Dr. Rocío Mercado Oropeza

Curriculum Vitae

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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

- **Swedish Research Council**, Starting Grant, *4M SEK (equiv 1 PhD student fully-funded for four 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 (equiv 1 PhD and 1 postdoctoral researcher fully-funded for three years)*, 2023
- **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 group startup costs for five years, including funding for 2 PhD students, 2 postdocs, and 80% self salary*, 2023
- **Gender Initiative for Excellence (Genie)**, Startup Funding, *2M SEK (equiv 1 PhD student for two 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; funding for one 4-year PhD student, to be recruited*, 2025
- **WASP**/**WISE**, Pilot Project, *with Anders Hellman; 1M SEK for a project duration of 1 year (0.5M SEK from WASP and 0.5M SEK from WISE)*, 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 four 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 four years*, 2023

RECENT PUBLICATIONS

1. *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, under review)
2. *A comprehensive review of emerging approaches in machine learning for de novo PROTAC design.* Yossra Gharbi, **R.M.**† *Digital Discovery*, 2024, 3, 2158-2176
3. *Contrastive learning for robust cell annotation and representation from single-cell transcriptomics.* Leo Andrekson, **R.M.**† *bioRxiv*, 2024. (preprint, under review)
4. *Modeling PROTAC degradation activity with machine learning.* Stefano Ribes, Eva Nittinger, Christian Tyrchan, **R.M.**† *Artificial Intelligence in the Life Sciences*, 2024, *6*, 100104.
5. *Do Chemformers dream of organic matter? Evaluating a transformer model for multi-step retrosynthesis.* Annie M. Westerlund, Siva Manohar Koki, Supriya Kancharla, Alessandro Tibo, Lakshidaa Saigiridharan, Mikhail Kabeshov, **R.M.**, Samuel Genheden. *J. Chem. Inf. Model.*, 2024, 64, 8, 3021–3033.

6. *Data sharing in chemistry: lessons learned and a case for mandating structured reaction data.* **R.M.**, Steven Kearnes, Connor W. Coley. *J. Chem. Inf. Model.*, 2023, 63, 14, 4253–4265.
7. *De novo PROTAC design using graph-based deep generative models.* Divya Nori, Connor W. Coley, **R.M.**† *AI4Science Workshop*, NeurIPS, 2022.
8. *De novo drug design using reinforcement learning with graph-based deep generative models.* Sara Romeo Atance, Juan Viguera Diez, Ola Engkvist, Simon Olsson, **R.M.**† *J. Chem. Inf. Model.*, 2022, 62, 20, 4863–4872.
9. *Amortized tree generation for bottom-up synthesis planning and synthesizable molecular design.* Wenhao Gao, **R.M.**, Connor W. Coley. *ICLR*, 2022. (conference paper)
10. *Graph networks for molecular design.* **R.M.**, Tobias Rastemo, Edvard Lindelöf, Günter Klambauer, Ola Engkvist, Hongming Chen, Esben J. Bjerrum. *Mach. Learn.: Sci. Tech.*, 2020.

†*indicates corresponding author*

PUBLICATION STATISTICS

Based on Google Scholar:

26	publications in total	*Total citations*: 2473
17	in peer-reviewed international journals	*h-index*: 17
4	in computer science conferences or workshops	*i10-index*: 17
9	with PhD supervisor	
16	as first and/or corresponding author	

RECENT INVITED TALKS

1. *AI in Drug Discovery and Biomedicine.* Barcelona, ES. Mar 31-Apr 02, 2025. *Engineering molecules to specification with generative AI.*
2. *2nd Nordic Computational Chemistry Conference.* Gothenburg, SE. Mar 18-19, 2025. *Engineering molecules to specification with generative AI.*
3. *Science Fika, Department of Chemistry, Chalmers.* Gothenburg, SE. Dec 11, 2024. *Engineering molecules with AI.*
4. *Workforce for Inclusive SciencE (WISE) Lunch Seminar, Department of Electrical Engineering, Chalmers.* Gothenburg, SE. Nov 21, 2024. *Engineering molecules to specification with AI.*
5. *Intel-Merck AWASES Program Kick-off Event.* Virtual. Apr 17, 2024. *An integrated molecular dynamics and deep learning framework for multi-modal materials data.*
6. *Generative AI in Life Science (GenLife).* Copenhagen, DN. Apr 16, 2024. *Next-gen drug design with machine learning.*
7. *WISE Dialogue 2024.* Gotheburg, SE. Mar 15, 2024. *Machine learning-accelerated electrolyte modelling and design.* Joint presentation with collaborator Chao Zhang.
8. *International Symposium on Machine Learning in Quantum Chemistry.* Uppsala, SE. Nov 29, 2023. *Deep generative models for biomolecular engineering.* link to recording
9. †*DDLS Annual Conference, Karolinska Institutet.* Stockholm, SE. Nov 16, 2023. *Transforming biomolecular engineering through AI.*
10. *Chemistry and Materials Science Department(s).* Aalto University. Helsinki, FI. Nov 13, 2023. *Deep generative models for biomolecular engineering.*

†*keynote presentation*

CURRENT STUDENTS AND POSTDOCS

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

Pablo Martínez Crespo *PhD Computer Science & Engineering (Sep 2024 – present)*
Chalmers University of Technology
Assistant advisors: Dr. 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: Dr. 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: Dr. Fredrik Johansson

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

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

CO-ADVISED STUDENTS AND POSTDOCS

Christopher Kolloff *PhD Computer Science & Engineering (Jan 2025 – present)*
Chalmers University of Technology
Main advisor: Dr. 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: Dr. 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: Dr. Simon Olsson, Dr. Alessandro Tibo (AstraZeneca), Dr. Jon-Paul Janet (AstraZeneca)

PAST STUDENTS AND POSTDOCS

Frederik Lizak Johansen *Guest PhD Researcher (Sep 2024 – Dec 2024)*
PhD Machine Learning
University of Copenhagen
- 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: Dr. 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)*
PhD Materials Science & Engineering

Polytechnic University of Madrid & IMDEA Materials Institute
- Project title: *Molecular dynamics and machine learning for copolymer property prediction*

María Nuria Peralta Moreno *Guest PhD Researcher (Oct 2023 – Feb 2024)*
PhD Theoretical Chemistry and Computational Modelling
University of Barcelona
- 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), Dr. 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: Dr. 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: Dr. 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: Dr. 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
- 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

Chemical Science, RSC Digital Discovery, AI4Science Workshop (NeurIPS, ICML), ML4Mat Workshop (NeurIPS), ML4Molecules Workshop, DGM4HSD (ICLR), 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 2023 StG, BOKU AI4Mat-Vienna-2024, NeurIPS 2024, AI4Mat (NeurIPS 2024 Workshop) Area Chair, ICLR 2025, AISTATS 2025, ELLIS ML4Molecules 2024, ICML 2025, FPI-ICLR2025

**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*, Gothenburg University 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*
- **Eric Anttila Ryderup** & **Yu-Ping Hsu**, *MSc Data Science & AI*, Chalmers, *Jun 2024*

Academic Service and Appointments

- **Profile Leader**, Health Engineering Area of Advance, Chalmers, *Feb 2024 – present* (link)
- **Organizer**, AI for Materials (AI4Mat) Workshop, ICLR 2025, *Oct 2024 – present*; *Role:* Co-organizer (with 5 international researchers); ∼1-3 hrs/mo
- **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); Ongoing organization of AI4Science Seminar and fika; ∼2-8 hrs/mo (seminar page; YouTube page)
- **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
- **Selection Committee**, Marie Skłodowska-Curie Actions (MSCA) COFUND Doctoral Training Program in Human-centric AI (HAIF), University of Turku, *Expected activity Fall 2024 – Sep 2025*
- **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

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

- "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*. link
- "Artificial Intelligence of Drug Discovery with Rocío Mercado." *Skype a Scientist LIVE*. link
- "Constructing an Edifice of Life and Science with Rocío Mercado." *Random Walks Podcast*. 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 February 23, 2025