Schedule at a Glance
MONDAY – 21 November

08:00  19:30  Registration
08:45  09:00  Morning Welcome
09:00  10:00  Keynote Presentation: *A Mechanistic View of Oncogenic K-Ras Biology*
   **Ruth Nussinov**, PhD, National Cancer Institute, Maryland, USA
10:00  10:30  Coffee Break
10:30  12:30  **Protein Session**

- **10:30** - 10:55  Biomolecular Dynamics in Complex in vivo Environments
   - **Garaging Papoian**

- **10:55** - 11:10  Discovery of Protein Isoforms for Different Stages of Prostate Cancer
   - **Luis Rueda**

- **11:10** - 11:25  Analysis of cell-cycle regulatory linear motifs bound by the pRb retinoblastoma tumor suppressor
   - **Lucia Chemes**

- **11:25** - 11:40  Identification and Substantiation of Specificity Determining Residue Networks using small Datasets and MI-promiscuity
   - **Facundo Orts**

- **11:40** - 11:55  Residue-covariation networks cluster similar functional domains
   - **Franco Simonetti**

- **11:55** - 12:10  Validation of Assembly and alignment-free method for chloroplast next generation sequences data
   - **Raúl Martin Amado Cattáneo**

- **12:10** - 12:20  SwissProt Select: The New Protein Superfamily Database for Reliable Function Assignment
   - **Nicolás Stocchi**

- **12:20** - 12:30  DEPICTViz - Differential Expression and Protein Interactions Visualization Tool
   - **Nalvo F. Almeida**

12:30  14:30  **Lunch on Own**
MONDAY - 21 November Cont.

14:30 16:30 Data Session

14:30 14:50 Tech Talk, EMBL-EBI, Overview of EMBL-EBI Services and How We Work with Industry

14:50 15:10 Systematic assessment of multi-gene predictors of pan-cancer tumour sensitivity to drugs exploiting gene expression data - Pedro J. Ballester

15:10 15:30 A Data-Driven Approach to Estimating the Number of Clusters in Hierarchical Clustering - Antoine Emil Zambelli

15:30 15:45 A novel approach for highly-diverse multi-omics data fusion applied to tomato germ plasm selection - Georgina Stegmayer

15:45 16:00 Pasteur_galaxy: An open and sustainable Galaxy instance for NGS data analysis - Oussama Souiai

16:00 16:15 Graphing genomes in 2D, applications of multivariate statistics on the genomic composition - María Camila Martínez

16:15 16:30 Coffee Break

17:00 18:00 Keynote Presentation: Coding for running speed and computing displacement in the mammalian brain's GPS

Emilio Kropff, PhD, Researcher at the National Research Council (CONICET), Leloir Institute IIBBA, Buenos Aires, Argentina

18:00 19:30 Networking and Posters Presentations, Odd numbered posters being presented, view poster abstracts at https://www.iscb.org/cms_addon/conferences/la2016/posterlist.php
Schedule at a Glance
TUESDAY – 22 November

08:30 19:30 Registration

08:45 09:00 Morning Welcome and Announcements

09:00 10:00 **Keynote Presentation**: Birdsong to study neural control and biomechanics in a learned sensorimotor task

*Ana Amador, PhD*, University of Buenos Aires and IFIBA, National Research Council (CONICET), Buenos Aires, Argentina

10:00 10:30 Coffee Break

10:30 12:30 **Machine Learning and Data Mining Session**

10:30 10.50 Tech-Talk, CITES, Latin American Business Incubator located in Sunchales, Santa Fe, Starting UP Bioinformatics

10:50 11:10 Ranking factors involved in diabetes remission after bariatric surgery using machine-learning integrating clinical and genomic biomarkers - Søren Brunak

11:10 11:30 Advanced data mining reveals a non-canonical mode of interaction for MHC class II ligands - Morten Nielsen

11:30 11:50 Novel microRNA discovery from genome-wide data: a computational pipeline with unsupervised machine learning - Georgina Stegmayer

11:50 12:03 NetPhosPan: a pan specific predictor for phosphorylation site predictions - Emilio Fenoy

12:03 12:16 Machine Learning Tools to Computationally Identify Genomic Elements - Melissa Woghiren

12:16 12:30 TAXOFOR: Taxonomic Assignment of 16S rDNA sequences using Fourier Analysis - Guillerm Luque y Guzman Saenz

12:30 14:30 Lunch on Own
14:30 16:30  **Disease Session**

14:30 14:50  Multi-Cohort Analysis Identifies Cross-Tissue Gene Signature to Predict Lung Function and TFS in Patients with Idiopathic Pulmonary Fibrosis - Scott Madeleine

14:50 15:10  Differential network analysis for the identification of common and specific regulatory mechanisms between idiopathic dilated cardiomyopathy and ischemic cardiomyopathy - Mariana Recamonde-Mendoza

15:10 15:30  A bioinformatics approach shows significant overlap of molecular pathology in early preeclampsia with endometrial diseases - Maria Rabaglino

15:30 15:45  Diagno: an online Clinical Genomics Diagnosis tool - Patricio Yankilevich

15:45 16:00  MultiOmics: an R package to infer genomics and epigenomics mechanisms involved with cancer disease progression - Martin Abba

16:00 16:15  In silico prediction of biological targets of small molecules by a chemical similarity approach - Andreas Schüller

16:15 16:30  Transcriptomic analysis of drug resistant isolates of the parasitic trematode Fasciola hepatica - Jose Tort

16:30 17:00  **Coffee Break**

17:00 18:00  **EMBO Lecture Keynote Presentation**: Systematic Patterns in Millions of 20 Yearlong Individual Patient Disease Trajectories

*Søren Brunak, PhD*, Professor, Research Director
Novo Nordisk Foundation Center for Protein Research, University of Copenhagen

18:00 19:30  **Networking and Posters, Even numbered posters to be presented, view poster abstracts at**
Schedule at a Glance

WEDNESDAY – 23 November

08:00 12:30  Registration

08:45 09:00  Morning Welcome and Announcements

09:00 10:00  **Keynote Presentation:** Data Visualization in Bioinformatics: Exploring the 'Dark' Proteome

  **Sean I. O'Donoghue, PhD,** CSIRO & Garvan Institute of Medical Research, Sydney, Australia

10:00 10:30  **Coffee Break**

10:30 12:30  **Genes Session**

  10:30 10:50  Tech Talk: Heritas, Bioinformatics for clinical diagnostics

  10:50 11:15  Extreme learning machines for discovering gene regulatory networks from temporal profiles of expression

  Mariano Rubiolo

  11:15 11:40  Dynamics of tRNA fragments and their targets in aging mammalian brain - Andrey Grigoriev

  11:40 12:05  Exploring the human virome, new tools, new insights

  Alejandro Reyes

  Seeking informative regions in viral genomes

  Jaime Leonardo Moreno

  12:05 12:17  Bioinformatic sequence analysis tools for the search for new short peptide in "non-coding" sequences - Luciana Ines Escobar

  12:17 12:30  Prediction of microRNA targets in Echinococcus

  Natalia Macchiaroli

12:30 14:30  **Lunch on Own**
**WEDNESDAY - 23 November Cont.**

<table>
<thead>
<tr>
<th>Time</th>
<th>Session</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>14:30 - 16:30</td>
<td><strong>Systems Session</strong></td>
<td></td>
</tr>
<tr>
<td>14:30 - 14:53</td>
<td>Bioinformatic mapping of microRNAs related with cervical cancer on Human Latinoamerican Genomic Variants</td>
<td>Milena Guerrero Flórez</td>
</tr>
<tr>
<td>14:53 - 15:15</td>
<td>An integrative method to unravel the host-parasite interactome: an orthology based approach</td>
<td>Yesid Cuesta Astroz</td>
</tr>
<tr>
<td>15:15 - 15:30</td>
<td>Universal attenuators and their interactions with feedback loops in gene regulatory networks</td>
<td>Dianbo Liu</td>
</tr>
<tr>
<td>15:30 - 15:45</td>
<td>Combining miRNA and their regulators to understand the formation of diapause as transgenerational defense against pathogens in C. elegant</td>
<td>Alberto Jesus Martin</td>
</tr>
<tr>
<td>15:45 - 16:00</td>
<td>Cellular Information Processing: pre-equilibrium signalling, cooperatively effects and membrane receptor trafficking</td>
<td>Federico Sevlever</td>
</tr>
<tr>
<td>16:00 - 16:15</td>
<td>Evaluation of Anti-biofilm activity of synthetic peptides analogous to human cathelicidin LL-37 in clinical isolates of Staphylococcus app</td>
<td>Fredy Alexander Guevara Agudelo</td>
</tr>
<tr>
<td>16:15 - 16:30</td>
<td>From in silico modelling to comprehension of agroecosystems: towards a complex index to study of microbial diversity and its relation of soil health</td>
<td>Arsenio J Rodríguez</td>
</tr>
<tr>
<td>16:30 - 17:00</td>
<td><strong>Awards and Closing</strong></td>
<td></td>
</tr>
</tbody>
</table>
Keynote Speakers

Ana Amador, PhD
Dept. of Physics
University of Buenos Aires and IFIBA
National Research Council (CONICET)
Buenos Aires, Argentina

*Birdsong to study neural control and biomechanics in a learned sensorimotor task*

Birdsong is a complex motor activity that emerges from the interaction between the peripheral system, the central nervous system and the environment. The similarities to human speech, both in production and learning, have positioned songbirds as unique animal models for studying this learned motor skill.

In this talk I will present a low dimensional dynamical system model of the vocal apparatus in which inputs could be related to physiological variables, being the output a synthetic song (SYN) that is a copy of the recorded birdsong (BOS). To go beyond sound comparison, we measured neural activity highly tuned to BOS and found that the patterns of response to BOS and SYN were remarkably similar. This work allowed to relate motor gestures and neural activity, making specific predictions on the timing of the neural activity. To study the dynamical emergence of this feature, we developed a neural model in which the variables were the average activities of different neural populations within the nuclei of the song system. This model was capable of reproducing the measured respiratory patterns and the specific timing of the neural activity. These results suggest that vocal production is controlled by a distributed recurrent network rather than by a top-down architecture.

Søren Brunak, PhD
Professor, Research Director
Novo Nordisk Foundation Center for Protein Research
University of Copenhagen

*EMBO Lecture
Systematic Patterns in Millions of 20 Yearlong Individual Patient Disease Trajectories*

Compared to the initial expectation human beings are gene-poor organisms. Many genes and pathways are likely to play a role in more than one disease, and numerous examples of gene pleiotropy and protein multi-functionality presumably await discovery. This situation contributes to the recent interest in clinical healthcare sector data and their accounts of fine-grained multi-morbidities. Patient record data remain a rather unexplored, but potentially rich data source for discovering correlations between diseases, drugs and genetic information in individual patients. A fundamental question in establishing biomarker-phenotype relationships is the basic definition of phenotypic categories. As an alternative to the conventional case-control, single disease model the talk will describe attempts to create phenotypic categories and patient stratification based on longitudinal data covering long periods of time. We carry out temporal analysis of clinical data in a more life-course oriented fashion. We use data covering 6-7 million patients from Denmark collected over a 20 year period and use them to “condense” millions of individual trajectories into a smaller set of recurrent ones. This set of trajectories can be interpreted as re-defined phenotypes representing a temporal diseaseome as opposed to a static one computed from non-directional comorbidities only. A special case is represented by disease co-occurrences which are treatment provoked, e.g. adverse drug reactions. An important issue is to resolve whether specific adverse drug reactions relate to variation in the individual genome of a patient, to drug/environment cocktail effects, or both. From patient records ADR profiles of approved drugs can be constructed using drug-ADR networks, or alternatively patients can be stratified from their ADR profiles and compared. This type of work can potentially gain importance in projects involving population-wide genome sequencing in the future.
Coding for running speed and computing displacement in the mammalian brain's GPS

The last decades have witnessed major discoveries concerning the brain mechanisms through which mammals compute their own location and orient in space. Hippocampal place cells provide maps that describe the position of the animal within a known environment, including a rich contextual description. Entorhinal grid cells provide instead a spatial map that is applied to all environments and is not altered by contextual variations. For this reason grid cells have been proposed to be the framework for an egocentric representation of location, where position is computed independently of contextual cues and based only on the animal's knowledge of its own movements. To achieve this, grid cells should receive information about orientation and speed of instantaneous movements. While neurons coding for the head orientation have been described in the entorhinal cortex, the entorhinal speed code has remained elusive for almost a decade. We present the Flintstone car, a new behavioral paradigm that allows the precise control of rat running speed. Using this device we have discovered a new functional entorhinal cell type: the speed cell. These neurons code for running speed in an instantaneous and linear way. The code is context-independent, allowing running speed to be decoded from the activity of a handful of speed cells even across environments. In addition, we found speed cells to be slightly ahead in time with respect to the actual running speed (~80 ms on average) and, consistently, we found grid cells to be ahead in time with respect to the actual position. Taken together, these observations point to entorhinal speed cells as a key component in the dynamic representation of self-location.

A Mechanistic View of Oncogenic K-Ras Biology

Ras proteins are small GTPases that act as signal transducers between cell surface receptors and several intracellular signaling cascades. KRAS is among the most frequently mutated oncogenes in human tumors. Ras proteins consist of highly homologous catalytic domains, and flexible C-terminal hypervariable regions (HVRs) that differ significantly across Ras isoforms. We have been focusing on key mechanistic questions in oncogenic Ras biology from the structural and signaling standpoints. These include whether Ras' disordered hypervariable region (HVR) has a role beyond membrane anchoring; Does Ras form dimers, and if so what is their structural landscape and how they help in activating Raf; What are Ras’ redundant pathways and importantly how to identify redundant pathways in cancer; What are the mechanisms of oncogenic mutations; Is RASSF5 - which links Ras and the MAPK pathway to the Hippo pathway - a tumor suppressor or activator as some experiments suggest, and what is the mechanism through which it works, and more. We believe that structural biology - computations and experiment – is uniquely able to tackle these fascinating and important questions.
Data Visualization in Bioinformatics: Exploring the 'Dark' Proteome

The rapidly increasing volume and complexity of biological data calls for new approaches to help life scientists gain insight from these data, rather than being overwhelmed. To address this, the application of modern data visualization principles and methods will be critical, in combination with improved data management, machine learning, and statistics. I will illustrate the power of this 'BioVis' approach by presenting several bioinformatics resources that empower biologists by making complex data easier to access and use. This includes Aquaria (http://aquaria.ws), Minardo (http://minardo.org/snapshot), and Rondo (http://rondo.ws). I will showcase how these resources are being used to explore the known and unknown ('dark') proteome, generating new insights into human biology and health. I will also discuss VIZBI, an international initiative aimed at raising the global standard of bioinformatics software (http://vizbi.org/). Finally, I'll discuss the use of visualization to create molecular and cellular-scale animations aimed at educating and inspiring the public about cutting-edge biomedical research (http://vizbi.org/plus).
Thank You Sponsors

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INTERNATIONAL SOCIETY FOR COMPUTATIONAL BIOLOGY
The primary mission of EMBL-EBI is to provide freely available data and bioinformatics services to all facets of the scientific community. The first part of the presentation will provide a high level overview of the core data, bioinformatics and cheminformatics services that are freely available from EMBL-EBI. The presentation will describe how we collaborate internationally and employ standards, integration tools and semantic technologies to make these data and services available to the global scientific community. The second part of the presentation will illustrate use cases with a pharmaceutical industry focus arising from some of our interactions with industry and illustrate how working with industry is important in the continual development of our services.

We will explore the experiences of a scientist turned entrepreneur who started a European technology company. The most important features will be considered and how to overcome common bottlenecks. We will contrast this situation with the existing opportunities for starting a technology based company with Cites in the “wild” Latin American Start Up ecosystem.

Heritas is a technology start-up aiming to translate clinical genomics into diagnostics for improved therapies and patient management in human health. Heritas is the result of a joint venture between the R&D Biotech company INDEAR and the clinical diagnostics lab CIBIC, both based in Rosario, Argentina. Heritas model is based on building an ecosystem with three key components: 1) Develop and produce high quality metrics of genomic raw data with Illumina systems, 2) Develop clinical genomic applications with key opinion leaders of the medical community, 3) Develop our own genetic counsellors group to assist medical doctors and patients to translate clinic genomic information into actionable results. Heritas is developing this ecosystem in three major areas: 1) clinical genomics for hereditary or acquired genetic diseases 2) clinical genomics for reproductive health, and 3) Human microbiome dysbiosis based diseases. A major challenge in clinical genomics is to translate genotype to phenotype correlations, and this premise escalates to a serious problem when dealing with intronic variants, one of the dark sides of the human genome. We will present our approaches in dealing with these major challenges in clinical genomics and our vision to translate this information into clinical actionable results.

Supported by: PROFIET – Programa de Fomento a la inversión Emprendedora en Tecnología, MINCyT
Odd numbered posters will be presented on MONDAY - 21 November.
Even numbered posters will be presented on TUESDAY - 22 November.

To view the poster abstracts visit

P001 Pasteur_galaxy: An open and sustainable Galaxy instance for NGS data analysis
Oussama Souiai

P002 Evaluation of Anti-biofilm activity of synthetic peptides analogous to human cathelicidin LL-37 in clinical isolates of Staphylococcus spp. - Fredy Guevara Agudelo

P004 An Exhaustive Feature Selection Approach for Blastocyst Differentiation
Elmer Fernandez

P006 In silico prediction of the thermolysin inhibition as antihypertensive model using artificial intelligent tools. - Yudith Cañizares Carmenate

P007 Fuzzy Clustering: Identification of Similar Compounds for Virtual Screening in Rational Drug Design - Ignacio Ponzoni

P008 On testing genetic covariance with the R package biotools - Anderson Silva

P010 Discovery of novel pre-miRNAs: unsupervised versus supervised machine learning
Georgina Stegmayer

P012 Computational Study of Bromopyrrole Alkaloids with Antimalarial Activity. A QSAR Approach - Edgar Brazon

P013 Parallel Bootstrap Consensus Clustering - Macarena Saenz

P014 Unsupervised Learning Based on Deep Learning Applied to the Identification of Applicability Domain of QSAR Models - Ignacio Ponzoni

P015 Prototype of deductive computing using deoxyribonucleic acid - Nelson Rivera

P016 Optimal threshold estimation in binary classifiers using game theory
Ignacio Sanchez

P017 Graphing genomes in 2D, applications of multivariate statistics on the genomic composition - Maria Martinez

P018 Novel microRNA discovery from genome-wide data: a computational pipeline with unsupervised machine learning - Georgina Stegmayer

P019 Drug targets prioritization for neglected diseases - Santiago Videla
A novel approach for highly-diverse multi-omics data fusion applied to tomato germplasm selection - Georgina Stegmayer

Development of analytic and visualization tools for linear B cell epitope mapping from peptide-arrays - Carolina Barra

The impact of RNA-Seq differential expression algorithms on Over-Representation Analysis of Gene Sets. - Juan Rodriguez

Bioinformatics workflow and assessment of software to seek secondary metabolites in Bacteria - Jose Alzate Ocampo

FastqCleaner: a Shiny web application for cleaning Illumina FASTQ files with R - Leandro Roser

UTRme: a tool to annotate UTRs in Trypanosoma cruzi - Santiago Radío

StructRNAfinder: Predicting RNA families from 3'UTR regions of Zika and related viruses through an automated tool - Raul Arias-Carrasco

Analysis of alternative splicing in timecourse experiments using Aspli R/Bioconductor package - Javier Iserte

Identification of multi-resistant bacteria through a machine learning approach using the whole genome - Harold Ballén Mejía

A platform for integration, data acquisition and data analysis in electronic medical records - Fernanda Almeida

Metagenomic binning of the uncultured fraction of the gut microbiome reveals neutral signature of rare taxa - Patricio Jeraldo

Analysis of a soil metagenome from the Argentine Northwest Monte and Thistle of the Prepuna region of the Province of Salta - Jorgelina Moreiras Clemente

Updates to the TDR Targets chemogenomics database - Lionel Uran Landaburu

Highly resolved phylogeny for Corynebacteriales - Nilson Da Rocha COimbra

Assessing bioinformatics strategies for de-novo transcriptome assembly - Sergio Gonzalez

Landscape of non-coding RNAs in Archaea: diversity, conservation and functional characterization. - Victor Aliaga-Tobar

TNSim: Simulating tumor-tissue sequencing data with wide-spectrum of somatic variant allelic fractions - Jiayin Wang

A bioinformatics approach shows significant overlap of molecular pathology in early preeclampsia with endometrial diseases - Maria Rabaglino

Differential network analysis for the identification of common and specific regulatory mechanisms between idiopathic dilated cardiomyopathy and ischemic cardiomyopathy - Mariana Recamonde-Mendoza
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P045 Identification, organization, and record of rhomboid proteases of Babesia and Theileria hemoprotozoans - Romina Gallenti

P048 Metagenomics in the identification of infectious agents - Liliane Conteville

P049 Towards a better cancer classification: mutational patterns of loci and cancer types - Soledad Ochoa

P050 Homology Modeling of T. cruzi Squalene Epoxidase. Estimation of Ligand-Binding Affinities by MM-PSBA - Guido Noguera

P051 Computational Study On Flavonoids With Anti-Hiv-1 Activity Employing The Density Fucctional Theory - José Malavé Guerra

P052 Bond-based Bilinear Indices in QSAR: Computational Discovery of Novel Trypanosomicidals Drug-Like Compounds - Juan Castillo-Garit

P054 Interactions of OHMLINE, a new lipid-antimetastatic agent, with different lipid membrane components. A molecular dynamics study - Natalia Piñeiro

P056 Glycosylated Flavonoids as Potential HIV-1 Reverse Transcriptase Inhibitors - Joseph Ortega

P057 Design and discovery of prodrugs of Zidovudine with high affinity to human serum albumin. - Esteban Schenfeld

P058 Regulatory molecular circuits in leukocytes of Juvenile Idiopathic Arthritis patients - César Prada-Medina

P059 Genome-Wide Prioritization Of Candidate Diagnostic Antigenic Markers In Human Pathogens - Diego Ramoa

P060 Metagenomic Analysis for identification of Viruses Associated with Neonatal Calf Diarrhea - Laura Avellaneda

P061 Identification of Potential Pancreatic Lipase Inhibitors by Structure-Based Repurposing - Irvyng Patrick Lanchero Barrios


P064 Differential TP73 exon usage in breast cancer molecular subtypes - Martin Guerrero

P065 Computational design of a Dengue virus sensor - Franco Tavella
P066  A Computational Methodology to Overcome Challenges Associated with the Search for Specific Targets to Develop Drugs against Leishmania major - Larissa Costa

P067  A comparative approach to identify discriminative DNA sequences. Case study: MTB Complex and Genus Mycobacterium - Iván Duque Aldana

P068  Inexpensive Mobile Diagnosis of Diabetic Retinopathy using Deep Learning - Kavya Kopparapu

P071  Non alcoholic fatty liver disease in Octodon degus. - Francisco Altimiras

P072  Dengue virus serotype 2 intra-host diversity in patients with different clinical outcomes - Maria Torres

P073  Exploring biological patterns in Anopheles associated microbiota: Is there a core bacterial assembly shared between African and American anophelines? - Luis Martinez

P074  Association of Tandem repeats to the pathogenicity of Gardnerella vaginalis in bacterial vaginosis - Fabian Tobar-Tosse

P075  Identification of unique nucleotide patterns between mucosal and cutaneous Human papillomaviruses using KM-Finder - Luciana Montera

P076  Perl for Biologists - An online tutorial - Huseyin Kocak

P078  Extreme learning machines for discovering gene regulatory networks from temporal profiles of expression - Mariano Rubiolo

P079  TAXOFO: Taxonomic Assignment of 16S rDNA sequences using Fourier Analysis - Guillermo Luque y Guzman Saenz

P080  Bioinformatic sequence analysis tools for the search for new short peptide in "non-coding" sequences. - Luciana Escobar

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P083  Seeking informative regions in viral genomes. - Jaime Moreno

P084  Impact of the Different Discretization Methods on Gene Expression Biclustering: Alzheimer Disease Progression Data as a Case Study - Ignacio Ponzoni

P085  Evaluation of the interaction networks of important Genes and microRNAs in HCV - Mohammad Navaderi

P086  Predicting Breast Cancer Drug Response via an Level-wise Gene Selection Approach - Dr. Alioune Ngom

P088  Improving the Uncertainty Estimation in PAM50: Impact on Subtype Assignment and ROR - Elmer A Fernandez

P090  Evolution of Proboscidea genomes illustrated by structural variant analysis
Abdul Grigoriev

P091 Evolution of Two Uncharacterized Non-catalytic Carboxylesterase Subfamilies Involved with Early Development of the Sensory Organs and Tracheal System in Insects
André Luiz Torres

P092 Comparative genomics of Acinetobacter baumannii international clone 1 reveals a high degree of synteny and gene sequence conservation
Verónica Álvarez

P093 Comparative genomics of miRNAs in Cestodes
Santiago Fontenla

P094 Loss and gain of genes in flatworms: adaptation of parasites to their way of life.
Santiago Fontenla

P095 The antimicrobial resistance determinants harbored in mobile elements collaborate with the genomic adaptation of P. aeruginosa during chronic infections
Maria Rapisardi

P096 The microsynteny of genes functionally related with the fruit ripening process in Solanaceae species
Paolo Cacchiarelli

P097 Transcriptomics of sensory stimuli detection in a Chagas disease vector
Jose Manuel Latorre

P098 Preliminary data on UTR prediction procedure of Piaractus mesopotamicus (pacu) aiming muscle development analysis.
Bruno Fantinatti

P099 HLA-MAPPER: an application to optimize the mapping of hla-related sequences produced by massively parallel sequencing procedures
Michelle Paz

P100 Variant Caller Assigner Comparison for Ion Torrent Data
Yanina Murua

P101 Whole genome SNPs analyses unravel Echinococcus species phylogeny
Lucas Maldonado

P102 Non-negative matrix factorization for prediction of gene annotations
Georgina Stegmayer

P103 Characterization of ABC-transporters, a detoxification-related gene family in the Chagas' disease vector Rhodnius prolixus
Lucila Traverso

P104 Using transcriptomic data to improve the annotation of Mesocestoides corti genome
Alicia Costábile

P105 Metatranscriptomic and transcriptomic analyses of the digestive tract of Spodoptera frugiperda larvae captured in the province of Tucumán
Gastón Rozadilla

P106 Elucidating gut microbiota of captive and wild Andean bears using comparative analysis of the 16S rDNA gene.
Andrea Borbon

P107 Analysis of the Microbial Community of Wastewater Stabilization Ponds from Small Dairy Industries using Whole Genome Shotgun Sequencing
José Irazoqui

P108 Identification of Bacteriophage crAssphage Through Hidden Markov Models
Laura Forero
P109 Using Oxford Nanopore MinION technology to deeply explore metagenome functions in the Argentine Human microbiome dataset characterised by Illumina 16s metagenomics pipeline - Cristian Rohr

P110 Effects of antibiotic use in clinical settings on environmental microbial communities of the Bogotá River (Colombia) - Carlos Posada

P111 Structure of bacterial community in the cecum of broiler chickens in response to growth promoters - Natalia Pin Viso

P112 Comparative analysis of Archean core promoter region information content and its relation with optimal growth temperature. - Ariel Aptekmann

P113 Estimating protein multifunctionality from gene ontology - Sayaka Fujio Vejar

P114 Differential Expression Analysis Of Uv Radiation Resistance In Deinococcus Swuensis, Isolated From Paramo Ecosystems. - Jorge Diaz-Riaño

P115 COVERT - COnserVEd Regulon Tool - Nalvo Almeida

P116 Automatic extraction of hairpin sequences from genome-wide data - Cristian Yones

P117 In-silico detection and characterization of non-coding RNAs from the non-fermenting gram-negative bacilli Shewanella and Acinetobacter - Cecilia Quiroga

P118 Cancer immunology of Cutaneous Melanoma: A Systems Biology Approach Mindy Muñoz

P119 Gene correlation networks with dual RNA-seq (Dual-seq) data - Caio Padoan

P120 Discover the most effective microRNA and Genes in pediatric brain tumors Samira Rahimi Rad

P122 tRNA Array Genomic Mining Revealed Their Occurrence and Diversity in Mycobacteria - Sergio Morgado

P124 Unraveling Reaction Mechanisms with QM/MM: Mycothiol MshA retaining glycosyltransferase reaction as a case study - Juan Blanco

P127 Discovery of Protein Isoforms for Different Stages of Prostate Cancer - Luis Rueda

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P132 DEPICTViz - Differential Expression and Protein InteracTions Visualization Tool Nalvo Almeida

P133 Cat-p-Data: Custom Analysis Tool for Protein Data - Karina Machado
P134  Analysis of Null Areas: void detection, calculation and tracking in molecular dynamics. - Patricio Barletta

P135  SwissProt Select: The New Protein Superfamily Database for Reliable Function Assignment - Nicolás Stocchi

P136  HMMER Performance Optimization for Protein Superfamily Classification with Reliable Cut-off - Agustin Amalfitano

P137  Benchmarking and parameter optimization of the GibbsCluster algorithm Bruno Alvarez

P138  TCRpMHC class II complex modeling and force field scoring with an application on peptide rankings for immunogenic response - Esteban Lanzarotti

P141  Helicobacter pylori AlpAB adhesin as potential target therapeutic based on camelid nanobodies - Diego Valencia

P142  Comparative degradome analysis of the human pathogens Cryptosporidium parvum and C. hominis - Tomás Poklépovich Caride

P144  Virtual screening and molecular dynamics simulations applied to design potent and selective caspase-1 inhibitors - Carlos Ramos Guzman

P145  FusionDB: Assessing Microbial Diversity and Environmental Preferences via Functional Similarity - Yana Bromberg

P146  High-density tiling peptide arrays for proteome-wide identification of new chagas disease antigens and mapping of antibody epitopes - Leonel Bracco

P147  Analisy of HCV peptides according to its ability to stimulate cytotoxic T cells Morten Nielsen

P148  Residue Geometry Networks: A Rigidity-Based Approach to the Amino Acid Network Alexander Fokas

P149  Dipole orientation of Aquaporin-4 pore-lining residues are possibly involved in an electrostatic gating mechanism - Yerko Escalona

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Heritas model is based on building an ecosystem with three key components:
1) Develop and produce high quality metrics of genomic raw data with Illumina systems, 2) Develop clinical genomic applications with key opinion leaders of the medical community , 3) Develop our own genetic counsellors group to assist medical doctors and patients to translate clinic genomic information into actionable results. Heritas is developing this ecosystem in three major areas: 1) clinical genomics for hereditary or acquired genetic diseases 2) clinical genomics for reproductive health, and 3) Human microbiome dysbiosis based diseases.

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