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Experience and Competencies

- Experienced Computational Biologist: 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

- Optimized 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.
- Developed 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 into the effects of charge distributions on ionic transport, constituting a step forward in better understanding GJCs.
- The work involved analyzing multiple datasets 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

- This degree focused on developing and implementing innovative biotechnological solutions while prioritizing environmental preservation and scientific advancement.

Work Experience

2023–Present **Data Engineer**, *Novasign GmbH*, Vienna, Austria

Developing a unified operations layer bridging multiple DataFrame libraries (Polars, PySpark, Modin, and Pandas), reducing code duplication and performance bottlenecks across large-scale data pipelines. Leveraging these enhanced frameworks to analyze large and diverse biological datasets associated with various bioprocesses. Optimizing simulation engines ranging from reactors to chromatography and filtration. These models use iterative step-by-step calculations to predict system behavior for bioprocess optimization.

2022–2023 **Computational Biologist**, *Fermify GmbH*, Vienna, Austria

Conducted simulations of casein proteins under different conditions using various 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
Performed free energy calculations of amino acids involved in a possible voltage gating response of a water channel (Aquaporin) using NAMD. Also explored the effects of the polarizability of graphene interacting with water molecules using GROMOS.

Skill Matrix

Languages:	Python	■■■■■	Extensive experience with OOP, scripting, data science pipelines, and web development
	C/C++	■■■■□	Developed simulation code (GROMOS package); solid background in compiled languages
	Perl	■■□□□	Basic usage for sequence analysis
	Bash	■■■■■	Experienced in shell scripting for automation, job scheduling, and pipelines
Data Wrangling:	Pandas, Modin, Polars, Spark	■■■■■	Expert in DataFrame operations, parallel computations, and large-scale data processing
	NumPy, SciPy	■■■■■	Core libraries for scientific computing and numerical methods
ML & AI:	Scikit-learn, PyTorch, TensorFlow, Keras	■■■■■	Design, training, and deployment of ML/DL models
	Matplotlib	■■■■■	Data visualization of complex datasets and simulation results
Web Dev:	Flask	■■■■■	Created production-level web apps and RESTful APIs
	FastAPI	■■■■□	Experience building asynchronous APIs for data-driven applications
	Django	■■■□□	Built smaller-scale applications with user authentication and databases
	JavaScript	■■□□□	Basic AJAX and dynamic UI functionality
	SQL	■■■□□	MySQL, SQLite, and PostgreSQL for web and analytics
DevOps:	GitLab CI/CD, Docker, Slurm	■■■■□	Set up pipelines, containerized environments, and HPC job schedulers
	GitHub, Azure DevOps	■■■■□	Managed repositories and workflow automation (Actions, Boards, etc.)
	Poetry, Ruff, Mypy, Black, Pytest	■■■■□	Handled Python packaging, linting, static typing, formatting, and parameterized testing
	Protocol Buffers	■■□□□	Basic usage for data serialization/RPC
AI Tools:	GitHub Copilot, Claude, Cline	■■■□□	Familiar with AI-based coding assistance, debugging, and brainstorming
Editors:	Markdown	■■■■■	Write clear documentation and READMEs
	LaTeX	■■■■■	Produce professional documents (articles, presentations, CV)
	Office	■■■■■	Microsoft Excel, PowerPoint, Word
OS:	Linux (Debian/Ubuntu/Arch)	■■■■■	Daily user; systems administration, package management, and shell scripting

Languages

Spanish	Mother tongue	
English	Academic	*Doctorate at BOKU*
German	Basic	*A2.2*

Academic Section

Teaching Experience

2023–Present **Lecturer**, *Biotech Campus Tulln at Fachhochschule Wiener Neustadt (FHWN)*, Vienna, Austria
Lecturer of the course "**Structural Bioinformatics**" at FHWN. Structural bioinformatics explores the principles and techniques used to analyze and interpret the three-dimensional structures of biomolecules. Students gain hands-on experience utilizing various bioinformatics tools, databases, and software to predict, model, and analyze biomolecules.

2020–2021 **Lecturer**, *BOKU*, Vienna, Austria
Lecturer of the course "**Programming with Python**" at BOKU. Together with Dr. Drazen Petrov, we taught Python for three semesters to numerous students with different backgrounds at BOKU.

2020–2021 **Co-supervisor**, *BOKU*, Vienna, Austria
Co-supervisor of two Bachelor's theses: "**Exploring the Interactions Between Amino Acids and Soil Organic Matter**" by Jonathan Shklarek and "**Free Energy Calculations of Glyphosate in Humic Substances**" by Christine Unterweger. Also co-supervised the Master's thesis "**Exploring the Structure and Dynamics of Proteins in Soil Organic Matter**" by Mathias Gotsmy.

July 2019, July 2020 **Lecturer Assistant**, *BOKU*, Vienna, Austria
Taught the usage of PyMOL to explain the structure of proteins and DNA in the context of the course "**Protein Chemistry and Protein Engineering**" by 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: Dr. Jose A. Garate, Dr. 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. *Agronomy (MDPI)*, 2023 https://doi.org/10.3390/agronomy13041044.

[2] Edgar Galica-Andres, **Escalona, Yerko**, Drazen Petrov, and Chris Oostenbrink. Molecular Dynamics Simulations up to Earth: Modeling of Soil Organic Matter. *Comprehensive Computational Chemistry*, 2023 https://doi.org/10.1016/B978-0-12-821978-2.00106-9.

[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.jpcb.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.