# ICBEB Courses “NMR for combating diseases: from cancer to SARS-CoV-2”

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

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<td>8.30-10.30</td>
<td>Lectures</td>
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<td>M. Piccioli, M. Fragai</td>
<td>F. Cantini, N. Bhavesh</td>
<td>F. Camponeschi, A. Rosato</td>
<td>R. Pierattelli, R. Konrat</td>
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<td>11.00-13.40</td>
<td>Arrival and registrations, Snacks</td>
<td>11.00-13.00</td>
<td>Lectures</td>
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<td>A. Bonvin</td>
<td>J. Hoch</td>
<td>E. Ravera</td>
<td>E. Luchinat</td>
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<td>13.40</td>
<td>Welcome L. Banci</td>
<td>Flash talks (4) Poster Session</td>
<td>Flash talks (4) Poster Session</td>
<td>Flash talks (5) Poster Session</td>
<td>Opportunities by ICGEB</td>
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<td>Course intro I. Felli/S. Cacciatore</td>
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<td>Writing an access proposal</td>
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<td>Lunch</td>
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<td>Closing</td>
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<td>14.00-16.00</td>
<td>Lectures L. Banci, H. Schwalbe</td>
<td>14.30-16.00</td>
<td>Practicals</td>
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<td>M. Schiavina (I), A. Bonvin(I)</td>
<td>N. Bhavesh (I), C. Richter (II)</td>
<td>J. Wirmer (I), L. Cerofolini (II)</td>
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<td>Departure</td>
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<td>16.30-18.00</td>
<td>Introduction of participants, Flash talks (12) Posters</td>
<td>16.30-18.00</td>
<td>Practicals</td>
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<td>M. Schiavina (II), A. Bonvin(I)</td>
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<td>Dinner in downtown Florence</td>
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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
16.00-16.40 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 $^{15}$N 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
8-Oxoguanine can form quartets with a large central ion cavity
Simon Aleksič

Metabolic reprogramming in immune cells: TGFβ1 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 Malagrinò

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 Clumeică
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