

Giacomo Fiorin

curriculum vitae

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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 Amantadine-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).