Mart van der Lugt

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Double master's student in Drug Discovery Sciences (VU Amsterdam) and Data Science & AI Technology (TU Delft). Research interests in computational approaches to drug discovery, with a focus on structure-based methods, graph neural networks for molecular representation, and ML-guided lead optimisation.

EDUCATION

MSc Drug Discovery Sciences Sep 2025 – Present
VU Amsterdam — Track: Computer-Aided Drug Design
Key coursework: Machine learning in Chemistry, Biomolecular Simulations

MSc Data Science and AI Technology Sep 2025 – Present
TU Delft — Tracks: Bioinformatics; Advanced Machine Learning
Key coursework: Graph-based Bioinformatics, Statistical Learning, Generative Modelling

BSc Pharmaceutical Sciences Sep 2022 – Aug 2025
VU Amsterdam — Cum Laude with Honours Programme
Honours: selective additional programme emphasising independent research and interdisciplinary study
Thesis: 9.5/10 — developed Pyrite, an open-source molecular docking framework (see Research & Projects)
Won both audience and jury prize for best poster presentation in the Molecular Toxicology course

BSc Computer Science and Engineering Sep 2018 – Jul 2023
TU Delft
Thesis: 9.0/10 — Error analysis of SARS-CoV-2 variant detection in wastewater (see Research & Projects)

PUBLICATIONS

Baaijens, J. A.; Zulli, A.; Ott, I. M.; Nika, I.; **van der Lugt, M. J.**; Petrone, M. E.; Alpert, T.; Fauver, J. R.; Kalinich, C. C.; Vogels, C. B.; et al. Lineage Abundance Estimation for SARS-CoV-2 in Wastewater Using Transcriptome Quantification Techniques. *Genome Biology* 2022, 23 (1), 236.
doi.org/10.1186/s13059-022-02805-9

RESEARCH & PROJECTS

Pyrite: Molecular Docking and Alignment Framework 2024 – Present
Open-source Python framework for structure-based virtual screening, developed as BSc thesis (grade: 9.5/10) and now being further developed within the group of Daan Geerke together with David Poole. Introduces a grid-based pocket detection and scoring algorithm, a crowding and niching strategy enforcing pose diversity, and seamless integration with RDKit, SciPy, and pygmo. Benchmarking on the 2024 PDBbind demo set shows that the Pocket function accelerates searching 2–6× compared to Vina and PLP scoring while maintaining or surpassing their accuracy in blind docking.
Presented at the NWO CHAINS conference, December 2025

Error Analysis: SARS-CoV-2 Variant Detection in Wastewater 2022 – 2023
BSc thesis (grade: 9.0/10) at TU Delft, contributing to a pipeline for estimating SARS-CoV-2 variant abundance from wastewater RNA sequencing. Demonstrated that prediction credibility depends on sequencing error rates and that contaminating human coronaviruses can significantly affect accuracy, though this effect is mitigated by including their reference genomes. Research published as part of Baaijens et al. (2022) in Genome Biology.

EXPERIENCE

Computer Scientist *Haaglanden Medisch Centrum* Mar 2022 – Present
The Hague
Maintaining and developing software in a clinical context within a small team. Statistical analysis and validation of patient and algorithm data. Independently organising and executing several R&D projects advancing patient care.

Teaching Assistant *Vrije Universiteit Amsterdam* Sep 2024 – Present

Amsterdam

Teaching tutorials and computer practicals for the second-year Statistics course across several bachelor programmes in the Faculty of Science. Assisting in practicals for the second-year Molecular Modeling course for Pharmaceutical Sciences. Coaching BSc students during four-week research projects.

Commissioner of External Affairs *VCSVU* Jun 2023 – Jun 2024

Amsterdam

Study association for Pharmaceutical Sciences, VU Amsterdam. Managed all external contacts and sponsorships; organised educational events; independently doubled sponsor contributions.

Team Manager *ALDI Nederland* Jun 2018 – Mar 2022

Boskoop

Managed a medium-sized team during peak hours.

TECHNICAL SKILLS

Programming: Python, C#, Delphi Pascal, Swift, SQL, JavaScript, R

ML / Data Science: PyTorch, scikit-learn, scipy, pandas, NumPy

Cheminformatics: RDKit, OpenBabel, AutoDock Vina/smina, AmberTools (antechamber, tLeap, cpptraj), UCSF ChimeraX

Other: Git, Linux, Docker, LaTeX, SwiftUI, iOS development

LANGUAGES

Dutch *(native)* English *(C2, native proficiency)*