

- Molecular modeling and structural analysis of the protein twitching motility a product of XF1633 gene of *Xylella fastidiosa*. EMBRAPA - CNPTIA

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2. R.C. Melo, C. Ribeiro, C.S. Murray, C.J.M. Veloso, C.H. da Silveira, Goran Neshich, W. Meira Jr, R.L. Carceroni and M.M. Santoro: "Finding protein-protein interactions by contact-maps matching." *Genet. Mol. Res.* 6 (4): 946-963 (2007)
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4. Stanley R. M. Oliveira, Gustavo V. Almeida, Kassius R. R. Souza, Diego N. Rodrigues, Paula R. Kuser-Falcão, Michel E. B. Yamagishi, Edgard H. Santos, Fábio D. Vieira, José G. Jardine and Goran Neshich: "STING_RDB: A relational database of structural parameters for protein analysis with support for Data Warehousing and Data Mining." *Genet. Mol. Res.* 6 (4): 911-922 (2007)
5. NESHICH, G: "Computational Biology in Brazil." *PLoS Comput Biol.* Oct; v3 (issue 10, e185), 2007.
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9. Janaina Gomide; Raquel Melo Minardi; Marcos Augusto dos Santos; Wagner Meira Jr.; Julio Cesar Dias Lopes; SANTORO, Marcelo; NESHICH, Goran: "Using Linear Algebra for Protein Structural Comparison and Classification." *Genet. Mol. Res.*, 2009.

Chilean EMBnet node: progress report



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In the past three years we have held a large number of activities related to bioinformatics and Systems Biology, which have had a big impact on the local scientific community. We have organized two mathematical modeling courses (1-2 weeks) aimed at the national biological research community.;

- the first one, Mathematical Modelling of Biological Systems, was offered in 2008 by local instructors with a solid background on biology, mathematics and computer science and was attended by over 70 participants;
- the second was an advanced course on Mathematical Models in Biology, was given by Benoit Perthame from Laboratoire J.-L. Lions, UPMC/INRIA, and it was attended by over 20 participants;
- in addition, we are planning on extending these outreach activities and offer a regional Latin American Systems Biology course next year (2010).

During this period, we have been awarded a major national grant (1 M\$ USD/yr) for the creation of the Institute for Cell Dynamics and Biotechnology: A Centre for Systems Biology (<http://www.icdb.uchile.cl/icdb>). This institute is composed by scientists whose background and area of expertise is very diverse. There has been a tremendous amount of cross-fertilization between the scientists participating in this institute, leading to a large number of collaborations, such as:



Figure 1. ICDB Institute - The Chilean node.

- mathematicians and bioengineers/biotechnologists (modelling of joint gene regulation and metabolic networks);
- cell biologists, bioengineers and mathematicians (modelling iron mediated oxidation and cell ageing at metabolic and genetic levels);
- mathematicians, bioengineers and microbiologists (modelling substrate and electron diffusional effects in biofilms with microbial populations in bioleaching);
- proteomics experts and cell biologists and biotechnologists, (applying modern computer tools in the analysis of proteomic and gene microarray expression data and in the use of a metabolic model to simulate and optimize virus production for gene therapy vector synthesis);
- molecular modellers/medicinal chemists and cell biologists (modulating interactions between HFE/transferrin receptor).

This scientific diversity has generated a very large number of scientific collaborations between mathematicians, biologists, bioengineers, computer scientists and chemists which have focused both on Systems Biology as well as Mathematical Biology, a young innovative discipline in our country and in Latin America. These interactions have generated several industrial patents and over 65 scientific publications in high impact factors journals. One of them was in fact published on the EMBnet's special issue of BMC bioinformatics

(2009, V10, S6). A full list of publications is available upon request.

In 2008 the institute supported and trained of 71 Ph.D. students, postdocs and young scientists in programmes ranging from bioengineering, mathematical modelling and computer science to biochemistry, neuroscience, microbiology and chemistry. These students are receiving formal training in biology, computer science and mathematics and most of them are doing part of their research projects abroad or in collaboration with top laboratories and research centres in US and Europe (Laboratoire Jacques-Louis Lions University of Paris VI, University of Cambridge, University of Kent, University of Delft, National Biotechnology Center of Spain, Functional Genomics Centre at the University of Manchester, the Bioengineering Laboratory at Northwestern University, the Metabolomics Laboratory at the University of Stuttgart and the Proteomics Laboratory at the University of Virginia and others).