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