

Extended Curriculum vitae: Luciano Andrés Abriata, PhD

Born 1981. Argentinian & Italian. Swiss permit B. e-mail: luciano.abriata@epfl.ch Website: <http://labriataphd.altervista.org/>

Languages: Native Spanish, Fluent English, Good Italian, Basic French.

Education and Research Positions

- **January 2017 - present: Biological NMR specialist**, Protein Expression and Structure Facility, EPFL, Switzerland.
- **June 2012 - present: Research assistant** (started with **EMBO long-term** postdoctoral fellowship), Dal Peraro lab, École Polytechnique Fédérale de Lausanne, Switzerland.
- **April 2010 – May 2012: Postdoctoral fellow** (CONICET fellowship), A. Vila lab, IBR-CONICET, Argentina.
- **March 2005 – March 2010: PhD in Chemistry** (ANPCyT/CONICET fellowships), A. Vila lab, IBR-CONICET, Argentina. Marked 10/10.
- **October 2004 – February 2005: Trainee** at the Magnetic Resonance Center, Italy.
- **March 1999 – September 2004: Lic. in Biotechnology** (5-year career): School of Biochemistry – University of Rosario, Argentina. Final thesis supported by an award from Fundación Josefina Prats. Marked 10/10.
- **Key extension courses:** EMBO course on biological NMR (2009), CECAM course on MD simulations (2012), “Dissolution Dynamic Nuclear Polarization” course at EPFL (2013), EMBO Laboratory Management course (2014), EMBO course on Biomolecular Simulations (2014)

Teaching and Academic Positions of Responsibility

- Ongoing: Reviewer** for grant agencies (ANPCyT, Argentina) and for international journals: *Nature Protocols*, *Scientific Reports* (NPG), *Bioinformatics*, *Briefings in Bioinformatics*, *Databases*, *PLoS One*, *ChemPhysChem*, *Biopolymers*, *J. Chem. Theor. Comp.* (ACS), *J. Phys. Chem. B* (ACS) - **Invited lecturer** at the course Biomolecular Structure and Mechanics at EPFL - **Cosupervision** of Master students.
- April 2010 – May 2012: **Evaluation of undergraduate theses** for the School of Biochemistry of the University of Rosario, Argentina.
 - March 2009 – December 2011: **Cosupervisor** of two **undergraduate theses** at the National University of Rosario, Argentina.
 - March 2001 – September 2009: **Laboratory assistant** at the School of Biochemistry of the University of Rosario, in the areas of Physical Chemistry, Biotechnological Processes and Biophysics, Argentina
 - 2007-2010: **Instructor of practical activities** for courses like the **EMBO NMR practical course** “Structure and dynamics of biomolecules by NMR spectroscopy” held in 2009 in Argentina.

Fellowships, Awards and Grants in the last 4 years

- November 2014: Award from **Sociedad Argentina de Biofísica** for the best PhD thesis on biophysics.
- September 2014: Granted access to **2 million CPU hours** from **CSCS** (Swiss National Supercomputing Center, estimated USD 40,000).
- November 2013: Granted access to **8 million CPU hours** from **PRACE** (Partnership for Advanced Computing in Europe) for 2014 (estimated USD 160,000).
- October 2013: **Travel grant** to attend the Black Forest Focus 9 conference *Protein Dynamics: From Water Hydration to Crowding Effects*, Germany.

- June 2012 – May 2014: **EMBO Long-Term** postdoctoral fellow.

Selected Conference and Invited Talks from the last 4 years

- **Abriata LA**, Proteins: from the Protein Data Bank and Structural Bioinformatics to Dynamics and Beyond, *IV Workshop em Métodos Computacionais Aplicados às Ciências Farmacêuticas*, UFRJ, Brasil, **2016**
- **Abriata LA** and Dal Peraro M, Understanding amino acid variation in terms of protein structure, dynamics and function, *CECAM Conference: Enzyme Engineering: Bright Strategies from Theory and Experiments*, Switzerland, **2016**
- **Abriata LA**, Spiga E and Dal Peraro M, Experimental and Computational Studies of the Effects of Highly Concentrated Solutes on Proteins: Insights Into the Causes and Consequences of Quinary Protein Structure and Cytoplasmic Organization. *The 29th Annual Symposium of the Protein Society*, Spain, **2015**
- **Abriata LA** Integrative and knowledge-based modeling of biomolecular systems. *Meeting of the Life Sciences PostDocs of the ETH domain*, Switzerland, **2015**
- **Abriata LA**. On the physicochemical traits that constrain the sequence space of functional proteins: insights from TEM lactamases, *12th β -Lactamase Meeting International Workshop*, Spain, **2014**
- **Abriata LA**. Data mining of protein structure, dynamics and function, *Joint Conference of the Argentinian and Latin American Associations for Biological Computing and Bioinformatics*, Argentina, **2013**

Full List of Peer-Reviewed Publications

(superscripts **1** and **#** indicate first and corresponding authorships, respectively)

All publications up to date in my [Google Scholar Profile](#)

- 33- Abriata LA[#]**, Spiga E and Dal Peraro M[#]. Molecular Effects of Concentrated Solutes on Protein Hydration, Dynamics, and Electrostatics. *Biophysical Journal* (**2016**) Aug 23;111(4):743
- 32- Abriata LA[#]**, Bovigny C and Dal Peraro M. Detection and sequence/structure mapping of biophysical constraints to protein variation in saturated mutational libraries and protein sequence alignments with a dedicated server. *BMC Bioinformatics* (**2016**) Jun 17;17(1):242.
- 31-** Song AS, Poor TA, **Abriata LA**, Jardetzky TS, Dal Peraro M, Lamb RA, Immobilization of the N-terminal helix stabilizes prefusion paramyxovirus fusion proteins. *Proc Natl Acad Sci U S A* (**2016**) Jul 5;113(27):E3844-51.
- 30- Abriata LA[#]**. Structural database resources for biological macromolecules. *Briefings in Bioinformatics* (**2016**) Jun 5. pii: bbw049
- 29-** Gonzalez M, **Abriata LA**, Tomatis P, and Vila A. Optimization of Conformational Dynamics in an Epistatic Evolutionary Trajectory. *Molecular Biology and Evolution* (**2016**) in press.
- 28-** Garavaglia BS, Zimaro T, **Abriata LA**, Ottado J, Gottig N. XacFhaB adhesin, an important *Xanthomonas citri* subsp. *citri* virulence factor, is recognized as a pathogen-associated molecular pattern. *Molecular Plant Pathology* (**2016**) in press.
- 27-** Morgada MN, **Abriata LA**, Cefaro C, Gajda K, Banci L, Vila AJ. Loop recognition and copper-mediated disulfide reduction underpin metal site assembly of CuA in human cytochrome oxidase. *Proc Natl Acad Sci U.S.A.* (**2015**) Sep 22;112(38):11771-6

- 26- Kolly GS, Mukherjee R, Kilacsková E, **Abriata LA**, Raccaud M, Blaško J, Sala C, Dal Peraro M, Mikušová K, Cole ST. GtrA Protein Rv3789 Is Required for Arabinosylation of Arabinogalactan in *Mycobacterium tuberculosis*. *Journal of Bacteriology* (2015)
- 25- Saita E¹, **Abriata LA**¹, Tsai Y, Trajtenberg F, Lemmin T, Buschiazzo A, Dal Peraro M, de Mendoza D and Albanesi D. A coiled coil switch mediates cold sensing by the thermosensory protein DesK. *Molecular Microbiology* (2015) Oct;98(2):258-71. (co-first author with E. Saita)
- 24- Zitare U, Álvarez-Paggi D, Morgada NM, **Abriata LA**, Vila AJ and Murgida DH, Reversible Switching of Redox-Active Molecular Orbitals and Electron Transfer Pathways in CuA Sites of Cytochrome *c* Oxidase. *Angewandte Chemie Intl Ed.* (2015) DOI: 10.1002/anie.201504188
- 23- **Abriata LA**[#] and Dal Peraro M[#], Assessing the potential of atomistic molecular dynamics simulations to probe reversible protein-protein recognition and binding. *Sci. Rep.* (2015) 5:10549
- 22- Tamò GE¹, **Abriata LA**¹ and Dal Peraro M, The importance of dynamics in integrative modeling of supramolecular assemblies. *Curr Opin Struct Biol* (2015) 31:28-34 (co-first author with GE Tamò)
- 21- **Abriata LA**[#], Palzkill T and Dal Peraro M, How structural and physicochemical determinants shape sequence constraints in a functional enzyme. *PLoS One* (2015) 10(2):e0118684
- 20- **Abriata LA**[#], Pontel LB, Vila AJ, Dal Peraro M and Soncini FC, A dimerization interface mediated by functionally critical residues creates interfacial disulfide bonds and copper sites in CueP. *J Inorg Biochem* (2014) 140:199-201
- 19- Spiga E¹, **Abriata LA**¹, Piazza F and Dal Peraro M, Dissecting the Effects of Concentrated Carbohydrate Solutions on Protein Diffusion, Hydration and Internal Dynamics *J. Phys. Chem. B* (2014) 118(20):5310-21 (co-first author with E Spiga)
- 18- Morgada MN, **Abriata LA**, Zitare U, Álvarez-Paggi D, Murgida DH and Vila AJ, Control of the electronic ground state on an electron transfer copper site by second-sphere perturbations *Angewandte Chemie Intl Ed.* (2014) 53(24):6188-92
- 17- **Abriata LA**[#], Vila AJ and Dal Peraro M, Molecular dynamics simulations of apocupredoxins: insights into the formation and stabilization of copper sites under entatic control. *J Biol Inorg Chem* (2014) 19(4-5):565-75
- 16- **Abriata LA**¹ and Vila AJ, Redox-state sensing by hydrogen bonds in the CuA center of cytochrome *c* oxidase. *J Inorg Biochem* (2014) 132:18-20
- 15- Sorrequieta A, **Abriata LA**, Boggio SB and Vale EM, Off-the-Vine Ripening of Tomato Fruit Causes Alteration in the Primary Metabolite Composition. *Metabolites* (2013) 3(4), 967-978
- 14- Alvarez-Paggi D, **Abriata LA**¹, Murgida DH and Vila AJ, Native CuA redox sites are largely resilient to pH variations within physiological range. *Chem Commun* (2013) 49(47):5381-3
- 13- **Abriata LA**¹, Spiga E, Dal Peraro M, All-atom simulations of crowding effects on ubiquitin dynamics. *Phys Biol* (2013) 10(4):045006
- 12- **Abriata LA**[#], Investigation of non-corrin Co(II)-containing sites in protein structures of the Protein Data Bank. *Acta Crystallogr B* (2013) 69(Pt 2):176-83
- 11- **Abriata LA**¹, Zaballa ME, Berry RE, Yang F, Zhang H, Walker FA and Vila AJ. Electron Spin Density on the Axial His Ligand of High-Spin and Low-Spin Nitrophorin 2 Probed by Heteronuclear NMR Spectroscopy. *Inorg Chem* (2013) 52(3):1285-95
- 10- **Abriata LA**¹, Alvarez-Paggi D, Ledesma GN, Blackburn NJ, Vila AJ and Murgida DH. Alternative ground states enable pathway switching in biological electron transfer. *Proc Natl Acad Sci U S A* (2012) 109(43):17348-53

- 9- **Abriata LA^{1#}**, Analysis of copper-ligand bond lengths in X-ray structures of different types of copper sites in proteins. *Acta Crystallogr D Biol Crystallogr* (2012) 68(9):1223-31
- 8- **Abriata LA^{1#}**, Salverda MLM, Tomatis PE. Sequence-function-stability relationships in proteins from datasets of functionally annotated variants: the case of TEM β -lactamases. *FEBS Lett* (2012) 586(19):3330-5
- 7- **Abriata LA^{1#}**, Utilization of NMR spectroscopy to study biological fluids and metabolic processes: Two introductory activities. *Conc Magn Reson A* (2012) 40A(4):171-178
- 6- Zaballa ME, **Abriata LA**, Donaire A, Vila AJ. Flexibility of the metal-binding region in apo-cupredoxins. *Proc Natl Acad Sci U S A* (2012) 109(24):9254-9
- 5- **Abriata LA^{1#}**, A simple spreadsheet program to simulate and analyze the far-UV circular dichroism spectra of proteins, *J Chem Educ* (2011) 88(9):1268-1273
- 4- **Abriata LA¹**, Ledesma GN, Pierattelli R and Vila AJ, Electronic Structure of the Ground and Excited States of the CuA Site by NMR Spectroscopy, *J Am Chem Soc* (2009) 131(5):1939-46
- 3- **Abriata LA¹**, Cassina A, Tórtora V, Marín M, Souza JM, Castro L, Vila AJ and Radi R, Nitration of solvent-exposed tyrosine-74 on cytochrome *c* triggers heme iron-methionine-80 bond disruption: Nuclear magnetic resonance and optical spectroscopy studies, *J Biol Chem* (2009) 284(1):17-26 (Journal Cover)
- 2- **Abriata LA¹**, Banci L, Bertini I, Ciofi-Baffoni S, Gkazonis P, Spyroulias G, Vila AJ and Wang S, Mechanism of CuA Assembly, *Nature Chem Biol* (2008) 4(10):599-601
- 1- **Abriata LA¹**, González LJ, Llarrull LI, Tomatis PE, Myers WK, Costello AL, Tierney DL and Vila AJ, Engineered Mononuclear Variants in *Bacillus cereus* Metallo-beta-lactamase BcII are Inactive, *Biochemistry* (2008) 47(33):8590-9

Unreviewed Preprints

- **Abriata LA**, Homology- and coevolution-consistent structural models of bacterial copper-tolerance protein CopM support a “metal sponge” function and suggest regions for metal-dependent protein-protein interactions (cited in *Elife* 2015, *Acta Cryst. D* 2016 and *Science* 2017)

Book Chapters

- **Abriata LA**, *Computational tools for structural analysis of proteins*, to appear in Elsevier's Reference Module in Life Sciences (2017)
- **Abriata LA**, Homology- and coevolution-consistent structural models of bacterial copper-tolerance protein CopM support a “metal sponge” function and suggest regions for metal-dependent protein-protein interactions
- **Abriata LA¹**, Zaballa ME and Vila AJ, *New Approaches for the Study of Paramagnetic Metalloproteins* in “*Advances in Biomedical Spectroscopy, volume 3: Biomolecular NMR Spectroscopy*”, S. Pascal and A. Dingley editors. (2011) IOS Press, The Netherlands, ISBN 1875-0656.
- Carraro F, Scarpeci T, **Abriata LA**, Vila AJ y Valle E, Capítulo 10 - *Metabólica*, in *Biotecnología y Mejoramiento vegetal II* (2009) ISBN 987-521-138-9