

## WORKSHOP DEFIS

# “Biophysics of large macromolecular assemblies experiments and simulations”

DAY 1: MONDAY 14TH OCTOBER 2013

08:30 - 09:00 Welcome Coffee

09:00 - 09:15 **Opening Session**

David PERAHIA (ENS de Cachan)

### Morning Session

09:15 – 09:55: Sergio MARCO (Institut Curie-Orsay)

*Questions asked by cryo-transmission electron microscopy in the understanding of molecular assemblies*

09:55 – 10:35: Liliane MOUAWAD (Institut Curie-Orsay)

*How does GTP stabilize microtubule? A case studied by Normal Mode Analysis*

10 :35-11 :05 Coffee break

11:05 – 11 :45 : Jean-Marie RUYSSCHAERT (ULB, Brussels)

*Emerging roles for lipids in Structure and Function of multidrug transporters*

11:45 – 12:25: Martine PREVOST (ULB, Brussels)

*Molecular origin of the voltage-dependent anion selective channel (VDAC)*

12:25 – 13:05: Paulo Mascarello. BISCH (IBCCF/UFRJ, Brésil)

*Pore Forming Membrane Proteins: Comparative Genomics Search for Sequence-Structure-Function Relationship*

13:05 - 14:15 Lunch + Poster session

### Afternoon Session

14:15 – 14:55: Michael NILGES (I. Pasteur)

*Inferential Structure Determination from Hybrid Data*

14:55 – 15:35: Patrice VACHETTE (IBBMC, Orsay)

*SAXS contribution to the study of macromolecule conformations. Coupling with high resolution results*

15:35 – 16:05 Coffee break

16:05 – 16h45: Nicolas FLOQUET (IBMM, Montpellier)

*Multi-scale dynamics of G-proteins Coupled Receptors and ligand/protein partners at the molecular scale : insights from in silico calculations*

16:45 – 17:25: Antoine TALY (IBPC, Paris)

*Signal transduction mechanism in ligand gated ion channels: interplay between modeling and experiments*

17:25 – 18:05: Nicolas FOLOPPE (England)

*Understanding the active-site of thiol-disulfide oxidoreductases with molecular dynamics and pKa calculations*

18:05 - 19:00 Cocktail

## DAY 2: TUESDAY 15TH OCTOBER 2013

### Morning Session

09:15 – 09:55: Jean-Marc VICTOR (U. Pierre et Marie Curie)  
*In silico single molecule manipulations unravel nucleosome dynamics*  
09:55 – 10:35: David BENSIMON (ENS-Paris)  
*Single molecule studies of DNA: from remodelling to sequencing*

10:35 – 11:05 **Coffee break**

11:05 – 11:45: Yves LANSAC (U. de Tours)  
*Formation of DNA-protamine bundles*  
11:45 – 12:25: Ahmad ELBAHNSI (ENS-Cachan)  
*Investigations on multi-scale dynamics of the nucleosome*  
12:25 – 13:05: Claude NOGUES (ENS-Cachan)  
*Sequence-Structure relationships in nucleosomes: a biophysical approach*

13:05 - 14:15 **Lunch + Poster session**

### Afternoon Session

14:15 – 14:55: Eric DEPREZ (ENS-Cachan)  
*Photoactivatable probes for imaging and triggering biological and enzymatic processes upon two-photon excitation*  
14:55 – 15:35: P. R. BATISTA (IOC- Rio de Janeiro, Brésil)  
*Evaluating and validating the interaction of MHC proteins with predicted epitopes from Leishmania amazonensis C-terminal CPB: insights from metadynamics*  
15:35 – 16:15: Luis Barbour SCOTT (ENS-Cachan & UFABC)  
*Protein-protein docking interactions taking into account global conformational changes*

16:15 - 16:30 **Concluding remarks**

