

CV | Jim Boelrijk

Data Scientist, Evonik

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PROFILE

Data scientist with a PhD in machine learning and chemistry. I develop machine-learning methods for chemical and analytical workflows, with a focus on Bayesian optimization, experimental automation, and liquid chromatography method development.

WORK EXPERIENCE

2024–now		Data Scientist · Evonik  Germany
2024		Senior Data Science Consultant · Valcon  Netherlands
2019–2020		Software Tester · Software for Chemistry & Materials (SCM)  Netherlands
2013–2015		Professional Rugby Player · Stade Montois Rugby  France

EDUCATION

2024		PhD Machine Learning & Chemistry  Amsterdam Machine Learning Lab, University of Amsterdam
2019		Master Chemistry (Cum Laude)  University of Amsterdam Track: Computational Chemistry
2017		Bachelor Chemistry  Vrije Universiteit Amsterdam Minor: Programming

SELECTED PUBLICATIONS

Shape-Aware Gaussian Process Kernels for Closed-Loop Bayesian Optimization of Gradients in Automated LC Method Development

ChemRxiv, 2026 Jim Boelrijk et al. Preprint

Comparison of optimization algorithms for automated method development of gradient profiles

Journal of Chromatography A, 2025 Gerben B. van Henten, Jim Boelrijk et al. DOI

Enhancing LC×LC separations through multi-task Bayesian optimization

Journal of Chromatography A, 2024 Jim Boelrijk et al. DOI

Closed-loop automatic gradient design for liquid chromatography using Bayesian optimization

Analytica Chimica Acta, 2023 Jim Boelrijk et al. DOI

Multi-objective optimization via equivariant deep hypervolume approximation

ICLR, 2023 Jim Boelrijk, Bernd Ensing, Patrick Forré arXiv

SELECTED TALKS & PRESENTATIONS

2026	Panelist, "AI-Ready Chemistry: From Hype to Implementation", <i>Amsterdam Chemistry Innovation Day (ACID)</i> .
2026	AI-driven LC method optimization, <i>Agilent Lab Productivity and Automation Days</i> , Waldbronn.
2026	Automated AI-driven LC Method Optimization, <i>Future-Ready Pharma Summit</i> .
2025	Chair, "Making Every Measurement Count: Adaptive Optimization in Analytical Technologies", <i>ChemAI 2025</i> , Amsterdam.
2021	Focus session on machine learning for chemical discovery, <i>CHAINS / KNCV</i> .
2020	Illustere Alumni event, <i>University of Amsterdam</i> .

TEACHING & REVIEWING

2021–2023	Molecular Simulation (PhD winter course).
2021	Deep Learning 1 (Master AI, UvA).
2020–2021	Machine Learning 2 (Master AI, UvA).
2020	Machine Learning 1 (Master AI, UvA).
	Role: Teaching Assistant.
2015–2019	Teacher & Exam Trainer, Physics, <i>Inwijls</i> , Netherlands.
Peer review: ICML (2024), NeurIPS (2023), AISTATS (2022, Top 10% Reviewer), ICLR (2022).	

SUMMER SCHOOLS & CONFERENCES

2024	Foundation Model Winter School, <i>University of Amsterdam</i> .
2023	ICML, ICLR and AutoML Conferences.
2023	Machine Learning Theory Boot Camp, <i>Centrum voor Wiskunde en Informatica (CWI)</i> .
2021	Deep Learning & Reinforcement Learning Summer School (DLRL), <i>CIFAR</i> .

SPORT ACHIEVEMENTS

2024	Captain and Dutch national champion with RC 't Gooi.
2018, 2013	Dutch national champion with RC 't Gooi.
2014–2024	Netherlands national rugby team player.
2012	Rugby Youth Player of the Netherlands; awarded best under-18 player.

PROGRAMMING

Python	● ● ● ● ● ●
PyTorch	● ● ● ● ● ●
GPyTorch, BoTorch, Ax	● ● ● ● ● ●
NumPy, pandas, scikit-learn	● ● ● ● ● ●
RDKit, ASE, CP2K, ADF	● ● ● ● ● ●

MACHINE LEARNING

Gaussian processes	● ● ● ● ● ●
Bayesian optimization	● ● ● ● ● ●
Multi-objective optimization	● ● ● ● ● ●
(Equivariant) deep learning	● ● ● ● ● ●
Molecular modeling	● ● ● ● ● ●

CERTIFICATES, LANGUAGES & INTERESTS

Certificates: Microsoft Certified: Azure AI Fundamentals (2024).	
Databricks Certified Machine Learning Associate (2024–2026).	
Languages:	Dutch (C2), English (C2), French (B2).
Hobbies:	Weightlifting, beer brewing.