



ICGEB International Centre for Genetic Engineering and Biotechnology

ICGEB Courses “NMR for combatting diseases: from cancer to SARS-CoV-2”

ICGEB training course - March 27-31, 2023
CERM/CIRMMP, Sesto Fiorentino (Florence), Italy



CERM • CIRMMP INFRASTRUCTURE



UNIVERSITÀ
DEGLI STUDI
FIRENZE

	March 27 th		March 28 th	March 29 th	March 30 th	March 31 st
		8.30-10.30	Lectures M. Piccioli M. Fragai	Lectures F. Cantini N. Bhavesh	Lectures F. Camponeschi A. Rosato	Lectures R. Pierattelli R. Konrat
		Coffee				
11.00-13.40	Arrival and registrations Snacks	11.00-13.00	Lectures A. Bonvin	Lectures J. Hoch	Lectures E. Ravera	Lectures E. Luchinat
13.40	Welcome L. Banci Course intro I. Felli/S. Cacciatore		Flash talks (4) Poster Session	Flash talks (4) Poster Session	Flash talks (5) Poster Session	Opportunities by ICGEB Writing an access proposal Closing I. Felli/S. Cacciatore
		Lunch				
14.00-16.00	Lectures L. Banci H. Schwalbe	14.30-16.00	Practicals M. Schiavina (I) A. Bonvin(II)	Practicals N. Bhavesh (I) C. Richter (II)	Practicals J. Wirmer (I) L. Cerofolini (II)	Departure
		Coffee				
16.30-18.00	Introduction of participants Flash talks (12) Posters	16.30-18.00	Practicals M. Schiavina (II) A. Bonvin(I)	Practicals N. Bhavesh (II) C. Richter (I)	Practicals J. Wirmer (II) L. Cerofolini (I)	
				Dinner in downtown Florence		

Topics covered through lectures and practicals (alphabetical order)

"Basic lectures" (45 minutes + 15 minutes for discussion)

- F. Camponeschi – Sample quality/properties – inspection of different cases
- F. Cantini – Protein structure and dynamics through NMR
- M. Fragai – NMR titrations / monitoring interactions
- M. Piccioli – From NMR basics to multidimensional biomolecular NMR
- E. Ravera – Tips and tricks for paramagnetic NMR acquisition
- A. Rosato - Protein dynamics by NMR spectroscopy

"Keynote lectures" (45 minutes + 15 minutes for discussion)

- L. Banci - NMR spectra as fingerprints of functional processes and of biological drugs and vaccines
- N. Bhavesh – Integration of NMR and X-ray for Covid19 research
- A. Bonvin – Solving 3D puzzles of biomolecular complexes by integrative modelling
- J. Hoch - Biological Magnetic Resonance Data Bank
- R. Konrat – NMR spectroscopy for studies of structural dynamics in IDPs and protein drug interactions
- E. Luchinat – In-cell NMR for real-time studies of protein-ligand interactions in human cells
- R. Pierattelli – Un-structural biology by NMR spectroscopy
- H. Schwalbe – New aspects of fragment-based drug discovery by NMR

"Practicals" (1.5 hours)

- N. Bhavesh – Drug protein titration studies using NMR
- A. Bonvin – HADDOCK tutorial on modelling antibody-antigen complexes
- L. Cerofolini – How flexible is my protein? - Local mobility from ^{15}N relaxation
- J. Wirmer – Setting up triple resonance experiments
- M. Schiavina – My first 1D and 2D NMR spectra – initial set-up, data acquisition and processing
- C. Richter – STD, water LOGSY to monitor interactions

"Flash talks"

5 minutes for the selected participants to introduce their background knowledge/research projects of interest

Isabella Felli, Stefano Cacciatore (Organizers)

Program

March 27th 2023

- 11.00-13.45 Arrival and registrations, Snacks
13-40-14.00 Welcome and course presentation
14.00-14.45 NMR spectra as fingerprints of functional processes and of biological drugs and vaccines
L. Banci, CERM, University of Florence, Italy
15.00-15.45 New aspects of fragment-based drug discovery by NMR
H. Schwalbe, BMRZ, Goethe University Frankfurt am Main, Germany
16-16.40 Coffee
16.30-18.00 Introduction of participants
Flash talks – session I
Posters

March 28th 2023

- 8.30-9.15 From NMR basics to multidimensional biomolecular NMR
M. Piccioli, CERM, University of Florence, Italy
9.30-10.15 NMR titrations / monitoring interactions
M. Fragai, CERM, University of Florence, Italy
10.30-11.00 Coffee
11.00-11.45 Solving 3D puzzles of biomolecular complexes by integrative modelling
A. Bonvin, Bijvoet Centre for Biomolecular Research, Utrecht University, The Netherlands
12.00-13.00 Flash talks – session II /Poster session
13.00-14.30 Lunch
14.30-16.00 Practical - My first 1D and 2D NMR spectra – initial set-up, data acquisition and processing
M. Schiavina, CERM, University of Florence, Italy
16.00-16.30 Coffee
16.30-18.00 Practical - HADDOCK tutorial on modelling antibody-antigen complexes
A. Bonvin, Bijvoet Centre for Biomolecular Research, Utrecht University, The Netherlands

March 29th 2023

- 8.30-9.15 Protein structure and dynamics through NMR
F. Cantini, CERM, University of Florence, Italy
- 9.30-10.15 Integration of NMR and X-ray for Covid19 research
N. Bhavesh, ICGEB, New Delhi, India
- 10.30-11.00 Coffee
- 11.00-11.45 Biological Magnetic Resonance Data Bank
J. Hoch, BMRB, University of Connecticut, USA
- 12.00-13.00 Flash talks – session III /Poster session
- 13.00-14.30 Lunch
- 14.30-16.00 Practical - Drug protein titration studies using NMR
N. Bhavesh, ICGEB, New Delhi, India
- 16.00-16.30 Coffee
- 16.30-18.00 Practical - STD, water LOGSY to monitor interactions
C. Richter, BMRZ, Goethe University Frankfurt am Main, Germany

Dinner in downtown Florence

March 30th 2023

- 8.30-9.15 Sample quality/properties – inspection of different cases
F. Camponeschi, CERM, University of Florence, Italy
- 9.30-10.15 Protein dynamics by NMR spectroscopy
A. Rosato, CERM, University of Florence, Italy
- 10.30-11.00 Coffee
- 11.00-11.45 Tips and tricks for paramagnetic NMR acquisition
E. Ravera, CERM, University of Florence, Italy
- 12.00-13.00 Flash talks – session IV /Poster session
- 13.00-14.30 Lunch
- 14.30-16.00 Practical - Setting up triple resonance experiments
J. Wirmer, BMRZ, Goethe University Frankfurt am Main, Germany
- 16.00-16.30 Coffee
- 16.30-18.00 Practical - How flexible is my protein? - Local mobility from ¹⁵N relaxation
L. Cerofolini, CERM, University of Florence, Italy

March 31st 2023

- 8.30-9.15 Un-structural biology by NMR spectroscopy
R. Pierattelli, CERM, University of Florence, Italy
- 9.30-10.15 NMR spectroscopy for studies of structural dynamics in IDPs and protein drug interactions
R. Konrat, University of Wien, Austria
- 10.30-11.00 Coffee
- 11.00-11.45 In-cell NMR for real-time studies of protein-ligand interactions in human cells
E. Luchinat, CERM, University of Florence, Italy
- 12.00-13.00 Opportunities by ICGEB
Writing an access proposal
Closing remarks
I. Felli/S. Cacciatore

Flash talks – session I
Monday March 27th 2023

8-Oxoguanine can form quartets with a large central ion cavity

Simon Aleksič

Metabolic reprogramming in immune cells: TGF β 1 signaling in primary human macrophages

Kareem Awad

Ruthenium(II) polypyridyl complexes with long-lived Nile Red-localised triplet states as potential candidates for use in photodynamic therapy

Claire Condon

Phen-DC3 Induces Refolding of Human Telomeric DNA into a Chair-Type Antiparallel G-Quadruplex through Ligand Intercalation

Anirban Ghosh

Fighting entropy: Enzyme active sites designed to minimize dynamics

Cristina López Gallego

Folding of a PDZ tandem repeat - a cryptic physiological role for a misfolded intermediate

Francesca Malagrino

Immunoinformatics design of multi-epitope vaccine candidate to combat Leptospirosis

Azira Muhamad

Preliminary studies on the biophysical characterization of RelP through nuclear magnetic resonance spectroscopy

Cristina Olivieri

Study of the impact of site-specific ubiquitination of the protein tau on its structural and aggregation propensities

Daniele Trivellato

Structural characterization of the postsynaptic Drebrin protein

Soma Varga

Peptides targeting EphA2-Sam/Ship2-Sam interaction: a multidisciplinary study

Marian Vincenzi

Monitoring the inhibition of copper chaperone Atox1 by NMR spectroscopy and molecular docking studies

Daniele Vitone

Flash talks – session II
Tuesday March 28th 2023

Biochemical and structural study of a zinc efflux pump involved in the adaptation of *M. tuberculosis* within infected macrophages

Louis-Alban Bénastre

Unravelling the biological role of membrane interaction by α -synuclein

Silvia Mansueto

Molecular insight into the PCNA-binding mode of FBH1

Antonio Ruiz-Albor

Insights into structural and dynamic properties of mitochondrial tRNA fragments

Vito Šuklje

Flash talks – session III
Wednesday March 29th 2023

Molecular Imaging of FLASH Radiation Effects on Cells

Andrei Ciumeică

A comprehensive assessment of the conformational ensembles through biophysical experimental data

Hamidreza Ghafouri

Phytochemical assessment of critically endangered Himalayan medicinal plants using multi-analytical platforms

Neetika Naudiyal

Characterization of the major pseudocoelomic globin of *Dioctophyme renale*.

Luciana Rodriguez Sawicki

Flash talks – session IV
Thursday March 30th 2023

Metabolites and lipoproteins profiles with associated immune responses of a pilot cohort of Pancreatic Ductal Adenocarcinoma patients

Nnenna Elebo

Study of biomarkers of radiation using magnetic resonance methods and Glioblastoma cells

Ioana Ileana Fidel

Multicore vs core-shell PFCE/PLGA NPs: impact of ultrastructure on particle stiffness and its influence on cell uptake mechanisms

Naiara Larreina

Stability of PLGA-PFCE nanoparticles

Navya U. Nayak