BIOGRAPHICAL SKETCH

Provide the following information for the key personnel and other significant contributors.
Follow this format for each person. **DO NOT EXCEED FOUR PAGES.**

NAME	POSITION TITLE
Provasi, Davide	Assistant Professor
eRA COMMONS USER NAME	

EDUCATION/TRAINING *(Begin with baccalaureate or other initial professional education, such as nursing, and include postdoctoral training.)*

INSTITUTION AND LOCATION	DEGREE *(if applicable)*	YEAR(s)	FIELD OF STUDY
University of Milano (Italy)	M.Sc.	1999	Physics
University of Milano (Italy)	Ph.D.	2003	Physics

A. Personal statement

My background spans a broad range of fields, from the statistical foundations of thermodynamics to physical and computational biology. In particular, I have contributed to develop novel simulation techniques for the effective study of the thermodynamic properties of molecular systems at atomistic resolution, in the general framework of molecular dynamics.

In the last years my interest has been focused on the study of the structural and dynamical determinants of molecular interactions and on the interplay between the formation of molecular complexes and conformational changes of the involved molecules, through the use of enhanced molecular simulation algorithms.

More recently, I have helped to adapt these state-of-the-art computational techniques to key research areas for this application, such as the combined use of different enhanced sampling algorithms to study both ligand recognition and ligand-induced conformational changes in membrane proteins. My skills include a strong expertise in high performance computing.

B. Positions and Honors.

Positions and Employment

1994-1999	M.Sc. in Physics, University of Milano (Italy)
1999-2000	Intern, Mario Negri Institute for Pharmacological Research, Milano (Italy) Epidemiology and Oncology Departments.
2000-2003	Ph.D. in Physics, University of Milano (Italy)
2003-2007	Research Assistant, Physics Department, University of Milano
2008-2009	Postdoctoral Fellow, Department of Structural and Chemical Biology, Mount Sinai School of Medicine, New York, NY.
2009-2012	Instructor, Department of Structural and Chemical Biology, Mount Sinai School of Medicine, New York, NY.
2012-	Assistant Professor, Department of Structural and Chemical Biology, Icahn School of Medicine at Mount Sinai (formerly Mount Sinai School of Medicine), New York, NY.

Other Experience and Professional Memberships

1996-	Member, Italian Physics Society
2000-	Member, Israeli Physics Society
2001-2006	Teaching assistant for Undergraduate courses of Physics for Biotechnology, School of Medicine, University of Milano,
2004-2006	Teaching assistant for Graduate courses of Quantum mechanics of molecules and clusters, Physics Department, University of Milano.

2006-2007	Teaching assistant for Graduate courses of Protein Physics, Physics Department, University of Milano.
2007-2008	Intern, Office of Technology and Business Development, University of Milano.
2008-	Member, Biophysical Society

C. Selected peer-reviewed publications (out of 26 total publications).

1. Camilloni, C., Provasi, D., Tiana, G. and Broglia, R. A. “Optical absorption of a Green Fluorescent Protein variant: environment effects in a density functional study”, J. Phys. Chem. B, 111(2007) 10807
2. Bonomi, M., Gervasio, F. L., Tiana, G., Provasi, D., Broglia, R. A. and Parrinello, M. “Insight in the folding inhibition of the HIV--1 Protease by a small peptide”, Biophys. J., 93(2007) 2813.
3. Camilloni, C., Provasi, D., Tiana, G., Broglia, R. A. “Exploring the Protein G Helix Free Energy Surface by Solute Tempering Metadynamics”, Proteins 71(2008) 1647.
4. Verkhivker, G., Tiana, G., Camilloni, C., Provasi, D. and Broglia, R. A. “Exploring the molecular basis of folding inhibition for unconventional HIV-1 protease inhibitors: a mechanism of structural mimicry in atomistic simulations of biomolecular binding”, Proteins 95(2008), 550-562.
5. Bonomi, M., Branduardi, D., Bussi, G., Camilloni, C., Provasi, D., Raiteri, P., Donadio, D., Marinelli, F., Pietrucci, F., Broglia, R., Parrinello, M., “PLUMED: A portable plugin for free-energy calculations with molecular dynamics”, Computer Physics Communications, 180 (2009) 1961-1972.
6. Provasi, D., Murcia, M., Coller, B.S., and Filizola, M. “Targeted Molecular Dynamics Reveals Overall Common Conformational Changes Upon Hybrid Domain Swing-Out in beta3 Integrins.” Proteins: Struct., Funct. & Bioinf. (2009) 77(2):447-489.
7. Bortolato, A., Mobarec, J.C., Provasi, D., Filizola, M. “Progress in Elucidating the Structural and Dynamic Character of G-Protein Coupled Receptor Oligomers for Use in Drug Discovery Current Pharmaceutical Design” (2009), 15(35):4017-4025.
8. Zhu, J., Zhu, J., Negri, A., Provasi, D., Filizola, M., Coller, B.S., Springer, T.A. “The closed headpiece of integrin aIIbb3 and its complex with an aIIbb3-specific antagonist that does not induce opening” Blood (2010) 116 (23): 5050-5059
9. Provasi, D. and Filizola, M. “Putative Active States of a Prototypic G-Protein Coupled Receptor from Biased Molecular Dynamics” Biophys. J. (2010) 19(10) 2347-2355.
10. Provasi, D., Johnston, J.M., Filizola, M. “Lessons from Free-Energy Simulations of delta-Opioid Receptor Homodimers Involving the Fourth Transmembrane Helix.” Biochemistry (2010) 49 (31): 6771–6776
11. Johnston, J.M., Aburi, M., Provasi, D., Bortolato, A., Urizar, E., Lambert, N.A., Javitch, J.A., Filizola, M. “Making Structural Sense of Dimerization Interfaces of Delta Opioid Receptor Homodimers” Biochemistry (2011) 50(10):1682-90
12. Wang, H., Barreyro, L., Provasi, D., Djemil, I., Torres-Arancivia, C., Filizola, M., Ubarretxena-Belandia, I. “Molecular determinants and thermodynamics of the amyloid precursor protein transmembrane domain implicated in Alzheimer’s disease” J. Mol. Biol. (2011); 408(5):879-895.
13. Fribourg, M., Moreno, J.L., Holloway, T., Provasi, D., Baki, L., Mahajan, R., Park, G., Adney, S.K., Hatcher, C., Eltit, J.M., Ruta, J.D., Albizu, L., Li, Z., Umali, A., Shim, J., Fabiato, A., MacKerell, A.D. Jr., Brezina, V., Sealfon, S.C., Filizola, M., Gonzalez-Maeso, J., Logothetis, D.E. “Decoding the Signaling of a GPCR Heteromeric Complex Reveals a Unifying Mechanism of Action of Antipsychotic Drugs” Cell (2011) 147 (5):1011-1023
14. Provasi, D., Camacho-Artacho, M., Negri, A., Mobarec, J.C., Filizola, M. “Ligand-Induced Modulation of the Free-Energy Landscape of G Protein-Coupled Receptors Explored by Adaptive Biasing Techniques.” PLOS Computational Biology (2011) 7(10):e1002193.
15. Johnston, J.M., Wang, H., Provasi, D., Filizola, M. “Assessing the Relative Stability of Dimer Interfaces in G Protein-Coupled Receptors.” PLOS Computational Biology (2012) 8(8):e1002649.
16. Coudray, N., Valvo, S., Hu, M., Lasala, R., Kim, C., Vink, M., Zhou, M., Provasi, D., Filizola, M., Tao, J., Fang, J., Penczek, P.A., Ubarretxena-Belandia, I., Stokes, D.L. “Inward-Facing Conformation of the Zinc Transporter YiiP revealed by Cryo-electron Microscopy” Proceedings of the National Academy of Science USA (2013) 110(6):2140-2145
17. Scarabelli, G., Provasi, D., Negri, A., and Filizola, M. “Bioactive Conformations of Two Seminal Delta Opioid Receptor Penta-peptides Inferred from Free-Energy Profiles” Biopolymers (2014) 101(1):21-27.

18. Provasi, D., Negri, A., Coller, B.S., Filizola, M. “Talin-driven inside-out activation mechanism of platelet αIIbβ3 integrin probed by multi-microsecond, all-atom molecular dynamics simulations” PROTEINS Proteins: Struct., Funct. & Bioinf. (2014) DOI: 10.1002/prot.24540.

C. Research Support

None