Carlos Vigil-Vásquez

Email: carlos.vigil.v@gmail.com Phone: +569 956447689 GitHub: github.com/cvigilv

Work experience

Microbiology's Platypus Lab (Institut Pasteur de Lille; France) Dr. Damien Devos, Ph. D.
PhD Student December '23 - today

- PhD researcher under the grant "International PhD call EGBSL, Universite de Lille, France".
- Project aiming to reconstruct the Tree-of-Life from biochemical networks (e.g. metabolic networks) and method development for reconstructing phylogenies from non-genomic data using novel computing paradigms and accelerated computing.

Protera Biosciences
Protein Designer September '23 - November '24

- Implementation, validation and maintenance of computational biology modules for madi™, Protera's proprietary SaaS platform for protein design applications.
- Conduct extensive analysis and modelling related to Protera's clients projects, utilizing bioinformatics, structural biology and protein design strategies.

Neurobiology of Aging Laboratory (USS; Chile) Dr. Cheril Tapia-Rojas, Ph. D.
Research Assistant May - August '23

- Conducted extensive bioinformatic analysis as part of a study investigating the correlation between mitochondrial protease Lonp1 and age-associated neurodegenerative diseases.
- Contributed writing and creating figures for a manuscript and poster presentation related to the previously mentioned work.

Molecular Design Laboratory (PUC; Chile) Dr. Andreas Schüller, Ph. D.
Research Assistant & Thesis Student July '17 - June '23

- *Summa cum laude* undergraduate thesis titled ''Weak-link paradox for *de novo* prediction of pharmacological targets'' between August 2020 and June 2022.
- Proposal and implementation of ''SimSpread'', a novel predictive model that combines graph theory and the concept of chemical similarity for drug discovery and repositioning, its optimization using different cross-validation schemes, and evaluation of the predictive performance of the proposed models.
- Related study on the discovery of drugs with antifungal activity using the SimSpread predictive model, discovering 4 new compounds with antifungal activity for 8 clinically relevant fungal organisms.
- Authored `SimSpread.j`, a software package for the Julia programming language that implements the SimSpread formalism for link prediction in graphs.
- Advised in the initiation and development of 3 projects related to the SimSpread model, related to increasing its predictive power, and extending the application domain and accessibility of the method.
- Authored a scientific publication, prepared multiple poster presentations and contributed to writing original research manuscript in the context of the SimSpread project and other projects developed at the laboratory.

REFRACT MSCA RISE PROJECT 2019 (UPO; Spain) Dr. Damien Devos, Ph. D.
Research Secondee September - December '22

- 3-month Research secondment carried out at the Microbiology's Platypus Lab at Universidad Pablo de Olavide in Sevilla, Spain.
- Proposal and implementation of ''ResidueFisher'', an open-source bioinformatics protocol to aid remote homology search between proteins using sequence and structural information.
- Lead the writing of the application note for the previously mentioned protocol.

Psychophysiology Laboratory (PUC; Chile) Dr. Diego Cosmelli, Ph. D.
Research Assistant January 2022 - December '22

- Implementation of analysis protocol based on machine learning, statistical modeling, and feature extraction of the trained models for a human study that resulted in the identification of the effect of different contemplative practices (e.g., meditation) on the well-being of the subjects studied.
- Contributed writing the methods and results sections of a paper related to the work previously mentioned.

Biostatistics (PUC; Chile) Dr. Andreas Schüller, Ph. D.
Teaching Assistant July - December '17

Academic productivity

Publications:

1. ''Movement-based Contemplative Practices positively impact overall well-being by developing a specific profile of cognitive, emotional, and self-awareness traits''; M. Villena-Gonzalez; F. Jaume-Guazzini; P. Oyarzo; **C. Vigil-Vásquez**; S. Walsen; J. Silva; V. López; D. Cosmelli. iScience, in review.
2. ''*De novo* prediction of drug targets and candidates by chemical similarity-guided network-based inference''; **C. Vigil-Vásquez** and A. Schüller.
IJMS (2022). DOI:10.3390/ijms23179666

Presentations:

1. ''madi™: From Machine Learning to Lab Bench - Advancing Protein Engineering''; **C. Vigil-Vásquez** (4th REFRACT Annual Latin America Visit: "Computational Methods for Structural Bioinformatics", Santiago, Chile 15 - 19 April 2024)

Poster presentations:

1. ''Changes in epigenetic control and loss of Lonp1 proteolytic protease activity induce abnormal protein accumulation and mitochondrial dysfunction in aging''; J. Llanquinao, C. Jara, M. Lira, **C. Vigil-Vásquez**, M. Sjöberg, A. Schüller, B. Kerr and C Tapia-Rojas. SBCCH (November, 2023)
2. ''De Novo Prediction of Pharmaceutical Targets Using Network-Based Inference Guided by Chemical and Structural Similarities.''; M. Saez-Ortega, V. Valdes, **C. Vigil-Vásquez** and A. Schüller. PUC-IIBM Symposium (November, 2023)
3. ''SimSpread Ensemble Model and SimSpread web server for prediction of drug-target interactions''; F. Melo, V. Valdes, **C. Vigil-Vásquez**, A. Schüller. PUC-IIBM Symposium (November, 2023)
4. ''Antifungal drug discovery by chemical similarity-guided network-based inference''; **C. Vigil-Vásquez**, M. Jimenez-Socha, P. Ortiz-Bermudez and A. Schüller. Chilean Bioinformatics Society (January, 2022)
5. ''DDTNBI: *de novo* target prediction using a social network-derived method''; **C. Vigil-Vásquez** and A. Schüller. International Society for Computational Biology/European Conference on Computational Biology (August, 2021)

6. ‘’A computational chemogenomics method for the prediction of off-target interactions with coagulation factor Xa’‘; A. Schüller and **C. Vigil-Vásquez**. European Hematology Association (August, 2020)
7. ‘’Limits and potential of in silico target prediction by chemical similarity’‘; M. Ruiz, **C. Vigil-Vásquez** and A. Schüller. International Society for Computational Biology-LA (October, 2018)

Awards:

1. **International PhD call EGBSL, Universite de Lille, France** PhD scholarship for a duration of 3 years.
1. **Undergraduate Research Contest - Summer 2020** Project titled ‘’Use of biochemical networks for the prediction of novel drugs for coagulation factor Xa.‘’
2. **Undergraduate Research Contest - Winter 2017** Project titled ‘’*In silico* prediction and prioritization of novel drug targets.‘’

Education

Licenciado en Bioquímica[1] Santiago, Chile
Pontificia Universidad Católica de Chile 2015 - 2022

Degree obtained after 4 years of studying, mainly focused on theoretical and practical courses.
- *Licenciatura* grade: 5.6/7.0
- Graduation exam grade: 6.3/7.0

Título profesional en Bioquímica Santiago, Chile
Pontificia Universidad Católica de Chile 2015 - 2022

Degree obtained after completing 5 years of study, obtained through the completion of a undergraduate research thesis.

- Undergraduate thesis grade: 7.0/7.0
- Graduation grade: 6.0/7.0
- Undergraduate thesis titled ‘’Weak-link paradox for *de novo* prediction of pharmacological targets‘‘

Skills

- **Human languages**: Spanish (native), English (TOEFL 101/120 points; over 24 points over all categories), French (reading)
- **Machine languages**: Julia, Python, Lua, LaTeX/Typst, Bash/Shell scripting
- **Predictive modelling**: Transfer learning, Machine learning (supervised and unsupervised models), conformal prediction, data processing, database management, REST API, data clustering and evaluation, predictive model evaluation, recommender systems, data visualization, biostatistics, statistics and probability, graph theory, network analysis, Scikit-Learn, Pandas, NumPy, Matplotlib, Seaborn, NetworkX, Pingouin
- **Bioinformatics**: Protein Language Models, Sequence alignment, MSA, structural alignment, molecular docking, structural biology, PyMOL scripting, AlphaFold modeling and evaluation, biostatistics, phylogenetic tree construction.
- **Cheminformatics**: Molecular descriptor preparation, chemical similarity analysis, confomer preparation, pharmacophoric modeling, RDKit, OpenBabel, computational representation of chemical compounds
- **Tools**: Git, GitHub, MySQL, SQLite, slurm, AWS, Pinecone
- **Platforms**: Linux, MacOS, `docker`

[1] Equivalent to a BSc. in Biochemistry, enables the recipient to apply for Master and Doctoral programs.

Extracurriculars

- Co-delegate of the National Association of Biochemistry Students (ANEB): 2018
- Member of the National Association of Biochemistry Students (ANEB): 2016 - 2021
- Member of the International Society for Computational Biology (ISCB): 2018 & 2021
- Author and maintainer of `SimSpread.jl`: 2022 - today