UNIMORE
UNIVERSITÀ DEGLI STUDI DI MODENA E REGGIO EMILIA

Dipartimento di Scienze della Vita

Proposta di insegnamento a scelta

Protein NMR Spectroscopy

Prof. Alejandro Josè Vila
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Instituto de Biologia Molecular y Celular de Rosario
Universidad Nacional de Rosario - Argentina

Protein NMR Spectroscopy

Il docente

Prof. Alejandro Vila

Laurea in Chimica industriale (1986)

Dottorato in Chimica (1990) (soggiorno a UNIFI per 18 mesi)

Docente di «Biofisica» e di «Spettroscopia di biomolecole» presso l'Università di Rosario (Argentina)

https://www.ibr-conicet.gov.ar/en/laboratorios/metalloproteins/

Sarà Visiting Professor dal 1 marzo al 3 maggio 2024

Ufficio a MO51, secondo piano, stanza 16

Protein NMR Spectroscopy

L'insegnamento

3 CFU = 24 ore di lezioni frontali a MO51

Erogato nel mese di marzo 2024

- martedì dalle 14 alle 17, aula B via Araldi
  giovedì dalle 14 alle 17 aula I via Araldi
- Lezioni in italiano e inglese

Forte carattere applicativo con esercitazioni e simulazioni al computer

Protein NMR Spectroscopy

Prerequisiti

Basics of NMR Spectroscopy applied to small molecules

Rudiments of trigonometry, vector properties, and electromagnetism.

Recommended prerequisite:

- Organic Chemistry I and II
- Biochemistry
- Physical Methods in Organic Chemistry (preferably)

Protein NMR Spectroscopy

Contenuti

Vectorial Model of the NMR phenomenon and NMR experiments (0,5 CFU, 4 hours)
Product Operator Formalism and application to NMR pulse sequences (0,5 CFU, 4 hours).

Multidimensional NMR Spectroscopy and Signal processing. HSQC Spectra, basics of triple resonance spectroscopy and protein backbone assignment. Protein-based strategies and heteronuclear-based strategies. Measurement of NMR constraints for structure determination. Assessment of the quality of an NMR-based protein structure. Study of intrinsically disordered proteins (1 CFU, 8 hours).

Nuclear Spin Relaxation. Relaxation mechanisms and impact on the NMR Spectral features. Study of protein backbone dynamics based on nuclear relaxation. Chemical exchange and study of protein dynamics within the time scale of chemical exchange phenomena (CPMG and CEST) (0,5 CFU, 4 hours).

Protein-ligand interaction. Different approaches: protein-centered and ligand-centered. Experimental approaches to study large proteins and large complexes by NMR. In-cell NMR (0,5 CFU, 4 hours).

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Metodi didattici

The lectures (32 hours) are **delivered in English/Italian** using Power point presentations. The product operator lessons involve exercises solved at the blackboard with participation of the students.

Part of the backbone assignment will be performed by the students in their own computers (PC or Mac) using academic free software with datafiles provided by the lecturer. This will be part of the final exam of the course.

The participation to the lectures is mandatory and the final participation assessment is conferred if the minimum of 75% participation to the lessons is achieved.

Protein NMR Spectroscopy

Modalità di verifica

The final exam will be divided into two parts.

One will consist of the **partial assignment of a protein backbone, during the lectures**, in a way that the students can **develop this skill** as well to allow the Professor to evaluate the impact of the classes.

The second one will be held **at the end of lessons** and consist in a short series of problems in which **the students will be challenged to interpret experimental NMR data** and suggest possible solutions, or will be posed a biochemical problem, and they will be asked to propose a series of NMR experiments aimed to solve this problem.

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Testi di riferimento

Copies of the pdf slides from the lecturer will be placed into the Moodle and MS Teams platform. This is copyrighted material, DO NOT disclose outside the University of Modena and Reggio Emilia.

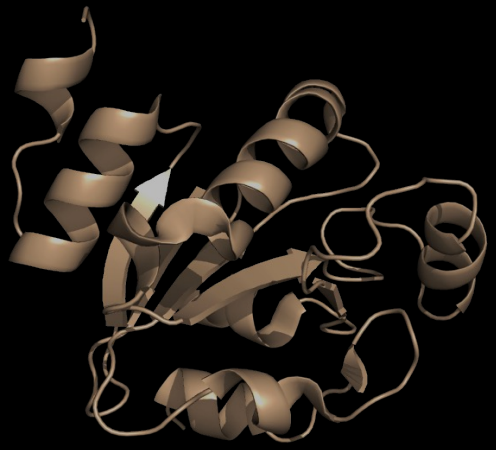
J. Keeler, Understanding NMR Spectroscopy, Wiley & Sons.

Book present in the Interdepartmental Scientific Library (BSI – UNIMORE)

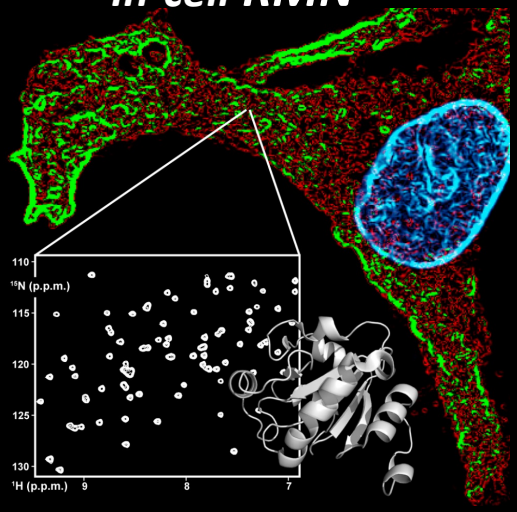
Protein NMR Spectroscopy

Un corso orientato a utenti non esperti interessati a metodi di indagine di struttura di proteine e delle interazioni farmaco-proteina

Struttura e dinamica di proteine



In-cell RMN



Interazioni farmaco-proteina