Eduardo Alberto Aguilar Bejarano

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Education

University of Nottingham, Nottingham, UK.
PhD, Chemistry, Artificial Intelligence Doctoral Training Centre. Expected: September 2026. Supervisors: Prof. Simon Woodward, Prof. Ender Özcan, and Dr. Grazziela Figueredo.

Universidad de Costa Rica, San José, Costa Rica.
Bachelor of Science with Honors, Chemistry; GPA: 9.23/10. March 2018 - June 2022
Relevant Coursework: Bio-organic Chemistry, Bio-inorganic Chemistry, Computational Tools for Physical Chemistry, Scientific Computation with Python, Introduction to Genomics and Metagenomics Data Processing, Automated Learning With Python.

Research Experience

PhD. Researcher, University of Nottingham.
Woodward-Figueredo-Özcan Research Groups member, October 2022 - present.
Advisors: Prof. Simon Woodward, Prof. Ender Özcan, Dr. Grazziela Figueredo.

1. *Prediction of internal energy of molybdenum carbides by a deep learning approach:* data pre-processing, design of representation of materials, development of graph neural networks models, and generation of software to interpret the models and understand the reasoning behind the computers' prediction.
2. *Prediction of selectivity of Rhodium-catalysed asymmetric 1,4 addition by a deep learning approach:* data pre-processing, design of reaction graph representations, development of graph neural networks models, and generation of interpretation software for the models.

Research Assistant, University of Costa Rica.
CBIO3 Research Group Member, January 2021 - October 2022.
Advisor: Prof. William Zamora-Ramírez

1. Prediction of physical-chemical profiles and rational design of bioactive compounds assisted by in silico methods:
    - *Prediction of $logP_{Water/Toluene}$ of bioactive molecules:* curation of databases, creation of molecular representation, variable selection algorithms, training the algorithms (multiple linear regression, support vector machine, random forest regressor and gradient boosting regressor) for logP prediction, data and results visualization, and model interpretation.
    - *Prediction of tautomers isomerization constant:* curation of tautomer databases, creation of molecular representations, development of different predictive models of the equilibrium constant of tautomers in different solvents.

Publications

Aguilar Bejarano E, Figueredo G, Woodward S, Lam HW, Özcan E, Rit R. HCat-GNet: An Interpretable Graph Neural Network for Catalysis Optimization. ChemRxiv. 2024; doi:10.26434/chemrxiv-2024-zjnkd This content is a preprint and has not been peer-reviewed.

Galvin D, **Aguilar Bejarano E**, Rogers DM, Woodward S, Özcan E, Guiry PJ, et al. Describing Chiral Ligands in Palladium-catalyzed Decarboxylative Asymmetric Allylic Allylation: A Critical Comparison of Three Machine Learning Approaches. ChemRxiv. 2024; doi:10.26434/chemrxiv-2024-gxvd9-v2 This content is a preprint and has not been peer-reviewed.

Ignacio Borge-Durán, **Eduardo Aguilar Bejarano**, Luis Arrieta Araya et al. Explainable GNN-Derived Structure-Property Relationships in Interstitial-Alloy Materials, 15 May 2024, PREPRINT (Version 1) available at Research Square `https://doi.org/10.21203/rs.3.rs-4295272/v1`

Conferences & presentations

University of Nottingham School of Chemistry Postgraduate Symposium, Nottingham, UK, July 2024. Aguilar, E; Özcan, E; Rit, R. K.; Lam, H. W.; Woodward, S.; Figueredo, G. "HCat-GNet: an Intepretable Graph Neural Network for Catalysis Optimization" (poster).

The GSK Prosperity Partnership, GSK, Stevenage, UK, March 2024. Aguilar, E. "HCat-GNet: An Interpretable Graph Neural Network for Catalysis Optimization" (lecture).

Faraday Community Poster Symposium, Burlington House, London, UK, November 2023. Aguilar, E; Arrieta, L; Gutierrez, M; Figueredo, G; Özcan, E; Borge, I; Woodward, S. "Feature Identification in Molybdenum Carbides: Graph Neural Networks vs. Human Empirical Search –

Who's the Winner?" (poster).

Machine Learning for Atomistic Modelling Autumn School, Daresbury Laboratory, Daresbury, UK, September 2023. Aguilar, E; Arrieta, L; Gutierrez, M; Figueredo, G; Özcan, E; Borge, I; Woodward, S. "Feature Identification in Molybdenum Carbides: Graph Neural Networks vs. Human Empirical Search – Who's the Winner?" (poster).

School of Chemistry Seminar Series, University of Costa Rica, San José, Costa Rica, August 2023. Aguilar, E. "Chemistry in the Artificial Intelligence Era" (lecture).

Sciences Week Scientific Poster Contest, San Jose, Costa Rica, September 2022. Aguilar, E; Ràfols, C; Ruiz, R; Zamora, W."Development of a Novel Lipophilicity Descriptor from Predictions of Partitions Coefficients Toluene/Water" (poster).

University Week Scientific Poster Contest, San José, Costa Rica, April 2022. Aguilar, E; Ràfols, C; Ruiz, R; Zamora, W. "Machine Learning Methods to Determine the Toluene/Water Partition Coefficient as an Efficient Lipophilic Descriptor" (poster).

Gulf Coast Undergraduate Research Symposium, Houston, TX, October 2021. Aguilar, E; Zamora, W. "Cheminformatic and Quantum Mechanics Approaches for Quantitative Prediction of Tautomerism in Bioactive Molecules" (lecture).

Honor & awards

Christopher J. Moody Synthesis and Catalysis Poster Prize.
University of Nottingham School of Chemistry, July 2024.
Second place PGR Symposium Poster Contest.

Artificial Intelligence Doctoral Training Centre Scholarship.
School of Computer Sciences, University of Nottingham, July 2022.
Scholarship that covers tuition fees and stipend for four years to pursue a PhD. degree.

Bachelor of Science with Honors.
University of Costa Rica, June 2022.
Award given to students graduating with academic excellence.

CeNAT-CONARE Research Fellowship.
National Center of High Technology, June 2022.
Grant conferred to outstanding research proposals from students from public Universities of Costa Rica. Award for the project: 'Cheminfor-

matic and Quantum Mechanics Approaches for Quantitative Prediction of Tautomerism in Bioactive Molecules'. Total grant received: $4300.

Best Scientific Poster.
Chemistry Students Association, April 2022.
Winner of the University Week Scientific Poster Contest.

GCURS Acceptance and Travel Award.
Rice University, October 2021
Award to cover travel expenses to the Gulf Coast Undergraduate Research Symposium held in Rice University in Houston, Texas, to present the research 'Cheminformatic and Quantum Mechanics Approaches for Quantitative Prediction of Tautomerism in Bioactive Molecules' of the CBIO3 Group.

Academic Excellence Scholarship.
Universidad de Costa Rica, 2019-Present.
Scholarship for a year given to students with Average Overall Score of 9/10 or more in the year before.

Teaching Experience

MSc Project Co-Supervisor *Co-supervisor of Machine Learning in Science MSc. students, May 2023 - July 2023.*
Co-supervisor with Dr. Grazziela Figueredo and Dr. Kristaps Ermanis on projects involving the use of deep learning for chemical sciences.

Programming, machine learning and data analysis tutor.
Tutor of programming and cheminformatics of students of the CBIO3 Group, July 2022 - September 2022.
Teaching assistance of prof. William Zamora of the course of Cheminformatics. I helped students in topics of programming, data visualization, machine learning algorithms and cheminformatic tools.

Organic Chemistry and Analytical Chemistry Tutor.
Tutor of Organic and Analytical Chemistry of students of the University of Costa Rica, September 2021 - November 2021.
Hired by the University of Costa Rica as a tutor to reinforce the classes of organic chemistry and analytical chemistry to students of the University, Campus Atlantic.

Chemistry Olympiad Tutor.
Olympiad tutor for students of the Scientific High School of San Pedro, March 2021 - October 2021.
Worked as chemistry tutor of high school students for their preparation for the Costa Rican Chemistry Olympiad. The work involves the prepa-

ration of classes corresponding to the Olympiad topics, teaching them and preparation of exercises for the students to practice for the Olympiad test.

Laboratory Teaching Assistant.
Assistant in laboratory courses of the Universidad de Costa Rica.
The work involved helping the professor to teach the laboratory techniques, evaluate the students' work in the laboratory and score the students' laboratory reports. Courses I have worked as an assistant:

- Physical Chemistry II Laboratory (QU0369, IS-2021)
- Analytical Chemistry I Laboratory (QU0247, IS-2021)
- Physical Chemistry I Laboratory (QU0367, IIS-2020)
- Chemical Experimentation II Laboratory (QU0112, IIS-2020)
- Organic Chemistry I Laboratory (QU212, IS-2020)
- General and Qualitative Chemistry Laboratory (QU0107, IIS-2019)
- General Organic Chemistry I Laboratory (QU0213, IIS-2019)

General Chemistry Tutor.
Tutor of new students of the Universidad de Costa Rica, March 2021, March 2022.
Tutor of new students of the University of Costa Rica with poor background in chemistry. The work involved the planning of classes, the generation of didactic material and teaching the lessons.

Physics Reinforcement Tutor.
Physics reinforcement tutor for students of the Scientific High School of San Pedro, March 2019 - July 2019.
Worked as reinforcement tutor for high school students that had issues with the physics subject. The work involved teaching various physics-related topics and developing teaching methods in order to help the students understand the subject and improve their scores.

Teaching Assistant.
Assistant of the professor Darío Chinchilla, March 2018-December 2018.
Worked as assistant of the professor in the course of General and Biological Chemistry of the University of Costa Rica and in the chemistry course at the Scientific High School of San Pedro, performing activities such as the preparation of exams and correction of evaluations.

Membership

- Royal Chemical Society (September 2023 - present)
- American Chemical Society (July 2021 - July 2022)
- Costa Rica ACS Student Chapter (June 2021 - June 2022)

Technical Skills

Computational:

- Software: DataWarrior, Obabel, Microsoft Office, MapleSoft, Pymol.
- Programming Skills: Bash (basic commands and scripts), C (basics), R (data analysis, data visualization and model development using machine learning algorithms), and Python (experience in the libraries: SciPy, NumPy, Pandas, Matplotlib, sklearn, RDKit, PyTorch, PyTorch-Geometric for data processing, data visualization, feature selection algorithms, machine learning model development, statistics, calculus, linear algebra, cheminformatics and object oriented programming).

Laboratory: HPLC, gas chromatography, atomic absorption, uv/vis spectrophotometry, fluorescence spectrophotometry.

Languages: Spanish (native) and English (fluent).