Derek van Tilborg

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

Education

5 First author papers
of which **7** Publications
300+ Citations
&
200+ Github stars

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

Mentored **4** MSc students
& **3** BSc students

16 Conference contributions
of which **9** Posters
6 Talks
1 Plenary lecture

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

2 Publications
of which **1** First author paper

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

Most exciting projects I've spearheaded:

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

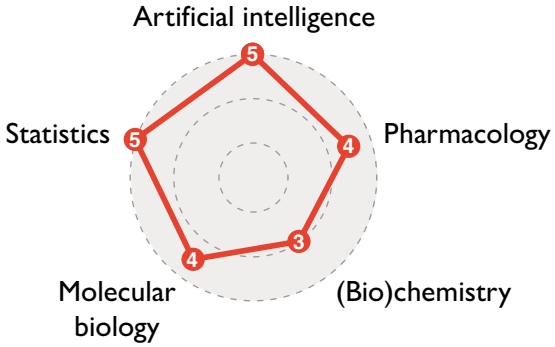
Molecular deep learning at the edge of chemical space.
I introduced a new method to estimate model reliability, which I validated experimentally.
Under review

Nanoparticle design with active learning.
I combined active learning with microfluidics and high-content imaging to design nanoparticles. A collaboration with A. Perez.
Published in Digital Discovery 3 (7), 1280-1291

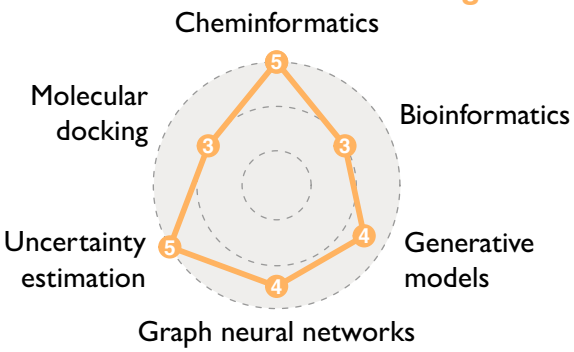
AI-guided evolution of immune cell-specific nanobiologics.
I designed nanobody binders using generative protein language models. A collaboration with A. Hokke and K. de Bruin.
Manuscript in preparation

Skills

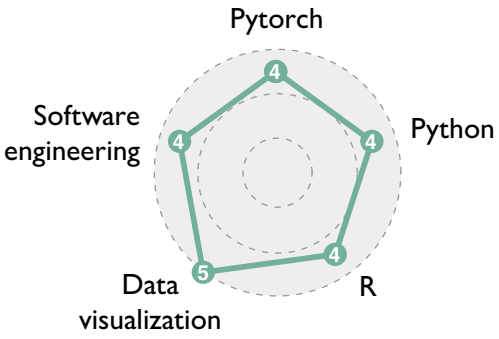
Scientific & domain knowledge



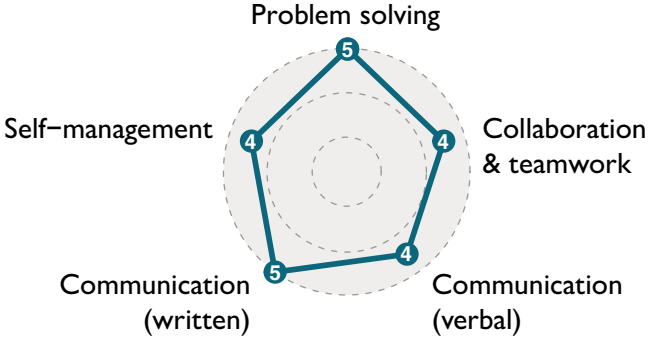
Molecular machine learning



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.

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

Machine learning-guided high throughput nanoparticle design.
Ana Ortiz-Perez, 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.

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.