

Nikolai Köhler

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- 2020 – 2023 Postdoctoral Researcher - ML for Spatial Omics (Velten Lab) HEIDELBERG UNIVERSITY
- 2023 Visiting Postgraduate Researcher
Manifold Learning for (Spatial) Metabolomics (Krishnaswamy Lab) YALE UNIVERSITY
- 2020 – 2023 Predoctoral Researcher - Computational Metabolomics TECHNICAL UNIVERSITY OF MUNICH (TUM)

EDUCATION

- 2020 – 2023 **Dr. rer. nat.** in Bioinformatics (*summa cum laude*) TUM (CHAIR OF EXPERIMENTAL BIOINFORMATICS)
Thesis Title: “Graph-Based Methods for the Analysis and Integration of Lipidome and Metabolome Data into the Omics-Landscape”
- 2018 – 2020 **M.Sc.** in Molecular Biotechnology (*with high distinction*) TECHNICAL 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*) TECHNICAL 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. Kolja Siebert, Tim Faro[†], **Nikolai Köhler[†]**, Hannes Hölz, Sebastian Jarosch, Monica Machado, Deborah Häcker, Federica De Zen, Mohammad Samer Hajji, Eberhard Lurz, Sibylle Koletzko, Josch K Pauling, Katja Steiger, Klaus Neuhaus, Caspar Ohnmacht, Markus List, Dirk H Busch, Dirk Haller, Tobias Schwerd *Endoscopic healing in pediatric IBD perpetuates a persistent signature defined by Th17 cells with molecular and microbial drivers of disease*. Cell Reports Medicine, 2025
2. Haecker D, Siebert K, Smith BJ, **Köhler N**, Riva A, Mahapatra A, Heimes H, Nie J, Metwaly A, Hölz H, Manz Q, De Zen F, Heetmeyer J, Socas K, Le Thi G, Meng C, Kleigrew K, Pauling JK, Neuhaus K, List M, Pollard KS, Schwerd T, Haller D: *Exclusive Enteral Nutrition Initiates Protective Microbiome Changes to Induce Remission in Pediatric Crohn's Disease* Cell Host & Microbe, 2024
3. 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
4. Damiani T, Bonciarelli S, Thallinger GG, **Köhler N**, Kretzler 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
5. Hoheneder F[†], Steidle CE[†], Messerer M, Mayer K, **Köhler N**, Wurmser C, Heß M, Gigl M, Dawid C, Stam R, Hüchelhoven R: *Barley shows reduced Fusarium Head Blight under drought and modular expression of differential expressed genes under combined stress*. Journal of Experimental Botany, 2023
6. 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

7. **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
8. **Köhler N**[†], Rose TD[†], Falk L and Pauling JK: *Investigating Global Lipidome Alterations with the Lipid Network Explorer*. Metabolites, 2021
9. 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
10. 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
11. Schramm S, **Köhler N**, Rozhon W: *Pyrrolizidine Alkaloids: Biosynthesis, Biological Activities and Occurrence in Crop Plants*. Molecules, 2019

Preprints

1. Felix Niedermaier, Konstantinos Mechteridis, Konstantin Pelz, Vivian Würf, **Nikolai Köhler**, Josch K Pauling *Navigating the Lipid Universe with LipidLibrarian: A Cross-Linked Database for Lipidomics Data Integration*. bioRxiv, 2025
2. Würf V, **Köhler N**, Molnar F, Hahnefeld L, Gurke R, Witting M, Pauling JK *LipidDetective-a deep learning model for the identification of molecular lipid species in tandem mass spectra* bioRxiv, 2024
3. **Köhler N**, Würf V, Rose TD and Pauling JK: *Identification and Integration of Key-Metabolic Reactions from Untargeted Metabolomics Data*. bioRxiv, 2023
4. 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, Janssen KP, Haller D: *ATF6 activation alters colonic lipid metabolism causing tumor-associated microbial adaptation*. bioRxiv, 2023

[†] These authors contributed equally to this work.

TALKS AND WORKSHOPS

Talks

- *Graph-Based Metabolic 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

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

TEACHING

Lectures

- Optimal Transport - Theory and Applications (M.Sc. Scientific Computing & M.Sc. Mathematics, 2025, Heidelberg University)
- Data Analysis for the Life Sciences (M.Sc. Biology, 2024, Heidelberg University)
- Data Analysis for RNA sequencing (B.Sc. Biology, 2024, Heidelberg University)
- Computational Biochemistry (M.Sc. Biochemistry, 2020-2022, TUM)

Practicals

- Systems BioMedicine (M.Sc. Bioinformatics, 2020-2022, TUM)
- Problem Based Learning (B.Sc. Bioinformatics, 2021, TUM)

THESIS SUPERVISION ---

Completed (Technical University of Munich)

- Bioinformatics (B.Sc.)
 - "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 (M.Sc.)
 - "A Network-based Meta-Analysis to Link Nutritional Metabolites to Lipid Metabolism and Related Diseases"

Ongoing (Heidelberg University)

- "Predicting RNA molecule localization from cellular neighborhood information" (M.Sc. Physics)
- "Incorporating subcellular localization into dimension reduction algorithms" (B.Sc. Biology)

HONORS AND SCHOLARSHIPS ---

Awards

- Best Presentation Award - Virtual Podium Asia Pacific 2021

Scholarships

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

REFERENCES ---

JProf. Dr. Britta Velten
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