Fabrizio Marinelli

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PERSONAL STATEMENT

The aim of my research is to characterize the molecular mechanisms of prominent biomolecules involved in membrane transport and/or cell signaling. The premise of my studies is that a deeper molecular understanding of such processes will help identifying more effective therapeutic agents for pathophysiological conditions.

My studies entail the use of computationally intensive molecular simulation techniques and are often performed in synergy with experimental collaborators such as structural biologists and biophysicists.

Part of my research efforts is devoted to the development of efficient and rigorous simulation methods to investigate the structural dynamics of biomolecules and to combine simulations and experimental/bioinformatics data.

POSITIONS

National Heart, Lung and Blood Institute, National Institutes of Health, Apr 2016-
Theoretical Molecular Biophysics Section, Bethesda, MD, USA
Staff Scientist.

National Heart, Lung and Blood Institute, National Institutes of Health, Aug 2013-Apr 2016
Theoretical Molecular Biophysics Section, Bethesda, MD, USA
Visiting Fellow. Advisor: Dr. José Faraldo-Gómez

Max Planck Institute of Biophysics, Frankfurt am Main, Germany, Nov 2009 – Aug 2013
Theoretical Molecular Biophysics Department
Postdoctoral Researcher. Advisor: Dr. José Faraldo-Gómez

International School for Advanced Studies (SISSA/ISAS), Statistical and Nov 2005 – Oct 2009
Biological Physics Sector. Trieste, Italy
PhD student. Advisor: Prof. Alessandro Laio

EDUCATION

PhD Statistical and Biological Physics, SISSA/ISAS, Trieste, Italy Nov 2005 – Oct 2009
MS Chemistry, "La Sapienza" University, Rome, Italy Oct 1998 – Feb 2005

PROFESSIONAL MEMBERSHIP & ACTIVITIES

- Member of the Biophysical Society 2009-
- Member of the American Chemical Society 2013, 2018-
- Member of the Society of General Physiologists 2018-

HONORS & AWARDS

- Selected for junior investigator presentation at the GRC conference 'Mechanisms of Membrane Transport'. Jun 2015
- Invited reviewer for the national grants of the Czech Science Foundation Jul 2014
- Selected for junior investigator presentation at the GRC conference 'Protons & Membrane reactions'. Feb 2014
- Max Planck Institute of Biophysics Postdoctoral Fellowship, Frankfurt am Main, Germany. Nov 2009 – Aug 2013
- SISSA/ISAS PhD Fellowship, Trieste, Italy Nov 2005 – Oct 2009
- *Magna cum laude* MS Chemistry Feb 2005

EDITORIAL & ACADEMIC SERVICE

EDITORIAL BOARD MEMBER (**publons.com/a/1375462/**)

- *Scientific Reports* (Nature Publishing Group) 2018-

REVIEWER (**publons.com/a/1375462/**)

- *eLife* 2018-
- *The Journal of General Physiology* 2018-
- *Communications Biology (Nature)* 2018-
- *Proteins: Structure, Function, and Bioinformatics (Wiley)* 2018-
- *BBA Biomembranes (Elsevier)* 2017-
- *Scientific Reports (Nature)* 2015-
- *European Biophysics Journal (Springer)* 2015-
- *The Journal of Physical Chemistry (ACS)* 2013-
- *Journal of Chemical Theory and Computation (ACS)* 2012-
- *Biophysical Journal (Cell Press)* 2010-

SCIENTIFIC SOFTWARE DEVELOPMENT

- Member of the PLUMED consortium [Link] 2019-
- Developer of the *Colvars* simulation software (C++) [Link] 2015-
- Co-contributor to the PLUMED (version 2) simulation software (C/C++) [Link] 2013-
- Co-developer of the METAGUI simulation analysis tool (Tcl/fortran) [Link] 2011-
- Co-developer of the PLUMED (version 1) simulation software (ANSI C) 2009 –2013

INVITED SEMINARS & CONFERENCE TALKS

POSTDOCTORAL

- **EPR Symposium, Rocky Mountain Conference**, Denver, CO, USA 2019
- **Snowmass Summer Biophysics Workshop**, Snowmass, CO, USA 2015
- **Gordon Research Conference**, *'Mechanisms of Membrane Transport'.* Lewiston, ME, USA. 2015
- **NIH Tenure-track investigator job interview.** National Institute on Drug Abuse, National Institutes of Health, Baltimore, MD, USA 2014

- **CNRS Research Scientist job interview.** Physical, Theoretical and Analytical Chemistry. Paris, France 2014
- **CNRS Research Scientist job interview.** Modeling and Analysis of Biological Data and Systems. Paris, France. 2014
- **CNRS Research Scientist job interview.** Chemistry for Living Systems and Medicinal Chemistry. Paris, France 2014
- **Gordon Research Conference**, *'Protons & Membrane reactions'.* Ventura, CA, USA. 2014
- **Membrane Protein Interest Group and Structural Biology Interest Group Postdoc Symposium**, NIH, Bethesda MD, USA 2014
- **Biophysical Society Annual Meeting**, San Francisco, CA, USA 2014
- **Assistant professor job interview** at Universidad de la República, Paysandú, Uruguay 2013
- **PLUMED developers and contributors meeting**, Trieste, Italy 2012
- **European Bioenergetics Conference (EBEC)**, Freiburg, Germany 2012
- **Universidad de la República**, Montevideo, Uruguay 2012
- **Pasteur Institute,** Montevideo, Uruguay
- **CECAM Workshop, '***Exploring Protein Interactions through Theory and Experiment's*, Lausanne, Switzerland 2012
- **Swiss Institute of Bioinformatics**, Laussane, Switzerland 2011
- **Biophysical Society Annual Meeting**, Baltimore MD, USA 2011
- **German Research School for Simulation Sciences**, Jülich, Germany 2010

PhD STUDENT

- **International Workshop (CECAM),** *'From Structure to Function: Influx and Efflux Systems'*, Cagliari, Italy. 2009
- **Mini symposium, Angelos Michaelides group, UCL university**, London, England. 2008
- **Marie Curie Training Course (CECAM),** *'Progress in simulating activated events'*, Casaprota, Italy. 2008

TEACHING & MENTORING

LECTURE SERIES & WORKSHOPS

- Course on Enhanced sampling techniques in classical MD simulations, QUITEL 2016, Montevideo, Uruguay. 2016
- Invited lectures on membrane protein atomistic simulations at the membrane transporters seminar series, Max Planck Institute of Biophysics, Max Planck Institute of Biophysics, Frankfurt, Germany 2013
- Computer Lab of the IMPReS course on modeling & simulation, Max Planck Institute of Biophysics, Frankfurt, Germany 2010
- Computer Lab of Current Techniques in Membrane Proteomics (Module C1) summer school, Goethe University of Frankfurt, Germany 2010
- Invited lectures on kinetics and thermodynamics from biased simulations at the advanced sampling techniques for numerical simulations Ph.D. course, SISSA, Trieste, Italy (in collaboration with Prof. Alessandro Laio). 2009
- Invited lectures on quantum chemistry methods at the computational chemistry course, University "La Sapienza", Rome, Italy (in collaboration with Dr. Luigi Bencivenni). 2005

- Teaching assistant at Physical Chemistry laboratory course, University "La Sapienza", Rome, Italy 2002-2004

MENTORING

- Co-supervisor of Dr. Rahul Banerjee and Dr. Wenchang Zhou in the Theoretical molecular biophysics section (NHLBI, NIH) Currently
- Co-supervisor of Dr. Richard Bradshaw in the Computational Structural Biology Section (NINDS, NIH) Currently
- Co-supervised Irina Shlosman, post baccalaureate in the Theoretical molecular biophysics section (NHLBI, NIH) 2016-2018
- Co-supervised Corinne Nief, summer student in in the Theoretical molecular biophysics laboratory (NHLBI, NIH) 2015
- Co-supervised the Ph.D. research of Carles Corbi-Verge (Ph.D. obtained in late 2012) 2011-2013

PUBLICATION LIST

(●) denotes corresponding authorship

(**#**) denotes equal first author contribution.

Research articles and reviews

POSTDOCTORAL

1. Fiorin G, Marinelli F and Faraldo-Gómez JD (2019). Direct derivation of free energies of membrane deformation and other solvent density fluctuations from molecular dynamics simulations. *J Comput Chem. Accepted.*
2. Bonomi M, Bussi G, Camilloni C, Tribello G, ..., Marinelli F, et al. (2019) Promoting transparency and reproducibility in enhanced molecular simulations. *Nature Methods* 16: 670–673. [Abstract]
3. Li M, Wang Y, Banerjee R, Marinelli F, Silberberg S, Faraldo-Gómez JD, Hattori M, Swartz KJ. Molecular mechanisms of human P2X3 receptor channel activation and modulation by divalent cation bound ATP (2019). *eLife* 8:e47060. [Abstract]
4. Marinelli F●, G. Fiorin (2018). Structural characterization of biomolecules through atomistic simulations guided by DEER measurements. *Structure* 27:359-370. [Abstract].
5. Hustedt E, Marinelli F**#**, Stein R, Faraldo-Gómez JD, Mchaourab H (2018). Confidence Analysis of DEER Data and its Structural Interpretation with Ensemble-Biased Metadynamics. *Biophys. J.* 115: 1200-16. [Abstract]
6. Shlosman I, Marinelli F, Faraldo-Gómez JD, Mindell JA (2017). The prokaryotic Na+/Ca2+ exchanger NCX_Mj transports Na+ and Ca2+ in a 3:1 stoichiometry. *J Gen Physiol*. 150:51-65. [Abstract]
7. Zhou W, Marinelli F●, Nief C, Faraldo-Gómez JD (2017). Atomistic simulations indicate the c-subunit ring of the F1Fo ATP synthase is not the mitochondrial permeability transition pore. *eLife* 6: e23781. [Abstract]
8. Liao J, Marinelli F**#**, Lee C, Huang Y, Faraldo-Gómez JD, Jiang Y (2016). Mechanism of extracellular ion exchange and binding-site occlusion in the sodium-calcium exchanger. *Nat. Struct. Mol. Biol.* 23: 590–599. [Abstract]

9. Marinelli F●, Faraldo-Gómez JD (2015). Ensemble-Biased Metadynamics: A Molecular Simulation Method to Sample Experimental Distributions. *Biophys. J.* 108:2779-82. [Abstract]

10. Branduardi D, Marinelli F, Faraldo-Gómez JD (2015). Atomic-resolution dissection of the energetics and mechanism of isomerization of hydrated ATP-Mg^{2+} through the SOMA string method. *J. Comput. Chem.*, DOI: 10.1002/jcc.23991. [Abstract]

11. Marinelli F, Almagor L, Hiller R, Giladi M, Khananshvili D, Faraldo-Gómez JD (2014). Sodium recognition by the Na^{+}/Ca^{2+} exchanger in the outward-facing conformation. *Proc Natl Acad Sci USA* 111:E5354-62. [Abstract]

12. Corbi-Verge C, Marinelli F**#**, Zafra-Ruano A, Ruiz-Sanz J, Luque I, Faraldo-Gómez JD (2013). Two-state dynamics of the SH3-SH2 tandem of Abl kinase and the allosteric role of the N-cap. *Proc Natl Acad Sci USA* 110:E3372-80. [Abstract]

13. Marinelli F● (2013). Following easy slope paths on a free energy landscape: the case study of the Trp- Cage folding mechanism. *Biophys J* 105:1236-47. [Abstract]

14. Marinelli F●, Sorrenti A, Corvaglia V, Leone V, Mancini G (2012). Molecular description of the propagation of chirality from molecules to complex systems: different mechanisms controlled by hydrophobic interactions. *Chem Eur J* 18:14680–88. [Abstract]

15. Biarnés X, Pietrucci F, Marinelli F, Laio A (2012). METAGUI. A VMD interface for analyzing metadynamics and molecular dynamics simulations. *Comput Phys Commun* 183:203-11. [Abstract]

16. Marinelli F, Kuhlmann SI, Grell E, Kunte HJ, Ziegler C, Faraldo-Gómez JD (2011). Evidence for an allosteric mechanism of substrate release from membrane-transporter accessory binding proteins. Proc Natl Acad Sci USA, 108:E1285-92. [Abstract]

17. Leone V, Marinelli F, Carloni P, Parrinello M (2010). Targeting biomolecular flexibility with metadynamics. *Curr Opin Struct Biol*, 20:148-54. [Abstract]. REVIEW (refereed)

PhD STUDENT

18. Crespo Y, Marinelli F●, Pietrucci F, Laio A (2010). Metadynamics convergence law in a multidimensional system. *Phys Rev E* 81:055701. [Abstract]

19. Cossio P, Marinelli F, Laio A, Pietrucci F (2010). Optimizing the performance of Bias-Exchange Metadynamics: folding a 48-residue LysM domain using a coarse-grained model. *J Phys Chem B* 114:3259-65. [Abstract]

20. Marinelli F, Pietrucci F, Laio A, Piana S (2009). A kinetic model of Trp-cage folding from multiple biased molecular dynamics simulations. *PLoS Comput Biol* 5:e1000452 doi:10.1371/journal.pcbi.1000452. [Abstract]

21. Pietrucci F, Marinelli F, Carloni P, Laio A (2009). Substrate binding mechanism of HIV-1 protease from explicit solvent atomistic simulations. *J Am Chem Soc* 131:11811–18. [Abstract]

22. Bonomi M, Branduardi D, Bussi G, Camilloni C, Provasi D, Raiteri P, Donadio D, Marinelli F, Pietrucci F, Broglia RA, Parrinello M (2009). PLUMED: A portable plugin for free-energy calculations with molecular dynamics *Comput Phys Commun* 180:1961-72. [Abstract]

23. Todorova N, Marinelli F, Piana S, Yarovsky I (2009). Exploring the folding free energy landscape of insulin using bias exchange metadynamics. *J Phys Chem B* 113:3556-64. [Abstract]

24. Piana S, Laio A, Marinelli F, Van Troys M, Bourry D, Ampe C, Martins JC (2008). Predicting the effect of a point mutation on a protein fold: the villin and advillin headpieces and their Pro62Ala mutants. *J Mol Biol* 375:460-70. [Abstract]

MS STUDENT

25. D'Abramo M, Aschi M, Marinelli F, Di Nola A, Amadei A (2007). Theoretical prediction of thermodynamic equilibrium constants of chemical reactions in water. *J Mol Structure Theochem* 811:197–201. [Abstract]
26. Amadei A, Marinelli F, D'Abramo M, D'Alessandro M, Anselmi M, Di Nola A, Aschi M (2005). Theoretical modeling of vibroelectronic quantum states in complex molecular systems: Solvated carbon monoxide, a test case. *J Chem Phys* 122:124506. [Abstract]
27. D'Alessandro M, Marinelli F, D'Abramo M, Aschi M, Di Nola A, Amadei A (2005). Ground and excited electronic state thermodynamics of aqueous carbon monoxide: A theoretical study. *J Chem Phys* 122:124507. [Abstract]

Conference Abstracts

1. Marinelli F, Ficici E, Faraldo-Gómez J (2019). Molecular Basis for Ion Recognition and Transport in a Na+/Ca2+ Exchanger. *62th Biophysical Society Annual Meeting*. Baltimore, MD, USA.
2. Marinelli F, Ficici E, Faraldo-Gómez J (2018). How the Substrate Occupancy of a Membrane Transporter Determines the Viability of its Alternating-Access Mechanism and thus its Functional Specificity. *61th Biophysical Society Annual Meeting*. San Francisco, CA, USA.
3. Marinelli F, (2017). Molecular Breakdown of Double Electron-Electron Resonance Data with Atomistic Simulations. *Biophysical Society Thematic Meeting: Conformational Ensembles from Experimental Data and Computer Simulations.* Berlin, Germany.
4. Marinelli F, Faraldo-Gómez JD (2017). Molecular mechanism of ion exchange and binding-site occlusion in a sodium/calcium exchanger. *Gordon Research Conference, Mechanisms of Membrane Transport.* Colby-Sawyer College, New London, NH, USA.
5. Marinelli F, Faraldo-Gómez JD (2017). Molecular Breakdown of Double Electron-Electron Resonance Data with Atomistic Simulations. *61th Biophysical Society Annual Meeting*. New Orleans, LA, USA.
6. Marinelli F, Faraldo-Gómez JD (2016). Keeping Secondary Transporters under Control: Lessons from a Na^+/Ca^{2+} Exchanger. *60th Biophysical Society Annual Meeting*. Los Angeles, CA, USA.
7. Marinelli F (2015). Ion Occupancy Shapes Conformational Free-Energy Landscape of a Na^+/Ca^{2+} Exchanger and Allosterically Controls Its Alternating-Access Mechanism. *Gordon Research Conference, Mechanisms of Membrane Transport.* Bates College, Lewiston, ME, USA.
8. Marinelli F, Faraldo-Gómez JD (2015). Minimally-biased Metadynamics method to sample conformational ensembles compatible with experimental measurements. *59th Biophysical Society Annual Meeting*. Baltimore MD, USA.
9. Marinelli F, Faraldo-Gómez JD (2014). Molecular basis for ion binding and conformational change in the Na^+/Ca^{2+} exchanger. *Gordon Research Conference, Protons & Membrane Reaction*. Ventura CA, USA.

10. Marinelli F, Faraldo-Gómez JD (2014). Molecular basis for sodium versus calcium binding in the sodium-calcium exchanger. 58th Biophysical Society Meeting. San Francisco CA, USA.
11. Marinelli F, Faraldo-Gómez JD (2013). *Molecular basis for Na^+ vs Ca^{2+} binding to the Na^+/Ca^{2+} exchanger*. *Gordon Research Conference, Mechanisms of Membrane Transport.* Mount Holyoke College South Hadley, MA, USA.
12. Marinelli F, Faraldo-Gómez, JD (2012). Insights into the mechanism of the Na^+/Ca^{2+} exchanger from atomistic dynamics simulations *16th. European Bioenergetics Conference*. Freiburg, Germany.
13. Marinelli F, Kuhlmann SI, Grell E, Bienert R, Kunte H-J, Ziegler C, Faraldo-Gómez J.D (2011). Enhanced substrate release from a TRAP transporter binding protein by allosteric reduction of Its affinity. *Gordon Research Conference, Mechanisms of Membrane Transport*. University of New England, Biddeford, ME, USA.
14. Marinelli F, Kuhlmann S.I., Grell E, Bienert R, Kunte H-J, Ziegler C, Faraldo-Gómez J.D. (2011). Enhanced substrate release from a trap transporter binding protein by remote modulation of its intrinsic conformational dynamics. 55th Biophysical Society Annual Meeting. Baltimore MD, USA.
15. Marinelli F, Piana S, Pietrucci F, Torodova N, Yarovsky I, Laio A (2009). Insights on protein structure and dynamics from multiple biased molecular dynamics simulations. 53rd Biophysical Society Annual Meeting. Boston MA, USA.

BIBLIOMETRICS (Source: Google scholar, 07/12/2019)
Since 2009: 2005 citations (average of 77 per article), H-index = 17