*Curriculum Vitae*


## Dr. Robin Schmid

PostDoctoral Researcher in Computational Mass Spectrometry
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## Research Interests

Metabolomics, Food Chemistry, Liquid Chromatography, Computational Mass Spectrometry, Open Data

## Background

I combine my background in food chemistry and analytical chemistry with computational mass spectrometry, developing new open tools to map and understand the complex chemical relationships between small molecules like metabolites and xenobiotics. My research focuses on non-target analysis, developing new integrative methods to link liquid chromatography-mass spectrometry with bioimaging and ion mobility spectrometry, applied in a broader chemical and biological context.

## Education

11/2019 – 12/2019 **Visiting researcher** (Biomedical Research)
Advisor: Professor Jing-Ke Weng, Massachusetts Institute of Technology, Cambridge, USA

09/2018 – 12/2018 **Visiting researcher** (Pharmacy and Pharmaceutical Sciences)
Advisor: Professor Pieter C. Dorrestein, University of California San Diego, USA

12/2016 – 09/2020 **PhD in Analytical Chemistry** (Chemiefonds FCI fellow)
Advisor: Professor Uwe Karst, University of Münster, Germany
Thesis: *New Computational Methods for Mass Spectrometry and Imaging Analysis*

09/2015 – 03/2016 **Research internship** (Forensic Science and the Elemental Bio-imaging Facility)
Advisor: Professor Philip Doble, University of Technology Sydney, Australia

10/2014 – 09/2016 **M.Sc. in Food Chemistry**
Advisor: Professor Hans-Ulrich Humpf, University of Münster, Germany
Thesis: *Novel Compound Discovery: Workflow Optimization and Algorithm Development for Data-Independent MS/MS Annotation, Applied to Differential Metabolomics Data of Fusarium fujikuroi*

10/2011 – 09/2014 **B.Sc. in Food Chemistry**
Advisor: Professor Uwe Karst, University of Münster, Germany
Thesis: Laser Ablation-Mass Spectrometric Analysis of Pharmaceuticals

05/2011 **Abitur** (general higher education entrance qualification) in Kassel, Germany

## Research Positions

01/2023 **Postdoctoral Researcher** (Computational Mass Spectrometry)
Advisor: Tomáš Pluskal, Institute of Organic Chemistry and Biochemistry, Prague, Czechia
Topic: *Automating Mass Spectrometry Data Processing*

10/2020 – 12/2022 **Postdoctoral Researcher** (Collaborative Mass Spectrometry Innovation Center)
Advisor: Professor Pieter C. Dorrestein, University of California San Diego, USA
Topic: *Repository Scale Metabolomics Data Analysis with GNPS and MZmine*

12/2016 – 09/2020 **PhD Student and Doctoral Research Associate**
University of Münster, Germany

04/2015 – 09/2015 **Student Assistant**
Advisor: Professor Uwe Karst, University of Münster, Germany
Topic: *Development of Mass Spectrometry Imaging Methods and Tools*

## Awards and Honors

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| 2019 | **Young Scientist Award** for the best oral presentation at the Young Scientist Meeting of the German Society for Mass Spectrometry (DGMS) |
| 2017 – 2019 | **Chemiefonds PhD fellowship** of the Chemical Industry Fund (FCI) |
| 11/2017 | **Scholarship for Mouse Imaging Academy 8 (MIA)** participation Cells in Motion (CiM) cluster of excellence, Münster |
| 2016 | **Food Chemistry Award** for the best master thesis at the University of Münster |

## Scientific Service and Membership

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| Reviewer | Nature Communications, Nature Methods, Analytical Chemistry |
| Since 2022 | Member, Virtual Multi-Omics Lab (VMOL) |
| Since 2019 | Admin and chief architect, MZmine open-source community |
| Since 2019 | Member, DGMS Young Scientists |
| Since 2018 | Member, Global Natural Products Social (GNPS) open-source community |
| Since 2017 | Member, German Society for Mass Spectrometry (DGMS) |
| Since 2017 | Member, German Chemical Society (GDCh) |
| 2016 – 2019 | Member, MZmine open-source community |

## Outreach

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| 2023 | Co-organization of the project "FAIRification of mass spectral libraries" at the Elixir BioHackathon in Barcelona |
| 2023 | Co-organization of International Summer School on Non-targeted Metabolomics, Copenhagen |
| 2022 | Co-organization of International Summer School on Non-targeted Metabolomics, Tübingen |
| 2021 | Co-organization of a Computational Mass Spectrometry Data Processing workshop, Prague |

## Cooperations

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| Since 2023 | Collaborative network for dynamic mass spectral libraries + Elixir BioHackathon<br>Prof. Jean-Luc Wolfender (University of Geneva), Prof. Nicola Zamboni (ETH Zürich), Prof. Gunda Köllensperger (University of Vienna), Prof. Asaph Aharoni (Weizmann Institute), Dr. Michael Zimmermann (EMBL), Dr. Justin J.J. van der Hooft (WUR), Prof. Florian Huber (Düsseldorf University of Applied Sciences), Dr. Thomas O. Metz (PNNL), Prof. Benedikt Warth |
| Since 2023 | Automatic extraction of retention times for RepoRT database<br>Dr. Michael Witting (Helmholtz Zentrum München), Prof. Sebastian Böcker (University of Jena) |
| Since 2019 | Data analysis and software for the timsTOF fleX mass spectrometer combining imaging and LC<br>Arne Fütterer (Bruker Daltonics GmbH Bremen), Steffen Heuckeroth (University of Münster) |
| Since 2018 | Methods and tools to identify siderophores and other ionophores<br>Dr. Allegra Aron (University of Denver) |
| Since 2018 | Development of computational metabolomics tools and the GNPS web platform<br>Prof. Pieter C. Dorrestein (UC San Diego), Dr. Mingxun Wang (UC Riverside), Dr. Daniel Petras (University of Tübingen), Prof. Louis-Felix Nothias (CNRS, Cote d'Azur University) |

2019 – 2020 Nanoparticle analysis by spICP-MS imaging
BMBF project NanoBioQuant, Münster

2019 Hybrid TOF-SIMS bioimaging tests and incorporation of support in ImaJar
IONTOF GmbH (Münster), Dr. Karsten Laman (tascon GmbH, Münster)

2018 – 2019 Testing and optimization of the iMScope mass spectrometer and software
Software Unit Shimadzu Japan, Dr. Ann-Christin Niehoff (Shimadzu Europe GmbH)

2017 – 2020 Development of imaging methods and the scientific imaging software ImaJar
Prof. Philip Doble (UTS), Bayer AG Berlin, Bundesanstalt für Materialforschung (BAM, Berlin), BASF Ludwigshafen, Elemental Scientific (ESI) USA, Charité Berlin

Since 2016 Development of MZmine for metabolomics and lipidomics,
Dr. Tomáš Pluskal (MIT, later IOCB)

## Third-Party Funding

2018 – 2019 **Chemiefonds PhD fellowship** of the Chemical Industry Fund (FCI)

## Peer-Reviewed Publication

* indicates equal contribution

22 **Evaluation of Data-Dependent MS/MS Acquisition Parameters for Non-Targeted Metabolomics and Molecular Networking of Environmental Samples: Focus on the Q Exactive Platform**
Stincone P, Pakkir Shah AK, **Schmid R**, Graves LG, Lambidis SP, Torres RR, Xia S-N, Minda V, Aron AT, Wang M, Hughes CC, Petras D
Analytical chemistry. 2023;95: 12673–12682. doi:10.1021/acs.analchem.3c01202

21 **Integrative analysis of multimodal mass spectrometry data in MZmine 3**
**Schmid R***, Heuckeroth S*, Korf A*, Smirnov A, Myers O, Dyrlund TS, Bushuiev R, Murray KJ, Hoffmann N, Lu M, Sarvepalli A, Zhang Z, Fleischauer M, Dührkop K, Wesner M, Hoogstra SJ, Rudt E, Mokshyna O, Brungs C, Ponomarov K, Mutabdžija L, Damiani T, Pudney CJ, Earll M, Helmer PO, Fallon TR, Schulze T, Rivas-Ubach A, Bilbao A, Richter H, Nothias L-F, Wang M, Orešič M, Weng J-K, Böcker S, Jeibmann A, Hayen H, Karst U, Dorrestein PC, Petras D, Du X, Pluskal T
Nature biotechnology. 2023;41: 447–449. doi:10.1038/s41587-023-01690-2

20 **Comparison of Cosine, Modified Cosine, and Neutral Loss Based Spectrum Alignment For Discovery of Structurally Related Molecules**
Bittremieux W*, **Schmid R***, Huber F, van der Hooft JJJ, Wang M, Dorrestein PC
Journal of the American Society for Mass Spectrometry. 2022;33: 1733–1744. doi:10.1021/jasms.2c00153

19 **Tattoo Pigment Identification in Inks and Skin Biopsies of Adverse Reactions by Complementary Elemental and Molecular Bioimaging with Mass Spectral Library Matching**
Brungs C*, **Schmid R***, Wolf C, Berg T, Korf A, Heuckeroth S, Hayen H, van der Bent S, Maijer K, Rustemeyer T, Karst U
Analytical chemistry. 2022;94: 3581–3589. doi:10.1021/acs.analchem.1c04922

18 **foodMASST a mass spectrometry search tool for foods and beverages**
West KA, **Schmid R**, Gauglitz JM, Wang M, Dorrestein PC
NPJ science of food. 2022;6: 22. doi:10.1038/s41538-022-00137-3

17 **GNPS Dashboard: collaborative exploration of mass spectrometry data in the web browser**
Petras D, Phelan VV, Acharya D, Allen AE, Aron AT, Bandeira N, Bowen BP, Belle-Oudry D, Boecker S, Cummings DA Jr, Deutsch JM, Fahy E, Garg N, Gregor R, Handelsman J, Navarro-Hoyos M, Jarmusch AK, Jarmusch SA, Louie K, Maloney KN, Marty MT, Meijler MM, Mizrahi I, Neve RL, Northen TR, Molina-Santiago C, Panitchpakdi M, Pullman B, Puri AW, **Schmid R**, Subramaniam S, Thukral M, Vasquez-Castro F, Dorrestein PC, Wang M
Nature methods. 2022;19: 134–136. doi:10.1038/s41592-021-01339-5

16 **Native mass spectrometry-based metabolomics identifies metal-binding compounds**
Aron AT, Petras D, **Schmid R**, Gauglitz JM, Büttel I, Antelo L, Zhi H, Nuccio S-P, Saak CC, Malarney KP, Thines E, Dutton RJ, Aluwihare LI, Raffatellu M, Dorrestein PC
Nature chemistry. 2022;14: 100–109. doi:10.1038/s41557-021-00803-1

15 **Ion identity molecular networking for mass spectrometry-based metabolomics in the GNPS environment**
**Schmid R***, Petras D*, Nothias L-F*, Wang M, Aron AT, Jagels A, Tsugawa H, Rainer J, Garcia-Aloy M, Dührkop K, Korf A, Pluskal T, Kameník Z, Jarmusch AK, Caraballo-Rodríguez AM, Weldon KC, Nothias-Esposito M, Aksenov AA, Bauermeister A, Albarracin Orio A, Grundmann CO, Vargas F, Koester I, Gauglitz JM, Gentry EC, Hövelmann Y, Kalinina SA, Pendergraft MA, Panitchpakdi M, Tehan R, Le Gouellec A, Aleti G, Mannochio Russo H, Arndt B, Hübner F, Hayen H, Zhi H, Raffatellu M, Prather KA, Aluwihare LI, Böcker S, McPhail KL, Humpf H-U, Karst U, Dorrestein PC
Nature communications. 2021;12: 3832. doi:10.1038/s41467-021-23953-9

14 **Feature-based molecular networking for identification of organic micropollutants including metabolites by non-target analysis applied to riverbank filtration**
Oberleitner D, **Schmid R**, Schulz W, Bergmann A, Achten C
Analytical and bioanalytical chemistry. 2021;413: 5291–5300. doi:10.1007/s00216-021-03500-7

13 **Auto-deconvolution and molecular networking of gas chromatography-mass spectrometry data**
Aksenov AA, Laponogov I, Zhang Z, Doran SLF, Belluomo I, Veselkov D, Bittremieux W, Nothias LF, Nothias-Esposito M, Maloney KN, Misra BB, Melnik AV, Smirnov A, Du X, Jones KL 2nd, Dorrestein K, Panitchpakdi M, Ernst M, van der Hooft JJJ, Gonzalez M, Carazzone C, Amézquita A, Callewaert C, Morton JT, Quinn RA, Bouslimani A, Orio AA, Petras D, Smania AM, Couvillion SP, Burnet MC, Nicora CD, Zink E, Metz TO, Artaev V, Humston-Fulmer E, Gregor R, Meijler MM, Mizrahi I, Eyal S, Anderson B, Dutton R, Lugan R, Boulch PL, Guitton Y, Prevost S, Poirier A, Dervilly G, Le Bizec B, Fait A, Persi NS, Song C, Gashu K, Coras R, Guma M, Manasson J, Scher JU, Barupal DK, Alseekh S, Fernie AR, Mirnezami R, Vasiliou V, **Schmid R**, Borisov RS, Kulikova LN, Knight R, Wang M, Hanna GB, Dorrestein PC, Veselkov K
Nature biotechnology. 2021;39: 169–173. doi:10.1038/s41587-020-0700-3

12 **Spatially and size-resolved analysis of gold nanoparticles in rat spleen after intratracheal instillation by laser ablation-inductively coupled plasma-mass spectrometry**
Nordhorn ID, Dietrich D, Verlemann C, Vennemann A, **Schmid R**, Elinkmann M, Fuchs J, Sperling M, Wiemann M, Karst U
Metallomics. 2021;13. doi:10.1093/mtomcs/mfab028

11 **Feature-based molecular networking in the GNPS analysis environment**
Nothias L-F*, Petras D*, **Schmid R***, Dührkop K, Rainer J, Sarvepalli A, Protsyuk I, Ernst M, Tsugawa H, Fleischauer M, Aicheler F, Aksenov AA, Alka O, Allard P-M, Barsch A, Cachet X, Caraballo-Rodriguez AM, Da Silva RR, Dang T, Garg N, Gauglitz JM, Gurevich A, Isaac G, Jarmusch AK, Kameník Z, Kang KB, Kessler N, Koester I, Korf A, Le Gouellec A, Ludwig M, Martin H C, McCall L-I, McSayles J, Meyer SW, Mohimani H, Morsy M, Moyne O, Neumann S, Neuweger H, Nguyen NH, Nothias-Esposito M, Paolini J, Phelan VV, Pluskal T, Quinn RA, Rogers S, Shrestha B, Tripathi A, van der Hooft JJJ, Vargas F, Weldon KC, Witting M, Yang H, Zhang Z, Zubeil F, Kohlbacher O, Böcker S, Alexandrov T, Bandeira N, Wang M, Dorrestein PC
Nature methods. 2020;17: 905–908. doi:10.1038/s41592-020-0933-6

10 **Reproducible molecular networking of untargeted mass spectrometry data using GNPS**
Aron AT, Gentry EC, McPhail KL, Nothias L-F, Nothias-Esposito M, Bouslimani A, Petras D, Gauglitz JM, Sikora N, Vargas F, van der Hooft JJJ, Ernst M, Kang KB, Aceves CM, Caraballo-Rodríguez AM, Koester I, Weldon KC, Bertrand S, Roullier C, Sun K, Tehan RM, Boya P CA, Christian MH, Gutiérrez M, Ulloa AM, Tejeda Mora JA, Mojica-Flores R, Lakey-Beitia J, Vásquez-Chaves V, Zhang Y, Calderón AI, Tayler N, Keyzers RA, Tugizimana F, Ndlovu N, Aksenov AA, Jarmusch AK, **Schmid R**, Truman AW, Bandeira N, Wang M, Dorrestein PC
Nature protocols. 2020;15: 1954–1991. doi:10.1038/s41596-020-0317-5

9 **Identification of potential human urinary biomarkers for tomato juice intake by mass spectrometry-based metabolomics**
Hövelmann Y, Jagels A, **Schmid R**, Hübner F, Humpf H-U
European journal of nutrition. 2020;59: 685–697. doi:10.1007/s00394-019-01935-4

8 **Digging deeper - A new data mining workflow for improved processing and interpretation of high resolution GC-Q-TOF MS data in archaeological research**
Korf A, Hammann S, **Schmid R**, Froning M, Hayen H, Cramp LJE
Scientific reports. 2020;10: 767. doi:10.1038/s41598-019-57154-8

7 **Fast Online Separation and Identification of Electrochemically Generated Isomeric Oxidation Products by Trapped Ion Mobility–Mass Spectrometry**
Fangmeyer J, Scheeren SG, **Schmid R**, Karst U
Analytical chemistry. 2020;92: 1205–1210. doi:10.1021/acs.analchem.9b04337

6 **Expanding the Kendrick Mass Plot Toolbox in MZmine 2 to Enable Rapid Polymer Characterization in Liquid Chromatography-Mass Spectrometry Data Sets**
Korf A, Fouquet T, **Schmid R**, Hayen H, Hagenhoff S
Analytical chemistry. 2020;92: 628–633. doi:10.1021/acs.analchem.9b03863

5 **Multimodal imaging of hallucinogens 25C- and 25I-NBOMe on blotter papers**
Lützen E, Holtkamp M, Stamme I, **Schmid R**, Sperling M, Pütz M, Karst U
Drug testing and analysis. 2020;12: 465–471. doi:10.1002/dta.2751

4 **Lipid Species Annotation at Double Bond Position Level with Custom Databases by Extension of the MZmine 2 Open-Source Software Package**
Korf A, Jeck V, **Schmid R**, Helmer PO, Hayen H
Analytical chemistry. 2019;91: 5098–5105. doi:10.1021/acs.analchem.8b05493

3 **Three-dimensional Kendrick mass plots as a tool for graphical lipid identification**
Korf A, Vosse C, **Schmid R**, Helmer PO, Jeck V, Hayen H
Rapid communications in mass spectrometry. 2018;32: 981–991. doi:10.1002/rcm.8117

2 **A Fungal N-Dimethylallyltryptophan Metabolite from Fusarium fujikuroi**
Arndt B, Janevska S, **Schmid R**, Hübner F, Tudzynski B, Humpf H-U
Chembiochem. 2017;18: 899–904. doi:10.1002/cbic.201600691

1 **Microfluidic high performance liquid chromatography-chip hyphenation to inductively coupled plasma-mass spectrometry**
Bishop DP, Blanes L, Wilson AB, Wilbanks T, Killeen K, Grimm R, Wenzel R, Major D, Macka M, Clarke D, **Schmid R**, Cole N, Doble PA
Journal of chromatography A. 2017;1497: 64–69. doi:10.1016/j.chroma.2017.03.025

## Preprints

[#] indicates corresponding author * indicates equal contribution

6 **On-tissue dataset-dependent MALDI-TIMS-MS2 bioimaging**
Heuckeroth S, Behrens A, Wolf C, Fütterer A, Nordhorn ID, Kronenberg K, Brungs C, Korf A, Richter H, Jeibmann A, Karst U, **Schmid R**[#]
ChemRxiv. 2023. doi:10.26434/chemrxiv-2023-nw5p3-v2

5 **A Taxonomically-informed Mass Spectrometry Search Tool for Microbial Metabolomics Data**
Zuffa S*, **Schmid R***, Bauermeister A, Gomes PWP, Caraballo-Rodriguez AM, El Abiead Y, Aron AT, Gentry EC, Zemlin J, Meehan MJ, Avalon NE, Cichewicz RH, Buzun E, Terrazas MC, Hsu C-Y, Oles R, Ayala AV, Zhao J, Chu H, Kuijpers MCM, Jackrel SL, Tugizimana F, Nephali LP, Dubery IA, Madala NE, Moreira EA, Costa-Lotufo LV, Lopes NP, Rezende-Teixeira P, Jimenez PC, Rimal B, Patterson AD, Traxler MF, de Cassia Pessotti R, Alvarado-Villalobos D, Tamayo-Castillo G, Chaverri P, Escudero-Leyva E, Quiros-Guerrero L-M, Bory AJ, Joubert J, Rutz A, Wolfender J-L, Allard P-M, Sichert A, Pontrelli S, Pullman BS, Bandeira N, Gerwick WH, Gindro K, Massana-Codina J, Wagner BC, Forchhammer K, Petras D, Aiosa N, Garg N, Liebeke M, Bourceau P, Kang KB, Gadhavi H, de Carvalho LPS, dos Santos MS, Pérez-Lorente AI, Molina-Santiago C, Romero D, Franke R, Brönstrup M, de León AVP, Pope PB, La Rosa SL, La Barbera G, Roager HM, Laursen MF, Hammerle F, Siewert B, Peintner U, Licona-Cassani C, Rodriguez-Orduña L, Rampler E, Hildebrand F, Koellensperger G, Schoeny H, Hohenwallner K, Panzenboeck L, Gregor R, O'Neill EC, Roxborough ET, Odoi J, Bale NJ, Ding S, Sinninghe Damsté JS, Guan XL, Cui JJ, Ju K-S, Silva DB, Silva FMR, da Silva GF, Koolen HHF, Grundmann C, Clement JA, Mohimani H, Broders K, McPhail KL, Ober-Singleton SE, Rath CM, McDonald D, Knight R, Wang M, Dorrestein PC
bioRxiv. 2023. p. 2023.07.20.549584. doi:10.1101/2023.07.20.549584

4 **Open Access Repository-Scale Propagated Nearest Neighbor Suspect Spectral Library for Untargeted Metabolomics**
Bittremieux W, Avalon NE, Thomas SP, Kakhkhorov SA, Aksenov AA, Gomes PWP, Aceves CM, Caraballo-Rodríguez AM, Gauglitz JM, Gerwick WH, Huan T, Jarmusch AK, Kaddurah-Daouk RF, Kang KB, Kim HW, Kondić T, Mannochio-Russo H, Meehan MJ, Melnik AV, Nothias L-F, O'Donovan C, Panitchpakdi M, Petras D, **Schmid R**, Schymanski EL, van der Hooft JJJ, Weldon KC, Yang H, Xing S, Zemlin J, Wang M, Dorrestein PC
bioRxiv. 2023. p. 2022.05.15.490691. doi:10.1101/2022.05.15.490691

3 **The Underappreciated Diversity of Bile Acid Modifications**
Mohanty I, Mannochio-Russo H, El Abiead Y, Schweer JV, Bittremieux W, Xing S, **Schmid R**, Zuffa S, Vasquez F, Muti VB, Zemlin J, Tovar-Herrera OE, Moraïs S, Desai D, Amin S, Koo I, Turck CW, Mizrahi I, Huan T, Patterson AD, Siegel D, Hagey LR, Wang M, Aron AT, Dorrestein P
SSRN, 2023. doi:10.2139/ssrn.4436846

2 **A multi-omics strategy for the study of microbial metabolism: application to the human skin's microbiome**
Nothias L-F, **Schmid R**, Garlet A, Cameron H, Leoty-Okombi S, André-Frei V, Fuchs R, Dorrestein PC, Ternes P
bioRxiv. 2023. doi:10.1101/2023.03.26.532286

1 **Two-Dimensional Liquid Chromatography Tandem-Mass Spectrometry Untangles the Deep Metabolome of Marine Dissolved Organic Matter**
Lambidis SP, Schramm T, Steuer-Lodd K, Farrell S, Stincone P, **Schmid R**, Koester I, Torres R, Aluwihare L, Simon C, Petras D
ChemRxiv. 2023. doi:10.26434/chemrxiv-2023-j1bxh

## Book Chapters

1 **Processing Metabolomics and Proteomics Data with Open Software: A Practical Guide**
**Chapter 7: Metabolomics Data Analysis Using MZmine**
Pluskal T, Korf A, Smirnov A, **Schmid R**, Fallon TR, Du X, Weng J-K
Royal Society of Chemistry, 2020, pp. 232–254.

## Oral Presentations

(as presenting author)

19 **Computational Mass Spectrometry Europe Tour 2023: MS Basics, Data Processing, Compound Annotation, Automatic Spectral Library Generation, Molecular Networking, microbeMASST & MZmine**
**R. Schmid**, C. Brungs (Series of Invited Talks)
Technical University of Denmark, Copenhagen, Denmark (Prof. Tilmann Weber)
European Molecular Biology Laboratory (EMBL), Heidelberg, Germany (Prof. Michael Zimmermann)
University of Geneva, Geneva, Switzerland (Prof. Jean-Luc Wolfender)
Eidgenössische Technische Hochschule (ETH) Zürich, Zürich Switzerland (Prof. Nicola Zamboni)
Wageningen University and Research, Wageningen, Netherlands (Dr. Justin J.J. van der Hooft)

18 **Enriching Molecular Networks by repository-scale MS searches in microbe, plant, and food extracts**
**R. Schmid**, S. Zuffa, M. Wang, T. Pluskal, P. Dorrestein
(Invited Talk) DGMS young scientists fall meeting 2023, Hünfeld, Germany

17 **Metabolomics Data Processing and Compound Annotation in MZmine**
**R. Schmid**, S. Heuckeroth, C. Brungs, D. Petras, M. Ernst
(Invited Talk) 3nd International Summer School on non-targeted Metabolomics Data Mining for Biomedical Research 2023, Copenhagen, Denmark, recordings: YouTube

16 **Enriching Molecular Networks by repository-scale MS searches in microbe, plant, and food extracts**
**R. Schmid**, S. Zuffa, M. Wang, T. Pluskal, P. Dorrestein
(Selected Talk) ANAKON 2023, Vienna, Austria

15 **Introduction to Mass Spectrometry-based Metabolomics**
**R. Schmid**, M. M. Zdouc, J. J.J. van der Hooft
(Invited Talk) Workshop on Natural Product Genome & Metabolome Mining, Wageningen, Netherlands

14 **Non-target Mass Spectrometry Data Processing in MZmine**
**R. Schmid**, S. Heuckeroth, D. Petras
(Invited Talk) 2nd International Summer School on non-targeted Metabolomics 2022, Tübingen, Germany
Recordings: YouTube

13 **Ion Identity Molecular Networking for Mass Spectrometry-based Metabolomics**
**R. Schmid**, D. Petras, L-F. Nothias, M. Wang, T. Pluskal, U. Karst, P. Dorrestein
(Selected Talk) Metabolomics Conference 2022, Valencia, Spain

12 **Representing the team of MZmine, SIRIUS, and GNPS at the CASMI workshop**
**R. Schmid**
(Invited Talk) Metabolomics Conference 2022, Valencia, Spain

11 **Non-target Mass Spectrometry and Ion Mobility Workshop in MZmine**
**R. Schmid**, S. Heuckeroth, T. Pluskal, T. Damiani
(Invited Talk) Metabolomics Conference 2022, Valencia, Spain

10 **Non-target MS Feature Finding, MZmine 3 Hands-on**
**R. Schmid**
(Invited Talk) CMFI Mass Spec Seminar, 2022, Online
Recordings: YouTube

9 **Mass Spectrometry Data Processing and Molecular Networking using MZmine, GNPS, and SIRIUS**
**R. Schmid**, S. Heuckeroth, T. Pluskal, T. Damiani, K. Dührkop, D. Petras
(Invited Talk) Computational Metabolomics Workshop, 2021, Prague, Czechia

8 **Mass Spectrometry Imaging: Multimodal Approaches, workshop**
**R. Schmid**, A. Römpp
(Invited Talk) DGMS conference 2020, Münster, Germany

7 **New Developments for Small Molecule Identification using Open Source Software**
**R. Schmid**, D. Petras, L.-F. Nothias, M. Wang, B. Arndt, F. Hübner, H.-U. Humpf, P. Dorrestein, U. Karst
(Award Lecture) DGMS Young Scientist Award, DGMS conference 2020, Münster, Germany

6 **Identification of small molecules by combination of ion identity and $MS^2$ molecular networking**
**R. Schmid**, D. Petras, L.-F. Nothias, M. Wang, B. Arndt, F. Hübner, H.-U. Humpf, P. Dorrestein, U. Karst
(Selected Talk) DGMS young scientists fall meeting 2019, Hünfeld, Germany

5 **Feature-based Molecular Networking in MZmine and GNPS hands-on tutorial**
**R. Schmid**, D. Petras, T. Pluskal
(Invited Talk) Molecular networking using MZmine and GNPS workshop, 2019, MIT, Cambridge, USA

4 **Ion Identity Molecular Networking: Linking MZmine and GNPS**
**R. Schmid**, L.-F. Nothias, M. Wang, JJJ. van der Hooft, R. C. Menezes
(Invited Talk) Mass Spectrometry-based Metabolomics Workshop 2019, MBU CAS Prague, Czechia

3 **Identification of small molecules by combination of ion identity and $MS^2$ molecular networking**
**R. Schmid,** D. Petras, L.-F. Nothias, M. Wang, B. Arndt, F. Hübner, H.-U. Humpf, P. Dorrestein, U. Karst
(Selected Talk) DGMS conference 2019, Rostock, Germany

2 **Feature correlation for HPLC-HRMS improves the identification of different ion adducts, multimers and in-source fragments in molecular networking**
**R. Schmid**, D. Petras, L.-F. Nothias, M. Wang, B. Arndt, F. Hübner, H.-U. Humpf, P. Dorrestein, U. Karst
(Selected Talk) ANAKON 2019, Münster, Germany

1 **A new software solution for imaging analysis, visualization, and single particle analysis**
**R. Schmid**, P. Doble, U. Karst
(Selected Talk) $BIMS^2$ 2018, Münster, Germany

# Teaching and Mentoring

(Total 447 h)

### Mentoring

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| Since 2018 | Steffen Heuckeroth during his B.Sc., M.Sc., and PhD in Analytical Chemistry | |
| 2023 | Student at Google Summer of Code. Open-source project: MZmine (4 months) | |
| 2019 | Student at Google Summer of Code. Open-source project: MZmine (4 months) | |
| 2019 | Carina Wolf, B.Sc. Analytical Chemistry (8 weeks) | |
| 2018 | Valentin Göldner, B.Sc. Food Chemistry (8 weeks) | |
| 2018 – 2020 | Two visiting high school students and a chemistry class project | |

### Practical Lab Courses

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|---|---|---|
| 2019 | Group mentor in Advanced Analytical Chemistry Master Courses, University of Münster | 30 h |
| 2019 | Tutor in instrumental analytical chemistry practical courses, University of Münster | 60 h |
| 2018 | Group mentor in Advanced Analytical Chemistry Master Courses, University of Münster | 30 h |
| 2018 | Tutor in instrumental analytical chemistry practical courses, University of Münster | 60 h |
| 2014 | Tutor in instrumental analytical chemistry practical courses, University of Münster | 60 h |

### Seminars on Data Science and Coding

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|---|---|---|
| 2022 | University of California San Diego, USA | 2 h |
| 2017 – 2019 | Institute of Inorganic and Analytical Chemistry, University of Münster, Germany | 6 h |
| 2015 | University of Technology Sydney, Australia | 2 h |
| 2014 | Institute of Inorganic and Analytical Chemistry, University of Münster, Germany | 2 h |

### Workshops on Mass Spectrometry-based Metabolomics and Data Analysis

| | | |
|---|---|---|
| 2023 | 3rd Summer School on Non-Targeted Metabolomics Data Mining for Biomedical Research Statens Serum Institute (SSI), Copenhagen, Denmark, recordings: NTMSS2023 | 40 h |
| 2023 | Technical University of Denmark, Copenhagen, Denmark | 6 h |
| 2023 | European Molecular Biology Laboratory, Heidelberg, Germany | 6 h |
| 2023 | University of Geneva, Geneva, Switzerland | 6 h |
| 2023 | Eidgenössische Technische Hochschule (ETH) Zürich, Zürich, Switzerland | 6 h |
| 2023 | Wageningen University and Research, Wageningen, Netherlands | 4 h |
| 2023 | Workshop on Natural Product Genome and Metabolome Mining, Wageningen | 40 h |
| 2022 | 2nd International Summer School on Non-Targeted Metabolomics University of Tübingen, Tübingen, Germany, recordings: NTMSS2022 | 40 h |
| 2022 | CMFI Mass Spec Seminar, Online, recordings: CMFI | 1 h |
| 2021 | Institute of Organic Chemistry and Biochemistry CAS, Prague, Czechia | 16 h |
| 2020 | GNPS workshops, Online, recordings: YouTube | 2 h |
| 2019 | Whitehead Institute for Biomedical Research, MIT, Cambridge, USA | 8 h |
| 2019 | Institute of Microbiology of the Czech Academy of Sciences, Prague, Czechia | 6 h |
| 2017 – 2020 | Institute of Inorganic and Analytical Chemistry, University of Münster, Germany | 12 h |

**Workshop on Mass Spectrometry Imaging: Multimodal Approaches**

2020 DGMS conference 2020, Münster, Germany 2 h