

# 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 ligand optimisation.

## EDUCATION

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### 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

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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](https://doi.org/10.1186/s13059-022-02805-9)

## RESEARCH & PROJECTS

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### 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

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### 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 and Research 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 first-year BSc students during four-week research projects. Developing websites for several research groups. Assisting BSc students with research methods during their thesis project in computational drug discovery.

**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.

**T E C H N I C A L   S K I L L S**

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**Programming:** Python, C#, Delphi Pascal, Swift, SQL, JavaScript, R, Julia**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**L A N G U A G E S**

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