Giacomo Fiorin
curriculum vitae

Mailing: 1900 North 12th Street
Institute for Computational Molecular Science
Biology-Life Sciences Building, Room 113B
Philadelphia, PA 19122-6078

Phone and fax: 215-204-4213, 215-204-2257

Email: giacomo.fiorin@gmail.com

NIH commons ID: **giacomo1**

Education

10/2002 – 12/2006	PhD in Statistical and Biological Physics SISSA - International School for Advanced Studies, Trieste, Italy Thesis advisor: Paolo Carloni
10/1997 – 02/2002	B.S.+M.S. ("Laurea") in Physics University of Padua, Italy Thesis advisor: Enrico Maglione

Appointments

07/2011 – present	Assistant Professor of Research College of Science and Technology and Institute for Computational Molecular Science (ICMS), Temple University
09/2009 – 06/2011	Postdoctoral Research Associate Institute for Computational Molecular Science (ICMS), Temple University Postdoctoral advisor: Michael L. Klein
05/2007 – 08/2009	Postdoctoral Research Associate Center for Molecular Modeling (CMM), University of Pennsylvania Postdoctoral advisor: Michael L. Klein

Publications

(asterisks, when present, indicate equal contributors)

1. **Fiorin G**, Klein ML, Hénin J.
"Using collective variables to drive molecular dynamics simulations."
Mol. Phys. (in press)

2. Wang J, Ma C, Wang J, Jo H, Canturk B, **Fiorin G**, Pinto LH, Lamb RA, Klein ML, DeGrado WF
"Discovery of Dual Inhibitors of WT and the Amatandine-Resistant Mutant, S31N of M2 from Influenza A Virus"
J. Med. Chem. (in press)

3. Wang J, Wu Y, Ma C, **Fiorin G**, Wang J, Pinto LH, Lamb RA, Klein ML, DeGrado WF
"Structure and inhibition of the drug-resistant S31N mutant of the M2 ion channel of influenza A virus"
Proc Natl Acad Sci USA **110**(4):1315-20 (2013)

4. Wang J, Ma C, **Fiorin G**, Carnevale V, Wang T, Hu F, Lamb RA, Pinto LH, Hong M, Klein ML, DeGrado WF.
"Molecular dynamics simulation directed rational design of inhibitors targeting drug-resistant mutants of influenza A virus M2."
J. Am. Chem. Soc. **133**(32):12834-41 (2011).

5. Donald JE*, Zhang Y*, **Fiorin G***, Carnevale V, Slochower DR, Gai F, Klein ML, Degrado WF.
"Transmembrane orientation and possible role of the fusogenic peptide from parainfluenza virus 5 (PIV5) in promoting fusion."
Proc Natl Acad Sci USA **108**(10):3958-63 (2011).

6. **Fiorin G**, Carnevale V, DeGrado WF.
"The flu's proton escort."
(comment on Science 330(6003):505-8 and Science 330(6003):509-12)
Science **330**(6003):456-8 (2010).

7. Carnevale V*, **Fiorin G***, Levine BG*, DeGrado WF and Klein ML.
"Multiple Proton Confinement in the M2 Channel from the Influenza A Virus."
J. Phys. Chem. C **114**(48):20856–20863 (2010).

8. Acharya R*. Carnevale V*, **Fiorin G***, Levine BG*, Polishchuck AL*, Balannik V, Samish I, Lamb RA, Pinto LH, Klein ML, DeGrado WF.
"Structure and mechanism of proton transport through the transmembrane tetrameric M2 protein bundle of the influenza A virus."
Proc Natl Acad Sci USA **107**(34):15075-80 (2010).

9. Vidossich P, **Fiorin G**, Alfonso Prieto M, Derat E, Shaik S, Rovira C.
"On the role of water in peroxidase catalysis: a theoretical investigation of HRP compound I formation."
J. Phys. Chem. B **114**(15):5161-9 (2010).

10. Balannik V, Carnevale V, **Fiorin G**, Levine BG, Lamb RA, Klein ML, DeGrado WF, Pinto LH.
"Functional studies and modeling of pore-lining residue mutants of the influenza A virus M2 ion channel."
Biochemistry **49**(4):696-708 (2010).

11. Hénin J, **Fiorin G**, Chipot C, Klein ML.
"Exploring Multidimensional Free Energy Landscapes Using Time-Dependent Biases on Collective Variables."
J. Chem. Theory Comput. **6**(1):35-47 (2010).

12. **Fiorin G**, Pastore A, Carloni P, Parrinello M.
"Using metadynamics to understand the mechanism of calmodulin/target recognition at atomic detail."
Biophys. J. **91**(8):2768-2777 (2006).

13. **Fiorin G**, Biekofsky RR, Pastore A, Carloni P.
"Unwinding the helical linker of calcium-loaded calmodulin: a molecular dynamics study."
Proteins **61**(4):829-39 (2005). (Cover article)

14. **Fiorin G**, Maglione E, Ferreira LS.
"Theoretical description of deformed proton emitters: nonadiabatic quasi-particle method."
Phys. Rev. C **67**(5):054302 (2003).

Current research interests

Advanced modeling of the human skin barrier

The immediate goal of the project is to refine a fully atomistic model of the lipid matrix of the stratum corneum of human skin, to identify the arrangement of the component molecules (ceramides, cholesterol, and free fatty acids). A secondary objective is to lay the groundwork for the use of modeling to investigate the permeation of chemicals through skin, using MD simulations as a complement to relatively low resolution structural experiments. Work performed in collaboration with Russell H. Devane and Michael Klein. Supported by a 65-million hours DOE-INCITE allocation on the Titan supercomputer (currently ranked as the #1 supercomputer).

Building computational models of membrane fusion.

The project involves using simulations on leadership–class computing resources to understand membrane fusion, a ubiquitous process enabling biological functions ranging from neurotransmitter release at the synapse to viral infection. Work performed in collaboration with Hemant Kashyap and Michael Klein at Temple. Supported by NSF grant CHE-1212416.

Mechanism of conduction by the M2 proton channel from influenza A virus and design of inhibitors against drug-resistant strains

This project is aimed at explaining the proton conduction mechanism of the M2 proton channel from the influenza A virus, and to develop portable molecular models to be used in rational drug design. A broad range of molecular dynamics-based techniques are involved, including simulation in a hydrated bilayer, quantum-mechanical simulations of proton transfers, refinement of NMR and crystallographic structures, and free energy calculations. The data are utilized within a multi-disciplinary approach to determine the structure-activity relationship of new inhibitors against resistant strains of the influenza A virus.
Work performed in collaboration with Hao Dong, Vincenzo Carnevale and Michael Klein at Temple, William DeGrado at UCSF, Robert Lamb and Lawrence Pinto at Northwestern.
Supported by NIH grant U01-AI-074571 (expired).

Enhanced sampling and biasing techniques in molecular dynamics.

This project began as the development of the Collective Variables Module, a software code for enhanced sampling and free energy calculations, and is a continued collaboration primarily with Jérôme Hénin at CNRS, France, and with James Phillips and Chris Harrison at UIUC.

Teaching responsibilities, synergistic activities and outreach

2011 – present	Primary instructor Biostatistics (3 credits) Undergraduate biology + PhD biology and bioengineering Temple University
2012	Experimental determination of protein structures (modulus within Introduction to Structural Bioinformatics) PhD in chemistry and biology, Temple University
2010	Statistical thermodynamics, teaching assistant PhD in chemistry, Temple University
2009	Physical chemistry II, two recitations Undergraduate chemistry, Temple University

2008 – present	End-user support on the NAMD mailing list
2007	Lecturer at the High Performance Computing workshop University of Pennsylvania

Grants and research support

01/2013 – 12/2013	Co-PI with Michael Klein (PI) and Russell DeVane on the project "*Advanced modeling of the human skin barrier*" under the DOE INCITE supercomputing program – 65,000,000 computing hours awarded over 1 year (project mentioned in National Geographic Daily News – 11/12/12)
07/2012 – 06/2015	Co-PI with Michael Klein (PI) and Axel Kohlmeyer on the NSF grant 1212416 "*Building Computational Models to Probe Membrane Fusion*" – $405,999 awarded
07/2011 – present	Allocation manager for ICMS under the NSF-XSEDE, DOE-INCITE and DOE-ERCAP supercomputing programs
01/2011 – 12/2012	Co-PI with Michael Klein (PI), Russell DeVane, Vincenzo Carnevale and Axel Kohlmeyer on the project CHM045 "*Coarse grained molecular dynamics studies of vesicle formation and fusion*" under the DOE INCITE supercomputing program – 48,000,000 computing hours awarded over 2 years

Collaborators

(collaborations more recent than 5 years are listed in boldface)

Mercedes Alfonso-Prieto (Temple); **Victoria Balannik** (Influmedix, Inc.); Paolo Carloni (German Research School – Jülich); **Vincenzo Carnevale** (Temple); **Lidia Cristian** (Influmedix, Inc); **Russell H. DeVane** (Procter & Gamble, Inc); **William F. DeGrado** (UCSF); **Jason E. Donald** (Agrivida, Inc.); Hao Dong (Temple); **Christopher B. Harrison** (University of Illinois at Urbana-Champaign); **Jérôme Hénin** (CNRS, Marseille France); **Robert A. Lamb** (Northwestern); **Benjamin G. Levine** (Michigan State); **Hemant Kashyap** (Temple); **Chunlong Ma** (Northwestern); Michele Parrinello (USI Lugano, Switzerland); Annalisa Pastore (National Institute for Medical Research, UK); **James C. Phillips** (University of Illinois at Urbana-Champaign); **Lawrence H. Pinto** (Northwestern); **Wataru Shinoda** (AIST, Japan); Pietro Vidossich (University of Barcelona); **Jizhou Wang** (Influmedix, Inc.); **Jun Wang** (UCSF), **Yao Zhang** (GlaxoSmithKline)