

# CURRICULUM VITAE

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## Academic Background

PhD in Biology. *Chemical Shifts-Driven Monte Carlo Simulations*. National University of San Luis. 2007-2012.

## Research positions

*Investigador Adjunto*. National Scientific and Technical Research Council (CONICET). 2017-present  
*Investigador Asistente*. National Scientific and Technical Research Council (CONICET). 2014-2017

## Recent scientific publications

Only last five years, visit [google scholar](#) for the entire list.

**Martin O.A.**, Vila J.A. *The Marginal Stability of Proteins: How Jiggling and Wiggling of Atoms are Connected to Neutral Evolution*. Journal of molecular evolution. 2020. (in press)

Arroyuelo A., **Martin, O.A** Scheraga H.A. Vila, J. A. *Assessing the One-Bond Ca-H Spin-Spin Coupling Constants in Proteins: Pros and Cons of Different Approaches*. The Journal of Physical Chemistry B. (2020)

Icazatti A.A, Loyola J.M., Szleifer I, Vila J.A. **Martin O.A.** *Classification of RNA backbone conformations into rotamers using  $^{13}\text{C}'$  chemical shifts: exploring how far we can go*. PeerJ 7, e7904 (2019)

**Martin O.A.** Vorobjev Y, Scheraga HA, Vila JA. Outline of an experimental design aimed to detect protein A mirror image in solution. PeerJ Physical Chemistry 1, e2 (2019)

Baldi G, Schauman S.A, Texeira M, Marinaro S, **Martin O.A**, Gandini P, Jobbágy E.G. *Nature representation in South American protected areas: country contrasts and conservation priorities*. PeerJ 7, e7155 (2019)

Kumar, R. Carroll C, Hartikainen A, **Martin, O.A** *ArviZ a unified library for exploratory analysis of Bayesian models in Python*. The Journal of Open Source Software (2019)

Icazatti, A. **Martin, O.A.** Villegas, M. Szleifer, I. Vila, J.A..  *$^{13}\text{C}$ Check\_RNA: A tool to evaluate  $^{13}\text{C}$  chemical shifts assignments of RNA*. Bioinformatics (2018)

Alonso, J.M. Arroyuelo, A. Garay, P.G. **Martin, O.A.** Vila J.A. *Finite Dimension: A Mathematical Tool to Analyse Glycans*. Scientific Reports (2018)

Garay, P.G. Vila, J. A. **Martin, O.A.** *CheSweet: An application to predict glycan's chemicals shifts*. The Journal of Open Source Software (2018)

Baldi G. Texeira M. **Martin O.A.** Grau R. Jobbágy E.G. *Opportunities drive the global distribution of protected areas*. Peerj (2017)

Arroyuelo A. **Martin O.A.** *Azahar: a PyMol plugin for construction, visualization and analysis of glycan molecules*. Journal of Computer-aided Molecular Design (2016)

Garay P.G. **Martin O.A.** Scheraga H.A. and Vila J.A. *Detection of methylation, acetylation and glycosylation of protein residues by monitoring  $^{13}\text{C}$  chemical-shift changes*. Peer J. (2016)

## Book

Bayesian Analysis with Python. Martin O.A. Packt Publishing.  
First Edition ISBN-13: 978-1785883804. 2016.  
Second Edition. ISBN-13: 978-1789341652. 2018

## Research projects funding as main researcher/principal investigator

Create educational material and give workshops related to exploratory analysis of Bayesian models with ArviZ. NumFOCUS small grants. (2019)

Probabilistic programming for Structural Bioinformatics FONCYT. PICT-Joven (2017-2019)

## Advisor for undergrad and graduate students

### Current projects

PhD Advisor: Lic. Tomás Capretto. *Exploratory Analysis of Bayesian Models*. National University of Rosario. (2019-2023)

PhD Advisor: Lic Agustina Arroyuelo. *Structural determination of biomolecules by statistical inference*. National University of San Luis. (2016-2020)

### Previous projects

Co-advisor Phd Thesis: Alejandro Icazatti. *Validation and determination of the structure of nucleic acids*. National University of San Luis. (2014-2019).

Co-advisor Phd Thesis: Pablo Garay. *CheSweet: Determination and validation of glycans and glycoproteins*. National University of San Luis. (2013-2017).

Advisor BSc Thesis: Agustina Arroyuelo. *Development of a software application for creating, viewing and analyzing models of macromolecules*. Thesis to get the degree of Bachelor in Molecular Biology. National University of San Luis. Approved September 2019.

Advisor BSc Thesis: Pedro Ramírez. *Protein structure refinement guided by  $^{13}\text{C}^{\alpha}$  y  $^{13}\text{C}^{\beta}$  chemical shifts*. Thesis to get the degree of Bachelor in Molecular biology. National University of San Luis. Approved December 2014.

Co-advisor BSc Thesis: Ezequiel Frigini. *Is the cell membrane, permeable to the diffusion of glyphosate?* Thesis to get the degree of Bachelor in Molecular biology. National University of San Luis. Approved December 2014.

## Software development

### Current projects

Core developer of [PyMC3](#). Probabilistic Programming in Python

Core developer of [ArviZ](#). Exploratory analysis of Bayesian models

Core developer of [Bambi](#). Bayesian Model-Building Interface in Python.

### Older projects

[CheShift](#): A web-server for protein-structure validation.

[PyMOL](#) Plugins: PyMOL is a molecular visualization system

## Google Summer of Code mentoring

Implementation of *Sequential Monte Carlo-Approximate Bayesian Computation* in PyMC3. May-July 2018. Mentor of Agustina Arroyuelo.

Implementation of *Bayesian additive Regression Trees* in PyMC3. May-July 2019. Mentor of Juan Martín Loyola.

Improve model comparison functionality in ArviZ. May-July 2019. Mentor of Oriol Abril Pla.

## Synergistic activities

Member of the PhD in Biology Committee. National University of San Luis. 2019-present.

Head of the organizing committee of PyData, San Luis, Argentina 2017. This was the first PyData in Latin-America. Member of the PyData San Luis chapter.

Co-host La Búsqueda, popular science radio-show and podcast.

Radio UNSL. 2008-2009

Radio Ciudad. 2010