

# ISCB Latin America 2012

## Conference on Bioinformatics Programme



An Official Conference of the  
International Society for Computational Biology



Santiago, Chile. March 17 - 21

### Topic Sessions

- Comparative Genomics and Evolution
- Genomics, Proteomics, Metagenomics and Metabolomics
- Macromolecule Structure/Function Prediction
- Computer Aided Drug Design and Docking Simulations
- Biomedicine and Immunoinformatics
- Functional Genomics and Systems Biology

### Tutorials

- Next generation sequencing
- Genome browsers with special emphasis in the ENSEMBL system
- Immunoinformatics
- Analysis, comparison and classification of protein structures
- Protein resources and tools
- Functional Genomics
- Computer Based Drug Design
- Algorithms and tools for transcriptomics and multiple gene profiling using the open source platforms R and Bioconductor

# About ISCB-Latin America

The International Society for Computational Biology (ISCB) is holding the ISCB Latin America Conference on Bioinformatics in Santiago, Chile, in March 17-21, 2012. This meeting constitutes the second regional ISCB Latin America meeting, with the first held in Montevideo, Uruguay, in March 2010.

Conferences are key to the development and exchange of new ideas in science. Over the years many thousands of participants have attended ISCB's annual ISMB conferences. As the majority of those attendees do their research in North America and Europe, the ISCB Regional Conferences aim to break the barrier imposed by high cost travel. How? By bringing a high quality conference, including lectures delivered by world-renowned scientists, to the regions of Latin America, Africa and Asia.

Toward this aim, in 2009 ISCB began organizing a newer series of smaller, regionally-based meetings as part of its mission to advance the science through world-wide education and training activities. These regional meetings have included ISCB-Africa (Mali 2009, South Africa 2011), ISCB-Latin America (Uruguay 2010) and ISCB-Asia (Malaysia 2011).

ISCB also aims to provide more students the opportunity to discuss and participate in the latest developments in bioinformatics and computational biology by bringing these meetings closer to home. We hope the ISCB-Latin America 2012 will be the second of many conferences that will contribute to the growth of the field within this region and support scientific innovation across Latin America.



# Organizing Committee

## Steering Committee of ISCB-Latin America 2012

**Francisco Melo**, Pontificia Universidad Católica de Chile,  
Conference Chair

**Cristina Marino**, Instituto Leloir, Argentina

**Alejandro Maass**, Universidad de Chile, Chile

**Guilherme Oliveira**, CEBio, Brazil

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**Gustavo Parisi**, Universidad de Quilmes, Argentina.

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**Mauricio González**, INTA, Chile.

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**Diego Ferreira**, Universidad de Buenos Aires, Argentina.

**Ignacio Sánchez**, Instituto Leloir, Argentina.

**Marc Marti-Renom**, Instituto de Investigación Príncipe Felipe, Spain.

**Andreas Schüller**, P. Universidad Católica de Chile, Chile.

**Tomás Pérez Aclé**, Universidad de Chile, Chile.

**Sergio Pantano**, Instituto Pasteur, Uruguay.

**Morten Nielsen**, Technical University of Denmark, Denmark.

**Andras Fiser**, Albert Einstein Medical School, USA.

**Fernan Aguero**, Universidad Nacional de San Martín, Argentina.

**Rodrigo Gutiérrez**, P. Universidad Católica de Chile, Chile.

**Luis Larrondo**, P. Universidad Católica de Chile, Chile.

**Alberto Dávila**, Instituto Oswaldo Cruz, Brazil.

## Local Organizing Committee of ISCB-Latin America 2012

**Juan José Cifuentes** (Universidad de Concepción, Chile)

**Rodrigo Gutiérrez** (Pontificia Universidad Católica de Chile, Chile)

**Alejandro Maass** (Universidad de Chile, Chile)

**Francisco Melo** (ISCB-LA-2012 Conference Chair)

**Tomás Norambuena** (Pontificia Universidad Católica de Chile, Chile)

**Andreas Schüller** (Pontificia Universidad Católica de Chile, Chile)

**Alex Slater** (Pontificia Universidad Católica de Chile, Chile)



# ISCB Latin America 2012

Conference on Bioinformatics

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8:30 AM - 9:00 AM

Tutorial Registration

9:00 AM - 12:30 PM

Practical Tutorials and Workshops (Morning Session)

Analysis, Comparison and Classification of Protein Structures

**Room Z06 FCBS**

Genome browsers with special emphasis in the ENSEMBL system

**Room CE1**

Protein resources and tools: sequence, architecture and protein interactions

**Room Z05 FCBS**

Algorithms and tools for transcriptomics and multiple gene profiling using the open source platforms R and Bioconductor

**Room CC1D**

12:30 PM - 2:00 PM

Lunch

2:00 PM - 5:30 PM

Practical Tutorials and Workshops (Afternoon Session)

Analysis, Comparison and Classification of Protein Structures

**Room Z06 FCBS**

Genome browsers with special emphasis in the ENSEMBL system

**Room CE1**

Protein resources and tools: sequence, architecture and protein interactions

**Room Z05 FCBS**

Algorithms and tools for transcriptomics and multiple gene profiling using the open source platforms R and Bioconductor

**Room CC1D**

## Day 2: Sunday - March 18, 2012

8:30 AM - 9:00 AM

Tutorial Registration

9:00 AM - 12:30 PM

Practical Tutorials and Workshops (Morning Session)

Immunoinformatics

**Room CC1D**

Next generation sequencing: an introduction for bioinformaticians

**Room Z06 FCBS**

Functional Genomics

**Room CE1**

Computer-Based Drug Design

**Room Z05 FCBS**

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Functional Genomics

**Room CE1**

Computer-Based Drug Design

**Room Z05 FCBS**

Three days ISCB-LatinAmerica-2012 Main Conference

Day 3: Monday - March 19, 2012

8:00 AM - 5:30 PM

Main Conference Registration

8:30 AM - 9:00 AM

Welcome/Opening Main Conference

**SESSION I. Comparative Genomics and Evolution.**

Chair of Session: Cristina Marino (Instituto Leloir, Argentina)

Location: Auditorium Juan Francisco Fresno (ground floor)

9:00 AM - 9:40 AM

**Keynote Lecture I: "Function prediction at different spatial scales"**

**Peer Bork.** EMBL, Heidelberg, Germany.

9:40 AM - 10:30 AM

Oral Presentations MM1-MM3

**MM1 » The PhyloFacts-SchistoDB Schistosoma Database**

**Presenting Author:** Kimmen Sjolander (University of California Berkeley)

**Co-authors:** Yaoqing Shen (University of California Berkeley, QB3); Ajithkumar Warriar (University of California Berkeley, QB3); Laila Nahum (FIOCRUZ Minas, Genomics and Computational Biology Group); Guilherme Oliveira (FIOCRUZ Minas, Genomics and Computational Biology Group)



**MM2 » Identification of transcription regulation associated proteins in plants and stramenopiles**

**Presenting Author:** Diego Mauricio Riaño Pachón (Universidad de los Andes)

**Co-authors:** Francisco J. Buitrago-Florez (Universidad de los Andes, Biological Sciences); Silvia Restrepo-Restrepo (Universidad de los Andes, Biological Sciences); Bernd Mueller-Roeber (Universität Potsdam, Institute of Biochemistry and Biology)

**MM3 » Molecular Phylodynamics and Protein Modeling of Infectious Salmon Anemia Virus (ISAV)**

**Presenting Author:** Eduardo Castro Nallar (Brigham Young University)

**Co-authors:** Marcelo Cortez-San Martín (Universidad de Santiago de Chile, Facultad de Química y Biología); Carolina Mascayano (Universidad de Santiago de Chile, Facultad de Química y Biología); Cristian Molina (Universidad de Santiago de Chile, Facultad de Química y Biología); Keith Crandall (Brigham Young University, Biology)

10:30 AM -11:00 AM

Coffee Break

11:00 AM - 11:40 AM

**Keynote Lecture II: “Orphan Orfogenic ORFs in the genomes of African trypanosomes”**

**Fernando Alvarez.** Universidad de la República, Uruguay.

11:40 AM - 12:30 PM

Oral Presentations MM4-MM6

**MM4 » Evolutionary events involved in pathogenic trait acquisition in Ascomycetes**

**Presenting Author:** Aminaël Sanchez-Rodriguez (Katholieke Universiteit Leuven)

**Co-authors:** Riet De Smet (Ghent University, Plant Systems Biology); Kristof Engelen (Katholieke Universiteit Leuven, Molecular and Microbial Systems); Qiang Fu (Katholieke Universiteit Leuven, Molecular and Microbial Systems); Yan Wu (Katholieke Universiteit Leuven, Molecular and Microbial Systems); Kathleen Marchal (Katholieke Universiteit Leuven, Molecular and Microbial Systems)

**MM5 » Novel Classes of Eukaryotic Aspartic Proteases and the Identification of their Specificity Determining Residues**

**Presenting Author:** María Revuelta (Universidad Nacional de Mar del Plata)

**MM6 » Conformational diversity: Relationship with protein evolution and designability**

**Presenting Author:** Diego Zea (Universidad Nacional de Quilmes)

**Co-authors:** Gustavo Parisi (Universidad Nacional de Quilmes, Centro de Estudios e Investigaciones); Cristina Marino Buslje (Fundación Instituto Leloir, Bioinformatics Unit)

12:30 PM - 2:00 PM

Lunch

12:40 PM - 2:00 PM

Business Presentation with free Lunch Sponsored by **Life Technologies** (open to any interested people)

Location: Sala Colorada (ground floor)

**SESSION II. Genomics, Proteomics, Metagenomics and Metabolomics.**

Chair of Session: David Holmes (Fundación Ciencia & Vida; Andrés Bello University, Chile)

Location: Auditorium Juan Francisco Fresno (ground floor)

2:00 PM - 2:40 PM

**Keynote Lecture III: “Challenges of Assembling Genomes from the Second Generation Sequencing data”**

**Aleksey Zimin.** University of Maryland, USA.

2:40 PM - 3:30 PM

Oral Presentations MA1-MA3

**MA1 » The ISA Commons – Towards interoperable data in bioscience**

**Presenting Author:** Susanna-Assunta Sansone (University of Oxford)

**Co-authors:** Philippe Rocca-Serra (University of Oxford, Oxford e-Research Centre); Eamonn Maguire (University of Oxford, Oxford e-Research Centre)

**MA2 » A Fast de novo Genome-Wide Tandem Repeat Discovery Algorithm**

**Presenting Author:** Marcelo Gonçalves Narciso (Embrapa)

**Co-authors:** Michel Yamagishi (Embrapa) Marcelo Gonçalves Narciso (Embrapa, Bioinformatics)

**MA3 » GOBOOT: testing set enrichment analysis robustness to background selection**

**Presenting Author:** Cristobal Fresno Rodríguez (Catholic University of Córdoba)

**Co-authors:** Andrea Llera (Leloir Institute, CONICET, Laboratory of Molecular and Cellular Therapy); María R Girotti (Leloir Institute, CONICET, Laboratory of Molecular and Cellular Therapy); María P Valacco (Leloir Institute, CONICET, Laboratory of Molecular and Cellular Therapy); Juan A López (National Center for Cardiovascular Research, Madrid); Osvaldo L Podhajcer (Leloir Institute, CONICET, Laboratory of Molecular and Cellular Therapy); Mónica G Balzarini (National University of Córdoba, Biometry Laboratory); Federico Prada (UADE, Institute of Technology, School of Engineering and Sciences); Elmer A Fernández (Catholic University of Córdoba, CONICET, BioScience Data Mining Group);

3:30 PM - 4:00 PM

Coffee Break

4:00 PM - 4:40 PM

**Keynote Lecture IV: "SABIA: A new version for next generation sequencing platforms"**

**Ana Teresa Ribeiro de Vasconcelos.** National Laboratory of Scientific Computation, Brazil.

4:40 PM - 5:30 PM

Oral Presentations MA4-MA6

**MA4 » Computational Pattern Recognition for the Identification of Transposases in Prokaryotic Genomes: Challenges and Advances.**

**Presenting Author:** Gonzalo Riadi (Talca University)

**Co-authors:** David Holmes (Fundacion Ciencia & Vida and Andres Bello University, Facultad Ciencias Biológicas); Gonzalo Riadi (Center of Bioinformatics and Molecular Simulation and Talca University, Engineering School)

**MA5 » Spinal Cord Regeneration in Xenopus: A Transcriptomics Analysis**

**Presenting Author:** Dasfne Lee-Liu (Pontificia Universidad Católica de Chile, Facultad de Ciencias Biológicas)

**Co-authors:** Juan Larrain (Pontificia Universidad Católica de Chile, Facultad de Ciencias Biológicas) Leonardo Almonacid (Pontificia Universidad Católica de Chile, Facultad de Ciencias Biológicas); Mauricio Moreno (Pontificia Universidad Católica de Chile, Facultad de Ciencias Biológicas); Rosana Muñoz (Pontificia Universidad Católica de Chile, Facultad de Ciencias Biológicas); Marcia Gaete (Pontificia Universidad Católica de Chile, Facultad de Ciencias Biológicas); Francisco Melo (Pontificia Universidad Católica de Chile, Facultad de Ciencias Biológicas)

**MA6 » High-resolution community genomics of a hypersaline microbial ecosystem**

**Presenting Author:** Juan Ugalde (University of California, San Diego)

**Co-authors:** Sheilla Podell (University of California, San Diego, Scripps Institution of Oceanography); Karla Heidelberg (University of Southern California, Department of Biological Sciences); Jill Banfield (University of California, Berkeley, Department of Earth and Planetary Sciences); Eric Allen (University of California, San Diego, Scripps Institution of Oceanography)

5:30 PM - 7:00 PM

**Poster Session I (Odd numbers)**

Location: Central Square (ground floor)

6:30 PM - 8:30 PM

Meeting of **SolBio** and **FreeBIT/CYTED**: Societies and Networks promoting Bioinformatics for Life Sciences and Biomedicine in IberoAmerica.

Location: Sala Colorada (ground floor)

Day 4: Tuesday - March 20, 2012

8:00 AM - 5:30 PM

Main Conference Registration

**SESSION III. Macromolecule Structure/Function Prediction.**

Chair of Session: Diego Ferreiro (Universidad de Buenos Aires, Argentina)

Location: Auditorium Juan Francisco Fresno (ground floor)

9:00 AM - 9:40 AM

**Keynote Lecture V: "Amazing Protein Folds"**

**Manfred Sippl.** University of Salzburg, Austria.

9:40 AM - 10:30 AM

Oral Presentations TM1-TM3

**TM1 » Modeling proteins using supersecondary structure library and NMR chemical shifts**

**Presenting Author:** Andras Fiser (Albert Einstein College of Medicine)

**Co-authors:** Vilas Menon (Albert Einstein College of Medicine, Systems and Computational Biology); Joseph Dybas (Albert Einstein College of Medicine, Systems and Computational Biology)

**TM2 » Using correlation data and network decomposition to obtain sub-class determinants in protein families**

**Presenting Author:** Lucas Bleicher (Universidade Federal de Minas Gerais)

**Co-authors:** Richard Garratt (Universidade de Sao Paulo, Instituto de Fisica de Sao Carlos); Ney Lemke (Universidade Estadual de Sao Paulo, Departamento de Fisica e Biofisica, Botucatu)

**TM3 » Evolution of linear motifs within the intrinsically disordered and globular domains of the papillomavirus E7 oncoprotein**

**Presenting Author:** Lucia Chemes (Fundación Instituto Leloir IIBBA-CONICET)

**Co-authors:** Juliana Glavina (Protein Physiology Laboratory, Facultad de Ciencias Exactas y Naturales, Universidad

de Buenos Aires, Argentina, Departamento de Química Biológica); Julian Faivovich (División Herpetología, Museo Argentino de Ciencias Naturales-CONICET, Buenos Aires, Argentina, Museo Argentino de Ciencias Naturales); Leonardo Alonso (Fundacion Instituto Leloir , Buenos Aires Argentina, IIBBA-CONICET); Cristina Marino-Buslje (Fundacion Instituto Leloir, IIBBA CONICET, Buenos Aires Argentina, Structural Bioinformatics Laboratory); Gonzalo de Prat Gay (Fundacion Instituto Leloir IIBBA CONICET, Buenos Aires Argentina, Protein Structure-Function and Engineering Laboratory); Sanchez Ignacio (Protein Physiology Laboratory, Facultad de Ciencias Exactas y Naturales, Universidad de Buenos Aires, Argentina, Departamento de Quimica Biologica)

10:30 AM - 11:00 AM

Coffee Break

11:00 AM - 11:40 AM

**Keynote Lecture VI: “Conformational diversity and the development of new tools in bioinformatics”**

**Gustavo Parisi.** Universidad Nacional de Quilmes, Argentina.

11:40 AM - 12:30 PM

Oral Presentations TM4-TM6

**TM4 » Cross talk between DNA and Transcription factors**

**Presenting Author:** Matias Machado (Institut Pasteur de Montevideo)

**Co-authors:** Pablo Dans (Institut Pasteur de Montevideo, Biomolecular Simulation Group); Sergio Pantano (Institut Pasteur de Montevideo, Biomolecular Simulation Group)

**TM5 » Standardized comparison of structural alignments of catalytic domains in DNA polymerases from different methods**

**Presenting Author:** Alex Slater (Molecular Bioinformatics Laboratory, Millennium Institute on Immunology and Immunotherapy. Pontificia Universidad Católica de Chile)

**Co-authors:** Manfred Sippl (University of Salzburg); Francisco Melo (Pontificia Universidad Católica de Chile, Depto. Genética Molecular y Microbiología)

**TM6 » A Multidisciplinary Strategy for Function Assignment: The Enzyme Function Initiative from a Bioinformatics Perspective**

**Presenting Author:** Daniel Almonacid (University of California)

**Co-authors:** Shoshana Brown (University of California San Francisco, Bioengineering and Therapeutic Sciences); Patricia Babbitt (University of California San Francisco, Bioengineering and Therapeutic Sciences)

12:30 PM - 2:00 PM

Lunch

12:40 PM - 2:00 PM

Business Presentation with free Lunch Sponsored by **Roche** (open to any interested people)

Location. Sala Colorada (ground floor)

**SESSION IV. Computer Aided Drug Design and Docking/ Molecular Dynamics Simulations.**

Chair of Session: Tomás Pérez-Acle (Universidad de Chile, Chile)

Location: Auditorium Juan Francisco Fresno (ground floor)

2:00 PM - 2:40 PM

**Keynote Lecture VII: “Coarse-Grain methods for molecular dynamics simulations: Actually bridging the gap between simulations and biological scales”**

**Sergio Pantano.** Instituto Pasteur de Montevideo, Uruguay.

2:40 PM - 3:30 PM

Oral Presentations TA1-TA3

**TA1 » Confidence Assessment of Candidate Drug Property Predictions by Subspace Mapping Methods**

**Presenting Author:** Axel Soto (Universidad Nacional del Sur)

**Co-authors:** Ignacio Ponzoni (Universidad Nacional del Sur) Gustavo Vazquez (Universidad Nacional del Sur, Laboratory of Research and Development in Scientific Computing (LIDeCC)); Marc Strickert (Siegen University, Institute for Vision and Graphics); Ignacio Ponzoni (Universidad Nacional del Sur, Laboratory of Research and Development in Scientific Computing (LIDeCC))

**TA2 » Docking Studies of a New Series of Analgesic and Anti-inflammatory Compounds (NSAIDs) with Cyclooxygenase**

**Presenting Author:** Lucas Saraiva (Federal University of Minas Gerais)

**Co-authors:** Ihosvany Camps (Federal University of Alfenas, Department of Exact Science); Raquel Melo-Minardi (Federal University of Minas Gerais, Department of Computer Science); Marcia Veloso (Federal University of Alfenas, Faculty of Pharmaceutical Science); Rodrigo Sailva (Federal University of São Carlos, Department of Chemistry)

**TA3 » Desintegrin-like domains in computer aided drug design of integrin-specific inhibitors**

**Presenting Author:** Jorge H. Fernandez (State University of North Fluminense)

**Co-authors:** Jorge Fernandez (State University of North Fluminense) Monika A. Coronado (UNESP-RP, Depto. de Física); Ana T.R. Vasconcelos (LNCC, BioInfo); Monica Lopes-Ferreira (Butantan Institute, LETA); Wilson Savino (Oswaldo Cruz Institute, Laboratory of Thymus Research)

3:30 PM - 4:00 PM

Coffee Break

4:00 PM - 4:40 PM

**Keynote Lecture VIII: "Molecular Simulation of Non-equilibrium Systems: The Dance of ions across the membrane"**

**Danilo González.** Universidad Andres Bello, Chile.

4:40 PM - 5:30 PM

Oral Presentations TA4-TA6

**TA4 » Using Computer Simulations to Understand Enzyme Mechanism: Application to Mycobacterium tuberculosis CYP121 Unusual Reaction**

**Presenting Author:** Victoria Dumas (University of Buenos Aires)

**Co-authors:** Adrián Turjanski (University of Buenos Aires, Química Inorgánica); Lucas Defelipe (University of Buenos Aires, Química Biológica); Marcelo Martí (University of Buenos Aires, Química Inorgánica)



**TA5 » Topological constraints and challenges imposed by knots in proteins**

**Presenting Author:** Cesar Ramirez (University of Chile)

**Co-authors:** Jeffrey K Noel (University of California San Diego, Center for Theoretical Biological Physics); Mauricio Baez (University of Chile, Department of Biology)

**TA6 » Combined structure- and ligand-based virtual screening in the search of novel 11beta-hydroxysteroid dehydrogenase inhibitors for the treatment of metabolic syndrome**

**Presenting Author:** Carlos Lagos (Pontificia Universidad Catolica de Chile)

**Co-authors:** Andrea Vecchiola (P. Universidad Catolica de Chile, Molecular Endocrinology Laboratory); Fidel Allende (P. Universidad Catolica de Chile, Clinical Laboratory); Carolina Valdivia (P. Universidad Catolica de Chile, Molecular Endocrinology Laboratory); Cristobal A. Fuentes (P. Universidad Catolica de Chile, Molecular Endocrinology Laboratory); Sandra Solari (P. Universidad Catolica de Chile, Clinical Laboratory); Carmen Campino (P. Universidad Catolica de Chile, Molecular Endocrinology Laboratory); Rene Baudrand (P. Universidad Catolica de Chile, Molecular Endocrinology Laboratory); Cristian A. Carvajal (P. Universidad Catolica de Chile, Molecular Endocrinology Laboratory); Carlos E. Fardella (P. Universidad Catolica de Chile, Molecular Endocrinology Laboratory); Mariana Cifuentes (Universidad de Chile, Institute of Nutrition and Food Technology (INTA))

5:30 PM - 7:00 PM

**Poster Session II (Even numbers)**

Location: Central Square (ground floor)

**SESSION V. Biomedicine and Immunoinformatics.**

Chair of Session: Alexis Kalergis (Pontificia Universidad Católica de Chile)

Location: Auditorium Juan Francisco Fresno (ground floor)

9:00 AM - 9:40 AM

**Keynote Lecture IX: “Immune Epitope Database and Analysis Resource Program: Proving Intuitive Access To Comprehensive Epitope Data And Tools”**

**Alessandro Sette.** La Jolla Institute for Allergy and Immunology, USA.

9:40 AM - 10:30 AM

Oral Presentations WM1-WM3

**WM1 » MHCcluster, and method for functional clustering of MHC molecules**

**Presenting Author:** Morten Nielsen (Center for Biological Sequence Analysis, BioCentrum, DTU)

**Co-authors:** Ole Lund (Center for Biological Sequence Analysis, BioCentrum, DTU, Department of Systems biology); Claus Lundegaard (Center for Biological Sequence Analysis, BioCentrum, DTU, Department of Systems biology)

**WM2 » A step towards pan-specific prediction methods for MHC class II molecules: a projection of HLA-DR on to HLA-DP and HLA-DQ**

**Presenting Author:** Edita Karosiene (Technical University of Denmark)

**Co-authors:** Morten Nielsen (Technical University of Denmark, Department of Systems Biology)

**WM3 » Systematic prediction of ligand-receptor pair across the immunoglobulin superfamily using a novel sequence homology measure**

**Presenting Author:** Eng Hui Yap (Albert Einstein College of Medicine)

**Co-authors:** Andras Fiser (Albert Einstein College of Medicine, Systems and Computational Biology); Tyler Rosche (Albert Einstein College of Medicine, Systems and Computational Biology)

10:30 AM - 11:00 AM

Coffee Break

11:00 AM - 11:40 AM

**Keynote Lecture X: "Using Genomics to Improve Response to Neoadjuvant Therapy in Patients with Rectal Cancer"**  
**Anamaría Camargo.** Ludwig Institute for Cancer Research, Brazil

11:40 AM - 12:30 PM

Oral Presentations WM4-WM6

**WM4 » Common features in damaged DNA detection**

**Presenting Author:** Juan José Cifuentes (Pontificia Universidad Católica de Chile)

**Co-authors:** Francisco Melo (Molecular Bioinformatics Laboratory, Depto. Genética Molecular y Microbiología. Pontificia Universidad Católica de Chile)

**WM5 » A bioinformatics strategy for the design of diagnostic epitope discovery tools: first generation peptide microarrays for Chagas Disease**

**Presenting Author:** Santiago Carmona (Universidad Nacional de San Martín)

**Co-authors:** Fernán Agüero (Universidad Nacional de San Martín) Paula Sartor (UBA, Dept. of Microbiology-Fac.Med.); Maria Susana Leguizamón (UBA, Dept. of Microbiology-Fac.Med.); Oscar Campetella (UNSAM, IIB); Fernán Agüero (UNSAM, IIB)

**WM6 » Annotation of putative AraC/XylS-family transcription factors of known structure but unknown function**

**Presenting Author:** Andreas Schüller (Pontificia Universidad Católica de Chile)

**Co-authors:** Alex W. Slater (Pontificia Universidad Católica de Chile, Depto. Genética Molecular y Microbiología); Tomás Norambuena (Pontificia Universidad Católica de Chile, Depto. Genética Molecular y Microbiología); Juan J. Cifuentes (Pontificia Universidad Católica de Chile, Depto. Genética Molecular y Microbiología); Francisco Melo (Pontificia Universidad Católica de Chile, Depto. Genética Molecular y Microbiología)

12:30 PM - 2:00 PM

Lunch

12:45 PM - 1:45 PM

The ISCB Open Member Meeting (open to any interested people)

Location: Sala Colorada (ground floor)

**SESSION VI. Functional Genomics and Systems Biology.**

Chair of Session: Rodrigo Gutiérrez (Pontificia Universidad Católica de Chile)

Location: Auditorium Juan Francisco Fresno (ground floor)

2:00 PM - 2:40 PM

**Keynote Lecture XI: "Using 'omics' data to study regulator-target interactions and organizational principles in networks"**

**Yves van de Peer.** University of Ghent, Belgium.

2:40 PM - 3:30 PM

Oral Presentations WA1-WA3

**WA1 » Evolution of domain architectures and catalytic functions of enzymes in metabolic systems**

**Presenting Author:** Chen-Hsiang Yeang (Academia Sinica)

**Co-authors:** Summit Suen (Academia Sinica, Institute of Statistical Science); Henry Horng-Shing Lu (National Chiao-Tung University, Institute of Statistics);

**WA2 » Unveiling combinatorial regulation through the combination of ChIP information and in silico cis-regulatory module detection**

**Presenting Author:** Kathleen Marchal (Ghent University)

**Co-authors:** Hong Sun (K.U.Leuven, Microbial and Molecular Systems); Tias Guns (K.U.Leuven, Computer Science); Ana Carolina Fierro (K.U.Leuven, Computer Science); Lieven Thorrez (K.U.Leuven, Interdepartmental Stem Cell Institute); Siegfried Nijssen (K.U.Leuven, Computer science)

**WA3 » LitProf – Gene Classifier: A text-mining gene function predictor for prokaryotes**

**Presenting Author:** Roney Coimbra (FIOCRUZ-Minas)

**Co-authors:** Raul Torrieri (FIOCRUZ-Minas, Center for

Excellence in Bioinformatics); Francislon Oliveira (FIOCRUZ-Minas, Center for Excellence in Bioinformatics); Guilherme Oliveira (FIOCRUZ-Minas, Center for Excellence in Bioinformatics)

3:30 PM - 4:00 PM

Coffee Break

4:00 PM - 4:40 PM

**Keynote Lecture XII: "On the evolution of PPI networks"**  
**Sandro José de Souza.** Ludwig Institute for Cancer Research, Brazil.

4:40 PM - 5:30 PM

Oral Presentations WA4-WA6

**WA4 » Discriminative local subspaces in gene expression data for effective gene function prediction**

**Presenting Author:** Tomas Puelma (Pontificia Universidad Católica de Chile)

**Co-authors:** Rodrigo Gutierrez (Pontificia Universidad Católica de Chile) Alvaro Soto (Pontificia Universidad Católica de Chile, Computer Science); Rodrigo Gutierrez (Pontificia Universidad Católica de Chile, Molecular Genetics and Microbiology)

**WA5 » The just-in-time expression of yeast ribosomal proteins**

**Presenting Author:** Andrzej Kudlicki (University of Texas Medical Branch)

**Co-authors:** Xueling Li (University of Texas Medical Branch, Institute of Translational Science); Gang Chen (Central South University, Computer Science)

**WA6 » Deciphering human protein interactome using structural complexes**

**Presenting Author:** Anna Panchenko (National Institutes of Health)

**Co-authors:** Manoj Tyagi (National Institutes of Health, NCBI); Kosuke Hashimoto (RIKEN, RIKEN); Benjamin Shoemaker (NIH, NCBI); Stefan Wuchty (NIH, NCBI)

5:30 PM - 6:00 PM

**Awards Ceremony**

Day 6: Thursday - March 22, 2012

6:00 PM – 6:30 PM

Closing Remarks

7:00 PM – 11:30 PM

### Conference Banquet

Location: Castillo Hidalgo, Cerro Santa Lucía, Santiago.

One day satellite Workshops and Round Tables

Day 6: Thursday - March 22, 2012

### SESSION VII. Workshops on Next Generation Sequencing Technologies and GRID Computing.

Chair of Session: Romilio Espejo (Omics Solutions, Chile)

Location: Auditorium Aula Magna Eleodoro Matte Ossa (second floor)

10:00 AM - 11:15 AM

#### “Ion Torrent – Open, Accessible, and Enabling”

**Matt Dyer.** Life Technologies, USA.

11:15 AM - 11:30 AM

Coffee Break

11:30 AM - 12:45 PM

#### “Introducing GS FLX+ System”

Xuemin Liu. 454 Sequencing/Roche, USA.

12:45 PM - 2:00 PM

Lunch

2:00 PM - 3:00 PM

#### “Optimization of bioinformatics applications to be executed on GRID platforms”

**Manuel A. Rodríguez-Pascual** and **Rafael Mayo-García**  
CIEMAT, Spain; SolBio, CYTED and FreeBIT

3:00 PM - 3:20 PM

Coffee Break

**SESSION VIII. Round Tables on Bioinformatics Research, Training and Education in Iberoamerica.**

Chair of Session: Danilo González (Universidad Andrés Bello, Chile)

Location: Auditorium Aula Magna Eleodoro Matte Ossa (second floor)

3:20 PM – 4:20 PM

**“Bioinformatics Education in Iberoamerica”**

**Alejandra Medina-Rivera** , **Juan Pablo Bustamante** (SolBio Student Council), **Daniel Almonacid** and **Priscila Grynberg** (ISCB Student Council).

4:20 PM – 4:40 PM

Coffee Break

4:40 PM – 5:40 PM

**“Bioinformatics Research and Training in Iberoamerica”**

**Guilherme de Oliveira** (Brazil), **Fernán Aguero** (Argentina), **Javier de las Rivas** (Spain), **Julio Collado-Vides** (México), **Allan Orozco** (Costa Rica) and **Francisco Melo** (Chile).

**Topic Session: *Comparative Genomics and Evolution***

**P1 » Identification of transcription regulation associated proteins in plants and stramenopiles**

**Presenting Author:** Diego Mauricio Riaño Pachón (Universidad de los Andes)

**Co-authors:** Francisco J. Buitrago-Florez (Universidad de los Andes, Biological Sciences); Silvia Restrepo-Restrepo (Universidad de los Andes, Biological Sciences); Bernd Mueller-Roeber (Universität Potsdam, Institute of Biochemistry and Biology)

**P2 » Novel Classes of Eukaryotic Aspartic Proteases and the Identification of their Specificity Determining Residues**

**Presenting Author:** María Revuelta (Universidad Nacional de Mar del Plata)

**P3 » Design-theoretical approach to homology assessment of DNA sequences**

**Presenting Author:** Andrzej Brodzik (The MITRE Corporation)

**P4 » Shedding light into bacterial pathogenicity prediction: a machine learning approach**

**Presenting Author:** Gregorio Iraola (Institut Pasteur Montevideo)

**Co-authors:** Lucía Spangenberg (Institut Pasteur Montevideo, Bioinformatics Unit); Gustavo Vazquez (Universidad Nacional del Sur, Departamento de Ciencias e Ingeniería de la Computación); Hugo Naya (Institut Pasteur Montevideo, Bioinformatics Unit)

**P5 » Identifying associations between amino acid changes and meta information in alignments**

**Presenting Author:** Lucía Spangenberg (Institut Pasteur de Montevideo)

**Co-authors:** Kay Nieselt (University of Tübingen, Center for Bioinformatics Tübingen); Florian Battke (University of Tübingen, Center for Bioinformatics Tübingen); Hugo Naya (Institut Pasteur de Montevideo, Bioinformatics Unit); Martín Graña (Institut Pasteur de Montevideo, Bioinformatics Unit)



**P6 » A phylogenomic approach to understand genomic and metabolic diversity in extreme acidophilic environments**

**Presenting Author:** Jorge Valdes (Fraunhofer Chile Research)

**P7 » Assessing the efficiency of multiple sequence alignment programs**

**Presenting Author:** Patrícia Ruy (Oswaldo Cruz Foundation)

**Co-authors:** Fabiano Sviatopolk-Mirsky Pais (Oswaldo Cruz Foundation, Center for Excellence in Bioinformatics); Guilherme Oliveira (Oswaldo Cruz Foundation, Center for Excellence in Bioinformatics / Genomics and Computational Biology Group); Roney Santos Coimbra (Oswaldo Cruz Foundation, Center for Excellence in Bioinformatics / Genomics and Computational Biology Group)

**P8 » Conformational diversity: Relationship with protein evolution and designability**

**Presenting Author:** Diego Zea (Universidad Nacional de Quilmes)

**Co-authors:** Gustavo Parisi (Universidad Nacional de Quilmes, Centro de Estudios e Investigaciones); Cristina Marino Buslje (Fundación Instituto Leloir, Bioinformatics Unit)

**P9 » On the particularities of Protozoa: a comparative genomics approach**

**Presenting Author:** Diogo Tschoeke (Oswaldo Cruz Institute)

**Co-authors:** Rodrigo Jardim (Computational and Systems Biology Lab, Oswaldo Cruz Institute, FIOCRU); Joana Lima (and Systems Biology Lab, Oswaldo Cruz Institute, FIOCRUZ); Sergio Serra (ICE / Federal Rural University of Rio de Janeiro, DEMAT ); Rafael Cuadrat (Computational and Systems Biology Lab, Oswaldo Cruz Institute, FIOCRUZ); Marta Mattoso (Federal University of Rio de Janeiro, COPPE/PESC ); Maria Luiza Campos (Federal University of Rio de Janeiro, PPGI); Alberto Dávila (Computational and Systems Biology Lab, Oswaldo Cruz Institute, FIOCRUZ)

**P10 » Genomic characterization of *Pseudomonas fluorescens* NCIMB11764, a bacteria strain with unique cyanide metabolism capabilities**

**Presenting Author:** Claudia Vilo (University of North Texas)

**Co-authors:** Michael Benedik (Texas A&M University, Biology); Daniel Kunz (University of North Texas, Biology); Qunfeng Dong (University of North Texas, Biology)

**P11 » Differential adaptive evolution in the *Helicobacter pylori* genome depending on human host population**

**Presenting Author:** Maria Soto-Giron (University of Puerto Rico)

**P12 » Evolution of 7SK RNA and Its Protein Partners in Metazoa**

**Presenting Author:** Nina Verstraete (Institut de Biologie de l'École Normale Supérieure)

**Co-authors:** Alexander Donath (University of Leipzig, Computer Science, and Interdisciplinary Center for Bioinformatics); Manja Marz (University of Leipzig, Computer Science, and Interdisciplinary Center for Bioinformatics); Peter F. Stadler (University of Leipzig, Computer Science, and Interdisciplinary Center for Bioinformatics); Van Trung Nguyen (Institut de Biologie de l'École Normale Supérieure, Génomique Fonctionnelle); Olivier Bensaude (Institut de Biologie de l'École Normale Supérieure, Génomique Fonctionnelle)

**P13 » Expression evolution of prokaryotic organisms**

**Presenting Author:** Pieter Meysman (KULeuven)

**Co-authors:** Kristof Engelen (KULeuven) Aminaél Sánchez-Rodríguez (KULeuven, Department Of Microbial And Molecular Systems (M2S)); Qiang Fu (KULeuven, Department Of Microbial And Molecular Systems (M2S)); Kathleen Marchal (KULeuven, Department Of Microbial And Molecular Systems (M2S))

**P14 » Analysis of genomic regions with abundant repetitive sequences using high-throughput genomic data: *Vibrio cholerae* superintegron**

**Presenting Author:** Michel Marín (Oswaldo Cruz Institute - Fiocruz)

**Co-authors:** Bas Dutilh (San Diego State University, Department of Biology and Department of Computer Science); Cristiane Thompson (Oswaldo Cruz Institute - Fiocruz, Laboratory of Molecular Genetics of Microorganisms); Robert Edwards (San Diego State University, Department of Computer Science)

**P15 » Genomic and computational analysis used for bacterial taxonomy: streptococci species as a test case**

**Presenting Author:** Michel Marín (Oswaldo Cruz Institute - Fiocruz)

**Co-authors:** Cristiane Thompson (Oswaldo Cruz Institute - Fiocruz) Vanessa Emmel (Oswaldo Cruz Institute - Fiocruz, Laboratory of Molecular Genetics of Microorganisms);

Michel Marin (Oswaldo Cruz Institute - Fiocruz, Laboratory of Molecular Genetics of Microorganisms); Ana Carolina Vicente (Oswaldo Cruz Institute - Fiocruz, Laboratory of Molecular Genetics of Microorganisms)

**P16 » Identification of transcription factor genes and their correlation with the high diversity of Stramenopiles**

**Presenting Author:** Francisco Buitrago (Universidad de los Andes)

**Co-authors:** Francisco Buitrago-Florez (Universidad de los Andes) Silvia Restrepo (Universidad de los Andes, Biological Sciences); Diego Riaño-Pachon (Universidad de los Andes, Biological Sciences)

**P17 » The phylogenomics of carbohydrate metabolism in Protozoa**

**Presenting Author:** Joana A. Lima Oliveira (Institute Oswaldo Cruz/Fiocruz)

**Co-authors:** Joana de Oliveira (Institute Oswaldo Cruz/Fiocruz) Diogo A. Tschoeke (Computational and Systems Biology Pole, Oswaldo Cruz Institute, FIOCRUZ); Alexandre Pittis (Center for Genomic Regulation/ CRG, CRG); Marina Marcet-Houben (Center for Genomic Regulation/ CRG, CRG); Toni Gabaldón (Center for Genomic Regulation/ CRG, CRG); Alberto M R Dávila (Computational and Systems Biology Pole, Oswaldo Cruz Institute, FIOCRUZ)

**P18 » Analysis of the Pathogen-Host relationship of Orthomyxoviruses**

**Presenting Author:** Mario Tello (Universidad de Santiago)

**Co-authors:** Jose Miguel Saavedra (Universidad de Santiago de Chile, Biología); Francisco Vergara (Universidad de Santiago de Chile, Biología); Eugenio Spencer (Universidad de Santiago de Chile, Biología)

**P19 » Comparative genomics of the oxidative stress response in acidophilic microorganisms**

**Presenting Author:** Juan Pablo Cárdenas (Fundacion Ciencia para la Vida & Universidad Andres Bello)

**Co-authors:** Juan Cárdenas (Fundacion Ciencia para la Vida & Universidad Andres Bello) David Holmes (Fundacion Ciencia para la Vida & Universidad Andres Bello, Center of Bioinformatics and Genome Biology); Raquel Quatrini (Fundacion Ciencia para la Vida & Universidad Andres Bello, Laboratorio de Ecofisiologia Microbiana); Gloria Levican (Universidad de Santiago de Chile, Facultad de Quimica y Biologia)

**P20 » A phylogenomic approach to understand genomic and metabolic diversity in extreme acidophilic environments**

**Presenting Author:** Jorge Valdes (Fraunhofer Chile Research)

**Co-authors:** Carolina Gonzalez (Center For Bioinformatics and Genome Biology, Fundacion Ciencia & Vida and Andrés Bello University, Departamento de Ciencias Biologicas); Paz Tapia (Fraunhofer Chile Research, Bio-Computing Division); O'car Campos (Fraunhofer Chile Research, Bio-Computing Division); David Holmes (Center For Bioinformatics and Genome Biology, Fundacion Ciencia & Vida and Andrés Bello University, Departamento de Ciencias Biologicas)

**P21 » Genome sequence analysis of Acinetobacter sp. Ver3 and Exiguobacterium sp. S17 isolated from High Altitude Andean Lakes**

**Presenting Author:** Daniel Kurth (PROIMI-CONICET)

**Co-authors:** Omar Ordoñez (PROIMI-CONICET, LIMLA); Virginia Albarracin (PROIMI-CONICET, LIMLA); Nestor Cortez (UNR-IBR-CONICET, Biología Molecular); Adrian Turjanski (Facultad de Ciencias Exactas-UBA, Departamento de Química Inorgánica, Analítica, y Química Física); Martin Vazquez (INDEAR-CONICET, Plataforma de Secuenciación Genómica y Bioinformática); Maria Eugenia Farias (PROIMI-CONICET, LIMLA)

**P22 » High dimensional multi-genomic investigation into the function and evolution of Eukaryotic single exon genes**

**Presenting Author:** Roddy Jorquera Cifuentes (Center for Bioinformatics and Genome Biology, Fundacion Ciencia & Vida and Facultad de Ciencias Biologicas, Universidad Andres Bello, Santiago Chile)

**Co-authors:** David Holmes (Center for Bioinformatics and Genome Biology, Fundacion Ciencia & Vida and Facultad de Ciencias Biologicas, Universidad Andres Bello, Santiago Chile) Rodrigo Ortiz Ortiz (Pontificia Universidad Católica de Chile, Facultad de Ciencias Biológicas); Aucán Pedroso Rovira (Universidad de Talca, Facultad de Ingeniería)

**P23 » Distribution of Fur family of transcriptional regulators in species belonging to the Lactobacillales order**

**Presenting Author:** Esteban Gárate (Universidad de Chile)

**Co-authors:** Mauricio González (Universidad de Chile, Laboratorio de Bioinformática y Expresión Génica, INTA); Angélica Reyes-Jara (Universidad de Chile, Laboratorio de Microbiología y Probióticos, INTA)

**P24 » Whole Genome Sequencing and Comparative Analysis of *Yersinia pestis*, the causative agent of a plague outbreak in northern Perú**

**Presenting Author:** Heinner Guio (Peruvian National Institute of Health)

**Co-authors:** Juan Montenegro (Peruvian National Institute of Health, Laboratorio de Biotecnología y Biología Molecular); Omar Cáceres (Peruvian National Institute of Health, Laboratorio de Biotecnología y Biología Molecular); Carlos Padilla (Peruvian National Institute of Health, Laboratorio de Biotecnología y Biología Molecular); Henri Bailón (Peruvian National Institute of Health, Laboratorio de Biotecnología y Biología Molecular); David Tarazona (Peruvian National Institute of Health, Laboratorio de Biotecnología y Biología Molecular); Patricia García (Peruvian National Institute of Health, Laboratorio de Zoonosis Bacteriana); Manuel Céspedes (Peruvian National Institute of Health, Centro Nacional de Salud Pública); Pedro Valencia (Peruvian National Institute of Health, Centro Nacional de Salud Pública)

**P25 » Molecular characterization of kinetoplast of three Venezuelan isolates of *Trypanosoma vivax***

**Presenting Author:** Alfredo Mijares (IVIC)

**Co-authors:** Iralis Cardozo (IVIC, CBB); Mary Isabel Gonzatti (Universidad Simon Bolivar, Departamento de Biología Celular)

**P26 » Evolutionary history of the Glucokinase/Phosphofruktokinase activity in the ADP-dependent sugar kinases family**

**Presenting Author:** Victor-Hugo Castro (Universidad de Chile)

**Co-authors:** Victoria Guixe (Universidad de Chile, Departamento de Biología)

**P27 » Whole Genome Sequencing and Comparative Analysis of the *Bartonella bacilliformis* strain INS, the causative agent of Carrion's disease**

**Presenting Author:** David Tarazona (Instituto Nacional de Salud)

**Co-authors:** Carlos Padilla (Instituto Nacional de Salud, Laboratorio de Biotecnología y Biología Molecular); Omar Cáceres (Instituto Nacional de Salud, Laboratorio de Biotecnología y Biología Molecular); Juan Montenegro (Instituto Nacional de Salud, Laboratorio de Biotecnología y Biología Molecular); Henri Bailón (Instituto Nacional de Salud, Laboratorio de Biotecnología y Biología Molecular);

Elizabeth Anaya (Instituto Nacional de Salud, Laboratorio de Metaxenicis Bacterianas); Giovanna Mendoza (Instituto Nacional de Salud, Laboratorio de Metaxenicis Bacterianas); Pedro Valencia (Instituto Nacional de Salud, Centro Nacional de Salud Pública); Heinner Guio (Instituto Nacional de Salud, Laboratorio de Biotecnología y Biología Molecular)

**P28 » Looking for orthologs for the sodium K<sup>+</sup>-independent, ouabain-insensitive Na<sup>+</sup>-ATPase**

**Presenting Author:** Luz Thomas (Instituto Venezolano de Investigaciones Científicas)

**Co-authors:** Miguel Rocafull (Instituto Venezolano de Investigaciones Científicas, Centro de Biofísica y Bioquímica); Jesús del Castillo (Instituto Venezolano de Investigaciones Científicas, Centro de Biofísica y Bioquímica)

**P29 » footprint-scan: Detecting conservation of regulatory interactions inside Gensor Units**

**Presenting Author:** Alejandra Medina Rivera (Centro de Ciencias Genómicas, Universidad Nacional Autónoma de México)

**Co-authors:** Jacques van Helden (Université d'Aix-Marseille (AMU), TAGC); Socorro Gama-Castro (Centro de Ciencias Genómicas-Universidad Nacional Autónoma de México, Programa de Genómica Computacional); Julio Collado-Vides (Centro de Ciencias Genómicas-Universidad Nacional Autónoma de México, Programa de Genómica Computacional)

**P30 » Whole Genome Sequencing and Comparative Analysis of *Yersinia pestis*, the causative agent of a plague outbreak in northern Perú**

**Presenting Author:** Juan D. Montenegro (Peruvian National Institute of Health)

**Co-authors:** Heinner Guio (Peruvian National Institute of Health) Juan D. Montenegro (Peruvian National Institute of Health, Laboratorio de Biotecnología y Biología Molecular); Omar Cáceres (Peruvian National Institute of Health, Laboratorio de Biotecnología y Biología Molecular); Carlos Padilla (Peruvian National Institute of Health, Laboratorio de Biotecnología y Biología Molecular); Manuel Céspedes (Peruvian National Institute of Health, Peruvian National Public Health Centre); Henri Bailón (Peruvian National Institute of Health, Laboratorio de Biotecnología y Biología Molecular); David Tarazona (Peruvian National Institute of Health, Laboratorio de Biotecnología y Biología Molecular); Patricia García (Peruvian National Institute of Health,

Laboratorio de Zoonosis Bacteriana); Pedro Valencia (Peruvian National Institute of Health, National Public Health Centre); Heinner Guio (Peruvian National Institute of Health, Laboratorio de Biotecnología y Biología Molecular)

**P31 » Mr.Cirrus: A Map-Reduce approach for High level Cloud Computing**

**Presenting Author:** Oswaldo Trelles (University of Malaga)

**Co-authors:** Juan Lago (Fundación Iavante, ; Consejería de Salud de la Junta de Andalucía); Daniel Ramet (University of Malaga, Computer Architecture); Oscar Torreño (University of Malaga, Computer Architecture); Johan Karlsson (University of Malaga, Computer Architecture); Juan Falgueras (University of Malaga, Languages and Computer Sciences); Noura Chelbat (Johannes Kepler University, Institute for Bioinformatics); Michael Krieger (RISC Software GmbH, Co-Location Center)

**Topic Session: *Genomics, Proteomics, Metagenomics and Metabolomics***

**P32 » A Fast de novo Genome-Wide Tandem Repeat Discovery Algorithm**

**Presenting Author:** Marcelo Gonçalves Narciso (Embrapa)

**Co-authors:** Michel Yamagishi (Embrapa) Marcelo Gonçalves Narciso (Embrapa, Bioinformatics)

**P33 » Gene expression in Schistosoma mansoni schistosomula in the presence of hamster's peripheral or portal serum**

**Presenting Author:** Fabiano Pais (Oswaldo Cruz Foundation)

**Co-authors:** Wander J Jeremias (Oswaldo Cruz Foundation, Schistosomiasis Laboratory); Flavio M G Araujo (Oswaldo Cruz Foundation, Center for Excellence in Bioinformatics); Paulo M Coelho (Oswaldo Cruz Foundation, Schistosomiasis Laboratory); Guilherme Oliveira (Oswaldo Cruz Foundation, Center for Excellence in Bioinformatics - Genomics and Computational Biology Group); Anna C Salim (Oswaldo Cruz Foundation, Center for Excellence in Bioinformatics); Fernando L Kamitani (Oswaldo Cruz Foundation, Center for Excellence in Bioinformatics); Renata Guerra-Sa (Ouro Preto Federal University, Biochemistry and Molecular Biology Laboratory); Roney S Coimbra (Oswaldo Cruz Foundation, Center for Excellence in Bioinformatics - Genomics and Computational Biology Group); Elio H Babá (Oswaldo Cruz Foundation, Schistosomiasis Laboratory)

**P34 » High-resolution community genomics of a hypersaline microbial ecosystem**

**Presenting Author:** Juan Ugalde (University of California, San Diego)

**Co-authors:** Sheilla Podell (University of California, San Diego, Scripps Institution of Oceanography); Karla Heidelberg (University of Southern California, Department of Biological Sciences); Jill Banfield (University of California, Berkeley, Department of Earth and Planetary Sciences); Eric Allen (University of California, San Diego, Scripps Institution of Oceanography)

**P35 » RNA-seq expression analyses in sweet cherries to try to understand cracking tolerance**

**Presenting Author:** Jonathan Maldonado (University of Chile)

**Co-authors:** Herman Silva (University of Chile) Herman Silva (University of Chile, Agricultural Production); Juan Carlos Rios (University of Chile, Agricultural Production)

**P36 » COLOMBOS: an ever expanding collection of bacterial expression compendia**

**Presenting Author:** Kristof Engelen (KULeuven)

**Co-authors:** Pieter Meysman (KULeuven, Department Of Microbial And Molecular Systems (M2S)); Aminaél Sánchez-Rodríguez (KULeuven, Department Of Microbial And Molecular Systems (M2S)); Qiang Fu (KULeuven, Department Of Microbial And Molecular Systems (M2S)); Kathleen Marchal (KULeuven, Department Of Microbial And Molecular Systems (M2S))

**P37 » Revealing new perspectives on the regulation of gene expression by trans-splicing mechanism in *S. mansoni***

**Presenting Author:** Mainá Bitar (Universidade Federal de Minas Gerais)

**Co-authors:** Marina Mourão (Fiocruz, Centro de Pesquisas René Rachou); Francisco Lobo (EMBRAPA, Bioinformática); Priscila Grynberg (Universidade Federal de Minas Gerais, Bioquímica); Andréa Macedo (Universidade Federal de Minas Gerais, Bioquímica); Carlos Renato Machado (Universidade Federal de Minas Gerais, Bioquímica); Glória Franco (Universidade Federal de Minas Gerais, Bioquímica)

**P38 » The marine metagenomic databases and computational analysis for the environmental resistome exploration**

**Presenting Author:** Michel Marin (Oswaldo Cruz Institute - Fiocruz)



**Co-authors:** Bruno Gabriel Andrade (Oswaldo Cruz Institute - Fiocruz) Erica Fonseca (Oswaldo Cruz Institute - Fiocruz, Laboratory of Molecular Genetics of Microorganisms); Michel Marín (Oswaldo Cruz Institute - Fiocruz, Laboratory of Molecular Genetics of Microorganisms); Ana Carolina Vicente (Oswaldo Cruz Institute - Fiocruz, Laboratory of Molecular Genetics of Microorganisms)

**P39 » MetaABC – an integrated Metagenomics platform for data Adjustment, Binning, and Clustering**

**Presenting Author:** Cheng-Yan Kao (National Taiwan University)

**Co-authors:** Chien-Hao Su (National Taiwan University, Dept. of Computer Science & Information Engineering); Huai-Kuang Tsai (Academia Sinica, Institute of Information Science)

**P40 » Towards a comprehensive search of putative chitinases sequences in environmental metagenomic databases**

**Presenting Author:** Aline Romao-Dumaresq (Fundação Oswaldo Cruz)

**Co-authors:** Rafael Cuadrat (Fundação Oswaldo Cruz, Instituto Oswaldo Cruz); Adriana Fróes (Fundação Oswaldo Cruz, Instituto Oswaldo Cruz); Floriano Silva Jr (Fundação Oswaldo Cruz, Instituto Oswaldo Cruz); Alberto Davila (Fundação Oswaldo Cruz, Instituto Oswaldo Cruz)

**P41 » Analysis of non-canonical introns in the human transcriptome**

**Presenting Author:** Guillermo Parada (Pontificia Universidad Católica de Chile)

**Co-authors:** Roberto Munita (Pontificia Universidad Católica de Chile, Departamento de Biología Celular y Molecular, Facultad de Ciencias Biológicas); Katia Gysling (Pontificia Universidad Católica de Chile, Departamento de Biología Celular y Molecular, Facultad de Ciencias Biológicas)

**P42 » FAIRE-seq data analysis of *Chlamydomonas reinhardtii* under carbon deprivation**

**Presenting Author:** David Urbina (Universidad de los Andes)

**Co-authors:** Diego Riaño-Pachón (Universidad de los Andes, Ciencias Biológicas)

**P43 » Bacterial Symbionts of the cochineal insect *Dactylopius coccus*, A Metagenomic Approach**

**Presenting Author:** Shamayim Tabita Ramirez-Puebla (Center for Genomic Sciences. National Autonomous University of Mexico)

**Co-authors:** Esperanza Martínez-Romero (Center for Genomic Sciences. National Autonomous University of Mexico, Genomic Ecology); Monica Rosenblueth-Laguette (Center for Genomic Sciences. National Autonomous University of Mexico, Genomic Ecology)

**P44 » Comparing the potential for identification of Lactobacillus spp of 16S rRNA variable regions**

**Presenting Author:** Laura Gonzalez (Universidad De Los Andes)

**Co-authors:** Consuelo Vanegas (Universidad De Los Andes, Bogota D.C); Diego Riaño (Universidad De Los Andes, Bogota D.C)

**P45 » Data Mining of Coffee Rust**

**Presenting Author:** David Boter-Rozo (Universidad de Los Andes, Colombia) **Co-authors:** David Boter-Rozo (Universidad de Los Andes, Colombia); William Giraldo (Cenicafé, Fitopatología); Álvaro Gaitán (Cenicafé, Biología); Marco Cristancho (Cenicafé, Fitopatología); Diego Riaño (Universidad de los Andes, Biología); Silvia Restrepo (Universidad de los Andes, Biología)

**P46 » Functional annotation pipeline for high-throughput sequencing microbiomes**

**Presenting Author:** Estefania Mancini (INDEAR)

**Co-authors:** Santiago Revale (INDEAR, Genomics and Bioinformatics); Nicolas Rascovan (INDEAR, Genomics and Bioinformatics); M. Belen Carbonetto (INDEAR, Genomics and Bioinformatics); Martin Vazquez (INDEAR, Genomics and Bioinformatics)

**P47 » Data Merge Annotation Pipeline (DMAP); Utilizing a sequence coordinate based approach to Prokaryotic annotation**

**Presenting Author:** Maximo Rivarola (Instituto de Biotecnología, Instituto Nacional de Tecnología Agropecuaria)

**Co-authors:** Sergio Gonzalez (Instituto Nacional de Tecnología Agropecuaria, Instituto de Biotecnología); Bernarndo Clavijo (Instituto Nacional de Tecnología Agropecuaria, Instituto de Biotecnología); Paula Fernandez (Instituto Nacional de Tecnología Agropecuaria, Instituto de Biotecnología); Maria Martinez (Instituto Nacional de Tecnología Agropecuaria, Instituto de Biotecnología); Maria Ceron Cuchi (Instituto Nacional de Tecnología Agropecuaria, Instituto de Patobiología); Silvio Cravero (Instituto Nacional de Tecnología

Agropecuaria, Instituto de Biotecnología); Joaquin Dopazo (Centro de Investigación Príncipe Felipe, Department of Bioinformatics); Marisa Farber (Instituto Nacional de Tecnología Agropecuaria, Instituto de Biotecnología); Norma Paniego (Instituto Nacional de Tecnología Agropecuaria, Instituto de Biotecnología)

**P48 » Bioinformatics analysis reveals the diverse and highly complex spinal cord regeneration transcriptome on *Xenopus laevis***

**Presenting Author:** Leonardo Almonacid (Pontificia Universidad Católica de Chile)

**Co-authors:** Dasfne Lee-Liu (Universidad de Chile, Center for Aging and Regeneration and Millennium Nucleus in Regenerative Biology); Francisco Melo (Pontificia Universidad Católica de Chile, Departamento de Genética Molecular y Microbiología); Juan Larrain (Pontificia Universidad Católica de Chile, Center for Aging and Regeneration and Millennium Nucleus in Regenerative Biology)

**P49 » SNP discovery with fuzzy inference through computational model for decision making**

**Presenting Author:** Wagner Arbex (Empresa Brasileira de Pesquisa Agropecuária)

**Co-authors:** Marta Martins (Empresa Brasileira de Pesquisa Agropecuária, Centro Nacional de Pesquisa de Gado de Leite); Marcos Vinícius Silva (Empresa Brasileira de Pesquisa Agropecuária, Centro Nacional de Pesquisa de Gado de Leite); Luís Alfredo Carvalho (Universidade Federal do Rio de Janeiro, Instituto Alberto Luiz Coimbra de Pós-Graduação e Pesquisa de Engenharia)

**Topic Session: *Macromolecule Structure/Function Prediction***

**P50 » Modeling proteins using supersecondary structure library and NMR chemical shifts**

**Presenting Author:** Andras Fiser (Albert Einstein College of Medicine)

**Co-authors:** Vilas Menon (Albert Einstein College of Medicine, Systems and Computational Biology); Joseph Dybas (Albert Einstein College of Medicine, Systems and Computational Biology)

**P51 » Using correlation data and network decomposition to obtain sub-class determinants in protein families**

**Presenting Author:** Lucas Bleicher (Universidade Federal de Minas Gerais)

**Co-authors:** Richard Garratt (Universidade de Sao Paulo, Instituto de Fisica de Sao Carlos); Ney Lemke (Universidade Estadual de Sao Paulo, Departamento de Fisica e Biofisica, Botucatu)

**P52 » Bacterial RNAs and host human cells interactions**

**Presenting Author:** Amir Shmaryahu (Fundación Ciencia para la Vida)

**Co-authors:** Pablo DT Valenzuela (Fundación Ciencia para la Vida, Bioinformatics)

**P53 » AFAL: a web service for profiling amino acids surrounding ligands in Protein Data Bank crystallographic data**

**Presenting Author:** Mauricio Arenas (Universidad de Talca)

**Co-authors:** Samuel Ortega (Centro de Bioinformática y Simulación Molecular, Universidad de Talca, Bioinformatica); Danilo Gonzalez-Nilo (Centro de Bioinformática y Simulación Molecular, Universidad de Talca, Bioinformatica); David Holmes (Center for Bioinformatics and Genome Biology, Fundación Ciencia & Vida and Facultad de Ciencias Biologicas, Universidad Andres Bello, Biology); Ehmke Pohl (Biophysical Sciences Institute, Durham University,, Chemistry); Raquel Quatrini (Center for Bioinformatics and Genome Biology, Fundación Ciencia & Vida and Facultad de Ciencias Biologicas, Universidad Andres Bello, Biology)

**P54 » Evolution of linear motifs within the intrinsically disordered and globular domains of the papillomavirus E7 oncoprotein**

**Presenting Author:** Lucia Chemes (Fundación Instituto Leloir IIBBA-CONICET)

**Co-authors:** Juliana Glavina (Protein Physiology Laboratory, Facultad de Ciencias Exactas y Naturales, Universidad de Buenos Aires, Argentina, Departamento de Química Biológica); Julian Faivovich (División Herpetología, Museo Argentino de Ciencias Naturales-CONICET, Buenos Aires, Argentina, Museo Argentino de Ciencias Naturales); Leonardo Alonso (Fundacion Instituto Leloir , Buenos Aires Argentina, IIBBA-CONICET); Cristina Marino-Buslje (Fundacion Instituto Leloir, IIBBA CONICET, Buenos Aires Argentina, Structural Bioinformatics Laboratory); Gonzalo de Prat Gay (Fundacion Instituto Leloir IIBBA CONICET, Buenos Alres Argentina,

Protein Structure-Function and Engineering Laboratory); Sanchez Ignacio (Protein Physiology Laboratory, Facultad de Ciencias Exactas y Naturales, Universidad de Buenos Aires, Argentina, Departamento de Quimica Biologica)

**P55 » Predicting Protein Function from Sequence and Structural Data: a Globin's Family Case**

**Presenting Author:** Juan Bustamante (University of Buenos Aires)

**Co-authors:** Dario Estrin (University of Buenos Aires, INQUIMAE); Marcelo Marti (University of Buenos Aires, INQUIMAE)

**P56 » Cross talk between DNA and Transcription factors**

**Presenting Author:** Matias Machado (Institut Pasteur de Montevideo)

**Co-authors:** Pablo Dans (Institut Pasteur de Montevideo, Biomolecular Simulation Group); Sergio Pantano (Institut Pasteur de Montevideo, Biomolecular Simulation Group)

**P57 » Protein folding using a HP model based on an octahedral core and genetic algorithms**

**Presenting Author:** Darío José (Universidad Industrial de Santander)

**Co-authors:** Darío Delgado Quintero (Universidad Industrial de Santander) Henry Arguello Fuentes (Profesor titular, School of System Engineering); Rodrigo Gonzalo Torres Sáez (Profesor Titular, School of Chemistry)

**P58 » Sulfenamide formation is a conserved mechanism of autoprotection among protein folds**

**Presenting Author:** Lucas A. Defelipe (Universidad de Buenos Aires)

**Co-authors:** Adrián Turjanski (Universidad de Buenos Aires) Esteban Lanzarotti (Universidad de Buenos Aires, Departamento de Química Biológica/INQUIMAE-UBA-CONICET); Marcelo Marti (Universidad de Buenos Aires, Departamento de Química Biológica/INQUIMAE-UBA-CONICET)

**P59 » Full-atom structure-based prediction of transcription factor binding sites**

**Presenting Author:** Tomas Norambuena (Molecular Bioinformatics Laboratory, Millennium Institute on Immunology and Immunotherapy, Pontificia Universidad Católica de Chile)

**Co-authors:** Francisco Melo (Pontificia Universidad Católica de Chile, Molecular Genetics and Microbiology)

**P60 » Annotation System based on Hydrophobic Cluster Analysis**

**Presenting Author:** Dario Delgado (Universidad Industrial de Santander)

**Co-authors:** Cindy Solano (Universidad Industrial de Santander) Cindy Solano (researcher, School of Computer and System Engineering); Narmer Fernando Galeano Vanegas (Development and research, CENICAFE); Alvaro Leon Gaitán (Researcher, CENICAFE); Cristian Blanco Tirado (Associate Professor, School of Chemistry - Universidad Industrial de Santander)

**P61 » Using protein conformational diversity increase protein stability estimation**

**Presenting Author:** Ezequiel Juritz (Universidad Nacional de Quilmes)

**Co-authors:** Gustavo Parisi (Universidad Nacional de Quilmes) Maria Silvina Fornasari (Universidad Nacional de Quilmes, Ciencia y Tecnología); Gustavo Parisi (Universidad Nacional de Quilmes, Ciencia y Tecnología)

**P62 » Structural bioinformatics on an enzyme involved in the synthesis of esters: The case of alcohol acyltransferase from the andean *Vasconcellea pubescens***

**Presenting Author:** Luis Morales-Quintana (Universidad de Talca)

**Co-authors:** Raul Herrera (Universidad de Talca) Carlos Gaete (Universidad de Talca, IBVB); Lida Fuentes (Universidad de Talca, IBVB); Maria Moya-Leon (Universidad de Talca, IBVB)

**P63 » Sea Anemone Neurotoxins: A computational approach**

**Presenting Author:** Samuel David Garcia (Pontificia Universidad Javeriana)

**Co-authors:** George Barreto (Pontificia Universidad Javeriana) Angelica Sabogal (Pontificia Universidad Javeriana, Nutrición y Bioquímica); Janneth Gonzalez (Pontificia Universidad Javeriana, Nutrición y Bioquímica); Ludis Morales (Pontificia Universidad Javeriana, Nutrición y Bioquímica)

**P64 » Dissecting alpha helices in HIV proteins**

**Presenting Author:** Hossein Fallahi (Razi University)

**Co-authors:** Ali Bidmeshkipour (Razi University, Biology)

**P65 » Dissecting relationships between sequence, structure and functions in the ankyrin repeat protein family**

**Presenting Author:** Rodrigo Gonzalo Parra (Universidad de Buenos Aires)

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**Co-authors:** Diego Ferreiro (Universidad de Buenos Aires)  
Diego Ferreiro (Universidad de Buenos Aires, Química Biológica)

**P66 » Sequence dependent elasticity of DNA heteropolymer**

**Presenting Author:** Sudipto Muhuri (Institute of Physics, Bhubaneswar, India)

**P67 » Computational analysis of the dominions CAH and FNIII of the Fosfacan DSD-1-PG and their union with the Tenascin R (TN-R)**

**Presenting Author:** Guillermo Villamil Mora (Pontificia Universidad Javeriana)

**Co-authors:** George Barreto (Pontificia Universidad Javeriana, Biology); Janneth Gonzalez (Pontificia Universidad Javeriana, Biology)

**P68 » VISUALDEP a tool to visualize differences in electrostatic potentials**

**Presenting Author:** Carlos Rios-Vera (Universidad de Concepcion)

**Co-authors:** Jose Martinez-Oyanedel (Universidad de Concepcion) Natalia Jaña-Perez (Universidad de Concepcion, Bioquímica y Biología Molecular); Marta Bunster (Universidad de Concepcion, Bioquímica y Biología Molecular)

**P69 » Prediction of Protein-Metal Binding Sites Using Machine Learning and Combining Diverse Types of Information**

**Presenting Author:** José Reyes (Universidad de Talca)

**Co-authors:** Alfredo Pereira (Universidad de Talca, Centro de Bioinformática y Simulación Molecular); Mauricio Arenas (Universidad de Talca, Centro de Bioinformática y Simulación Molecular)

**P70 » Neural Network Detection of Viral Structural Proteins**

**Presenting Author:** Victor Seguritan (San Diego State University)

**P71 » Potv2, a program that allows to plot the electrostatic potential of the minor groove of DNA.**

**Presenting Author:** Fernando Gutierrez (P. Universidad Católica de Chile)

**Co-authors:** Francisco Melo (P. Universidad Católica de Chile); Tomas Norambuena (P. Universidad Católica de Chile)

**P72 » The salmonid selenotranscriptome: in silico and in vivo characterization**

**Presenting Author:** Francisco J. Altimiras (Universidad de Chile)

**Co-authors:** Verónica Cambiazo (Universidad de Chile, Laboratorio de Bioinformática y Expresión Génica, INTA.); Rodrigo Pulgar (Universidad de Chile, Laboratorio de Bioinformática y Expresión Génica, INTA)

**P73 » Bioinformatic and Biophysical Characterization of Fur (Ferric Uptake Regulator) from an Extreme Acidophile Thriving in an Iron Rich Environment**

**Presenting Author:** Mauricio Arenas (Universidad de Talca/ Universidad Andrés Bello)

**Co-authors:** ehmke pohl (Biophysical Sciences Institute, Durham University, Chemistry); Narcizo Marquez (Laboratório Nacional de Luz Síncrotron, XAFS); David S Holmes (Center for Bioinformatics and Genome Biology, Fundación Ciencia & Vida and Facultad de Ciencias Biológicas, Universidad Andres Bello, biología); Raquel Quatrini (Center for Bioinformatics and Genome Biology, Fundación Ciencia & Vida and Facultad de Ciencias Biológicas, Universidad Andres Bello, biología)

**P74 » Comparative Modeling of B-DNA**

**Presenting Author:** Ignacio Ibarra (P. Universidad Católica de Chile)

**Co-authors:** Francisco Melo (P. Universidad Católica de Chile); M.S. Madhusudhan (Bioinformatics Institute, Biomolecular Modeling and Design Division)

**P75 » FragProt, a database of short protein fragments clustered by structural similarity**

**Presenting Author:** Felipe Rodríguez (P. Universidad Católica de Chile)

**Co-authors:** Francisco Melo (P. Universidad Católica de Chile) Alex Slater (P. Universidad Católica de Chile, Molecular Genetics and Microbiology)

**P76 » Implementation of a new methodology for the 2D representation and visualization of 3D interfaces in protein-DNA complexes.**

**Presenting Author:** Jaime Riquelme (P. Universidad Católica de Chile)

**Co-authors:** Francisco Melo (P. Universidad Católica de Chile)



**P77 » Using protein conformational diversity increase protein stability estimation**

**Presenting Author:** Ezequiel Juritz (Universidad Nacional de Quilmes)

**Co-authors:** Silvina Fornasari (Universidad Nacional de Quilmes, Structural Bioinformatics Group); Gustavo Parisi (Universidad Nacional de Quilmes, Structural Bioinformatics Group)

**P78 » On the conformational diversity of proteins and its relationship with biological properties**

**Presenting Author:** Alexander Monzon (National University of Quilmes)

**Co-authors:** Ezequiel Juritz (National University of Quilmes, Departamento de Ciencia y Tecnologia); Gustavo Parisi (National University of Quilmes, Departamento de Ciencia y Tecnologia)

**P79 » BeEP and the BeEP Server: using evolutionary information to help in protein structure modeling and characterization**

**Presenting Author:** Nicolás Palopoli (Universidad Nacional de Quilmes)

**Co-authors:** Gustavo Parisi (Universidad Nacional de Quilmes, Departamento de Ciencia y Tecnología)

**P80 » Modular anatomy of the Ribokinase family fold**

**Presenting Author:** Pablo Villalobos (Universidad de Chile)

**Co-authors:** Jorge Babul (Universidad de Chile, Bioquímica y Biología Molecular); Ricardo Cabrera (Universidad de Chile, Bioquímica y Biología Molecular); Mauricio Baez (Universidad de Chile, Bioquímica y Biología Molecular)

**P81 » WebRASP: A novel web tool to assess and explore RNA structures based on the Ribonucleic Acids Statistical Potential**

**Presenting Author:** Jorge Cares (P. Universidad Católica de Chile)

**Co-authors:** Tomas Norambuena (Pontificia Universidad Católica de Chile, Molecular Genetics and Microbiology); Francisco Melo (Pontificia Universidad Católica de Chile, Molecular Genetics and Microbiology)

**P82 » Clustering of Proteins based on their Three-dimensional Shape using Maximum Common Subgraph**

**Presenting Author:** Cristian López (San Pablo Catholic University)

**Co-authors:** July Banda-Tapia (San Pablo Catholic University)

**P83 » Curvature and Flexibility as Promoter Regions Classifiers in Gram-Negative Bacteria**

**Presenting Author:** Ivaine Sauthier Sartor (University of Caxias do Sul)

**Co-authors:** Tahila Andrighetti (University of Caxias do Sul, Biotechnology Institute); Günther Gerhardt (University of Caxias do Sul, Biotechnology Institute); Sergio Echeverrigaray (University of Caxias do Sul, Biotechnology Institute); Scheila de Avila e Silva (University of Caxias do Sul, Biotechnology Institute)

**Topic Session: Computer Aided Drug Design and Docking/ Molecular Dynamics Simulations**

**P84 » Molecular ordering of dotriacontane supported on silica surfaces**

**Presenting Author:** Sebastián Gutiérrez-Maldonado (Computational Biology Lab (DLab), Centro de Modelamiento Matemático (CMM), Facultad de Ciencias Físicas y Matemáticas (FCFM), Universidad de Chile, Santiago, Chile)

**Co-authors:** Raul Araya-Secchi (Computational Biology Lab (DLab), Centro de Modelamiento Matemático (CMM), Facultad de Ciencias Físicas y Matemáticas (FCFM), Universidad de Chile, Santiago, Chile) Maria Jose Retamal (Laboratorio de Superficies (SurfLab), Facultad de Física, Pontificia Universidad Católica de Chile, Santiago, Chile) Ulrich Volkmann (Laboratorio de Superficies (SurfLab), Facultad de Física, Pontificia Universidad Católica de Chile, Santiago, Chile) Tomas Perez-Acle (Computational Biology Lab (DLab), Centro de Modelamiento Matemático (CMM), Facultad de Ciencias Físicas y Matemáticas (FCFM), Universidad de Chile, Santiago, Chile)

**P85 » Study of the differences in activity between structurally similar protein kinase inhibitors by using docking, molecular dynamics, and fragment-based de novo design**

**Presenting Author:** Julio Caballero (Universidad de Talca)

**P86 » Docking Studies of a New Series of Analgesic and Anti-inflammatory Compounds (NSAIDs) with Cyclooxygenase**

**Presenting Author:** Lucas Saraiva (Federal University of Minas Gerais)

**Co-authors:** Ihosvany Camps (Federal University of Alfenas, Department of Exact Science); Raquel Melo-Minardi (Federal University of Minas Gerais, Department of Computer Science); Marcia Veloso (Federal University of Alfenas, Faculty of Pharmaceutical Science); Rodrigo Sailva (Federal University of São Carlos, Department of Chemistry)

**P87 » How does a specific drug bind to an ion channel?**

**Presenting Author:** Wendy Gonzalez (Universidad de Talca)

**P88 » Efficient selection of flexible receptor snapshots applied in molecular docking simulations**

**Presenting Author:** Karina Machado (Universidade Federal do Rio Grande)

**Co-authors:** Ana Winck (Pontifícia Universidade Católica do Rio Grande do Sul, GPIN-PPGCC-FACIN); Duncan Ruiz (Pontifícia Universidade Católica do Rio Grande do Sul, GPIN-PPGCC-FACIN); Osmar Norberto de Souza (Pontifícia Universidade Católica do Rio Grande do Sul, LABIO-PPGCC-FACIN)

**P89 » Semi-flexible Protein-Ligand Docking Using a Controlled Genetic Algorithm**

**Presenting Author:** Paola Rondon-Villarreal (PhD Student-Universidad Industrial de Santander)

**Co-authors:** Rodrigo Torres (Professor - Universidad Industrial de Santander, School of Chemistry)

**P90 » Structural databases: A way of improving knowledge-based docking**

**Presenting Author:** Esteban Lanzarotti (Universidad de Buenos Aires)

**Co-authors:** Adrián Turjanski (Universidad de Buenos Aires) Lucas A. Defelipe (Universidad de Buenos Aires, Departamento de Química Biológica/INQUIMAE-UBA-CONICET); Marcelo Marti (Universidad de Buenos Aires, Departamento de Química Biológica/INQUIMAE-UBA-CONICET)

**P91 » Molecular Docking Simulation of RILUZOLE complex with Structural Model of Human alpha subunit of voltage-gated sodium channel Nav 1.6.**

**Presenting Author:** Omar Sierra Bello (Pontificia Universidad Javeriana)

**Co-authors:** Janeth Gonzalez (Pontificia Universidad Javeriana, Nutrition and Biochemistry); George Barreto (Pontificia Universidad Javeriana, Nutrition and Biochemistry)

**P92 » Molecular Modeling Interactions among Sea Anemone Toxins and Kv1 Channel**

**Presenting Author:** Angélica Sabogal (Pontificia Universidad Javeriana)

**P93 » Topological constraints and challenges imposed by knots in proteins**

**Presenting Author:** Cesar Ramirez (University of Chile)

**Co-authors:** Jeffrey K Noel (University of California San Diego, Center for Theoretical Biological Physics); Mauricio Baez (University of Chile, Department of Biology)

**P94 » Molecular basis of the mechanism of thiol oxidation by hydrogen peroxide in aqueous solution: challenging the SN2 paradigm**

**Presenting Author:** Ari Zeida (Facultad de Ciencias Exactas y Naturales, Universidad de Buenos Aires)

**Co-authors:** Ryan Babbush (Harvard University, Department of Chemistry ); Mariano C. González Lebrero (Facultad de Farmacia y Bioquímica, Universidad de Buenos Aires , IQUIFIB-Dpto. Química Biológica ); Madia Trujillo (Facultad de Medicina, Universidad de la República , Departamento de Bioquímica and Center for Free Radical and Biomedical Research ); Rafael Radi (Facultad de Medicina, Universidad de la República , Departamento de Bioquímica and Center for Free Radical and Biomedical Research ); Dario Estrin (Facultad de Ciencias Exactas y Naturales, Universidad de Buenos Aires , Departamento de Química Inorgánica, Analítica y Química-Física and INQUIMAE-CONICET)

**P95 » Binding Studies and Quantitative Structure–Activity Relationship of 3-Amino-1H-Indazoles as Inhibitors of GSK3beta**

**Presenting Author:** Julio Caballero (Universidad de Talca)

**Co-authors:** William Tiznado (Universidad Andres Bello, Facultad de Ecología y Recursos Naturales)

**P96 » Molecular Dynamics Simulations of Cx26-Wt and deafness related mutants M34A, A40G and V37I**

**Presenting Author:** Raul Araya-Secchi (Computational Biology Lab, Center for Mathematical Modeling, Facultad de Ciencias Físicas y Matemáticas, Universidad de Chile)

**Co-authors:** Carlos Lagos (Departamento de Farmacia, Facultad de Química, P. Universidad Católica de Chile); Fernando Abarca (Computational Biology Lab, Center for Mathematical Modeling, Facultad de Ciencias Físicas y Matemáticas, Universidad de Chile); Agustin Martinez

(Centro Interdisciplinario de Neurociencias de Valparaíso); Tomas Perez-Acle (Computational Biology Lab, Center for Mathematical Modeling, Facultad de Ciencias Físicas y Matemáticas, Universidad de Chile)

**P97 » Multi template homology modeling improves the model for type II-NADH: menaquinone oxidoreductase from *Mycobacterium tuberculosis*: validation by antagonist docking**

**Presenting Author:** Nitin Chitranshi (Rameshwaram Institute of Technology & Management)

**Co-authors:** Shipra Gupta (Biotech Park, Bioinformatics); Pushendra Tripathi (Rameshwaram Institute of Technology & Management, Pharmacy)

**P98 » De novo modeling and replica exchange molecular dynamic simulation of lipoprotein Licanantase of strain *Licanantay*: *Acidithiobacillus thiooxidans* DSM 17318**

**Presenting Author:** Fernando Abarca (Universidad de Chile)

**Co-authors:** Raul Araya-Secchi (Computational Biology Lab, Center for Mathematical Modeling (CMM), Facultad de Ciencias Físicas y Matemáticas (FCFM), Universidad de Chile, Santiago, Chile.) Pilar Parada (BioSigma 'S.A.', Loteo Los Libertadores, Lote 106, Colina, Chile.) Tomas Perez-Acle (Computational Biology Lab, Center for Mathematical Modeling (CMM), Facultad de Ciencias Físicas y Matemáticas (FCFM), Universidad de Chile, Santiago, Chile)

**P99 » Study and molecular characterization of the hypothetical representative of a third subfamily of aquaporins, AqpF from *Acidithiobacillus ferrooxidans***

**Presenting Author:** Sebastián Flores J (Centro de Modelamiento Matemático. Universidad de Chile.)

**Co-authors:** Raúl Araya-Secchi (Centro de Modelamiento Matemático. Universidad de Chile, Computational Biology Lab.); Tomás Perez-Acle (Centro de Modelamiento Matemático. Universidad de Chile, Computational Biology Lab); David Holmes (Fundación Ciencia para la Vida , Center for Bioinformatics and Genome Biology (CBBG))

**P100 » Theoretical study of the interaction between Zidovudine (and novel derivatives) and human serum albumin**

**Presenting Author:** Ileana Tossolini (National University of Entre Ríos)

**Co-authors:** María Cecilia Gómez (National University of Entre Ríos, Faculty of Engineering); Mario Alfredo Quevedo (National University of Córdoba, Department of Pharmacy)

**P101 » 3D-QSAR and molecular docking studies of 2-Pyrimidinecarbonitrile derivatives as inhibitors against falcipain**

**Presenting Author:** Angamba Potshangbam (University Of Hyderabad)

**P102 » Discovering of small molecules designed to prevent ethanol-induced potentiation of GlyR by G-beta/gamma**

**Presenting Author:** Fabián Cerda (University of Concepción)  
**Co-authors:** Verónica Jimenez (University de Concepción, Group of computational Chemistry); José Guzmán (University of Concepcion, Departament of Physiology)

**P103 » Docking study of LipL32-human plasminogen complex: insights contributing to knowledge of the host invasion by pathogenic leptospire**

**Presenting Author:** Leidy Viviana Barreto (Pontificia Universidad Javeriana)

**Co-authors:** Janneth González (Pontificia Universidad Javeriana) George Barreto (Pontificia Universidad Javeriana, Nutrition and Biochemistry); Ludis Morales (Pontificia Universidad Javeriana, Nutrition and Biochemistry)

**P104 » Non-equilibrium molecular dynamics: An approach to understand conductance in Shaker P475D potassium channel**

**Presenting Author:** Romina V. Sepúlveda (Universidad Andres Bello)

**Co-authors:** Romina Sepúlveda (Universidad Andres Bello) David Naranjo (CINV, Universidad de Valparaiso, CINV); Danilo González-Nilo (CINV - Universidad Andrés Bello, CBIB)

**P105 » Studying binding free energies of protein kinase inhibitors combining molecular dynamic simulations and MM-GBSA methods**

**Presenting Author:** Camila Muñoz Gutierrez (Universidad de Talca)

**Co-authors:** Jans Alzate-Morales (Universidad de Talca) Julio Caballero (Universidad de Talca, Escuela de Ingeniería en Bioinformática, Centro de Bioinformática y Simulación Molecular)

**P106 » Study of the Binding Strength and Selectivity of Inhibitors by CDK2/CDK4 Protein Systems: QM/MM Interaction Energy as a Descriptor of Biological Activity**

**Presenting Author:** Ingrid Araya (Universidad de Talca)

**Co-authors:** Jans Alzate-Morales (Universidad de Talca)

**P107 » Computational study of CDK2-ligand interactions: Search of new energy descriptors from MM-GBSA calculations**

**Presenting Author:** Camila Navas (University of Talca)

**Co-authors:** Jans Alzate (University of Talca)

**P108 » Molecular modelling, docking simulations and substrate specificity of the protein alcohol acyltransferase from *Vasconcellea pubescens***

**Presenting Author:** Luis Morales-Quintana (Universidad de Talca)

**Co-authors:** Maria Alejandra Moya-León (Universidad de Talca, Instituto de Biología Vegetal y Biotecnología); Raúl Herrera (Universidad de Talca, Instituto de Biología Vegetal y Biotecnología)

**P109 » Structural bases of P2X4r and P2X2r allosteric modulation**

**Presenting Author:** Camilo Navarrete (CARE - Pontificia Universidad Católica de Chile)

**Co-authors:** Carlos F Lagos (Pontificia Universidad Católica de Chile, Farmacia); Natali Garcia (CARE-Pontificia Universidad Católica de Chile, Fisiología); Juan Pablo Huidobro-Toro (CARE-Pontificia Universidad Católica de Chile, Fisiología); Alex Slater (Molecular Bioinformatics Laboratory, Millennium Institute on Immunology and Immunotherapy Pontificia Universidad Católica de Chile, Genética Molecular y Microbiología); Francisco Melo (Molecular Bioinformatics Laboratory, Millennium Institute on Immunology and Immunotherapy Pontificia Universidad Católica de Chile, Genética Molecular y Microbiología); Paulina Bull (Pontificia Universidad Católica de Chile, Genética Molecular y Microbiología)

**Topic Session: *Biomedicine and Immunoinformatics***

**P110 » Analyzing Clinical data and Genetic data for the classification of Alzheimer's Disease using Bayesian networks**

**Presenting Author:** Yomaira Guzmán Paredes (Universidad Nacional de Colombia)

**Co-authors:** Luis Fernando Niño Vásquez (Universidad Nacional de Colombia, Bogota D.C.); Humberto Arboleda Granados (Universidad Nacional de Colombia, Bogotá D.C.); Ludwig Segura Bermúdez (Universidad Nacional de Colombia, Bogotá D.C.)

**P111 » Bioinformatics software development in Central America: A growth alternative in education and computer technology on the molecular modeling of protein and DNA virtual structures field.**

**Presenting Author:** Allan Orozco (University of Costa Rica)

**P112 » Systematic prediction of ligand-receptor pair across the immunoglobulin superfamily using a novel sequence homology measure**

**Presenting Author:** Eng Hui Yap (Albert Einstein College of Medicine)

**Co-authors:** Andras Fiser (Albert Einstein College of Medicine, Systems and Computational Biology); Tyler Rosche (Albert Einstein College of Medicine, Systems and Computational Biology)

**P113 » Modeling Cancer Metastasis by Using GGH Model in CompuCell3D**

**Presenting Author:** Ismael Fortuna (Universidade Federal do Rio Grande do Sul)

**Co-authors:** Rita Maria Cunha De Almeida (Universidade Federal Do Rio Grande Do Sul, Instituto De Física); Gilberto Lima Thomas (Universidade Federal Do Rio Grande Do Sul, Instituto De Física); Fares Zeidán-Chuliá (Universidade Federal Do Rio Grande Do Sul, Instituto De Ciências Básicas Da Saúde, Departamento De Bioquímica); José Cláudio Fonseca Moreira (Universidade Federal Do Rio Grande Do Sul, Instituto De Ciências Básicas Da Saúde, Departamento De Bioquímica)

**P114 » Developing new drugs and vaccines for schistosomiasis**

**Presenting Author:** Guilherme Oliveira (Oswaldo Cruz Foundation)

**Co-authors:** Adhemar Zerlotini (Fiocruz, CEBio); Larissa Silva (Fiocruz, Genomics and Computational Biology Group); Luiza Andrade (Fiocruz, Genomics and Computational Biology Group); Marina Mourão (Fiocruz, Genomics and Computational Biology Group); Fernanda Ludolf (Fiocruz, Genomics and Computational Biology Group); Rômulo Morais (Fiocruz, Genomics and Computational Biology Group); Lívia Avelar (Fiocruz, Genomics and Computational Biology Group); Eric Aguiar (Fiocruz, CEBio); Rosângela Hickson (Inforium, Computer Science); Rosiane Pereira (Fiocruz, Genomics and Computational Biology Group); Raymond Pierce (Pasteur Institute, Lille, Centre d'Infection et d'Immunité de Lille); Franco Falcone (University of Nottingham, School



of Pharmacy); Marina Marcet-Houben (Center for Genomic Regulation, Bioinformatics and Genomics Programme); Huayong Xu (Shanghai Center for Bioinformation Technology, Bioinformatics); Fudong Yu (Shanghai Center for Bioinformation Technology, Bioinformatics); Robin Gasser (University of Melbourne, Parasitology); Neil Young (University of Melbourne, Parasitology); Jessica Kissinger (University of Georgia, Genetics); Toni Gabaldon (Center for Genomic Regulation, Bioinformatics and Genomics Programme); Roney Coimbra (Fiocruz, CEBio); Laila Nahum (Fiocruz, Genomics and Computational Biology Group)

**P115 » Analysis of DNA Sequences of HIV Virus Using Information Theory**

**Presenting Author:** Tahila Andrighetti (Universidade de Caxias do Sul)

**P116 » Using feature extraction to find biomarkers in Parkinson's disease**

**Presenting Author:** Elinor Velasquez (University of California, Santa Cruz)

**P117 » Characterizing the binding motifs of 11 common human HLA-DP and HLA-DQ molecules using NNAlign**

**Presenting Author:** Massimo Andreatta (Technical University of Denmark)

**Co-authors:** Morten Nielsen (Technical University of Denmark, Center for Biological Sequence Analysis)

**P118 » Immune activation in Fragile X Mental Retardation 1 (FMR1) premutation carriers : Levels of IL-10 as a prognostic marker for Fragile X-associated Tremor/Ataxia Syndrome (FXTAS) progression**

**Presenting Author:** Diana Marek (University of Lausanne & Swiss Institute of Bioinformatics)

**Co-authors:** Stephanie Papin (University of Lausanne, Medical Genetics Department); Kim Ellefsen (Lausanne University Hospital, Division of Immunology and Allergy); Julien Niederhauser (Lausanne University Hospital, Department of Clinical Neuroscience); Nathalie Isidor (Lausanne University Hospital, Medical Genetics Service); Adriana Ransijn (University of Lausanne, Medical Genetics Department); Lucienne Poupon (Lausanne University Hospital, Division of Immunology and Allergy); Francois Spertini (Lausanne University Hospital, Division of Immunology and Allergy); Giuseppe Pantaleo (Lausanne University Hospital, Division of Immunology and Allergy); Sven Bergmann (University

of Lausanne & Swiss Institute of Bioinformatics, Medical Genetics Department); Jacques S. Beckmann (University of Lausanne & Lausanne University Hospital, Medical Genetics Department & Service); Sebastien Jacquemont (Lausanne University Hospital, Medical Genetics Service); Goranka Tanackovic (University of Lausanne, Medical Genetics Department)

**P119 » Hierarchical clustering of pMHC complexes based on the electrostatic potential of the TCR-interacting surface**

**Presenting Author:** Dinler Amaral Antunes (Federal University of Rio Grande do Sul)

**Co-authors:** Danieli Forgiarini Figueiredo (Federal University of Rio Grande do Sul, Genetics); Mauricio Menegatti Rigo (Federal University of Rio Grande do Sul, Genetics); Jader Peres da Silva (Federal University of Rio Grande do Sul, Genetics); Jose Bogo Chies (Federal University of Rio Grande do Sul, Genetics); Marialva Sinigaglia (Federal University of Rio Grande do Sul, Genetics); Gustavo Fioravanti Vieira (Federal University of Rio Grande do Sul, Genetics)

**P120 » Analysis of interaction residues between HLA-A\*02:01 cleft and epitopes**

**Presenting Author:** Mauricio Menegatti Rigo (Federal University of Rio Grande do Sul)

**Co-authors:** Mauricio Menegatti Rigo (Federal University of Rio Grande do Sul); Dinler Amaral Antunes (Federal University of Rio Grande do Sul, Genetics); Roberto Minozzo (Federal University of Rio Grande do Sul, Genetics); Jader Peres da Silva (Federal University of Rio Grande do Sul, Genetics); Danieli Forgiarini Figueiredo (Federal University of Rio Grande do Sul, Genetics); Jose Artur Bogo Chies (Federal University of Rio Grande do Sul, Genetics); Marialva Sinigaglia (Federal University of Rio Grande do Sul, Genetics); Gustavo Fioravanti Vieira (Federal University of Rio Grande do Sul, Genetics)

**P121 » Protein-disease association significance from candidate ranking lists**

**Presenting Author:** Ariel Berenstein (University of Buenos Aires)

**Co-authors:** Irene Ibanez (University Buenos Aires, Physics); Ariel Chernomoretz (Fundacion Instituto Leloir, Integrative Systems Biology)

**P122 » Gene expression profiling of human epithelial ovarian cancer**

**Presenting Author:** Gladys Ramos (Universidad de Chile)

**Co-authors:** Ulises Urzúa (Universidad de Chile) Sandra Ampuero (Universidad de Chile, Programa de Virología); Nelson Peña (Universidad de Chile, Laboratorio de genómica aplicada); Ulises Urzua (Universidad de Chile, Laboratorio de genómica aplicada); Carmen Romero (Universidad de Chile, Laboratorio de endocrinología y reproducción)

**P123 » Immunohistochemistry quantification using support vector machine**

**Presenting Author:** Raquel Pezoa (Universidad Tecnica Federico Santa Maria)

**Co-authors:** Rodrigo Rojas-Moraleda (Universidad Tecnica Federico Santa Maria, Informatics)

**P124 » Integration of mRNA and miR profiles identified restricted and unique patterns in Breast & Colon cancer cell lines**

**Presenting Author:** Benjamin Garcia (Pontificia Universidad Catolica de Chile)

**Co-authors:** Alejandro Corvalan (Pontificia Universidad Catolica de Chile); Alejandra Sandoval (Pontificia Universidad Catolica de Chile, Hematology and Oncology); Rodrigo Droguett (Pontificia Universidad Catolica de Chile, Hematology and Oncology); Jose Diaz (Pontificia Universidad Catolica de Chile, Hematology and Oncology)

**P125 » In silico isolation of natural products: obtaining 1H NMR spectra of pure compounds from spectra of mixtures that contain them**

**Presenting Author:** Ivana Ayelen Ramallo (Universidad Nacional de Rosario)

**Co-authors:** Ivana Ramallo (Universidad Nacional de Rosario); Pablo Gatti (Facultad de Ciencias Exactas, Ingeniería y Agrimensura, CIFASIS); Ricardo Furlan (Facultad de Ciencias Bioquímicas y Farmacéuticas, Farmacognosia); Elizabeth Tapia (Facultad de Ciencias Exactas, Ingeniería y Agrimensura, CIFASIS); Gabriela Ibañez (Facultad de Ciencias Bioquímicas y Farmacéuticas, IQUIR); Alejandro Olivieri (Facultad de Ciencias Bioquímicas y Farmacéuticas, IQUIR)

**P126 » Comparative Identification of Novel genes from Non Coding Regions of Plasmodium**

**Presenting Author:** Anandakumar Shanmugam (Bharathiar University)

**P127 » Unveiling combinatorial regulation through the combination of ChIP information and in silico cis-regulatory module detection**

**Presenting Author:** Kathleen Marchal (Ghent University)

**Co-authors:** Hong Sun (K.U.Leuven, Microbial and Molecular Systems); Tias Guns (K.U.Leuven, Computer Science); Ana Carolina Fierro (K.U.Leuven, Computer Science); Lieven Thorrez (K.U.Leuven, Interdepartmental Stem Cell Institute); Siegfried Nijssen (K.U.Leuven, Computer science)

**P128 » Integrative approaches for mode of action determination**

**Presenting Author:** Ana Carolina Fierro Gutierrez (K.U. Leuven)

**Co-authors:** Riet De Smet (Ghent University, Plant Biotechnology and Bioinformatics); Yan Wu (Ghent University, Microbial and Molecular Systems); Lore Cloots (Ghent University, Microbial and Molecular Systems); Dries De Maeyer (Ghent University, Microbial and Molecular Systems); Peyman Zarrineh (Ghent University, Microbial and Molecular Systems); Qiang Fu (Ghent University, Microbial and Molecular Systems); Kristof Engelen (Ghent University, Microbial and Molecular Systems)

**P129 » An integrative methodology for the classification of genes into pathways using a novel text mining approach**

**Presenting Author:** Julieta Dussaut (Universidad Nacional del Sur)

**Co-authors:** Ignacio Ponzoni (Universidad Nacional del Sur) Rocío Cecchini; (Universidad Nacional del Sur, Laboratory of Research and Development in Scientific Computing (LIDeCC)); Ignacio Ponzoni (Universidad Nacional del Sur, Laboratory of Research and Development in Scientific Computing (LIDeCC)); Ana Maguitman (Universidad Nacional del Sur, Artificial Intelligence Research and Development Laboratory (LIDIA))

**P130 » Network complexity evolves as an efficient mechanism for the acquisition of robustness in gene regulatory networks**

**Presenting Author:** Mario Pujato (Albert Einstein College of Medicine)

**Co-authors:** Thomas MacCarthy (Albert Einstein College of Medicine, Systems and Computational Biology); Andras Fiser (Albert Einstein College of Medicine, Systems and Computational Biology); Aviv Bergman (Albert Einstein College of Medicine, Systems and Computational Biology)

**P131 » LitProf – Gene Classifier: A text-mining gene function predictor for prokaryotes**

**Presenting Author:** Roney Coimbra (FIOCRUZ-Minas)

**Co-authors:** Raul Torrieri (FIOCRUZ-Minas, Center for Excellence in Bioinformatics); Francislon Oliveira (FIOCRUZ-Minas, Center for Excellence in Bioinformatics); Guilherme Oliveira (FIOCRUZ-Minas, Center for Excellence in Bioinformatics)

**P132 » Strategy for the Detection of Functional Clusters of Genes using Data Mining Techniques**

**Presenting Author:** Liliana Olarte (Universidad Nacional de Colombia)

**Co-authors:** Luis Niño (Universidad Nacional de Colombia, Systems and Industrial Engineering); Liliana López (Universidad Nacional de Colombia, Statistics Department)

**P133 » Discriminative local subspaces in gene expression data for effective gene function prediction**

**Presenting Author:** Tomas Puelma (Pontificia Universidad Católica de Chile)

**Co-authors:** Rodrigo Gutierrez (Pontificia Universidad Católica de Chile); Alvaro Soto (Pontificia Universidad Católica de Chile, Computer Science); Rodrigo Gutierrez (Pontificia Universidad Católica de Chile, Molecular Genetics and Microbiology)

**P134 » Gene Functional Annotation beyond Enrichment Analysis: moving from gene lists to functional metagroups and gene networks**

**Presenting Author:** Celia Fontanillo (Centro de Investigacion del Cancer)

**Co-authors:** Sara Aibar (Centro de Investigacion del Cancer, Bioinformatics and Functional Genomics Group); Javier De Las Rivas (Centro de Investigacion del Cancer, Bioinformatics and Functional Genomics Group)

**P135 » Computational Flux Balance Analysis (FBA) of new representative objective functions using a multiple compartmental objective approach and its application to *Saccharomyces cerevisiae* biological behavior**

**Presenting Author:** Carlos García (Universidad Industrial de Santander)

**Co-authors:** Rodrigo Torres (Universidad Industrial de Santander); Carlos García (Universidad Industrial de Santander, Chemical Engineering); César Vargas (Universidad Industrial de Santander, System Engineering); Henry Argüello (Universidad Industrial de Santander, System Engineering)

**P136 » The just-in-time expression of yeast ribosomal proteins**

**Presenting Author:** Andrzej Kudlicki (University of Texas Medical Branch)

**Co-authors:** Xueling Li (University of Texas Medical Branch, Institute of Translational Science); Gang Chen (Central South University, Computer Science)

**P137 » Deciphering human protein interactome using structural complexes**

**Presenting Author:** Anna Panchenko (National Institutes of Health)

**Co-authors:** Manoj Tyagi (National Institutes of Health, NCBI); Kosuke Hashimoto (RIKEN, RIKEN); Benjamin Shoemaker (NIH, NCBI); Stefan Wuchty (NIH, NCBI)

**P138 » SNPpower, an integrative platform for the analysis and visualization of human disease-associated short mutations, genes, and protein interactions**

**Presenting Author:** Cheng-Yan Kao (National Taiwan University)

**Co-authors:** Theresa Tsao (Department of Computer Science and Information Engineering & Graduate Institute of Biomedical Electronics and Bioinformatics, National Taiwan University); Sheng-An Lee (Department of Information Management, Kainan University)

**P139 » A search for probiotic yeast: comparison of transcriptional profile in *S. cerevisiae* strain W303 and *S. boulardii* using microarray**

**Presenting Author:** Priscila Grynberg (Universidade Federal de Minas Gerais)

**Co-authors:** Leonardo Dias (Universidade Federal de Minas Gerais, Departamento de Bioquímica e Imunologia); Mariana Boroni (Universidade Federal de Minas Gerais, Departamento

de Bioquímica e Imunologia); Daiane de Laat (Instituto Agronômico de Campinas, Divisão de Biologia Fitotécnica); Ieso Castro (Universidade Federal de Ouro Preto, Núcleo de Pesquisas em Ciências Biológicas - NUPEB); Gloria Franco (Universidade Federal de Minas Gerais, Departamento de Bioquímica e Imunologia)

**P140 » A Rule-based Model for a Stochastic Simulation of a Zombie Outbreak**

**Presenting Author:** Felipe Nuñez (Universidad de Chile)

**Co-authors:** Cesar Ravello (Universidad de Chile, Computational Biology Lab. Center for Mathematical Modeling. Facultad de Ciencias Físicas y Matemáticas.); Hector Urbina (Universidad de Chile, Computational Biology Lab. Center for Mathematical Modeling. Facultad de Ciencias Físicas y Matemáticas.); Tomas Perez-Acle (Universidad de Chile, Computational Biology Lab. Center for Mathematical Modeling. Facultad de Ciencias Físicas y Matemáticas.)

**P141 » Another Tool for Genomic Comprehension (ATGC): an ontology driven database and web interface applied to Sunflower Microarray Project**

**Presenting Author:** Paula Fernandez (Instituto Nacional de Tecnología Agropecuaria)

**Co-authors:** Sergio Gonzalez (Instituto Nacional de Tecnología Agropecuaria, Instituto de Biotecnología); Maximo Rivarola (Instituto Nacional de Tecnología Agropecuaria, Instituto de Biotecnología); Ruth Heinz (Instituto Nacional de Tecnología Agropecuaria, Instituto de Biotecnología); Marisa Farber (Instituto Nacional de Tecnología Agropecuaria, Instituto de Biotecnología); Norma Paniago (Instituto Nacional de Tecnología Agropecuaria, Instituto de Biotecnología); Bernardo Clavijo (Instituto Nacional de Tecnología Agropecuaria, Instituto de Biotecnología)

**P142 » Computational Flux Balance Analysis (FBA) of new representative objective functions using a multiple compartmental objective approach and its application to *Saccharomyces cerevisiae* biological behavior**

**Presenting Author:** Carlos García Sánchez (Universidad Industrial de Santander)

**Co-authors:** César Augusto Vargas García (Universidad Industrial de Santander, Santander); Henry Argüello Fuentes (Universidad Industrial de Santander, Santander); Rodrigo Gonzalo Torres Sáez (Universidad Industrial de Santander, Santander)

**P143 » Comparing Stochastic Models of Gene Expression**

**Presenting Author:** Pablo Gutierrez (Centro Regional de Estudios Genómicos - Universidad Nacional de La Plata)

**Co-authors:** Luis Diambra (Centro Regional de Estudios Genómicos - Universidad Nacional de La Plata, Laboratorio de Biología de Sistemas)

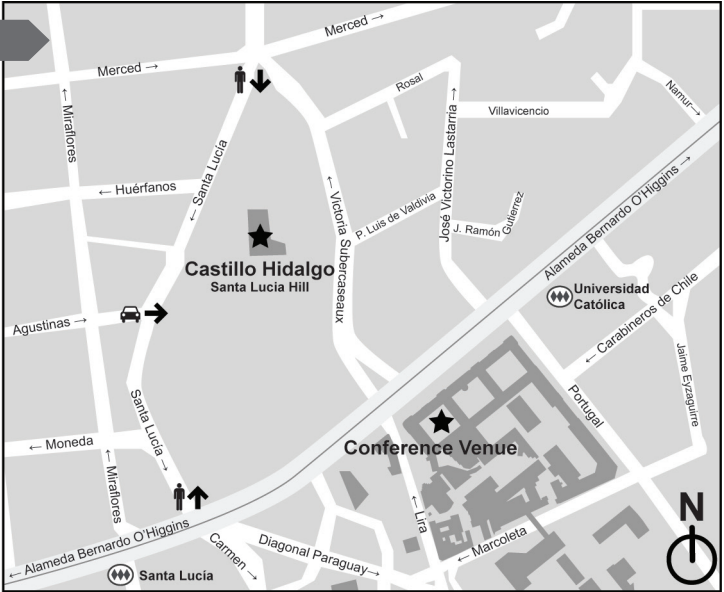
**P144 » Modeling the emergence of circadian rhythms in a clock network**

**Presenting Author:** Luis Diambra (Universidad Nacional de La Plata)

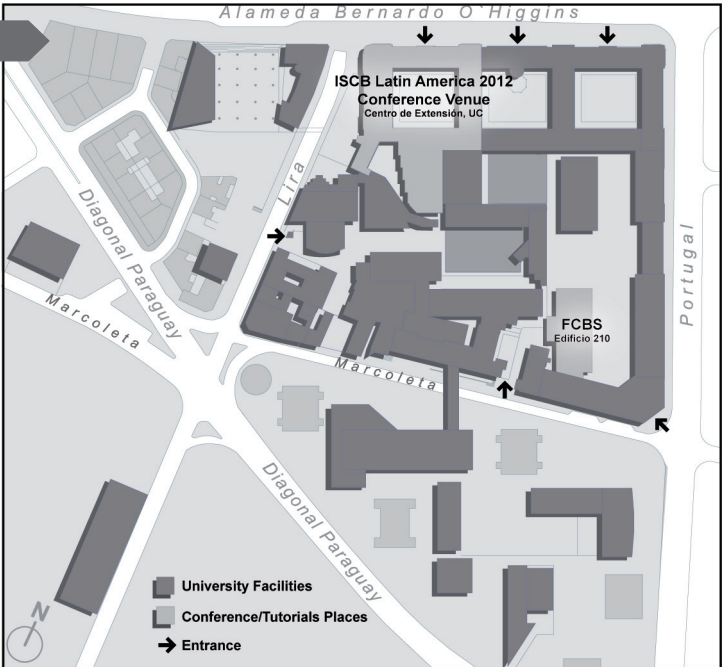




Reference Maps



- Subway station
- Pedestrian entrance
- Car entrance



Ground floor level



Second floor level











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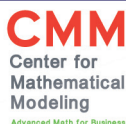
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