



NMR relaxometry for biomedicine and advanced materials

HORIZON-MSCA-DN-2021 — FC-RELAX 101072758



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FC-RELAX, HIRES-MULTIDYN, IMF-NMR Joint Research Workshop: From Fast Field-Cycling to Ultrafast High-Resolution Relaxometry

13-15 March 2025

*Department of Chemistry, Ecole Normale Supérieure – PSL,
24, rue Lhomond, 75005 Paris, France*

Thursday March 13

- 8:50-9:00 Welcome by Fabien Ferrage and Giacomo Parigi
Chair: Giacomo Parigi
- 9:00-9:30 Fabien Ferrage (ENS)
Dynamics of biomolecular systems by high-resolution relaxometry
- 9:30-10:00 Dermot Brougham (University College Dublin)
NMR relaxometry in guiding magnetic nanoparticle synthesis and
colloidal stabilisation for applications in MRI and hyperthermia
- 10:00-10:15 Mamoona Riffat (LUT)
Adsorption Phenomenon of colloidal system by NMR relaxometry
- 10:15-10:30 Kahinga Kamau (UWM)
Spin-lattice and spin-spin relaxation – a consistent model for trypsin
- 10:30-11:00 *Coffee break*
Chair: Guillaume Bouvignies
- 11:00-11:30 Giacomo Parigi (UNIFI)
Field-cycling relaxometry of olive oil
- 11:30-11:45 Ana Paula Aguilar Alva (ENS)
Side-chain dynamics in the kinase p38g by ultrafast high-resolution
relaxometry
- 11:45-12:00 Muhammad Muntazir Mehdi (IST)
Data Processing Software for FC NMR Relaxometry and
Characterization of Advanced Materials



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- 12:00-12:30 Arthur G. Palmer (Columbia University)
Relaxometry using the Field Cycling Technology Shuttle at NYSBC:
New Science on the Horizon?
- 12:30-14:00 Lunch break*
- 13:30-14:00 Small group visit of the NMR laboratory @ ENS - PSL
Chair: Claudio Luchinat
- 14:00-14:30 Jakob Teetz (ETH Zürich)
Leveraging Molecular Dynamics for Enhanced Interpretation of High-
Resolution Relaxometry
- 14:30-14:45 Adam Kubrak (UNIFI)
Sensing molecular interactions in blood serum by high-resolution
relaxometry
- 14:45-15:00 Rajka Pejanovic (ENS)
A Deep Learning Approach for Removing Vibration Artifacts in Shuttled
NMR Experiments
- 15:00-15:30 Jorge Villanueva-Garibay (Bruker BioSpin)
Ultrafast high-resolution relaxometry
- 15:30-16:00 Coffee break*
- 16:00-18:00 **Complementary Training Course**
Manoj Nimbalkar (STELAR)
Navigating Your Career Path After a PhD
- 19:30 Dinner (@ Lilane)*

Friday March 14

- Chair: Pedro Sebastiao
- 9:00-9:30 Zsolt Baranyai (BRACCO)
Thermodynamic and Kinetic Differences in the Proton Exchange
Processes of Stereoisomers Formed by [M(HP-DO3A)] ($M^{3+} = \text{Eu}^{3+}$,
 Gd^{3+} and Y^{3+})
- 9:30-10.00 Manoj Nimbalkar (STELAR)
FFC relaxometry and its applications



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- 10:00-10:15 Danuta Kruk (UWM)
Fluoroniline as an almost perfect heteronuclear spin system
- 10:15-10:30 Claudio Luchinat (UNIFI)
Interactions between small molecules and macromolecules through high-resolution relaxometry
- 10:30-11:00 *Coffee break*
Chair: Zsolt Baranyai
- 11:00-11:30 Céline Henoumont (UMONS)
NMR, a toolbox to characterize nanoparticulate contrast agents for MRI
- 11:30-11:45 Angel Mary Chiramel Tony (UROS)
Molecular picture behind the frequency-dependant NMR relaxation rates
- 11:45-12:00 Madeleine Rhodes (UNIABDN)
Elucidating Water Dynamics Driving T_1 Relaxation below 200 mT in Biological Filamentous Structures
- 12:00-12:30 Frans Mulder (Johannes Kepler University Linz)
Investigation of co-solute paramagnetic relaxation using field shuttling
- 12:30-14:00 *Lunch break*
- 13:30-14:00 Small group visit of the NMR laboratory @ ENS - PSL
Chair: Anne-Laure Rollet
- 14:00-14:30 Éva Jakab Toth (Centre de Biophysique Moléculaire, CNRS, Orléans)
Towards safer and more specific MRI agents
- 14:30-14:45 Valeriia Baranauskaite (RS)
Slow motion dynamics in polymers according to TD NMR and FFC
- 14:45-15:00 Giulia Licciardi (ENS)
Exploring dynamics in alpha-synuclein: what can high-resolution relaxometry reveal?
- 15:00-15:30 Pedro Sebastiao (IST)
OneFit-Engine at the core of the different NMR model fitting tools for data analysis
- 15:30-16:00 *Coffee break*
Chair: Philippe Pelupessy



NMR relaxometry for biomedicine and advanced materials

- 16:00-16:30 Danuta Kruk (UWM)
The theoretical challenge of combining low and high-frequency relaxation data for ionic liquids
- 16:30-16:45 Denis Burov (STELAR)
Novel coil designs and practical compromises in modern NMR instrumentation. Academic approach to industrial R&D
- 16:45-17:00 Alessandro Ruda (ENS)
High-resolution NMR relaxometry of small molecules, perspectives and applications
- 17:00-17:30 Anne-Laure Rollet (Sorbonne Université)
Cover this interface that should not be seen
- 17:30-18:30 Visit of the FFC relaxometry platform at Sorbonne University
- 19:00 *Dinner ([@ Polidor](#))*

Saturday March 15

- Chair: Danuta Kruk
- 9:00-9:30 Leonid Grunin (RS)
Phases Composition Analysis by TD-NMR
- 9:30-10.00 Erkki Lähderanta (LUT)
Theory and molecular dynamics simulations of NMR relaxation of dendrimers for biomedical applications
- 10:00-10:30 Angelo Galante (UNIVAQ)
Metamaterials enhanced NMR
- 10:30-11:00 *Coffee break*
Chair: Frans Mulder
- 11:00-11:30 Lionel Broche (UNIABDN)
Data structures and methods for field-cycling NMR analysis
- 11:30-11:45 Madalina Ranga (BRACCO)
Characterization of the Proton Exchange Processes Between [Gd(DOTP)]⁵⁻ with Meglumine, D-Glucamine, and Dimeglumine



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- 11:45-12:00 Guru Kiran (UMONS)
Synthesis, Equilibrium, Kinetic, and Relaxation Properties of Mn(II)
Complexes
- 12:00-12:30 Ralf Ludwig (UROS)
Predicting NMR dipolar relaxation rates from theory: The example of
water and perspective for ionic liquids
- 12:30-14:00 Lunch break*
- 13:00-14:30 **FC-RELAX Supervisory Board meeting**
- 14:30-15:30 **FC-RELAX Steering Board meeting**



FC-RELAX and HIRES-MULTIDYN Joint Training Course High resolution NMR relaxometry of biological samples

17-19 March 2025

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Monday March 17

- 9:00-10:30 Fabien Ferrage *et al.* (ENS)
High-resolution relaxometry instrumentation and experiment design
- 10:30-11:00 *Coffee break*
- 11:00-12:00 Philippe Pelupessy (ENS)
Cross-relaxation in NMR: mechanisms (auto- and cross-correlated),
measurement methods, how to suppress its effects
- 12:00-13:30 *Lunch break*
- 13:30-15:30 Practical 1 and 2 in parallel for small groups
Practical 1: Running a high-resolution relaxometry experiment
Practical 2: Analysis of high-resolution relaxometry datasets
- 15:30-16:00 *Coffee break*
- 16:00-18:00 Practical 1 and 2 in parallel for small groups
- 19:00 *Dinner*

Tuesday March 18

- 9:00-10:30 Arthur G. Palmer (Columbia University)
ps-ns dynamics in biomolecules: high-field approaches and additional
information from relaxometry
- 10:30-11:00 *Coffee break*
- 11:00-12:00 Guillaume Bouvignies *et al.* (ENS)
Relaxation experiments beyond exponential decays: Integrating the
Master equation. Numerical methods, applications to chemical
exchange, relaxometry
- 12:00-13:30 *Lunch break*
- 13:30-15:30 Practical 1 and 2 in parallel for small groups



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Practical 1: Running a high-resolution relaxometry experiment

Practical 2: Analysis of high-resolution relaxometry datasets

15:30-16:00 Coffee break

16:00-18:00 Practical 1 and 2 in parallel for small groups

19:00 Dinner

Wednesday March 19

9:00-10:30 Claudio Luchinat and Giacomo Parigi (UNIFI)

Relaxation profiles and correlation times of paramagnetic systems

10:30-11:00 Coffee break

11:00-12:30 Lucas Siemons (ENS)

Combining NMR relaxation and molecular dynamics simulations in biomolecules

12:30-14:00 Lunch break

14:00-15:30 **Complementary Training Course**

Fabien Ferrage (ENS)

How to write a scientific article?

15:30-16:00 Coffee break

16:00-18:00 **Complementary Training Course**

Mathias Girel (ENS)

Ethics of the scientist

19:00 Dinner