Mart van der Lugt

MSc student Data Science and AI & Drug Discovery Sciences

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PROFILE

Computational scientist trained in both pharmaceutical sciences and computer science, now completing a double master's in Drug Discovery Sciences (VU Amsterdam) and Data Science & AI Technology (TU Delft). I work on structure-based drug discovery, graph neural networks for molecular representation and ML-guided ligand optimisation, and bring five years of experience building and validating software in a hospital setting. Author of the open-source docking toolkit *Pyrite*.

EDUCATION

MSc Data Science and Artificial Intelligence Technology Sep 2025 – present
TU Delft · tracks Bioinformatics and Advanced Machine Learning Delft

- Coursework: Graph-based Bioinformatics, Statistical Learning, Generative Modelling

MSc Drug Discovery Sciences Sep 2025 – present
VU Amsterdam · track Computer-Aided Drug Design Amsterdam

- Part of the AIMMS talent programme
- Coursework: Physical Organic Chemistry, Biomolecular Simulations

BSc Pharmaceutical Sciences — *cum laude*, Honours Programme Sep 2022 – Aug 2025
VU Amsterdam Amsterdam

- Thesis (9.5/10): developed *Pyrite*, an open-source molecular docking framework
- Honours Programme: selective extra-curricular programme in independent and interdisciplinary research

BSc Computer Science and Engineering Sep 2018 – Jul 2023
TU Delft Delft

- Thesis (9.0/10): error analysis of SARS-CoV-2 variant detection in wastewater; published as part of a paper in *Genome Biology*

RESEARCH & PROJECTS

Pyrite: molecular docking and alignment framework 2025 – present
Biomolecular Simulation group (Dr. D. P. Geerke), VU Amsterdam · with Dr. D. A. Poole III Amsterdam

- Open-source Python toolkit for molecular docking, started as BSc thesis and grown into a documented, tested package
- Designed a grid-based pocket detection and scoring algorithm and a crowding/niching strategy for pose diversity
- Modular by design: scoring functions and search strategies can be swapped or extended
- Presented at the NWO CHAINS conference (Dec 2025)

SARS-CoV-2 variant detection in wastewater 2022 – 2023
Delft Bioinformatics Lab, TU Delft · with Dr. J. A. Baaijens Delft

- Error analysis of a pipeline estimating variant abundance from wastewater RNA sequencing
- Showed that prediction reliability depends on sequencing error rates, and that contaminating human coronaviruses reduce accuracy unless their reference genomes are included

PUBLICATIONS

Baaijens, J. A., Zulli, A., Ott, I. M., Nika, I., **van der Lugt, M. J.**, Petrone, M. E., et al. (2022). Lineage abundance estimation for SARS-CoV-2 in wastewater using transcriptome quantification techniques. *Genome Biology*, 23(1), 236. doi:10.1186/s13059-022-02805-9

EXPERIENCE

Computer Scientist — Mar 2022 – present
Haaglanden Medisch Centrum — The Hague

- Develop and maintain clinical software within a small team
- Perform statistical analysis and validation of patient and algorithm data
- Independently initiate and run R&D projects to improve patient care

Teaching and Research Assistant — Sep 2024 – present
Vrije Universiteit Amsterdam, Faculty of Science — Amsterdam

- Teach tutorials and computer practicals for the second-year Statistics course across several BSc programmes
- Assist in Molecular Modelling practicals (Pharmaceutical Sciences) and supervise BSc thesis students in computational drug discovery
- Coach first-year students through four-week research projects
- Built websites for research groups

Commissioner of External Affairs (full board year) — Jun 2023 – Jun 2024
VCSVU, study association for Pharmaceutical Sciences, VU Amsterdam — Amsterdam

- Managed all external relations and sponsorships; doubled sponsor contributions
- Organised educational events for members

Team Manager — Jun 2018 – Mar 2022
ALDI Nederland — Boskoop

- Led a store team during peak hours, alongside BSc studies

SKILLS

Programming	Python, Swift, C#, R, SQL, JavaScript, Julia, Delphi Pascal
Machine learning	PyTorch, scikit-learn, SciPy, pandas, NumPy
Cheminformatics	RDKit, OpenBabel, AutoDock Vina/smina, AmberTools (antechamber, tLeap, cpptraj), UCSF ChimeraX
Tools	Git, Linux, HPC clusters, Docker, LaTeX, SwiftUI / iOS development

LANGUAGES

Dutch	Native
English	Fluent (C2)

INTERESTS

Road cycling, cooking, photography.

References available on request.