Course Specifications
Valid as from the academic year 2018-2019

Advanced Chromatography and Organic Mass Spectroscopy (C002555)

Course size
Credits 6.0
Study time 150 h
Contact hrs 55.0 h

Course offerings and teaching methods in academic year 2018-2019
A (semester 1)
English
lecture 20.0 h
demonstration 2.5 h
seminar: coached exercises 10.0 h
practicum 22.5 h

Lecturers in academic year 2018-2019
Lynen, Frederic WE07 lecturer-in-charge
Desmet, Gert VUB co-lecturer

Offered in the following programmes in 2018-2019 crdts offering
Master of Science in Chemistry 6 A
Exchange Programme in Chemistry (master's level) 6 A

Contact hrs Study time 150 h

Teaching languages
English

Keywords
Separation science, mass spectrometry

Position of the course
Theoretical and practical education in modern analytical techniques related to chromatography, electrophoresis and mass spectrometry for the analysis of organic and biomolecules

Contents
1 Fundamentals of State-of-the-Art Gas Chromatography
2 Fundamentals of State-of-the-Art Liquid Chromatography
3 High Throughput and High Resolution 1D Separation approaches
4 Kinetic plots in Liquid Chromatography
5 High Throughput and High Resolution 2D Separation approaches
6 Recent Developments in Sample Preparation for Gaseous, Liquid and Solid Samples
7 Fundamentals of Organic Mass Spectroscopy
8 Gas Chromatography - Mass Spectroscopy for small Molecules
9 Mass Spectroscopy - structural elucidation of small Molecules - principles I
10 Mass Spectroscopy - structural elucidation of small Molecules - principles II
11 Mass Spectroscopy - structural elucidation of small Molecules - implementation I
12 Mass Spectroscopy - structural elucidation of small Molecules - implementation II
13 Mass Spectroscopy - structural elucidation of small Molecules - implementation III
14 Gas Chromatography - Isotope ratio Mass Spectroscopy
15 Liquid Chromatography - Mass Spectroscopy for Small Molecules
16 Liquid Chromatography - Mass Spectroscopy for Biomolecules
17 Selection of a Chromatographic Technique for a Given Application
18 Pressure versus Electroosmotic Driven Chromatographic Techniques
19 Stationary phase as an adaptable tool for selectivity tuning in chromatography

(Approved)
• 20 non-linear versus linear chromatography – principles of preparative chromatography
• 21 Advanced chromatographic method validation techniques for improved quantitative analysis

Tutorials
1 Constructing Kinetic Plots
2 Interpretation of MS Data. Part 1. Small volatile molecules, ionization, molecular ion, link elemental composition, nitrogen rule, isotopic clusters
3 Interpretation of MS Data. Part 2: factors influencing ion abundance, fragmentography, fragmentation types, sigma electron ionization, radical site initiation, McLafferty rearrangement
4 Interpretation of MS Data. Part 3: alkanes, polyaromatic hydrocarbons, alcohols, esters, aldehydes and ketones, amines, allocation of structures to spectra, interpretation of unknown spectra
5 Interpretation of MS Data. Part 4: (high resolution) MS analysis of non-volatile, LC-compatible solutes.

Practicals
qualitative and quantitative analysis of mixtures of organic solutes. The course participant is provided with controlled mixtures of samples for which he or she is challenged to practically select the optimal analysis methods, develop the optimal separation and to identify and quantify the solutes. Strong emphasis is set on the development of student self-reliance.

Initial competences
Fundamental aspects of chromatography and mass spectrometry

Final competences
1 The student is able to select adequate sample preparation, separation and detection techniques to address qualitative and quantitative issues in organic analysis.
2 The student is able to implement in a theoretical and practical way adequate sample preparation, separation and detection techniques to address qualitative and quantitative issues in organic analysis.
3 The student is able to interpret electron ionisation (EI) mass spectra of molecules containing the most important functional groups.
4 The student is able to to select the most suitable separation and detection technique to allow qualitative and quantitative analysis of beforehand unknown samples.
5 The student is able to perform without supervision qualitative and quantitative HPLC and GC-MS analyses and to intrepret the data.
6 The student is able to propose solutions for sampling, separation and detection issues both in theory and in practice.
7 The student is able to interpret electrospray- and (atmospheric pressure) chemical ionization mass spectra of small organic molecules and of biomolecules.

Conditions for credit contract
Access to this course unit via a credit contract is determined after successful competences assessment

Conditions for exam contract
This course unit cannot be taken via an exam contract

Teaching methods
Demonstration, lecture, practicum, seminar: coached exercises

Extra information on the teaching methods
Classes on the most recent developments via powerpoint presentations
Practical exercises on chromatographic instrumentation

Learning materials and price
PowerPoint presentations (Minerva)
Recent literature
The following textbooks below are useful regarding the section of mass spectrometry and structural elucidation. These books do not need to be purchased. Students can a copy on demand.

References
Analytical Chemistry

(Approved)
Course content-related study coaching
   Individual monitoring by tutor and assistants on request
   Questions during practicals and tutorials

Evaluation methods
   end-of-term evaluation and continuous assessment

Examination methods in case of periodic evaluation during the first examination period
   Written examination

Examination methods in case of periodic evaluation during the second examination period
   Written examination

Examination methods in case of permanent evaluation
   Participation, skills test, report

Possibilities of retake in case of permanent evaluation
   examination during the second examination period is possible

Extra information on the examination methods
   Written exam

Calculation of the examination mark
   Period based evaluation (70%), non-period based evaluation (30%).

   Students who are absent without any well-justified reason or who do not participate in
   (part of) the permanent evaluation, do not pass the exam for this course unit. The
   marks resulting from the permanent evaluation are retained in the second examination
   period, as the second examination period only consists of a periodic evaluation.