Curriculum Vitæ

Nikolai Köhler

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Education

2020 – 2023 **Ph.D.** in Bioinformatics — TUM School of Life Sciences (Chair of Experimental Bioinformatics)

Working Title: "Graph-Based Methods for the Analysis and Integration of Lipidome and Metabolome Data into the Omics-Landscape"
Expected Submission Date: January 2024

2023 **Visiting Researcher** — Yale University

Visiting research stay in the lab of Prof. Smita Krishnaswamy working on manifold learning and topological data analysis

2018 – 2020 **M.Sc.** in Molecular Biotechnology (***with high distinction***) — Technichal University of Munich (TUM)

Thesis: "Analysis of Organ-specific Lipidome Compositions and their Network Interactions in Mice"

2014 – 2018 **B.Sc.** in Agricultural Science (***with distinction***) — Technichal University of Munich (TUM)

Thesis: "Regulation of Pyrrolizidine Alkaloid Biosynthesis in *Crassocephalum crepidioides*"

Extra-curricular Education

Oxford Machine Learning Summer School 2022

Publications

Journal Publications

1. Rose TD†, **Köhler N**†, Falk L, Klischat L, Lazareva OE and Pauling JK: *Lipid network and moiety analysis for revealing enzymatic dysregulation and mechanistic alterations from lipidomics data.* Briefings in Bioinformatics, 2023
2. Damiani T, Bonciarelli S, Thallinger GG, **Köhler N**, Krettler CS, Salihoğlu AK, Korf A, Pauling JK, Pluskal T, Ni Y, and Goracci L: *Software and Computational Tools for LC-MS-Based Epilipidomics: Challenges and Solutions.* Analytical Chemistry, 2023
3. Rose TD, Bechtler T, Ciora O, Lilian Le KA, Molnar F, **Köhler N**, Baumbach J, Roettger J, Pauling JK: *MoSBi: Automated signature mining for molecular stratification and subtyping.* Proceedings of the National Academy of Science 2022
4. **Köhler N**†, Höring M†, Czepukojc B†, Rose TD†, Buechler C, Kröhler T, Haybaeck J, Liebisch G, Pauling JK, Kessler SM, Kiemer AK: *Kupffer cells are protective in alcoholic steatosis.* Biochimica et Biophysica Acta (BBA) - Molecular Basis of Disease, 2022
5. **Köhler N**†, Rose TD†, Falk L and Pauling JK: *Investigating Global Lipidome Alterations with the Lipid Network Explorer.* Metabolites, 2021
6. Dieckmann S, Strohmeyer A, Willershäuser M, Maurer S, Wurst W, Marschall S, Hrabe de Angelis M, Kühn R, Worthmann A, Fuh MM, Heeren J, **Köhler N**, Pauling JK, Klingenspor M: *Susceptibility to diet induced obesity at thermoneutral conditions is independent of UCP1.* American Journal of Physiology-Endocrinology and Metabolism, 2021
7. Haberl EM, Weiss TS, Peschel G, Weigand K, **Köhler N**, Pauling JK, Wenzel JJ, Höring M, Krautbauer S, Liebisch G, Buechler C: *Liver Lipids of Patients with Hepatitis B and C and Associated Hepatocellular Carcinoma.* International Journal of Molecular Sciences, 2021
8. Schramm S, **Köhler N**, Rozhon W: *Pyrrolizidine Alkaloids: Biosynthesis, Biological Activities and Occurrence in Crop Plants.* Molecules, 2019

Preprints

1. **Köhler N**, Würf V, Rose TD and Pauling JK: *Identification and Integration of Key-Metabolic Reactions from Untargeted Metabolomics Data.* bioRxiv, 2023; under review in Communications Biology
2. Hoheneder F†, Steidele CE†, Messerer M, Mayer K, **Köhler N**, Wurmser C, Heß M, Gigl M, Dawid C, Stam R, Hückelhoven R: *Barley shows reduced Fusarium Head Blight under drought and modular expression of differential expressed genes under combined stress.* bioRxiv, 2023; under review in Journal of Experimental Botany
3. Coleman OI†, Sorbie A†, Bierwirth S, Kövilein J, von Stern M, **Köhler N**, Wirbel J, Schmidt C, Kacprowski T, Dunkel A, Pauling JK, Plagge J, Miedel-Cuadra D, Wagner S, Peng T, Metzler T, Schafmayer C, Hinz S, Röder C, Röcken C, Stecher B, Rosenstiel P, Steiger K, Jesinghaus M, Liebisch G, Ecker J, Zeller G, Jansse KP, Haller D: *ATF6 activation alters colonic lipid metabolism causing tumor-associated microbial adaptation.* bioRxiv, 2023;

† These authors contributed equally to this work.

Internships

2017 – 2018 Roessner Lab (Chair for Plant Biochemistry), Unversity of Melbourne/Metabolomics Australia

2015 Julius Kühn Insitute, Federal Research Centre for Cultivated Plants, Institute for Grapevine Breeding

Work Experience

2019 – 2020 Student Research Assistant — LipiTUM/Chair of Experimental Bioinformatics (TUM)

2018 – 2019 Student Research Assistant — Chair for Biotechnology of Horticultural Crops (TUM)

2017 Student Research Assistant — Chair of Plant Breeding (TUM)

Honors and Scholarships

Awards

- Best Presentation Award - Virtual Podium Asia Pacific 2021

Scholarships

- PROMOS Travel Scholarship - German Academic Exchange Service (Oct. 17 - Mar. 18)

Talks and Workshops

Talks

- *Graph-Based Metaboilc Reaction-Centered Multi-Omics Data Integration*, 72nd ASMS Annual Conference, 2023
- *Reaction-Centered Metabolic Network Analysis*, 4th Munich Metabolomics Meeting, 2022
- *Lipid network and moiety analysis for revealing enzymatic dysregulation and mechanistic alterations from lipidomics data*, International Conference on Systems Biology, 2022
- ***Keynote:** "Lipid metabolic network analysis for inferring mechanistic changes in enzyme activity* 10th Workshop in Lipidomics, 2022
- *Network-based Lipidomics Analysis using the Lipid Network Explorer.* Virtual Podium Asia Pacific, 2021
- *Investigating Global Lipidome Alterations with the Lipid Network Explorer.* 1st International Lipidomics Society Conference, 2021

Co-Organized Workshops

- LipiTUM Workshop on Patient Stratification and Lipid Metabolic Network Analysis. 1st International Lipidomics Society Conference, 2021
- Workshop on Lipidomics Data Analysis. 8th Lipidomics Forum, 2023

Skills

Programming Languages:	Python, C++, R	ML Frameworks:	PyTorch, JAX
Containerization:	Docker, Podman	HPC administration:	slurm

BSc/MSc Thesis Supervision

Bioinformatics

- "Development of a Deep Learning Model for the Detection and Prediction of Characteristic Fragmentation Patterns in Lipid Mass Spectra"
- "Network Integration of Metabolome and Microbiome Data using Local Search Optimisation"
- "Evaluating Linear Model-based Reaction Approximation and Multi-Omics Integration"
- "Imputing Unmeasured Lipids to Improve the Connectivity of Lipid Metabolic Networks"

Molecular Biotechnology

- "A Network-based Meta-Analysis to Link Nutritional Metabolites to Lipid Metabolism and Related Diseases"

References

Prof. Dr. Smita Krishnaswamy
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Dr. Bastian Rieck
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