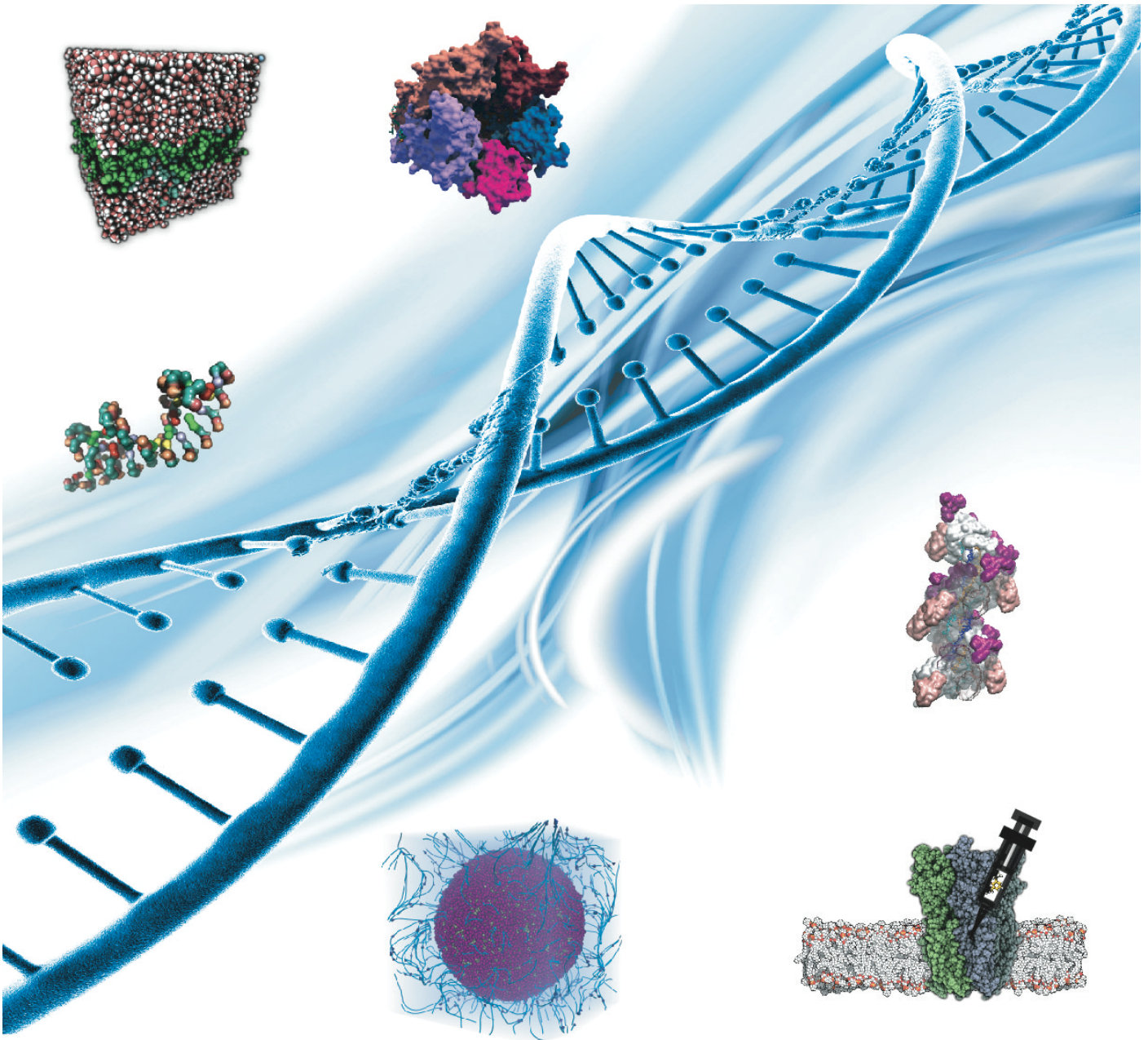


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2019



60 ans du Laboratoire de Biochimie Théorique

9 – 11 avril 2019

Note: all presentations will take place in the main library (ground floor) and the coffee breaks just outside the library. The reception/dinner for Tuesday and Wednesday's lunch will be in the common room of the 3rd floor.

Tuesday, April 9th

- 14h **Welcome and Introduction**
- 14h10 *Historical perspectives: the LBT from 1977 to 2007*
Richard Lavery, IBCP Lyon
- 15h *The multiple faces of DNA simulations*
Modesto Orozco, Univ. Barcelona (invited)
- 16h Coffee Break
- 16h20 *Constant pH coarse-grained simulations for RNA molecules*
Samuela Pasquali, Univ. Paris Descartes
- 16h45 *Neuron-like networks between ribosomal proteins in the ribosome*
Youri Timsit, Institut Méditerranéen d'Océanologie, Marseille
- 17h10 *DNA structure and its applications in high-throughput genome analysis*
Remo Rohs, Univ. Southern California
- 17h35 *Molecular dynamics and normal mode analysis for structural and functional characterization of biomolecules*
David Perahia, ENS Paris-Saclay
- 18h *On the role of chromatin geometry in epigenetic domain formation*
Marina Katava, IBPC
- 18h30 **Reception and dinner**

Wednesday, April 10th (morning)

- 9h *Historical perspectives: the LBT from 2007 to 2016*
Philippe Derreumaux, IBPC
- 9h50 *The molecular dynamics of potassium channel permeation, selectivity and gating*
Bert de Groot, MPI Göttingen (invited)
- 10h50 Coffee Break
- 11h10 *Navigating in the RNA World*
Guillaume Stirnemann, IBPC
- 11h30 *Theoretical studies of fireflies bioluminescence*
Isabelle Navizet, Univ. Paris Est
- 11h55 *Development, validation and applications of a polarizable molecular dynamics approach*
Nohad Gresh, Sorbonne Université
- 12h20 *Some perspectives from the non-academic world*
Anne Dagallier, Sanofi
- 12h45 Lunch

(afternoon)

- 14h15 *Theoretical biochemistry: present and future of our lab*
Marc Baaden, IBPC
- 15h05 *Integrative structural biology*
Michael Nilges, Institut Pasteur (invited)
- 16h05 Coffee Break
- 16h25 *Modeling membrane proteins from mitochondria to synapse*
Antoine Taly, IBPC
- 16h45 *From Cryo-EM map to atomistic interpretation of the bacterial translational machinery*
Emmanuel Giudice, Univ. Rennes
- 17h10 *3-dimensional structure and genome: how to leave 3rd floor of IBPC and come back*
Ingrid Lafontaine, IBPC

Thursday, April 11th

- 9h *From toy membrane peptide to membrane complexes: A long story initiated in LBT*
Catherine Etchebest, Univ. Paris Diderot
- 9h25 *RESPIRE: Repository of Enhanced Structures of Proteins Involved in Red blood cell Environment*
Stéphane Téletchéa, Univ. Nantes
- 9h50 *m1A modification in tRNAs*
Carine Tisné, IBPC
- 10h15 *Ultrafast electron transfer in cryptochrome/photolyases*
Fabien Cailliez, Univ. Paris Saclay
- 10h40 Coffee Break
- 11h *A distance geometry approach to determine the conformational space of flexible proteins from chemical shift measurements*
Thérèse Malliavin, Institut Pasteur
- 11h25 *MD simulation combined to fragment based approach for protein-peptide complex structure prediction*
Samuel Murail, Univ. Paris Diderot
- 11h50 *Udock: a free interactive protein docking system*
Benjamin Boyer, CNAM
- 12h15 *Multi-scale simulations yield insight into protein diffusion and stability in crowded environments*
Stepan Timr, IBPC
- 12h35 **Conclusions and Farewell**

DNA strand by Freepik from www.flaticon.com
All other images are courtesy of LBT members

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 FONDATIONS
EDMOND DE ROTHSCHILD



Depuis 80 ans, nos connaissances
bâtissent de nouveaux mondes

