Molecular structural characterization and analysis

Lecturers
Gilles BRUYLANTS (Coordinator) and Sebastiaan EELTINK

Course mnemonic
CHIM-H407

ECTS credits
5 credits

Language(s) of instruction
English

Course period
Second term

Campuses
Solbosch and Other campus

Course content

Introduction: Raison d'être of the course

I. Molecules

II. Non Covalent Interactions

III. Importance of Separation Sciences

A. Separation Sciences

A.I. HPLC instrumentation and hyphenation to detectors

A.II. Types of Liquid Chromatography

A.III. Optimization of HPLC separations

A.IV. Band broadening in LC

A.V. Kinetic performance limits

A.VI. Multi-dimensional separations

A.VII. Chip Technology

A.VIII. Gas chromatography

B. Molecular Structure Characterization

B.I. Spectroscopy: general considerations

B.II. Electronic spectroscopies

B.III. Vibrational spectroscopies

B.IV. NMR spectroscopy

Objectives (and/or specific learning outcomes)

The aim of the course is to give you insight into the chromatographic methods available for the isolation and purification of molecules of industrial importance. In addition, we aim to teach you the fundamentals and application possibilities of different spectroscopic methods available for the determination and characterization of molecular structures.

Pre-requisits and co-requisits

Required knowledge and skills

Basic knowledge in organic chemistry and intermolecular interactions.

Teaching method and learning activities

Interactive course with powerpoint presentations.

Seminars and practicals illustrate the theory seen during classes.

Contribution to the teaching profile

This teaching unit contributes to the following competences:

- In-depth knowledge and understanding of exact sciences with the specificity of their application to (bio)engineering
- A creative, problem-solving, result-driven and evidence-based attitude, aiming at innovation and applicability in industry and society
- The flexibility and adaptability to work in an international and/or intercultural context
- An integrated insight in (bio)chemical process technology and materials' technology
- Insight in chemistry as a link between process and materials technology

References, bibliography and recommended reading

Separation Sciences

www.chromacademy.com

HPLC Columns: Theory, Technology, and Practice; U.D. Neue

Wiley-VCH (1997)

Contemporary Instrumental Analysis; K.A. Rubinson and J.F. Rubinson

Prentice-Hall (2000)

Molecular Structure Determination

Introduction to Organic Spectroscopy; L.M. Harwood and T.D.W Claridge

Oxford Chemistry Primers, Oxford Science Publications (1997)

Molecular Spectroscopy; J.M. Brown

Oxford Chemistry Primers, Oxford Science Publications (1998)

Spectrometric Identification of Organic Compounds; R. M. Silverstein, F. X. Webster

John Wiley & Sons Inc (7th edition, 2005 or any other edition)

Understanding NMR Spectroscopy, J. Keeler

Wiley–Blackwell; 2nd Edition (2010)

Course notes

Podcast and Université virtuelle

Other information

Place(s) of teaching

Other campus and Solbosch

Contact(s)

Prof. Gilles Bruylants: gilles.bruylants@ulb.be; Office: P2.2.110 (ULB)

Prof. Sebastiaan Eeltink: Sebastiaan.Eeltink@vub.be (VUB)

Evaluation method(s)

written examination and Group work

Evaluation method(s) (additional information)

The exercices and practicals illustrate the content of the courses and are as important as the theory.

Written examination Spectroscopy: students have to elucidate the structure of a molecule on the basis of spectra (IR, UV-Vis, NMR) and to ba able to answer to theoretical questions regarding the conditions to record a quantitative spectrum.

Determination of the mark (including the weighting of partial marks)

A graded practical will account for 20 % of the final mark. Modalities will be given during class.

A written examination, covering all the material seen during classes and exercise sessions, accounts for the remaining 80% of the final mark.

This grade is the weighted average of two grades, one for each of the teaching units (40% separation science - 60% spectroscopy).

Main language(s) of evaluation

English

Programmes

Programmes proposing this course at the Brussels School of Engineering

MA-IRBC | Master in Chemistry and Bio-industries Bioengineering | finalité Professional/unit 2 and MA-IRMA | Master of Science in Chemical and Materials Engineering | finalité Professional/unit 1

Programmes proposing this course at the faculty of Sciences

MA-IRBC | Master in Chemistry and Bio-industries Bioengineering | finalité Professional/unit 2