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Dr. sc. Simon L. Dürr

Curriculum vitae

Professional Working Proficiency: German, English, French Limited working proficiency

Work experience

Mar '25 – now **Assistant Professor UAS for Digital Life Science**, *HES-SO Valais-Wallis*, Sion, Switzerland, 25%, full time from June 2025

Mar '25 – now **AdaptyvBio**, *Science Product Engineer*

Dec '24 – Jun' 25 **PostDoc in the group of Prof. Ursula Röthlisberger**, *EPFL*, Switzerland

Education

Nov '19 – Nov' 24 **Doctorate in the group of Prof. Ursula Röthlisberger**, *EPFL*, Switzerland, Doctoral school of Chemistry and Chemical Engineering
Engineering of functional metalloenzymes using evolutionary computation, deep learning and simulation

2016 – 2019 **Master of Science**, *Universität Konstanz*, Germany
Life Science with focus on biophysical and computational chemistry

2017 – 2018 **Exchange studies**, *Uppsala University*, Sweden
Focus on theoretical chemistry and computational biology

2013 – 2016 **Bachelor of Science**, *Universität Konstanz*, Germany
Life Science

Research experience

Feb '23 – now **Fellow**, *Huggingface Inc*, USA, Protein Design and AI

Aug '22 – Oct '22 **Visiting Researcher in the group of Prof. Possu Huang**, *Stanford University*, USA, Deep learning based protein sequence design for metalloproteins

Nov '18 – Jul '19 **Masterthesis in the group of Prof. Ursula Röthlisberger**, *EPFL*, Switzerland, Genetic algorithm optimization and QM/MM simulations of metalloproteins

Jan '18 – May '18 **Research internship in the group of Prof. Lynn Kamerlin**, *Uppsala University*, Uppsala, Sweden, Structural bioinformatics of phosphate binding

Jan '17 – Jun '17 **Research internship in the groups of Prof. Kay Diederichs and Prof. Christine Peter**, *Universität Konstanz*,
Konstanz, Deutschland, QM/MM refinement

Jun '16 – Sep '16 **Bachelorthesis in group of Dr. Edina Rosta**, *Kings College London*, London, United Kingdom, QM/MM simulations of HIV-1 reverse transcriptase

Aug '15 – Oct '15 **Research internship in the group of Prof. Joelle Pelletier**, *University of Montréal*, Montréal, Canada, Implicit ligand sampling of cytochrome P450s

Review activity and panel memberships

JCIM	2 articles reviewed	**ICML-ML4LMS**	3 articles reviewed
Nature Comm.	4 articles reviewed	**STAR Protocols**	2 articles reviewed
NeurIPS MLSB	12 articles reviewed	**Protein Science**	4 articles reviewed

SciPy Conf Reviewer for Materials & Chemistry track, 3 submissions reviewed

NeurIPS, *Workshop co-organizer, leaderboard/challenge for docking predictions in collaboration with NVidia, UBasel & Vant.ai*, `https://mlsb.io`

Open Science and Open Source

Founder of Bioicons.com, *Open source clipart library*, Nuxt, Vue, SVG, 1425 stars, *>800k impressions, 100+ contributors*

Protein Design Webapps, *FAIR implementations of ProteinMPNN, DiffDock, Boltz-1*, Huggingface Spaces

Inkscape, *Contributed to new import webresource extension*, Python

Gradio, *Improvements to core and custom component (e.g Molecule3D, Molecule1D, CofoldingInput)*, Python

RadialScope, *A utility to plot radial substrate scopes easily with RDKit and Matplotlib*, Python

Invited Talks

2023 **Bonn Conference on Mathematical Life Sciences**, *Designing stable metalloproteins using deep learning*
Bonn, 17-20.4.2023

2023 **ML4Proteins**, *Deploying protein machine learning models on the web*
virtual, 28.3.2023

Selected Talks

2024 **German Open Science Festival**, *Open scientific illustrations*
Mainz, 17.-18.9.2024

2023 **European RosettaCon**, *Designing stable metalloproteins using deep learning*
Leipzig, 27.-29.9.2023

2023 **Directions in AI for Structural Biology**, *Designing stable metalloproteins using deep learning*
Marseille, 20.-24.3.2023

2022 **Neurips MLSB**, *Metal3D: Accurate prediction of transition metal ion location via deep learning*
New Orleans, 3.12.2022

2022 **European RosettaCon**, *Metal3D: Accurate prediction of transition metal ion location via deep learning*
Warsaw, 10.-13.5.2022

2022 **Advances in Protein Folding, Evolution, and Design**, *Metal3D: Accurate prediction of transition metal ion location via deep learning*
Bayreuth, 6.-8.4.2022

Preprints

2025 **AllMetal3D: joint prediction of localization, identity and geometry of common metal ions in proteins** , Simon L. Dürr, Ursula Rothlisberger
https://doi.org/10.1101/2025.02.05.636627

2024 **Predicting metal-protein interactions using cofolding methods: Status quo**, *Simon L. Dürr*, Ursula Rothlisberger, bioRxiv
https://doi.org/10.1101/2024.05.28.596236

Peer-reviewed publications

2023 **Metal3D: a general deep learning framework for accurate metal ion location prediction in proteins** , Simon L. Dürr, Andrea Levy, Ursula Rothlisberger *Nature Communications* , **2023** DOI: https://doi.org/10.1038/s41467-023-37870-6

2021 **The Role of Conserved Residues in the DEDDh Motif: the Proton Transfer Mechanism of HIV-1 RNase H**, Simon L. Dürr, Olga Bohuszewicz, Reynier Suardiaz, Pablo G. Jambrina, Christine Peter, Yihan Shao, Edina Rosta, *ACS Catalysis* , **2021** 11, pp. 7915-7927 DOI: 10.1021/acscatal.1c01493

2020 **Radial Scope: A New Visualization Tool for Structure–Data Relationships**, Attabey Rodríguez Benítez Simon L. Dürr Alison R.H.Narayan *Trends in Chemistry*, **2020**
2 (7), 2020, pp.587-589 DOI: 10.1016/j.trechm.2020.04.003

2018 **Snapshots of modified nucleotide ”moving” through the confines of a DNA polymerase**, Heike Kropp,Simon L. Dürr, Christine Peter, Kay Diederichs, Andreas Marx *Proceedings of the National Academy of Sciences*, **2018**
115 (40), pp. 9992-9997 DOI: 10.1073/pnas.1811518115

2016 **Evolution of P450 Monooxygenases toward Formation of Transient Channels and Exclusion of Nonproductive Gases**, Maximilian C. C. J. C. Ebert, Simon L. Dürr, Armande A. Houle, Guillaume Lamoureux, Joelle N. Pelletier, *ACS Catalysis*, **2016**
6 (11), pp 7426–7437 DOI: 10.1021/acscatal.6b02154

Teaching activities

2020 - 2024 **Assistant in CH-351 and CH-353 courses**, *EPFL*, Computational Chemistry, Transformation of course into Jupyter Notebook format and transition to PSI4 DFT code, Open Source Toy MD code, teaching, exercise sessions. (1 exercise session per week)
lcbc-epfl.github.io/iesm-public lcbc-epfl.github.io/mdmc-public

2021 - 2023 **Research Data Management**, *CUSO*, Course on good practices for research data management (1 full day). Designed course content and teaching material.

2020 **Assistant in CHE-437**, *Bioprocesses and downstream processing*

2019-2024 **Direct student supervision**, *Supervision of 1 master thesis (30 ECTS), 2 large master projects (12 ECTS), 1 small master project (6 ECTS), 1 student internship (30 ECTS) and 2 bachelor projects (2 ECTS)*