

Dr. Rocío Mercado Oropeza

Curriculum Vitae

Contact info:

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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

- *LeMaterial Scientific Community Lead* Mar 2026 – present
- *SciLifeLab Group Leader* Nov 2025 – present
- *National Allocations Committee (NAC) Member, NAISS* Nov 2025 – present
- *Health Engineering AoA Profile Leader, Chalmers* Feb 2024 – present

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
Laboratoire de simulation moléculaire, Faculty of Basic Sciences
École polytechnique fédérale de Lausanne, Sion, CH & Aug 2016 – Nov 2016
& Jul 2015 – Nov 2015

PhD Researcher Aug 2013 – Dec 2017
Molecular Simulation Group, Department of Chemical & Biomolecular Engineering
University of California, Berkeley, 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 Supercomputing in Sweden (NAISS)**, various Compute and Storage allocations: Small Compute (Aug 2023 – Sep 2023), Medium Compute (Oct 2023 – Jun 2026; renewed as *AI for Molecular Engineering*, NAISS 2026/3-549, 2026), Medium Storage (Oct 2023 – Jun 2025), Large Storage (Jul 2025 – Jun 2026), Medium Compute+Storage (Jul 2026 – 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. *AI-guided discovery for low-resource peptide engineering using evolutionary scale modeling*. Leo Andrekson, Robin Rydbergh, **R.M.**,[†] Michaela Wenzel.[†] *bioRxiv*, 2026. (preprint, under review) [link](#)
2. *AI-accelerated design and modeling of organic electrochemical energy materials: from redox-active molecules to polymer electrolytes*. Zhan-Yun Zhang, Giannis Savvas, Jichen Li, Yue Zhou, Thanh Trung Le, Daniel Brandell, **R.M.**, Chao Zhang. *ChemRxiv*, 2026. (preprint, under review) [link](#)
3. *Biologically-driven generative chemistry: using biological data to guide de novo drug design*. Philip John Harrison, **R.M.**[†] *ChemRxiv*, 2026. (preprint, under review) [link](#)
4. *TACK: A statistical evaluation of degradation activity on a novel Targeting Chimeras Knowledge dataset*. Stefano Ribes, Nils Dunlop, **R.M.**[†] *KDD*, 2026. [link](#)
5. *Boltzmann-expected molecular design with decoupled annealing flows*. Selma Moqvist, Richard Beckmann, Ross Irwin, **R.M.**, Simon Olsson. *arXiv*, 2026. (preprint, under review) [link](#)
6. *Beyond manual curation: Augmenting targeted protein degradation databases via agentic literature extraction workflows*. Yaochen Rao, Farzaneh Jalalypour, N. M. Anoop Krishnan, **R.M.**[†] *arXiv*, 2026. (preprint, under review) [link](#)
7. *QT-Net: Rethinking evaluation of AI models in atomic chemical space*. Pablo Martínez Crespo, Stefano Ribes, Martin Rahm, Richard Beckmann, Robert S. Jordan, Marisa Gliège, Santiago Miret, Vijay Kris Narasimhan, **R.M.**[†] *arXiv*, 2026. (preprint, under review) [link](#)
8. *SurfKit: Multi-property surfactant prediction combining experimental data and molecular dynamics simulations*. Richard Beckmann, Pablo Martínez Crespo, Robert S. Jordan, Marisa Gliège, Santiago Miret, Vijay Kris Narasimhan, **R.M.**[†] *ChemRxiv*, 2026. (preprint, under review) [link](#)
9. *Do humans and large language models agree on the quality of synthesis plans?* Varvara Voinarovska, **R.M.**, Mikhail Kabeshov, Samuel Genheden. *ChemRxiv*, 2026. (preprint, under review) [link](#)
10. *Unlocking the chemical space for rechargeable batteries with a generative solvent design system*. Zhan-Yun Zhang, **R.M.**, Thanh Trung Le, Chao Zhang. *ACS Nano*, 2026. (in press) [link](#)

[†] indicates corresponding author (two or more [†] on a paper indicate co-corresponding authors); * indicates co-first authors

PUBLICATION STATISTICS

Based on [Google Scholar](#):

45	publications in total	Total citations: 3338
27	in peer-reviewed international journals	<i>h</i> -index: 20
2 (6)	in computer science conferences (workshops)	<i>i10</i> -index: 22
26	as first and/or corresponding author	

RECENT INVITED TALKS

1. *ChemAI NYC 2026 (NYC AI4Chemistry Summit)*. NYU, New York, NY, USA. Jun 29 – Jul 1, 2026. *Invited talk*. [link](#)
2. *AoA Materials Science Day*. Säröhus, SE. Jun 8, 2026. *Invited talk and panel discussion on AI in Materials Science*.
3. *Chalmers–NTU Workshop in Materials Science for Sustainability*. Chalmers, Gothenburg, SE. May 27–28, 2026. *Designing Molecules with AI: Synthesis, Degradation, and Beyond*.
4. *AI4b.io Webinar*. Virtual. Apr 30, 2026. *Designing Molecules with AI: Synthesis, Degradation, and Beyond*. [link](#)
5. *AI4Chem Seminar, Caltech*. Virtual. Apr 28, 2026. *Designing Molecules with AI: Synthesis, Degradation, and Beyond*.
6. *SciLifeLab Day Gothenburg*. Gothenburg, SE. Apr 17, 2026. *Chemical Language Models for Drug Design and Engineering*. [link](#)
7. *Chemical Compound Space Conference (CCSC) 2026*. Munich, DE. Mar 12, 2026. *Generative AI for Molecular Design: From Drugs to Sustainable Materials*.

8. *International Workshop on Polymer Data (IWPDP)*. Washington, DC, USA. Mar 6, 2026. *Attendance, discussion, and session moderation.*
9. *Chalmers Health Science Day 2026*. Gothenburg, SE. Feb 26, 2026. *Chemical Language Models for Drug Design and Engineering.*
10. *Applied Machine Learning Days (AMLD) 2026, AI and the Molecular World track*. EPFL, Lausanne, CH. Feb 10, 2026. *Invited talk.*
11. *WASP Winter Conference*. Örebro, SE. Jan 14–15, 2026. *AI for Molecular Design and Engineering.*
12. *ML4Molecules ELLIS Unconference Workshop*. Copenhagen, DK. Dec 2, 2025. *Generative AI for Molecular Design: From Drugs to Sustainable Materials.*
13. *Chalmers International Office Virtual Research Seminar ("Master Class")*. Virtual. Nov 24, 2025. *Generative AI for Molecular Engineering.*
14. *Women in Machine Learning Workshop (WASP)*. Chalmers, Gothenburg, SE. Nov 14, 2025. *Keynote.*
15. *Data-Driven Life Sciences (DDLs) Annual Meeting*. Uppsala, SE. Nov 12, 2025. *Introduction to TIMED NEST Project (with co-PI Ola Spjuth).*
16. *Computer-Aided Drug Discovery (CADD) Gordon Research Conference (GRC)*, Portland, Maine, USA. July 14, 2025. *Generative AI for PROTAC design.*

CURRENT STUDENTS AND POSTDOCS

Currently supervising 19: 11 PhD students, 4 postdoctoral researchers, and 4 MSc research assistants.

Varun Ajith *PhD Computer Science & Engineering (Jun 2026 – present)*
Chalmers University of Technology
Co-advisor: Prof. Simon Olsson; PhD examiner: Prof. Vincenzo Gulisano

Kevin George *PhD Computer Science & Engineering (May 2026 – present)*
Chalmers University of Technology
Co-advisor: Prof. Simon Olsson; PhD examiner: Prof. Vincenzo Gulisano

Lukáš Hudec *Research Assistant, MSc Data Science & AI (Feb 2026 – present)*
Chalmers University of Technology

Giannis Savvas *PhD Computer Science & Engineering (Nov 2025 – present)*
Chalmers University of Technology & AstraZeneca
Assistant advisors: Prof. Chao Zhang (Uppsala), Prof. Esther Galby (Chalmers), Prof. Peter Damaschke (Chalmers); PhD examiner: Prof. Miquel Pericas

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

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

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; PhD examiner: Prof. Richard 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);
PhD examiner: Prof. Morteza Chehreghani

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; PhD examiner: Prof. Ross King

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; PhD examiner: Prof. Ross King

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

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

CO-ADVISED STUDENTS AND POSTDOCS

Co-advising 10: 9 PhD students and 1 postdoctoral researcher.

Mehdi Babaeivavdare *PhD Computer Science & Engineering (Jan 2026 – present)*
Chalmers University of Technology
Main advisor: Prof. Ashkan Panahi; PhD examiner: Prof. Richard Johansson

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; PhD examiner: Prof. Richard Johansson

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); PhD examiner: Prof. Martin Högbom

Valter Schütz

PhD Computer Science & Engineering (Sep 2024 – present)

Chalmers University of Technology

Main advisor: Prof. Morteza Chehreghani; PhD examiner: Prof. Richard Johansson

Selma Moqvist

PhD Computer Science & Engineering (Sep 2024 – present)

Chalmers University of Technology

Main advisor: Prof. Simon Olsson; PhD examiner: Prof. Morteza Chehreghani

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); PhD examiner: Prof. Ross King

PAST STUDENTS AND POSTDOCS (REVERSE CHRONOLOGICAL)

41 in total: 1 co-advised PhD student, 3 guest PhD researchers, 34 MSc students, and 3 BSc students.

Christopher Kolloff

PhD Computer Science & Engineering (Jan 2025 – Jun 2026)

Chalmers University of Technology; main advisor: Prof. Simon Olsson; PhD examiner: Prof. Devdatt Dubhashi

Noah Márquez Vara

MSc Data Science & AI (Jan 2026 – Jun 2026)

& Siyu (Zoe) Hu

Research Assistant & MSc Complex Adaptive Systems (Jun 2025 – Jun 2026)

Chalmers University of Technology (Noah) & University of Gothenburg (Zoe); main advisor: Télió Cropsal

Tingting Mo

MSc Applied Data Science (Jan 2026 – Jun 2026)

& Andrea (Jia Xin) Zhu

Research Assistant & MSc Applied Data Science (Jan 2026 – Jul 2026)

University of Gothenburg; main advisor: Stefano Ribes

Alexander Persson

Research Assistant & MSc Algorithms, Languages & Logic (Jan 2026 – Aug 2026)

& Felix Erngård

Research Assistant & MSc Data Science & AI (Jan 2026 – Jul 2026)

Chalmers University of Technology; main advisor: Stefano Ribes

Hannes Öhman

MSc Complex Adaptive Systems (Jan 2026 – Jun 2026)

Chalmers University of Technology; main advisor: Dr. Richard Beckmann

Frida Jacobson

2026 MSc Applied Data Science

University of Gothenburg & AstraZeneca; main advisors: Dr. Richard Beckmann (Chalmers) and Dr. Mikhail Kabeshov (AstraZeneca)

Yihuai Cai

Research Assistant (Jun 2025 – Aug 2025)

Chalmers University of Technology

MSc Data Science & AI

Main advisor: Dr. Farzaneh Jalalypour

Francisco Alejandro Erazo Piza & Nils Dunlop

2025 MSc Applied Data Science

University of Gothenburg; co-advisor: Dr. Farzaneh Jalalypour

**Dadi Andrason
& Marcus Johansson**

2025 MSc Data Science & AI

2025 MSc Complex Adaptive Systems

Chalmers University of Technology; co-advisor: Dr. Philip John Harrison

Miranda Carlsson & Sofia Larsson

2025 MSc Complex Adaptive Systems

Chalmers University of Technology & AstraZeneca; co-advisors: Dr. Filip Miljković (AstraZeneca), Dr. Richard Beckmann (Chalmers)

Ranxuan Zhang

2025 MSc Biotechnology

Chalmers University of Technology; co-advisor: Stefano Ribes

Frederik Lizak Johansen

Guest PhD Researcher (Sep 2024 – Dec 2024)

University of Copenhagen

PhD Machine Learning

Main advisor: Prof. Raghavendra Selvan

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)

Jin Ahmad

2024 BSc Chemistry

Karlstad University; co-advisor: Prof. Angela Grommet (Chalmers)

Pär Aronsson & Amanda Dehlén

2024 MSc Data Science & AI / Algorithms, Languages & Logic

Chalmers University of Technology & AstraZeneca; co-advisor: Dr. Filip Miljković (AstraZeneca)

Leo Andrekson

2024 MSc Biotechnology

Chalmers University of Technology

Anders Källberg

2024 MSc Biotechnology

Chalmers University of Technology & AstraZeneca; co-advisors: Dr. Eva Nittinger, Dr. Christian Tyrchan (AstraZeneca)

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

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

Mert Yurdakul

2023 MSc Data Science & AI

Chalmers University of Technology & AstraZeneca; co-advisors: Dr. Martin Priessner, Dr. Anna Tomberg (AstraZeneca)

Kinga Jenei

2023 MSc Data Science & AI

University of Gothenburg & AstraZeneca; co-advisor: Dr. Vignesh Subramanian (AstraZeneca)

Stefano Ribes *2023 MSc Computer Science & Engineering*
Chalmers University of Technology & AstraZeneca; co-advisors: Dr. Eva Nittinger, Dr. Christian Tyrchan (AstraZeneca)

Edwin Holst & Preetha Mutharasu *2023 MSc Computer Science & Engineering*
Chalmers University of Technology & AstraZeneca; co-advisor: Dr. Jon Paul Janet (AstraZeneca)

Siva Manohar & Supriya Kancharla *2023 MSc Data Science & AI*
University of Gothenburg & AstraZeneca; co-advisors: Dr. Samuel Genheden, Dr. Annie Westerlund (AstraZeneca)

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)

Divya Nori *2025 BSc Electrical Eng. & Computer Science, Minor Mathematics*
Massachusetts Institute of Technology; co-advisor: Prof. Connor Coley

Sara Romeo Atance & Juan Viguera Diez *2021 MSc Complex Adaptive Systems*
Chalmers University of Technology & AstraZeneca; co-advisor: Prof. Simon Olsson (Chalmers)

Julio Ponte Hernández *2021 MSc Computer Science & Engineering*
Chalmers University of Technology & AstraZeneca; co-advisor: Prof. Simon Olsson (Chalmers)

Tobias Rastemo *2020 MSc Computer Science & Engineering*
Chalmers University of Technology & AstraZeneca; co-advisor: Dr. Shirin Tavera (Chalmers)

Rueih-Sheng (Ray) Fu *2018 BSc Chemical Engineering*
University of California, Berkeley; Molecular Simulation Group

RECENT TEACHING EXPERIENCE

Course Responsible & Examiner, DAT675 – AI for Molecules Jan 2026 – Mar 2026
Computer Science & Engineering (CSE) Department
Chalmers University of Technology, Gothenburg, SE
• Created this course from scratch (16 lectures and 5 graded assignments) for a 25-student class ($\approx 2/3$ MSc and $\approx 1/3$ PhD students), with TA Stefano Ribes leading recitation sections

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, Molecular Systems Biology, AI4Mat-ICLR-2026 Area Chair, KDD 2026 AI4Sciences, NeurIPS 2026 Area Chair, NAISS Large Spring 2026 (NAC reviewer)

**indicates received reviewer award from publisher*

RECENT PROFESSIONAL SERVICE

PhD, Lic./Halfway Seminar, and MSc Defenses

- **Muhammad Arslan Masood**, *PhD (pre-examiner)*, Aalto University, May 2026
- **James Urban**, *PhD*, University of Gothenburg, Apr 2026
- **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 PhD Seminar Electrical Engineering*, Chalmers, Jun 2024
- **Filip Ekström Kelvinius**, *Halfway PhD Seminar Computer & Information Science*, Linköping University, Feb 2024
- **Gökçe Geylan**, *Halfway PhD Seminar Systems Biology*, Linköping University, Feb 2024
- **Noah Márquez Vara & Siyu Hu**, *MSc Data Science & AI (Chalmers) and MSc Complex Adaptive Systems (University of Gothenburg)*, Jun 2026
- **Tingting Mo & Andrea Zhu**, *MSc Applied Data Science*, University of Gothenburg, Jun 2026
- **Alexander Persson & Felix Erngård**, *MSc Algorithms, Languages & Logic and MSc Data Science & AI*, Chalmers, Jun 2026
- **Hannes Öhman**, *MSc Complex Adaptive Systems*, Chalmers, Jun 2026
- **Borja Medina de las Heras**, *MSc Bioinformatics (opponent)*, Lund University, Jun 2026
- **Frida Jacobson**, *MSc Applied Data Science*, University of Gothenburg, Jan 2026
- **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

- **Scientific Committee**, Faraday Discussion on Digital Chemistry Discovery, Edinburgh, UK, Sep 8–10, 2027
- **Organizer**, Machine Learning for Molecular and Materials Discoveries (ML2MD) Symposium, biannually co-organized with Prof. Chao Zhang. **2026** at Uppsala University, Jun 17–19, 2026 (lead: Chao Zhang; [event page](#)); **2024** in Gothenburg, SE, Jan–Sep 2024 (lead: **R.M.**; [event page](#))
- **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 – Dec 2025*; *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*

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

- “Intensive collaborations to secure new research funding.” *Chalmers Communications*. Dec 2025. [link](#)
- “Designing molecular recipes: Rocío Mercado Oropeza’s push for smarter molecular AI.” *WASP Sweden*. Nov 2025. [link](#)
- “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)*. 2019. [link](#)

Scientific talks

- *AI4b.io Webinar Recording. Designing Molecules with AI: Synthesis, Degradation, and Beyond*. Apr 30, 2026. [link](#)
- “Lightning talks from selected poster presenters; Joshua Meier, Divya Nori, Rocío Mercado, Xuetao Shi.” *Broad Institute MLinDD Symposium*. [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](#)

Miscellaneous

- Recorded talks for the Chalmers AI4Science Seminar. *YouTube*. [link](#)

LANGUAGES

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

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