



INSTITUTE
FOR RESEARCH
IN BIOMEDICINE

Barcelona BioMed Conference

From genomes to structures: looking at big data with an atomic perspective

November 28-30, 2016

Programme

Monday, November 28, 2016

8.30 - 9.00 Registration

9.00 - 9.15 Welcome by Joan J. Guinovart

9.15 - 9.30 **Overview of the meeting**
Maria J. Macias and Hartmut Oschkinat

Session I: Genomes: SNPs, Mutations associated with diseases
Chair: Chris Sander

9.30 - 10.10 **From genotype to phenotype using evolutionary couplings. Part I.**
Chris Sander, DFCI & HMS, Boston (Boston, MA, USA)

10.10 - 10.40 *Coffee break and poster session*

10.40 - 11.20 **Hospital-based cohorts, Genomic Discovery and Personalized
Medicine**
Erwin Boettinger, CEO of Berlin Institute of Health (Berlin, Germany)

11.20 - 12.00 **Clinical impact of global genomic studies in lymphoid neoplasms**
Elias Campo, Hospital Clínic - Biomedical Diagnostic Center - Pathology
(Barcelona, Spain)

12.00 - 12.15 **SHORT TALK 1 The rules and impact of nonsense-mediated mRNA
decay in human cancers**
Fran Supek, CRG (Barcelona, Spain)

- 12.15 - 12.30 **SHORT TALK 2 Single cell analysis tracks clonal selection during acquired chemoresistance in cancer**
Holger Heyn, CNAG-CRG (Barcelona, Spain)
- 12.30 - 13.10 **Co-evolution based methods in the prediction and analysis of protein interaction networks**
Alfonso Valencia, Spanish National Cancer Research Centre (Madrid, Spain)
- 13.10 - 15.00 **Lunch (FrescCo, C/ Carme, 16)**

Session II: Quantitative Approaches (Systems Biology)

Chair: Leo Cheng

- 15.00 - 15.40 **Metabolomics: From Disease Mechanisms to Imaging**
Leo Cheng, Massachusetts General Hospital / Harvard Medical School (Boston, MA, USA)
- 15.40 - 16.20 **From spectrometric data to metabolic networks: An integrated quantitative view of cell metabolism**
Oscar Yanes, Universitat Rovira i Virgili (Tarragona, Spain)
- 16.20 - 16.50 **Coffee break and poster session**
- 16.50 - 18.00 **Round table, chair person Ada Yonath**
- 18.00 **End of session**

Tuesday, November 29, 2016

Session III: Cellular Structural Biology

Chair: Hartmut Oschkinat

- 9.00 - 9.40 **The molecular genetic translation machinery in contemporary medicine, resistance to antibiotics, environmental aspects and the microbiome**
Ada Yonath, Helen and Milton A. Kimmelman Center for Biomolecular Structure and Assembly, Weizmann Institute of Science (Rehovot, Israel)
- 9.40 - 10.20 **Cell-free protein synthesis methods to produce mammalian multiple transmembrane domain proteins**
Shigeyuki Yokoyama, RIKEN Systems and Structural Biology Center, (Yokohama, Japan)
- 10.20 - 10.50 **Coffee break and poster session**
- 10.50 - 11.30 **Probing the epigenome with structural and chemical biology**
Cheryl Arrowsmith, Structural Genomics Consortium (Toronto, Canada)

- 11.30 - 11.45 **SHORT TALK 3** **PICH and BEND3 Co-operate to Maintain Chromosome Stability**
Guillermo Montoya, NNF-CPR (Copenhagen, Denmark)
- 11.45 - 12.00 **SHORT TALK 4** **Structural basis for the recruitment of the general transcription factor TFIIF by the androgen receptor in castration resistant prostate cancer**
Elzbieta Szulc, IRB Barcelona (Barcelona, Spain)
- 12.00 - 12.15 **SHORT TALK 5** **Structural landscape of the human full-length SMAD4 protein - the hub in the TGF- β protein family signaling pathway**
Tiago Lopes, IRB Barcelona (Barcelona, Spain)
- 12.15 - 12.55 **Open science to promote protein research**
Aled Edwards, Structural Genomics Consortium (Oxford, UK)
- 12.55 - 13.35 **Cellular structural biology of human general transcription factor TFIID assembly**
Imre Berger, University Walk (Bristol, UK)
- 13.35 - 15.00 **Lunch (FresCo, C/ Carme, 16)**

Session IV: Structural "genomics" approaches

Chair: Debora Marks

- 15.00 - 15.40 **From genotype to phenotype using evolutionary couplings. Part II**
Debora Marks, The Raymond and Beverley Sackler Laboratory for Computational Biology at Harvard Medical School (Boston, MA, USA)
- 15.40 - 16.20 **Structural perspectives on RNA polymerase I and III transcription**
Christoph Müller, EMBL (Heidelberg, Germany)
- 16.20 - 16.50 **Coffee break and poster session**
- 16.50 - 17.30 **CrPV-IRES: the dynamic tale of a molecular pirate**
Israel S. Fernández, Columbian University (New York, USA)
- 17.30 - 17.45 **SHORT TALK 6** **Oligomerization mechanism of Alzheimer A β 40 peptides deciphered through extensive atomistic replica exchange molecular dynamics**
Josep M. Campanera, Universitat de Barcelona (Barcelona, Spain)
- 17.45 - 18.00 **SHORT TALK 7** **Molecular mechanism of canonical activation of p38 α MAP Kinase**
Antonija Kuzmanic, IRB Barcelona (Barcelona, Spain)
- 18.00 - 18.15 **SHORT TALK 8** **Considering thermal motion in protein structure prediction**
Martin Goethe, Universitat de Barcelona (Barcelona, Spain)

18.15 - 18.55 **Protein NMR methodology for efficient structure determination**
Thomas Szyperski, University of Buffalo (New York, USA)

18.55 *End of session*

20.30 *Speakers dinner "Restaurant Citrus" (Passeig de Gràcia, 44)*

Wednesday, November 30, 2016

Session V: Methodological developments

Chair: Stephan Grzesiek

9.00 - 9.40 **Insights into GPCR function from new NMR techniques**
Stephan Grzesiek, University of Basel (Basel, Switzerland)

9.40 - 10.20 **The emerging role of native mass spectrometry in investigating macromolecular complexes**
Fabienne Hans, Institut de Biologie Structurale (Grenoble, France)

10.20 - 10.50 *Coffee break and poster session*

10.50 - 11.30 **In-situ NMR studies of membrane protein complexes**
Marc Baldus, Utrecht University (Utrecht, The Netherlands)

11.30 - 12.10 **Statistical analysis of high-throughput data: interdisciplinarity is the new black**
Camille Stephan-Otto, IRB Barcelona (Barcelona, Spain)

12.10 - 12.50 **Microscopy studies of protein misfolding, aggregation and disaggregation in cellular models of amyloid disease**
Helen Saibil, Birkbeck College University of London (London, UK)

12.50 - 13.30 **Towards a new generation of integrated facilities for macromolecular crystallography**
Jose A. Márquez, EMBL (Grenoble, France)

13.30 - 13.45 **Closing remarks:** Hartmut Oschkinat, Leibniz-Institut für Molekulare Pharmakologie (Berlin, Germany)

13.45 *End of session*