

4ο Συνέδριο Ελληνικής Εταιρείας Υπολογιστικής Βιολογίας και Βιοπληροφορικής  
18-20 Δεκεμβρίου 2009, ΕΙΕ, Αθήνα

# HSCBB\_09

## Πρόγραμμα

## Program

4th Conference of the Hellenic Society for Computational Biology and Bioinformatics  
18-20 December 2009, NHRF, Athens



# HSCBB09

## Co-organized by



Hellenic Society for Computational Biology and Bioinformatics (HSCBB)



Biophysics and Bioinformatics Laboratory, Faculty of Biology, University of Athens



Institute of Biological Research and Biotechnology, National Hellenic Research Foundation

## ORGANIZING COMMITTEE

Hamodrakas Stavros - University of Athens, Greece  
Iliopoulos Ioannis - University of Crete, Greece  
Kolisis Fragiskos - National Hellenic Research Foundation, Greece  
Ouzounis Christos - King's College, London, U.K.  
Promponas Vasilis - University of Cyprus, Nicosia, Cyprus  
Stamatakis Alexandros - Ludwig-Maximilians Universität, Munich, Germany

## PROGRAM COMMITTEE

Bagos Pantelis - University of Central Greece, Lamia, Greece  
Chanalaris Anastasios - Royal Free and UCL Medical School London, U.K.  
Chatziioannou Aristotelis - National Hellenic Research Foundation, Greece  
Hamodrakas Stavros - University of Athens, Greece  
Iliopoulos Ioannis - University of Crete, Greece  
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Poirazi Yiota - IMBB Crete, Greece  
Promponas Vasilis - University of Cyprus, Nicosia, Cyprus  
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## LOCAL ORGANIZING COMMITTEE

Chatziioannou Aristotelis - National Hellenic Research Foundation, Greece  
Hamodrakas Stavros - University of Athens, Greece  
Iconomidou Vasiliki - University of Athens, Greece  
Kolisis Fragiskos - National Hellenic Research Foundation, Greece

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# Welcome message

Dear colleagues and students,

This is the 4th conference of the Computational Biology and Bioinformatics community in Greece, following previous meetings in Crete, Athens and the great success of the HSCBB08 meeting in Thessaloniki.

Apart from the scientific program, the conference will also have as a primary goal the expansion of the Hellenic Society for Computational Biology and Bioinformatics.

The conference is co-organized by the HSCBB, the University of Athens and the National Hellenic Research Foundation.

We truly hope you will enjoy the conference!

The HSCBB09 Organizing Committee

**Hamodrakas Stavros**

University of Athens, Greece

**Iliopoulos Ioannis**

University of Crete, Greece

**Kolisis Fragiskos**

National Hellenic Research Foundation, Greece

**Ouzounis Christos**

King's College, London, U.K.

**Promponas Vasilis**

University of Cyprus, Nicosia, Cyprus

**Stamatakis Alexandros**

Ludwig-Maximilians Universität, Munich, Germany

# Program at a glance

## Friday 18/12/2009

10:30 – 11:30	Registration
11:30 – 12:00	Opening Session
12:00 – 13:45	Session 1 – Biological Sequence Analysis (I): Sequence comparison and modeling
13:45 – 14:45	Lunch break
14:45 – 16:00	Session 2 – Structural Bioinformatics (I): Structure-based design and modeling
16:00 – 16:15	Short break
16:15 – 18:00	Session 3 – Other (I): Mathematical modeling of biological systems
18:00 – 18:30	Coffee break – Poster Session (I)
18:30 – 20:30	Session 4 – Other (II): Computational and statistical methods in genetics and genomics

## Saturday 19/12/2009

10:00 – 11:45	Session 5 - Inference and Visualization of Large Biological Networks
11:45 – 12:00	Short break
12:00 – 13:00	Invited lecture
13:00 – 14:00	Lunch break
14:00 – 17:00	HSCBB General assembly and elections
17:00 – 18:30	Session 6 - Structural Bioinformatics (II): Protein structure prediction & modeling
18:30 – 19:00	Coffee break – Poster Session (II)
19:00 – 20:30	Round table discussion: <i>The future role and goals of HSCBB</i>

## Sunday 20/12/2009

09:30– 10:30	Session 7 - Text Analysis and Ontology Data Mining
10:30–10:45	Short break
10:45 – 12:00	Session 8 - Biological Sequence Analysis (II): Genome Sequence Analysis
12:00–12:15	Short break
12:15 – 13:30	Session 9 – Other (III): Data analysis techniques in biomedical informatics and bioinformatics
13:30–14:30	Lunch break
14:30 – 16:15	Session 10: High Performance Computing in Bioinformatics
16:15–16:45	Coffee break
16:45 – 19:00	Session 11 - Structural Bioinformatics (III): Protein folding and interactions
19:00–19:15	Short break
19:15 – 20:00	Session 12 – Other (IV): Computational systems to assess biological diversity
19:45 – 20:15	Best student poster award – Closing remarks
21:00++	Social event at “Karavitis”

# HSCBB09 Program

## Friday 18/12/2009

- 10:30 – 11:30 Registration
- 11:30 – 12:00 **Opening Session**
- 12:00 – 13:45 **Session 1 – Biological Sequence Analysis (I):  
Sequence comparison and modeling**  
Chairs: Pantelis Bagos and Vasilis Promponas
- 12:00 – 12:30 Manolis Christodoulakis, S. M. Shabab Hossain, Md. Mahmudur Rahman and M Sohel Rahman  
*Comparing weighted sequences using LCSs*
- 12:30 – 12:45 Anastasis Oulas, Ioannis Iliopoulos and Panayiota Poirazi  
*Development of a MicroRNA Target Prediction Tool*
- 12:45 – 13:00 Ioannis Kirmitzoglou and Vasilis Promponas  
*Is ASTRAL the proper data set to benchmark sequence similarity search methods?*
- 13:00 – 13:15 Verena Tischler, Christos A. Ouzounis and D. Fear  
*Sequence Analysis of Activation-Induced Cytidine Deaminase (AID) using CHIP-seq Data*
- 13:15 – 13:45 Stavros Hamodrakas  
*Computational Studies of GPCR's, G-proteins, Effectors and their Interactions*
- 13:45 – 14:45 Lunch break
- 14:45 – 16:00 **Session 2 – Structural Bioinformatics (I):  
Structure-based design and modeling**  
Chairs: Elias Eliopoulos and Stavros Hamodrakas
- 14:45 – 15:00 Christos Lamprakos, Joseph Hayes, Demetres Komiotis and Demetres Leonidas  
*Structure based design of hypoglycaemic agents:  
in silico studies of 3'-substituted glucose derivatives as inhibitors of glycogen phosphorylase*
- 15:00 – 15:15 Michail Mamais, Joseph Hayes, Thanasis Gimisis and Evangelia Chrysina  
 *$\beta$ -D-glucose pyrimidine derivatives binding at the catalytic site of Glycogen Phosphorylase:  
the role of ligand ionization/tautomeric states*
- 15:15 – 15:30 Nikolaos Dimitropoulos, Georgios Dalkas, Athanasios Papakyriakou, Christos Chasapis and Georgios Spyroulias  
*Conformational dynamics of the  $\alpha$ 1 nicotinic acetylcholine receptor subunit bound to  $\alpha$ -bungarotoxin,  $\alpha$ -cobratoxin and  $\alpha$ -conotoxin*
- 15:30 – 15:45 Athanasios Papakyriakou, Michael Karpusas and Dionisios Vourloumis  
*Targeted Molecular Dynamics of the EGFR Kinase Domain Reveals Structural Features Involved in Activation*
- 15:45 – 16:00 Vassilios Myriantopoulos, Olivier Losach, Laurent Meijer and Emmanuel Mikros  
*Consensus scoring-assisted virtual screening of the NCI-diversity II library and identification of inhibitors of the dual specificity kinase DYRK1A*
- 16:00 – 16:15 Short break

# HSCBB09 Program

## Friday 18/12/2009 (contd.)

- 16:15 – 18:00 **Session 3 – Other (I):**  
**Mathematical modeling of biological systems**  
Chairs: Anastasios Chanalaris and Christos Ouzounis
- 16:15 – 16:30 Konstantinos Exarchos, Georgios Rigas, Yorgos Goletsis and Dimitrios Fotiadis  
*Dynamic Bayesian Networks for disease evolution monitoring: the test case of oral cancer reoccurrence*
- 16:30 – 16:45 George Lambrou and Aristotelis Chatziioannou  
*A Modeling Approach to the Detection of Cellular Pharmacogenomic Phenotypic Traits Through Microarray Screening of the Early Expressional Profile*
- 16:45 – 17:00 Maria Kalimeri, Labrini Athanasopoulou and Konstantinos Eftaxias  
*Epileptic activity recognition in EEG recordings using concepts of entropy and tools of information theory*
- 17:00 – 17:15 Labrini Athanasopoulou, Maria Kalimeri and Konstantinos Eftaxias  
*A unified approach of catastrophic phenomena by means of complexity*
- 17:15 – 17:30 Athanassios Tartas, Theodore Georgomanolis and Evangelia D. Chrysina  
*PERC: A new graphical tool based on molecular visualization programs*
- 17:30 – 18:00 Spyros Papageorgiou  
*An explanation of the puzzling HOX gene collinearity*
- 18:00 – 18:30 Coffee break – Poster Session (I)
- 18:30 – 20:30 **Session 4 – Other (II):**  
**Computational and statistical methods in genetics and genomics**  
Chairs: Anastasios Bezerianos and Ioannis Iliopoulos
- 18:30 – 19:15 Perspective  
Christos Ouzounis  
*Recent developments in phylogenetic profiling across multiple genomes and metagenomes*
- 19:15 – 19:30 Konstantinos Karagiannis, Fotis Psomopoulos and Pericles Mitkas  
*Multi Level Clustering of Phylogenetic Profiles*
- 19:30 – 19:45 Ioannis Melas, Aikaterini D. Chairakaki, Alexander Mitsos, Julio Saez-Rodriguez and Leonidas G Alexopoulos  
*Drug Effects Identification using an Integer Linear Programming Optimization Formulation*
- 19:45 – 20:00 Vassiliki Gkantouna, Sophia Douzgou, Ioannis Tzimas, Konstantinos Poulas, Michael B. Petersen, Athanassios K. Tsakalidis and George Patrinos  
*Application of Internet Technologies and Relational Databases in Clinical Genetics – A Case Study*
- 20:00 – 20:30 Pantelis Bagos and Theodore Liakopoulos  
*A multivariate method for meta-analysis of association studies using different sets of markers*

# HSCBB09 Program

## Saturday 19/12/2009

- 10:00 – 11:45 **Session 5 - Inference and Visualization of Large Biological Networks**  
Chairs: Anastasios Chanalaris and Fragkiskos Kolisis
- 10:00 – 10:30 Dimitris Goussis, Panayotis Kourdis and Ralf Steuer  
*Analysis of Complex Biochemical Networks: Glycolysis in Saccharomyces cerevisiae*
- 10:30 – 10:45 Georgios Pavlopoulos, Charalampos Moschopoulos, Evangelos Pafilis and Reinhard Schneider  
*Visualization and Data Integration Techniques in Systems Biology*
- 10:45 – 11:00 Eleftherios Pilalis, Aristotelis Chatziioannou and Fragkiskos Kolisis  
*Systemic regulatory analysis of Rapeseed central metabolism using an in silico compartmented model*
- 11:00 – 11:15 Kalliopi Tsafo, E. Theodoridis, Christos Makris, Maria Klapa, Athanassios Tsakalidis and Nikolaos Moschonas  
*Towards the development of a knowledge base (PICKLE\_DB) for the human protein interactome*
- 11:15 – 11:30 Hariklia Eleftherohorinou, Victoria Wright, Clive Hoggart, Marjo-Riitta Jarvelin, David Balding, Lachlan Coin and Michael Levin  
*Pathway Analysis of GWAS Provides New Insights into Genetic Susceptibility to 3 Inflammatory Diseases*
- 11:30 – 11:45 Spiros Kostopoulos, Dimitrios Glotsos and Dionisis Cavouras  
*Stochastic modeling of intracellular dynamics on the basis of Fluorescent Recovery After Photobleaching experiments*
- 11:45 – 12:00 Short break
- 12:00 – 13:00 Invited lecture  
Chairs: Fragkiskos Kolisis  
Vassily Hatzimanikatis  
*The Systems Engineering of Systems Bio/Technology*
- 13:00 – 14:00 Lunch break
- 14:00 – 17:00 HSCBB General assembly and elections
- 17:00 – 18:30 **Session 6 - Structural Bioinformatics (II):  
Protein structure prediction & modeling**  
Chairs: Elias Eliopoulos and Vassiliki Iconomidou
- 17:00 – 17:15 Evangelia Petsalaki, Alexander Stark, Eduardo García-Urdiales and Robert Russell  
*Prediction of peptide-protein interactions and their structures*
- 17:15 – 17:30 Renate Gessmann, Nikos Kourtis, Kyriacos Petratos and Nektarios Tavernarakis  
*Homology-based modeling of mechanosensory ion channel structural and functional features*
- 17:30 – 17:45 Eythymios Pournaras, Vassiliki Iconomidou, Nikolaos Panousis and Stavros Hamodrakas  
*Calculation of the "Mean Packing Density" for each of the 20 common amino acid residues on a 30% non-redundant set of transmembrane proteins*



# HSCBB09 Program

## Saturday 19/12/2009 (contd.)

- 17:45 – 18:00 Panagiotis L. Kastritis, Thodoris K. Karamanos, Nikolaos C. Papandreou, Constantinos E. Vorgias and Stavros J. Hamodrakas  
*Computational studies on the Temperature Adaptation Mechanisms of Dihydrofolate Reductases from Psychrophiles*
- 18:00 – 18:30 Vasilis J. Promponas and Stavros Hamodrakas  
*Structural analysis and an instance-based learning approach for the prediction of tightly interacting, successive in sequence, transmembrane  $\alpha$ -helices in polytopic transmembrane proteins*
- 18:30 – 19:00 Coffee break – Poster Session (II)
- 19:00 – 20:30 Round table discussion: *The future role and goals of HSCBB*

# HSCBB09 Program

## Sunday 20/12/2009

- 09:30 – 10:30 **Session 7 - Text Analysis and Ontology Data Mining**  
Chairs: Ioannis Iliopoulos and Vasilis Promponas
- 09:30 – 09:45 Michalopoulos, I., Pavlopoulos, G., Karelis, A., and Kostadima, M.A.  
*Human Gene Correlation Analysis: A web-based tool for the coexpression of genes in Humans*
- 09:45 – 10:00 Konstantions Tsirigos, Pantelis Bagos and Stavros Hamodrakas  
*OMPdb: a database of  $\beta$ -barrel outer membrane proteins from Gram-negative bacteria*
- 10:00 – 10:30 Christos Louis, Pantelis Topalis, Emmanuel Dialynas, Elvira Mitraka, Elena Deliyanni and Inga Siden-Kiamos  
*A set of ontologies to drive tools for the control of vector-borne diseases*
- 10:30 – 10:45 Short break
- 10:45 – 12:00 **Session 8 - Biological Sequence Analysis (II):  
Genome Sequence Analysis**  
Chairs: Aristotelis Chatziioannou and Christos Ouzounis
- 10:45 – 11:00 Georgios Tsaousis, Pantelis Bagos and Stavros Hamodrakas  
*A computational approach to the optimal placement of a topology reporter: Implications to large-scale analysis*
- 11:00 – 11:15 Danaï Fimereli, Zoi Litou, Pantelis Bagos and Stavros Hamodrakas  
*A HMM model for the prediction of the cell wall proteins (CWPs) of Gram positive bacteria*
- 11:15 – 11:30 Margarita Theodoropoulou, Venkata Satagopam, Chris Stampolakis, Georgios Pavlopoulos, Nikolaos Papandreou, Pantelis Bagos, Reinhard Schneider and Stavros Hamodrakas  
*Human-gpDB: A database of Human GPCRs, G-Proteins, Effectors and their interactions*
- 11:30 – 12:00 Nikolaos Papanikolaou, Kaliopi Trachana, Theodosios Theodosiou, Vasilis Promponas and Ioannis Iliopoulos  
*Gene socialization: Gene order, GC content and gene silencing in Salmonella*
- 12:00 – 12:15 Short break
- 12:15 – 13:30 **Session 9 – Other (III):  
Data analysis techniques in biomedical informatics and bioinformatics**  
Chairs: Pantelis Bagos and Ilias Maglogiannis
- 12:15 – 12:30 Panayotis Katsaloulis  
*2-D and 3-D Fractal Analysis of Diffusion Tensor Images of the Human Brain*
- 12:30 – 12:45 Panagiotis Moulos, Hendrik G. Stunnenberg and Fragiskos N. Kolisis  
*Challenges in the analysis of Next Generation Sequencing data: a proposed workflow*
- 12:45 – 13:00 Panagiotis Moulos, Olga Papadodima, Aristotelis Chatziioannou, Heleni Loutrari, Charis Roussos and Fragiskos N. Kolisis  
*A proposed analysis workflow for Illumina BeadChips*
- 13:00 – 13:30 George M. Spyrou  
*Building a BioServer on the Biomedical Research Foundation of the Academy of Athens*

# HSCBB09 Program

## Sunday 20/12/2009 (contd.)

- 13:30 — 14:30 Lunch break
- 14:30 — 16:15 **Session 10: High Performance Computing in Bioinformatics**  
Chairs : Pantelis Topalis and Fragkiskos Kolisis
- 14:30 — 15:15 Perspective  
Christos Nicolaou  
*The HPC project of the Cyprus Institute: Opportunities for Life Sciences Research*
- 15:15 — 15:30 Nikolaos Alachiotis and Alexandros Stamatakis  
*Future Reconfigurable Architectures for Phylogenetic Inference*
- 15:30 — 15:45 Panagiotis Bougioukos, Spiros Kostopoulos, Dimitris Glotsos, Ioannis Kalatzis, Dionisis Cavouras, George Nikiforidis and Anastasios Bezerianos  
*Classification of prostate MS spectra based on peak intensity regions generation*
- 15:45 — 16:15 Aristotelis Chatziioannou, Ioannis Kanaris, Ilias Maglogiannis, Charalampos Doukas, Panagiotis Moulos, Eleftherios Pilalis and Fragiskos Kolisis  
*GRISSOM web based Grid portal: Exploiting the power of Grid infrastructure for the interpretation and storage of DNA microarray experiments*
- 16:15 — 16:45 Coffee break
- 16:45 — 19:00 **Session 11 - Structural Bioinformatics (III): Protein folding and interactions**  
Chairs: Vassiliki Iconomidou and Vasilis Promponas
- 16:45 — 17:15 George Papamokos, George Tziatzos, Dimitrios Papageorgiou, Anastasia Politou and Efthimios Kaxiras  
*Computational Epigenetics: Molecular simulations of the structure of HP1 bound to a variably modified H3 tail: A binary switch or a modification cassette?*
- 17:15 — 17:30 Georgios Tziatzos, George Papamokos and Dimitrios Papageorgiou  
*Molecular Dynamics study of post-translational modifications in the H3-HP1 complex*
- 17:30 — 17:45 Lykourgos Chiniadis, Athanassios Hountas and Kostas Bethanis  
*Unbound docking studies of Aflatoxin B1 binding to human Glutathione S-transferase A1-1*
- 17:45 — 18:00 Maria Anna Rapsomaniki, Xenia Orkopoulou, Konstantinos Kovas, Athanasios Tsitsoulis, Vasilis Haidinis, Vassiliki Gkantouna, Eleni Christodouloupoulou, Ioannis Tzimas, George Patrinos, Athanasios Tsakalidis and Konstantinos Poulas  
*Modeling the neuromuscular junction*
- 18:00 — 18:15 Panagiota Georgoulia  
*Quest for foldable tetrapeptides*
- 18:15 — 18:30 Phanourios Tamamis and Georgios Archontis  
*Computational and experimental insights into the self-assembly of diphenylalanine and triphenylalanine peptides*
- 18:30 — 19:00 Phanourios Tamamis and Georgios Archontis  
*From adenovirus peptidic sequences self assembly to nanocircuitry: Can MD simulations bridge up the gap?*

# HSCBB09 Program

## Sunday 20/12/2009 (contd.)

- 19:00 — 19:15 Short break
- 19:15 — 20:00 **Session 12 – Other (IV):  
Computational systems to assess biological diversity**  
Chairs: Aristotelis Chatziioannou and Ioannis Iliopoulos
- 19:15 — 19:30 Michael Gioutlakis and Persefoni Megalofonou  
*Tagging european sea bass with implantable archival tags: an experimental trial in tank*
- 19:30 — 19:45 Nikos Nikolaou, Pantelis Sampaziotis, Marilena Aplikioti, Andreas Drakos, Ioannis Kirmitzoglou, Marina Argyrou, Nikos Papamarkos and Vasilis Promponas  
*Development of a prototype computer-aided system for semi-automatically identifying key species of the marine benthic macrofauna of Cyprus*
- 19:45 — 20:15 **Best student poster award – Closing remarks**
- 21:00 ++ Social event at “Karavitis”



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