Curriculum Vitae Hilda Sandström

Full name	**Hilda Sandström**
E-mail	hilda.sandstrom@aalto.fi
Research IDs	ResearchGate, ORCID, Web of Science
Homepage/Social Media	hilsan.github.io, LinkedIn

Expertise

Cheminformatics | Computational Chemistry | Enhanced Molecular Dynamics | Molecular Modelling | Structure Prediction | Machine Learning for Molecular Sciences

Professional and Academic Career

Since 9/2022 — **Postdoc**, Aalto University

- Development of machine learning based compound identification with mass spectrometry
- Development of machine learning methods for property prediction of atmospheric compounds
- Development of molecular descriptors for atmospheric compounds
- Development of machine learning interatomic potentials for atmospheric compounds

Academic Studies

9/2017 – 5/2022 — **PhD** in Chemistry with a specialization in theoretical chemistry
Chalmers University of Technology, Sweden. PhD award date 02/06/2022
Thesis – *Nitriles in Prebiotic Chemistry and Astrobiology* Supervisor – Prof Martin Rahm.

8/2012 – 9/2017 — **MEng** in Chemical engineering with engineering physics, Chalmers University of Technology, Sweden. **Award date** 08/11/2017.
Thesis – *Understanding the Mechanism of PAQR-2 Through Modeling and Simulations*
Supervisor – Dr. Samuel Genheden.

8/2015 – 9/2017 — **MSc** in Engineering physics (Nanotechnology master program, integrated), Chalmers University of Technology, Sweden. Integrated within MEng program. **Award date** 08/11/2017.

8/2012 – 6/2015 — **BSc** in Chemical engineering with engineering physics (integrated), Chalmers University of Technology, Sweden. Integrated withing MEng program. **Award date** 12/06/2015.

Software and Modeling Skills

Programming languages	OpenBabel, RDKit, Atomistic Simulation Environment (ASE) – Well Experienced
Machine learning toolkits	Scikit-learn, TensorFlow – Experienced
Development	Git – Experienced
Cheminformatics	OpenBabel, RDKit, Atomistic Simulation Environment (ASE) – Well experienced
Molecular dynamics and simulation	CP2K, Gromacs, PLUMED – Expert; xTB, QCxMS, VMD (visualization) – Experienced
Structure prediction and conformational Sampling	CALYPSO, CREST – Well Experienced
Quantum chemistry and mass spectrometry simulation	Gaussian, Orca – Expert; QCxMS, QCxMS2, NEIMS – Experienced

Peer-Reviewed Scientific Publications

(Google Scholar, 25/08/2025, 12 publications, 6 first author)
Total citations: 93, h-index: 5 , i-index: 4

12. J. Brean, F. Bortolussi, A. Rowell, D. C. S. Beddows, K. Weinhold, P. Mettke, M. Merkel, A. Kumar, S. Barua, S. Iyer, A. Karppinen, **Sandström, H**., P. Rinke, A. Wiedensohler, M. Pöhlker, M. Dal Maso, M. Rissanen, Z. Shi, & R. M. Harrison, *ACS ES&T Air*, 2, 1704–1713 (2025). DOI: 10.1021/acsestair.5c00119 [Supervised PhD student F. Bortolussi in developing and evaluating the machine learning model
11. F. Izquierdo-Ruiz, M. L. Cable, R. Hodyss, T. H. Vu, **Sandström, H**., A. Lobato, & M. Rahm, *Proc. Natl. Acad. Sci. U.S.A.*, 122, e2507522122 (2025). DOI: 10.1073/pnas.2507522122 [Developed and tested crystal structure prediction program workflow for molecular cocrystals of hydrogen cyanide.]
10. R. R. Valiev, R. T. Nasibullin, **Sandström, H**., P. Rinke, K. Puolamäki, & T. Kurten, *Physical Chemistry Chemical Physics*, 27, 14804–14814 (2025). DOI: 10.1039/d5cP01101a [Co-advisor for ML workflow; developed MBTR model.]
9. Bortolussi, F., **Sandström, H**., F. Partovi, J. Mikkilä, P. Rinke, & M. Rissanen, *Atmospheric Chemistry and Physics*, 25, 685–704 (2025). DOI: 10.5194/acp-25-685-2025 [Co-designed study, supervised, and contributed to programming and model testing.]
8. Malaska, M. J., **Sandström, H**., A. E. Hofmann, R. Hodyss, L. Rensmo, M. van der Meulen, M. Rahm, M. L. Cable, & J. I. Lunine, *Astrobiology*, 25 (2025). DOI: 10.1089/ast.2024.0125 [Performed geometry optimizations and molecular measurements and student supervision.]
7. **Sandström, H**., P. Rinke, *Geoscientific Model Development*, 18, 2701–2724 (2025). DOI: 10.5194/gmd-18-2701-2025
6. **Sandström, H.**, M. Rissanen, J. Rousu, P. Rinke, *Advanced Science*, 11, 2306235 (2024). DOI: 10.1002/advs.202306235
5. **Sandström, H**., F. Izquierdo-Ruiz, M. Cappelletti, R. Dogan, S. Sharma, C. Bailey, & M. Rahm, *ACS Earth and Space Chemistry*, 8, 1272–1280 (2024). DOI: 10.1021/acsearthspacechem.4c00088
4. **Sandström, H**., & Rahm, M., *The Journal of Physical Chemistry A*, 127, 4503–4510 (2023). DOI: 10.1021/acs.jpca.3c01504
3. **Sandström, H.**, & Rahm, M., *ACS Earth and Space Chemistry*, 5, 2152–2159 (2021). DOI: 10.1021/acsearthspacechem.1c00195
2. **Sandström, H**., & Rahm, M., *Science Advances*, 6, eaax0272 (2020). DOI: 10.1126/sciadv.aax0272
1. Lindblom, A., K. K. Sriram, V. Müller, R. Öz, **Sandström, H.**, C. Åhrén, F. Westerlund, & N. Karami, *Diagnostic Microbiology and Infectious Disease*, 93, 380–385 (2019). DOI: 10.1016/j.diagmicrobio.2018.10.014 [Performed fluorescence microscopy assays where I stained, trapped, and photographed plasmids in nanochannels.]

Teaching, Pedagogical Experience and Supervision of Students

Lectures and Excercises

Year	Subject	Degree	Type	Week hours
2018 – 2020	Quantum engineering	1st year MSc Nanotechnology	Computer labs	2
2018 – 2021	Physical chemistry	2nd year BSc Biotechnology	Tutorials and experimental labs	12
2018 – 2021	Theoretical chemistry	3rd year Bsc Chemical engineering with engineering physics	Computer labs	4
2017 – 2018	Chemistry and biochemistry	1st year BSc Chemical engineering	Experimental labs	8
2014	Calculus	1st year BSc Chemical engineering with engineering physics	Exercise	1

Pedagogical Training

2019	Teaching, learning and evaluation at Chalmers University of Technology (3 ECTS)

Supervision of Students

Since 2024	Supervisor of MSc student at Aalto University
Since 2024	Advisor of PhD student at Aalto University
Since 2022	Co-supervisor of PhD student at University of Helsinki
11/2024 – 5/2024	Supervisor of BSc student at Aalto University
5/2021 – 9/2021	Co-supervisor of 2 visiting and 3 BSc students at Chalmers University of Technology
1/2021 – 6/2021	Co-supervisor of 6 BSc students at Chalmers University of technology
6/2020 – 8/2020	Supervisor of 2 BSc students at Chalmers University of Technology
1/2020 – 6/2020	Supervisor of 6 BSc students at Chalmers University of Technology
4/2019 – 7/2019	Supervisor of visiting BSc students at Chalmers University of Technology
4/2018 – 6/2018	Supervisor of one BSc student at Chalmers University of Technology

Funding and Resource Acquisition

2025	202k EUR Marie Skłodowska-Curie postdoctoral fellowship
2024 – 2025	LUMI extreme scale access resource allocation
2021	17,000 SEK Nils Philblad's foundation travel grant
2019	3,650 SEK Nils Philblad's foundation travel grant
2018	3,850 SEK Karl and Annie Leon's foundation travel grant

Conference Contributions

2025	**Invited talk** Nordic Workshop on AI for Climate Change, Sweden. *Machine learning for atmospheric mass spectrometry*
2024	**Invited talk** FysKemDagarna (Physics and Chemistry Days), Sweden. *AI in Chemistry: Solving experimental challenges with artificial intelligence*
2023	International Aerosol Modeling Algorithms Conference, USA. *Characterizing Atmospheric Molecules for Machine Learning*
2023	European Aerosol Conference, Spain. *Characterizing Atmospheric Molecules for Machine Learning*
2023	Physics Days, Finland. *Characterizing atmospheric molecules for machine learning*
2022	AbSciCon, USA. *Untangling hydrogen cyanide polymerization using quantum chemistry*

Academic Service and Outreach

2025	Reviewer for *ACS Earth Space Chem, ACS Omega* and *Atmospheric Chemistry and Physics*.
2025	Organizing committee. *Nordic Workshop on AI for Climate Change*, Sweden.
2025	Core member, organizer and Finland representative. *Climate AI Nordics Network.*
2024	Panelist on AI in chemistry, physics, and education, *FysKemDagarna (Physics and Chemistry Days).*
2023	Organizer of workshop hands-on session. *Shaking Up Tech 2013.* Workshop for underrepresented groups in STEM, Aalto University, Finland.
2023	Session chair and organizer. *ESTML*, Levi, Finland.
2022	Session chair. *AbSciCon*, USA.