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 heads the AI Lab for Molecular Engineering (AIME) at Chalmers, where she and her team seek to bridge methods from machine learning, chemistry, and the 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 researchers, 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

- **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. *A comprehensive review of emerging approaches in machine learning for de novo PROTAC design.* Yossra Gharbi, **R.M.**† *arXiv*, 2024. (preprint)
2. *Contrastive learning for robust cell annotation and representation from single-cell transcriptomics.* Leo Andrekson, **R.M.**† *bioRxiv*, 2024. (preprint)
3. *Modeling PROTAC degradation activity with machine learning.* Stefano Ribes, Eva Nittinger, Christian Tyrchan, **R.M.**† *Artificial Intelligence in the Life Sciences*, 2024, ASAP.
4. *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.
5. *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.
6. *De novo PROTAC design using graph-based deep generative models.* Divya Nori, Connor W. Coley, **R.M.**† *AI4Science Workshop*, NeurIPS, 2022.
7. *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.
8. *Amortized tree generation for bottom-up synthesis planning and synthesizable molecular design.* Wenhao Gao, **R.M.**, Connor W. Coley. *ICLR*, 2022. (conference paper)
9. *Exploring graph traversal algorithms in graph-based molecular generation.* **R.M.**, Esben J. Bjerrum, Ola Engkvist. *J. Chem. Inf. Model.*, 2022, 62, 9, 2093–2100.

10. *A transferable Boltzmann Generator for small molecules.* Juan Viguera Diez, Sara Romeo Atance, Ola Engkvist, **R.M.**, Simon Olsson. *ELLIS Machine Learning for Molecule Discovery Workshop*, 2021. (workshop paper)
11. *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.**† *RL4RealLife Workshop*, ICML, 2021.
12. *Comparative study of deep generative models on chemical space coverage.* Jie Zhang, **R.M.**, Ola Engkvist, Hongming Chen. *J. Chem. Inf. Model.*, 2021, *61*, **6**, 2572–2581.
13. *Molecular representations in AI-driven drug discovery: a review and practical guide.* Laurianne David, Amol Thakkar, **R.M.**, Ola Engkvist. *J. Cheminf.*, 2020, 12, 56.
14. *Practical notes on building graph generative models.* **R.M.**, Tobias Rastemo, Edvard Lindelöf, Günter Klambauer, Ola Engkvist, Hongming Chen, Esben J. Bjerrum. *Applied AI Letters*, 2020.
15. *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*; **indicates co-first authors*

PUBLICATION STATISTICS

Based on Google Scholar:

26	publications in total	*Total citations*: 2178
17	in peer-reviewed international journals	*h-index*: 15
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. *2nd Nordic Computational Chemistry Conference.* Gothenburg, SE. Mar 18-19, 2024. *Talk title TBD.*
2. *Intel-Merck AWASES Program Kick-off Event.* Virtual. Apr 17, 2024. *An integrated molecular dynamics and deep learning framework for multi-modal materials data.*
3. *Generative AI in Life Science (GenLife).* Copenhagen, DN. Apr 16, 2024. *Next-gen drug design with machine learning.*
4. *WISE Dialogue 2024.* Gotheburg, SE. Mar 15, 2024. *Machine learning-accelerated electrolyte modelling and design.* Joint presentation with collaborator Chao Zhang.
5. *International Symposium on Machine Learning in Quantum Chemistry.* Uppsala, SE. Nov 29, 2023. *Deep generative models for biomolecular engineering.* link to recording
6. †*DDLS Annual Conference, Karolinska Institutet*. Stockholm, SE. Nov 16, 2023. *Transforming biomolecular engineering through AI.*
7. *Chemistry and Materials Science Department(s).* Aalto University. Helsinki, FI. Nov 13, 2023. *Deep generative models for biomolecular engineering.*
8. *18th Scandinavian Symposium on Chemometrics (SSC) 2023.* Gothenburg, SE. Oct 2, 2023. *Deep generative models for biomolecular engineering.*
9. *Girls Code Club.* Chalmers University of Technology. Gothenburg, SE. Jun 21, 2023. *From Coding to Cures: How Computers Help Scientists Design Better Medicines.*
10. *Condensed Matter Seminar.* Chalmers University of Technology. Gothenburg, SE. Jun 20, 2023. *Deep generative models for biomolecular engineering.*
11. *IMDEA Materials.* Madrid, ES. Jun 13, 2023. *Deep generative models for biomolecular engineering.*
12. *Machine Learning for Multiscale Molecular Modeling Workshop.* SIMPLAIX 2023. Heidelberg, DE. May 2-4, 2023. *Deep generative models for biomolecular engineering.*
13. *MLLS Seminar Series.* Center for Basic Machine Learning Research in Life Science. Copenhagen, DK. Apr 21, 2023. *Deep generative models for biomolecular engineering.*

14. *AI for Accelerated Materials Design (AI4Mat) Workshop.* NeurIPS 2022. New Orleans, LA, USA. Dec 2, 2022. *Panelist: Everyday research challenges in AI for automated materials design.*
15. *ML for Science Seminar Series.* EPFL. Virtual. Nov 8, 2022. *Exploring new frontiers in drug discovery using deep generative models.*

† *keynote presentation*

CURRENT STUDENTS AND POSTDOCS

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 Rydholm *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

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

Ross Irwin *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

Cristian-Catalin Pop *2024 MSc Bioinformatics*
Uppsala University
Main advisors: Prof. Ola Spjuth, Dr. Philip John Harrison

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*

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*

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*

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*

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*

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*

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*

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*

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*

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*

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*

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

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

Course Responsible & Examiner, DAT565 – Introduction to Data Science & AI Aug 2023 – Nov 2023
Computer Science & Engineering 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

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, AI4Mat-Vienna-2024, NeurIPS 2024

** indicates received reviewer award from publisher*

RECENT PROFESSIONAL SERVICE

PhD 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*

Licentiate Defenses ("Halfway PhD")

- **David Hagerman**, *PhD Electrical Engineering*, Chalmers, *Jun 2024*
- **Filip Ekström Kelvinius**, *PhD Computer & Information Science*, Linköping University, *Feb 2024*

MSc Defenses

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

Faculty Recruitment

- **DDLS Professorship Recruitment Group**, Chalmers CSE Department, *Jun 2023 – Mar 2024*
- **WASP AI/MATH Professorship Recruitment Group**, Chalmers CSE Department, *Feb 2023 – Mar 2024*

Event Planning

- **WASP/WISE Machine Learning for Molecular and Materials Discoveries (ML2MD) Symposium**, Gothenburg, SE, *Jan 2024 – present*
  - *Role:* Co-organizer (with Chao Zhang, Uppsala University)
  - Ongoing event organization for ML2MD Symposium (Aug 2024); ∼8 hrs/mo
- **CSE Department Colloquium**, Chalmers, *Dec 2023 – present*
  - *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; organizing Spring 2025 colloquium with speaker Sanjit Seshia; ∼1-2 hrs/mo
- **CHAIR Theme on Structured Learning**, Chalmers, *Oct 2022 – present*
  - *Role:* Co-organizer (with 3 other faculty from Chalmers CSE & MATH)
  - Ongoing organization for Structured Learning Workshop (Oct 2023; Oct 2024); ∼1-3 hrs/mo
  - Ongoing organization of AI4Science Seminar (and fika) and speaker hosting; ∼2-6 hrs/mo
- **Broad Institute Machine Learning in Drug Discovery (MLinDD) Symposium**, Virtual, *Dec 2022 – present*
  - *Role:* Co-organizer (with 10 other scientists, mainly Broadies)
  - Ongoing organization for MLinDD Symposium (Oct 2023; Nov 2024); speaker, sponsorship, and poster sub-committees; ∼1-3 hrs/mo

Past Events

- **NeurIPS 2023 AI4Science Workshop**, *Jan 2023 – Dec 2023*
  - *Role:* Faculty co-organizer
  - Provided feedback on workshop application, nominated potential speakers; ∼2 hrs
- **Wallenberg Advanced Scientific Forum 2023**, *Feb 2023 – Oct 2023*
  - *Role:* Co-organizer (with 3 other faculty from Chalmers & OIST)
  - *Theme:* Nobel-Turing Grand Challenge Workshop
  - Nominated and invited attendees, with a focus on gender balance and diversity; ∼4 hrs

Other Engagements

- **Profile Leader**, Health Engineering Area of Advance, Chalmers, *Feb 2024 – present*
- **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*
- **Guest Editor**, 'Good Practices in AI: Democratization of Open Science' Themed Article Collection, *Artificial Intelligence in the Life Sciences*, *Dec 2023 – present*

IN THE MEDIA

Interviews

- "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

Scientific talks

- "Deep generative models for biomolecular engineering." *2nd International Symposium in Machine Learning in Quantum Chemistry*. link
- "Lightning talks from selected poster presenters; Joshua Meier, Divya Nori, Rocío Mercado, Xuetao Shi." *Broad Institute MLinDD Symposium*. link
- "Accelerating molecular design using graph-based deep generative models." *Graph Machine Learning in Industry*. link
- "Discovering New Molecules Using Graph Neural Networks by Rocío Mercado." *GAIA 2020 Conference*. link
- "Applying graph neural networks to molecular design." *NeurIPS 2020 ML4Molecules Workshop*. link
- "Disrupting the pharma industry with AI." *GAIA Meet-up*. link

News articles

- "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 August 1, 2024