

# AILM2024

## Advanced Isotope Labelling Methods for Integrated Structural Biology

Organization

THE UNIVERSITY  
*of York*

igbmc  
institut de génétique et de  
biologie moléculaire et cellulaire

IBPC

 ibs  
Institut de Biologie Structurale

 cnrs  
advancing the frontiers

May 28-31  
Grenoble – France.

## **International Workshop Advanced Isotopic Labelling Methods**

**May 28-31 in Grenoble (France)  
[www.ailm2024.org](http://www.ailm2024.org)**

In recent years, isotope labeling technologies have undergone considerable development, enabling them to be applied to a wide range of biological systems. Appropriate use of recent labeling methods has made it possible to address some fundamental biological questions, revealing the dynamics of molecular systems irrespective of their size or location within a cell. The application of labeling technologies is expected to continue to expand, as the possibilities offered by these methods are only just beginning to be explored. The AILM2024 workshop aims to provide an overview of current developments in isotope labeling techniques and their applications to the study of biomolecule structure and dynamics. This interdisciplinary meeting brings together researchers in NMR spectroscopy, neutron scattering and diffraction to promote scientific exchange on the latest labeling technologies. The number of participants and the very high quality of the lectures are a gratifying sign of the great interest aroused by such an event in the biophysics and structural biology research communities. We hope that this meeting, in the heart of the French Alps, will live up to your expectations and help spread the productive use of isotope labeling technologies for integrated structural biology.

The organizers would like to warmly thank Drs. P. Bernado, K. Frederick, A Gossert and K. Petzold for their contribution to the preparation of the program, as well as our generous sponsors and exhibitors for their support of AILM2024. We would also like to thank the IBS staff for their help in organizing the event.

We wish you a pleasant stay in Grenoble and fruitful scientific exchanges.

The AILM2024 organizing committee,  
Jérôme Boisbouvier (IBS – Grenoble )  
Bruno Kieffer (IGBMC – Strasbourg)  
Michael Plevin (Univeristy of York)  
Carine Tisné (IBPC - Paris)

Exhibitors & Sponsors



## GENERAL INFORMATION

Registration and Venue

EPN SCIENCE CAMPUS – 71 AVENUE DES MARTYRS – 38000 GRENOBLE - FRANCE



The AILM2024 conference takes place on the EPN Campus in Grenoble in IBS building. **To access the site, you must go to the entrance of the site (access map) with a valid ID (passport or ID card, driver's license refused).** Badges for access to the conference site and to the conference buffets and dinners will be given at the registration desk.

Registration:

Registration takes place at the IBS Central Building on Tuesday May 28<sup>th</sup> from 9 am to noon. Late registration will be possible at the Help Desk situated in the IBS Entrance Hall.

Venue:

- **from Lyon Airport:** Lyon Saint Exupery Airport is an hour's drive from Grenoble and regular shuttle buses ('Navette Aéroport') operate to and from the Grenoble bus station, which is located next to the Grenoble train station. Buses run every hour, seven days a week.

Two bus companies offer trips from Lyon to Grenoble:

FLIXBUS: You must reserve your seat in advance via the link below. The bus will stop near the ESRF/ILL/EMBL site upon request. You must tell the bus driver when you board the bus at the airport that you want to be dropped off at "Grenoble - Oxford". The bus stop is a few minutes walk from the EPN campus (see the access map on the previous page).

<https://www.flixbus.com>

BLABLABUS: You must reserve your seat in advance via the link below. The bus stops near the Grenoble train station. Take the tramway line B to its terminus (Oxford) which is a few steps from the EPN Campus. (See the map on the previous page).

<https://www.blablacar.fr>

- **from Geneva Airport:** Geneva Airport is a two-hour drive from the EPN campus. FLIXBUS : Please note that there is no bus every day.

<https://www.flixbus.com/>

BLABLABUS : Shuttles run between Grenoble train station and Geneva airport. There is at least one per day but they are not that frequent.

<https://www.blablacar.fr>

In addition, train connections from Geneva Central Station (Genève Cornavin) to Grenoble exist but are not very frequent and there are with transfers.

<https://www.sncf.com/en>

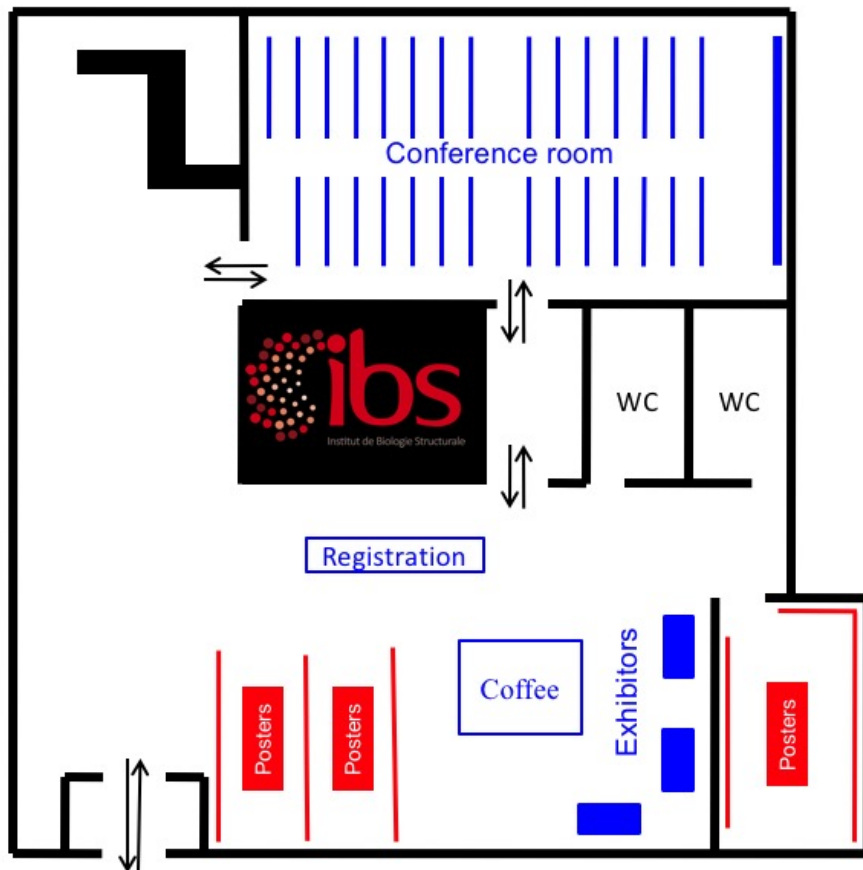
- **from Grenoble train/coach station:** take the tramway line B to its terminus (Oxford) which is a few steps from the EPN campus. (See the access map on the previous page).
- **from Lyon or Valence by car:** stay on the A48 as you approach Grenoble, following the signs "Grenoble Bastille-Gares-Europole". Leave the A48 at exit N°16 ("Polygone Scientifique") and cross the suspension bridge over the Isère. At the end of the bridge, turn right and go north on *Avenue des Martyrs*. The entrance to the site is on the left after a few hundred meters.
- **from Geneva by car:** take the Rocade Sud/N87 in the direction of Lyon, which brings you to the A480. Take the A480 direction "Lyon". Leave the A480 at the exit N°1 for the Polygone Scientifique. At the first traffic circle, turn right. The entrance of the site is on your right after a few hundred meters.

## Public Transportation

### Tram:

Line B connects EPN campus to downtown Grenoble with a frequency of 3 to 10 minutes from 6 am to 8 pm. In the evening, the tramways run every 30 minutes until 1 am. The tramway stop is located only 400 m from the entrance of the EPN site, and corresponds to the tramway B terminus called "Oxford".

Conference Organization



### Lectures:

Lectures will be held in the IBS conference room.

### Poster Sessions and Exhibition:

Company booths will be in the IBS Entrance Hall. Posters will be on display in the IBS entrance hall and room next to the IBS hall. Poster should be set up on Tuesday morning. Odd and even numbered posters will be presented on Wednesday and Thursday, respectively.

### Coffee Breaks:

Coffee will be served inside the IBS Hall.

### Lunches:

Outdoor lunch and dinner buffets are offered in front of IBS building on from Tuesday to Thursday. On Friday, lunches will be served in the EPN campus restaurant. You will need to present your AILM2024 badge at checkout.

### WiFi Access:

Free access is provided by eduroam IBS buildings using your personal login and password (<https://www.eduroam.org/>). For those who do not have an eduroam access, a visitor login and password can be requested at the IBS Help Desk (IBS building only).



## PROGRAM AILM2024

Tuesday May 28<sup>h</sup>

8:30 - 10:00 *Arrival / Registration / Coffee*

**Isotopic Labeling for the Study of Nucleic Acids and Complexes I - Chair W. Weissenhorn**

10:00 **Welcome**

10:20 **Frédéric Allain** (ETH Zurich – CH) - *Structural insights into protein-RNA interactions within biomolecular condensates using UV cross-linking and mass spectrometry of isotopically labeled RNA*

11:00 **Victoria D'Souza** (Harvard Medical School – Boston, USA) - *Extending the toolbox for RNA biology*

11:40 **Darren Hart** (ISBG - Grenoble – FR) - *User access to high-level research platforms through Instruct-ERIC and French FRISBI programs*

12:10-13:40 *Lunch will be served in front of IBS*

**Isotopic Labeling for Neutron Sciences - Chair P. Bernado**

13:40 **Giovanna Fragneto** (European Spallation Source, Lund –SE) - *Neutron structural characterisation of model membranes from natural lipids*

14:20 **Karyn Wylde** (National Deuteration Facility – ANSTO – AU) - *Enabling biomolecular investigations using neutrons and more: isotopic labelling strategies of the Australian National Deuteration Facility*

14:40 **Franck Gabel** (ILL, Grenoble – FR) - *Deuteration and neutrons: a perfect couple for studying complex biomacromolecular systems in solution*

15:20 **Suzanne Zoe Fisher** (European Spallation Source, Lund –SE) - *Botryococcus braunii autolysate for the production of deuterium-labeled recombinant protein production*

15:40-16:10 *Coffee Break*

**Spin Labeling for DNP & EPR – Chair R. Schneider**

16:10 **Bjorn Corzilius** (University of Rostock – DE) - *Site-specific dynamic nuclear polarization in uniform and sparsely labeled biomolecules*

16:50 **Sabine Hediger** (CEA – Grenoble - FR) - *SelDNP: Focusing on a selected protein site by DNP-enhanced solid-state NMR*

17:30 **Elisabetta Mileo** (Bioénergétique et Ingénierie des Protéines, Marseille, FR) – *Structural dynamics insights from in-cell EPR of proteins*

17:50 **Kendra Frederick** (University of Southwestern, Dallas – USA) - TBA

18:30- 20:00 *Drinks & Dinner will be served in front of IBS*

Wednesday May 29<sup>th</sup>**In Cell NMR – Chair N. Wolff**

- 8:45** François-Xavier Theillet (I2BC – Gif sur Yvette - FR) - *In-cell NMR of  $\alpha$ -Synuclein and Tau at 310K and 10  $\mu$ M: the actual powers of  $^{13}$ C-labeling &  $^{13}$ C-detection*
- 9:25** Enrico Luchinat (CERM, Florence – IT) - *Expression of fluorinated proteins in human cells for  $^{19}$ F in-cell NMR*

*10:05-10:35 Coffee Break*

**Membrane Proteins – Chair H. Déméné**

- 10:35** Alvar Gossert (ETH Zurich – CH) - *Labeling in eukaryotic cells enables NMR studies of GPCR activation and deactivation*
- 11:15** Lauriane Lecoq (MMSB – Lyon - FR) - *Deciphering the Structure of SARS-CoV-2 ORF6 Membrane Protein Using Selective Labeling and combination of solution and solid-state NMR*
- 11:35** Clemens Glaubitz (University of Frankfurt – DE) - *Solid-state NMR and DNP approaches for the study of transporter and receptor proteins within the membrane*
- 12:15** Sun Zhiyu (CRMN – Villeurbanne - FR) - *Isotopic labelling of the human copper transporter hCTR1 for structural dynamics study with NMR*

*12:35-14:35 Lunch and Poster session*

**Chemical Biology for NMR – Chair M. Jensen**

- 14:35** Galia Debelouchina (University of California, San Diego – USA) - *Chemical biology tools for NMR spectroscopy of gels and cells*
- 15:15** Darja Rhoden (University of Vienna –AT) - *Unraveling Protein Dynamics with Selectively Labeled Arginine in NMR Spectroscopy*
- 15:35** Martina Rosati (CERM-University of Florence, IT) - *Towards cost-effective side-chain isotope labelling of proteins expressed in human cells*
- 15:55** Giorgia Toscano (University of Vienna –AT) – *Isotope Labeling to probe Biomolecular Interactions*

*16:15-16:45 Coffee Break*

**Isotopic Labelling for the Study of Nucleic Acids and Complexes II – Chair I. Lebars**

- 16:45** Sarah Keane (University of Michigan – FR) - *Structure-based regulation of microRNAs biogenesis*
- 17:25** Laura Troussicot (CRMN – Lyon –FR) -  *$^{19}$ F NMR - a gateway towards complex dynamical processes in RNA*
- 17:45** Katja Petzold (Uppsala University – SE) - *What label for what experiment: RNA dynamics*
- 18:25** Loïc Salmon (CRMN – Lyon) - *Assessing extreme flexibility in RNA by combining selective labeling, ultra-high-field NMR spectroscopy and advanced molecular modeling*

*19:00- 20:00 Dinner will be served in front of IBS*

**Thursday May 30<sup>th</sup>****Integrated Structural Biology – E. Lescop**

- 8:45** **Nadia Izadi-Pruneyre** (Pasteur Institute, Paris – FR) - *Integrative structural biology of bacterial membrane nanomachines*
- 9:25** **Maximilian Zinke** (Pasteur Institute, Paris – FR) - *TONB RAIDER – Discovering the Secrets of the Ton System's Order*
- 9:45** **Hélène Déméné** (CBS – Montpellier – FR) - *Activation of the vasopressin type 2 receptor seen by an integrative approach*

*10:05-10:35 Coffee Break*

**Therapeutic Proteins and Drug Discoveries – Chair F.X. Theillet**

- 10:35** **Julien Orts** (University of Vienna – AT) - *Lead Generation without an X-Ray Crystal Structure: An NMR Method to Probe Protein-Ligand Complexes*
- 11:15** **Maria Pia Lenza** (University of Naples –FR) - *Siglec-8 complex structures with a therapeutic antibody and a high-affinity sialoside analog*
- 11:35** **Faustine Henot** (Sanofi –FR) - *Development of a fast and efficient assignment transfer strategy: from a first Fab fragment to other ones*
- 11:55** **Ulrich Hommel** (Novartis, Basel – CH) - *Drugging the Undruggable: Can Protein Dynamics guide Drug Discovery ?*

*12:35-14:35 Lunch and Poster session*

**NMR of Proteins I – Chair N. Izadi-Pruneyre**

- 14:35** **Elise Delaforge** (IBS, Grenoble –FR) - *Intrinsic disorder in the human 3'-end pre-mRNA polyadenylation machinery*
- 14:55** **Tessa Bolognesi** (CERM, University of Florence - IT) - *Expression of the nucleocapsid protein (N) from SARS-COV 2 and its characterization through high-field NMR spectroscopy*
- 15:15** **Stepanka Nedvedova** (ICSN, CNRS –FR) - *Unveiling the Enigma: Structural Insights into Schistosoma mansoni MEG Proteins*
- 15:35** **Stefan Nebl** (IBS, Grenoble - FR) - *Deciphering Electron Flow in Neisserial DsbD by Mutagenesis and NMR Dynamics*

*15:55-16:25 Coffee Break*

**Isotopic Labeling and Cell-Free Protein Expression – Chair L. Lecoq**

- 16:25** **Frank Bernhard** (University of Frankfurt – DE) - *Cell-Free protein synthesis tools for the production of NMR samples*
- 17:05** **Astrid Audibert** (IBS, Grenoble – FR) - *Towards an atomic-resolution functional study of the ClpXP machinery in action using cell free and NMR technologies.*
- 17:25** **Pau Bernado** (CBS, Montpellier – FR) - *Cell-Free approaches for the incorporation of structural probes for <sup>19</sup>F-NMR and SANS*
- 18:05** **Morgan Callon** (MMSB – Lyon - FR) - *Proton detected fast MAS solid-state NMR studies of the hepatitis D virus S and L proteins*

*18:30-20:00 –Dinner will be served in front of IBS*

**Friday May 31<sup>st</sup>****NMR of Proteins II – Chair S. Hediger**

- 8:45** **Sebastian Hiller** (Biozentrum, Basel – CH) - *The dynamic chaperone network in the endoplasmic reticulum*
- 9:25** **Benoit Odaert** (CNRS, Bordeaux –FR) - *Biochemical and Biophysical Characterization of the Mechanism of Activation for the pro-apoptotic death domain receptor DR5 by multivalent agonist.*
- 9:45** **Ewen Lescop** (ICSN Gif-sur Yvette – FR) - *Probing lipid/protein coupled dynamics in membranes by High-Pressure NMR spectroscopy*

*10:25-10:55 Coffee Break*

**<sup>19</sup>F Labeling Methodologies – Chair L. Salmon**

- 10:55** **Ronald Micura** (University of Innsbruck - AT) - *Chemical Synthesis of Modified RNA*
- 11:35** **Davy Sinnaeve** (CNRS, Lille - FR) - *A library of fluorinated prolines to study proline-rich motifs with <sup>19</sup>F NMR*
- 11:55** **Haribabu Arthanari** (Harvard Medical School – Boston, USA) - *Leveraging Fluorine as Atomic Beacons in Biomolecular NMR: Challenges and Opportunities*

*12:35 Closing of AILM2024*

*12:45-13:30 Lunch at the EPN Campus Restaurant*