Dr. Rocío Mercado Oropeza

Curriculum Vitae

Contact info:
Elektrogården 1
412 58 Göteborg, SE
rocio.mercado@chalmers.se
+46 (0)76 854-7752

Webpage: ailab.bio
ORCID: 0000-0002-6170-6088
Born: October 9, 1992
Nationality: American

RESEARCH INTERESTS

Dr. Mercado Oropeza heads the AI Lab for Molecular Engineering (AIME) at Chalmers, where she and her team seek to bridge methods from machine learning, chemistry, and life sciences to engineer molecular systems for therapeutic applications and sustainable materials, focusing on new AI method development. She and her team maintain active collaborations with industry, including AstraZeneca, Intel, and Merck.

ACADEMIC EDUCATION

Doctor of Philosophy, Chemistry — Aug 2018
University of California, Berkeley, CA, USA
Thesis title: *Computationally-driven investigations towards better gas adsorption materials*

Bachelor of Science, Chemistry — Jun 2013
California Institute of Technology, Pasadena, CA, USA
Thesis title: *Fluorinated cobaloximes for electrocatalytic proton reduction*

PROFESSIONAL APPOINTMENTS

WASP AI/MLX Assistant Professor — Jan 2023 – present
AI laboratory for Molecular Engineering (AIME)
Section for Data Science and AI, Department of Computer Science and Engineering
Chalmers University of Technology, Gothenburg, SE

Postdoctoral Associate — Aug 2021 – Dec 2022
Coley Group, Department of Chemical Engineering
Massachusetts Institute of Technology, Cambridge, MA, USA

Postdoctoral Researcher — Oct 2018 – Jul 2021
Molecular AI, Discovery Sciences R&D
AstraZeneca, Gothenburg, SE

Visiting PhD Researcher — Jan 2018 – Aug 2018 & Aug 2016 – Nov 2016 & Jul 2015 – Nov 2015
Laboratoire de simulation moléculaire, Faculty of Basic Sciences
École polytechnique fédérale de Lausanne, Sion, CH

PhD Researcher — Aug 2013 – Dec 2017
Molecular Simulation Group, Department of Chemical & Biomolecular Engineering
University of California, Berkeley, CA, USA

Undergraduate Researcher — Apr 2011 – Jul 2013
Gray Group, Department of Chemistry & Chemical Engineering
California Institute of Technology, Pasadena, CA, USA

SELECT FUNDING AND AWARDS

Main applicant

- **European Research Council (ERC)**, Starting Grant (StG), *1.5M €, including funding for two 5-year PhD students and two 3-year postdocs*, 2026–2030
- **WASP**/**WISE**, NEST, *main applicant with Chao Zhang; co-applicant: Daniel Brandell; ≈10M SEK, including funding for two 5-year PhD students and one 2-year postdoc*, 2025–2030
- **WASP**/**DDLS**, NEST, *main applicant with Ola Spjuth; co-applicants: Prashant Singh, Brinton Seashore-Ludlow, Ashkan Panahi; 15M SEK from WASP and 15M SEK from DDLS (30M SEK total), including funding for four 5-year PhD students & three 2-year postdocs*, 2025–2030
- **Swedish Research Council**, Starting Grant, *4M SEK (≈1 PhD student fully-funded for 4 years)*, 2023
- **Intel-Merck AWASES Award**, Intel-Merck Joint Academic Research Center for AI-Aware Pathways to Sustainable Semiconductor Process and Manufacturing Technologies (AWASES), *6.4M SEK (≈1 PhD and 1 postdoctoral researcher fully-funded for three years)*, 2023
- **National Academic Infrastructure for Super computing in Sweden (NAISS)**, various Compute and Storage allocations: Small Compute (Aug 2023 – Sep 2023), Medium Compute (Oct 2023 – present), Medium Storage (Oct 2023 – Jun 2025), Large Storage (Jul 2025 – present)
- **Chalmers Health Engineering Area of Advance**, Seed Funding, *50K SEK (MSc student summer research project)*, 2023
- **Wallenberg AI, Autonomous Systems, and Software Program (WASP)**, Startup Funding, *research startup costs for 5 years, including funding for 2 PhD students, 2 postdocs, and 80% self salary*, 2023
- **Chalmers Gender Initiative for Excellence (Genie)**, Startup Funding, *2M SEK (≈1 PhD student for 2 years)*, 2023
- **National Science Foundation (NSF) Graduate Research Fellowship Program (GRFP)**, *$34,000 stipend per Fellowship Year for three years, plus $12,000 Cost of Education Allowance per year for three years; 12% acceptance rate in 2015*, 2015

Co-applicant

- **DDLS**, Industrial PhD Funding, *with Filip Miljković and Susanne Winiwarter (AstraZeneca); funding for one 4-year PhD student, to be recruited*, 2025
- **WASP**/**WISE**, Pilot Project, *with Anders Hellman; 500K SEK per partner*, 2025
- **WASP**, Industrial Postdoc Funding, *with Samuel Genheden and Varvara Voinarovska; funding for one 2-year postdoc*, 2024
- **Data-Driven Life Sciences (DDLS)**, Industrial PhD Funding, *with Erik Lindahl (main applicant, Stockholm University), Ola Engkvist (main applicant, AstraZeneca), and Werngard Czechtizky (AstraZeneca); funding for 1 industrial PhD student fully-funded for 4 years*, 2024
- **WASP**/**WISE**, Pre-Project Grant, *with Chao Zhang (Uppsala University); 500K SEK per partner*, 2023
- **WASP**, Industrial PhD Funding, *with Samuel Genheden (AstraZeneca) and Emma Rydholm (PhD applicant); funding for 1 industrial PhD student fully-funded for 4 years*, 2023

RECENT PUBLICATIONS

1. *LeMat-GenBench: Bridging the gap between crystal generation and materials discovery.* Alexandre Duval, Siddharth Betala, Samuel P. Gleason, Andy Xu, Georgia Channing, Daniel Levy, Ali Ramlaoui, Clémentine Fourrier, Chaitanya K. Joshi, Nikita Kazeev, Sékou-Oumar Kaba, Félix Therrien, Alex Hernández-García, **R.M.**, N. M. Anoop Krishnan. *AI4Mat Workshop @ NeurIPS*, 2025.
2. *TopoMole: Topological Message Passing Meets Hyperedge Messages.* Pablo Martínez Crespo, Robert S. Jordan, Marisa Gliege, Santiago Miret, Vijay K. Narasimhan, **R.M.**† *AI4Mat Workshop @ NeurIPS*, 2025.

3. *Compressing Biology: Evaluating the Stable Diffusion VAE for Phenotypic Drug Discovery.* Télio Cropsal, **R.M.**† *Imageomics Workshop @ NeurIPS*, 2025.
4. *Descriptor and graph-based molecular representations in prediction of copolymer properties using machine learning.* Elaheh Kazemi-Khasragh, **R.M.,**† Carlos Gonzalez, Maciej Haranczyk.† *arXiv*, 2025. (preprint)
5. *LAGOM: A Transformer-based chemical language model for drug metabolite prediction.* Sofia Larsson Author, Miranda Carlsson, Richard Beckmann, Filip Miljković,† **R.M.**† *AILSCI*, 2025.
6. *Predicting PROTAC-mediated ternary complexes with AlphaFold3 and Boltz-1.* Nils Dunlop*, Francisco Erazo*, Farzaneh Jalalypour, **R.M.**† *Digital Discovery*, 2025.
7. *PROTAC-Splitter: A machine learning framework for automated identification of PROTAC substructures.* Stefano Ribes, Ranxuan Zhang, Télio Cropsal, Anders Källberg, Christian Tyrchan, Eva Nittinger,† **R.M.**† *ChemRxiv*, 2025. (preprint, under review)
8. *Prediction of permeability and efflux using multi-task learning.* Philip Ivers Ohlsson, Gianmarco Ghiandoni, Susanne Winiwarter, **R.M.**,† Vigneshwari Subramanian.† *ACS Omega*, 2025.
9. *RetroSynFormer: Planning multi-step chemical synthesis routes via a Decision Transformer.* Emma Granqvist, **R.M.**, Samuel Genheden, *ChemRxiv*, 2025. (preprint, under review)
10. *deCIFer: Crystal structure prediction from powder diffraction data using autoregressive language models.* Frederik Lizak Johansen, Ulrik Friis-Jensen, Erik Bjørnager Dam, Kirsten Marie Ørnsbjerg Jensen, **R.M.**, Raghavendra Selvan. *arXiv*, 2025. (preprint)

† *indicates corresponding author*

PUBLICATION STATISTICS

Based on Google Scholar:

35	publications in total	*Total citations*: 2876
19	in peer-reviewed international journals	*h-index*: 18
7	in computer science conferences or workshops	*i10-index*: 20
24	as first and/or corresponding author	

RECENT INVITED TALKS

1. *Chemical Compound Space Conference (CCSC) 2026.* Munich, DE. Mar 12, 2026. *Generative AI for Molecular Design: From Drugs to Sustainable Materials.*
2. *Applied Machine Learning Days (AMLD) 2026.* Lausanne, CH. Feb 10, 2026. *Invited talk (title TBD).*
3. *WASP Winter Conference.* Örebro, SE. Jan 14–15, 2026. *Invited talk (title TBD).*
4. *ML4Molecules ELLIS Unconference Workshop.* Copenhagen, DK. Dec 2, 2025. *Generative AI for Molecular Design: From Drugs to Sustainable Materials.*
5. *Chalmers International Office Virtual Research Seminar ("Master Class").* Virtual. Nov 24, 2025. *Generative AI for Molecular Engineering.*
6. † *Women in Machine Learning Workshop (WASP).* Chalmers, Gothenburg, SE. Nov 14, 2025. *Keynote (title TBD).*
7. *Data-Driven Life Sciences (DDLS) Annual Meeting.* Uppsala, SE. Nov 12, 2025. *Introduction to TIMED NEST Project (with co-PI Ola Spjuth).*
8. *Fakultetsdagen (speed presentations)*, University of Gothenburg, Gothenburg, SE. Nov 3, 2025. *How AI can help us design better molecules.*
9. *Computer-Aided Drug Discovery (CADD) Gordon Research Conference (GRC)*, Portland, Maine, USA. July 14, 2025. *Generative AI for PROTAC design.*
10. *IRB Barcelona Biomed Conferences: AI in Drug Discovery and Biomedicine.* Barcelona, ES. Apr 1, 2025. *Engineering molecules to specification with generative AI.*

† *keynote presentation*

CURRENT STUDENTS AND POSTDOCS

Sofia Larsson *PhD Computer Science & Engineering (Nov 2025 – present)*
Chalmers University of Technology & AstraZeneca
Assistant advisors: Dr. Filip Miljković (AstraZeneca), Dr. Susanne Winiwarter (AstraZeneca)

Nils Dunlop *PhD Computer Science & Engineering (Oct 2025 – present)*
Chalmers University of Technology
Assistant advisor: Prof. Ashkan Panahi

Frida Jacobsson *MSc Applied Data Science (Aug 2025 – Dec 2025)*
Chalmers University of Technology & AstraZeneca
Main supervisors: Dr. Richard Beckmann (Chalmers) and Dr. Mikhail Kabeshov (AstraZeneca)

Siyu (Zoe) Hu *Research Assistant (Jun 2025 – present)*
Chalmers University of Technology *MSc Complex Adaptive Systems*

Dr. Varvara Voinarovska *Industrial Postdoctoral Researcher (Apr 2025 – present)*
Chalmers University of Technology & AstraZeneca
Co-advisor: Dr. Samuel Genheden (AstraZeneca), Dr. Mikhail Kabeshov (AstraZeneca)

Yaochen Rao *PhD Computer Science & Engineering (Dec 2024 – present)*
Chalmers University of Technology
Assistant advisor: Prof. Fredrik Johansson

Pablo Martínez Crespo *PhD Computer Science & Engineering (Sep 2024 – present)*
Chalmers University of Technology
Assistant advisors: Prof. Simon Olsson, Dr. Santiago Miret (Intel), Dr. Vijay Narasimhan (EMD Electronics)

Dr. Richard Beckmann *Postdoctoral Researcher (Aug 2024 – present)*
Chalmers University of Technology
Assistant advisors: Dr. Santiago Miret (Intel), Dr. Vijay Narasimhan (EMD Electronics)

Dr. Farzaneh Jalalypour *Postdoctoral Researcher (May 2024 – present)*
Chalmers University of Technology

Stefano Ribes *PhD Computer Science & Engineering (Mar 2024 – present)*
Chalmers University of Technology
Assistant advisor: Prof. Moa Johansson

Dr. Philip John Harrison *Postdoctoral Researcher (Jan 2024 – present)*
Chalmers University of Technology

Emma Granqvist *Industrial PhD Computer Science & Engineering (Oct 2023 – present)*
Chalmers University of Technology & AstraZeneca
Co-advisor: Dr. Samuel Genheden (AstraZeneca); assistant advisor: Prof. Fredrik Johansson

Télio Cropsal *PhD Computer Science & Engineering (Sep 2023 – present)*
Chalmers University of Technology
Assistant advisor: Prof. Simon Olsson

Yossra Gharbi *PhD Computer Science & Engineering (Sep 2023 – present)*
Chalmers University of Technology
Assistant advisor: Prof. Simon Olsson

CO-ADVISED STUDENTS AND POSTDOCS

Robin Rydbergh *PhD Life Sciences (Oct 2025 – present)*
Chalmers University of Technology
Main advisor: Prof. Michaela Wenzel; co-supervisor: Prof. Annikka Polster

Leo Andrekson *PhD Life Sciences (Oct 2025 – present)*
Chalmers University of Technology
Main advisor: Prof. Michaela Wenzel; co-supervisor: Prof. Annikka Polster

Beatrice Pavesi *PhD Computer Science & Engineering (Apr 2025 – present)*
Chalmers University of Technology
Main advisor: Prof. Simon Olsson

Christopher Kolloff *PhD Computer Science & Engineering (Jan 2025 – present)*
Chalmers University of Technology
Main advisor: Prof. Simon Olsson

Jessica Bair *PhD Chemistry (Dec 2024 – present)*
Chalmers University of Technology
Main advisor: Prof. Christian Müller

Camille Penot *PhD Biophysics (Oct 2024 – present)*
Stockholm University & AstraZeneca
Co-advisors: Prof. Erik Lindahl, Dr. Ola Engkvist (AstraZeneca), Dr. Marco Klähn (AstraZeneca), Dr. Werngard Czechtizky (AstraZeneca)

Valter Schütz *PhD Computer Science & Engineering (Sep 2024 – present)*
Chalmers University of Technology
Main advisor: Prof. Morteza Chehreghani

Selma Moqvist *PhD Computer Science & Engineering (Sep 2024 – present)*
Chalmers University of Technology
Main advisor: Prof. Simon Olsson

Zhan-Yun Zhang *Postdoctoral Researcher (Jan 2024 – present)*
Uppsala University
Main advisor: Prof. Chao Zhang

Ross Irwin *Industrial PhD Computer Science & Engineering (Oct 2023 – present)*
Chalmers University of Technology & AstraZeneca
Main advisors: Prof. Simon Olsson, Dr. Alessandro Tibo (AstraZeneca), Dr. Jon-Paul Janet (AstraZeneca)

PAST STUDENTS AND POSTDOCS

Nils Dunlop *Research Assistant (Jul 2025 – Aug 2025)*
University of Gothenburg *2025 MSc Applied Data Science*

Yihuai Cai *Research Assistant (Jun 2025 – Aug 2025)*
Chalmers University of Technology *MSc Data Science & AI*
Main supervisor: Dr. Farzaneh Jalalypour

Francisco Alejandro Erazo Piza & **Nils Dunlop** *2025 MSc Applied Data Science*

University of Gothenburg
Co-advisor: Dr. Farzaneh Jalalypour
- Thesis title: *Ligand-Enhanced Prediction of PROTAC and Molecular Glue Complexes Using AlphaFold 3 and Boltz-1*

Dadi Andrason *2025 MSc Data Science & AI*
& **Marcus Johansson** *2025 MSc Complex Adaptive Systems*
Chalmers University of Technology
Co-advisor: Dr. Philip John Harrison
- Thesis title: *Data Engineering and Image Analysis for JUMP Cell Painting Data for Drug Discovery*

Miranda Carlsson & **Sofia Larsson** *2025 MSc Complex Adaptive Systems*
Chalmers University of Technology & AstraZeneca
Co-advisors: Dr. Filip Miljković (AstraZeneca), Dr. Richard Beckmann (Chalmers)
- Thesis title: *AI for Metabolite Prediction in Drug Discovery*

Ranxuan Zhang *2025 MSc Biotechnology*
Chalmers University of Technology
Co-advisor: Stefano Ribes
- Thesis title: *Machine Learning for PROTAC Decomposition and Enhanced Degradation Prediction*

Frederik Lizak Johansen *Guest PhD Researcher (Sep 2024 – Dec 2024)*
University of Copenhagen *PhD Machine Learning*
Main advisor: Prof. Raghavendra Selvan
- Project title: *Expanding generative AI capabilities for crystal structure generation with language models*

Cristian-Catalin Pop *2024 MSc Bioinformatics*
Uppsala University
Main advisors: Prof. Ola Spjuth, Dr. Philip John Harrison
- Thesis title: *Using ADME/PK models to improve generative molecular design with reinforcement learning* link

Philip Ivers Ohlsson *2024 MSc Data Science & AI*
Chalmers University of Technology & AstraZeneca
Co-advisor: Dr. Vignesh Subramanian (AstraZeneca)
- Thesis title: *Refining permeability forecasts in drug discovery*

Jin Ahmad *2024 BSc Chemistry*
Karlstad University
Co-advisor: Prof. Angela Grommet (Chalmers)
- Thesis title: *Engineering coordination cages with generative AI* link

Pär Aronsson & *2024 MSc Data Science & AI*
Amanda Dehlén *2024 MSc Algorithms, Languages & Logic*
Chalmers University of Technology & AstraZeneca
Co-advisor: Dr. Filip Miljković (AstraZeneca)
- Thesis title: *Prediction of drug metabolites using a deep learning language model*

Leo Andrekson *2024 MSc Biotechnology*
Chalmers University of Technology
- Thesis title: *Learning meaningful representations of cells* link

Anders Källberg *2024 MSc Biotechnology*

Chalmers University of Technology & AstraZeneca
Co-advisors: Dr. Eva Nittinger (AstraZeneca), Dr. Christian Tyrchan (AstraZeneca)
- Thesis title: *Machine learning for structural predictions of PROTACs* link

Elaheh Kazemi Khasragh *Guest PhD Researcher (Feb 2024 – May 2024)*
Polytechnic University of Madrid & IMDEA Materials Institute *PhD Materials Science & Engineering*
Main advisor: Dr. Maciej Haranczyk, Prof. Carlos González
- Project title: *Molecular dynamics and machine learning for copolymer property prediction*

María Nuria Peralta Moreno *Guest PhD Researcher (Oct 2023 – Feb 2024)*
University of Barcelona *PhD Theoretical Chemistry and Computational Modelling*
Main advisor: Prof. Jaime Rubio Martínez
- Project title: *Machine learning for binding site identification*

Mert Yurdakul *2023 MSc Data Science & AI*
Chalmers University of Technology & AstraZeneca
Co-advisors: Dr. Martin Priessner (AstraZeneca), Dr. Anna Tomberg (AstraZeneca)
- Thesis title: *Automating molecular structure elucidation using machine learning*

Kinga Jenei *2023 MSc Data Science & AI*
University of Gothenburg & AstraZeneca
Co-advisor: Dr. Vignesh Subramanian (AstraZeneca)
- Thesis title: *Machine learning for molecular property prediction and drug safety* link

Stefano Ribes *2023 MSc Computer Science & Engineering*
Chalmers University of Technology & AstraZeneca
Co-advisors: Dr. Eva Nittinger (AstraZeneca), Dr. Christian Tyrchan (AstraZeneca)
- Thesis title: *Machine learning for predicting targeted protein degradation* link

Edwin Holst & **Preetha Mutharasu** *2023 MSc Computer Science & Engineering*
Chalmers University of Technology & AstraZeneca
Co-advisor: Dr. Jon Paul Janet (AstraZeneca)
- Thesis title: *Human-in-the-loop control of molecular reinforcement learning with online adaptive classifiers* link

Siva Manohar & **Supriya Kancharla** *2023 MSc Data Science & AI*
University of Gothenburg & AstraZeneca
Co-advisors: Dr. Samuel Genheden (AstraZeneca), Dr. Annie Westerlund (AstraZeneca)
- Thesis title: *Evaluating and optimizing Transformer models for predicting chemical reactions* link

Christian Ulmer *2023 MSc Computer Simulations for Science & Engineering*
KTH Royal Institute of Technology & Technical University Berlin (dual degree)
Co-advisors: Wenhao Gao (MIT), Prof. Connor Coley (MIT), Prof. Elias Jarlebring (KTH)
- Thesis title: *SynNet 2.0: Improved Synthesizable Molecular Design* link

Divya Nori *2025 BSc Electrical Eng. & Computer Science, Minor Mathematics (exp.)*
Massachusetts Institute of Technology
Co-advisor: Prof. Connor Coley
- Project title (UROP): *De novo design PROTAC design using graph-based deep generative models*

Sara Romeo Atance & **Juan Viguera Diez** *2021 MSc Complex Adaptive Systems*
Chalmers University of Technology & AstraZeneca
Co-advisor: Prof. Simon Olsson (Chalmers)
- Thesis title: *Towards molecular design with desired property profiles and 3D conformer generation*

using deep generative models link

Julio Ponte Hernández *2021 MSc Computer Science & Engineering*
Chalmers University of Technology & AstraZeneca
Co-advisor: Prof. Simon Olsson (Chalmers)
- Thesis title: *Deep learning a transferable model for drug-receptor binding-energy* link

Tobias Rastemo *2020 MSc Computer Science & Engineering*
Chalmers University of Technology & AstraZeneca
Co-advisor: Dr. Shirin Tavara (Chalmers)
- Thesis title: *Sampling a subset of chemical space with GNN-based generative models* link

Rueih-Sheng (Ray) Fu *2018 BSc Chemical Engineering*
University of California, Berkeley
Molecular Simulation Group
- Thesis title: *In silico design of covalent organic frameworks for applications in methane storage*

RECENT TEACHING EXPERIENCE

Course Responsible & Examiner, DAT565 – Introduction to Data Science & AI — Aug 2023 – Nov 2023
Computer Science & Engineering (CSE) Department — & Aug 2024 – Nov 2024
Chalmers University of Technology, Gothenburg, SE — & Aug 2025 – Nov 2025
- Course responsible, examiner, and principal lecturer for a 200-student introductory data science course for bachelors and masters students from various Chalmers programs

Guest Lecturer, SK00037 – Artificial Intelligence in Healthcare — Feb 2024 – Apr 2024
Gothenburg University & Sahlgrenska Academy, Gothenburg, SE
- PhD course led by Robert Feldt, Eric Hamrin Senorski, Justin Schneiderman, and Linn Söderholm
- Prepared a 3 hr lecture delivered on Mar 7, 2024 on generative models in drug discovery

REVIEWING SERVICE

ACS Nano, AILSCI, Chemical Science, RSC Digital Discovery, AI4Science Workshop (NeurIPS, ICML), ML4Mat Workshop (NeurIPS), ML4Molecules Workshop, DGM4HSD (ICLR), Microbial Drug Resistance, Journal of Cheminformatics, Communications Chemistry*, Machine Learning: Science and Technology*, Nature Communications, Nature Machine Intelligence, Nature Computational Science, IEEE Transactions on Neural Networks and Learning Systems, Journal of Chemical Information and Modeling, Journal of Computer-Aided Molecular Design, ACS Industrial & Engineering Chemical Research, Wiley Chemistry Select, WIREs Computational Molecular Science, NDiSTEM Session Proposals (SACNAS), Research Presentations and Travel Scholarship Abstracts (SACNAS), WASP Academic PhD Call 2023, WASP Academic PhD Call 2024, ICML 2023 Workshop Selection, ERC StG 2023, BOKU AI4Mat-Vienna-2024, NeurIPS 2024, AI4Mat-NeurIPS-2024 Area Chair, AI4Mat-NeurIPS-2025 Area Chair, ICLR 2025, AISTATS 2025, ELLIS ML4Molecules 2024, ELLIS ML4Molecules 2025, ICML 2025, FPI-ICLR-2025, NeurIPS 2025

**indicates received reviewer award from publisher*

RECENT PROFESSIONAL SERVICE

PhD, Lic./Halfway Seminar, and MSc Defenses
- **Nedra Mekni**, *PhD Computational Chemistry*, University of Vienna, *Jan 2024*
- **Juan Inda Diaz**, *PhD Mathematical Sciences*, University of Gothenburg and Chalmers, *Nov 2023*
- **Giulia Lo Dico**, *PhD Material Science & Engineering*, Universidad Carlos III de Madrid, *Jun 2023*

- **David Hagerman**, *Halfway Seminar Electrical Engineering*, Chalmers, *Jun 2024*
- **Filip Ekström Kelvinius**, *Halfway Seminar Computer & Information Science*, Linköping University, *Feb 2024*
- **Gökçe Geylan**, *Halfway Seminar Systems Biology*, Linköping University, *Feb 2024*
- **Ranxuan Zhang**, *MSc Biotechnology*, Chalmers, *Jun 2025*
- **Dadi Andrason** & **Marcus Johansson**, *MSc Data Science & AI* and *MSc Complex Adaptive Systems*, Chalmers, *Jun 2025*
- **Miranda Carlsson** & **Sofia Larsson**, *MSc Complex Adaptive Systems*, Chalmers, *Jun 2025*
- **Francisco Alejandro Erazo Piza** & **Nils Dunlop**, *MSc Applied Data Science*, University of Gothenburg, *Jun 2025*
- **Dimitrios Stefanou**, *MSc Data Science and AI*, Chalmers, *Aug 2024*
- **Eric Anttila Ryderup** & **Yu-Ping Hsu**, *MSc Data Science & AI*, Chalmers, *Jun 2024*

Academic Service and Appointments

- **National Allocations Committee (NAC) Member**, National Academic Infrastructure for Supercomputing in Sweden, *Oct 2025 – present* (link)
- **Mentor**, Chemistry Women Mentorship Network (ChemWMN), *Sep 2025 – present*
- **Profile Leader**, Health Engineering Area of Advance, Chalmers, *Feb 2024 – present* (link)
- **Organizer**, AI for Accelerated Materials Design (AI4Mat) Workshop, NeurIPS 2025, *May 2025 – present*; *Role:* Co-organizer (with 7 international researchers); previously also co-organized AI4Mat-ICLR-2025; ∼1-4 hrs/mo (event page)
- **Organizer**, CHAIR Theme on Structured Learning, Chalmers, *Oct 2022 – present*; *Role:* Co-organizer (with 3 other faculty from Chalmers CSE & MATH); ∼1-3 hrs/mo (2023 event page; 2024 event page; 2025 event page); Ongoing organization of AI4Science Seminar and fika; ∼2-8 hrs/mo (seminar page; YouTube page)
- **Selection Committee**, Marie Skłodowska-Curie Actions (MSCA) COFUND Doctoral Training Program in Human-centric AI (HAIF), University of Turku, *Fall 2024 – present*
- **Organizer**, CSE Department Colloquium, Chalmers, *Dec 2023 – Apr 2025*; *Role:* Co-organizer (with 4 other faculty from Chalmers CSE) and DSAI representative, organized Apr 2024 colloquium titled "Entrepreneurship in Academia" with speakers Per Stenström, Devdatt Dubhashi, and Yinan Yu; coordinated Apr 2024 colloquium with speaker Ricardo Baeza Yates; coordinated Nov 2024 colloquium with Kenny Smith; ∼1-2 hrs/mo
- **Organizer**, Broad Institute Machine Learning in Drug Discovery (MLinDD) Symposium, Virtual, *Dec 2022 – Sep 2024*; *Role:* Co-organizer (with 10 other scientists, mainly Broadies) for MLinDD Symposium Oct 2023 and Nov 2024; speaker, sponsorship, and poster sub-committees; ∼1-3 hrs/mo (2024 event page)
- **Organizer**, WASP/WISE Machine Learning for Molecular and Materials Discoveries (ML2MD) Symposium, Gothenburg, SE, *Jan 2024 – Sep 2024*; *Role:* Co-organizer with Chao Zhang (Uppsala University); ∼8 hrs/mo (2024 event page)

**FoAss: Swedish equivalent of assistant professor ("forskarassistent")*

SELECT HONORS AND AWARDS

Supervisor of the Year Finalist, Chalmers Doctoral Students' Guild, *2025*. link
Reviewer of the Month, Communications Chemistry, *2021*.
Outstanding Reviewer Award, IOP Publishing, *2021*.
Outstanding Graduate Student Instructor Award, UC Berkeley, *2015*.

IN THE MEDIA

Interviews and news articles

- "Rocío Mercado receives ERC Starting Grant." *WASP Sweden*. Sep 2025. link
- "Distinguished EU grant to promising Chalmers researchers." *Chalmers News*. Sep 2025. link
- "A double win for AI in this year's Noble prize" by Natalija Sako. *Chalmers News*. Oct 2024. link
- "Department Interview: Meet Assistant Professor Rocío Mercado." *Chalmers CSE*. Nov 2022. link
- "Artificial Intelligence of Drug Discovery with Rocío Mercado." *Skype a Scientist LIVE*. Feb 2022. link
- "Constructing an Edifice of Life and Science with Rocío Mercado." *Random Walks Podcast*. Nov 2021. link
- "Mentorship creates lasting bonds" by Lisa Muñoz. *Scholar News (Amgen Scholars Program)*. link

Miscellaneous

- Recorded talks for the Chalmers AI4Science Seminar. *YouTube*. link

LANGUAGES

English (fluent), Spanish (fluent), and Swedish (C1)

Last updated November 9, 2025