

BIOINFORMATICS: PRESENT APPLICATIONS AND FUTURE CHALLENGES

Barcelona (Spain) 19-21 May 2003

Monday, 19 May 2003

Program:

Tuesday, 20 May 2003

9:00 - 9:30. *Registration*

9:30 - 9:50. *Inauguration*

Andreu Mas-Colell
Minister for Universities, Research and the Information Society. Government of Catalonia

Salvador Barberà
Director. Catalan Institution for Research and Advanced Studies (ICREA)

Lluís Jofre
Director. Catalan Research Foundation (FCR)

Màrius Rubiralta
Director. Barcelona Science Park

9:50 - 10:00. *Welcome address*

Xavier de la Cruz
ICREA researcher. Molecular Modeling and Bioinformatics Unit, Institute of Biomedical Research of Barcelona, Barcelona Science Park

Session 1: BIOINFORMATICS IN BIOMEDICINE

Chairman: **Federico Gago**. University of Alcalá de Henares, Spain

10:00 - 10:50. **Hugo Kubinyi**. Heidelberg University, Germany
"Drug Research in the Genomics and Proteomics Area"

11:00 - 11:40. **Modesto Orozco**. Institute of Biomedical Research of Barcelona, Barcelona Science Park, University of Barcelona, Spain
"Drug Design: a Multidisciplinary Problem"

11:45 - 12:00. *Coffee Break*

12:00 - 12:40. **Xavier Estivill**. Center of Genomic Regulation, Spain
"Segmental Duplications of the Genome and Its Relation to Disease"

12:45 - 13:25. **Xavier de la Cruz**. ICREA. Institute of Biomedical Research of Barcelona, Barcelona Science Park, Spain
"Prediction of Pathological Mutations"

Session 2: STRUCTURAL BIOINFORMATICS

Chairman: **Ernest Giralt**. Institute of Biomedical Research of Barcelona, Barcelona Science Park, University of Barcelona, Spain

15:30 - 16:20. **Janet M. Thornton**. European Bioinformatics Institute, United Kingdom
"The Evolution of Enzymes - from a Structure and Function Perspective: Analysis and Prediction"

16:30 - 17:00. **Miquel Coll**. Center for Research and Development, Spanish Council for Scientific Research, Spain
"Protein Crystallography in the Postgenomic Era"

17:05 - 17:20. *Coffee Break*

17:20 - 17:50. **Maria Macias**. ICREA. Institute of Biomedical Research of Barcelona, Barcelona Science Park, Spain
"De Novo Design of Proteins with a Native Fold: the WW Prototype"

17:55 - 18:25. **Xavier Daura**. ICREA. Autonomous University of Barcelona, Spain
"Peptide Folding: What Have We Learned from Molecular Dynamics Simulations?"

18:30 - 19:00. **Angel Ortiz**. Centre for Molecular Biology, Spanish Council for Scientific Research, Spain
"On the Limits of Fold Recognition"

Session 3: DATABASES AND DATAMINING IN BIOINFORMATICS

Chairman: **Ferran Sanz**. Municipal Institute of Medical Research. Pompeu Fabra University, Spain

10:00 - 10:45. **José María Carazo**. National Center for Biotechnology, Spanish Council for Scientific Research, Spain
"Expanding Knowledge Discovery: Data Base Mediation over Different Resolution Levels"

10:55 - 11:25. **Alex Bateman**. Sanger Institute, United Kingdom
"The Pfam Database of Protein Domains"

11:30 - 11:45. *Coffee Break*

11:45 - 12:15. **Christian Blaschke**. National Center for Biotechnology, Spain Council for Scientific Research, Spain
"Application of Information Extraction Technology to Biology"

ROUND-TABLE

12:20 - 14:20. *"The Challenge of the Use of Human Genome"*

Moderator: **Màrius Rubiralta**. Director. Barcelona Science Park, Spain

Participants:
José María Carazo. General Subdirector of Planification and Monitoring. Spanish Ministry of Science and Technology
Joaquim Casal. General Director of Research. Government of Catalonia
Miquel Huguet. Director. Supercomputing Center of Catalonia
Modesto Orozco. Professor of Biochemistry and Molecular Biology. Institute of Biomedical Research of Barcelona, University of Barcelona, Barcelona Science Park, Spain
Alfonso Valencia. Senior Researcher. National Center for Biotechnology, Spanish Council for Scientific Research, Spain
Narcís Fornés. Responsible of Education and Research. SGI
Juan José Porta. Head of Europe for Strategy and Tecnology for Sciences Life. IBM

Session 4: BIOINFORMATICS IN EVOLUTION

Chairman: **Montserrat Aguadé**. University of Barcelona, Spain

16:00 - 16:50. **Jaume Bertranpetit**. Pompeu Fabra University, Spain
"The Structure of Diversity in the Human Genome"

17:00 - 17:50. **Javier Castresana**. Center of Genomic Regulation, Spain
"Evolutionary Rate Variation in Lineages, Genes and Genomes"

18:00 - 18:15. *Coffee Break*

18:15 - 19:15. Extraordinary address. **Hugo Kubinyi**. Heidelberg University, Germany
"Virtual Screening for Biologically Active Compounds"

Wednesday, 21 May 2003

Session 5: BIOINFORMATICS AND GENOMICS

Chairman: **Manuel Palacín**. Institute of Biomedical Research of Barcelona, Barcelona Science Park, University of Barcelona, Spain

10:00 - 10:50. **Alfonso Valencia**. National Center for Biotechnology, Spanish Council for Scientific Research, Spain

"Annotating Protein Function: Challenges and Difficulties"

11:00 - 11:50. **Joaquín Dopazo**. Spanish National Cancer Center, Spain
"DNA Microarrays: New Challenges for Bioinformatics"

12:00 - 12:50. **Pere Puigdomènech**. Center for Research and Development, Spanish Council for Scientific Research, Spain
"Arabidopsis, Rice and Other Species"

End of the conference

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