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Main areas of research

Research activities focus on the comprehensive analysis of (bio)organic molecules (i.e. drugs, pharmaceuticals, industrial chemical, endogenous compounds, and metabolites thereof) in human and environmental specimens. The analytical method of choice is mass spectrometry (MS). In most cases, MS is hyphenated to chromatographic methods (liquid chromatography or gas chromatography). Research activities are indented to optimize the complete analytical process. These efforts include the optimization of chromatographic techniques, the improvement of the mass spectrometric detection of biomolecules, the perfecting of sample preparation procedures, and the advancement of data mining strategies. The developed analytical techniques find application in fields like human biomonitoring, environmental analysis, forensic analysis, wastewater-based epidemiology, metabolomics, diagnostics, and therapeutic drug monitoring.

Academic milestones and positions held to date

2022-	Professor for Metabolomics and Bioanalytical Mass Spectrometry at the Medical University of Innsbruck, Austria
2011-2021	Associate Professor at the Institute of Legal Medicine of the Medical University of Innsbruck, Austria
2011-	Scientific head of the Core Facility Metabolomics of the Medical University of Innsbruck, Austria
2008-	Leader of the "Bioanalytical Mass Spectrometry" group, Institute of Legal Medicine of the Medical University of Innsbruck, Austria
2007-	Venia Docendi of the Medical University of Innsbruck, Austria, for "Bioanalysis"
2003-2011	Senior researcher at the Institute of Legal Medicine of the Medical University of Innsbruck, Austria, by Prof. Dr. Richard Scheithauer
2002-2003	Postdoctoral fellow at the Institute of Instrumental Analysis and Bioanalysis, Saarland University, Saarbrücken, Germany
2000-2002	Research assistant at the Institute of Analytical Chemistry und Radiochemistry of the Leopold-Franzens-University Innsbruck, Austria
2002	PhD with distinction
1999-2002	PhD thesis at the Institute of Analytical Chemistry and Radiochemistry of the Leopold-Franzens-University Innsbruck, Austria
1999	MSc with distinction
1994-1999	Study of chemistry at the Leopold-Franzens-University Innsbruck, Austria

Publications (Ten most important regarding the research topic)

1. Reinstadler, V., Gutmann, R., Pitterl, F., Winkler, K., **Oberacher, H.*** Gas Chromatography – High-Temperature Proton-Transfer Reaction Mass Spectrometry as Novel Tool for Forensic Drug Testing. Separations, 9 (2022), 328.

2. Huber, C., Krauss, M., Reinstadler, V., Denicolò, S., Mayer, G., Schulze, T., Brack, W., **Oberacher, H.*** In-Silico Deconjugation of Glucuronide Conjugates Enhances Tandem Mass Spectra Library Annotation of Human Samples. *Analytical and Bioanalytical Chemistry*, 414 (2022), 2629-2640.
3. Reinstadler, V., Lierheimer, S., Boettcher, M., **Oberacher, H.*** A Validated Workflow for Drug Detection in Oral Fluid by Non-targeted Liquid Chromatography-Tandem Mass Spectrometry. *Analytical and Bioanalytical Chemistry*, 411 (2019), 867-876.
4. Arnhard, K., Gottschall, A., Pitterl, F., **Oberacher, H.*** Applying 'Sequential Windowed Acquisition of All Theoretical Fragment Ion Mass Spectra' (SWATH) for Systematic Toxicological Analysis with Liquid Chromatography – High-Resolution Tandem Mass Spectrometry. *Analytical and Bioanalytical Chemistry*, 407 (2015), 405-414.
5. Steger, J., Arnhard, K., Haslacher, S., Geiger, K., Singer, K., Schlapp, M., Pitterl, F., **Oberacher, H.*** Successful Adaption of a Forensic Toxicological Screening Workflow Employing Non-targeted Liquid Chromatography-Tandem Mass Spectrometry to Water Analysis. *Electrophoresis*, 37 (2016), 1085-1094.
6. **Oberacher, H.** Wiley Registry of Tandem Mass Spectral Data, MSforID. John Wiley & Sons, Hoboken, NJ, USA, ISBN: 978-1-1180-3744-7, 2011.
7. **Oberacher, H.***, Sasse, M., Antignac, J.-P., Guitton, Y., Debrauwer, L., Jamin, E. L., Schulze, T., Krauss, M., Covaci, A., Caballero-Casero, N., Rousseau, K., Damont, A., Fenaille, F., Lamoree, M., Schymanski, E. L.* A European Proposal for Quality Control and Quality Assurance of Tandem Mass Spectral Libraries. *Environmental Science Europe*, 32 (2020), 43.
8. **Oberacher, H.***, Reinstadler, V., Kreidl, M., Stravs, M. A., Hollender, J., Schymanski, E. L.* Annotating Non-targeted LC-HRMS/MS Data with Two Complementary Tandem Mass Spectral Libraries. *Metabolites*, 9 (2019), 3.
9. González-Mariño, I. and 70 coauthors Spatio-temporal Assessment of Illicit Drug Use at Large Scale: Evidence from Seven Years of International Wastewater Monitoring. *Addiction*, 115 (2020), 109-120.
10. van Nuijs, A. *, Lai, F. Y., Been, F., Andres-Costa, M. J., Barron, L., Baz-Lomba, J. A., Berset, J.-D., Benaglia, L., Bijlsma, L., Burgard, D., Castiglioni, S., Christophoridis, C., Covaci, A., de Voogt, P., Emke, E., Fatta-Kassinos, D., Fick, J., Hernandez, F., Gerber, C., González-Mariño, I., Grabic, R., Gunnar, T., Kannan, K., Karolak, S., Kasprzyk-Hordern, B., Kokot, Z., Krizman-Matasic, I., Li, A., Li, X., Löve, A. S. C., Lopez de Alda, M., Meyer, M. R., **Oberacher, H.**, O'Brien, J., Quintana, J. B., Reid, M., Schneider, S., Sadler Simoes, S., Thomaidis N. S., Thomas, K., Yargeau, V., Ort, C. Multi-year Interlaboratory Exercises for the Analysis of Illicit Drugs and Metabolites in Wastewater: Development of a Quality Control System. *Trends in Analytical Chemistry*, 103 (2018), 34-43.

Achievements (Ten most important)

- 144 papers in peer-reviewed journals (4045 citations, h-index 34) and 97 oral presentations.
- Another important scientific publication is the "Wiley Registry of Tandem Mass Spectral Data, MSforID", which represented one of the first tandem mass spectral libraries available for immediate application in NTS.
- Four patent applications.
- Ten research grants as PI or Co-I (H2020, COST, FWF, FFG, ÖNB, Tiroler Innovationsförderung) and several research projects with corporate partners (e.g. Applied Biosystems, Antex Leyden, Lipomed, Ionicon)
- Development and organization of the 'Core Facility Metabolomics' of the Medical University of Innsbruck. The CFM serves as an enabling resource for research and development programs with partners in and out of MUI. +1000 samples are analyzed per year.
- Supervisor of +40 students working on their MSc, PhD, or MSc thesis.

- Ten honors/awards including the Fachgruppenpreis der Fachgruppe Analytische Chemie der Gesellschaft Deutscher Chemiker (2003), the Austrian Life Science Award (2006), the Mattauch-Herzog Förderpreis der Deutschen Gesellschaft für Massenspektrometrie (2008), “Top 40 under 40” presented by “The Analytical Scientist” (2014).
- Ad hoc reviewer for 20+ journals including Analyst, Analytical and Bioanalytical Chemistry, Analytical Chemistry, Bioanalysis, Metabolites, Proteomics, International Journal of Mass Spectrometry, Rapid Communications in Mass Spectrometry, Trends in Analytical Chemistry.
- Selected memberships in academic societies: *Österreichische Plattform für Humanbiomonitoring*, *Austrian Society of Toxicology (ASTOX)*, *Austrian Society for Analytical Chemistry (ASAC)*, *Austrian Chemical Society (GOECH)*, *Gesellschaft für Toxikologische und Forensische Chemie (GTFCh)*.

Key cooperation partners for project-related research (<https://biomassspec.gmi.tirol/>)

(a) NTS for human biomonitoring

Maria Uhl and Sigrid Scharf, Environmental Agency Austria, Vienna, Austria
 Jean-Philippe Antignac, LABERCA, INRAE, Nantes, France
 Jana Klanova, RECETOX Centre, Masaryk University, Brno, Czech Republic
 Adrian Covaci, University of Antwerp, Belgium
 Laurent Debrauwer, TOXALIM, INRAE, Toulouse, France

(b) Tandem mass spectral libraries and bioinformatics

E. L. Schymanski, University of Luxembourg, Luxembourg
 Antony J. Williams, U.S. Environmental Protection Agency, Research Triangle Park, NC, USA
 Martin Krauss and Tobias Schulze, UFZ, Leipzig, Germany
 G. Whitley, B. Berger, John Wiley & Sons, Hoboken, NJ, USA

(c) Wastewater-based epidemiology

SCORE group - <https://score-cost.eu/>