng

Current Pure and Applied Chemistry, 15 credits

### **Main field of study**

Chemistry

### **Subject Group**

Chemistry

### **Level of classification**

Second Level

### **Progression**

A1N

### **Date of Ratification**

Approved by Faculty of Health and Life Sciences 2014-12-19

The course syllabus is valid from autumn semester 2015

### **Prerequisites**

Bachelor's degree within a subject area of Natural Science, or equivalent, including at least 90 credits Chemistry, or equivalent.

English proficiency equivalent to the level of TOEFL ibt 90 or IELTS 6.5.

## Objectives

During the course the student should acquire solid knowledge and skills in methods within chemistry and applied chemistry.

After completing the course the student should be able to:

- Apply chosen methods within chemistry and applied chemistry
- Make a case for and draw conclusions regarding the possibilities and limits of the chosen methods, based on the scientific literature
- Give an account of and argue for the effects of different methods on the environment and on society based on the scientific literature, legislation and ethical considerations.

The course consists of 7 subcourses where subcourses 4A and 4B, and 5A and 5B respectively can be chosen as options.

After completing subcourse 1 (Beräkningskemi – Computational Chemistry – see below) the student should be able to:

- Give an account of the theoretical description of an atom/molecule as well as a simulation of a molecular system;
- Give a general account of the use of multivariate methods of analysis as well as the interpretation of results using these methods;
- Give a basic account of the concept of experiment planning and how this method can

be used during optimization,

- Use visualization tools within molecular modelling during oral and written presentations;
- Critically evaluate the scientific work of others, and
- Present aspects of the above in oral and written presentations.

After completing subcourse 2 (Molekylär spektroskopi – Molecular spectroscopy – see below) the student should be able to:

- Give an account of some of the commonly used methods of spectroscopy;
- Give a basic account of the theory behind some of the commonly used methods of spectroscopy;
- Interpret data obtained using some of the commonly used methods of spectroscopy;
- Make a case for the choice of different spectroscopic methods used in the determination of molecular structure and in the analysis of molecular systems;
- Conduct UV/fluorescence spectroscopy studies of biomolecules
- Present aspects of the above in oral and written presentations.

After completing subcourse 3 (Organisk kemi – Organic chemistry – see below) the student should be able to:

- Give an account of the concept of solid-phase peptide synthesis
- Give an account of the methods for creating carbon-carbon bonds, including their limitations and areas of application;
- Give an account of the concept of the use of biomolecules in organic synthesis, including their limitations and areas of application;
- Give an account of the concept of asymmetric synthesis, including methods for creating optically active substances and the characterization of optical purity;
- Conduct solid-phase peptide synthesis, including isolation and characterization of the product;
- Conduct organic synthesis with the help of enzymes, including isolation and characterization of the product, and
- Present aspects of the above in oral and written presentations.

After completing subcourse 4A (Makromolekylär kemi – Macromolecular chemistry – see below) the student should be able to:

- Give a general account of the structure and function of the most common types of macromolecules, both biological and synthetic (carbon-based);
- Give an account of methods for producing synthetic polymers and dendrimers;
- Give a general account of methods used to characterize synthetic polymers;
- Give a general account of methods used to produce proteins.
- Conduct a polymer synthesis, including isolation and characterization of the product; and
- Present aspects of the above in oral and written presentations.

After completing subcourse 4B (Biomaterial – Biomaterials – see below) the student should be able to:

- Give an account of some of the common types of biomaterials and their areas of use;
- Give an account of the interaction between cells and non-biological material (in vitro);
- Give an account of the interaction between tissue (blood) and non-biological material (in vitro);
- Give an account of test systems for measuring the activation of blood's cascade system and cells, and
- Present aspects of the above in oral and written presentations.

After completing subcourse 5A (Analytisk kemi med inriktning mot sensorer – Analytical chemistry with a focus on sensors – see below) the student should be able to:

- Give an account of the physical principles used in sensor technology;
- Give an account of the technical structure of a sensor;
- Use different sensor techniques for qualitative and quantitative characterization of molecular interactions;

- Make a case for the choice of sensor techniques for molecular detection, and
- Present aspects of the above in oral and written presentations.

After completing subcourse 5B (Enzymteknik – Enzyme engineering – see below) the student should be able to:

- Give an account of the basic properties of different types of biocatalysts;
- Give an account of the possibility of customizing biocatalysts;
- Give an account of the production, cleaning and use of biocatalysts on an industrial scale;
- Give an account of the properties of immobilized biocatalysts och their application in technical processes, and
- Present aspects of the above in oral and written presentations.

## Content

### *Subcourse 1 Computational chemistry, 3 credits*

- The quantum-mechanical description of an atom/molecule: orbital theory and wave functions.
- Force field-based empirical description of a molecule and a molecular system (Amber, Opis, Charmm, Gromos, Gaff).
- Molecular dynamics and its applications in biomolecular systems.
- Multivariate analysis methods such as PCA, MLR, PCR and PLSR.
- Chemometrics, experiment design (fractional factorial, full factorial, central composite, Box-Behnken and Doehlert design) as well as optimization (simplex and simulated annealing)
- Computational programs (AMBER, GROMACS, NAMD, GAUSSIAN, AVOGADRO, MOLEKEL, R).
- Visualization tools: VMD

### *Subcourse 2 Molecular spectroscopy, 3 credits*

- Spectroscopic methods such as NMR, FR-IR, UV-VIS and fluorescence spectroscopy.
- NMR and FT-IR for structure determination.
- NMR, fluorescence spectroscopy and UV-VIS for interaction studies.

### *Subcourse 3 Organic chemistry, 3 credits*

- Solid phase peptide synthesis, Merrifield synthesis, modern Fmoc and BOC strategies, orthogonal protecting group strategy.
- Some central reactions for the creation of carbon-carbon bonds: Aldol, Wittig, Diels-Alder, Suzuki and Heck reactions.
- Enzymes in organic synthesis: protein stability, use in organic synthesis
- Asymmetric synthesis: strategies and some principally important reactions.

### *Subcourse 4A Macromolecular chemistry, 3 credits*

- Structure and function of biomolecular and synthetic macromolecules.
- Principles for polymer and dendrimer synthesis.
- Physical characterization of polymers (MW, NMR, IR, SEM, BET, rheology, interactions).

### *Subcourse 4B Biomaterials, 3 credits*

- Common types of biomaterials and their areas of use.
- Interaction between artificial materials and cells.
- Interaction between artificial materials and tissue (blood)
- Composition of blood: protein systems and cells.
- In vitro systems for studies of the interaction between blood and artificial materials.
- ELISA, western blot, flow cytometry.

### *Subcourse 5A Analytical chemistry with a focus on sensors, 3 credits*

- Physical principles for generating measurement signals: piezoelectricity, surface plasmon resonance and luminescence.

- The technical construction of a sensor: sample introduction, flow cell, detector, amplifier, translator, computer.
- Sensor techniques: QCM, SPR, fluorescence spectroscopy
- Electronic nose/tongue, glucose sensor, aerosol sensor and powder sensor.

#### *Subcourse 5B Enzyme engineering, 3 credits*

- Different biocatalysts (single-enzyme systems, multi-enzyme systems, whole cell systems) used for technical applications as well as their properties.
- Use of molecular biological methods for the creation of customized biocatalysts.
- How different biocatalysts (single-enzyme systems, multi-enzyme systems, whole cell systems) are produced, cleaned and used in technical processes.
- How the properties of biocatalysts (single-enzyme systems, multi-enzyme systems, whole cell systems) are affected by immobilization. Advantages and disadvantages of immobilized biocatalysts.

### Type of Instruction

The instruction consists of seminars, exercises and laboratory work. Participation in seminars, exercises and laboratory work is obligatory; all obligatory elements are presented in the schedule. The course is designed to train the student to actively seek, gather and evaluate knowledge, apply knowledge in practice as well as present and discuss results in association with exercises and seminars.

### Examination

The course is assessed with the grades A, B, C, D, E, Fx or F.

The grade A constitutes the highest grade on the scale and the remaining grades follow in descending order where the grade E is the lowest grade on the scale that will result in a pass. The grade F means that the student's performance is assessed as fail.

Examination of each respective subcourse is either conducted continuously (active participation by the students in particular elements of the course) or by written examination at the end of the subcourse. The number of opportunities for examination is limited to five. Resubmission of an examination should as a general rule occur within 10 days of feedback.

The subcourses are evaluated with the grades A to F. The theoretical and practical elements of the course respectively are assessed in their entirety. The criteria for a passing grade are listed in Objectives (see above).

The language of instruction is normally English but the course may be conducted in Swedish if only Swedish speaking students participate.

### Course Evaluation

A written course evaluation is conducted at the end of the course. The results of the evaluation are compiled in a course report that is archived by the department's administration. The results and any measures taken are communicated to the head of department and presented to the students at the next occasion.

### Credit Overlap

This course cannot be part of a degree in combination with another course in which the content fully or partly correspond to the content of this course: 4KE003 Current Pure and Applied Chemistry 15 credits

### Other

Grade criteria for the A–F scale are communicated to the student through a special document. The student is to be informed about the grade criteria for the course by the start of the course at the latest.

### Required Reading and Additional Study Material

*SUBCOURSE 1 (Computational Chemistry)*

Schlick, Tamar (2002). *Molecular modeling and simulation: an interdisciplinary guide*. Springer, New York. ISBN 978-0-3879-5404-2 (E-book available via the university library).

Plus scientific articles.

*SUBCOURSE 2 (Molecular spectroscopy)*

Albani, Jihad Rene (2008). *Principles and Applications of Fluorescence Spectroscopy*. John Wiley & Sons, Oxford. ISBN 978-1-4051-3891-8 (E-book available via the university library).

Plus scientific articles.

*SUBCOURSE 3 (Organic Chemistry)*

Bloch, Daniel (2006). *Organic Chemistry Demystified*. McGraw-Hill Professional Publishing. ISBN 9780071487108 (E-book available via the university library).

Carey, Francis A. Sundberg, Richard J. (2000). *Advanced Organic Chemistry, Part A: Structure and Mechanisms (4th Edition)*. Kluwer Academic/Plenum Publishers. ISBN 9780306462429 (E-book available via the university library).

Carey, Francis A. Sundberg, Richard J. (2001). *Advanced Organic Chemistry, Part B: Reactions and Synthesis*. Kluwer Academic Publishers. ISBN 9780306473807 (E-book available via the university library).

Plus scientific articles.

*SUBCOURSE 4A (Macromolecular Chemistry)*

Carey, Francis A. Sundberg, Richard J. (2000). *Advanced Organic Chemistry, Part A: Structure and Mechanisms*. Kluwer Academic/Plenum Publishers. ISBN 978-0-30646-242-9 (E-book available via the university library).

Carey, Francis A. Sundberg, Richard J. (2001). *Advanced Organic Chemistry, Part B: Reactions and Synthesis*. Kluwer Academic Publishers. ISBN 978-0-30647-380-7 (E-book available via the university library).

Hill, A.J., Hannink, H. J. (Eds) (2006). *Nanostructure Control of Materials*. Woodhead Publishing, New York. ISBN 978-1-84569-118-9 (E-book available via the university library).

Plus scientific articles.

*SUBCOURSE 4B (Biomaterials)*

Ratner, Buddy D., Hoffman, Allan S., Schoen, Fredrick J., Lemons Jack E. Eds (2004). *Biomaterials Science: An Introduction to Materials in Medicine*, pp. 1-19 (distributed electronically).

Plus scientific articles.

*SUBCOURSE 5A (Analytical chemistry with a focus on sensors)*

Eggins, Brian R. (2008). *Chemical sensors and biosensors*. John Wiley & Sons, Chichester. ISBN 978-0-4718-9914-3 (E-book available via the university library).

Plus scientific articles.

*SUBCOURSE 5B (Enzymtechnik) Enzyme Technology – Web book*  
(<http://www.lsbu.ac.uk/biology/enztech/>). Plus scientific articles.