Module Title:
Mass spectrometry

Module Code:
AM-09-12

Maximum Number of Students:
25

Total ECTS Credits
2

Notional Learning Hours
(a) Contact Time - 10 h
(b) Private Study - 40 h

Format of Teaching:

Lectures	10 h
Laboratories or Practicals	0 h
Other	0 h

Teaching Strategy:
Formal lectures in 60/90 min timetable.

Convener:
Encarnación Moyano

University / Department:
University of Barcelona. Analytical Chemistry Department

Language of Tuition:
English

Module Description - The Purpose or Aims:
- To introduce the fundamentals aspects of mass spectrometry
- To recognize and understand the main components of a mass spectrometer
- To fully understand the fundamentals and the main characteristics of the most common mass analyzers
- To understand the fundamentals of tandem mass spectrometry
- To understand basic concepts and practical aspects of coupling mass spectrometry to separation techniques: GC-MS, LC-MS, CE-MS
- To explore the fundamentals of mass spectrometry data interpretation
- To explore the principles of quantitative analysis in mass spectrometry
- To acquire basic knowledge to use the technology in different application fields (environmental, food analysis, pharmaceutical industry, etc.)

Specific Learning Outcomes for this module: (contributing to general learning outcomes GLO 1 – GLO 10)
At the end of the module the learner is expected to be able to:
1. Critically select the most appropriate ionization technique taking into account the chemical characteristics of the analytes
2. Critically select the most suitable mass analyzer taking into account the structural information and the selectivity required for a given analytical problem
3. Design the most appropriate tandem mass spectrometry experiments to obtain the structural information required
4. Critically select the most suitable coupling technique (separation technique-mass spectrometry) to solve a given analytical problem
5. Full understanding and effective use of mass spectrometric data (mass spectral data interpretation to identity functional groups, to estimate elemental composition and to propose chemical structures).
6. Full understanding the validation and quantitative/confirmatory analysis using mass spectrometry in a regulated environment

Summary of Course Content:
This module explores the fundamental aspects of mass spectrometry and topics that will be discussed include: (a) mass spectrometry basics, (b) theoretical and practical aspects of the most popular ionization techniques, (c) the basics of the main mass analyzers, (d) fundamentals of tandem mass spectrometry and an introduction to popular MS/MS instrument types (e.g., QqTOF, QqQ, QIT, LIT, FTICR), (e) basic aspects of coupling mass spectrometry to separation techniques (GC-MS, LC-MS, CE-MS), (f) mass spectrometry of small and large molecules, (g) the principles of quantitative analysis using mass spectrometry and (h) an overview of mass spectral interpretation.

Transferable Skills Taught:

Information Technology:

Advances in mass spectrometry instrumentation and mass spectrometry database search (NIST)

Communications:

Communication with use of mass spectrometry terminology

Assessment Methods:

LO1-LO6 – Written Examination (80%)

LO1-LO6 – Resolution of practical exercises: real situation-real MS solutions (20%)

Assessment Criteria:

Threshold:

LO1, LO2 and LO4: to understand the principles of the ionization techniques, the mass analyzers and the coupling of separation techniques to mass spectrometry

LO3: to understand the fundamentals of tandem mass spectrometry

LO5: to have a general knowledge about the information than can be obtained from mass spectral data

LO6: to have a general knowledge about quantitative/qualitative analysis using mass spectrometry

Good:

LO1, LO2 and LO4: to be able to choose the most adequate ionization technique, mass analyzer and coupling technique to solve an analytical problem

LO3: to be able to correctly design a tandem mass spectrometry experiment to provide the structural information required

LO5: to identify the possible structure of and organic compound from the interpretation of the mass spectral data

LO6: to design the experimental work to determine a target compound using mass spectrometry under regulated environment

Excellent:

LO1-LO4 and LO6: given a set samples, to choose the best available ionization technique, mass analyzer and coupling technique to analyze each sample and devise an experimental protocol to perform the respective study

LO5: given a set spectral data, to interpret: to correctly assign fragments, to calculate elemental composition, to propose a chemical structure.

Resource Implications of Proposal and Proposed Solutions:

Lectures notes will be available for students.

Recommended reading:

- F.W. McLafferty and F. Turecek. ***Interpretation of mass spectra.*** University Science Books, 4th edition, 1993.
- E. de Hoffmann and V. Stroobant. ***Mass Spectrometry. Principles and Applications.*** J. Wiley and Sons, 3rd edition, 2007.
- J. Barker, D.J. Ando, R. Davis, M.J. Frearson. ***Mass Spectrometry. ACOL,*** 1999.
- B. Ardrey. ***Liquid Chromatography-Mass Spectrometry: An introduction.*** J. Wiley and Sons, 2004.
- www.spectroscopynow.com

Pre-Requisites: