UNIVERSITÀ
DEGLI STUDI DI MILANO-BICOCCA

SYLLABUS DEL CORSO

Analisi di Biomolecole

2425-1-F0802Q043

Aims

The main aim of the course is providing the description of the main spectroscopic and spectrometric methods used the analysis of small and medium-sized molecules (primary and secondary metabolites, small synthetic molecules, peptides, oligonucleotides, oligosaccharides). In particular, infrared spectroscopy (IR), mass spectrometry (MS) and Nuclear magnetic resonance (NMR) spectroscopy will be described.
Practical exercises will allow the student to familiarize with the identification of the chemical structure of an organic molecule starting from the corresponding spectra, also by the use of web resources of spectra available for educational purposes.

Knowledge and understanding skills
At the end of this training activity, the student will be able to:
1. describe the basic principles underlying IR spectroscopy, MS and NMR spectroscopy;
2. describe the main features of an IR, MS and NMR spectrum and the information contained therein;
3. describe the fundamental components of MS instrumentation;
4. describe the main fragmentation reactions of organic molecules that can take place in an ionization source;
5. identify NMR active nuclei;
6. describe the main features of mono- and two-dimensional NMR spectra and the information contained therein;
7. describe the main applications of IR, MS and NMR to the study of biomolecules.

Ability to apply knowledge and understanding
At the end of this training activity, the student will be able to:
1. correlate the frequency and intensity of the bands present in an IR spectrum to the structure of organic compounds and to the secondary structures of proteins;
2. provide the appearance of the MS and NMR spectra of simple organic biomolecules;
3. correlate experimental data obtained from MS and NMR spectra to the structural properties of bioorganic molecules;
4. analyze spectra of MS and NMR by determining useful quantities such as the m / z ratio, the relative abundances of the ions, the chemical shift, the coupling constants.

Making judgements
At the end of this training activity, the student will be able to:
1. choose the best analytical techniques for the structural analysis of a molecule of interest;
2. select the most suitable techniques to obtain specific structural and conformational information, as well as to study molecular interaction phenomena;
4. assign the signals present in the 1H-NMR spectrum of a low molecular weight biomolecule on the basis of mono- and bi-dimensional NMR spectra (COSY, 2D-TOCSY, 2D-NOESY, HSQC).

Communication skills
Use of an appropriate scientific/chemical vocabulary and ability in oral reports.

Learning skills
At the end of this training activity, the student will be able to:
1. to collect and understand the new information useful for rationalizing the structural properties of organic compounds of biological interest;
2. to collect and understand information about the evolution of spectroscopic and spectrometric techniques in the context of the analysis of biomolecules and their molecular interactions.

Contents

Theory and applications of IR and NMR spectroscopy and mass spectrometry to the analysis of biomolecules.

Detailed program

IR spectroscopy
IR resonance theory; characteristic bands of the classes of organic compounds; detailed discussion of correlation between the absorption and emission of IR radiation and the molecular structure.

Mass spectrometry
Basic principles of mass spectrometry; exact mass; sources and analyzers used in mass spectrometry; mass spectroscopy applications to the study of proteins

NMR spectroscopy
Nuclear spin and NMR; chemical shift; spin-spin coupling; 1H and 13C spectroscopy; Fourier transform NMR spectrometer; data acquisition and spectrum processing; NOE effect; two-dimensional spectra (COSY, TOCSY, NOESY and HSQC); interpretation of spectra of small organic molecules (metabolites, synthetic compounds); applications of NMR spectroscopy to molecular recognition studies and to the rational design of drugs.

Prerequisites

Background. Basic knowledge of organic chemistry.
Prerequisites. None

Teaching form

17 2 hours-lectures and 1 1 hour-lecture composed by:

- a section of delivered didactics (Didattica erogativa, DE) focused on the presentation-illustration of contents by the lecturer;
- a section of interactive teaching (Didattica Interattiva, DI) including teaching interventions supplementary to delivered didactic activities, short interventions by
  trainees, demonstrations, practical applications.
  Didactic activities are conveyed by means of face-to-face lectures.

10 hours of Tutorial activities on spectroscopic data interpretation aimed at guiding and assisting students throughout their studies in view of the exam preparation delivered by interactive teaching (Didattica Interattiva, DI) 16 through in-person tutorials, 4 through distance learning.

Lectures and tutorials are delivered in Italian.

Textbook and teaching resource

Slides. Available at the e-learning platform.
Handout. Available at the e-learning platform. Recommended text books.
Spectrometric Identification of Organic Compounds" R. M. Silverstein, F. X. Webster, D. Kiemle
Guide to the interpretation of NMR Spectra, Antonio Randazzo.

Semester

First semester

Assessment method

Written examination, based on questions on the basics and applications of IR, MS and NMR, and the resolution of an exercise concerning the assignment of the resonances of a low molecular weight biomolecule based on mono- and bi-dimensional NMR spectra, to be completed in two hours.

Office hours

Contact: on demand by mail to the lecture

Sustainable Development Goals