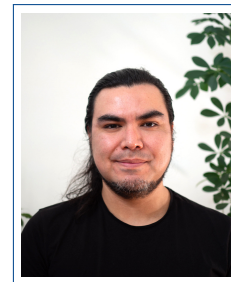


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Experience and Competencies

- Experienced Computational Biologist: an expert in applying computational techniques and methodologies to address biological research questions.
- Well-versed in data analysis, algorithm development, and statistical modeling to extract meaningful insights from biological datasets.
- Proficient in programming languages commonly used in structural bioinformatics and computational biology, such as PYTHON and C++.
- Demonstrated ability to communicate scientific findings effectively and contribute to the advancement of biological understanding through computational approaches.

Education

- 2017–2021 **Doctor in Natural Resources and Life Sciences**, *University of Natural Resources and Life Sciences (BOKU) Vienna, Austria*
- Optimization of the Vienna Soil Organic Matter Modeler (VSOMM) tool to generate molecular systems of soil organic matter (SOM) using experimental input parameters. This expanded understanding of SOM at a molecular level, shedding light on its macroscopic properties and interactions with proteins and pesticides.
 - Web development of the website <https://somm.boku.ac.at> using PYTHON, which controls a GROMOS pipeline for molecular modeling and simulation of biomolecules. The website runs under a DOCKER image for efficient development and production.
- 2012–2017 **Master of Biological Sciences**, *Universidad de Chile, Santiago, Chile*
- Performed molecular dynamics simulations to study the behavior of dual-membrane systems resembling gap junction channels (GJCs) under external electric fields. Our results provide insights on the effects of charge distributions over ionic transport, constituting a step forward into a better understanding of GJCs.
 - The work implies the analysis of multiple data associated with ionic currents and thermodynamics.
- 2010–2015 **Molecular Biotechnology Engineer (Diploma Thesis)**, *Universidad de Chile, Santiago, Chile*
- Employed structural bioinformatics methods to identify crucial residues involved in the interaction between β - and γ -tubulin with the chaperonin CCT.
- 2005–2010 **Bachelor of Molecular Biotechnology Engineering**, *Universidad de Chile, Santiago, Chile*
- Career focused on developing and implementing innovative biotechnological solutions while prioritizing environmental preservation and scientific advancement.

Work Experience

- 2022–2023 **Computational Biologist**, *Fermify GmbH, Vienna, Austria*
Simulations of casein proteins under different conditions using different force fields for Intrinsically Disordered Proteins (MARTINI-IDP and MOFF-IDP) with the simulation program GROMACS.
- 2016–2017 **Research assistant**, *dLab, Fundación Ciencia & Vida, Santiago, Chile*
Free energy calculations of amino acids involved in a possible voltage gating response of a water channel (Aquaporin) using NAMD. Also, exploring the effects of the polarizability of graphene interacting with water molecules using GROMOS.

Skill matrix

Language:	Python	■■■■■	Experience with objected oriented programming associated with data science and web development.
	C/C++	■■■■■	Experience coding with C++ associated with the GROMOS package.
	Perl	■■■■■	Basic experience associated with sequence analysis.
	Bash	■■■■■	Experience handling multiple jobs and pipelines with bash.
Data Science:	Numpy Scipy Pandas	■■■■■	Experience using core-functions for Data Science.
	Scikit-learn PyTorch Keras TensorFlow	■■■■■	Experience with the usage of machine learning modules.
	Matplotlib	■■■■■	Experience plotting data with Matplotlib.
Web Development:	Flask	■■■■■	Experience developing a website with Flask.
	Django	■■■■■	Experience developing simple websites with Django.
	Javascript	■■■■■	Experience using AJAX on a website.
	SQL	■■■■■	Use of SQL databases (MySQL, SQLite, PostgreSQL).
OS:	Linux	■■■■■	Experience with Debian, Ubuntu and Archlinux.
	Gitlab CI/CD	■■■■■	Experience in the configuration of Continuous Integration.
	Docker	■■■■■	Experience creating different virtual images for web development purposes.
	Slurm	■■■■■	Experience related to the configuration and installation of Slurm.

Languages

Spanish	Mothertongue
English	Academic
German	Basic

Doctorate at BOKU
A2+ (Ibis acam Bildungs GmbH, Wien)

Interests

Music	Making music is my passion
Sports	I like to practice Chess and Muay Thai
Photography	I enjoy making macrophotography @yerkoescalona.macro

Academic Section

Teaching Experience

- 2020–2021 **Lecturer**, BOKU, Vienna, Austria
Lecturer of the course “**Programming with Python**” at BOKU. Together with Dr. Drazen Petrov, we have taught Python for three semester to numerous students with different backgrounds at BOKU.
- 2020–2021 **Co-supervisor**, BOKU, Vienna, Austria
Co-supervisor of two Bachelor Theses : “**Exploring the Interactions Between Amino Acids and Soil Organic Matter**” of Jonathan Shklarek and “**Free energy calculations of Glyphosate in Humic Substances**” of Christine Unterweger. Also, co-supervisor of the Master thesis “**Exploring the Structure and Dynamics of Proteins in Soil Organic Matter**” of Mathias Gotsmy.
- July 2019, July 2020 **Lecturer assistant**, BOKU, Vienna, Austria
Teaching the usage of a program called PyMOL, in order to explain the structure of proteins and DNA, in the context of the course “**Protein chemistry and protein engineering**” of Dr. Chris Oostenbrink.
- July 2019 **Tutor**, BOKU, Vienna, Austria
Tutor in the CECAM School “**Introduction to biomolecular simulation with GROMOS**”. Teachers: Prof. Chris Oostenbrink, Prof. Niels Hansen and Prof. Wilfred van Gunsteren. Vienna, Austria.
- November 2017 **Tutor**, BOKU, Vienna, Austria
Tutor in the International Spring School for Graduate Students: “**Applied Statistical Thermodynamics 2017: from theory to molecular dynamics simulation**”. Teachers: PhD. Jose A. Garate, PhD. Drazen Petrov, Prof. Chris Oostenbrink and Prof. Wilfred van Gunsteren. Santiago, Chile.

List of Publications

- [1] **Escalona, Yerko**, Drazen Petrov, and Chris Oostenbrink. Exploring the Macroscopic Properties of Humic Substances using Modeling and Molecular Simulations [accepted]. *Agronomy (MDPI)*, 2023.
- [2] Edgar Galica-Andres, **Escalona, Yerko**, Drazen Petrov, and Chris Oostenbrink. Molecular Dynamics Simulations up to Earth: Modeling of Soil Organic Matter [accepted]. *Comprehensive Computational Chemistry*, 2023.
- [3] **Escalona, Yerko**, Nicolas Espinoza, Mateo Barria-Urenda, Chris Oostenbrink, and Jose Antonio Garate. On the effects of induced polarizability at the water-graphene interface via classical charge-on-spring models. *Physical Chemistry Chemical Physics*, 24:7748–7758, 2022 <https://doi.org/10.1039/D1CP05573A>.
- [4] **Escalona, Yerko**, Drazen Petrov, and Chris Oostenbrink. Modeling soil organic matter: Changes in macroscopic properties due to microscopic changes. *Geochimica et Cosmochimica Acta*, 307:228–241, 2021 <https://doi.org/10.1016/j.gca.2021.05.035>.
- [5] **Escalona, Yerko**, Drazen Petrov, and Chris Oostenbrink. Vienna soil organic matter modeler 2 (VSOMM2). *Journal of Molecular Graphics and Modelling*, 103:107817, 2021 <https://doi.org/10.1016/j.jmgm.2020.107817>.
- [6] Edgar Galicia-Andrés, **Escalona, Yerko**, Chris Oostenbrink, Daniel Tunega, and Martin H. Gerzabek. Soil organic matter stabilization at molecular scale: The role of metal cations and hydrogen bonds. *Geoderma*, 401(June):115237, 2021 <https://doi.org/10.1016/j.geoderma.2021.115237>.
- [7] Mathias Gotsmy, **Escalona, Yerko**, Chris Oostenbrink, and Drazen Petrov. Exploring the structure and dynamics of proteins in soil organic matter. *Proteins: Structure, Function and Bioinformatics*, (February):925–936, 2021 <https://doi.org/10.1002/prot.26070>.
- [8] Jose Antonio Garate, Alejandro Bernardin, **Escalona, Yerko**, Carlos Yanez, Niall J. English, and Tomas Perez-Acle. Orientational and Folding Thermodynamics via Electric Dipole Moment Restraining. *Journal of Physical Chemistry B*, 123(12):2599–2608, 2019 <https://doi.org/10.1021/acs.jpcc.8b09374>.
- [9] Anibal A Vargas, Bruno A Cisterna, Fujiko Saavedra-Leiva, Carolina Urrutia, Luis A Cea, Alex H Vielma, Sebastian E Gutierrez-Maldonado, Alberto J M Martin, C Pareja-Barrueto, **Escalona, Yerko**, Oliver Schmachtenberg, Carlos F Lagos, Tomas Perez-Acle, and Juan C Sáez. On Biophysical Properties and Sensitivity to Gap Junction Blockers of Connexin 39 Hemichannels Expressed in HeLa Cells. *Frontiers in physiology*, 2017 <https://doi.org/10.3389/fphys.2017.00038>.

- [10] F Villanelo, **Escalona, Y**, C Pareja-Barrueto, J A Garate, I M Skerrett, and T Perez-Acle. Accessing gap-junction channel structure- function relationships through molecular modeling and simulations. *BMC Cell Biology*, 28(Suppl 1):1–15, 2017 <https://doi.org/10.1186/s12860-016-0121-9>.
- [11] **Escalona, Yerko**, Jose A Garate, Raul Araya-Secchi, Tien Huynh, Ruhong Zhou, and Tomas Perez-Acle. Exploring the Membrane Potential of Simple Dual-Membrane Systems as Models for Gap-Junction Channels. *Biophysical Journal*, 110(12):2678–2688, 2016 <https://doi.org/10.1016/j.bpj.2016.05.005>.
- [12] Matthew J Brennan, Jennifer Karcz, Nicholas R Vaughn, Yvonne Woolwine-Cunningham, Adam D DePriest, **Escalona, Yerko**, Tomas Perez-Acle, and I Martha Skerrett. Tryptophan scanning reveals dense packing of connexin transmembrane domains in gap junction channels composed of connexin32. *Journal of Biological Chemistry*, 290(28):17074–17084, 2015 <https://doi.org/10.1074/jbc.M115.650747>.
- [13] **Escalona, Yerko**, Jose A Garate, and Tomas Perez-Acle. Exploring the membrane potential of a simple dual membrane system by using a constant electric field. *BMC Bioinformatics*, 16(Suppl 8):A5, 2015 <https://doi.org/10.1186/1471-2105-16-S8-A5>.
- [14] Raul Araya-Secchi, Tomas Perez-Acle, Seung Gu Kang, Tien Huynh, Alejandro Bernardin, **Escalona, Yerko**, Jose Antonio Garate, Agustin D Martínez, Isaac E García, Juan C Sáez, and Ruhong Zhou. Characterization of a novel water pocket inside the human Cx26 hemichannel structure. *Biophysical Journal*, 107(3):599–612, aug 2014 <https://doi.org/10.1016/j.bpj.2014.05.037>.

Participation in Scientific Conferences and Workshops

- August 2021 Poster “Structural and Dynamic Analysis of Humic Substances by using the Vienna Soil Organic Matter Modeler 2 (VSOMM2)” in the Eurosoil 2021 conference, Geneva, Switzerland
- September 2019 Oral presentation “Soil Organic Matter: Challenges in modeling and molecular dynamic simulations” in the 29th Intl. BIOMOS Symposium on Biomolecular Simulation in Ausserberg, Switzerland
- September 2018 Oral presentation “Exploring properties of SOM at the nanoscopic level using molecular dynamics” in the 28th Intl. BIOMOS Symposium on Biomolecular Simulation in Ausserberg, Switzerland
- August 2018 Poster presentation in the 14th Greta Pifat Mrzljak International School of Biophysics, Split, Croatia
- August 2018 Poster presentation in the 21st World Congress of Soil Science, Rio de Janeiro, Brazil
- November 2015 Participation in the International Spring School for Graduate Students: “Applied Statistical Thermodynamics 2015: from theory to molecular dynamics simulation”. Teachers: PhD. Jose A. Garate, PhD. Maria Reif, Prof. Chris Oostenbrink and Prof. Wilfred van Gunsteren. Santiago, Chile.
- May 2015 Learning Coarsed-Grained in the Workshop: “OpenLab: Performing Molecular Simulations with SIRAH force field”. Teachers: PhD. Sergio Pantano and PhD. Matías Machado. Montevideo, Uruguay.
- Septembre 2015 Oral presentation “Exploring the membrane potential of a simple dual membrane system by using a constant electric field” in the IV Meeting Millenium Institute CINV. Valparaíso, Chile
- March 2015 Poster presentation “Exploring the membrane potential of a simple dual membrane system by using a constant electric field” in the International Gap Junction Conference (IGJC), Valparaíso, Chile
- October 2014 Oral presentation “Exploring the membrane potential of a simple dual membrane system by using a constant electric field” in the ISCB LA / X-Meeting / BSB/ SolBio 2014. Belo Horizonte, Brazil