

# Nancy Computational Structural Biology Meeting (NCSB)

July 9<sup>th</sup>, 2024

## Program:

- 9:30 - 9:45      Welcome and introduction
- 9:45 - 10:30     Massimiliano Bonomi (Institut Pasteur, CNRS, Paris) - Protein structural ensembles from 3D and 2D cryo-EM data
- 10:30 - 11:00    Coffee break
- 11:00 - 11:30    Chris Chipot (Université de Lorraine, CNRS, LPCT, Nancy) - Modeling rare events. Discovering reaction pathways, slow variables, and committor probabilities with machine learning
- 11:30 - 12:00    Alessandra Carbone (Sorbonne Université, LCQB, Paris) - Sequence, structure and population allele frequency accurately predict mutational effects in proteins
- 12:00 - 14:00    Lunch and poster session
- 14:00 - 14:30    Lars Malmstrom (University of Zurich, Switzerland) - Using proteomics and digital twin modeling to predict sepsis patient outcomes
- 14:30 - 15:00    Elodie Laine (Sorbonne Université, LCQB, Paris) - Explaining Conformational Diversity in Protein Families through Molecular Motions
- 15:00 - 16:00    Coffee break and poster session
- 16:00 - 16:30    Sergei Grudinin (CNRS, LJK, Grenoble) - On the simplification of dynamics in molecular systems
- 16:30 - 17:00    Nicolas Soler (Université de Lorraine, Dynamic, Nancy) - DNA processing during conjugative transfer of ICEs from Firmicutes

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