Leonardo Boechi

Contact Information

Intendente Güiraldes 2160, Ciudad Universitaria
Edificio Cero*Infinito
Ciudad Autónoma de Buenos Aires, C1428EGA, Argentina
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Professional Experience

Research associate CONICET — 2014-Present
Instituto de Cálculo
University of Buenos Aires, Argentina

Postdoctoral scholar
Advisor: Prof. J. Andrew McCammon — 2012-2014
University of California, San Diego (UCSD)

Advisor: Prof. Peter G. Wolynes — 2011-2012
University of California, San Diego (UCSD)

Grants

Pew Latin American Repatriation Award — 2015
The Pew Charitable Trusts, $35.000

Award of repatriation — 2016
The Bunge & Born Fundation, $35.000

Young researcher grant (PICT) — 2016-2018
ANPCyT$5.000

Honors

Pew Latin American Fellow, U.S.A. — 2012-2014

CONICET Doctoral Fellowship (type II), Argentina — 2008-2011

ANPCyT Doctoral Fellowship, Argentina — 2006-2008

Education

Ph.D., Physical Chemistry — March 2011
Advisor: Prof. Darío Estrin
University of Buenos Aires, Argentina

Lic. Biology (M.S. equivalent) — April 2006
Area of specialization: Molecular Biology
University of Buenos Aires, Argentina

Publications

Somacal A, Barrera Y, Boechi L, Jonckheere M, Lefieux V, Picard D, Smucler E. *Uncovering differential equations from data with hidden variables* Physical Review E. 2022;105(5-1):054209

Barrera A, Boechi L, Jonckheere M, Lefieux V, Picard D, Smucler E, Somacal A, Umfurer A. *Clustering high dimensional meteorological scenarios: results and performance index* International Journal of Approximate Reasoning. 2021;139:1-11

Boubeta FM, Bieza SA, Bringas M, Palermo JC, Boechi L, Estrin DA, Bari SE. *Hemeproteins as Targets for Sulfide Species* Antioxid Redox Signal 2019;32(4):247-257

Boubeta FM, Contestin Garcia RM, Lorenzo EN, Boechi L, Estrin D, Sued M, Arrar M. *Lessons learned about steered molecular dynamics simulations and free energy calculations* Chemical Biology and Drug Design 2019;93(6):1129-1138

Arrar M, Boubeta FM, Szretter ME, Sued M, Boechi L*, Rodriguez D. *On the accurate estimation of free energies using the jarzynski equality* Journal of Computational Chemistry 2019; 40(4):688-696

Boubeta FM, Boechi L, Estrin D, Patrizi B, Di Donato M, Iagatti A, Giordano D, Verde C, Bruno S, Abbruzzetti S, Viappiani C. *Cold-Adaptation Signatures in the Ligand Rebinding Kinetics to the Truncated Hemoglobin of the Antarctic Bacterium Pseudoalteromonas haloplanktis TAC125* J Phys Chem B. 2018;282(15):2948-65

Boubeta FM, Bieza SA, Bringas M, Estrin DA, Boechi L, Bari SE. *Mechanism of Sulfide Binding by Ferric Hemeproteins.* Inorg. Chem. 2018;57(13):7591-7600

Boubeta FM, Bari S, Estrin DA and Boechi L*. *Access and binding of H2S to hemeproteins: the case of HbI of Lucina pectinata* J. Phys. Chem. B 2016;120(36):9642-53

Bustamante JP, Szretter ME, Sued M, Marti MA, Estrin DA and Boechi L*. *A quantitative model for oxygen uptake and release in a family of hemeproteins* Bioinformatics. 2016;32(12):1805-13

Bustamante JP, Radusky L, Boechi L, Estrin DA, Ten Have A, Martí MA. *Evolutionary and Functional Relationships in the Truncated Hemoglobin Family* PLoS Comput Biol. 2016;12(1):4701

Boron I, Bustamante JP, Davidge KS, Singh S, Bowman LA, Tinajero-Trejo M, Carballal S, Radi R, Poole RK, Dikshit K, Estrin DA, Marti MA and Boechi L*. *Ligand uptake in Mycobacterium tuberculosis truncated hemoglobins is controlled by both internal tunnels and active site water molecules* F1000research. 2015;23(4):22-37

Bieza SA, Boubeta F, Feis A, Smulevich G, Estrin DA, Boechi L, Bari SE. *Reactivity of inorganic sulfide species toward a heme protein model* Inorg Chem. 2015;54(2):527-533

Howes BD, Boechi L, Boffi A, Estrin DE, Smulevich G. *Bridging Theory and Experiment to Address Structural Properties of Truncated Haemoglobins: Insights from Thermobifida fusca HbO* Adv Microb Physiol. 2015;67:85-126.

Giordano D, Pesce A, Boechi L, Bustamante JP, Caldelli E, Howes BD, Riccio A, di Prisco G, Nardini M, Estrin D, Smulevich G, Bolognesi M, Verde C.*Structural flexibility of the heme cavity in the cold-adapted truncated hemoglobin from the Antarctic marine bacterium Pseudoalteromonas haloplanktis TAC125* FEBS J. 2015;282(15):2948-65

Pesce A, Bustamante JP, Bidon-Chanal A, Boechi L, Estrin DA, Luque FJ, Sebilo A, Guertin M, Bolognesi M, Ascenzi P, Nardini M. *The N-terminal pre-A region of Mycobacterium tuberculosis 2/2HbN promotes NO-dioxygenase activity* FEBS J. 2016;283(2):305-322

Bustamante JP, Bonamore A, Nadra AD, Sciamanna N, Boffi A, Estrin DA, Boechi L. *Molecular basis of thermal stability in truncated (2/2) hemoglobins* BBA. 2014;1840(7):2282-2288

Boechi L, Pierce L, Komives E, McCammon JA. *Trypsinogen activation as observed in accelerated molecular dynamics simulations* Protein Sci. 2014;23(11):1550-1558

Tanner JJ, Boechi L, McCammon JA, Sobrado P. *Insights into the dynamics of UDP-Galactopyranose mutase: towards a rational drug design.* Arch. Biochem. Biophys. 2014;544:128-141

Bustamante JP, Abbruzzetti S, Marcelli A, Gauto D, Boechi L, Bonamore A, Boffi A, Bruno S, Feis A, Foggi P, Estrin DA, Viappiani C. *Ligand uptake modulation by internal water molecules and hydrophobic cavities in hemoglobins* J. Phys. Chem. B 2014;118(5):1234-1245

Boechi L, de Oliveira CA, Da Fonseca I, Kizjakina K, Sobrado P, Tanner JJ, McCammon JA. *Substrate-dependent dynamics of UDP-galactopyranose mutase: Implications for drug design.* Protein Sci. 2013;22(11):1490-1501

Boechi L, Arrar M, Martí MA, Olson JS, Roitberg AE, Estrin DA. *Hydrophobic effect drives oxygen uptake in myoglobin via histidine E7.* J. Biol. Chem. 2013;288(9):6754-6762

Capece L, Boechi L, Perissinotti LL, Arroyo-Mañez P, Bikiel DE, Smulevich G, Marti MA, Estrin DA. *Small ligand-globin interactions: Reviewing lessons derived from computer simulation.* BBA 2013;1834(9):10394-10402

Ferreiro DN, Boechi L, Estrin DA, Martí MA. *The key role of water in the dioxygenase function of Escherichia coli flavohemoglobin.* J. Inorg. Biochem. 2013;119:75-84

Oliveira A, Singh S, Bidon-Chanal A, Forti F, Martí MA, Boechi L, Estrin DA, Dikshit KL, Luque FJ. *Role of PheE15 gate in ligand entry and nitric oxide detoxification function of mycobacterium tuberculosis truncated hemoglobin N.* PLoS One. 2012;7(11):49291

Nicoletti F, Droghetti E, Boechi L, Bonamore A, Sciamanna N, Estrin D, Feis A, Boffi A, Smulevich G. *Fluoride as a probe for H-bonding interactions in the active site of heme proteins: the case of Thermobifida fusca hemoglobin.* J. Am. Chem. Soc. 2011;133(51):8834-41

Forti F, Boechi L, Bikiel D, Martí MA, Nardini M, Bolognesi M, Viappiani C, Estrin DA, Luque FJ. *Ligand Migration in Methanosarcina acetivorans Protoglobin: Effects of Ligand Binding and Dimeric Assembly.* J. Phys Chem B 2011;115(46):13771-13780

Arroyo-Mañez P, Lu C, Boechi L, Martí MA, Shepherd M, Wilson JL, Poole RK, Luque FJ, Yeh SR, and Estrin DA. *Role of the Distal Hydrogen-Bonding Network in Ligand Binding in Campylobacter jejuni truncated hemoglobin III.* Biochemistry 2011;50(19):3946-56

Forti F, Boechi L, Estrin DA, Martí MA. *Combining Implicit ligand sampling (ILS) with Multiple Steered Molecular Dynamics (MSMD) to study ligand migration processes in heme proteins.* J. Comput. Chem. 2011;32(10):2219-2231

Boechi L, Martí MA, Vergara A, Sica F, Mazzarella L, Estrin DA, Merlino A. *Protonation of Histidine 55 affects the oxygen access to heme in the alpha chain of the hemoglobin from the Antarctic fish Trematomus bernacchii.* IUBM Life 2011;63(3):175

Boron I, Russo R, Boechi L, Cheng C, Di Prisco G, Estrin DA , Verde C and Nadra AD. *Structure and dynamics of Antarctic fish Neuroglobin assessed by computer simulations.* IUBMLife 2011;63(3):206

Moreno DM, Martí MA, De Biase PM, Estrin DA, Demicheli V, Radi R, and Boechi L. *Role of Tyr34 nitration in Human MnSOD reactivity* Arch. Biochem Biophys. 2011; 507(2):304-9

Howes BD, Giordano D, Boechi L, Russo R, Mucciacciaro S, Ciaccio C, Sinibald F, Fittipaldi M, Martí MA, Estrin DA, di Prisco G, Coletta M, Verde V, and Smulevich G. *The Peculiar Heme Pocket of the 2/2 Hemoglobin of Antarctic cold-adapted Pseudoalteromonas haloplanktis TAC125.* J. Biol. Inorg. Chem. 2010;16(2):299-311

Droghetti E, Nicoletti FP, Bonamore A, Boechi L, Arroyo Mañez P, Estrin DA, Boffi A, Smulevich G, and Feis A. *Heme pocket structural properties of a bacterial truncated hemoglobin from Thermobifida fusca.* Biochemistry. 2010;49(49):10394-402

Arroyo-Mañez P, Bikiel D, Boechi L, Capece L, Di Lella S, Martí MA, Moreno DM, Nadra A, Petruk A and Estrin D. *Proteins dynamics and ligand migration interplay as studied by computer simulation.* Biochem. Biophys Acta. 2010;1814(8):1054-64.

Bikiel D, Forti F, Boechi L, Nardini M, Luque FJ, Martí MA, Estrin, DA. *Role of heme distortion on oxygen affinity in heme proteins: the Protoglobin case.* J. Phys. Chem. B. 2010;114(25):8536-43.

Nicoletti FP, Comandini A, Bonamore A, Boechi L, Boubeta FM, Feis A, Smulevich G, and Boffi A. *Sulfide Binding properties of truncated hemoglobins.* Biochemistry. 2010;49(10):2269-78.

Boechi L, Arroyo Mañez P, Luque J, Martí MA and Estrin DA. *Unraveling the molecular basis for ligand binding in truncated hemoglobins: the trHbO B. subtilis case.* Proteins. 2010;78(4):962-70.

Giordano D, Boechi L, Vergara A, Martí MA, Samuni U, Dantsker D, Grassi L, Estrin DA, Friedman JM, Mazzarella L, di Prisco G, Verde C. *The hemoglobins of the sub-Antarctic fish Cottoperca gobio, a phyletically basal species–oxygen-binding equilibria, kinetics and molecular dynamics.* FEBS J. 2009;276(8):2266-77.

Boechi L, Martí MA, Milani M, Bolognesi M, Luque FJ, Estrin DA. *Structural determinants of ligand migration in Mycobacterium tuberculosis truncated hemoglobin O.* Proteins. 2008;73(2):372-9.

Bikiel DE, Boechi L, Capece L, Crespo A, De Biase PM, Di Lella S, Gonzalez Lebrero MC, Martí MA, Nadra AD, Perissinotti LL, Scherlis DA, Estrin DA. *Modeling heme proteins using atomistic simulations.* Phys. Chem. Chem. Phys. 2006;8(48):5611-28.

Martí MA, Crespo A, Capece L, Boechi L, Bikiel DE, Scherlis DA, Estrin DA. *Dioxygen affinity in heme proteins investigated by computer simulation.* J. Inorg. Biochem. 2006; 100(4):761-70.

Invited Talks

Antartic Thresholds, Spring Course *Computer simulations of adapted and non-adapted organisms* September 2018. Buenos Aires, Argentina

University of Tehran, "Sulfide binding and reactivity to hemeproteins". September 2017. Tehran, Iran

Institute for Research in Fundamental Sciences, "A quantitative model of oxygen uptake and release in Truncated Hemoglobins". September 2017. Tehran, Iran

Departamento de Química Orgánica, FCEN-UBA *"Mecanismos enzimáticos estudiados a partir de simulaciones computacionales".* November 2013. Buenos Aires, Argentina.

Departamento de Química Biológica, FCEN-UBA *"Plegamiento de proteínas de membrana".* December 2012. Buenos Aires, Argentina.

Universitá degli Studi Roma Trè *"Structure and dynamics of TrHb investigated through Computer Simulation".* September 2010. Roma, Italia.

Universitá degli Studi di Firenze. *"Simulazione computazionale della reattività chimica in emoproteine".* July 2009. Florencia, Italia.

Fundación Instituto de Inmunología de Colombia (FIDIC). *"Simulaciones Computacionales en hemoproteínas".* September 2009. Bogotá, Colombia.

Universidad de Entre Ríos. *"Simulaciones computacionales de hemoproteínas".* September 2009. Paraná, Argentina.

German Research School for Simulation Sciences *"Ligand migration in heme proteins".* August 2010. Jülich, Germany. *Paolo Carloni's group*

University of Florida - QTP. *"Is the simple protonation of HisE7 sufficent to control the oxygen uptake in Myoglobin?"* February 2010. Gainesville, USA. *Adrián Roitberg's group*

Universidad de la República. *"Bases moleculares de la afinidad de Hemoglobinas Truncadas por oxígeno".* June 2009. Montevideo, Uruguay. *Rafael Radi's group*

Conferences

VII Applied math conference (MACI) 2019, Córdoba, Argentina.

XV internacional conference of oxygen binding protein. September 2018, Barcelona, Spain (oral presentation)

Latin American Crosstalk in Biophysics and Physiology. Noviembre 2015. Salto, Uruguay (Poster)

XVIII internacional conference of oxygen binding protein. July 2014. Scheffield, Inglaterra (oral presentation)

58th Annual Meeting Biophysical Society. February 2014. San Diego, USA (Poster)

XLI Reunión Anual de la Sociedad Argentina de Biofísica. December 2012, Tucumán. (Poster)

56th Annual Meeting Biophysical Society. February 2012. San Diego, USA (Poster)

Gordon Research Conference - Proteing Folding Dynamics. January 2012. Ventura, USA (Poster)

XVI International Conference on Oxygen Binding and Sensing Proteins (O2 BIP). August 2010. Antwerp, Belgium. (Poster)

3rd Latin American Protein Society Meeting and Reunión Anual de la Sociedad Argentina de Biofísica. October 2010 - Salta. Argentina. (Poster)

239th ACS National Meeting & Exposition - March 2010. San Francisco, USA.

50th Sanibel Symposium. February/March 2010 - St Simon Island, USA. (Poster)

XXXV Congreso de Quḿicos Teóricos de Expresión Latina (Quitel). September 2009. San Andrés, Colombia (Poster).

VII European Biophysics Congress (EBSA). July 2009. Genova, Italia (Poster).

XVI Congreso Argentino de Fisicoquḿica y Quḿica Inorgánica. May 2009. Salta, Argentina. (oral presentation)

XV International Conference on Oxygen Binding and Sensing Proteins (O2 BIP). August 2008. Aarhus, Denmark. (Poster)

VI International Conference of Biological Physics– 2007. Montevideo - Uruguay (Poster).

XIV Congreso Argentino de Fisicoquḿica y Quḿica Inorgánica – October 2007. Tandil. Argentina (Poster).

XXV Annual Meeting of the Argentinean Biophysical Society – 2006. Rosario. Argentina (oral presentation)

Workshop on Metalloproteins and Biomimetics Coordination Complex - 2006. San Nicolás. Argentina. (oral presentation)

XIV Congreso Argentino de Fisicoquḿica, April 2005. Río Hondo, Argentina (Poster)

Congreso Argentino de Sociedades Biomédicas, November - 2004, Mar del Plata, Argentina. (Poster).

University Involvement and Service

Faculty representative
Instituto de Calculo Advisory Board 2014-2019

Student body representative
INQUIMAE Advisory Board 2009

Grant proposal reviewer
Universidad de Los Andes, Colombia; CSIC, Uruguay; PICT-Mincyt, Argentina 2009-2015

PhD committee member
Dr. Herman Schinca, Universidad de Buenos Aires, Argentina 2015

Dr. Veronica Tortora, Universidad de la República, Uruguay 2014

Peer review for scientific journals
Free Radical Biology and Medicine, Archives of Biochemistry and Biophysics, Biochimica et Biophysica Acta, Journal of Molecular Modeling, Chemical Physics Letters, Journal of Chemical Information and Modeling

Theses directed

Co-director, M.S. 2008-2010
Juan Pablo Bustamante
Universidad Nacional de Entre Rios
Rating: 10/10

Co-director, Ph.D. 2010-2015
Lic. Juan Pablo Bustamante
Universidad de Buenos Aires
Rating: 10/10

Co-director, Ph.D. 2011-2016
Lic. Fernando Boubeta
Universidad de Buenos Aires
Rating: 10/10

Languages

Spanish (native), English, Italian