



Scientific Programme
26 June, 2007

9.00 – 9.45 Opening

- 9.00 – 9.15 **Ferran Sanz** – GRIB, IMIM/Universitat Pompeu Fabra, Barcelona, Spain.
9.15 – 9.30 **Hans Åhlfeldt** – Linköping University, Sweden.
9.30 – 9.45 **Joël Bacquet** - European Commission DG INFSO, Brussels, Belgium.

9.45 – 11.30 Session A: Systems Biology Insight into Human Disease and Treatment
Chairperson: Jordi Villà-Freixa - GRIB, IMIM/Universitat Pompeu Fabra, Barcelona, Spain.

- 09.45 – 10.10 **Marta Cascante** - Universitat de Barcelona, Barcelona, Spain.
Fragilities in a Robustly Specialized Metabolism Could Become New Targets for Novel Designed Therapies.
- 10.10 – 10.35 **Ricard V. Solé** - GRIB, IMIM/Universitat Pompeu Fabra, Barcelona, Spain.
Cancer Dynamics: from Stem Cells to Error Catastrophes.
- 10.35 – 10.50 **Fernando Martin** - Instituto de Salud Carlos III, Madrid, Spain.
Biomedical Informatics and Convergent Technologies (NBIC): Interactions in Pursuit of Better Healthcare.
- 10.50 – 11.05 **Kevin Robertson** - University of Edinburgh, Edinburgh, Scotland, UK.
Transforming Pathway Biology into Pathway Medicine.
- 11.05 – 11.20 **Baldo Oliva** - GRIB, IMIM/Universitat Pompeu Fabra, Barcelona, Spain.
Protein-Protein Interactions Reveal Molecular Details of Proteins and Provide Biological Insights.
- 11.20 – 11.30 Discussion

11.30 – 12.00 Coffee Break

12:00 – 13:45 Session B: Biocomputation and Knowledge Management in Drug Discovery and Development
Chairperson: Maria Isabel Loza – Universidad de Santiago de Compostela, Santiago de Compostela, Spain.

- 12.00 - 12.25 **Martin Stahl** - F. Hoffmann-La Roche Ltd., Basel, Switzerland.
Tools and Methods of Proven Value in Molecular Design.
- 12.25 - 12.50 **Tudor I. Oprea** - University of New Mexico School of Medicine, Albuquerque, New Mexico, USA.
From Digital to Experimental Bioactivity.
- 12.50 - 13.05 **Angelo Carotti** - University of Bari, Bari, Italy.
The Role of Structural Biology and Chemoinformatics in the Discovery of New Clinical Candidates for Neurodegeneration.
- 13.05 - 13.20 **Gerhard F. Ecker** - University of Vienna, Vienna, Austria.
Predicting Ligands for ABC-transporter – Structure-based vs. Ligand-based Approaches.
- 13.20 - 13.35 **Manuel Pastor** - GRIB, IMIM/Universitat Pompeu Fabra, Barcelona, Spain.
How Useful are the Results of Computational Chemistry Methods in Drug Discovery?
- 13.35 - 13.45 Discussion

13.45 - 14.45 Lunch



14.45 – 16.30 Session C: **Data and Knowledge Mining in Biomedical Research**
Chairperson: Roderic Guigó – Centre de Regulació Genòmica, Barcelona, Spain.

- 14.45 - 15.10** **Anthony J. Brookes** - University of Leicester, Leicester, UK.
New Developments in Genotype-To-Phenotype Databasing
- 15.10 - 15.35** **Alfonso Valencia** - CNIO, Madrid, Spain.
Computational Methods for the Analysis of Biomedical Information.
- 15.35 - 15.50** **Jordi Mestres** - GRIB, IMIM/Universitat Pompeu Fabra, Barcelona, Spain.
Knowledge-Based Approaches to Pharmacological Profiling.
- 15.50 - 16.05** **Patrick Ruch** - Geneva University Hospitals, Geneva, Switzerland.
Automatic Annotation of Pathological Functions in UniProt.
- 16.05 - 16.20** **Dietrich Rebholz-Schumann** - European Bioinformatics Institute, Cambridge, UK.
Streaming Facts from Scientific Publications to the Scientist.
- 16.20 - 16.30** Discussion

16.30 - 17.00 Coffee Break

17.00 – 18.45 Session D: **Modelling and Simulation in Biomedical Research**
Chairperson: Ferran Sanz - GRIB, IMIM/Universitat Pompeu Fabra, Barcelona, Spain.

- 17.00 - 17.25** **Alex Frangi** - Universitat Pompeu Fabra, Barcelona, Spain.
An Integrative Approach to Cerebral Aneurysms Disease Management: the @neurIST Project.
- 17.25 - 17.50** **Peter J. Bond** - University of Oxford, Oxford, UK.
Coarse-Grained Molecular Dynamics Simulations of Membrane Proteins.
- 17.50 - 18.05** **Amin Rostami – Hodjegan** - University of Sheffield, Sheffield, UK.
Modelling ADME in Drug Development and Linking in vitro Data to in vivo Outcome: Integrating Known-knowns to Assess Impact of Known-unknowns.
- 18.05 - 18.20** **James Sharpe** – Centre de Regulació Genòmica, Barcelona, Spain.
Towards a 4D Computer Simulation of Vertebrate Limb Development.
- 18.20 - 18.35** **Gianni de Fabritiis** - GRIB, IMIM/Universitat Pompeu Fabra, Barcelona, Spain.
PS3GRID.NET: A Distributed Computing Environment for Molecular Simulations on the PlayStation3.
- 18.35 - 18.45** Discussion



27 June, 2007

9.00 – 10.45 Session E: Standards and Ontologies in Biomedical Informatics

Chairperson: Hans Åhlfeldt- Linköping University, Sweden.

- 09.00 - 09.25** **Gunnar Klein** - Karolinska Institute, Stockholm, Sweden.
Standards and Ontologies in Biomedical Informatics.
- 09.25 - 09.50** **Dipak Kalra** - University College London, London, UK.
Advancing the Realisation of EHR Interoperability.
- 09.50 - 10.05** **Susanna-Assunta Sansone** - The European Bioinformatics Institute, Cambridge, UK.
Reporting Standards for Omics Data – An Overview.
- 10.05 - 10.20** **Arne Kverneland** - National Board of Health, Denmark.
SNOMED CT – New International Governance – New Possibilities?
- 10.20 - 10.35** **Miguel García** - Universidad Politécnica de Madrid, Madrid, Spain.
Using Ontologies in Clinico-Genomic Applications. The INFOBIOMED and ACGT Experiences.
- 10.35 - 10.45** Discussion

10.45 - 11.15 *Coffee Break*

11.15 – 13.25 Session F: Case Studies of Biomedical Informatics Applications

Chairperson: Johan van der Lei - Erasmus University Medical Center, The Netherlands.

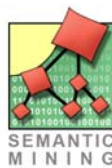
- 11.15 - 11.30** **Jose Luis Oliveira** - Universidade de Aveiro, Aveiro, Portugal.
On the Integration of Biomedical Databases: A Naive Approach.
- 11.30 - 11.45** **Francesca Incardona** - Informa Srl, Rome, Italy.
Multiple Modelling Techniques.
- 11.45 - 12.00** **Dimitris Kafetzopoulos** - FORTH-ICS/ Heraklion, Crete, Greece.
Protein Profiling and Diagnosis with Lab-on-Chip and Proteomics Technology: The LOCCANDIA Integrated Clinico-Proteomics Environment.
- 12.00 - 12.15** **Bruno G. Loos** - University of Amsterdam, Amsterdam, The Netherlands.
Biomedical Informatics in Chronic Infectious and Inflammatory Disease Research: Periodontitis as a Model.
- 12.15 - 12.30** **Inge Bernstein** - Hvidovre Hospital, Copenhagen, Denmark.
INFOBIOMED: the Danish Pilot – Genomics and Colon Cancer.
- 12.30 - 12.45** **George Potamias** - FORTH-ICS/ Heraklion, Crete, Greece.
Cancer, Clinico-Genomics and Biomedical Informatics: The ACGT Approach.
- 12.45 – 13.00** **Magi Lluch** – MicroArt, Barcelona, Spain.
HealthAgents: Distributed Decision Support System for Brain Tumour Diagnosis and Prognosis using Agent Technology.
- 13.00 - 13.15** **Vassilis Moustakis** - FORTH-ICS/ Heraklion, Crete, Greece.
Excellence in Biomedical Informatics Development and Implementation.
- 13.15 - 13.25** Discussion



Meeting Venue

Auditorium of the PRBB
(Barcelona Biomedical Research Park)
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Additional Information

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