Programme prévisionnel AMMIB du 20 Avril 2023

Institut de Biologie Intégrative de la Cellule, I2BC
Amphi Bâtiment 21, 1 avenue de la Terrasse, 91190 Gif-sur-Yvette.

Machine Learning applied to Molecular Modelling

9:15 – 09:30	Introduction de la journée
9:30 – 9:50	**Clément Fauchereau**, I2BC, CNRS/CEA, Gif-Sur-Yvette (15' talk + 5' questions) *Artificial intelligence: overview and prospects*
9:50 – 10 :20	**Mehdi Munim**, Université Paris-Cité, Paris (25' talk + 5' questions) *Evaluation of the prediction of amyloid fibrillar structures by AlphaFold 2*
Pause	
10:50 – 11:20	**Satya Prakash Tripathi**, I2BC, CNRS/CEA, Gif-Sur-Yvette (15' talk + 5' questions) *AlphaFold assisted Structural insights into NOS: A computational biology perspective*
11:20 – 11:50	**Ivan Reveguk**, école Polytechnique (25' talk + 5' questions) *Classifying kinase structures using machine learning*
11:50 – 12:20	**Thibault Tubiana**, I2BC, CNRS, Gif-sur-Yvette (25' talk + 5' questions) *Molecular modelling, homo-oligomerisation and membrane interactions of hepatitis E virus pORF1 replication polyprotein*
Déjeuner	
13:50 – 14:00	Hommages Stéphane Abel & Jean Cognet

Structure and Molecular Dynamic

14:00 – 14:20	**Thibaud Dieudonné**, I2BC, CNRS, Gif-sur-Yvette (15' talk + 5' questions) *Cryo-EM investigation of the catalytic cycle of a human lipid transporter*
14:20 – 14:40	**Neha Tripathi**, I2BC, CNRS/CEA, Gif-Sur-Yvette (15' talk + 5' questions) *Study of the formation of a peptide corona around a plastic nanoparticle by molecular dynamics*
14:40 – 15:10	**Jiang Yingmin**, Université Paris Saclay, Orsay (25' talk + 5' questions) *Coarse-grained molecular dynamics simulations of liquid-liquid phase separation of intrinsically disordered proteins*
15:10 – 15:40	**Cagla Okyay,** Université Paris Saclay, Orsay (25' talk + 5' questions) *Coarse-grained modelling of ssDNA translocation through a protein nanopore*
Pause	
16:10 – 16:40	**Liuba Mazzanti**, Université Paris Saclay, Orsay (25' talk + 5' questions) *Understanding passive membrane permeation of peptides: physical models and sampling methods compared*.
16:40 – 17:10	**Raphaëlle Versini**, LBT/LB, CNRS/Sorbonne Université, Paris (25' talk + 5' questions) *Molecular dynamics based prediction of Fzo1 transmembrane domains*
17:10 – 17:20	Conclusion