Daniel Felipe Victoria Muñoz

PhD Student

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Current Research Interest

Main interest

The main areas of my research comprise the development and use of state-of-the-art methodologies to assist ligand- and structure-based drug discovery campaigns. This involves the prediction of the most probable targets for a compound (ligand profiling) and the search and design of novel compounds for a given target (virtual screening).

Research skills by Keywords

Cheminformatics, Data Mining, Drug Discovery, Virtual Screening, Ligand Profiling, Computational Chemistry, Machine-Learning, Deep Learning

Education

University of Münster — *Correnssstraße 48, Münster, Germany*

PhD Medicinal Chemistry and Computational Drug Discovery — *03/2022 - 03/2025*

- Advisor: Prof. Dr. Oliver Koch

National University of Colombia — *Sede Bogotá, Bogotá D.C., Colombia*

MSc Pharmaceutical Science — *02/2020 - 12/2021*

- Advisor: Dr. Fabian Lopez-Vallejo

National University of Colombia — *Sede Bogotá, Bogotá D.C., Colombia*

BS Pharmaceutical Chemistry — *02/2011 - 03/2017*

- Undergrad research advisor: Dr. Mary Trujillo Gonzales

Professional Experience

2022-2025	**PhD fellow with Prof. Dr. O. Koch**, University of Münster
2020-2021	**Graduate Teaching Assistant**, Department of pharmacy, National University of Colombia
2019-2021	**Researcher Assistant**, National University of Colombia – Fundación para la promoción de la investigación y la tecnología
2017-2019	**Technological transfer analist**, Tecnoquimicas S.A.
2016-2017	**Undergraduate Research Assistant**, Pharmaceutical analysis laboratory, Department of Pharmacy, National University of Colombia
2015	**Undergraduate Research Assistant**, Ministry of Health - Department of Pharmacy, National University of Colombia

Publications

Published

Victoria-Muñoz, F.; Sánchez-Cruz, N.; Medina-Franco, J. L; Lopez-Vallejo, F. Cheminformatics analysis of molecular datasets of transcription factors associated with quorum sensing in Pseudomonas aeruginosa. RSC Adv., 2022,12, 6783-6790, DOI: https://doi.org/10.1039/D1RA08352J

In Review

Victoria-Muñoz, F.; Menke, J.; Sánchez-Cruz, N.; Koch. O.; Efficient Decoy Selection to Improve Virtual Screening Using Machine Learning Models. 2024.

Victoria-Muñoz F.,Torres-García A., Koch O., Sierra C., Sánchez-Cruz N.; Harnessing the Potential of Natural Products in Insecticide Discovery: A Cheminformatics Approaches. 2024.

In Prep

Victoria-Muñoz, F.; Menke, J.; Sánchez-Cruz, N.; Koch. O.; Automatic workflow for specific target scoring function in molecular docking. 2024.

Presentations

** presenting author; + mentored undergraduate*

Oral presentations

Victoria-Muñoz, F.; Menke, J.; Sánchez-Cruz, N.; Koch. O. 2024. Machine Learning based Scoring Functions: Reasonable Decoy Selection for Automated Docking-based model creation. 2nd School of Chemoinformatics in Latin America, Flash talk, Virtual.

Victoria-Muñoz, F.; Menke, J.; Sánchez-Cruz, N.; Koch. O. 2024. Machine Learning based Scoring Functions: Reasonable Decoy Selection for Automated Docking-based model creation. 18th German Conference on Cheminformatics (GCC 2024), Bad Soden am Taunus, Germany.

Victoria-Muñoz, F.; Menke, J.; Sánchez-Cruz, N.; Koch. O. 2024. Beyond the active: Integrating decoys in machine learning models, PADIF case. Oral presentation: ACS Fall 2024, Denver, Colorado.

Torres-Garcia, A.;, **Victoria-Muñoz, F.**; Plazas-Gonzales, E.; Sánchez-Cruz, N.; Sierra-Avila, C. 2023. Natural volatile compounds as possible insecticides. ACS Fall 2023, Virtual.

Victoria-Muñoz, F.; Sánchez-Cruz, N.; Medina-Franco J.L.; López-Vallejo F. 2021. Key aminoacidic residues for agonist or antagonist activity against PqsR transcriptional factor from *P. aeruginosa*. ACS Spring 2021, Virtual.

Poster Presentations

Victoria-Muñoz, F.; Menke, J.; Sánchez-Cruz, N.; Koch. O. 2024. Machine learning based scoring functions: Reasonable decoy selection for automated docking-based model creation. 24th European Symposium on Quantitative Structure-Activity Relationship, Barcelona, Spain.

Victoria-Muñoz, F.; Menke, J.; Sánchez-Cruz, N.; Koch. O. 2024. Decoy Selection in Bioactivity Classification Models: Exploring Protein-Ligand Interaction Fingerprints with PADIF. 7th RSC-CICAG/RSC-BMCS Artificial Intelligence in Chemistry, Cambridge, United Kingdom

Victoria-Muñoz, F.; Sánchez-Cruz, N.; Medina-Franco J.L.; López-Vallejo F. 2020. Cheminformatics analysis on molecular datasets of transcription factors associated with quorum sensing in *Pseudomonas aeruginosa*. EFMC-ISMC and EFMC-YMCS 2020, Virtual.

Victoria-Muñoz, F.; López-Vallejo F. 2019. Cheminformatics analysis of agonist and antagonist of the transcriptional regulators of LasR, PqsR and RhlR in *Pseudomonas aeruginosa*. Poster presentation: XXII Latin-American Meeting on Pharmacology, Cali, Colombia.

Undergrad, **Victoria-Muñoz, F.**, Orozco-López F. 2015. Rational design of new Spiro-beta-lactames as potentials inhibitors of Penicillin binding protein 4. XVI National Congress of Students of Pharmaceutical Chemistry, Cartagena, Colombia.

Computational skills

Programming languages: Python (advanced), R (basic)

Cheminformatic Modules: RDKit, Datamol, Molfeat, Openbabel, Biopython

Machine-Learning Modules: Scikit-Learn, Pytorch, TensorFlow, DeepChem, PyCaret

Molecular modelling software: CCDC, MOE, AutoDock, AutoDock VINA

Molecular Dynamics Simulations software: AMBER, Desmond

Research Funding (participated as collaborator)

University of Münster - Institute of Pharmaceutical and Medicinal Chemistry *Münster, Germany*
PI: Prof. Dr. Oliver Koch *Mar. 2022 - Present*

- Project tittle: "Analysis of the selectivity and promiscuity of ligand binding for fragment-based design"
- Funding institution: Deutsche Forschungsgemeinschaft / DFG (German research society)

National University of Colombia - Sede Bogotá - Dept of Chemistry *Bogotá, Colombia*
PI: Dr. Cesar Sierra *Jun. 2024 - Present*

- Project tittle: "Cacao On Capable Options for Common Agriculture Problems (COCOA)"
- Funding institution: The CLIMA/IE Colombia Innovation Fund Grant Competition: Grupo energia de Bogotá, Fundación Santo Domingo, Department of Agriculture (USDA)

National University of Colombia - Sede Bogotá - Dept of Chemistry *Bogotá, Colombia*
PI: Dr. Fabian Lopez-Vallejo *Sep. 2020 - Sep. 2021*

- Project tittle: "Chemoinformatic analysis of active molecules against transcription factors associated with quorum sensing in *Pseudomonas aeruginosa*"
- Funding institution: FPIT - Fundación para la promoción de la investigación y la tecnología, and National University of Colombia

National University of Colombia - Sede Bogotá - Dept of Chemistry *Bogotá, Colombia*
PI: Dr. Fabian Lopez-Vallejo *Sep. 2020 - Sep. 2021*

- Project tittle: "Identification of lead molecules of natural resources with multitarget activity as quorum sensing inhibitors in *Pseudomonas aeruginosa*"
- Funding institution: Ministry of Science, Technology and Innovation, and National University of Colombia

Awards, Fellowships, & Grants

2024	**AGRO Education Awards for Student Travel**, AGRO division ACS scholarship, Bayer US LLC, Crop Science Division
2020	**Directory for international affairs for Student Travel**, National University of Colombia

Teaching Experience

2024-II	**Computational drug discovery / Toxicology**, Teaching Fellow Position - Salesiana University	*Bogotá - Virtual*
2024-I	**Computational drug discovery / Toxicology**, Teaching Fellow Position - Salesiana University	*Bogotá - Virtual*
2023-II	**Computational drug discovery / Toxicology**, Teaching Fellow Position - Salesiana University	*Bogotá - Virtual*
2023-I	**Computational drug discovery**, Teaching Fellow Position - Salesiana University	*Bogotá - Virtual*
2021-II	**Medicinal Chemistry / Introduction of Pharmacy**, Teaching Fellow Position - University in applied and environmental science	*Bogotá*
2021-I	**Medicinal Chemistry / Introduction of Pharmacy**, Teaching Fellow Position - University in applied and environmental science	*Bogotá*
2019 - 2020	**Phytochemistry**, Teaching Assistant - National University of Colombia	*Bogotá*

Mentoring

2021-2022	**Maria Paula Cubides**, Teaching Fellow - University in applied and environmental science	*Bogotá*
2021-2022	**Rafael Mejía Marín**, Teaching Fellow - University in applied and environmental science	*Bogotá*

Outreach & Professional Development

Service and Outreach

2024 **2st international summer school - AI4MedChem**, Organizer and Lecturer *Münster, Germany*

2023 **Mexican International Conference on Artificial Intelligence - MICAI**, Committe Member *Merida, Mexico*

Development

Computational biomolecular simulation workflows with BioExcel building blocks, training and management of BioExcel building blocks for Molecular Dynamics.

Professional Memberships

ACS (American Chemical Society) member 2021
DPhG (Deutsche Pharmazeutische Gesellschaft) member 2024