aviesan

alliance nationale
pour les sciences de la vie et de la santé

ITMO MOLECULAR AND STRUCTURAL BASIS OF LIFE SCIENCES

DECIPHERING THE FUNCTIONAL MECHANISMS OF BIOLOGICAL MACROMOLECULES:

Upcoming challenges in Bioinformatics, Modelling and Experimental validations

October 7-8th, 2019

BIOPARK
11, rue Watt - Paris 13e
France

OCTOBER 7th, 2019

- 8:30 a.m.-9:00 a.m. **Coffee**
- 9:00 a.m.-9:30 a.m. **Welcome and housekeeping notes by the organizers**

Theme 1: Molecular design and Statistical approaches

- 9:30 a.m.-10:15 a.m. **Computational design of antibodies, enzymes and vaccine immunogens**
  Sarel FLEISHMAN, Weizmann Institute, Rehovot, Israël
- 10:15 a.m.-10:45 a.m. **Protein sequence landscapes: from data-driven models to protein design**
  Martin WEIGT, Sorbonne Université, Paris, France
- 10:45 a.m.-11:15 a.m. Coffee break
- 11:15 a.m.-11:45 a.m. **Structure-based computational methods & tools for protein design**
  Sophie BARBE, INSA, Toulouse, France
- 11:45 a.m.-12:15 p.m. **Stories of virtual screening for drug design**
  Esther KELLENBERGER, Université de Strasbourg, France
- 12:15 p.m.-12:45 p.m. **Design principles of respiratory chain complexes**
  Chris CHIPOT, Université de Lorraine, Nancy, France
- 12:45 p.m.-2:00 p.m. Lunch

Theme 2: Capturing Complexity and Dynamics

- 2:00 p.m.-2:45 p.m. **Using simulations to decipher the molecular choreography within the bacterial cell envelope**
  Syma KHALID, University of Southampton, UK
- 2:45 p.m.-3:15 p.m. **Polymers in the cell nucleus**
  Maria BARBI, Sorbonne Université, Paris, France
- 3:15 p.m.-3:45 p.m. **Exploring Chemo-mechanical Transduction in the Myosin molecular motor: Emerging mechanisms and Chemical modulation by Computer simulations**
  Marco CECCHINI, Université de Strasbourg, France
- 3:45 p.m.-4:15 p.m. Coffee break

- 4:15 p.m.-4:45 p.m. **Bioinformatics and Modelling for Glycosciences**
  Anne IMBERTY, CNRS, Grenoble, France
- 4:45 p.m.-5:30 p.m. **Prototyping multiscale cellular visualization & modeling techniques**
  Graham JOHNSON, Allen Institute, Seattle, USA

OCTOBER 8th, 2019

Theme 3: Integrative and Multiscale modelling

- 9:00 a.m.-9:45 a.m **Integrative modelling of biomolecules complexes**
  Alexandre BONVIN, Utrecht University, The Netherlands
- 9:45 a.m.-10:15 a.m **Combining cryo-EM image analysis and molecular mechanics simulation methods to study biomolecular conformational dynamics**
  Slavica JONIC, CNRS, Sorbonne Université, Paris, France
- 10:15 a.m.-10:45 a.m. **Deep learning and artificial intelligence applied to the prediction of protein structure and interactions**
  Sergei GRUDININ, INRIA/CNRS, Grenoble, France
- 10:45 a.m.-11:00 a.m. Coffee break
- 11:00 a.m.-11:30 a.m. **Realistic models of intrinsically disordered proteins by a combination of experimental and computational methods**
  Juan CORTES, LAAS-CNRS, Toulouse, France
- 11:30 a.m.-12:00 p.m. **Deciphering actin (dis)assembly, one reaction at a time**
  Guillaume ROMET-LEMONNE, Institut J. Monod, Paris, France
- 12:00 p.m.-12:30 p.m. **Stochastic modeling and analysis of massive amount of super-resolution trajectories reveals the sub-cellular organization and the nanophysiology**
  David HOLCMAN, Ecole Normale Supérieure, Paris, France