Alejandro Giorgetti, PhD.

Assistant Professor

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Curriculum Vitae

Since 2007	*Assistant Professor (tenured)* at the University of Verona. Faculty of Mathematical, Physical and Natural Sciences, Department of Biotechnology. Verona, Italy
2011 - 2014	*Visiting Scientist* at the German Research School for Simulation Sciences (GRS). Juelich, Germany
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 (tenured) 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 Alejandro Giorgetti 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. Alejandro Giorgetti 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. Structural neuroinformatics: Modelling of proteins/receptors of neurological interest. Those include
   a) Receptors involved in chemoperception: Bitter taste receptors and olfactory receptors.
   b) Receptors involved in neurodegenerative diseases: GPR3 receptors.
   c) Oxytocin receptors.
2. Development of multiscale approaches for gaining insights into the structure function of receptors of neurobiological interest: GOMODO server for modelling and docking of GPCR receptors and the coarse-grained/molecular mechanics (CG/MM) hybrid approach
3. Chemoinformatics: Deorphanizing olfactory receptors by the use of bioinformatics techniques and chemoinformatic approaches.
4. **Membrane protein modelling at genomic level:** 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.

5. Interaction of HIV-1 proteins with its human counterpart, i.e. hTE8/Nef and HLA-C/env.
6. Effects of mutation on protein structure and disease. This project is carried out in collaboration with the Personal Genomics at the University of Verona. The aim is to analyse the effect of mutations detected by Next Generation Sequencing approaches.

Publications[1] *(*: corresponding author).*

- Last five years (2010 - 2014)

1. A. Grison, S. Zucchelli, A. Urzì, I. Zamparo, D. Lazarevic, G. Pascarella, P. Roncaglia, **A. Giorgetti**, P. Garcia-Esparcia, C. Vlachouli, R. Simone, F. Persichetti, A.R.R. Forrest, Y. Hayashizaki, P. Carloni, I. Ferrer, C. Lodovichi, C. Plessy, P. Carninci, S. Gustincich. Mesencephalic dopaminergic neurons express a repertoire of olfactory receptors and respond to odorant-like molecules ***BMC Genomics***, vol. 15, ***2014***, pp. 729-744

2. Piccoli S., Musiani F. and **Giorgetti A***. (2014). "Dynamic characterization and substrate binding of cis-2,3-dihydrobiphenyl-2,3-diol dehydrogenase, an enzyme used in bioremediation". ***Journal of Molecular Modeling. 20(12):2531***

3. Astegno, A. Allegrini, Piccoli S., **Giorgetti A.** and Dominici P. (2014). "Role of Active-Site Residues Tyr55 and Tyr114 in Catalysis and Substrate Specificity of Corynebacterium diphtheriae C-S Lyase." ***Proteins***, 83(1):78-90

4. Montioli R, Dindo M, **Giorgetti A**, Piccoli S, Cellini B, Voltattorni CB. A comprehensive picture of the mutations associated with aromatic amino acid decarboxylase deficiency: from molecular mechanisms to therapy implications. ***Hum Mol Genet.*** **2014** Oct 15;23(20):5429-40

5. Costantini S, Malerba G, Contreas G, Corradi M, Marin Vargas SP, **Giorgetti A**, Maffeis C. Genetic and bioinformatics analysis of four novel GCK missense variants detected in Caucasian families with GCK-MODY phenotype. ***Clin Genet.*** **2014** Apr 16. doi: 10.1111/cge.12406. [Epub ahead of print]

6. S. Piccoli, M. Andreolli, **A. Giorgetti**, F. Zordan, Silvia Lampis, G. Vallini, Identification of aldolase and ferredoxin reductase within the dbt operon of Burkholderia fungorum DBT1. ***Journal Of Basic Microbiology***, vol. 54, n. 5, **2014**, pp. 464-469

7. **Giorgetti, A.** "Membrane Proteins: Insights from computational biology" (2014) ***Biology and Medicine***, 6 (1), art. no. 1000e101

8. **Giorgetti, A.** Multi-scale computational biology (2014) Biology and Medicine, 6 (1), art. no. 1000e102

9. Sandal, M.; Paltrinieri, D.; Carloni, P.; Musiani, F.; **Giorgetti, A***. "Structure/Function Relationships of Phospholipases C Beta". ***Curr Protein Pept Sci.*** 2013 Dec;14(8):650-7

10. Sandal, M.; Duy, T.P.; Cona, M.; Zung, H.; Carloni, P.; Musiani, F.; **Giorgetti, A.*** **(2013)** "GOMoDo: a GPCRs online modeling and docking webserver". ***PLOS ONE***, vol. 8, p. 1-12

11. Alessandra Astegno, **Alejandro Giorgetti**, Alessandra Allegrini, Barbara Cellini and Paola Dominici. **(2013)** "Characterization of C-S Lyase from C.diphtheriae: a possible target for new antimicrobial drugs". ***BioMed Research International. vol. 2013, p. 1-13.***

[1] H-index= 11 and total number of citations= 415 as from Scopus database (14/11/2014).

12. Stefano Piccoli, Eda Suku, Marianna Garonzi and **Alejandro Giorgetti*** (2013). Genome-wide Membrane Protein Structure Prediction. *Current Genomics* (14), pp: 324 – 329.

13. Alessandro Marchiori, Luciana Capece, **Alejandro Giorgetti,** Paolo Gasparini, Maik Behrens,Paolo Carloni,Wolfgang Meyerhof, Coarse-Grained/Molecular Mechanics of the TAS2R38 Bitter Taste Receptor: Experimentally-Validated Detailed Structural Prediction of Agonist Binding «*PLoS ONE*» , vol. 8 , n. 5 , 2013 , pp. 1-12

14. Bisha I, Laio A, Magistrato A, **Giorgetti A** and Sgrignani J. (2013). A Candidate Ion-Retaining State in the Inward-Facing Conformation of Sodium/Galactose Symporter: Clues from Atomistic Simulations. *J. Chem. Theory Comput.*, 2013, *9* (2), pp 1240−1246

15. 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

16. **Giorgetti A.**, P. Ruggerone, S. Pantano, and P. Carloni, Advanced Computational Methods in Molecular Medicine, *Journal of Biomedicine and Biotechnology*, 2012: p. 709085.

17. 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.

18. 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

19. Piccoli, S. and **Giorgetti A***. Perspectives on Computational Structural Bio-Systems. **J Bioproces Biotechniq 2011,1:104e**

20. 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

21. Griguoli M.; Maul A.; Nguyen C.; **Giorgetti A.**; Carloni P.; Cherubini E. (2010). *Nicotine blocks the hyperpolarization-activated current Ih and severely impairs the oscillatory behavior of orienslacunosum molecular interneurons.* ***THE JOURNAL OF NEUROSCIENCE***, pp. 10773-10783 Vol.30

22. 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

23. 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

24. Mazzolini M.; Marchesi A.; **Giorgetti A.**; Torre V. (2010). *Gating in CNGA1 channels.* ***PFLUGERS ARCHIV***, pp. 547- 555 Vol.459

- Previous: 2003 - 2009

25. 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

26. 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

27. 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

28. Cozzetto D, **Giorgetti A**, Raimondo D, Tramontano A. (2008). *The Evaluation of Protein Structure Prediction Results..* ***MOLECULAR BIOTECHNOLOGY***, pp. 1- 8 Vol.39

29. 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

30. Tramontano, D. Cozzetto, **A. Giorgetti**, D. Raimondo.(2007) *The assessment of methods for protein structure prediction.* **Methods in Molecular Biology** 413, pp. 43-57

31. 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

32. 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

33. **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.

34. 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

35. **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.

36. **Giorgetti A**, Carloni P, Mistrik P, Torre V. *A Homology Model of the Pore Region of HCN channels.* ***BIOPHYSICAL J.*** 89(2):932-944.

37. **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.

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

Book chapters

1. Musiani F, Rossetti G, **Giorgetti A***, Carloni P. *Chemosensorial G-proteins-coupled receptors: a perspective from computational methods. Adv Exp Med Biol. 2014;805:441-57.*

2. **Giorgetti A.** and Carloni P. *"Molecular Mechanics/Coarse-Grained models". 2014 pag 165 - 174. In 'Protein Modelling'; editor: Gábor Náray-Szab. Springer. ISBN: 978-3-319-09975-0*

3. **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).*

4. *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*

5. *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*

Editorial activities

- *Member of the editorial board* of the journal: *Scientific Reports* (Nature group).
- *Guest editor for the special issue on* "Advanced Computational Methods in Molecular Medicine". Journal of Biomedicine and Biotechnology.
- *Guest editor* of the special issue on "Bioinformatics Applications in Life Sciences and Technologies". *BioMed Research International.*
- *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. 'Ligand binding mechanisms of bitter taste receptors: Insights from multiscale computational approaches'. 9th International Conference on Computational Physics; Symposia on Multiscale Modeling and Simulations. 7 - 11 January **2015**, Singapore National University, Singapore.
2. 'Multiscale simulation approaches: Insights into the ligand binding mechanisms of bitter taste receptors'. IBBI14 Conference on Isolated Biomolecules and Biomolecular Interactions. May 18th-23rd, **2014**. Location: Porquerolles, France.
3. 'Molecular mechanics/coarse-grained simulations: Insights into the ligand binding mechanisms of GPCRs'. Computational Driven Drug Discovery. 3rd Meeting, March 4th-5th-6th, **2014**. Location: Verona, Italy.
4. '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.
5. 'Structural Bioinformatics approaches to chemical senses'. The International Conference in Computational Medicine*Ho Chi Minh City, Vietnam, January 11-12th,* **2012**
6. 'Chemical Senses: Insights from Structural Bioinformatics'. AIMS seminar series. AICES RWTH Aachen University, Aachen, Germany. 5th December **2011**.
7. '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.

8. '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.

9. "Membrane Transporters: Insights from Bioinformatics". International Workshop: From Structure to Function: Influx and Efflux Systems. 6Th - 8th May 2009, Cagliari (IT)

10. Perspectives on Computational Structural/Molecular Systems Biology. March 31st 2009. Dept. of Informatics, University of Verona, Verona, Italy.

11. '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

12. 'Molecular Systems Biology Insights from Bioinformatics'. Computer Design and Discovery of Potential Drugs for Developing Countries'. ICS-UNIDO, 8th - 12nd June. 2009, Trieste, Italy.

13. 'El Proyecto ENCODE: Desde el genoma a las proteinas: un viaje de ida y vuelta'. July 11th 2008. Universidad del Sur, Bahia Blanca, Argentina

14. 'New perspectives in protein landscape of the human genome: the Encode project'. April 11th 2008. University of Padova, Padova , Italy

15. Bioinformatica: dalla genomica alla farmacogenomica.XVII Settimana della cultura scientifica e tecnologica. April 20th 2007. Cagliari, Italy

16. "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.

17. "Evaluating the usefulness of protein structure models for molecular replacement. ECCB 2005 - Madrid, Spain.

18. "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 (Adjunct) 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 lasts years include:

- Professor of the postgraduate course: Biofisica Molecular Computacional. Universidad Nacional del Sur, Bahia Blanca, Argentina. June 2012.
- 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

- 2007 – 2008. Professor of Bioinformatica, Laurea Specialistica in Biotecnologie Agro-Industriali (4CFU)
- 2007 – 2008. Professor of Lab. di Bioinformatica I, Laurea in Bioinformatica (4CFU)
- 2008 – 2010. Professor of Lab. di Bioinformatica I, Laurea in Bioinformatica (4CFU)
- 2008 – 2013. Professor of Lab. di Bioinformatica II, Laurea in Bioinformatica (4CFU)
- 2008 – 2013. Professor of Computational Biology, Laurea Magistrale in Bioinformatica e Biotecnologie Mediche. (6 CFU)

Professorships in Italian universities:

• Professor of **'Bioinformatica Strutturale'** (SSD Bio/10). 2013-2014. PhD school: Physics and Chemistry of Biological Systems. Scuola Internazionale di Studi Superiori Avanzati (SISSA/ISAS) Trieste, Italy. (30 ore)

• Professor of **'Bioinformatica Strutturale'** (SSD Bio/10). 2012-2013. PhD school: Physics and Chemistry of Biological Systems. Scuola Internazionale di Studi Superiori Avanzati (SISSA/ISAS) Trieste, Italy. (30 ore)

• Professor of **'Bioinformatica Strutturale'** (SSD Bio/10). 2011-2012. PhD school: Physics and Chemistry of Biological Systems. Scuola Internazionale di Studi Superiori Avanzati (SISSA/ISAS) Trieste, Italy. (30 ore)

• Professor of: 'Database search'. Master in Biotecnologie Bioinformatiche applicate alla Medicina personalizzata. Pula (CA) - Italy; June, 2007

• Professor of: 'Structure Prediction'. Master in Biotecnologie Bioinformatiche applicate alla Medicina personalizzata. Pula (CA) , Italy; July, 2007.

• Professor of: 'Database search'. Master in Biotecnologie Bioinformatiche applicate alla Medicina personalizzata. Pula (CA) - Italy; June 5th - 15th, 2006.

• Professor of: 'Structure Prediction'. Master in Biotecnologie Bioinformatiche applicate alla Medicina personalizzata. Pula (CA), Italy; July 3rd - 7th , 2006.

PhD thesis director.

- PhD thesis tutor: Dr. Stefano Piccoli, Università degli Studi di Verona (2010 - 2013)

- PhD thesis tutor: Ivan Sciascia, Università degli Studi di Verona (2012 -)

- PhD thesis tutor: Sergio Marin Vargas, Università degli Studi di Verona (2013 -)

- PhD thesis tutor: Mirko Busato, Università degli Studi di Verona (2014 -)

- Co-tutor PhD thesis: Chuong Nguyen. German Research School for Atomistic Simulations e University of Aachen, Germany.(2009 -2012)

- Co-tutor PhD thesis: Massimo Sandal. German Research School for Atomistic Simulations e University of Aachen, Germany