

Alejandro Giorgetti, PhD.

Assistant Professor

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Official Visiting Scientist

*German Research School for Simulation Sciences (GRS)
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Curriculum Vitae

- Since 2011** *Adjunct Visiting Scientist* at the German Research School for Simulation Sciences (GRS). Juelich, Germany.
- Since 2007** *Assistant Professor* at the University of Verona. Faculty of Mathematical, Physical and Natural Sciences, Department of Biotechnology. Verona, Italy
- 2004 - 2007** Postdoctoral research fellow at the Department of Biochemical Sciences, University of Rome "La Sapienza". Rome, Italy.
- 2006-2009** Research fellow at the Bioinformatics Program, CRS4, Pula (CA). Sardegna, Italy
- 2004** PhD in Statistical and biological Physics, cum laude. SISSA (Scuola Internazionale Superiore di Studi Avanzati. Trieste, Italy (10-10-2004)
- 1999 - 2000** Quality Control expert of the SPECT system. Sanatorio Privado del Sur. Bahia Blanca, Argentina
- 2000** Master degree in Medical Physics at the Universidad de Buenos Aires (UBA), Argentina
- 1997 - 1999** Internship for Medical Physics activities supported by the Universidad Nacional del Sur. Bahia Blanca, Argentina.
- 1996** Licenciado en Fisica (Degree in Physics) at the Universidad Nacional del Sur (UNS). Bahia Blanca, Argentina (18-12-1996).

Research Activities

Dr. Alejandro Giorgetti has been appointed as Assistant Professor of Biochemistry at the University of Verona, Italy since 2007. Since his appointment, he is the Principal Investigator of the *Applied Bioinformatics Group*. The main research interests of the group include: protein modelling from sequence, in particular using comparative modelling techniques; protein structure analysis; protein sequence analysis; protein design; and the development of tools aimed at the investigation and understanding of the relationship between protein sequence, structure and function. The group is actively involved in different collaboration projects both within the national territory and with scientists abroad. Recently he has been also appointed as Adjunct Visiting scientist (2011-2014) at the German Research School for Simulation Sciences (GRS), Juelich, Germany.

Specific projects include:

1. **Membrane protein modelling:** My group counts with an important expertise in the field of membrane protein modelling, comprising the modelling of mammalian ion channels (CNG and HCN), modelling of odorant and bitter taste receptors (GPCR), modelling of efflux pumps.
2. Interaction of HIV-1 proteins with its human counterpart, i.e. hTE8/Nef and HLA-C/env.

3. Effects of mutation on protein structure and disease.
4. Development of pipelines to optimize the template search in homology modelling approaches.
5. Multiscale approach for protein function: from a molecular description to a systemic point of view. Insights into the bitter and olfactory signalling pathways and into the naphthalene degradation pathway.

Publications (* corresponding author).

1. Leguèbe M, Nguyen C, Capece L, Hoang Z, Giorgetti A*, et al. (2012). Hybrid Molecular Mechanics/Coarse-Grained Simulations for Structural Prediction of G-Protein Coupled Receptor/Ligand Complexes. *PLoS ONE* 7(10): e47332. doi:10.1371/journal.pone.0047332
2. Giorgetti A., P. Ruggerone, S. Pantano, and P. Carloni, Advanced Computational Methods in Molecular Medicine, *Journal of Biomedicine and Biotechnology*, 2012. 2012: p. 709085.
3. Zanzoni, S.; Assfalg, M.; Giorgetti, A.; D'Onofrio, M.; Molinari, H.. Structural Requirements for Cooperativity in Ileal Bile Acid Binding Proteins. 2011. *J Biol Chem*. 2011 Nov 11;286(45):39307-17.
4. Modena, D.; Trentini, M.; Corsini, M.; Bombaci, A.; Giorgetti, A*. OlfactionDB: A Database of Olfactory Receptors and Their Ligands. *Advances in Life Sciences* 2011; 1(1): 9-13
5. Piccoli, S. and Giorgetti A*. Perspectives on Computational Structural Bio-Systems. 2011. *J Bioprocess Biotechniq* 2011,1:104e
6. Biarnés X.; Marchiori A.; Giorgetti A.*; Lanzara C.; Gasparini P.; Carloni P.; Born S.; Brockhoff A.; Behrens M.; Meyerhof W. (2010). *Insights into the Binding of Phenyltiocarbamide (PTC) Agonist to Its Target Human TAS2R38 Bitter Receptor*. *PLOS ONE*, pp. 1- 6 Vol.5
7. Griguoli M.; Maul A.; Nguyen C.; Giorgetti A.; Carloni P.; Cherubini E. (2010). *Nicotine blocks the hyperpolarization-activated current I_h and severely impairs the oscillatory behavior of orienslacunosum molecular interneurons*. *THE JOURNAL OF NEUROSCIENCE*, pp. 10773- 10783 Vol.30
8. Heller D.M.; Giorgetti A.* (2010). *NMR Constraints Analyser: a web-server for the graphical analysis of NMR experimental constraints*. *NUCLEIC ACIDS RESEARCH*, pp. W628- W632 Vol.38
9. Saga G.; Giorgetti A.; Fufezan C.; Giacometti G.M.; Bassi R.; Morosinotto T. (2010). *Mutation analysis of violaxanthin De-epoxidase identifies substrate-binding sites and residues involved in catalysis*. *THE JOURNAL OF BIOLOGICAL CHEMISTRY*, pp. 23763- 23770 Vol.285
10. Mazzolini M.; Marchesi A.; Giorgetti A.; Torre V. (2010). *Gating in CNGA1 channels*.

PFLUGERS ARCHIV, pp. 547- 555 Vol.459

11. Maullu C.; Raimondo D.; Caboi F.; Giorgetti A.; Sergi M.; Valentini M.; Tonon G.; Tramontano A. (2009). *Site-directed enzymatic PEGylation of the human granulocyte colony-stimulating factor*. *THE FEBS JOURNAL*, pp. 6741- 6750 Vol.276
12. Lupieri P.;Nguyen C.H.H. ;Bafghi Z.G.;Giorgetti A.;Carloni P. (2009). *Computational molecular biology approaches to ligand-target interactions*. *HFSP JOURNAL*, pp. 228-239 Vol.3
13. Raimondo D., Giorgetti A., Bernassola F., Melino G., Tramontano A. (2008). *Modelling and molecular dynamics of the interaction between the E3 ubiquitin ligase Itch and the E2 UbcH7*. *BIOCHEMICAL PHARMACOLOGY*, pp. 1620- 1627 Vol.76
14. Cozzetto D, Giorgetti A, Raimondo D, Tramontano A. (2008). *The Evaluation of Protein Structure Prediction Results..* *MOLECULAR BIOTECHNOLOGY*, pp. 1- 8 Vol.39
15. Albiero E., Madeo D., Ruggeri M., Bernardi M., Giorgetti A., Rodeghiero F. (2008). *Loss of the JAK2 intramolecular auto-inhibition mechanism is predicted by structural modeling of a novel exon 12 insertion mutation in a case of Idiopathic Erythrocytosis* . *BRITISH JOURNAL OF HAEMATOLOGY*, pp. 986- 990 Vol.142
16. Moutran A, Balan A, Ferreira LC, Giorgetti A, Tramontano A, Ferreira RC. (2007). *Structural model and ligand interactions of the Xanthomonas axonopodis pv. citri oligopeptide-binding protein*. *GENETICS AND MOLECULAR RESEARCH*, pp. 1169-1177 Vol.6
17. Tress, M., Martelli, P.L., Frankish, A., Reeves, G., Wesselink J.J., Yeats, C., Olason, P.I., Albrecht, M., Hegyi H., Giorgetti, A., Raimondo, D., Lagarde, J., Laskowski, R., Lopez, G., Sadowski, M.I., Watson, J., Fariselli, P., Rossi, I., Nagy, A., Kai, W., Stoerling, Z., Orsini, M., Assenov, Y., Blakenburg, H., Huthmacher, C., Ramirez, F., Schlicker, A., Denoued, F., Jones, P., Kerrien, S., Orchard, S., Birney, E., Brunak, S., Casadio, R., Guigo, R., Harrow, J., Hermjakob, H., Jones, D.T., Lengauer, T., Orengo, C., Patthy, L., Thornton, J., Tramontano, A., Valencia, A. 2007. *The implications of alternative splicing in the ENCODE protein complement* *PROC. NATL ACAD SCI* 104: 5495 - 5500
18. Giorgetti, A., Raimondo, D., Bosi, S. and Tramontano, A. 2007. *An automatic procedure for using models of proteins in molecular replacement*. *PROTEINS*. 15;66(3):689-96.
19. Nair, A.V., Mazzolini, M., Codega, P., Giorgetti, A. and Torre, V. 2006. *Locking CNGA1 channels in the open and closed state*. *BIOPHYSICAL J.* 90: 3599-3607
20. Giorgetti, A., Raimondo, D., Miele, A. and Tramontano, A. 2005. *Evaluating the usefulness of protein structure models for molecular replacement*. *BIOINFORMATICS*, 21(suppl_2):ii72-ii76.
21. Giorgetti A, Carloni P, Mistrik P, Torre V. *A Homology Model of the Pore Region of HCN channels*. *BIOPHYSICAL J.* 89(2):932-944.
22. Giorgetti, A., A.V. Nair, P. Codega, V. Torre and P. Carloni. 2005. *Structural Basis of Gating of CNG channels*. *FEBS LETTERS*. 579(9):1968-1972.

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23. **Giorgetti, A., Carloni, P. 2003. Molecular Modeling of Ion Channels: Structural Predictions. *Current Opinion in Chemical Biology*. 7: 150-156.**

Book chapters

1. **Giorgetti A., S. Piccoli, Knowledge Based Membrane Protein Structure Prediction: From X-Ray Crystallography to Bioinformatics and Back to Molecular Biology, in *Current Trends in X-Ray Crystallography*, edited by Annamalai Chandrasekaran, InTech Publisher (2011).**
2. **Tress M., Casadio R., Giorgetti A., Hallin PF., Juncker AS., Kulberkyte E., Martelli PL., Raimondo D., Reeves GA., Thornton JM., Tramontano A., Wang K., Wesselink JJ., Valencia A., *Alternative Splicing in the ENCODE Protein- Complement*, Frishman D., Valencia A. *Modern Genome Annotation: the Biosapiens Network*, Wienn, Springer-Verlag, 2008**
3. **Tramontano A., Jones D., Rychlewski L., Casadio R., Martelli PL., Raimondo D., Giorgetti A., *Protein structure prediction*, Frishman D., Valencia A. *Modern Genome Annotation: the Biosapiens Network*, Wienn, Springer-Verlag, 2008**
4. **Tramontano, D. Cozzetto, A. Giorgetti, D. Raimondo. *The assessment of methods for protein structure prediction in 'Protein methods and protocols'*. 2nd edition. Edited by Chris Bystroff and Mohammed Zaki: The Humana Press, Inc, 2008**

Editorial activities

- **Member of the Editorial board of the 'Journal of Bioprocessing and Biotechniques'**
- **Member of the Editorial board of the 'American Journal of Bioinformatic research'**
- **Guest editor for the special issue on "Advanced Computational Methods in Molecular Medicine". *Journal of Biomedicine and Biotechnology*.**
- **Reviewer: *FEBS journal; Bioinformatics; Proteins; Biophysical journal; Amino Acids; EBJO; Protein Engineering, Design, and Selection (PEDS); Current Bioinformatics; Plos Computational Biology; Plos One*.**
- **Expert Reviewer for the French National Research Agency "Blanc SVSE 5" call for proposals.**

Invited Speaker

1. **'Bitter taste sensing: Insights from computational biology'. CECAM meeting: Molecular Simulations of Membrane Proteins: From Biophysics to Pharmacological Application, March 7, 2012 to March 9, 2012. Location : CECAM-HQ-EPFL, Lausanne, Switzerland.**
2. **'Structural Bioinformatics approaches to chemical senses'. The International Conference in Computational Medicine *Ho Chi Minh City, Vietnam, January 11-12th, 2012***
3. **'Chemical Senses: Insights from Structural Bioinformatics'. AIMS seminar series. AICES RWTH Aachen University, Aachen, Germany. 5th December 2011.**

4. 'Structural determinants of bitter taste perception: insights from a combined *in silico* and *in vitro* Study ' 25th August 2010. German Research School (GRS), Jülich, Germany.
5. 'Applicazioni biomediche e farmaceutiche'. Sessione di Dinamica Molecolare nel Master in Comunicazione della Scienza. International School for Advanced Studies (SISSA), 24th June. 2010, Trieste, Italy.
6. "Membrane Transporters: Insights from Bioinformatics". International Workshop: From Structure to Function: Influx and Efflux Systems. 6th - 8th May 2009, Cagliari (IT)
7. Perspectives on Computational Structural/Molecular Systems Biology. March 31st 2009. Dept. of Informatics, University of Verona, Verona, Italy.
8. 'Hands on Session on Bioinformatics'. 2nd Conference on Drug Development for the Third World: from Computational Molecular Biology to Experimental Approaches. 1st -5th June 2009. Trieste, Italy
9. 'Molecular Systems Biology Insights from Bioinformatics'. Computer Design and Discovery of Potential Drugs for Developing Countries'. ICS-UNIDO, 8th - 12nd June. 2009, Trieste, Italy.
10. 'El Proyecto ENCODE: Desde el genoma a las proteínas: un viaje de ida y vuelta'. July 11th 2008. Universidad del Sur, Bahia Blanca, Argentina
11. 'New perspectives in protein landscape of the human genome: the Encode project'. April 11th 2008. University of Padova, Padova , Italy
12. Bioinformatica: dalla genomica alla farmacogenomica.XVII Settimana della cultura scientifica e tecnologica. April 20th 2007. Cagliari, Italy
13. "Aspetti chiave nella bioinformatica delle proteine e la loro utilità pratica". 12 Maggio 2006 Villa Mondragone, Frascati (Roma). Università degli Studi di Roma 'Tor vergata'. Simposio dei dottorandi.
14. "Evaluating the usefulness of protein structure models for molecular replacement. ECCB 2005 - Madrid, Spain.
15. "Structural models of HCN ion channels". CECAM Discussion Meeting 'Ion Channels: from Biology to Physic'. Lyon -France (2002)

Teaching activities

Alejandro Giorgetti is an *Assistant Professor of the University of Verona*. The teaching activities regard principally the different areas of bioinformatics, in particular much emphasis is given to protein structural bioinformatics. A detailed list of the teaching activities during the last years include:

- Professor of the postgraduate course: Biofisica Molecular Computacional. Universidad

Nacional del Sur, Bahia Blanca, Argentina. June 2012.

- Professor of the course: Structural Bioinformatics. 2012. PhD course: Physics and Chemistry of Biological Systems. International School for Advanced Studies (SISSA/ISAS) Trieste, Italy.
- 2011 and 2012 Teaching of the Protein Bioinformatics module of the elective course: 'Computational Molecular Biology', German Research School for Simulation Sciences, Jülich, Germany.
- 'DNA Software'. BioNoCo extension courses: Software Tools. Aachen University, Aachen, Germany. 27th - 28th October 2011.
- Since 2007 : Lecturer (Adjunct Professor) of the Bioinformatic courses (laboratories I and II) in the Mathematical, Physical and Natural Sciences Faculty of the University of Verona.

Details (Italian):

- 2007 - 2008. Titolare corso Bioinformatica, Laurea Specialistica in Biotecnologie Agro-Industriali (4CFU)
 - 2007 - 2008. Titolare corso Lab. di Bioinformatica I, Laurea in Bioinformatica (4CFU)
 - 2008 - 2009. Titolare corso Lab. di Bioinformatica I, Laurea in Bioinformatica (4CFU)
 - 2008 - 2009. Titolare corso Lab. di Bioinformatica II, Laurea in Bioinformatica (4CFU)
 - 2008 - 2009. Titolare corso Banche Dati Biomolecolari, Laurea in Biotecnologie Agro-Industriali (3 CFU)
 - 2008 - 2009. Titolare corso Bioinformatica Strutturale e Genomica, Laurea in Biotecnologie Molecolari e Industriali (4CFU)
 - 2009 - 2010. Titolare corso Lab. di Bioinformatica I, Laurea in Bioinformatica (6CFU)
 - 2009 - 2010. Titolare corso Lab. di Bioinformatica II, Laurea in Bioinformatica (6CFU)
 - 2009 - 2010. Titolare corso Bioinformatica e Banche Dati Biologiche, Laurea in Biotecnologie (6 CFU)
 - 2009 - 2010. Titolare corso Bioinformatica Avanzata, Laurea Magistrale in Biotecnologie Agro-Industriali (6 CFU)
 - 2010 - 2011 Titolare corso Lab. di Bioinformatica II, Laurea in Bioinformatica (6CFU)
 - 2010 - 2011 Titolare corso Biologia Computazionale, Laurea Magistrale in Bioinformatica e Biotecnologie Mediche. (6 CFU)
 - 2011 - 2012 Titolare corso Lab. di Bioinformatica II, Laurea in Bioinformatica (6CFU)
 - 2011 - 2012 Titolare corso Biologia Computazionale, Laurea Magistrale in Bioinformatica e Biotecnologie Mediche. (6 CFU)
 - 2012 - 2013 Titolare corso Lab. di Bioinformatica II, Laurea in Bioinformatica (6CFU)
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- Professor: 'Database search'. Master in Biotecnologie Bioinformatiche applicate alla Medicina personalizzata. Pula (CA) - Italy; June, 2007
 - Professor: 'Structure Prediction'. Master in Biotecnologie Bioinformatiche applicate alla Medicina personalizzata. Pula (CA) , Italy; July, 2007.
 - Professor: 'Database search'. Master in Biotecnologie Bioinformatiche applicate alla Medicina personalizzata. Pula (CA) - Italy; June 5th - 15th, 2006 -
 - Professor: 'Structure Prediction'. Master in Biotecnologie Bioinformatiche applicate alla Medicina personalizzata. Pula (CA), Italy; July 3rd - 7th , 2006.
 - Tutor in the "Continuing Professional Development - Bioscience Programme" . Module: "The Experimental-Bioinformatics Interface - Key Issues in Protein Bioinformatics". Oxford University, UK from 16th to 20th January 20 .
 - Instructor of the 3rd Biosapiens Permanent European School in Bioinformatics. Madrid - Spain (2005).-

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- Instructor of the 1st Biosapiens Permanent European School in Bioinformatics. Verona, Italy (2004).

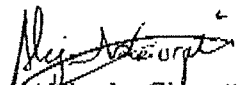
Program Committee member

- BIRD08, ECCB08, ITBAM 2009, BMIC 2009, BIOINFORMATICS 2010

Local Organizing committee:

- ECCB08, September 2008, Cagliari, Italy

19-10-2012
Verona, Italy


Alejandro Giorgetti

