Derek van Tilborg

www.derekvantilborg.com

PhD-trained scientist specialized in molecular machine learning for drug discovery. Experienced in deep learning, chem/bioinformatics, and interdisciplinary collaboration with wet-lab teams.

Education

2021-2025 (expected, thesis submitted)
PhD, Biomedical Engineering
Eindhoven University of Technology
Molecular machine learning group of F. Grisoni

2019-2021
MSc, Bioinformatics
Wageningen University & Research
Average grade of 8.5, MSc thesis 9.5 out of 10

2015-2019
BSc, Biomedical science
Avans University of Applied Sciences, Breda
Average grade of 8.0, BSc thesis 9.0 out of 10

Conference contributions **16**

6 First author papers
of which
7 Publications

Mentored
4 MSc students
&
3 BSc students

Other experience

2021
Internship - Radboud Medical Hospital
Developed a computational framework for homology modeling of peptide:MHC complexes, aimed at immunotherapy design.

2018-2019
Internship - Crossfire Oncology
Predicted drug response on an in house panel of cancer cell lines using multimodal machine learning.

Most exciting projects I've spearheaded

ML-guided evolution of immune cell-specific nanobiologics
I successfully designed multiple nanobody binders for CD25 using a home-made protein language model. Experimental work is done in collaboration.
Manuscript in preparation

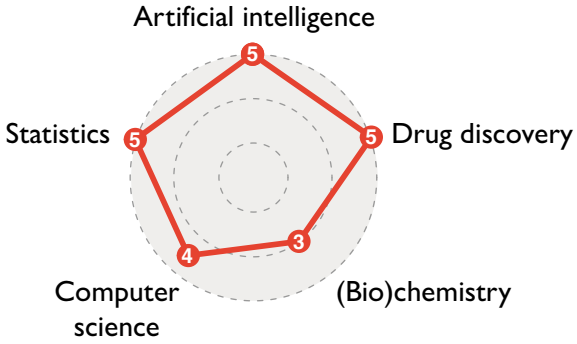
Molecular deep learning at the edge of chemical space
I discovered multiple novel bioactive molecules across two protein targets by engineering a deep learning architecture that natively models prediction reliability. My proudest project.
Under review at Nature Machine Intelligence

Molecular property prediction with active learning
A computational study for active learning in low-data regimes.
Published in Nature Computational Science 4 (10), 786-796

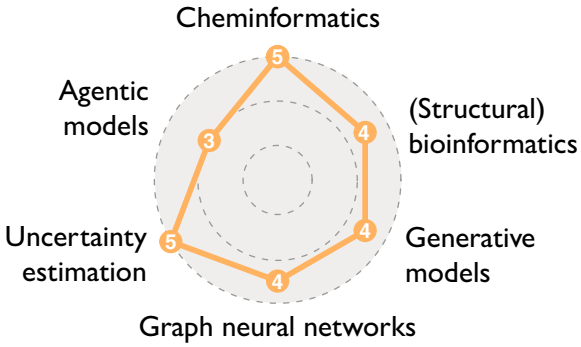
Nanoparticle design with active learning.
I used active learning to design nanoparticles for drug delivery in cancer cells. Experimental work is done in collaboration.
Published in Digital Discovery 3 (7), 1280-1291

Skills

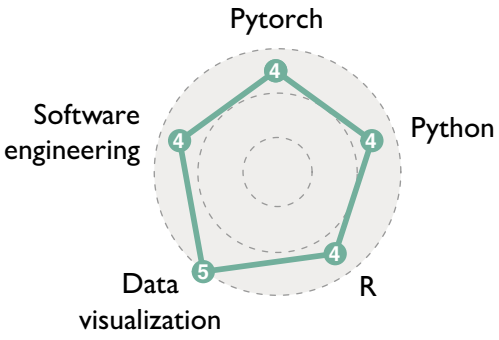
Scientific & domain knowledge



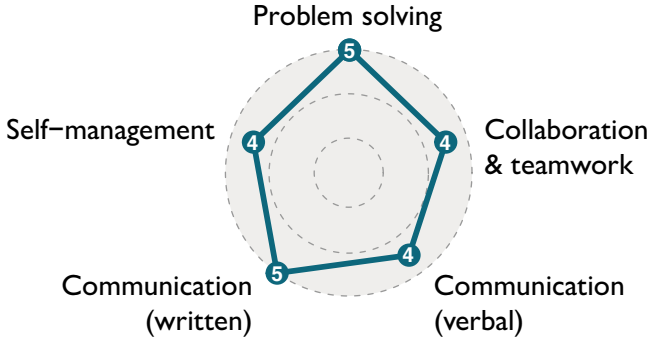
Molecular machine learning



Data science / programming skills



Soft skills



Levels of competence are scored according to the Dreyfus model:
1. Novice, 2. Advanced beginner,
3. Competent, 4. Proficient, 5. Expert

List of first author journal articles

Cancers in Agreement? Exploring the Cross-Talk of Cancer Metabolomic and Transcriptomic Landscapes Using Publicly Available Data.
Derek van Tilborg and Edoardo Saccenti.
Cancers 13 (3), 393, 2021.

Exposing the Limitations of Molecular Machine Learning with Activity Cliffs.
Derek van Tilborg et al.
Journal of Chemical Information and Modeling 62 (23), 5938-5951, 2022.

This project has well over 200 citations and almost 200 GitHub stars. The included benchmarking datasets are now widely used in computational drug discovery.

Structure-based Drug discovery with Deep Learning.
Rıza Özçelik and Derek van Tilborg, et al.
ChemBioChem, e202200776, 2023.

Machine learning-guided high throughput nanoparticle design.
Ana Ortiz-Perez and Derek van Tilborg, et al.
Digital Discovery 3 (7), 1280-1291, 2024.

Deep learning for low-data drug discovery: Hurdles and opportunities.
Derek van Tilborg et al.
Current Opinion in Structural Biology 86, 102818, 2024.

Traversing chemical space with active deep learning for low-data drug discovery.
Derek van Tilborg and Francesca Grisoni.
Nature Computational Science 4 (10), 786-796, 2024.

Molecular deep learning at the edge of chemical space.
Derek van Tilborg et al.
ChemRxiv, 2025 (preprint, under review).

Selected conference contributions

Poster presentation (best poster prize)
MoleculeACE – a benchmark for molecular machine learning with activity cliffs
Molecular Graphics and Modelling Society - Young Modeller Forum, online, February 2022

Invited talk
Exposing the limitations of molecular machine learning with activity cliffs.
Valence labs, Molecular Modeling and Drug Design, online, May 2022.

Poster presentation
MoleculeACE: a benchmark for machine learning with activity cliffs.
International Conference on Chemical Structures, Noordwijkerhout, The Netherlands, June 2022.

Poster presentation
Self-supervised learning with graph neural networks for drug discovery.
NWO CHAINS, Veldhoven, The Netherlands, September 2022.

Poster presentation
Traversing Chemical Space with Active Learning.
Institute of Complex Molecular Systems - Annual Symposium, Eindhoven, The Netherlands, March 2023.

Poster presentation (best poster prize)
Traversing Chemical Space with Active Learning.
20th IEEE Conference on Computational Intelligence in Bioinformatics and Computational Biology, Eindhoven, The Netherlands, August 2023.

Plenary lecture
Traversing Chemical Space with Active Learning,
International Symposium on Bioinformatics and Computer-Aided Drug Discovery, online, September 2023.

Invited talk
Traversing Chemical Space with Active Learning.
Figon Dutch medicine days, Oss, The Netherlands, September 2023.

Poster presentation
Machine learning-guided high throughput design.
ELLIS machine learning for molecules, online, December 2023.

Poster presentation
Traversing Chemical Space with Active Learning.
Institute of Complex Molecular Systems - Annual Symposium, Eindhoven, The Netherlands, March 2024.

Oral presentation
Drug discovery at the edge of chemical space.
NWO CHAINS, Veldhoven, The Netherlands, December 2024.

Invited talk
Molecular deep learning at the edge of chemical space.
École Polytechnique Fédérale de Lausanne, online, April 2025.

Poster presentation (best poster prize)
Molecular deep learning at the edge of chemical space.
Institute of Complex Molecular Systems - Annual Symposium, Eindhoven, The Netherlands, March 2025.