

Report 2019-2021

Department of Chemistry

University of Natural Resources and Life Sciences, Vienna

Acknowledgements

Support in data collection and proof-reading by

Univ. Prof. Paul Kosma Ao. Univ. Prof. Paul Furtmüller and Dipl.-Ing. Hannelore Schopfhauser

is gratefully acknowledged.

Pictures were kindly provided by department members.

Imprint

Publisher Department of Chemistry University of Natural Resources and Life Sciences, Vienna Muthgasse 18 A-1190 Vienna Austria

www.chemie.boku.ac.at

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University of Natural Resources and Life Sciences, Vienna Department of Chemistry



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Preface

Continuing a tradition, the Department of Chemistry presents a triennial summary of its activities covering the years 2019-2021. This timeframe coincides with the corresponding period of the performance agreement ("Leistungsvereinbarung") of the University of Natural Resources and Life Sciences, Vienna (BOKU) with the Federal Ministry of Education, Science and Research (BMBWF).

Located in three buildings at two sites (Vienna and Tulln; respectively at the VIBT and UFT), approximately 110 persons in scientific, technical and administrative positions contribute to the excellent achievements of the department in research and teaching. The scientific areas are focused on the biotechnology of proteins, all aspects of glycobiology and glycochemistry, the chemistry of renewable materials and their application in bio-economy, and advanced analytical approaches such as ultratrace analysis and mass spectrometry-based fingerprinting for challenging applications. The high competence in modern analytical analysis and the impressive instrumentation completes the portfolio of our expertise. Our research areas fit well into the competence fields of the university and are highly recognized by the international scientific community. In this report, we present our research topics as well as an overview on our teaching portfolio and other activities that connect us with society.

The period 2019-2021 was very challenging for all staff members. Nevertheless, it was also characterised by successful acquisition of large projects and improvements in infrastructure. Our excellent performance was confirmed by a number of independent evaluations including an evaluation of the whole department, employee satisfaction survey, and the ISO45001 audit. The heads of two institutes retired (Paul Kosma, Organic Chemistry; Gerhard Stingeder, Analytical Chemistry) and we welcomed their successors Fabian Pfrengle and Stephan Hann in 2020 – all against the backdrop of a challenging surrounding with lockdowns, home office and restricted access to laboratories and facilities due to the SARS-CoV-2 pandemic situation.



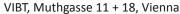
UFT, Konrad Lorenz Strasse 24, Tulln/Donau

Being a central unit for the theoretical and practical education in basic and advanced chemistry for nearly all bachelor and several master curricula of the university, the adequate supervision of students at bachelor, master and doctoral levels is of utmost importance to our staff. Therefore, during the first lockdown in early spring 2020, we adapted our teaching programmes from lab courses and lecture halls to Zoom sessions and online exams within few days. However, chemistry is a field for which hands-on experience is essential, so we switched back as soon as possible to practical courses in small groups, with appropriate distancing and wearing of masks.

Eager to return to regular research and teaching conditions, we will continue our high level of research and motivating a new generation of scientists to develop the broad field of chemistry with their curiosity and new ideas.

On behalf of the Department I want to thank all people and institutions of BOKU, cooperation partners and funding institutions for their continuous support and assistance.

A very big **THANK YOU** to all members of the Department! Our excellent performance in teaching and research is the product of many motivated and hard-working people. YOUR immense flexibility dealing with completely new situations, combined with friendly and patient interaction is the basis of our success.







Erika Staudacher Head of Department

For an online version of this document see <u>https://boku.ac.at/chemie/aktuelles/departmentreports</u>

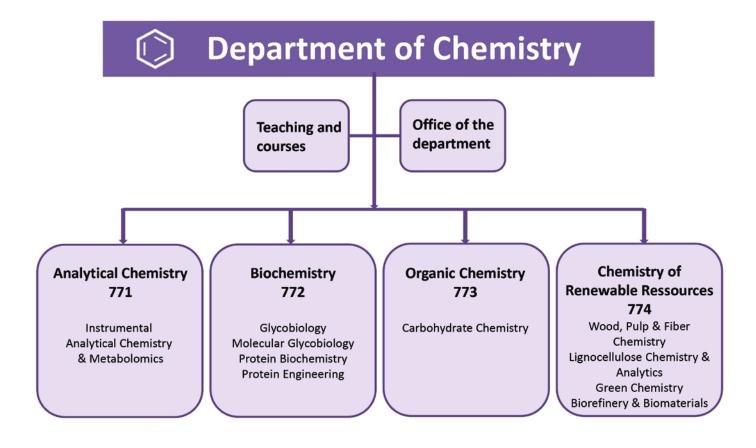
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Chapter 1 Mission Statement & Structure

The Department of Chemistry serves as a central unit in teaching basic and advanced chemistry within most curricula of the university. Research activities are focussed on the biotechnology of proteins and glycans, the chemistry of renewable materials and competence in state-of-the-art analytical instrumentation.



Personnel

* Names of persons who already left the department are printed in colour.

Head of Department

Ao. Univ. Prof. Dipl.-Ing. Dr. Erika Staudacher

Deputy Heads of the Department

Univ.Prof. Dipl.-Ing. Dr. Stephan Hann Univ.Prof. Dipl.-Chem. Dr. DDr. h.c. Thomas Rosenau

Full professors

- 771 Univ. Prof. Dipl.-Ing. Dr. Gerhard Stingeder (retired) Univ. Prof. Dipl.-Ing. Dr. Stephan Hann
- 772 Univ. Prof. Dipl.-Ing. Dr. Friedrich AltmannO.Univ. Prof. Dipl.-Ing. Dr. Dr.h.c. Leopold März (emer.)Univ. Prof. Mag. Dr. Christian Obinger
- 773 Univ. Prof. Dipl.-Ing. Dr. Paul Kosma (retired) Univ. Prof. Dipl.-Chem. Dr. Fabian Pfrengle
- 774 Univ. Prof. Dipl.-Chem. Dr. Antje Potthast Univ. Prof. Dipl.-Chem. Dr. DDr. h.c. Thomas Rosenau

Associate professors

- 771 Assoc. Prof. Dipl.-Ing. Dr. Stephan Hann (until 2020)
- 772 Ao.Univ.Prof. Dipl.-Ing. Dr. Paul G. Furtmüller Ao.Univ.Prof. Dipl.-Ing. Dr. Erika Staudacher Ao.Univ.Prof. Dr. Iain B.H. Wilson
- 773 Assoc. Prof. Dr. Alla Zamyatina
- 774 Assoc. Prof. Dipl.-Chem. Dr. Falk Liebner

Assistant professors and Senior Scientists

- Ass. Prof. BSc., Tim Causon, PhD Univ. Ass. Dr. David Cocovi Solberg Senior Scientist Mag. Dr. Elisabeth Fischer Univ. Ass. Dipl.-Ing. Dr. Zora Jandric Univ. Ass. Dr. Sven Kochmann Univ. Ass. Dipl. Ing. Dr. Teresa Steininger-Mairinger Univ. Ass. Dipl.-Ing. Dr. Anastassiya Tchaikovsky Senior Scientist Dipl.-Ing. Dr. Christine Troyer
- 772 Priv.Doz. Dipl.-Ing. Stefan Hofbauer, PhD Univ. Ass. Dipl.-Ing. Dr. Johannes Stadlmann Senior Scientist Dipl.-Ing. Dr. Michael Traxlmayr
- 773 Univ. Ass. Ignacio Jose Alvarez Martinez, MSc. Univ. Ass. Dipl.-Ing. Dr. Markus Blaukopf Ass. Prof. Dipl.-Ing. Dr. Andreas Hofinger-Horvath Univ. Ass. Irene Pasini, MSc. Univ. Ass. Dr. Colin Ruprecht
- 774 Senior Scientist Mag. Dr. Markus Bacher, part time Univ. Ass. Dr. Marco Beaumont, part time Senior Scientist Dipl.-Ing. Dr. Stefan Böhmdorfer Senior Scientist Mag. Dr. Hubert Hettegger

Senior Lecturers (770)

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- 772 Matthäus Böhm Ing. Thomas Dalik Rudolf Figl Daniel Maresch, BSc. Ing. Karin Polacsek Valeria Stefania Anja Wagner, MSc. Jakob Wallner, BSc.
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- 774 Christiane Gollner Daniel Kofi Owusu Dickson Dipl.-Ing. Dr. Sonja Schiehser Dipl.-Ing. Philipp Vejdovszky

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- 771 Maximilian Wrede
- 773 Helena Boulaxis
- 774 Tobias Dvorak

Assistant lecturers

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External Lecturers

Ao.Univ.Prof. Dipl.-Ing. Dr. Karl Stich Univ. Prof. Dipl.-Ing. Dr. Viktoria Weber Dr. Shi Yan, MSc.

Here we thank all the numerous colleagues from other departments for their contributions to our courses!

(Project) Personnel

771 Alexandra Bennett Dr. Martina Burnik-Sturm Univ. Ass. Dr. David Cocovi Solberg Hung Si Le, MSc. Max Lennart Feuerstein, MSc. Kaan Georg Kutlucinar, MSc. Barbara Mahlberg Miralem Mešić, BSc. Dipl.-Ing. Bernd Mitic Bernadette Moser, MSc. Dipl.-Ing. Lisa-Marie Petje Michael Santangeli, MSc. Michael Schober, BSc. Anna Urbanetz Dr. Younes Valadbeigi Dipl.-Ing. Lukas Zeh 772 Alex Alton, BSc. Alina-Sophie Destinger, Bakk.techn. Dipl.-Ing. Markus Dobersberger Zuzanna Dutkiewicz, MSc. Caroline Eigner, BSc. Dipl.-Ing. Dr. Margareta Furtmüller, part time Dipl.-Ing. Johannes Führer Dipl.-Ing. Thomas Gabler, BSc. Dipl.-Ing. Dr. Clemens Grünwald-Gruber Dipl.-Ing. Johannes Helm Dipl.-Ing. Dr. Alba Hykollari Jonatan Kendler, BSc. Urban Leitgeb, BSc. Elisabeth Lehner, BSc. Daniel Malzl Dipl.-Ing. Hanna Michlits, PhD Mara Mitstorfer, BSc. Dr. Reka Tünde Mócsai, MSc. Dipl.-Ing. Dr. Katharina Paschinger Gaurav Patil, MSc. Dipl.-Ing. Vera Pfanzagl, PhD Dipl.-Ing. Barbara Rothwangl-Eckmair, PhD Dr. Benjamin Salzer Dipl.-Ing. Irene Schaffner, PhD Dipl.-Ing. Daniel Schmidt Fabian Schubert, BSc. Lorenz Schwaiger, BSc. Jacqueline Seigner, MSc. Dipl.-Ing. Benjamin Sevcnikar, PhD Dipl.-Ing. David Stenitzer

Dipl.-Ing. Magdalena Teufl Julia Thoma, MSc. Nina Valente. BSc. Dr. Jorick Vanbeselaere Florian Wöls Dr. Shi Yan. MSc. Dipl.-Ing. Charlotte Zajc, PhD Dr. Marcel Zamocky Dipl.-Ing. Marilica Zemkollari 773 Aleksandra Arezina Matteo Cattin, MSc. Angela Del Prete, MSc. Dipl.-Ing. Dr. Philipp Gritsch Mag. Dr. Lukas Kerner Dipl.-Ing. Simon Krauter Dipl.-Ing. Charlie Lim Alessandro Monti, MSc. Marlene Neulinger Charlotte Olagnon, MSc. Uwe Osswald, MSc. Paul Pilwax Jakob Raffler, BSc. Brian Sachini, MSc. Sebastian Strobl, MSc. Dr. Nino Trattnig, MSc. Tomás Vasícek, MSc. Daniele Zucchetta, MSc. 774 Dr. Hassan Amer Mahmoud Hassan Abdelzaher Amer Stefano Barbini, MSc. Dipl.-Ing. Florian Bausch Elisabeth Billich, BSc. Dipl.-Ing. David Budischowsky Enkhjargal Budjav, MSc. Katharina Dorninger, BSc. Samira Galler, BSc. Patrick Geiger, BSc. Silvano Gollner Matthias Guggenberger, MSc. Takaaki Goto, MSc. Martin Grömmer Dr. Saida Ibragic Dipl.-Ing. Paul Jusner Hajar Khaliliyan, MSc. Dipl.-Ing. Nadine Kohlhuber Davood Kolahreez, MSc. Anna Florentina Lehrhofer, MSc. Markus Löcker, BSc. Maximilian Lubitz, BSc. Dr. Arianna Lucia Ivan Melikhov, MSc. Karolina Mlynarczyk, MSc. Dipl.-Ing. Oliver Musl Dipl.-Ing. Dr. Josua Timotheus Oberlerchner Dipl.-Ing. Dr. Sven Plappert Dimitrii Rusakov, MSc. Paulina Sacken Martin Schäfferling, BSc. Elisabeth Schaubmayr, BSc.



Anna-Maria Schnegg, BSc. Jonas Simon, MSc. Dr. Dev Sriranganadane Dr. Irina Sulaeva Dr. Ivan Sumerskii Dr. Otogontuul Tsetsgee Miriam Vogt, BSc. Laura Völkel, M.A. Tilmann Wohlgenannt, BSc. Dipl.-Ing. Gerhild Wurzer Mag. Natalia Yelavik Dr. Sara Zaccaron Johanna Zieher, BSc. Grigory Zinovyev, MSc.

INCOMING MOVERS



Colin Ruprecht obtained his PhD in 2011 at the Max Planck Institute of Molecular Plant Physiology in Potsdam. Working in Fabian Pfrengle's group on synthetic plant carbohydrates as a Postdoc, he joined the Department of Chemistry as a University Assistant in March 2020. His research focuses on enzymes involved in plant cell wall biosynthesis.

Some years ago **Johannes Stadlmann** obtained his PhD at BOKU. For more than 10 years he worked as a Postdoc at the Institute of Molecular Pathology in Vienna, the Analytical Development Division of Baxter and, finally, in Prof. Josef Penninger's laboratory at IMBA, where he focused on the development of novel glycoproteomics methodologies and computational tools to identify intact glycopeptides in complex biological samples. In 2020 he rejoined the Department of Chemistry and has recently accepted a tenure track position in the fields of glyco/proteomics. His research focuses on the development of mass spectrometric analysis platforms to explore complex protein modifications.





Teresa Steininger-Mairinger completed the master's degree programs "Analytical chemistry, food chemistry and environmental chemistry" and "Nutritional sciences, with focus on molecular nutrition" at the University of Vienna. In 2017, she completed her dissertation on "Mass spectrometry-based analysis of primary metabolites in ¹³C-based metabolic flux analysis experiments" at BOKU Vienna, followed by a Postdoc position under the supervision of Prof. Juliane Hollender at the Swiss Institute of Aquatic Science and Technology (Eawag). Since 2020, Dr. Steininger-Mairinger holds a tenure track position, where she is focusing on the development of advanced HRMS-based workflows for the investigation of chemicals of concern in the aquatic environment as well as fingerprinting for food authentication.

David Cocovi-Solberg completed his master's degree in Chemical Science and Technology at the University of the Balearic Islands (UIB) in 2012 and obtained his Doctor in Chemical Science and Technology at UIB with his thesis on "Real-time monitoring of bioaccessibility tests for solid samples using automatic flow methods". He was awarded an FWF Lise Meitner fellowship and started his research project at the Institute of Analytical Chemistry, BOKU in April 2019. In 2020 he successfully applied for a Senior Scientist position on "Miniaturization" at the Institute, where he is working on the design and implementation of new pump and valve prototypes to reduce the footprint of the benchtop instrumentation; his future project applications aim toward micro total analysis systems.



Anastassiya Tchaikovsky studied technical chemistry at the at the Technical University Vienna and obtained her master's degree in 2013. She performed her dissertation on "Strontium isotopic and elemental fingerprints as tools for source determination in aquatic ecosystems" from 2013 to 2019 at BOKU in cooperation with the Austrian Competence Centre for Feed and Food Quality, Safety and Innovation (FFoQSI). After a Postdoc time at the University of Vienna, she took up a position as lab head at Glock Health Science and Research GmbH before successfully applying for a Senior Scientist position on "Elemental analysis and isotope ratio analysis" at the Institute of Analytical Chemistry in autumn 2020. She is now performing research on the development, implementation and validation of analytical methods based on ICP-MS for accurate elemental and isotope amount ratio analysis.



NEW FULL PROFESSORS

Organic Chemistry – Fabian Pfrengle

2020 Professor for Organic Chemistry, BOKU, Vienna 2019 Habilitation (*venia docendi*) "Organic Chemistry" 2010 Dr. rer. nat. Freie Universität Berlin, Germany 2006 Dipl.-Chem. Freie Universität Berlin, Germany

Fabian Pfrengle joined the Department as Professor for Organic Chemistry and Head of the Institute of Organic Chemistry in March 2020. He obtained his PhD in synthetic organic chemistry from Freie Universität Berlin in 2010. Afterwards he joined the Scripps Research Institute in La Jolla (USA), where he worked on new methods to tolerize cells against specific antigens and thus dampen un-

wanted immune responses with the help of carbohydrate-decorated nanoparticles. In 2013 he started his independent career as a group leader at the Max Planck Institute of Colloids and Interfaces in Potsdam (Germany). Supported by an Emmy Noether grant of the German Research Foundation (DFG) his research group used chemical and enzymatic methods for the synthesis of glycans ranging in the size from oligo- to polysac-charides, with a particular focus on plant glycans. At BOKU he continues his studies on synthetic plant cell wall glycans as tools to investigate cell wall biosynthesis and plant immunity.

Analytical Chemistry – Stephan Hann

2020 Professor for Analytical Chemistry, BOKU, Vienna 2005 Habilitation (*venia docendi*) "Analytical Chemistry" 2001 Dr. techn. Technical University Vienna 1999 Dipl.-Ing. Technical University Vienna

Stephan Hann is Professor of Analytical Chemistry and Head of the Institute of Analytical Chemistry since October 2020. He obtained his PhD in analytical chemistry in 2001 from the Technical University of Vienna. In the same year he took a position as University Assistant at BOKU where he established his research group and obtained his Habilitation on the field of elemental speciation analysis in 2005. His main areas of research are separation sciences, elemental and



molecular mass spectrometry, environmental analysis, metabolomics, elemental ultra-trace and speciation analysis, authenticity of food and beverages as well as uncertainty of measurement. Prof. Hann has published more than 180 SCI-papers (h-index 42). He is head of the advisory board of the BOKU Core Facility Mass Spectrometry, PI and faculty member of the Doctoral School AgriGenomics, PI and associated faculty member of the PhD Program BioToP, key researcher of the Austrian COMET Centres "Centre of Industrial Biotechnology (acib)" and "Austrian Competence Centre for Feed and Food Quality (FFoQSI)". Additionally, Stephan Hann is board member of Austrian Society of Analytical Chemistry and an Austrian delegate in the Division of Chemistry and the Environment of the European Chemical Society.



OBITUARY FRANK MICHAEL UNGER



Frank Michael Unger - a long-term supporter of carbohydrate chemistry and biochemistry at the Department - passed away on 29th April 2019.

Frank M. Unger earned his PhD in 1968 at Georgetown University, Washington DC and after two years working in Experimental Cancer Research (Vienna) and Organic Chemistry (Basel) he became group leader at the former SANDOZ Research Institute in Vienna. In 1987 he left to work as vice director of research at Chembiomed and Biomira in Edmonton, Canada, before returning to Austria in 1993 as a guest professor at the Department (until 2000) and eventually as adjunct professor at the Department of Pharmaceutical Technology and Biopharmaceuticals, University of Vienna. Frank Unger has been a pioneer and mentor of carbohydrate chemistry in Austria and the Vienna region. He served as the first president of the European Carbohydrate Organization (ECO) and organizer of the first European Carbohydrate Symposium at BOKU together with Leopold März in 1981, which initiated the implementation and successful development of carbohydrate related research topics at the department.

RETIRED PROFESSORS

Paul Kosma, the former long-term head of the Department and Institute of Organic Chemistry retired in October 2019.

Paul Kosma has been key to the development of glycobiochemistry, glycochemistry and cellulose research at the department documented by one of the first Christian-Doppler Laboratories at BOKU (CDL of Pulp Reactivity), national representation of Austria in the European and International Carbohydrate Organizations and as organizer of conferences and workshops. He was also involved in the acquisition of advanced analytical infrastructure and new lab-space at the VIBT and UFT campus and the implementation of Thomas Rosenau as chair for wood-, pulp- and fibre chemistry. He has published > 280 SCI papers, 14 book chapters, 4 books and holds 14 patents. He was presented with the



Grand Decoration of Honour in Silver for Services to the Republic of Austria (2013) and the Austrian Cross of Honour for Science and Art (2018). His main research interests are in synthesis of complex oligosaccharides and neoglycoconjugates of biomedical importance, nucleotide-activated sugars and structural analysis of glycans by NMR spectroscopy.



Gerhard Stingeder was full professor of Analytical Chemistry and headed the Institute of Analytical Chemistry (former Division of Analytical Chemistry) from 1993 until 2020. From the beginning, he was organizing all teaching activities on general and analytical chemistry in the Bachelor programme *Food Science and Biotechnology*. Within this period, he introduced almost 10 000 students to the basic principles of chemistry. His research was focused on mass spectrometry developments and applications reflected in his 130 peer-reviewed publications. He also mentored four successful Habilitations (*venia docendi*), three of which have been appointed full professors of analytical chemistry at University of Vienna, Montanuniversität Leoben, and at BOKU in recent years. Gerhard Stingeder retired on Sept 30th, 2020 and is now fully occupied by supporting his family, in particular his three grandchildren.

Chapter 2 Institutes

Institute of Analytical Chemistry

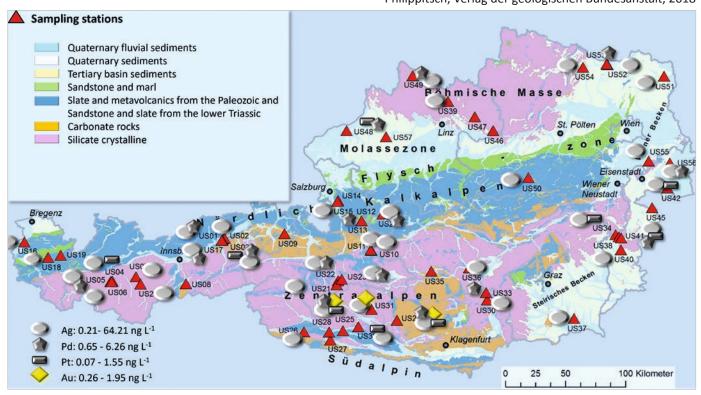
The scientific competencies of the Institute of Analytical Chemistry include elemental, isotope ratio, speciation and molecular analysis. Analytical methods and procedures with a focus on the combination of separation science with inorganic and molecular mass spectrometry are developed and refined for the research fields *of bio(techno)logy, environmental sciences and food sciences*. The overall goal is the development and implementation of new, fit-for-purpose analytical methodologies in interdisciplinary projects and collaborations. The Institute of Analytical Chemistry is equipped with high-end instrumentation for mass spectrometry and interacts with the Core Facility Mass Spectrometry on a scientific and administrative basis.

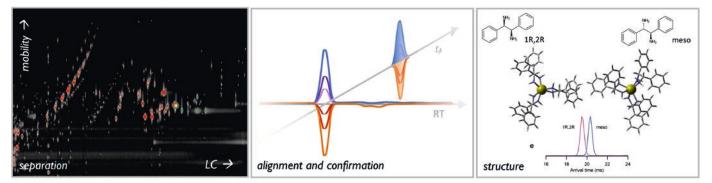
In the research field of **elemental analysis**, the group performs **elemental ultratrace analysis down to sub-ng** L^{-1} concentrations via ICP-MS in clean room laboratories targeting mainly surface water, ground water and seawater. Moreover, online separation techniques, i.e., HPLC, CE and GC are combined with ICP-MS for **elemental speciation analysis**.

Method development is implemented into a range of environmental projects (iron transport in the ocean, analysis of natural waters, platinum group elements and compounds), soil/plant research (root exudates, metal complexes in the rhizosphere, plant and microbial siderophores) and the field of metal/protein interactions.

Molecular mass spectrometry has been applied in the context of **metabolomics** for many years, particularly for biotechnology. Here, the institute strongly collaborates with the BOKU Department of Biotechnology and the COMET Centre Austrian Centre of Industrial Biotechnology (**acib**). Tandem mass spectrometry (LC-MS/MS and GC-MS/MS) is used for targeted quantification of primary metabolites and intermediates in biological systems (e.g., microbial cell factories). The emerging topic of ¹³C **metabolic flux analysis** has been a focus including method development for the measurement of accurate isotopologue and isotopomer ratios of selected metabolites in cell extracts including use of high resolution mass spectrometry (LC-HRMS and GC-HRMS). After calculation of isotopologue fractions, these data are transfer-

For the first time, concentrations of Ag, Pd, Pt and Au have been assessed by ultratrace analysis in highly mineralized groundwater sources in Austria. Source: D. Elster, L. Fischer, S. Hann, J. Goldbrunner, G. Schubert, R. Berka, G. Hobiger, P. Legerer & R. Philippitsch, Verlag der geologischen Bundesanstalt, 2018





Ion mobility-mass spectrometry is used for analytical and physical characterisation applications.

red to bioinformatic modelling of metabolic fluxes and for validation of pathway engineering; a highlight being the publication in *Nature Biotechnology* (Gassler et al., (2020), **38**, 210–216). Quantitative data are also generated using advanced quantification strategies based on elemental labelling or isotope dilution mass spectrometry. Two ongoing PhD projects on metabolomics in biotechnology at the institute are part of the FWF doctoral program **BioToP**.

New research on the behaviour of **anthropogenic pollutants in aquatic environments** has been recently started by Teresa Steininger-Mairinger. A focus will be placed on studying pharmaceuticals and personal care products and their respective transformation products in the water cycle. These transformation products can be of chemical and/or biological/microbial origin. Here, tools of metabolomics, including isotope tracer studies and non-targeted analysis, are going to be employed (<u>https://www.sciencedirect.com/science/article/pii/</u> <u>S0043135420312781</u>). In this context, the Institute of Analytical Chemistry is participating in the **NORMAN Network**, which is a platform enhancing the exchange of information and research strategies on emerging environmental substances.

A central research topic on advanced technologies is ion mobility-mass spectrometry, where the group obtained several research grants from Agilent Technologies (Santa Clara USA) and has performed research at the forefront of this emerging technology. Accurate determination of collision cross section (CCS) values, standardization of measurement, and new hardware supporting novel acquisition strategies such as ion mobility-quadrupole resolved all ions (IM-QRAI) are performed in collaboration with Dr. Ruwan Kurulugama. Tim Causon is well embedded in the research community of ion mobility-mass spectrometry in the context of application developments and fundamental studies including the FWF Lise Meitner project ("Ion Formation in Ion Mobility-Mass Spectrometry" with Dr. Younes Valadbeigi, Iran) that commenced in 2021.

Research into the field of **food authenticity and origin** is part of projects within the COMET Centre Austrian Competence Centre for Feed and Food Quality, Safety and Innovation (**FFoQSI**) using a broad combination of



Institute of Analytical Chemistry at BOKU VIBT.

different analytical techniques. Isotope ratio analysis of strontium by multi-collector ICP-MS, multielement analysis by ICP-MS and molecular fingerprinting by HRMS are combined utilizing sophisticated chemometric data analysis methods in order to assess the authenticity of different food and feed commodities. Similar analytical techniques and data analysis tools are applied in an FWF project in the field of rhizosphere research focused on the discovery of compounds responsible for belowground communication of plants, for example between cover crops and crop plants with the final aim to reduce the use of pesticides. Two PhD projects corresponding to the above-mentioned topics are performed within the BOKU doctoral school **Agrigenomics**.

HABILITATION: TIM CAUSON

Tim Causon completed his BSc (Hons) and PhD at the University of Tasmania (Australia) between 2005 and 2012. He then worked at the Johannes Kepler University Linz until 2014 including a Lise Meitner Fellowship. After joining BOKU in late 2014, he worked as Senior Scientist and later as Assistant Prof. at the Institute of Analytical Chemistry. His research has focused on separation sciences and mass spectrometry, particularly liquid chromatography-mass spectrometry and ion mobility-mass spectrometry. In addition to fundamental investigations with these techniques, analytical method development for quantitative metabolomics for biotechnology and related small molecule questions are a major focus. In December 2021 he held his Habilitation colloquium to obtain his *venia docendi* in the field of Analytical Chemistry.

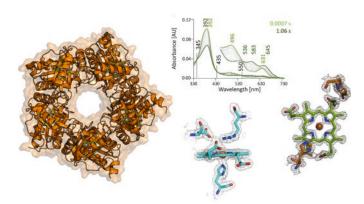


Institute of Biochemistry

The Institute of Biochemistry focuses on basic and applied research in the fields of **Protein Biochemistry** and **Glycobiology**. During 2019-2021 **18 FWF stand-alone projects**, a **Christian Doppler Laboratory for CAR-T cell engineering** and several other §27 projects have been conducted by members of this Institute.

The **Protein Biochemistry Group** (Christian Obinger, Paul Furtmüller, Michael Traxlmayr, Stefan Hofbauer) is active in two main fields:

(A) Bioinorganic chemistry and biochemistry of metal-containing oxidoreductases with a focus on heme enzymes like peroxidases, catalase-peroxidases, peroxidasins, chlorite dismutases and enzymes involved in bacterial heme biosynthesis (coproporphyrin ferrochelatases and coproheme decarboxylases). Typical research questions in this field of molecular enzymology include (i) structure-function relationships and (un)folding pathways of metal-containing oxidoreductases, (ii) kinetics and thermodynamics of electron transfer reactions, (iii) impact of the protein matrix and post-translational modifications of both the protein and/or the prosthetic group(s) on catalysis and (iv) elucidation of mechanisms of reactions mediated by these enzymes.

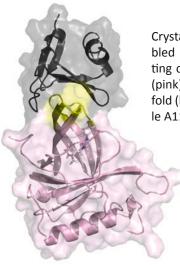


Structure-function relationship of enzymes are investigated with manifold biochemical and biophysical methods.

B) **Protein engineering and design** with a focus on the development of novel molecular tools for the construction of next generation CAR T cells. In particular, the group focuses on the design of molecular ON-switches, i.e. a system where the interaction between two proteins can be turned on by administering a small molecule. Furthermore, it has been demonstrated that this molecular ON-switch can be used to regulate the function of CAR T cells by adding the respective small molecule. This project has been performed in close collaboration with the Children's Cancer Research Institute (CCRI) and three patent applications have been filed based on this collaborative and interdisciplinary project. Moreover, the group engineer specific mini-binders, which can be used



as alternatives to antibodies, thereby enabling the specific detection and purification of endogenous proteins.



Crystal structure of the assembled ON-switch complex consisting of the human lipocalin RBP4 (pink), an engineered binder scaffold (black) and the small molecule A1120 (pink sticks).

Established methods and techniques in the Protein Biochemistry Group include recombinant protein production in *Escherichia coli, Pichia pastoris*, mammalian lines (HEK and CHO), site-directed mutagenesis, random mutagenesis and directed evolution strategies, protein library design, yeast display and screening of libraries by fluorescent activated cell sorting (FACS). Several biophysical methods are well established including (time-resolved) circular dichroism, fluorescence, UV-vis, FTIR- and resonance Raman spectroscopy, static light scattering, electron paramagnetic resonance spectroscopy, multimixing stopped-flow spectroscopy, spectro-electrochemistry (Ottle cell), differential scanning calorimetry and isothermal titration calorimetry.

Scientific highlights of the Protein Biochemistry Group include (i) the discovery of novel bacterial halogenating peroxidases with posttranslationally modified and co-

valently bound heme, (ii) elucidation of structure and function of pentameric and dimeric chlorite dismutases, (iii) characterization of the homotrimeric multidomain human enzyme peroxidasin, which represents an important player in the extracellular matrix formation; (iv) revealing the reaction mechanism of coproheme decarboxylase that catalyzes the key step in the coproporphyrin-dependent heme biosynthesis pathway of Grampositive bacteria and coproporphyrin ferrochelatase that is responsible for the penultimate step in this pathway; (v) development of protocols for the elucidation of the stability landscape and for stability engineering of proteins, and (vi) development of novel molecular ON-switches with improved properties compared to previously existing ones, and (vii) selection of mini-binders for the detection and purification of human peroxidasin.

The Glyco-bio-analysis and Molecular Glycobiology groups deal with the biosynthesis and biological role of protein-glycans from all kingdoms of life. Glycosylation of proteins is the most complex post-translational modification and its biological functions - the so called "glycocode" - remain to be fully deciphered. Oligosaccharides on secreted proteins differ by the number and position/linkage of several different sugar residues, which requires highly sophisticated analysis in the form of liquid chromatography and mass spectrometry. The Glyco-bio-analysis Group (Johannes Stadlmann, Erika Staudacher and Friedrich Altmann) operates an ion-trap with CID and ETD capability (Bruker, amaZone Speed ETD) plus the necessary nano- and capillary HPLC systems. More importantly, it is the scientific anchor of the proteomics part of the BOKU Core Facility Mass Spectrometry with its brand new Orbitrap Exploris top level mass spectrometer. This equipment allows tackling of an infinite variety of analytical problems such as protein identification via peptide mapping, characterization of pharmaceutically relevant of (glyco)-proteins, quantita-

HABILITATION: STEFAN HOFBAUER

Stefan Hofbauer finished his Master's in Biotechnology at BOKU in 2011 and graduated from the international doctoral school BioToP in 2014. From 2014 to 2016 he was a Post-Doc in the Max Perutz Labs affiliated with the University of Vienna. After rejoining the Institute of Biochemistry as an FWF-fellow in November of 2016, Stefan Hofbauer was employed as Univ. Ass. starting in February 2018. He investigates structure-function relationships of enzymes involved in the heme biosynthesis of Gram-positive bacteria, which are also promising targets in the quest to find highly needed novel antibiotic substances. In January 2021 he held his habilitation colloquium to obtain his *venia docendi* in the field of Molecular Enzymology.

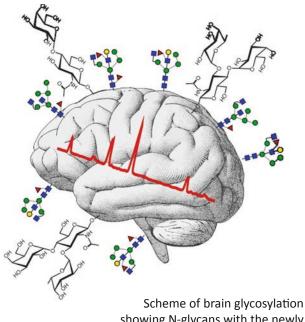


tive proteomics and – at the heart of the group's competence – isomer resolved N- and O-glycan analysis. To this end, reference glycans are synthesized using recombinant glycosyltransferases and stable isotope-labeled sugars. Separation of isobaric structures is achieved by chromatography on the unusual stationary phase graphitic carbon and glycans are characterized by retention time and negative mode fragmentation. Application of this novel methodology to brain N-glycans led to the discovery of structures that had so far escaped attention.

Relevant achievements evolved around the peculiar structure of protein-linked glycans of plants and insects, where a particular fucose residue (core-1,3-fucose) was identified as being immunogenic. This led – on the one hand - to the identification of the responsible enzyme and later on to the generation of "humanized" plants for the production of biopharmaceuticals by a BOKU partner group (Keyword: anti-Ebola antibody ZMAPP). In the field of allergy diagnosis - on the other hand – we could develop a strategy to minimize false-positive diagnostic results that are due to this fucose residue. This transitional research culminated in the foundation of the spin-off *Proglycan* in autumn 2021.

Given the variety of the roles of glycans in host-pathogen interactions, where sugars are receptors or defense shields against the host immune system, there is need for more research with "exotic" organisms. One focus of the group is protein glycosylation in snails (more exactly gastropods). Investigation of microalgae of the Chlorella clade revealed fundamental differences in the N-glycans of what was until now considered the same species. Apart from the discovery of many novel structural fea-

The Glyco-bio-analysis group



showing N-glycans with the newly discovered bisecting Lewis X determinants.

tures, the fact that apparently similar algal strains exhibit differences in N-glycan structures by far exceeding that observed for all land plants demands for a new consideration of microalgal species assignments. Microalgae are considered important tools for the development of a sustainable supply chain and thus reliable strain identification constitutes a vital step towards successful application of these organisms.

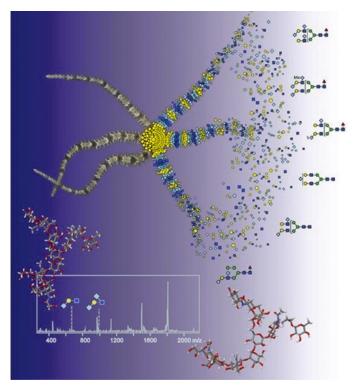
The **Molecular Glycobiology & Glycophylogeny Group** (headed by lain Wilson) encompasses the use of molecular biological, cell biological, enzymological and glycomic methods to understand the types, basis and import-

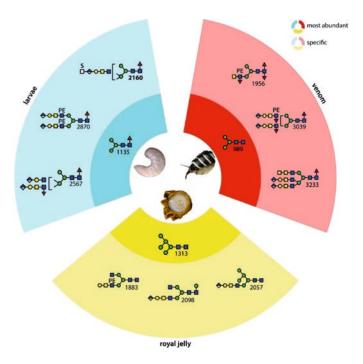


ance of glycoconjugates in a range of systems. The group is particularly interested in the **biosynthesis and developmental roles of protein glycosylation in various model organisms**, especially *Drosophila*, *Dictyostelium* and *Caenorhabditis*, as well as in various parasitic worms, fungi, molluscs and protists. Seeking parallels between model and parasitic organisms in addition to determining the unique nature of parasite glycomes constitute a major part of the work. In the last three years, this attracted international guests to our lab, Jaclyn Swan from Australia and Prof. Nicola Pohl, who both unfortunately had to leave early due to the COVID-19-related lockdown in 2020.

In order to uncover the "secrets" of these not so primitive organisms, knock-out strategies are utilized in order to study the effect of gene deletions on glycan biosynthesis and the resulting glycomes in model organisms. Thereby, a major focus is on N-glycomic analyses with HPLC, MALDI-TOF MS, MS/MS and chemical/enzymatic digestions; the group also has a tradition in glycoenzymology and, over the years, has identified unusual glycosidases and glycosyltransferases. The interactions of lectins (carbohydrate-binding proteins) and antibodies with glycans as exemplified by our approaches to generate non-mammalian glycan arrays. In this context, our ongoing collaboration with the Institute of Organic Chemistry is to be highlighted, as exemplified by joint publications (the latest in ACS Chemical Biology) and joint projects, in which array tools for detecting interactions between host proteins and parasite glycans are being developed.

Depiction of N-glycan diversity in the brittle star as defined by mass spectrometry (Eckmair *et al., J Biol Chem.* 2020, 295(10), 3173).





Depiction of N-glycan diversity in honeybee samples (*Hykollari* et al., *Mol Cell Proteomics*. 2018, 17(11), 2177 and *Hykollari* et al. Biochim Biophys Acta. 2019, 1863(11), 129409).

Also, our joint project with the Medical University of Vienna on Entamoeba involves development of a glycan array in addition to other methods.

Scientific highlights of the Wilson Group include recent publications in "top" journals, e.g. *Molecular & Cellular Proteomics, Journal of Biological Chemistry* and *Nature Communications* describing the isomeric and isobaric complexities of the protein-linked glycans of a range of organisms including nematodes, insects and echinoderms, including discovery of new N-glycan structures in bee venom.

In the past three years we have also written a number of commissioned reviews in top journals and our group is also the only one in Austria with contributions in the forthcoming fourth edition of the key textbook in the field – *Essentials of Glycobiology*. Another reflection of our group's strengths is that a number of new projects were funded in the last three years: four to our postdocs (Katharina Paschinger on bivalves, Alba Hykollari on flukes, Shi Yan on nematodes, Jorick Vanbeslaere on trichomonads) as well as two to Iain (an FWF grant and a WWTF joint with Alla Zamyatina from the Institute of Organic Chemistry on development of glycan arrays).

Glycans, biodiversity and climate change

Whether it be climate change or it be human activities, such as transport or exploitation, the geographic range of species can increase or decrease. In the past few years, we have analysed the glycomes of a broad range of species, so contributing to the overall understanding of the molecular aspects of glycobiology.

One example is our study on the canine heartworm, Dirofilaria immitis; with climate change, certain mosquitoes can now live in more temperate climates, which in turn, this contributes to the spread of certain diseases - one example being dirofilariasis. Dirofilaria requires Aedes mosquitoes as a vector and so it was of interest to find some parallels between the glycomes of the heartworm and its insect intermediate host; in particular, glucuronic acid was found in addition to other unique features on the N-glycans of Dirofilaria. Together with glycan array data showing recognition of immobilized native sugars with dog sera, lectins and pentraxins, our publication in Nature Communications suggests that the parasite's native sugar modifications mediate immunomodulation of the host and offer the ability to avoid host immune surveillance.

Another comparative glycomics study was the topic of two of our papers published back-to-back in the *Journal of Biological Chemistry*. While the brittle star is an invasive species, sea cucumbers are endangered due to their use in Asian cuisine. Furthermore, both are echinoderms, a group of organisms at the nexus between the invertebrates and vertebrates. Despite their relatedness, the anionic and neutral N-glycans of these two species were rather different, hinting that sugar chains may be responsible for reproductive isolation and speciation of these marine organisms. All these studies indicate the power of glycan analysis using off-line MALDI-TOF MS based on the accumulated experience of the postdoctoral FWF Fellows in the group.

The Molecular Glycobiology & Glycophylogeny Group





Institute of Organic Chemistry

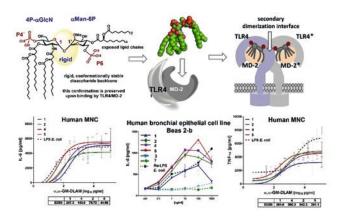
Research in the Institute of Organic Chemistry focuses on the chemical synthesis of carbohydrates and their application in the biomedical and agricultural sciences. One major research scheme is investigating the role of carbohydrates in eliciting or modulating the adaptive as well as the innate human immune response against pathogenic microorganisms. In particular we are interested in the immunochemistry and structural biology of complex carbohydrates from viruses, bacteria, parasites and plants. Bacterial cell-wall carbohydrates, termed lipopolysaccharides (endotoxins) from Gram-negative bacteria and secondary cell wall polysaccharides from Gram-positive ones are one of our main target molecules. A long-term goal is seen in the development of glycan-based tools for diagnostic and therapeutic applications such as novel antimicrobial and antisepsis drugs, e.g. by preparing biosynthetic intermediates as potent inhibitors that might interfere with the assembly of these cell-wall glycans. In addition, structurally conserved bacterial higher-carbon sugars and their biosynthetic precursors are key components in immune recognition, including antibodies, the innate immune response and lectin binding. A special emphasis is placed on creation of carbohydrate-based molecules able to upregulate cellular pro-inflammatory responses with potential application as safe vaccine adjuvants and immunotherapeutics.

A second research scheme is investigating plant cell wall glycan biosynthesis and plant immunity. Plant biomass, which is comprised of carbohydrate-rich plant cell walls, represents the most abundant renewable resource on Earth. Plant cell walls represent a cellular exoskeleton that provides mechanical support for growth and development of the plant. Oligosaccharide fragments of cell wall polysaccharides are valuable molecular tools for investigating structure and function of this complex matrix of biopolymers. They can serve as acceptor molecules for glycosyltransferases, substrates for glycosyl hydrolases, epitopes for antibodies and glycan binding modules, and as ligands for plant immune receptors. Despite the importance of such molecules, the availability of well-defined and pure oligosaccharide samples is very limited. We aim to chemically synthesize these oligosaccharide samples as well as nucleotide-activated sugars in order to advance the field of plant glycobiology. The long-term goal is to provide enabling knowledge for breading plants with improved material properties and resistance to pathogens.

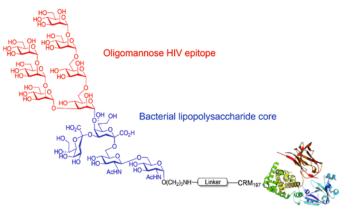
All these endeavors require basic studies of carbohydrate-protein interactions including antibodies, receptors and lectins on a molecular level using well-defined synthetic ligands and neoglycoconjugates. Key questions are investigated within national and international collaborations in the fields of crystallography, molecular biology, biochemistry, enzymology and immunobiology.



Group members of the Institute of Organic Chemistry (2020)



Tailored modulation of the TLR4-mediated pro-inflammatory cellular responses with synthetic glycolipids (Heine et al., Front Immunol. 2021, 12, 631797).



Structure of a neoglycoconjugate connected to an HIV-1-oligomannose epitope and a bacterial lipopolysaccharide subunit designed as inbuilt adjuvant (N.Trattnig et al., J. Am. Chem. Soc. 2019, 141, 7946).

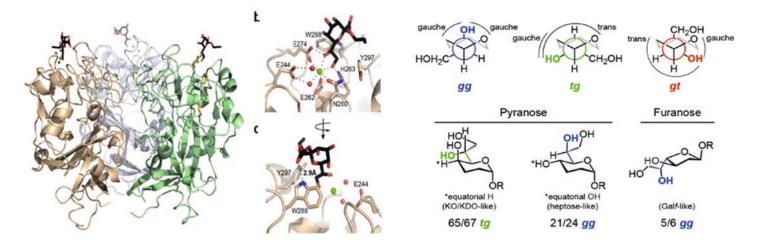
Highlights

Targeting innate immune receptors with synthetic glycan-based probes.

Using crystal structure-based design and advanced synthetic chemistry we created a set of versatile glycolipid probes for studying the structural basis for activation of mammalian innate immune receptors Toll-like receptor 4 (TLR4) and caspase-4/11. Our highly potent glycan-based immunostimulants with picomolar affinity for TLR4 could interact with a newly discovered cytosolic LPS-receptor caspase-4/11 and promote caspase-4/11 oligomerization while abolishing caspase-11 protease activity. Modulation of innate immune responses through controlled induction of the TLR4 signaling without triggering caspase-4/11 activation opens new perspectives in the development of safe vaccine adjuvants and immunotherapeutics.

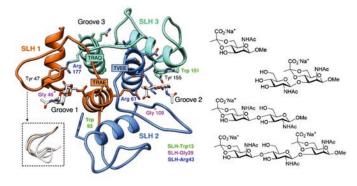
The expertise in Kdo chemistry has been used to assemble an undecasaccharide as a bacterial mimetic of HIV-1 oligomannose glycans for immunization studies. Additional oligomannoside constructs have been made and were shown to induce modest neutralizing anti-HIV-1 activities (J.-F. Bruxelle et al. Sci Rep. 2021, 11, 4637). Vaccine development based on these oligomannose epitopes, however, has to overcome their rapid degradation by mannosidases in serum (J.-F. Bruxelle et al. Sci Rep. 2020, 10, 7582).

Ligands and neoglycoconjugates containing D- and L-qlycero-D-manno-heptose, Kdo and D-glycero-D-talo-octulosonic acid (Ko) were used to prove that binding of these bacterial sugars to human intelectin-1 is governed by stereoelectronic effects induced by the side chain conformers of these higher-carbon sugars.



X-ray structure of Ko bound via a Ca²⁺ ion to human intelectin-1 (left) and side-chain conformers of bacterial sugars (C. M. McMahon et al., J. Am. Chem. Soc. 2020, 142, 2386).

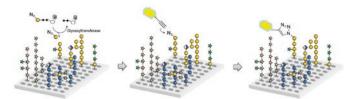




Dynamic cell surface protein anchoring by SLH domains explored by using synthetic substrates and SLH mutants. (R. Blackler, *et al. Nat Commun.* 2018, 9, 3120)

Plant glycan array-based characterization of plant glycosyltransferases

We have established a high-throughput assay for the identification and characterization of plant cell wall biosynthetic GTs based on the use of azido-functionalized sugar nucleotide donors on glycan microarrays that are equipped with synthetic cell wall oligosaccharides. Utilizing glycan microarray technology, the interactions of more than 100 different acceptor oligosaccharides with several enzymes and sugar nucleotide donors were investigated simultaneously on a single glass slide. Current efforts are directed at the synthesis of further donor and acceptor substrates to enable comprehensive screens for new plant GT activities.



Glycan array-based assay for the identification and characterization of plant GTs. The array is incubated with a chemically modified nucleotide sugar donor and a putative GT, followed by visualization of any transferred monosaccharide by an "on chip" reaction with an alkynyl-functionalized dye (C. Ruprecht *et al., Angew. Chem. Int. Ed.* 2020, 59 (30), 12493-12498).

Institute of Chemistry of Renewable Resources (NAWARO)

The Institute of Chemistry of Renewable Resources (NA-WARO) is concerned with the structure, identification, and chemistry of natural products. Having a background in synthetic and mechanistic organic chemistry, the research addresses current topics from the borderline region of natural product chemistry and organic, polymer, materials as well as analytical chemistry. The NAWARO group consists currently of approximately 35 members including BSc, Master, Ph.D. and visiting students, senior scientists, and lecturers.

The institute regards itself as one of the central units of BOKU for research in the fields of renewable resources and biorefineries. Originating as a result of the establishment of a chair of Wood, Pulp, and Fibre Chemistry in 2005 to the Institute of Organic Chemistry, the unit became a separate institute in 2012.

In recent years, the institute has developed into an internationally renowned centre for the chemistry of renewable resources, pulp & paper, and biorefinery chemistry. This is reflected by several indicators: the fact that the highest scientific awards in these fields were awarded on three occasions to group leaders of the institute – the Hayashi Jisuke International Cellulose Award in 2007 and again in 2012, as well as the Anselme Payen Award of the American Chemical Society in 2014. The integration into an extensive network of active international cooperations with leading institutions, and the involvement in the organization committees of the most important conference series in these fields: the International Symposium on Wood, Fiber and Pulping Chemistry [ISWFPC], the European Workshop on Lignocellulosics and Pulp (EWLP), the International Cellulose Conference (ICC) and the American Chemical Society meetings (ACS, CELL division).

The institute represents an attractive target for visiting scientists and visiting professors (30 and 16, respectively, staying for one semester or more over the past seven years). The institute's group leaders are active in the editorial boards of numerous relevant journals, and the heads are also engaged in prestigious advisory functions, such as the University Council of Shinshu University, Ja-

Bacterial secondary cell wall polysaccharides

A fruitful collaboration with the glyconanobiotechnology group of Christina Schäffer (Dept. Nanobiotechnology) has allowed the identification of pyruvylated ManNAc in a secondary cell wall polymer from *Paenibacillus alvei* as anchoring mechanism for surface-layer proteins. Moreover, the ManNAc unit is bound to two mutually exclusive binding grooves, thereby supporting dynamic changes during bacterial cell wall assembly and cell division. pan, the University Council of Aalto University, Helsinki, Finland, and the National Finnish Bioeconomy Council. In addition, the institute's research group leaders are very active in acquisition of research funding. They have acted as the academic head for the flagship project, Future Lignin and Pulp Processing Research (FLIPPR II, 2018-2021), and are the leading initiative in the Advanced Biorefinery Center Tulln (ABCT, 2018-2022). The ABCT combines basic research and applied sciences in the field of biorefineries, the chemistry of renewable raw materials, material sciences, new biomaterials, biotechnology, and analysis of biorefinery streams; and is closely linked to the ABCM (Advanced Biorefineries: Chemistry and Materials) Doctoral School, which has a special curriculum tailored to biorefinery topics. The institute is also involved in several international projects, e.g., FunEnzFibres funded by the ERA-NET Cofund ForestValue, and Grete Project, which has received funding from the Bio-based

Industries Joint Undertaking under the European Union's Horizon 2020 research and innovation program.

In regards to the scientific topics, the institute attempts to cover the field of chemistry of renewable resources and biorefineries as comprehensively as possible, which is also reflected in a considerable breadth of the research topics. The classical areas of cellulose chemistry, pulping and bleaching, paper and fibre chemistry, and analysis, as represented by the institute heads Thomas Rosenau and Antje Potthast, are well established and internationally well-regarded. The same applies to the fields of antioxidant and vitamin E chemistry; two vitamin E-based medications for the treatment of intestinal diseases have been approved for use in Europe and the US in 2009 and 2011. Since 2011, the fields of lignin chemistry, analysis, and utilization have been strengthened in

Institute of Chemistry of Renewable Resources (NAWARO) Group Retreat 2020 in St. Gilgen at Wolfgangsee, and beach group logo acquired during the International Conference on Renewable Resources and Biorefineries (RRB) in Aveiro, Portugal (2021).





order to keep up with international developments and to complement the well-established cellulose research performed at the institute.

The research area "Biopolymer and Paper Analytics" (Antje Potthast) covers the whole range of analytical issues related to lignocelluloses and polysaccharides. This includes both the application of established analytical tools to different species and tasks as well as the development of new analytical methodologies for modern lignocellulose science. Size-exclusion chromatography (SEC) with multiple methods of detection is the central tool in this endeavour, running on independent lines for routine analysis and special analytical tasks, respectively. SEC is combined with different fluorescence labelling techniques that allow recording of functional groups, substituents, or special moieties not only as sum parameters, but as profiles along with the molar mass distribution. These methods are apt for monitoring oxidative changes in cellulosic substrates occurring as a consequence of processing, environmental stress, or aging. Research on lignin focuses on the development of fast analytical tools to characterize natural and technical lignins in order to support questions related to quality and function-property relationships. High-throughput purification and model compound studies are equally important in that context.

Conversion of the renewable biopolymers cellulose, hemicellulose, and lignin into novel value-added products is the focus of the research area "Biomaterials Chemistry" (Falk Liebner). Non-energetic utilization of lignin encompasses projects such as the conversion of technical lignins or ligneous raw materials into environmentally friendly humus substitutes or water-storing hydrogels which can be used for large-scale rehabilitation of degraded soils. Chemical activation and fixation of carbon dioxide by different systems, among them lignoid structures and quinones, are also studied. Research in the field of cellulose modification is dedicated to the synthesis of ultralight-weight cellulose aerogels in different application scenarios, such as bone replacement materials or true volumetric displays. Advanced techniques in chemical engineering, such as supercritical drying, ultrasonic activation, or micro-wave-mediated derivatization are employed.

Two additional Junior working groups are part of the Institute of Chemistry of Renewable Resources, led by Stefan Böhmdorfer and Hubert Hettegger.

The research area "Biorefinery Analytics" (Stefan Böhmdorfer) is concerned with the chemical characterization of plant biomass, especially in complex mixtures as they are formed in biorefinery approaches. Plant biomass is a particularly complex mixture of a broad range of compounds with very heterogeneous properties.

Therefore, specialized methods have to be developed for each analytical problem. When current technologies are insufficient to answer the question, methods need to be developed further. The focus lies, in this regard, on high-performance thin-layer chromatography hyphenated to mass spectrometry (HPTLC-MS), bioactivity screening on HPTLC plates, or selective fluorescence labelling. Exemplary sample materials include extracts from leaves and bark, essential oils, mono- and oligosaccharides, non-cellulosic polysaccharides, secondary metabolites of plants and fungi, and natural antioxidants.

The group "Hybrid Materials and Green Chemistry" (Hubert Hettegger) is mainly concerned with the production of materials made up both of organic and inorganic components for applications in material science and analytical chemistry. A special focus is placed on chiral stationary phases (CSP) for enantiomer separation, based on silica gel as the carrier matrix and different polysaccharide derivatives as chiral selectors. Further key aspects are the development of sustainable and resource-saving reactions and processes and the molecular mechanisms of aging processes of lignocellulosic materials.

Recent cover stories from publication in 2020-2021 in the toptier journals: Small, ACS Sustainable Chemistry & Engineering, ChemSusChem and Journal of the American Chemical Society.



Chapter 3 Flagship projects

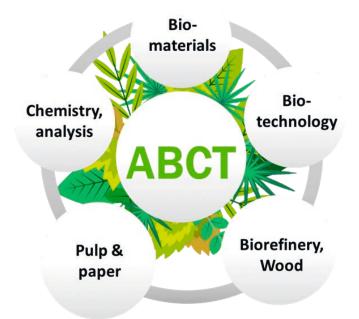
Austrian Biorefinery Center Tulln

The Austrian Biorefinery Center Tulln (ABCT) is dedicated to scientific excellence and research on an internationally competitive level, based on the leading positions of the involved research units. It bundles fundamental and applied research in the fields of biorefineries, the chemistry of renewable resources, biomaterials, and analysis of biorefinery streams.

The ABCT is designed as a leading international center on fundamental and applied research in the field of biorefineries and chemistry of renewable resources, deriving from the renowned expertise of the participating research institutes and the concentration of expertise and industrial cooperation at the Tulln location. In terms of research organization, the ABCT is based on the model of Christian Doppler laboratories. This combines training at the dissertation level with industry-related basic research.

The ABCT is linked to the doctoral school ABC&M ("Advanced Biorefineries: Chemistry and Materials" see Chapter 4). The long-term education of outstanding scientists is seen as the most important "export product" of the ABCT/ABC&M twin. BOKU is the first university to offer this tight pairing of research and PhD education in the biorefinery field. Research, excellence and innovation can only succeed if top research and PhD training at an international level go hand in hand.

The planning of the ABCT began in 2015 at the Institute of Chemistry of Renewable Resources at the UFT during the phasing-out of the Christian-Doppler laboratory "Advanced Cellulose Chemistry and Analysis" with continuing great interest of the company partners in long-term and fundamental research. At the same time, the BOKU Bioeconomy/Biorefinery Evaluation (2016) was concluded, with the recommendation of the international experts to further bundle and expand the existing concentration of expertise at the Tulln site into a lighthouse project.



The ABCT is headed by Prof. Thomas Rosenau and Prof. Antje Potthast from the Institute of Chemistry of Renewable Resources (Department of Chemistry). Collaborating faculty members are Dr. Stefan Böhmdorfer from the same research unit, as well as researchers from the Department of Materials Science and Process Technology (Prof. Wolfgang Gindl-Altmutter, Assoc.Prof. Ulrich Müller) and the Department IFA Tulln (Prof. Georg Gübitz).

The partner companies of the ABCT comprise local SMEs as well as big national and international players in the field of chemistry, renewable resources, textiles, and sustainable processing. The ABCT is

supported by equal matching funds from BOKU and the participating institutes, the partner companies, and the province of Lower Austria. Sappi Lenzing Austropapier Sappi Lenzing Austropapier Concord Clanzstoff El Weitzer



FLIPPR II – Future Lignin and Pulp Processing Research

Products made from renewable resources carry the potential to solve pressing global problems in the field of climate change and fossil resource utilization. The pulp and paper industry - as one of the main industries of Austria and the major user of wood as the most important renewable resource - is playing a key role in this regard.

The collaboration between BOKU (Department of Chemistry, Institute of Chemistry of Renewable Resources), Graz University of Technology (Institute of Paper and Pulp Technology) and the University of Graz (Wegener Institute) and the four largest cellulosic pulp producers in Austria, Mondi, Sappi, Heinzel Pulp (Zellstoff Pöls) and Norske Skoog, started in 2018 its second four-year project phase ("FLIPPR II").

The project develops the scientific basis of optimized material use for novel cellulose and lignin products based on wood according to different pulping processes. With the Institute of Chemistry of Renewable Resources as the academic lead, the project brings together industrial partners - and even competitors - in a concerted effort to tackle fundamental tasks regarding the "classical" products, pulp and fibers, and to find new utilization ways for the hitherto neglected second major product of wood biorefineries, the technical lignins. This, however, requires major analytical efforts before meaningful utilization paths can be taken.



EPNOE – European Polysaccharide Network of **Excellence**



Network Of Excellence

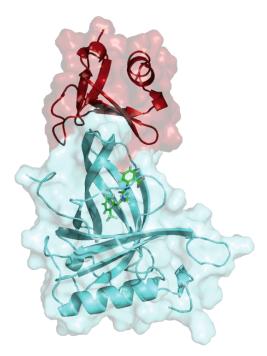
Polysaccharides, such as cellulose and starch as the most well-known ones, are fully biodegradable and renewable raw materials produced by nature on a large scale (1000 times the amount of synthetic polymers). To organize and integrate the European scientific community to promote the use of these materials as industry feedstocks for the manufacturing of advanced multifunctional materials is the mission of the European Polysaccharide Network of Excellence (EPNOE). Applications of these materials pertain to the pulp and paper industries, fibers, textiles, construction, and packaging materials as well as to hygiene and medical fields.

The network started in 2005, funded by the European Commission within the thematic priority "Nanotechnologies and Nanosciences-Multifunctional Materials, Processes and Production" of the Network of Excellence initiative, with a consortium of 17 European research groups from 9 different countries, including the Institute of Chemistry of Renewables Resources at BOKU. Since 2010, the network has been transformed into an Association with 32 academic groups and 10 international company partners.

CD Laboratory for Next Generation CAR T Cells

T cells that are genetically modified to express chimeric antigen receptors (CAR T cells) are among the most promising approaches in cancer immunotherapy. Briefly, the synthetic CAR receptor redirects human T cells to recognize and kill cancer cells. A huge advantage of this therapeutic approach is the ability of the CAR T cells to proliferate and to persist in the patient for long time (i.e., up to years). However, this persistence and expansion of CAR T cells *in vivo* is also associated with a drawback, i.e., the poor controllability of this therapeutic product after administration to the patient.

In this CD Laboratory, which is a joint project together with the St. Anna Children's Cancer Research Institute (CCRI) and Miltenyi Biotec, we develop molecular ONswitches to be able to regulate CAR T cell activity in vivo using small molecule drugs. First proof-of-principle data have already been published in top ranking journals (Zajc et al., *PNAS* 2020; Salzer et *al.*, *Nature Communications* 2020) and we have also filed three patent applications covering these novel technologies.



X-ray structure of a molecular ON-switch consisting of human retinol binding protein 4 (hRBP4, cyan), an engineered binder (red) and the small molecule drug A1120 (green). In this switch, addition of the drug A1120 triggers the protein-protein interaction between hRBP4 and the engineered binder.

Feed and Food Quality Safety and Innovation (FFoQSI) - COMET-K1 competence center



The COMET-K1 competence centre FFoQSI was funded by the Austrian ministries BMVIT, BMDW and the provinces Lower Austria, Upper Austria and Vienna within the scope of COMET - Competence Centers for Excellent Technologies operated through the Austrian Research Promotion Agency FFG.

The BOKU, the University of Veterinary Medicine and the Fachhochschule Wels are the scientific partners. The Research Program of Areas 1 and 2 was jointly developed by industry and science and covers selected topics along the value chain of plant food and food (green value chain) and animal food (red value chain) with a focus on sustainable improvements in production. Area 3 (blue area) involves strategic research and is an innovation platform for technology development, wherein the Institute of Analytical Chemistry has been a major contributor.

The research of the Institute of Analytical Chemistry within FFoQSI primarily deals with the determination of origin and authenticity of primary agricultural products (e.g. vegetables, meat and fish) by using a combination of multi-elemental, isotopic and molecular fingerprinting methods. During the last years, especially with the second period starting in 2020, the portfolio and expertise has been expanded to molecular fingerprinting and spectroscopic methods, as well as to advanced chemometric and data fusion strategies.



Global Center of Excellence (GCoE) Fiber Science

The Global Center of Excellence in Fiber Science (GCo-EFS) is a network of scientifically leading academic institutions in this field headed by Shinshu University, Japan. The selection of the members is highly competitive and takes place in a three-stage international expert procedure.

European partners are the Institute for Textile and Fiber Research Stuttgart-Denkendorf (D), the School of Textiles/Manchester University (UK), and the BOKU, Institute of Chemistry of Renewable Resources. The BOKU division covers the field of chemistry of cellulosic fibers. In addition to the training and exchange of scientists, strategic research, and the transfer of research results into industrial practice, the international networking of research institutions through joint scientific activities is one of the main goals of the Center of Excellence. In the first funding phase that concluded in 2020, joint projects in the field of intelligent cellulosic fibers and textiles (e.g. products with electrical conductivity, controlled release of active substances, or photoelectroactivity) are underway.

Apart from the GCoE, BOKU and Shinshu University are linked by a general Memorandum of Understanding which is much more than just a piece of paper. It has al-

ready been renewed for the third time and has produced a lively exchange of students and staff on all levels. In the framework of the GCoE, the Japanese Ministry of Science and Academy of Science has approved the doctorate school "Global Leader Program for Fiber Renaissance" for a period of 10 years, which accepts 10 Japanese and international candidates per year, thus enabling the education of 100 scientists in different fields of modern fiber science. The Institute of Chemistry of Renewable Resources at BOKU is responsible for the education in the field of cellulosic fibers within the doctorate school's curriculum. Since commencing in 2012, annual excursions of the Japanese PhD students have been organized with the help of BOKU International Relations (BOKU-IR) and include a stay at BOKU for 2 weeks, filled with lectures, visits to two companies, and workshops.

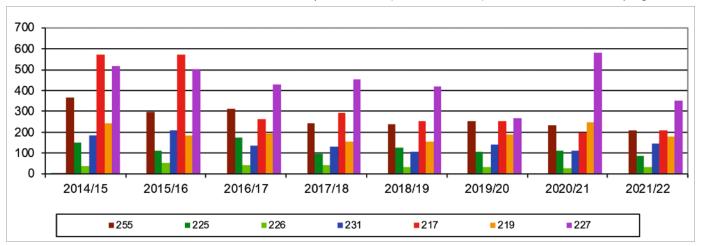
The lectures are presented by group leaders from BOKU and Shinshu University and are also open to PhD students from BOKU and Shinshu University. Apart from the scientific aspects, cultural and social experiences are also a mainstay of the excursions, and quite some personal friendship between BOKU and Shinshu students has resulted from these visits over the years.



Chapter 4 Teaching

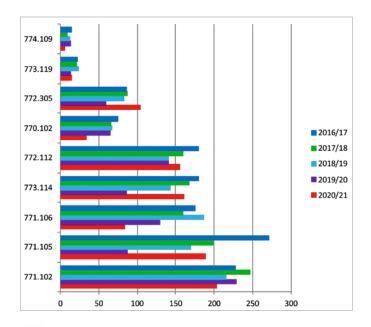
Bachelor and master programmes

The Department offers compulsory courses in 6 out of 7 bachelor study programmes of BOKU: *Food Science & Biotechnology* (217), *Forestry* (225), *Wood & Fibre Technology* (226), *Environment and Bioresources* Management (227), Environmental Engineering (231) and Agricultural Sciences (255). Only the bachelor programme Landscape Architecture & Landscape Planning (219) does not involve courses in chemistry.



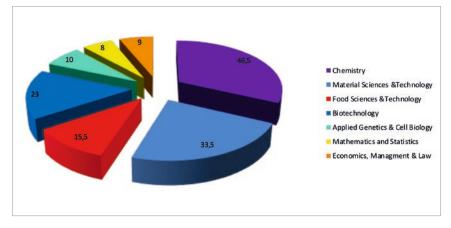
Number of first-year students (winter semester) in the different bachelor programmes.

BOKU is an attractive university which has observed an increasing number of students during the last decade. This was particularly seen for the student numbers of the bachelor programme *Food Science & Biotechnology*, where the department is responsible for about one third of the total curriculum, which increased dramatically during the years 2014 and 2015. This was (and remains) a challenge in the laboratory courses in terms of space, equipment, and supervision capacity. Due to restrictions on the number of students, the situation has somewhat returned to manageable levels since 2016. However, still many laboratory courses need to run in multiple parallel groups which have to be jointly scheduled with courses of the Department of Biotechnology and the Department of Applied Genetics & Cell Biology in order to optimise the use of facilities and limit the time demand on students.





Number of participants in laboratory courses of the department. 771 102 Einführung in die Chemie Übungen, 771 105 Analytische Chemie Übungen, 771 106 Instrumentelle Analytische und Physikalische Chemie Übungen, 773 114 Organische Chemie Übungen, 772 112 Biochemie Übungen I, 770 102 Chemische Übungen (Agrarwissenschaften), 772 305 Practical course in biochemistry II, 773 119 Chemische Übungen, 774 109 Chemie NAWAROS.



Bachelor programme *Food Science & Biotechnology*. Compulsory courses (in ECTS) offered by BOKU- departments.

BACHELOR THESES COMPLETED

2019

CERNY Angelika, FALB Nikolaus, FASCHINGEDER Felix Oliver, FEURSTEIN Gabriela Julia, FIGL Rudolf, HORAK Sophia, HÜLSNER Katharina Marie, HUMMEL Ferdinand, ICKA ARAKI Noah, KILLINGER Jennifer, LUNZER Katharina, MAGENBAUER Verena, MAYER Jasmin Sharon, OBERREITER, Samuel Pascal Christian, PACHSCHWÖLL Paul, SCHMIDT Katharina, SEEBER Angelika, SZIKORA Tanja, WEBHOFER Katharina Johanna, WINTER Martina Christine, WOKUREK Carina

2020

DORFNER Simon Philipp, GRÖSSING Philip Samuel, HEVES Gergely, HUBER Saskia, KLAMBAUER Jakob, KLAMING Kristin, PARZER Bianca, PERTILLER Matthias Bernhard, PFAFFENEDER Katharina (FH-Krems), RAUSCH Lisa (FH-Krems), STROHMAIER Anika, TAMGUE CHRAKRO.OH Tasha (FH-Krems), TEUBL Marcel, TIMMEL Philipp, URBANETZ Anna, WILD Isabella

2021

ALCARVA-PONTES Cristiana (FH-Krems), AUSSERER Magdalena, FRÖHLICH Flavia (FH-Krems), GISMONDI Alexander (FH-Krems), GUO Wei (FH-Krems), HAMZIC Alan (FH-Krems), KELZ Theres (FH-Krems), KREITSCHITZ Nadja, MEŠIĆ Miralem, NEULINGER Marlene, OBETZHAUSER Elena, PANZENBÖCK Richard, PILWAX Paul, RINDERER Dominik, SAILER Klara, SCHWARZ Laetitia (FH-Krems), SUPPARITSCH Stephanie, STAMPFL Karina Elena, TERZER Filipp, UNTERLEITNER Katja, VRABLICZ Patrick (FH-Krems), WÖLS Florian, ZOBERNIG Max

On master level compulsory and elective courses are offered in the programmes *Biotechnology* (418) and *Material & Energetic Exploitation of Renewable Raw Materials* (471) and elective courses in *Natural Resources Management & Ecological Engineering* (416), *Wood Technology & Management* (426), *Environmental Sciences – Soil, Water & Biodiversity* (449) and *Food Science & Technology* (417). The courses cover characterisation (structure and functionality of bioproducts) as well as an introduction into bioanalytical techniques (biospectroscopy, NMR, mass spectrometry, GPC of biopolymers). Students doing their master thesis at the department are integrated into scientific projects and learn – alongside specific methods and background of the topic – the framework of research and the basics how to run a laboratory.



In total the department offers 70 different courses, which account for 180 semester hours (one semester hour = one hour per week during the whole semester of approximately 14 weeks). Some of the courses are held in winter as well as in summer semester, some of the courses (nearly all laboratory courses) need to be held in

several parallel groups which results in a teaching load of approximately 320 semester hours. 39 (112 semester hours) courses are held in English.

For detailed information on the courses offered by the department see appendix D.

MASTER THESES COMPLETED

2019

BUDISCHOWSKY David – Ozone bleaching of cellulosic chromophores.

DOBERSBERGER Markus - Regulating the function of chimeric antigen receptor (CAR) T cells by small molecules.

GABLER Thomas - The forge of the tetrapyrrole to rule them all - Biochemical characterisation of Coproheme Decarboxylase from *Listeria monocytogenes*.

HELM Johannes - Biochemical and biophysical characterization of coproporphyrin ferrochelatase from *Listeria monocytogenes*.

JAHN Elisabeth – Cellulose/Silica Nanocomposites.

LEDERMÜLLER Sebastian – Screening of small compounds for improving the safety of Chimeric Antigen Receptors.

MOSER Bernadette - Online matrix separation/preconcentration of selected technology critical and hazardous elements in natural waters by ICP-SFMS (University of Vienna)

SCHWAIGER Lorenz – A novel role for the B-type dyedecolourising peroxidase in the Kef-system in E. coli.

SELINGER Julian – Waste chicken feathers as raw material for carbon fibers.

STENITZER David – Purification and characterisation of β -galactosidases from molluscs.

TARNOCZI Nicole - Higher complexes of the pneumococcal PsrP-BR domain with extracellular DNA and their function in shaping biofilm structures.

WURZER Gerhild Katharina – Cellulose containing materials for the purification of virus-like particles and proteins.

2020

DORNINGER Katharina – Chemometric models for the analysis of kraft lignin.

GEIGER Patrick – Chemical and mechanical analysis of Danubian Myriophyllum spicatum.

GOLD Lukas – Screening for drug resistance and activation mutations EGFR using mammalian cell surface display.

KOHLHUBER Nadine – Preparation of thermally super-insulating Celllulose I Aerogels: up-scaling and optimization.

PETJE Lisa-Marie – Impact of iron on allergic sensitization.

SCHAUBMAYR Elisabeth – Succinylated nanocellulose for application in silica composites.

SCHÖBER Michael - Exploiting avidity in chimeric antigen receptors (CARs) to increase safety and specificity of CAR T cell therapy.

2021

ALTON Alex – Development of an assay for reducing non-specific binding of engineered proteins.

HARTLMAYR David Nikolaus – Process optimization of sub μ L cellular digests towards single cell proteomics.

MITSTORFER Mara – Elucidating of biochemical parameters of scFvs influencing tonic CAR signalling.

SCHACHINGER Tobias – Quantification of factor VIII antigens bioencapsulated in lettuce cells for oral tolerance induction in hemophilia A patients.

SCHOBER Michael – Species specific sulfur isotope amount ratios of sulfur-containing amino acids using HPLC and MC ICP-MS (TU Vienna)

SCHUSTER Christian – Quantifizierung von Lignin in Kochlaugen.

SIPOS Timea – Alkali stressing of the API dimetindene maleate and investigation of its degradation products using GC-FID and GC-MS.

ZOLLNER Alexander – Analytical methods for the characterization and improvement of mammalian cell culture media stability.



2019

LE Si Hung – Selectivity considerations for analytical method development in metabolomics.

MIMINI Vebi – Lignofoams: potential for 100% biobased matrices and resins.

OLAGNON Charlotte - Synthesis and biological studies of phospho-lipid linked donor substrates for L-Ara4N transferases involved in Gram-negative bacteria antibiotic resistance.

PFANZAGL Vera – Biochemistry of B-type dye decolorizing peroxidases.

SALZER Benjamin – Safety and specificity engineering of chimeric antigen receptor T cells (CAR-T cells) by exploitation of avidity.

TCHAIKOVSKY Anastassiya – Strontium isotopic and elemental fingerprints as tools for source determination in aquatic ecosystems.

URBAN Michael - GC-MS/MS and two-dimensional LC-MS/MS approaches for the determination of contaminants and residues in food.

ZINOVYEV Grigory – Advanced molar mass characterization of technical lignins.

2020

BREY Charlotte Ulrike – Engineering of a conformation-specific On-switch for the regulation of CAR T cells.

ECKMAIR Barbara – From structural to functional Nglycomics: N-glycan analysis using mass spectrometry and carbohydrate microarrays.

FENDL Birgit – Interaction of extracellular vesicles with immune cells.

FÜHRER Johannes – Stable isotope labelling of O-glycans for improved tumor biomarker analysis.

JAXEL Julien – Tailoring of supercritical carbon dioxide technologies for the coloration of solid wood.

LUCIA Arianna – Dialdehyde cellulose-based binder for mineral wool. Development and optimization of an environmentally friendly, and non-toxic alternative to phenolic resin adhesive.

RETZMANN Anika – Method development for (multi-)isotopic analysis of bioapatites. SEVCNIKAR Benjamin – Biochemistry of human peroxidasin 1.

2021

BURGER Dennis – Silk fibroin-cellulose hybrids composite materials (Shinshu University, Japan).

ESPAÑA OROZCO Sebastian – Characterization and quantification of wood extractives during sulphite pulping and TCF bleaching.

KORNTNER Philipp – Method development for the analysis of technical lignins.

KRAUTER Simon – Molecular basis of binding interactions of pyruvylated cell wall polymers.

MICHLITS Hanna – Biochemistry of actinobacterial coproheme decarboxylase from *Corynebacterium diphtheriae*.

MOCSAI Reka Tunde – Structures, occurrence, immunogenicity and biosynthesis of methylated N-glycans in non-vascular plants.

NAUER Stefan – Chemische Charakterisierung des pfeffrigen Aromas ("Rotundon") von Weinen der Sorte Grüner Veltliner sowie Untersuchung der technologischen Beeinflussbarkeit.

QURAISHI Sakeena – Photoluminescent and light weight porous materials from oxidatively modified cellulose for sensing and thermal insulation applications.

SAROSI Oliver Pascal – Elucidating the effects of electron beam irradiation on cellulose and lignin and the consequences for woodbased biorefineries.

SCHIMPER Christian – Advancing the properties of cellulosic aerogels with particular focus on cell scaffolding materials.

WANG Luyao – Lignin fractionation and utilization (Åbo Akademi University, Finnland).

WASITO Hendri – Targeted and non-targeted metabolomics with separation sciences and accurate mass spectrometry in biotechnology.

ZHANG Jiaping – Approaches to preparation of highstrengths and ultrafine regenerated cellulose fibers using ionic liquid solvents (Åbo Akademi University, Finnland).

Doctorate

Besides individual doctorate studies in the programme H788 Doctoral studies of Natural Resources & Life Sciences with the degree Dr. nat. techn., BOKU offers a structured PhD programme (BioToP) which was organised and chaired until 2018 by the Department of Chemistry (see below). Now the chair moved to the Department of Material Sciences & Process Engineering, but several faculty members from the Department are still involved. Since 2018 a new doctoral school "Advanced Biorefineries: Chemistry & Materials (ABC&M)" (see below) is chaired by the Department of Chemistry. In the doctoral schools "AgriGenomics" and "Biomaterials and Biointerfaces" one faculty member is provided by the Department of Chemistry, respectively. Furthermore, the department is partner in the international doctorate programme "Fibre Science" with Shinshu University, Japan (see below). With respect to doctorate studies, the policy of the department is to attract qualified students also from other chemistry departments in Austria and abroad (which is a must, since students from BOKU have only a limited background in chemical sciences), but also to jointly supervise PhD theses with other groups in Austrian and foreign laboratories. Although being fully subsidized by the department, these cases are not listed in the statistics of the university.

Doctoral School -Advanced Biorefineries: Chemistry & Materials (ABC&M)



DOCTORAL SCHOOL ADVANCED BIOREFINERIES: CHEMISTRY & MATERIALS

Biorefineries play a central role in the field of the bioeconomy. The issue here is that, in the long term, the entire material flows of the chemical industries will have to be converted from fossil to renewable raw materials - a revolution for which there are no parallels in history so far. Due to the rapid basic scientific, technological, and applied industrial developments in this field, there will be an enormous demand for biorefinery experts in the medium term, both in university and industrial research as well as in industrial application. This need is proactively addressed by the BOKU doctoral school "Advanced Biorefineries: Chemistry & Materials (ABC&M)" - the only doctoral school in Austria that specifically addresses the

Excursion to Japan 2019



future field of biorefineries / bioeconomy. ABC&M offers an intensive, specialized doctoral education that focuses on scientific issues of the bioeconomy and provides indepth knowledge in the fields of the chemistry of renewable resources, lignocelluloses, and their modification and analysis, as well as in the field of materials science. Here, the application on an industrial scale also plays a special role. Most of the PhD students of the ABC&M are financed by third-party funded projects with industrial participation, e.g., in the framework of the Austrian Biorefinery Center Tulln (ABCT).

The curriculum comprises 40 ECTS of scientific/technological basics, socio-economic aspects, and, among other things, techniques of scientific work, presentation, and publishing. A central aspect is internationalization, especially the close thematic integration with doctoral colleges in Japan (Shinshu) and Finland (Turku), where tailor-made excursions will also take place. The last excursion took place in 2019, 17 PhD students from the ABC&M doctorate school visited three internationally leading Japanese institutes: Shinshu University, Kyoto University, and Kyoto University – Uji Campus.

Contact ABC&M:

Univ.Prof. Dr. Antje Potthast; Website: abcm.boku.ac.at

Doctoral School - BioToP



The international PhD programme BioToP (Biomolecular Technology of Proteins, https://biotop.boku.ac.at) focuses on research in the field of modern recombinant protein science and technology (from gene to product). Structural and functional analysis, design and engineering as well as recombinant production of proteins require inter- and multidisciplinary training in fields ranging from biochemistry and cell biology to production systems based on different organisms of varying complexity, up to bioinformatics and downstream processing. BioToP is a joint project of the Departments of Applied Genetics and Cell Biology, Biotechnology, Chemistry, Food Sciences & Technology, Nanobiotechnology and Material Sciences & Process Engineering. In the funding period (2010-2014, 2015-2018; Speaker: Christian Obinger), 101 doctoral candidates (39 % international; 51 % female) were selected by a competitive and transparent admission procedure. Funding was secured by FWF (14+14 doctoral candidates), BOKU (7+9) and third-party funds (57).

In September 2018, the program was positively evaluated by the FWF and in January 2019 the third funding period started (2019-2022; Speaker: Chris Oostenbrink). 47 doctoral students (44 % from abroad; 57 % women) were additionally selected in a competitive and transparent selection process. Currently (as of February 2022), 51 students (55 % female; 47 % international) are trained by a faculty of 15 Principal Investigators and 11 Associated Faculty Members who support the Principal Investigators in research and teaching. Funding is provided by the FWF (19 students), BOKU (9 students) and thirdparty funds (23 students).

Based on permanent internal (e.g. thesis committee meetings, evaluation of lectures and courses, curriculum committee activities) and external monitoring (e.g. by the Scientific Advisory Board) the program is continuously upgraded to cope with new developments in the relevant fields.

The visibility and dissemination of the scientific achievements of BioToP PhD students are accomplished by 378 SCI publications, as well as participation in many international conferences (521 presentations, including 151 talks). 13 conferences even included dedicated BioToP sessions.

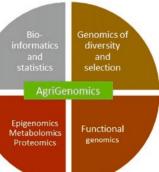
So far, 94 students successfully completed PhD programme, of which 69 % had research stays abroad. Their funding was provided by the FWF (14+14 doctoral candidates), BOKU (7+8) and third-party funds (52).

Contact BioToP:

Univ.Prof. Dr. Chris Oostenbrink; Website: biotop.boku.ac.at

Doctoral School -AgriGenomics

The Doctoral School AgriGenomics "performs multi-disciplinary research to create a more holistic picture of agricultural genomics by exploiting the strong relationships between research in plants, animals and microbes in combination



with research in gene expression mediated metabolomic processes and modern bio-informatics and statistics."

Stephan Hann supervises two PhD students in the Doctoral School: Bernadette Moser is working on the PhD topic "Evaluation of spectral methods for assessing food authenticity and quality" and Alexandra Bennett on the PhD topic "Assessment of below ground chemical communication by allelopathic cover crops in response to heterospecific neighbours", which is financed by FWF.

Contact AgriGenomics: Univ.Prof. Dr. Hermann Bürstmayr; Website: <u>agrigenomics.boku.ac.at</u>

Doctoral School – Biomaterials and Biointerfaces



The research focus of the Doctoral School "Biomaterials and Biointerfaces" (Bio-Mat-Int) is centered around the interaction between engineered materials and biological structures when they come into close contact. The Faculty of this School consists of 9 Principal Investigators (PIs) and 5 Associated Faculty Members, recruited from 7 Departments of BOKU, among them the Department of Chemistry (Falk Liebner, PI). As of December 2021, already 16 doctoral candidates have enrolled in Bio-Mat-Int.

The interdisciplinary topic linking fundamental and biosciences with technological and legal aspects is of immense importance in medicine due to the increased request for novel, more biologically oriented tools and materials for use in human medicine. These include minimum invasive diagnostics and therapy, targeted drug delivery as well as tissue replacement and restoration. In all these applications bio-compatible materials get into very close contact with patient cells or tissue. Challenges arising from this interaction include pathogen invasion, biofilm formation, inflammatory response, and tissue alterations due to changed chemical and mechanical environments. On the other hand, the interaction also opens a variety of promising opportunities, such as biosensing and simultaneous diagnostic and therapy (theranostics). Furthermore, cell culture technologies and tissue engineering can also contribute to reduce animal testing and to enhance the reliability of diagnostic or therapeutic approaches.

According to complexity, research is developed in three steps, i) patient cells and tissue: imaging, characterization and modelling of patient tissue and tissue culture, ii) interface: characterization of biomaterial-tissue interactions, prevention of adverse effects (biofilms, pathogens), exploitation of interactions for sensing, diagnostics and therapy, iii) biomaterials: mechanical performance testing, optimization and tailoring of biomaterials.

Contact Bio.Mat.Int: Univ.Prof. Dr. Helga Lichtenegger; Website: <u>biomatint.boku.ac.at</u>

Doctoral School -Programme Fibre Science

The Division of Chemistry of Renewable Resources is full member of the network "Global Center of Excellence in Fibre Science", headed by Shinshu University. For further information see Chapter 3.



Further teaching

Several staff members are also engaged in teaching activities at Colleges of Higher Education (Fachhochschule) such as FH *Biotechnical Processing* at Tulln (http://www.tulln.fhwn.ac.at) and FH *Bioengineering & Biomedical Science* in Vienna (http://www.fh-campuswien.ac.at) with lectures and courses being offered in evening hours and holiday seasons in the latter case.

In addition to lecturing at these polytechnics by staff members, public lectures and seminars are held. Regularly, members of the department take part in the teaching of foreign universities (Shinshu University, Japan; Åbo Akademi, Turku, Finland; Royal Society International Scientific Seminar, London, UK; SABK Stuttgart, Germany; Aveiro University, Portugal), summer schools or joint courses.



Quality assurance

At the department level, experienced staff is responsible for coordinating and performing teaching including lecturing, laboratory courses and examinations. Due to lab-space and time limitations, the organization of laboratory courses for the students of Food- & Biotechnology has to be tightly scheduled jointly with the Department of Biotechnology and the Department of Applied Genetics & Cell Biology (DAGZ). Several teaching assistant positions are allocated to the department by the university who are responsible for the internal organization of the first- and second-year laboratory courses. Further support comes from tutorial assistantships mostly given to experienced students, as well as master or PhD students at the department. Even with increasing activities using e-learning and on-line tools, university staff has to spend considerable time in the preparation and supervision of lab courses including oral examinations and corrections of protocols. Due to the pandemic situation in summer term 2020 all courses switched within days into various online formats (see below).

The quality of lectures and lab courses is routinely being evaluated by students, the results are open to the public and serve as a means for quality control. Evaluations by the students are taken very seriously. Although the use of this assessment instrument by the students is declining, reports reveal a high appreciation of the teaching performance of the department by the community of undergraduates.

Teaching quality is a concern of all lecturers of the department. Courses in didactics, new teaching methods, e-learning and exam preparation are a valuable part of their qualification.

DEPARTMENT EVALUATION 2020

In 2020 a department evaluation took place. Five international peers examined and commented the achievements of the department during the period of 2014-2019. The inspection covered research and teaching activities as well as administrative aspects, international reputation and communication with the society.

Proudly we can announce that the reviewers were very pleased with our accomplishments.

Peers:

Prof. Luc Moens - Faculty of Sciences,
Department of Sciences, Univ. Ghent, Belgium
Prof. Pauline Rudd - Emeritus Fellow, Conway
Institute, University College Dublin, Ireland
Prof. Jonathan Davies - Department of
Biomedical Sciences, København, Denmark
Prof. Joachim Thiem (Head of Peers) Universität Hamburg, Fachbereich Chemie, Institut für Organische Chemie, Hamburg
Prof. Monica Ek - Division of Wood Chemistry
and Pulp Technology, Stockholm, Sweden

The department participates regularly in external evaluations and audits, in the period 2019-2021 it has been evaluated completely (see box), participated in EMAScertification and was ISO 45001 certified (see chapter 9).

"QUALITY ASSURANCE IN THE CHEMICAL LABORATORY"



is offered by the University of Leoben as a post graduate course. The course was initiated by Prof. Wolfhard Wegscheider, who was Professor of General and Analytical Chemistry at the University of Leoben and is a past chair of EURACHEM. In the framework of the course, Stephan Hann taught "Documentation requirements of EN ISO 17025 and EN ISO 17020" in the year 2019. The 3-day module covers the contents of a quality assurance manual. As a practical exercise, a quality audit of an accredited laboratory is performed.

Teaching during the COVID-19 pandemic

Since the summer term 2020 we face an extraordinary teaching situation due to the SARS-CoV-2 pandemic. Due to lockdowns and distancing, all courses had to be adapted to the new safety conditions. In order to avoid a detailed list of changes, two teachers share their personal experiences of the situation: one for lectures and exams (Falk Liebner) and one for laboratory exercises (Erika Staudacher).

Lectures and exams by Falk Liebner

Asked to write a few lines about conversion of teaching to online operation, with the example of one of the biggest lectures at BOKU, one needs to think back to the tense days at the beginning of March 2020 when the first serious signs of the pandemic popped up and it became evident that COVID-19 would not spare Europe. I remember the almost eerily empty terminals at Porto airport, when returning from a longer stay in Portugal on the 6th of March, imposing the first shadows of what would follow. Even on Wednesday 11th of March, when we offered our monthly written exam for about 100 students of the courses in General Chemistry (altogether 1300 registered students in WS 2019), no one expected that just a few days later a complete lockdown would strike the summer semester. After few days of paralysis, intensive work started on finding solutions for setting up the appropriate environment for online teaching and meetings, which was hampered by missing and difficultto-purchase infrastructure like webcams, headsets, tablets. Besides choosing the right meeting software (Teams,

Zoom, Skype, Jitsi etc.) and challenges related to operation of the latter (virtual meeting rooms, desktop sharing, chat functions, etc.) a series of didactic adaptions had to be made for each form of teaching. Soon in April, the first requests for online exams were made, giving rise to further challenges like how to use the tools of BOKU-Learn properly and how to design a virtual exam ensuring a maximum of trust, honesty and support. Altogether, these activities consumed a great deal of time. Instead of holding a two-hours written exam in presence for 200 students in BOKU's biggest lecture hall, 23 online exam dates were offered in June, July and September 2020 for General Chemistry alone due to the limited number of places per exam, since every student had to log in with two devices. To cope with the continuing COVID-19 situation, additional efforts were made from October 2020 onwards to accompany the Monday morning webinar lectures (3.5 h) with introductory courses in September, in the form of Zoom meetings for questions immediately after the webinars, by opening the weekly online consultation hour also for exam reviews, and by offering a monthly 2-3 hour online tutorial. Now that there is cautious optimism that in-person teaching will return, it can be summarized that the Department of Chemistry not only mastered the changeover from in-person to fully online teaching in a short time while maintaining high quality, but it is also well-prepared should circumstances require shifting teaching again to online formats.

Laboratory courses by Erika Staudacher

Flying to London in February 2020, I watched the passengers of a Taiwan-flight who boarded close to mine. All persons in the queue were equipped with masks. It looked totally strange and unbelievable for me at the time.







Three weeks later we were ahead of our first lockdown. On Thursday March 12th, we were told to end all laboratory courses until next day. Within two busy days all students had to clean and empty their benches and collect their labcoats - this affected first-year-students in laboratory courses as well as bachelor, master and PhDstudents working in the research groups. At that time, we were still optimistic and expected just a break of 2-3 weeks. The following units of some elective courses were changed to an online format, while the main practical courses were shifted to the end of the term. Chemistry is a "hands-on" competence. Laboratory skills cannot be acquired by watching videos. 9 weeks (!!) later the first limited number of scientists was allowed to come back to the research groups. A strict timetable guaranteeing just few persons in each laboratory, obligatory masks, disinfection guidelines and distance rules allowed to continue some practical work at least for thesis-students. By the end of June also lab courses started. Small groups got all their introductory teaching by Zoom and could then gain at least some practical experience. We held those groups all over summer to compensate the loss of the

summer term partially. The university year 2020/2021 was characterised by a number of lockdowns with more or less restricted rules. However, going to work or going to study was allowed all the time and so we could process all of our courses, still in multiple runs with smaller groups.

Now (summer term 2022) most members of the staff and of the students are fully vaccinated and therefore the disease lost its fright. The infection rates are higher than ever, nevertheless we are back at normal frequency of our lab-courses. Though, high flexibility is necessary, because of high infection rates among students and staff causing numerous cancellations. Even when the course offer is back at a normal level, the pandemic situation has left marks in our general social behaviour. The social life of the research groups is still rather reduced. Big events were not possible for more than two years. Some of the PhD-students or new staff members never attended a department Christmas party or a department excursion. What a pity! What a loss!





Chapter 5 **Awards and Achievements**



Charlotte Zajc (Brey) and Vera Pfanzagl

Best Student Award of the **FWF-funded International**

Doctoral School BioToP,

2019

Réka T. Mócsai

Sven Plappert

Award 2019

Best Poster Award at the 25th International Symposium on Glycoconjugates, Milano, Italy, 2019

Christiane Gollner, Arianna Lucia, Stefan Böhmdorfer, Hubert Hettegger, Julien Jaxel, **Paul Jusner** Georg Haberhauer Administration Award 2019

Matthias Guggenberger 2nd place at the DocDay

Heinzel-Mondi-Sappi

Irina Sulaeva

Award 2020



Arianna Lucia 3rd place at the DocDay



Charlotte Zajc Life Science Research Awards Austria, 2021

Charlotte Zajc BOKU Talent Awards for her dissertation, 2021



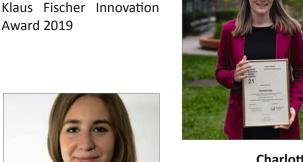
Thomas Gabler BOKU Talent Awards for his master thesis, 2021



Nele Zwirchmayr Dissertation Award, American Chemical Society, CELL division,



Grigory Zinovyev



Charlotte Zajc BOKU Best Paper Awards, 2021

Heinzel-Mondi-Sappi Award 2019

Hubert Hettegger Science Fair Award of Niederösterreich 2019



Falk Liebner Energy Globe Award Niederösterreich: category: "Luft", 2019

Benjamin Salzer Life Science Research Awards Austria, 2021









THOMAS ROSENAU NAMED FELLOW OF THE ROYAL SOCIETY OF CHEMISTRY (FRSC)



Thomas Rosenau, Professor of Wood, Pulp and Fiber Chemistry at the Institute of Chemistry of Renewable Resources, has been appointed fellow of the Royal Society of Chemistry, the oldest international chemical society, for his work on the chemistry of lignocellulosic materials and the 1st prize of the International Green Chemistry Challenge (2018).

INVITED CHAIR POSITION FOR BIOECONOMY AND BIOREFINERY, DEPARTMENT OF CHEMISTRY, AVEIRO UNIVERSITY, PORTUGAL

Assoc. Prof. Falk Liebner, Institute for Chemistry of Renewable Resources accepted a call for an Invited Chair (Full Professor, part-time) Position for Bioeconomy and Biorefinery at the Department of Chemistry, University of Aveiro, Portugal. Complementing his research and teaching at BOKU, Falk Liebner will work four months a year for the period of 2019-2024 at the University of Aveiro in research and teaching, in the framework of a large EU structural fond project (InPaCTus, Innovative Products and Technologies from Eucalyptus). Topics of this project, which is promoted by major national and international research partners and companies, are pulps with innovative features, new paper products with different specificities and functions, tissue paper with innovative properties, and new bio-based materials obtained from deconstruction and conversion of forest biomass and by-products of the pulping industry.





HONORARY DOCTORATE FOR BOKU SCIENTIST

Thomas Rosenau, Professor of Wood, Pulp and Fiber Chemistry at the Institute of Chemistry of Renewable Resources, was awarded an honorary doctorate from the National University of Malaysia at Kuala Lumpur, for his work on biorefinery concepts, in particular the sustainable use of oil palms and palm oil-based bulk chemicals, and in recognition of many years of fruitful collaboration.

BOKU SCIENTIST ACCEPTED INTO THE INTERNATIONAL ACADEMY OF WOOD SCIENCE

Antje Potthast, Professor of Chemistry of Lignocellulosic Materials at the Institute of Chemistry of Renewable Resources, has been appointed a member of the International Academy of Wood Science (IAWS) in recognition of her contributions to cellulose analysis and restoration/ preservation of historical cellulosic objects.



International Academy of Wood Science



BOKU INVENTION 2020

The award went to the inventors, Dr. Charlotte Zajc and Dr. Michael TraxImayr from the Department of Chemistry, Institute of Biochemistry, with the technology "A lipocalin fold-based inducible dimerization system ("Lipocalin-Switch")". The invention is the result of excellent scientific research in cooperation with St. Anna Children's Cancer Research, and it was also made possible by the cooperation with the globally active biotechnology and biomedicine company Miltényi Biotec. It is characterized by the wide range of possible applications, which makes economic exploitation possible in many areas. With the help of this invention, the safety and tumor specificity of CAR-T cell therapy will be further developed so that more effective therapies can be brought into broad clinical use and new decisive impulses for cancer therapy can be made possible worldwide.

TOP-PAPER 2021

Dr. Johannes Stadlmann and **a team of Austrian researchers** release the "sugar brake" and develop highly effective SARS-CoV-2 receptor mock-up. An interdisciplinary research team with the participation of BOKU has calculated and experimentally determined the influence of sugar structures on the docking of the coronavirus to the receptor protein ACE2. It has been shown that some of these sugar chains of the receptor protein stand in the way of the virus and thus "brake" its docking, which has far-reaching significance in the fight against the coronavirus (<u>eLife 2021;10:e73641 doi: 10.7554/eLife.73641</u>).





Chapter 6 Instrumentation

NMR INFRASTRUCTURE

The Institute of Organic Chemistry and the Institute of Chemistry of Renewables operate four NMR cryomagnet systems at different magnetic fields (600 MHz, 2 x 400 MHz, 300 MHz). NMR spectroscopy can be performed either in solution using deuterated solvents (**liquid state NMR** @ all systems) as well as with gel-like or solid compounds (**solid state NMR** @ 400 MHz), which requires different hardware. The NMR facilities require dedicated and specialized staff and regular maintenance to supply liquid N₂ and liquid He. NMR spectroscopy is also available as an analytical service for in-house collaborations as well as for external customers.



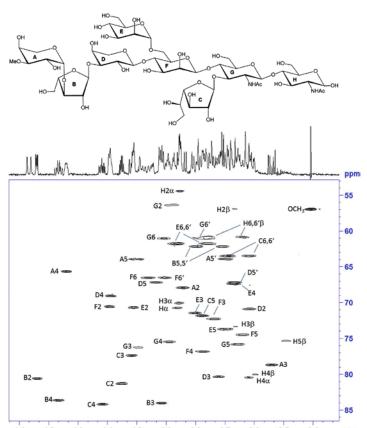
He-refill of the 600 MHz magnet



The 400 MHz instrument equipped with a liquid N_2 cooled cryoprobe (Prodigy) located at UFT

By using state-of-the-art one- and multidimensional homo- and heteronuclear experiments in the **liquid state**, structure elucidation, conformational analysis or purity confirmation of synthesized products or biological samples is done. Measurements of reaction kinetics, analysis of complex mixtures such as plant metabolites, bacterial and parasite glycans and technical lignins or cellulose derivatives are also performed. Additional techniques beyond ¹H and ¹³C spectroscopy such as measurements of heteronuclei such as ¹⁹F, ³¹P or ¹⁵N, experiments at variable temperatures, diffusion experiments, binding studies and many more are performed according to requirements.

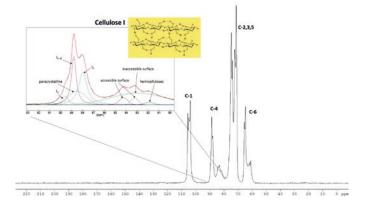
As an example, the structural elucidation of an N-glycan from an algal *Chlorella* species is shown. Based on the analysis of NMR data using a combination of COSY, TOC-SY, HSQC, HMBC, HSQC-TOCSY and ROESY experiments, the chemical structure of a reducing octasaccharide, including linkage sites and anomeric configuration of the constituent sugars could be solved (in collaboration with F. Altmann). Novel structural features were observed for β -linked galactofuranose attached to the chitobiose core



4.4 4.3 4.2 4.1 4.0 3.9 3.8 3.7 3.6 3.5 3.4 ppn HSQC correlations and structure of the octasaccharide from Chlorella pyrenoidosa

and a trisaccharide of arabinosyl units containing α - and β -linked arabinopyranosyl units, an internal arabino-furanose and capping 3-O-methylatoin.

For the characterization of insoluble materials, one of the 400 MHz magnets is equipped for solid state NMR. Gel-like samples like many carbohydrates or aerogels can be investigated with the HR-MAS probe (high resolution magic angle spinning) whereas all variants concerning CP-MAS (cross polarization magic angle spinning) is the method of choice for solids.



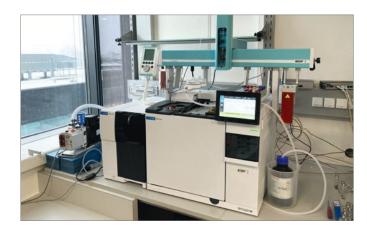
Determination of crystallinity index of cellulose I by solid state NMR

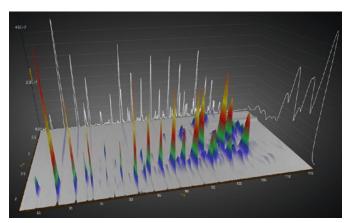
GCxGC

The extraction of plant biomass by solvents yields a variety of small molecules. The exact composition depends on the source material, the extraction method, harvesting time, and storage conditions. These mixtures can contain bioactive molecules with potential uses in food and pharmaceutical applications, and they also influence the technological properties of plant biomass (hydrophobization, durability, processability during pulping). For the determination of the exact composition of an extractive fraction, the Institute of Chemistry of Renewable Resources operates in the framework of the Interreg Project Valid a state-of-the-art Agilent 8890 system for comprehensive, multidimensional gas chromatography (GCxGC) with single-quadrupole mass-spectrometry detection. In this setup, the high separation power of conventional gas chromatography (GC) is multiplied by immediately subjecting all molecules to a second separation. This way, molecules that were not separated in the first dimension can be resolved in the second separation dimension, which allows a clear separation of almost all compounds in the extract. The singled-out components are then subjected to mass spectrometry and identified by commercial and dedicated in-house databases. Simultaneously, a conventional flame ionization detector is used for compound quantification. The entire system is capable of high temperature separation to widen the scope of analytes to steryl esters and triglycerides. The modulator, the key component that joins the second to the first separation, operates without cryogenic conditions and is very flexible. Therefore, the system can also be used for other complex samples, such as essential oils, fatty acids, glycerides, or mixtures of mono- and disaccharides. The multifunctional sampler allows the analysis of sample solutions and volatiles extracted from the gas-phase. Together with supercritical fluid chromatography and high-performance thin-layer chromatography, a comprehensive picture can be obtained of complex mixtures of small molecules.

MALDI-TOF MS

Matrix-assisted laser-desorption-ionisation time-offlight mass spectrometer (MALDI-TOF MS): the Bruker Autoflex Speed (installed in 2012) is the latest of this type of instrument in the department (the first one arrived in 1998). A particular focus is on "off-line" HPLC-MSbased glycomics, which means that glycans from various sources are chromatographically separated before spotting onto a metal target, which is then introduced into the MALDI-TOF MS for analysis including MS/MS fragmentation in positive and negative ion modes. Having this instrument "on-site" is key to the work of the Molecular Glycobiology & Phylogenetics group (headed by lain Wilson), but also supports work by other research groups within the Department. To be highlighted in particular are recent publications in "top" Journals descri-







lain Wilson and the MALDI TOF MS

bing the isomeric and isobaric complexities of the protein-linked glycans of a range of organisms; such studies would not have been possible in such fine detail without this instrument, indicating its importance for the discovery of unexpected glycan epitopes.

GLYCAN ARRAY PRINTING AND SPOTTING

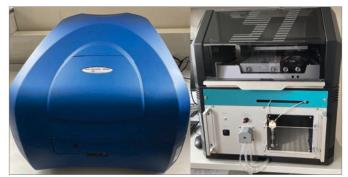
In the past few years, the Molecular Glycobiology & Phylogenetics has established the use of glycan arrays as a tool to determine interactions between glycans and antibodies, lectins or pentraxins. For this purpose, we have both a non-contact printer (Scienion Flexarrayer S1) and an array reader (Molecular Devices Genepix 4400) – devices also used by the group of Fabian Pfrengle in the Institute of Organic Chemistry. With such instrumentation, we can ask questions about the physiologically- and pathologically-relevant partners of glycans from invertebrates and their role in interactions with host immune systems.



Clean room

ELEMENTAL MASS SPECTROMETRY

The Institute of Analytical Chemistry performs research with high-end elemental and isotope ratio mass spectrometry (ICP-MS) and molecular mass spectrometry (LC-MS, GC-MS). The sector field ICP-MS system of the Institute is used in the context of elemental ultra-trace and speciation analysis. The instrument is situated in a class 10 000 clean room environment, which allows the accurate measurement of sub-ng/L element concentrations for a variety of research questions. An SEC-ICP-MS (Waters H-Class Bio - PerkinElmer Nexion 2000) system is also situated in the clean room. This combination of instruments was acquired in the framework of the granted HRSM project "Bioresource Analysis". The SEC-ICP-MS is used for the analysis of metal- (or hetero-element)containing compounds, or biopolymers and for the investigation of metal/biomolecule interactions. A special focus is the interaction of metals with proteins and the characterisation of metalloproteins.



Glycan array printer

BOKU Core Facilities and the Department of Chemistry

In the past few years the vice-rectorate for research and innovation re-organized instrumentation infrastructure at BOKU by focusing resources into Core Facilities in order to make them accessible to the entire scientific community and to raise the usage time of each instrument. Many instruments from the Department of Chemistry have been transferred to BOKU Core Facilities. Thus, the Department of Chemistry is heavily involved in organisational issues and also delivers scientific input. The following researchers of the Department of Chemistry are key contributors to BOKU Core Facilities:

- Johannes Stadlmann, Scientific Head of Core Facility Mass Spectrometry
- Teresa Steininger-Mairinger, Deputy Scientific Head of Core Facility Mass Spectrometry
- Stephan Hann, Chair of the Advisory Board of the Core Facility Mass Spectrometry
- Friedrich Altmann, Deputy Chair of the Advisory Board of the Core Facility Mass Spectrometry
- Antje Potthast, Scientific Head of the Core Facility ALICE
- Stefan Böhmdorfer, Deputy Scientific Head of the Core Facility ALICE
- Thomas Rosenau, Chair of the Advisory Board of the Core Facility ALICE
- Michael Traxlmayr, Scientific Head of the Core Facility BmCA
- Stefan Hofbauer, Deputy Chair of the Advisory Board BmCA

BOKU CORE FACILITY MASS SPECTROMETRY (MS)



Within the Core Facility Mass Spectrometry (CF MS), BOKU offers internal and external users a state-of-theart equipment park for performing analyses in the fields of isotope, elemental and molecular mass spectrometry. Measurements are carried out both by the CF MS staff and, after appropriate training, by the users themselves. The extensive MS instrumentation can be viewed at the website (<u>https://boku.ac.at/cf/ms</u>).

The CF MS is supervised by experienced staff, which are highly competent in sample preparation, chromatography and mass spectrometry and have a broad knowledge in the field of biological, food and environmental sciences. These synergies ensure that the existing and future questions and requirements of BOKU scientists and the scientific community at large can be met efficiently and with the highest quality standards.

The excellent equipment of the CF MS enables the development of fit-for-purpose methods and their application in routine. The broad method portfolio ranges from targeted absolute and relative quantification by molecular and elemental mass spectrometry as well as the possibility of non-targeted analysis by high-resolution mass spectrometry and proteomics, glycomics and metabolomics. The CF MS receives scientific support from the Institute of Analytical Chemistry and the Institute of Biochemistry at the Department of Chemistry.

In summer 2022, the CF MS will move to a newly developed area with high-tech laboratory infrastructure on more than 400 m² in Muthgasse 11 (MG III), where it will enable the unique combination of elemental, isotopic and molecular mass spectrometry at one location including laboratories for sample preparation, an ICP-MS clean room laboratory and several measuring stations with LC-MS and GC-MS instruments.

RESEARCH SERVICES -

THE FOLLOWING INSTRUMENTATION IS AVAILABLE TO ACADEMIA AND INDUSTRY:

I. Proteomics and glycomics

In the fields of proteomics and glycomics, we provide electrospray time-of-flight and high-resolution spectrometers with different tuning configurations as well as various source options to address a broad variety of research questions. The combination of on-line liquid chromatography as a separation technique allows for in-depth identification and quantification of complex sample mixtures. The analysis of glycosylated peptides as well as free glycans and many other post translational modifications is one of our core competences. Recently an Orbitrap Exploris[™] 480 Mass Spectrometer was installed at the CF MS, facilitating ultra-high-resolution experiments in combination with several fragmentation options.





LC-IM-QTOFMS, 6560, Agilent Technologies, LC-TOFMS, 6230B, Agilent Technologies, LC-MS/MS, TSQ Vantage, Thermo Scientific

II. Small molecules

CF MS provides LC and GC separations in combination with triple quadrupole mass spectrometry systems for quantification of a broad range of small organic molecules covering a wide scope of applications. One of the specializations is metabolomics for biotechnology applications, in particular the delivery of high-quality data for cellular metabolism studies.

Furthermore, the high-resolution time of flight instruments allow non-targeted analysis and support identity confirmation and screening workflows using accurate mass, ion mobility, and fragmentation-supported workflows. Methods covering a range of sample types and research questions can be developed upon request.

III. Elemental and isotope ratio analysis

CF MS provides sector-field and quadrupole-based ICP-MS systems for quantification of almost all elements of the periodic system in various matrices. The high-end MC ICP-MS will enable *accurate isotope ratio analysis* of stable isotopes of strontium, sulfur, and lead.

WHERE AND HOW:

MS core facility is located at Muthgasse 11/1st floor. For requests please contact us at any time per email to: *ms@boku.ac.at*

Detailed information on our equipment and services can be found at <u>https://boku.ac.at/cf/ms</u>.

BOKU CORE FACILITY BIOMOLECULAR AND CELLULAR ANALYSIS (BMCA)



The BOKU Core Facility Biomolecular & Cellular Analysis (BmCA) is one of currently eight highly specialized facilities at BOKU (two located in Tulln and six located at the campus Muthgasse). BmCA is a state-of-the-art analytical laboratory with focus on biomolecular characterization and characterization of biomolecular interactions, protein crystallography as well as flow cytometry. Besides high-end instrumentation, BmCA offers the possibility to prepare your samples in the most optimal way. BmCA provides basic laboratory equipment, and offers two PC workstations which are accessible for all Core Facility users to utilize the (licenced) special software of the various instruments. Apart from the provision of instruments, professional training for certain techniques as well as consultation regarding experimental setup and design are offered. Further, it is possible to make use of our full service, which comprises the measurements of your samples by trained staff and the generation of experimental reports.

GC-QTOFMS, 7200B, Agilent Technologies, GC-MS/MS, 7010B, Agilent Technologie



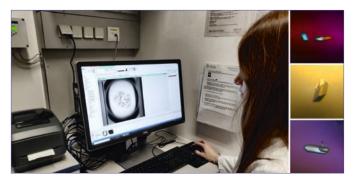
RESEARCH SERVICES -THE FOLLOWING INSTRUMENTATION IS AVAILABLE TO ACADEMIA AND INDUSTRY:

I. Biomolecular analysis

A strong focus is put on the investigation and characterization of all kinds of biomolecular interactions. For that purpose, we are equipped with a *surface plasmon resonance spectrometer* (SPR, Biacore T200, GE Healthcare), a *biolayer interferometer* (BLI, Octet RED96e, Pall FortéBio) and an *isothermal titration calorimeter* (PEAQ-ITC Automated, Malvern Panalytical).

Prior to the application of the above-described techniques, a comprehensive sample characterization is prerequisite. BmCA offers the possibility to check for aggregation behaviour of your (protein) sample (Zetasizer Nano ZSP equipped with an autotitrator, Malvern Panalytical). The instrument is also useful to determine the zeta potential and molecular weight of particles. The measurement principle is *dynamic light scattering*. Additionally, we offer a multi-detector GPC/SEC system (OMNISEC, Malvern Panalytical) to accurately determine the molecular weights and concentrations of proteins. It can be used to analyze the purity of a sample, to determine the oligomeric state of proteins and protein complexes, and to quantify the different species present in a sample. The system combines analytical SEC with an integrated triple-detector (Refractive Index, Light Scattering and UV/ VIS PDA). Moreover, the temperature-controlled column oven is equipped with different columns for high-resolution analysis of proteins and other biomolecules covering a broad fractionation range.

A very informative quality parameter is the thermal stability of proteins and other biomolecules. BmCA offers *differential scanning calorimetry* (DSC) to determine thermal transition values (T_m) and thermodynamics of



Formulatrix Crystal Hotel – RockImager 1000

unfolding (PEAQ-DSC Automated, Malvern Panalytical). This technique is very versatile since it can be used to solve various kinds of research questions, e.g. oligomeric state determination of proteins, reversibility/irreversibility of unfolding, screening for optimal buffer conditions, indirect investigation of ligand binding etc.

II. Cellular analysis

BmCA further offers techniques for the analysis of cells or cellular components. This part is mainly covered by *flow cytometry*. BmCA is equipped with two analysis instruments (CytoFLEX-S: in 2 and 4 laser configuration, Beckman Coulter) and two sorting instruments (SH800S: easy-to-use and chip-based cell sorting system, Sony; MoFlow Astrios EQ: high-speed cell sorting, Beckman Coulter).

Furthermore, it is possible to measure size distribution and zeta potential of primarily extracellular vesicles using **nano particle tracking analysis** (ZetaView, particle-metrix). However, this technique can be applied to practically any particles of between 10 nm and 3 μ m in size.

Formulatrix pipetting robot - Formulator





III. Crystallization of proteins and X-ray diffraction analysis

The latest expansion of the facility is in the field of protein X-ray crystallography. BmCA provides state-of-the-art infrastructure for the crystallization of proteins and subsequent analysis. BmCA is equipped with:

- Pipetting robot (Mosquito LCP, SPT Labtech)
- Crystal imaging hotel (Rock Imager 1000, Formulatrix)
- Stereomicroscope (SteREO Discovery.V12, Zeiss)
- Protein formulation screen builder (FORMULATOR 10, Formulatrix)

Tools and equipment for crystal harvesting, freezing, storage and dry shippers for sending crystals to the synchrotron are also available. Shipment of crystals, data collection, the processing of diffraction data and the generation of 3D models of your proteins under study are all part of the services offered.

WHERE AND HOW:

BmCA is located at Muthgasse 11/1st floor/room B01-015. For requests please contact us at any time per email to: *bmca@boku.ac.at*

Condensed information on our equipment and services can be found at <u>www.boku.ac.at/cf/bmca</u>.

BOKU CORE FACILITY ALICE (ANALYSIS OF LIGNOCELLULOSICS)

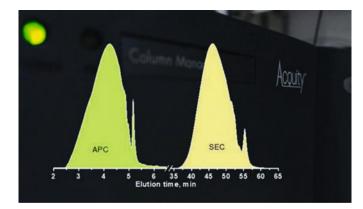


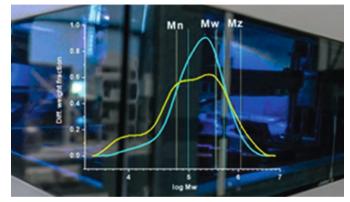
The BOKU Core Facility "ALICE" (Analysis of Lignocellulosics) offers method development and state-of-the-art chromatographic, spectroscopic and chemical analysis for the advanced characterization of lignocellulosics and biorefinery products.

The special feature of this core facility is its connection to the twin Core Facility at Åbo Akademi University Turku, Finland. While ALICE is specialized in celluloses and lignins, Abo focuses on hemicelluloses and extracts, so that together the whole spectrum of important components in post-growing raw materials can be covered. This specialization and a common customer base will promote considerable synergies.

A largely unique combination of methods is available for the analysis of celluloses, covering the entire range of cellulosic materials, from cellulosic pulp and paper, via nanostructured celluloses and cellulosic fibres, to textiles, cellulose derivatives and historical cellulosic objects of art. Solubility studies are part of the portfolio as well as the determination of molar mass distributions by multidetector-chromatography, the determination of cellulose allomorphs and crystallinity by solid-state NMR spectroscopy, the analysis of hemicellulosic components, as well as thermal and mechanical properties. The recording of profiles of oxidized groups (carbonyls and carboxyls) in relation to the molar mass distribution with group-selective fluorescence labeling is unique and performed worldwide only here, the same applies to the isolation and identification of cellulosic trace chromophores. One of the largest cellulose databases, on an international scale, with data of more than 3000 different cellulose samples, is available for data matching and comparison.

Lignins are analyzed by several spectroscopic, chromatographic and wet chemical methods, which in combination far exceed the information provided by conventional or individual analytical techniques. Native lignins, nearnative lignins (e.g., milled-wood lignin) and all types of technical lignins (Kraft, lignosulfonate, organosolv, biorefinery lignins) are covered.





The first step is the isolation of lignins from their complex matrices and their separation from organic and inorganic accompanying substances, if needed. The lignins' molar mass distribution is measured by different approaches, using the latest methodology which avoids conventional error-prone calibrations. The determination of the lignins' functional groups is performed both NMR-spectroscopically and by wet- chemical/chromatographic means with robot-automated methods optimized towards higher throughput. Based on an extensive lignin database, which represents the counterpart of the cellulose database, fast methods by NIR/IR/chemometrics are available.

In the field of diverse biorefinery scenarios, several separation and extraction techniques, both for fractionation and purification, are available. Extractives, secondary metabolites or dyes can be obtained both by solvent extraction and supercritical extraction, which can be combined with supercritical chromatographic separation (SFC) and identification (QTOF-MS) if required. For all the offered analytical methods and services, additional advanced data interpretation as well as professional training sessions are offered on request. Further services include special, tailor-made investigations of chromophore chemistry, aging and analysis of conservation methods of cellulosic materials as well as studies of modification, properties and utilization of lignins.

WHERE AND HOW:

Core Facility ALICE is located at Universitäts- und Forschungszentrum Tulln, Konrad-Lorenz-Str. 24, 3430 Tulln. For requests please contact us at any time per email to: *alice@boku.ac.at*

Condensed information on our equipment and services can be found at <u>https://boku.ac.at/cf/alice</u>.



Chapter 7 International Activities

Incoming

Visiting Professors appointed by the Senate of BOKU



Photograph Courtesy of Alex Berg

Alex Berg University of Concepcion, Coronel, Chile

Alex Berg from the University of Concepción (UdeC, Concepción, Chile) visited BOKU as a guest professor in March 2020. He is the Executive Director of the Technological Development Unit (UDT) at UdeC, and an expert in wood chemistry, bioproducts, and biorefineries. During his visit, he gave lectures and valuable scientific support to BOKU students and researchers.



© Stephen V. Evans

Stephen V. Evans University of Victoria, Victoria, Canada

Stephen Evans is Professor at the Department of Biochemistry and Microbiology at the University of Victoria. He graduated in 1986 from the Department of Chemistry, University of British Columbia and, after 4 years at the Department of Biochemistry, he moved to the renowned Institute for Biological Sciences - National Research Council of Canada in Ottawa with a research focus on the structural biology of protein-carbohydrate interactions. In 2003 he returned to British Columbia at the University of Victoria followed by promotion to full professor in the Department of Biochemistry and Microbiology in 2007. He is an internationally renowned expert in the structure determination of glycobiology-relevant proteins, with his contributions focused on glycosyltransferases and carbohydrate-specific antibodies.



Luis Laglera Universitat de les Illes Balears, Palma de Mallorca, Spain

Luis Laglera is a Marine Scientist and Professor at the Department of Chemistry at the University of the Balearic Islands (UIB). He is a member of the group FI-TRACE (Flow Injection and Trace Analysis) at UIB and his research interests are focused on the study of the biogeochemical cycles of trace metals in ocean, coastal and estuarine waters (with emphasis in iron, copper, lead, cobalt and mercury), and in particular in the characterization and quantification of natural organic ligands.



Ken Kitajima Nagoya University, Nagoya, Japan

Ken Kitajima is Professor at the Bioscience and Biotechnology Center & Graduate School of Bioagricultural Sciences at Nagoya. His research focuses on the fundamental biological processes regulating cell adhesion and signalling with particular emphasis on the functions of glycans in glycoproteins and other glycoconjugates; a particular focus is on the occurrence and role of sialic acid in a wide range of organisms. After his doctorate from the University of Tokyo in 1987, he was assistant professor first at the University of Tokyo, then associate professor at Nagoya University. Since 2004, he has been Professor at the Bioscience and Biotechnology Center & Graduate School of Bioagricultural Sciences at Nagoya. He was awarded a Research Award for a Young Researcher by the Japanese Society of Carbohydrate Research in 1999.

Guest Professors



Nicola Pohl Indiana University, Bloomington, USA

Nichola Pohl is the Marvin Carmack Chair in Bioorganic Chemistry. She received her Ph.D. in chemistry from the University of Wisconsin-Madison in 1997. Following an NIH Postdoctoral Fellowship at Stanford University, she joined the faculty at Iowa State University in the fall of 2000 and was a professor of chemistry and of chemical and biological engineering and held the Wilkinson Professor of Interdisciplinary Engineering there before moving to Indiana University in 2012. She was a Fulbright U.S. Scholar in 2020 at the Department of Chemistry.



Vlad Panin Texas A&M University, USA

Prof. Vlad Panin is Professor at the Department of Biochemistry & Biophysics, Texas A&M University where his group studies the neuroglycobiology of the fruit fly. He received his Ph.D. in Biophysics from Moscow State University (Russia) in 1990 and was a postdoc in Ken Irvine's laboratory at Rutgers University, NJ before joining Texas A&M University in 2002. He has twice held a research seminar at the Department of Chemistry, most recently in December 2019.



Invited Lecturers

John Beale, Paul Scherrer Institute, Switzerland Blaise Tardy, Aalto University, Helsinki, Finland

Guest Scientists

2019

Ruwan Kurulugama, Agilent Technologies, USA Chu Dinh Binh, Hanoi University of Science and Technology, Vietnam Christine Gallampois, Umeå University, Sweden Tuba Recap, Hacettepe University, Turkey Ilenia Serra, University of Antwerp, Belgium Chiara Bernini, University of Modena and Reggio Emilia Marja Stanojkovic, University of Niš, Serbia Ashna Rawat, National Museum Institute of History of Art, Conservation and Museology, India Hanna de la Motte, RISE Research Institutes of Sweden Saida Ibragic, University of Sarajevo, Bosnia and Herzegovina Hiroko Ninoyu, Hokkaido University, Japan Pavel Vostreis, Brno University of Technology, Czech Republic Peter Sekandi, Makerere University, Uganda Masaaki Aoki, Shinshu University, Japan Davood Kolahreez, Isfahan University of Technology, Iran Alice Merio, ENSAIA, France Karolina Młynarczyk, Uniwersytet Szczeciński, Szczecin, Poland Entela Celiku-Hodaj, Agricultural University of Tirana, Albania

2020

Mariana Aparicio, Eindhoven, The Netherlands Jaclyn Swan, Latrobe University, Melbourne, Australia Tasha Tamgue Chakro-oh, FH Krems Lisa Rausch, FH Krems Katharina Pfaffeneder, FH Krems Cornelia Bußlehner, Institute for Conservation and Restoration, Academy of Fine Arts Vienna Muhamad Nur Ghoyatul Amin, Airlangga University, Indonesia Davood Kolahreez, Isfahan University of Technology, Iran Ute El Nahawi, HAWK University of applied sciences and art, Hildesheim, Germany Maryam Allahdady, University of Teheran, Iran Seng Joe Lim, Universiti Kebangsaan, Malaysia Rebecca Whetton, University College Dublin, Ireland Barbora Benetkova University of Prague, Czech Republic

2021

Noemae Lim, University of Tartu, Estonia Selorm Torgbo, Kasetsart University Bangkok, Thailand Lukas Fliri, Aalto University, Finland Natthawadi Wongthet, Kasetsart University Bangkok, Thailand Justine Lin, Sorbonne University, France Nohman Arshad Iqbal, Sorbonne University, France Salma Daoufa, IMT Mines Alès, France Bruna Alves, Coimbra University, Portugal

Outgoing - Lectures, Teaching and Research

2019

Stephan Hann – University of Balearic Islands, Palma de Mallorca, Spain

Stephan Hann – Vietnam National University, Hanoi, Vietnam

Iain Wilson – University of Georgia, USA Iain Wilson – Limburg/Lahn, Germany Katharina Paschinger – Milano, Italy Katharina Paschinger – Adelaide, Australia Benjamin Sevcnikar – University of Copenhagen, Denmark Charlotte Brey – Stanford University, USA Hanna Michlits – University of Firenze, Italy Paul Kosma – Borstel, Germany Grigory Zinovyev – Pardubice, Czech Republic

2020

Tim Causon – Agilent IMS User Meeting, Essen, Germany Iain Wilson – Mainz, Germany Fabian Pfrengle – TU-Vienna, Austria Fabian Pfrengle – University of Vienna Antje Potthast – EPNAT Meeting, Brazil, online Falk Liebner–University of Aveiro, Portugal (see Chapter 5)

2021

Stephan Hann – University of Balearic Islands, Palma de Mallorca, Spain Max Feuerstein – INRAE, LABERCA, Nantes, France Tim Causon - Virtual Ion Mobility Spectrometry Mini-Symposium, online Tim Causon – Separation Science: State of the Art (LC GC) Seminar, online Reka T. Mocsai – European Chlorella Conference 2021, online Iain Wilson – Göteborgs Universitet, Sweden, online Paul Furtmüller – Zaragoza, Spain Fabian Pfrengle – CiLST lecture Series, online Fabian Pfrengle – ACS Carbohydrate Division Young Investigator Symposium, online Fabian Pfrengle – 6th Latin American Glycobiology Congress, online Alla Zamyatina – 16th Meeting of the International Endo-

toxin and Innate Immunity Society, Kobe, Japan, online Alla Zamyatina – 4th ENOVA Adjuvant Workshop, online

Hajar Khaliliyan – University of Copenhagen, Denmark Jonas Simon – University of Florida, Gainsville, USA David Budischovsky – NMBU, Norway Nadine Kohlhuber – Aalto Helsinki, Finland Takaaki Goto - Kyoto Prefectural University, Japan Cuong Viet Bui – University of Science and Technology, Danang City, Vietnam Hubert Hettegger – Workshop on "Chemicals for woodbased materials", Krems Hubert Hettegger – Invited lecturer at Euroleague for Life Sciences Summer School on "Bioeconomy", BOKU Antje Potthast - University of Jember, Indonesia, online Antje Potthast – University of Leeds, UK, online Antje Potthast – GRETE Biobased Industries Consortium, online Antje Potthast – SMART Conference, online Antje Potthast – Seminar für Philosophie, Ringvorlesung, TU Braunschweig, Germany Thomas Rosenau – GRETE stakeholder lecture, online Thomas Rosenau – Papierfabrik Wattens, online Thomas Rosenau – LigninReSurf Kick-off, Abo Akademi University, Turku, Finland, online Thomas Rosenau - Meeting with Head R&D and lab heads of SAPPI, South Africa, online Thomas Rosenau - EPNOE workshop "Horizon projects", online Thomas Rosenau – FLIPPR-Abschluss-Meeting, online Thomas Rosenau – Meeting with Alchimia Nova, online Thomas Rosenau - Meeting with Head R&D, OFA Bamberg, Germany, online

Organisation and Co-Organisation of Conferences

2019

- 15th Annual Conference of the Metabolomics Society, The Hague, Netherlands
- FFoQSI Mini-Symposium: "Neue analytische Strategien zur Prüfung der Authentizität und Qualität von Lebensmitteln", Linz, Austria
- 11th Human Peroxidase Meeting, Brno, Czech Republic

2020

- 24th Austrian Carbohydrate Workshop, TU Vienna
- International Conference on Aerogels for Biomedical and Environmental Applications, Santiago de Compostela, Spain
- EPNOE Workshop "Modern analytical approaches in biopolymer characterization", Tulln, Austria
- ACS Spring Meeting and Exhibition, Philadelphia, USA

2021

- XXIIIrd International Symposium on Advances in Extraction Technologies (ExTech)
- Session at the Annual AAAS Meeting: "Complex Glycans in Coronavirus Biology: The "Sweet" Secrets of a Pandemic", online
- 7th EPNOE International Polysaccharide Conference, Nantes, France (session co-organizer)



Chapter 8 Outreach activities

Besides research articles in scientific journals, we communicate our results to the public via print media and contributions to broadcasts, TV and film. In addition, outreach is performed in the form of guided tours, visits and workshops for students. The period of 2020-2021 limited our ability to engage on-site with visiting students or attend events in person, but some outreach activities were held when permitted.

Print media

Articles in national newspapers during period of 2019-2021 included: APA press report (01/2019): "Wiener Forscher erstellen chemischen "Fingerabdruck" von Weinen", (Die Presse, Oe24, Der Standard, Wiener Zeitung, Neue Züricher Zeitung, Tiroler Tageszeitung, Bauernzeitung, LISAvienna life science Austria, Forschung und Wissen, Bauernladen, Economy, BBJ Wein-Newsletter 2019 03 and Der Winzer); "Herzwurm von Hund enttarnt" (Die Presse, 12/01/2019); "Nutzung von Lignin: Erwähnung des FLIPPR2 Projekts" (Die Presse, 24/02/2019); "Einzigartige Musikalien vor dem Zerfall retten" (Die Presse, 28/03/2020); "Der Fingerabdruck des Merlots" (Die Presse, 04/05/2019); "Es ist nicht alles Kellergold" (Süddeutsche Zeitung, 14/05/2020); "Was Badende in der Alten Donau stört, wird sinnvoll verwertet" (Die Presse 15/05/2021); "Naschen aus der Seegrasschale" (Der Standard, 02/07/2021); and "Neue Wege zu Supermaterialien aus Cellulose" (Der Standard, 04/11/2021).

Further printed articles included "Gibt es schon bald einen Impfstoff gegen die Herzwurmerkrankung?" in Vet-Journal (03/2019); "Preis (GÖCH) für Masterarbeit Erika Schaudy "Synthese von Hydrotyrosol" (Bezirksblätter & NÖN Woche 13/2019); Land NÖ fördert Forschung – Förderung des NMR Probenkopfes; Bericht über die Weihnachtsvorlesung/Chemie-Show (Bezirksblätter Tulln, 2019); Gemeindezeitung Raabs an der Thaya: Science Fair Award NÖ Bericht (Hubert Hettegger); "Molekularer Fingerprint" in Vinaria österreichische Zeitschrift für Weinkultur (2020, Number 7); "Virtuelle Realität und digitale Lehre an der BOKU: E-learning und Didaktik in Zeiten von Corona" in BOKU-Das Magazin der Universität des Lebens (06/2020), "E-Examinations im Großprüfungskontext: Rechtsprüfungen im Distanzmodus an der Universität für Bodenkultur Wien" (fnma Magazine, 18/12/2020); JungforscherInnen Kalender 2020 Niederösterreich (Hubert Hettegger); "Mähboote sind unterwegsVerpackungsmaterial aus Wasserpflanzen", PUSH-Dein tägliches Info-Magazin, 11/3/2021); "Bioraffinerie und viele Bäume" (Mein Bezirk, 15/03/2021); "An Interview with Max Lennart Feuerstein" (Agilent Science Futures, 17/11/2021); "New platform for exposome analysis" (EU Research, 06/2021); "Verpackung aus Wasserpflanzen erhält Energy Globe Award" (APA, 10/03/2021); "Beste Umweltprojekte prämiert" Energy Globe Award (NÖN Woche 03/2021)); "Jungforscher Hubert Hettegger im Porträt: "Cellulose in der Chromatographie-Säule" (03/2021: Chemiereport); "Rechercheplattform für Nachhaltigkeit und gegen Greenwashing" & "Nachhaltige Fasern: Grün, Grün, grün sind alle meine Kleider", (Inspektorin Grün, 27/11/2021).

"Chemieolympiade" 2019 and 2021

Continuing with an outreach started by Prof. Paul Kosma several years ago, the visit of groups of pupils from the Am Puls "Chemie Camp" program took place in 2019 and 2021. The program is organised by Verband der Chemielehrer Österreichs (VCÖ) and the Fachverband der Chemischen Industrie Österreichs (FCIO). The program is open to graduates of the "Chemistry Olympics" and provides them with opportunities to visit research laboratories in Vienna and obtain an insight into the everyday work of researchers, including at the Department of Chemistry, BOKU. The visit of pupils to DCh/BOKU was organised by Prof. Kosma in 2019 and supported by Gerhard Stingeder (Institute of Analytical Chemistry), Irene Schaffner (CF Biomolecular and Cellular Analysis) and Markus Blaukopf (Institute of Organic Chemistry). After an enforced hiatus in 2020, Tim Causon took over the organisation in 2021 and pupils were engaged in activities and discussions with Michael Traxlmayr (Biochemistry, CD-Lab for next generation CAR-T Cells), Georg Mlynek (CF Biomolecular and Cellular Analysis) and again Markus Blaukopf.

Science Talk

Michael Traxlmayr was an invited speaker at the Science Talk "Moderne Krebsforschung -Neue Chancen durch personalisierte Medizin?" organised by the Austrian Federal Ministry of Education Science and Research (BMBWF). He was joined by Ulrich Jäger (AKH Wien) and Petra Heffeter (Medical University Vienna) in the podium discussion moderated by Mario Wasserfaller (APA) at the Aula der Wissenschaft in Vienna (23/09/2019). A focus of the discussion was the current research efforts toward pushing the boundaries of what is feasible, so that what is considered unfeasible today will be feasible in twenty or thirty years for the treatment of cancer, particularly the prospects of personalized medicine.



Chemistry for kids at BOKU

The Department of Chemistry hosted approximately 50 students (8-11 years old) over two days in April 2019 for a "Chemistry for kids at BOKU" day. Organised by Viktoriya Vasilieva and Christina Steiner-Friedmann, the students were introduced in a workshop format to the world of chemistry in the context of teaching and research at BOKU including hands-on activities based on

our lab courses. The practical part of the workshop included the identification of an unknown sample (salt) using classical analytical tests. The students were introduced to the basics of scientific work and presented with a certificate upon successful identification of the unknown sample.



An additional goal of the workshop was to improve the understanding and appreciation of chemistry among students. Participating students responded after the workshop that they felt significantly better informed about what working in the field of "chemistry" means.

Broadcast, TV and film

Servus AKTUELL (*Flippr*), ServusTV Doku, ("*Bestäuben*, *befruchten*, *bewahren* - *Bienen* in *Gefahr*...", 10/07/2019), Ö3 Nachrichten: ("*Verpackung aus Wasserpflanzen*", 10/03/2021); and Radio Arabella ("*Verpackungsmaterial aus Wasserpflanzen*", 10/03/2021).





Chapter 9 Management and administration

The members of the Department of Chemistry see their duties mainly in teaching and research. However, to make these run properly, a lot of time must be spent on administration issues. Members of the department are representatives in local university committees and boards and also cover legal commitments. They are active members of national and international boards, evaluation committees as well as editors and reviewers for international journals.

University administration

- Department evaluation 2020
- ISO 45001 certification
- Members in habilitation committees
- Contributions to evaluations of other departments
- Contributions to the evaluation of the University's quality management
- Members of appointment committees for professorships
- EMAS Re-certification of the University

Members in university committees and boards

Friedrich Altmann:

• Member of the curricula committee *Food and Biotechnology*

Stephan Hann:

- Member of the curricula committee *Food and Biotechnology*
- Member of the VIBT steering group
- Chair of the CF Mass spectrometry advisory board

Hubert Hettegger:

• Member of the curricula committee Green Chemistry

Andreas Hofinger-Horvath:

- Member of the curricula committee for doctoral studies
- Member of the curricula committee *Food and Biotechnology*

Paul Kosma:

• Deputy chair of the "Ombudsstelle"

Falk Liebner:

• Member of BiRT steering group Tulln

Christian Obinger:

Vice Rector for Research and Innovation

Antje Potthast :

- Speaker of doctorate programme ABC-M (from 2020)
- Member of BiRT steering group Tulln
- Scientific Head of the CF ALICE

Thomas Rosenau:

- Member of the Senate/Deputy member of the Senate
- Member of Qualifizierungsbeirat
- Member of BiRT steering group Tulln
- Member of the curricula committee Green Chemistry
- Chair of the CF ALICE advisory board

Johannes Stadlmann:

• Scientific Head of the CF Mass spectrometry

Erika Staudacher:

- Dean of Studies (until 2020)
- Member of the VIBT steering group

National scientific community services

- Member of the Austrian Science Fund Kuratorium (lain Wilson)
- Christian-Doppler-Research Association, Board member (Paul Kosma)
- Member of the Austrian Agency for Scientific Integrity (Paul Kosma)
- Project evaluations (CD-labs, COMET, ÖAD, Austrian Academy of Sciences)
- Member of the Austrian National Bioeconomy Platform (Thomas Rosenau)
- Beirat Technisches Museum (Antje Potthast, Thomas Rosenau)
- Accreditation commission "Applied Chemistry" FH Krems (Thomas Rosenau)
- Wood Kplus board member (Antje Potthast)
- Austrian Society of Analytical Chemistry ASAC Board member and treasurer (Stephan Hann)
- Austrian Proteomics Association AUPA Board member (Stephan Hann)
- Austrian Green Chemistry Platform (Hubert Hettegger, Thomas Rosenau)
- Accountant and member of the Austrian Proteomics Association AUPA (Friedrich Altmann)



ISO 45001:2018

The Department of Chemistry is the first department at the University of Natural Resources and Life Sciences Vienna successfully certified for meeting all the requirements of a modern, operational occupational health and safety management system within the framework of ISO45001:2018 under the leadership of Andreas Hofinger-Horvath (Department of Chemistry), Marie-Christine Bruckner and Erik Griebl (both staff section for employment protection) since March 2020. In the meantime, the annually required reaudit has also been successfully passed.

Aim of this certification is to achieve the following goals

- Risk reduction
- Safer and healthier workplaces
- Easier incorporation of new employees
- Increase in motivation and gualification

ZERTIFIKAT Universität für Bodenkultur Wien Konrad Lore A-3430 Tullr 調証書 e Che ein Managementsy ngeführt hat und an rch ein Audit, Bericht-Nr. 1531844 eis erbracht, dass die Fo ISO 45001 : 2018 ind. Dieses Zertifikat ist gültig bis 31. Mai 2023 Zertifikat-Registrier-Nr. ASM1531368

CERTIFICAT

CERTIFICADO

СЕРТИФИКАТ

CERTIFICATE +

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ZERTIFIKAT

Certificate handover. Vice rector Gerhard Mannsberger (fourth from right), the team of the Department (Erika Staudacher, left; Andreas Hofinger-Horvath, holding certificate) and representatives of the staff section for employment protection.





International scientific community services

- Editorial Board Memberships or Editorial Advisory Panel Members in peer-reviewed SCI-journals: Analytical Chimica Acta, Chemical Monthly, Glycobiology, Glycoconjugate Journal, Journal of Biological Chemistry, Hydrogels, International Journal of Polymer Science, Holzforschung, Cellulose, Restaurator, Wood Science and Technology, Journal of Renewable Materials, Arkivoc, Current Organic Synthesis, Current Chromatography, The Open Macromolecules Journal, The Open Natural Products Journal, Current Organic Synthesis, Mini-Reviews in Organic Chemistry, Innate Immunity, Trends in Carbohydrate Chemistry, Biochemical Biophysical Acta
- Editors of Special Issues: Archives of Biochemistry and Biophysics, Biomolecules
- Reviewer for SCI journals several hundred per year
- Evaluator of international funding organisations (Deutsche Forschungsgemeinschaft DFG, Finland Academy of Sciences, Swedish Science Fund, National Science Foundation USA, US Department of Agriculture, US Department of Energy, USA, Netherlands Organisation for Scientific Research NWO, French CNRS, European Research Council (ERC), Canadian Research Council, Science Foundation Argentina, Israel Science Foundation, Slovenian National Research Council, Royal Irish Society, Institut Pasteur, Croatian Science Fund, MEraNet, Flandern Science Fund, KU Leuven Fund, Canadian Nat. Sci. and Engin. Research Concil, Swiss Science Fund, Deutsche Bundesstiftung Umwelt, Fund for Scientific Research - FNRS - Belgium, Romanian Executive Agency for Higher Education, Research, Development and Innovation Funding, Edene - European Doctoral Program in Energy and Environment, BMBF - Basis Bioeconomy International, Hungarian Scientific **Research Funds**

Member of evaluation commissions for professorship and senior scientist appointments (University of Vienna, Austria; "Sustainable chemistry", "Organic Chemistry", Barcelona Univ., Spain; Professorship, "Biological chemistry", The University of Kyoto, Japan; Professorship, "Biochemistry", Helsinki University, Finland; Tenure-track position "Renewable materials", Freiburg Univ., Germany; Tenure-track position "Organic Chemistry", RWTH Aachen, Germany; "Physical chemistry", The University of Tokyo, Japan; "Biomaterial chemistry", Lund University, Sweden; "Organic chemistry", Cologne Univ., Germany; "Biobased materials", FH Rosenheim, Germany, "Mikrobiologie" FH Hildesheim, Germany, "Color chemistry and material science", Academy of Fine Arts, Vienna; "Sustainable Bioproducts Innovation", Aalto University, Finland; "Reversible Chemistry", Chalmers University/WWSC, Gothenburg, Sweden; "Lignocellulose chemistry and Engineering" Aalto University, Finland

- Austrian delegate of the *Division of Chemistry and the Environment* in EuChemS (Stephan Hann)
- Representative of Austria in the International Carbohydrate Organization ICO (Paul Kosma, until 2019)
- Representative of Austria in the European Carbohydrate Organization ECO (Paul Kosma, until 2019)
- Member of the University Council of Shinshu University, Ueda, Japan (Thomas Rosenau)
- National Finnish Bioeconomy Council, member (Thomas Rosenau)
- Elected Member of the Executive Committee of the Cellulose and Renewable Materials Division (CELL) of the American Chemical Society (Falk Liebner)
- Adjunct Professor of Fiber Chemistry, Shinshu University, Japan (Thomas Rosenau)
- Adjunct Professor at the Johan Gadolin Process Chemistry Center, Abo Academy, Turku, Finland (Thomas Rosenau)
- Advisory Board "Klassik Stiftung Weimar" and Anna Amalia Library, Germany (Antje Potthast)
- Advisory Board, Basel University Library, Switzerland (Antje Potthast)
- Advisory Board "Förderverein Papierrestaurierung" (Association for the Promotion of Paper Conservation), Stuttgart, Germany (Antje Potthast)
- Implementation and maintaining of the website of the International Glycoconjugate Organization (2013-2017)
- Scientific Councilor in chemistry of the International Endotoxin and Innate Immunity Society (Alla Zamyatina)
- Member EC stakeholder group "Single use plastics directive" (Antje Potthast)
- Austrian Representative in COST Action 18125 "Aerogels" (Falk Liebner)

DEPARTMENT REPRESENTATIVES AND OFFICERS

First Aid

Markus Bacher Thomas Grasi Stefan Hofbauer Philip Lackner Christoph Luef Katharina Paschinger Bruna Pekec Antje Potthast Sonja Schiehser Thomas Schmidt Christina Steiner-Friedmann Philipp Tondl Viktoriya Vasilieva Petra Viehauser

Fire protection (Brandschutzwart)

Markus Blaukopf Rudolf Figl Hubert Hettegger Alexandra Hofinger Thomas Schmidt Christina Steiner-Friedmann Philipp Tondl

Michael Traxlmayr Viktoriya Vasilieva Petra Viehauser

Safety Officer Stefan Böhmdorfer Thomas Dalik Andreas Hofinger-Horvath

Chemicals Stefan Böhmdorfer Andreas Hofinger-Horvath

Disposal Christiane Gollner Andreas Hofinger-Horvath Sonja Schiehser

Biological Safety Michael Traxlmayr Iain Wilson **Gases** Thomas Dalik

IT-Masteruser Markus Blaukopf Stefan Böhmdorfer Stefan Hofbauer

Teaching Andreas Hofinger-Horvath

e-learning Andreas Zitek

Department report Tim Causon Paul Furtmüller Stefan Hofbauer

Department homepage Luzia Kneisz

Research Stephan Hann Michael Traxlmayr

Laser safety Tim Causon

Ethics Tim Causon Sonja Schiehser

Internationalisation Falk Liebner Alla Zamyatina

Data Protection Markus Blaukopf Stefan Böhmdorfer Stefan Hofbauer

Infosec Markus Blaukopf Stefan Böhmdorfer Stefan Hofbauer



Appendix A Projects

For further information please visit the research information system (FIS) of our university: <u>https://forschung.boku.ac.at/fis</u>

771 Analytical Chemistry

Already running 2019

Title: ISOfood – Tracing provenance and authenticity of food (ISOfood)
Project leader: Hann Stephan
Financing: austrian companies (2017-2031)
Grant amount: € 300.000,-

Title: Modern mass spectrometry strategies for metabolomics (MS-STRAT)
Project leader: Hann Stephan
Financing: Agilent Technologies Inc. (2018-2022)
Grant amount: € 144.495,-

Title: Entwicklung eines multi-methodischen Ansatzes für das Studium von Wildtierverhalten: Untersuchung von Mensch-Bär-Konflikten in gegensätzlichen europäischen Landschaften (SLObear)
Project leader: Hann Stephan
Financing: EU (2017-2020)
Grant amount: € 20.900,-

Title: Investigation of migration and provenance of eel using multielement and Sr – isotope pattern. (IsoEel)
Project leader: Hann Stephan
Financing: Sustainable Eel Group, London (2017-2020)
Grant amount: € 38.564,-

Title: "ISOprint" - Development of "Diffusive Gradient in Thin Films (DGT) – multi-collector ICP-MS techniques" for location-specific isotopic fingerprinting of S, Sr and Pb in soils as a tool for the provenance determination of primary agricultural products (ISOprint)
Project leader: Hann Stephan
Financing: FWF (2017-2020)
Grant amount: € 358.699,-

Title: Development and application of separation methods and mass spectrometric methods in the field of non-targeted analysis of water (WV-NTA-DAC)
Project leader: Hann Stephan
Financing: Stadt Wien, Österreich (2016-2021)
Grant amount: € 72.000,-

Title: Analysis of technology-related metals in the environment (TRM) Project leader: Hann Stephan

Financing: Solutions 4 Science Handels GmbH, Mitterndorf an der Fischa, Österreich (2016-2022) Grant amount: € 14.400,-

Title: Feed and Food Quality Safety and Innovation (FFoQSI)

Project leader: Hann Stephan
Financing: K1-Projekt im Rahmen einer strategischen
Beteiligung COMET (2016-2021)
Grant amount: € 776.000,-

Title: Austrian Centre of Industrial Biotechnology (acib)
Project leader: Hann Stephan
Financing: K1-Projekt im Rahmen einer strategischen
Beteiligung COMET (2015-2019)
Grant amount: € 300.000,-

Title: Monitoring of nitrate and nitrite during sugar production and reduction of nitrite in molasses (MoNiSu) II
Project leader: Domig Konrad, Hann Stephan
Financing: Agrana Research (2018-2021)
Grant amount: € 25.000,-

Title: Monitoring of nitrate and nitrite during sugar production and reduction of nitrite in molasses (MoNiSu) III
Project leader: Domig Konrad, Hann Stephan
Financing: Agrana Research (2018-2021)
Grant amount: € 25.000,-

Title: Classification of wine by determination of bioactive phenolic compounds using high resolution mass spectrometry

Project leader: Causon Tim
Financing: OeAD-GmbH, Vienna, Austria (2017-2019)
Grant amount: € 5.960,-

Title: Bestimmung der Elementmobilisierung in bioabbaubaren Implantaten (DegSTRUT)
Project leader: Hann Stephan
Financing: BIOTRONIK AG, Erlangen, Germany (2016-2020)
Grant amount: € 163.000,-



2019-2021 - new

Title: Renewable turbulent flow chromatography for exposomics (TFC)
Project leader: Cocovi Solberg David, Stephan Hann
Financing: FWF (2019-2021)
Grant amount: € 156.140,-

Title: Collision cross section as an identification point for steroids in chemical exposure studies
Project leader: Causon Tim
Financing: OeAD (2020-2022)
Grant amount: € 5.300,-

Title: Below ground crop/weed interaction (CROP/WEED) Project leader: Hann Stephan Financing: FWF (2020-2023) Grant amount: € 175.527,-Title: Analytical μ-Platform for Automated Cell Factory Screening (μ-CFS) Project leader: Causon Tim Financing: Agilent Technologies (2021-2022) Grant amount: € 45.000,-

772 Biochemistry

Already running 2019

Title: Nicotiana prolyl hydroxylase acting on proteins Project leader: Altmann Friedrich Financing: FWF (2017-2021) Grant amount: € 278.841,-

Title: Developing Multipurpose Nicotiana crops for molecular farming using new plant breeding techniques (NEWCOTIANA)
Project leader: Stöger Eva (DAGZ), Altmann Friedrich
Financing: EC (2017-2020)
Grant amount: € 103.000,-

Title: Structure and function of invertebrate Golgi hexosaminidases

Project leader: Wilson lain Financing: FWF (2016-2021) Grant amount: € 349.671,-

Title: Biosynthesis of helminth N-glycoproteins in insect cells
Project leader: Wilson Iain, Shi Yan
Financing: FWF (2017-2021)
Grant amount: € 32.320,- (partner VetMed)

2019-2021 - new

Title: N-glycan epitopes in bivalve self/non-self recognition Project leader: Paschinger Katharina Financing: FWF (2019-2023) Grant amount: € 408.000,- Title: Ion formation in ion mobility-mass spectrometry Project leader: Valadbeigi Younes, Causon Tim Financing: FWF (2021-2023) Grant amount: € 175.780,-

Title: Rock glaciers as groundwater storages in alpine catchments and their impact on downstream river systems with regard to climate change (AlpCatch)
Project leader: Fischer Lisa
Financing: Federal Ministry Republic of Austria, Agriculture, Regions and Tourism (2020-2023)
Grant amount: € 31.733,-

Title: "FFoQSI: Authenticity and Quality" within FFoQSI Blue Area: Smart Technologies - Scientific innovations for sustainable food chains (FFoQSI - C30-P11-W01) Project Leader: Hann Stephan Financing: FFG (2021-2024) Grant amount: € 430.571,-

Title: Doktoratskolleg plus "Biomolecular Technology of Proteins"

Project leader: Oostenbrink Chris Financing: FWF/BOKU (2019-2023) Grant amount: € 4.612.230,-

Title: Biochemistry of HemQ Project leader: Hofbauer Stefan Financing: FWF (2016-2021) Grant amount: € 272.506,-

Title: Unravelling the function in chlorite dismutases and related peroxidases by EPR
Project leader: Obinger Christian
Financing: FWF (2016-2019)
Grant amount: € 152.271,-

Title: Structural and mechanistic studies on a dimeric chlorite dismutase
Project leader: Obinger Christian
Financing: FWF (2018-2020)
Grant amount: € 327.678,-

Title: Glycan structure and biosynthesis in Entamoeba Project leader: Wilson Iain, Duchene Michael Financing: FWF (2019-2023) Grant amount: € 174.760,- (partner MUW)

Department of Chemistry

Title: Metabolic degradation of methylated glycans Project leader: Staudacher Erika Financing: FWF (2020-2024) Grant amount: € 398.480,-

Title: The dipteran glycan array Project leader: Wilson Iain Financing: FWF (2021-2025) Grant amount: € 406.087,-

Title: Multi-omics analysis of the fluke parasite Opisthorchis felinus (fluke multiomics)
Project leader: Hykollari Alba, Paschinger Katharina
Financing: FWF (2021-2024)
Grant amount: € 55.205,- (partner VetMed)

Title: Next generation CAR-T cells
Project leader: TraxImayr Michael (cooperation with St. Anna Kinderspital)
Financing: FFG - Christian Dopper Laboratory (2019-2026)
Grant amount: € 1.401.237,-

Title: SPIN – a novel scaffold for the design of inhibitors
for human peroxidases
Project leader: Obinger Christian
Financing: FWF (2020-2024)
Grant amount: € 364.288,-

Title: Biochemistry of coproporphyrin ferrochelatases Project leader: Hofbauer Stefan Financing: FWF (2020-2025) Grant amount: € 354.947,-

Title: Molecular evolution of heme peroxidases from Cephalochordata
Project leader: Zamocky Marcel, Furtmüller Paul
Financing: FWF (2020-2023)
Grant amount: € 169.694,-

Title: In-depth studies of actinobacterial ChdC Project leader: Hofbauer Stefan Financing: FWF (2021-2025) Grant amount: € 386.925,-

773 Organic Chemistry

Already running 2019

Title: Molecular basis of binding interactions of pyruvylated cell wall polymers Project leader: Schäffer Christina (DNBT) in coop. (Kosma Paul) Financing: FWF (2014-2019) Grant amount: ~110.000,- (part)

Title: Synthetic bacterial analogs of mammalian oligomannose Project leader: Kosma Paul Financing: NIH (2017-2022) Grant amount: \$ 485.068,-

2019-2021 – new

Title: Synthetic glycolipids for exploration of inflammation and sepsis.
Project leader: Zamyatina Alla
Financing: FWF (2019-2023)
Grant amount: € 406.108,-

Title: Molecular basis of cell wall polymer pyruvylation
Project leader: Schäffer Christina (DNBT) in coop. Kosma
Paul, Blaukopf Markus
Financing: FWF (2019-2024)
Grant amount: €~110.000,- (part)

Title: Synthetic conformationally confined Lipid A mimetics for exploration of lipopolysaccharide recognition by the proteins of the innate immune system Project leader: Zamyatina Alla Financing: FWF (2016-2019) Grant amount: € 352.779,-

Title: Synthesis of donor substrates of 4-amino-4-deoxy-L-arabinose transferases Project leader: Kosma Paul Financing: FWF (2016-2019) Grant amount: € 349.960,-

Title: Synthesis of functionalized sugar nucleotide donors for the glycan microarray-based identification and characterization of plant glycosyltransferases.
Project leader: Pfrengle Fabian
Financing: DFG (2020-2023)
Grant amount: € 171.617,-

Title: Homogeneous bicomponent glycoconjugate vaccines Project leader: Trattnig Nino Financing: FWF (2021-2022) Grant amount: € 84.630,- (part)

Title: The dipteran glycan array Project leader: Wilson Iain, coop. Zamyatina Alla Financing: FWF (2021-2025) Grant amount: € 130.000,- (part)



774 Chemistry of Renewable Ressources

Already running 2019

Title: K plus WOOD
Project leader: Rosenau Thomas, Potthast Antje, Böhmdorfer Stefan, Liebner Falk
Financing: FFG – Forschungsförderungsgesellschaft, Bundesländer, Industriepartner (2011-2014, 2015-2023)
Grant amount: € 80.000,-

Title: Future Lignin and Pulp Processing Research (FLIPPR II) Project leader: Rosenau Thomas, Potthast Antje, Böhmdorfer Stefan, Gindl-Altmutter Wolfgang, Konnerth Johannes Financing: FFG - Österreichische Forschungsförderungsgesellschaft (2017-2021) Grant amount: € 5.825.414,-

Title: Lignin Shaping (Shaping)
Project leader: Potthast Antje, Rosenau Thomas
Financing: FFG – Forschungsförderungsgesellschaft (2017-2021)
Grant amount: € 192.500,-

Title: Lignin and Liquor Utilization Pllatform (Liliput) Project leader: Potthast Antje, Rosenau Thomas Financing: FFG – Forschungsförderungsgesellschaft (2017-2021) Grant amount: f 522 500 -

Grant amount: € 532.500,-

Title: Fiber platform, BOKU part (Fiber) Project leader: Rosenau Thomas, Potthast Antje Financing: FFG – Forschungsförderungsgesellschaft (2017-2021) Creat amount: 6 150 000

Grant amount: € 150.000,-

Title: Complexing agents (Complexing Agents)
Project leader: Rosenau Thomas
Financing: FFG – Forschungsförderungsgesellschaft (2017-2021)
Grant amount: € 192.500,-

Title: Odour Reduction in Biorefinery Products (Odour)
Project leader: Böhmdorfer Stefan
Financing: FFG – Forschungsförderungsgesellschaft (2017-2021)
Grant amount: € 195.200,-

Title: FunEnzFibers: Von Grundlagen zur Nutzung;
Enzymatische Oxidation von Cellulose
Project leader: Potthast Antje
Financing: Forest Value call (EU) (2018-2023)
Grant amount: € 286.000,-

Title: Nanocell: Einsatz von nano-oder microfibrillierten Cellulosen für die Stabilisierung und Restaurierung von historischem Papier

Project leader: Potthast Antje Financing: Anna Amalia Bibliothek/Eigenforschung (2018-2021)

Grant amount: € 65.000,-

Title: Lignin als Bindemittelkomponente für Holzwerkstoffe
Project leader: Potthast Antje
Financing: Industry (2017-2019)
Grant amount: € 116.500,-

Title: Austrian Biorefinery Center Tulln (BOKU-ABCT) Project leader: Rosenau Thomas, Potthast Antje Financing: NÖ, 10 Companies, BOKU (2017-2022) Grant amount: € 2.400.000,-

Title: ABCT_Tissue: Modification of cellulosics towards high performance tissues
Project leader: Potthast Antje
Financing: 10 Companies, BOKU (2017-2022)
Grant amount: € 120.000,-

Title: ABCT_Bark: Processing of bark towards green biorefinery applications
Project leader: Potthast Antje
Financing: 10 Companies, BOKU (2017-2022)
Grant amount: € 120.000,-

Title: ABCT_Lignosulfonates: Lignosulfonates as starting compounds in future biorefineries
Project leader: Rosenau Thomas
Financing: 10 Companies, BOKU (2017-2022)
Grant amount: € 120.000,-

Title: ABCT TrafoPaper: Special papers with high thermal resistace Project leader: Rosenau Thomas

Financing: 10 Companies, BOKU (2017-2022) Grant amount: € 120.000,-

Title: ABCT_Textile: Chemistry of novel, environmentally benign textile treatments
Project leader: Rosenau Thomas
Financing: 10 Companies, BOKU (2017-2022)
Grant amount: € 120.000,-

Title: ABCT_NIR: NIR – fast process control Project leader: Böhmdorfer Stefan Financing: 10 Companies, BOKU (2017-2022) Grant amount: € 180.000,- Title: Doktoratskolleg Advanced Biorefineries: Chemistry & Materials (ABC&M) Project leader: Potthast Antje Financing: BOKU (2018-2022) Grant amount: € 375.000,-

Title: Auslöser und Angriffspunkte der Ascaridol-Wirkung in Leishmanien
Project leader: Rosenau Thomas
Financing: FWF (2015-2021)
Grant amount: € 268.300,-

Title: Endophytic Sebacinales and arbuscular mycorrhiza: putative synergists in plant growth promotion and biocontrol of Fusarium oxysporum f. sp. Lycopersici
Project leader: Böhmdorfer Stefan
Financing: FWF (2017-2020)
Grant amount: € 14.000,-

2019-2021 – new

Title: GRETE Project leader: Potthast Antje Financing: EU H2020 (2019-2023) Grant amount: € 290.000,-

Title: POLIGOM – Porous lignin organic materials
Project leader: Smirnova (DE, Konsortialführung und Gesamt-PL), Liebner (AT, Partner)
Financing: FFG (2019-2022)
Grant amount: € 215.685,- (BOKU part)

Title: LIBIKO II – Lignin als Bindemittelkomponente
Project leader: Potthast Antje
Financing: Industry (2020-2023)
Grant amount: € 116.000,-

Title: Oxidative modification of cellulose Project leader: Potthast Antje Financing: Industry (2020-2022) Grant amount: € 200.000,-

Title: 5D-click-printing Project leader: Beaumont Marco Financing: FWF (2020-2022) Grant amount: € 43.190,-

Title: Science Call Nadine Kohlhuber Project leader: Potthast Antje Financing: NFB (2020-2024) Grant amount: € 61.339,- Title: Dechiffering the chemical language of fungi and their resoinses to the chemical environment (Fungal Language)
Project leader: Böhmdorfer Stefan
Financing: WWTF (2017-2021)
Grant amount: € 50.413,-

Title: TALKoutTOXINS: Understanding fungal communication to modulate production of antibiotics and mycotoxins
Project leader: Böhmdorfer Stefan
Financing: FWF (2017-2021)
Grant amount: € 7.200,-

Title: Triboelectric reduction of particulate air pollution and formation of dust clouds in wood processsing Project leader: Frömel-Frybort, Liebner Falk (partner) Financing: Wood K plus (2020-2022) Grant amount: € 22.000,-

Title: Bilateral Mobility Project CZ Project leader: Liebner Falk Financing: OEAD (2019) Grant amount: € 6.000,-

Title: Traditional Monoglian medicinal plants Project leader: Rosenau Thomas Financing: OEAD (2022) Grant amount: € 7.950,-

Title: NFB Chirality Project leader: Hettegger Hubert Financing: NFB NÖ (2021-2025) Grant amount: € 257.277,-

Title: Diacetyl Schnelltest Project leader: Böhmdorfer Stefan Financing: FFG (2021-2022) Grant amount: € 12.121,-

Title: Valid GCxGC Project leader: Rosenau Thomas Financing: Interreg (2021-2024) Grant amount: € 192.400,-

Title: POLYSTAB Project leader: Rosenau Thomas Financing: ATHENOE (2021-2024) Grant amount: € 197.334,-



Appendix B Publications

For further information please visit the research information system (FIS) of our university: <u>https://forschung.boku.ac.at/fis</u>

771 Analytical Chemistry

Original articles and reviews in refereed journals

2019

Belina-Aldemita, MD; Opper, C; Schreiner, M; D'Amico, S. (2019) Nutritional composition of pot-pollen produced by stingless bees (*Tetragonula biroi Friese*) from the Philippines. J Food Compos Anal. 2019; 82, UNSP 103215.

Carrasco-Correa, EJ; Kuban, P; Cocovi-Solberg, DJ; Miro, M. (2019) Fully automated electric-field-driven liquid phase microextraction system with renewable organic membrane as a front end to high performance liquid chromatography. Anal Chem. 2019; 91(16): 10808-10815.

Causon, TJ; Ivanova-Petropulos, V; Petrusheva, D; Bogeva, E; Hann, S. (2019) Fingerprinting of traditionally produced red wines using liquid chromatography combined with drift tube ion mobility-mass spectrometry. Anal Chim Acta. 2019; 1052: 179-189.

Causon, TJ; Si-Hung, L; Newton, K; Kurulugama, RT; Fjeldsted, J; Hann, S. (2019) Fundamental study of ion trapping and multiplexing using drift tube-ion mobility time-of-flight mass spectrometry for non-targeted metabolomics. Anal Bioanal Chem. 2019; 411(24):6265-6274.

Cindric, IJ; Zeiner, M; Starcevic, A; Stingeder, G. (2019) Metals in pine needles: characterisation of bio-indicators depending on species. IntJ Environ Sci Te. 2019; 16(8): 4339-4346.

Fikarova, K; Cocovi-Solberg, DJ; Rosende, M; Horstkotte, B; Sklenalova, H; Miro, M. (2019) A flow-based platform hyphenated to on-line liquid chromatography for automatic leaching tests of chemical additives from microplastics into seawater. J Chromatogr A. 2019; 1602: 160-167.

Gabelica, V; Shvartsburg, AA; Afonso, C; Barran, P; Benesch, JLP; Bleiholder, C; Bowers, MT; Bilbao, A; Bush, MF; Campbell, JL; Campuzano, IDG; Causon, T; Clowers, BH; Creaser, CS; De Pauw, E; Far, J; Fernandez-Lima, F; Fjeldsted, JC; Giles, K; Groessl, M; Hogan, CJ; Hann, S; Kim, HI; Kurulugama, RT; May, JC; McLean, JA; Pagel, K; Richardson, K; Ridgeway, ME; Rosu, F; Sobott, F; Thalassinos, K; Valentine, SJ; Wyttenbach, T. (2019) Recommendations for reporting ion mobility Mass Spectrometry measurements. Mass Spectrom Rev. 2019; 38(3):291-320.

Le, SH; Troyer, C; Causon, T; Hann, S. (2019) Sensitive quantitative analysis of phosphorylated primary metabolites using selective metal oxide enrichment and GC- and IC- MS/MS. Talanta. 2019; 205, 120147.

Mairinger, T; Sanderson, J; Hann, S. (2019) GC-QTOFMS with a lowenergy electron ionization source for advancing isotopologue analysis in C-13-based metabolic flux analysis. Anal Bioanal Chem. 2019; 411(8): 1495-1502.

Mairinger, T; Kurulugama, R; Causon, TJ; Stafford, G; Fjeldsted, J; Hann, S. (2019) Rapid screening methods for yeast sub-metabolome analysis with a high-resolution ion mobility quadrupole time-of-flight mass spectrometer. Rapid Commun Mass Spectrom. 2019; 33 Suppl 2:66-74.

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Rottensteiner, H; Kaufmann, S; Rathgeb, A; Kink, B; Plaimauer, B; Matthiessen, P; Hann, S; Scheiflinger, F. (2029) Temperature-dependent irreversible conformational change of recombinant ADAMTS13 upon metal ion chelation. J Thromb Haemost. 2019; 17(6):995-1002.

Ruano, A; Zitek, A; Hinterstoisser, B; Hermoso, E. (2019) NIR hyperspectral imaging (NIR-HI) and mu XRD for determination of the transition between juvenile and mature wood of *Pinus sylvestris* L. Holzforschung 2019; 73(7): 621-627.

Schneider, M; Keiblinger, KM; Paumann, M; Soja, G; Mentler, A; Golestani-Fard, A; Retzmann, A; Prohaska, T; Zechmeister-Boltenstern, S; Wenzel, W; Zehetner, F. (2019) Fungicide application increased copper-bioavailability and impaired nitrogen fixation through reduced root nodule formation on alfalfa. Ecotoxicology. 2019; 28(6):599-611.

Shoham, E; Prohaska, T; Barkay, Z; Zitek, A; Benayahu, Y. (2019) Soft corals form aragonite-precipitated columnar spiculite in mesophotic reefs. Sci Rep. 2019; 9(1):1241.

Strashnov, I; Izosimov, I; Gilmour, JD; Denecke, MA; Almiral, J; Cannavan, A; Chen, G; Dissanayake, C; Doroshenko, I; Elghali, T; Enston, E; Fernando, BR; Kasozi, G; Kelly, S; Maqsood, M; Muhammad, SA; Muryn, C; Pomerantsev, AL; Singh, DK; Smith, G; Taous, F; Webb, C; Williamson, D; Xu, ZZ; Yangg, SM; Zitek, A. (2019) A laser ablation resonance ionisation mass spectrometer (LA-RIMS) for the detection of isotope ratios of uranium at ultra-trace concentrations from solid particles and solutions. J Anal Atom Spectrom. 2019; 34(8): 1630-1638.

Tchaikovsky, A; Häusler, H; Kralik, M; Zitek, A; Irrgeher, J; Prohaska, T. (2019) Analysis of $n(^{87}Sr)/n(^{86}Sr)$, $\delta^{88}Sr/^{86}Sr_{SRM987}$ and elemental pattern to characterise groundwater and recharge of saline ponds in a clastic aquifer in East Austria. Isotopes Environ Health Stud. 2019; 55(2):179-198.

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Theiner, S; Schoeberl, A; Fischer, L; Neumayer, S; Hann, S; Koellensperger, G. (2019) FI-ICP-TOFMS for quantification of biologically essential trace elements in cerebrospinal fluid - high-throughput at low sample volume. Analyst. 2019; 144(15):4653-4660.

Urban, M; Hann, S; Rost, H. (2019) Simultaneous determination of pesticides, mycotoxins, tropane alkaloids, growth regulators, and pyrrolizidine alkaloids in oats and whole wheat grains after online clean-up via two-dimensional liquid chromatography tandem mass spectrometry. J Environ Sci Heal B. 2019; 54(2): 98-111.

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Zeiner, M; Kuhar, A; Cindric, IJ. (2019) Geographic differences in element accumulation in needles of Aleppo Pines (*Pinus halepensis* Mill.) grown in mediterranean region. Molecules. 2019; 24(10), 1877.

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2020

Bauer, R; Tondl, P; Schneider, WJ. (2020) A differentiation program induced by bone morphogenetic proteins 4 and 7 in endodermal epithelial cells provides the molecular basis for efficient nutrient transport by the chicken yolk sac. Dev Dynam. 2020; 249(2): 222-236.

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Delgado-Povedano, MDM; de Villiers, A; Hann, S; Causon, T. (2020) Identity confirmation of anthocyanins in berries by LC–DAD–IM-QTOFMS. Electrophoresis, 2020. Fischer, L; Hann, S; Worsfold, PJ; Miro, M. (2020) On-line sample treatment coupled with atomic spectrometric detection for the determination of trace elements in natural waters. J Anal Atom Spectrom. 2020; 35(4): 643-670.

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Oliver, M; Roca-Jimenez, M; Miro, M; Cocovi-Solberg, DJ. (2020) In quest of effect directed analysis in the smart laboratory: Automated system for flow-through evaluation of membranotropic effects of emerging contaminants. Talanta. 2020; 209, 120600.

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Széliová, D; Schoeny, H; Knez, Š; Troyer, C; Coman, C; Rampler, E; Koellensperger, G; Ahrends, R; Hann, S; Borth, N; Zanghellini, J; Ruckerbauer, DE. (2020) Robust analytical methods for the accurate quantification of the total biomass composition of mammalian cells. Methods Mol Biol. 2020; 2088:119-160.



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Books and book chapters

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Conferences and workshop proceedings, abstracts

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Appendix C Cooperation partners

771 Analytical Chemistry

Rebekka Birke

AGRANA Research & Innovation Center GmbH, Monitoring of nitrate and nitrite in the course of sugar production and reduction of nitrite in molasses (MoNiSu)

Elisabeth Bondar-Kunze

Institute of Hydrobiology and Aquatic Ecosystem Management, BOKU

The trophic cascade of herbicides: Effects of herbicides and their metabolites on non-target organisms (periphyton & macroinvertebrates) (HINT)

Heike Brielmann

Umweltbundesamt Österreich, Wien, Österreich; Spurenstoffe im Grundwasser

Hermann Bürstmayr

Institute of Plant Breeding, BOKU cooperation partner Dokoratskolleg "AgriGenomics"

David Bunt

Sustainable Eel Group, Fishmongers Hall, London, UK Investigation of the migration and origin of eel using Sr isotopes and multi-element fingerprints (IsoEel)

Ruwan Kurulugama

Agilent Technologies, Santa Clara, USA Modern Mass Spectrometric Strategies for Metabolomics (MS-STRAT)

Eva Oburger

Institute of Soil Research, BOKU cooperation partner Mysterium Root Exudates - New Insights into Ecologically Relevant Exudate Sampling Approaches (REX), The biogeochemistry of tungsten (W) in the soil-plant continuum (FWF-W), Wanted: Micronutrients! Phytosiderophore-mediated acquisition strategies in grass crops (PhytoTrace)

Chris Oostenbrink

Institute of Molecular Modeling and Simulation (MMS), BOKU cooperation partner Doktoratskolleg plus "Biomolecular Technology of Proteins" (BioToP)

Markus Puschenreiter

Institute of Soil Research, BOKU cooperation partner Interaction of crops and weeds in the soil (CROP/WEED)

Florian Stein

Technical University Braunschweig, Deutschland Investigation of the migration and origin of eel using Sr isotopes and multi-element fingerprints (IsoEel)

Clive Trueman

University of Southampton, UK Investigation of the migration and origin of eel using Sr isotopes and multi-element fingerprints (IsoEel)

Franz Weigang

Agilent Technologies GmbH, Austria Modern Mass Spectrometric Strategies for Metabolomics (MS-STRAT)

Gerfried Winkler

Karl Franzens Universität Graz, Universitätsplatz 2, 8010 Graz, Österreich;

Blockgletscher als Grundwasserspeicher in alpinen Einzugsgebieten und ihr Einfluss auf übergeordnete Flusssysteme unter dem Einfluss des Klimawandels (AlpCatch)

Judith Wirth

AGROSCOPE, Nyon, Switzerland Interaktion von Nutzpflanzen und Beikraut im Boden (Markus Puschenreiter)

Wolfgang Zerobin

MA 31 Wiener Wasserwerke, Wien, Österreich Development and application of separation methods and mass spectrometric methods in the field of untargeted analysis of water (WV-NTA-DAC)

772 Biochemistry

Daniel Abed-Navandi Haus des Meeres Wien, Austria Glycoepitopes of N-Glycans in Echinodermata

Coenraad M. Adema University of New Mexico, Albuquerque, USA Metabolic degradation of methylated glycans

Gianantonio Battistuzzi

University of Modena and Reggio Emilia, Italy Redox thermodynamics of chorite dismutase, peroxidasins and dye-decolorizing peroxidases

Pedro Bonay Miarons

Universidad Autónoma de Madrid, Spain Metabolic degradation of methylated glycans

Jin Chunsheng Göteborgs Universitet, Sweden LC-MS analyses of N- and O-glycans

Mike Davies

Department of Biomedical Sciences, University of Copenhagen, Denmark The leucine-rich repeat domain of human peroxidasin 1 promotes binding to laminin in basement membranes

Kristina Djinović-Carugo

University of Vienna, Austria Molecular mechanisms and catalysis of oxidoreductases

Michael Duchene Medizinische Universität Wien, Austria Glycan structure and biosynthesis in Entamoeba

Reingard Grabherr Department of Biotechnology, BOKU cooperation partner Metabolic degradation of methylated glycans

Alba Hykollari Veterinärmedizinische Universität Wien Multi-omics analysis of the fluke parasite *Opisthorchis felinus*

Tony Kettle, Christin Winterbourn University of Otago, New Zealand Peroxidasin protein expression and enzymatic activity in metastatic melanoma cell lines

Daria Kokova

Tomsk State University, Russia Multi-omics analysis of the fluke parasite *Opisthorchis felinus*

Manfred Lehner

CCRI – Children's Cancer Research Institute, Austria Engineering next generation CAR T Cells

Chris Oostenbrink

Chair of Molecular Simulation, BOKU cooperation partner Modelling

Nina Siragusa

Merck KGaA, Germany Polysaccharide in *Pichia*

Giulietta Smulevich

Università degli Studi di Firenze, Italy Resonance Raman spectroscopy studies on peroxidases, chlorite dismutases, and coproheme decarboxylases and ferrochelatases

Stefan Tögel

Meduni Wien, Austria Role of glycosylation in joint cell function

Pierre Van Antwerpen

Université Libre de Bruxelles, Belgium Ligand-based pharmacophore modelling and structurebased virtual screening for the discovery of novel myeloperoxidase inhibitors

Sabine Van Doorslaer

Department of Physics, University of Antwerp, Belgium. Role of the flexible arginine in chlorite dismutases.

Gerardo Vasta

University of Maryland, USA Glycosylation of bivalves and their parasites

Shi Yan

Veterinärmedizinische Universität Wien Biosynthesis of helminth N-glycoproteins in insect cells



773 Organic Chemistry

Youssef Belkhadir Gregor Mendel Institute, Vienna, Austria Plant Innate Immunity

Rudi Beyaert University Ghent, Belgium TLR4 ligands

Jesus Arenas Busto Utrecht University, Belgium LPS B. pertussis

Stephen Evans University of Victoria, Canada LPS ligands; SCWP-S-Layer interaction

Jean-Baptiste Farcet Takeda, Vienna, Austria NMR of polysialylated glycoconjugates

Dietmar Haltrich Department of Food Sciences and Technologies, BOKUcooperation partner NMR of milk oligosaccharides

Arvand Haschemi Medical University Vienna, Austria Biochemistry and metabolism of sedoheptulose phosphate

Holger Heine Research Center Borstel, Germany Innate Immune response in primary immune cells

Laura Kiessling University of Wisconsin-Madison, USA LPS ligands for human intelectin binding studies

Renate Kunert Department of Biotechnology, BOKU-cooperation partner HIV antibodies

Thomas Meyer Max-Planck Institute of Infectious Biology, Berlin, Germany Heptosyl bisphosphate (HBP) Antonio Molina, Hugo Melida University of Madrid, Spain Title of the project: Plant Immune Activation

Chris Oostenbrink Chair of Molecular Simulation, BOKU-cooperation partner Modelling

Ralph Pantophlet Simon Fraser University, Canada Synthesis of bacterial mimetics of HIV gp120 glycan epitopes

Irma Schabussova Medical University of Vienna, Austria Toxocara antigens

Christina Schäffer Department of Nanobiotechnology, BOKU-cooperation partner NMR of S-Layer glycans and SCWP, Liposomes

Herbert Strobl Medical University Graz, Austria Immune response, Bacterial OMV

Breeanna Urbanowicz, Michael Hahn University of Georgia, USA Plant Cell Wall GTs

Peter Van der Ley Intravacc, The Netherlands Title of the project: LPS B. pertussis

Miguel A. Valvano Queen's University Belfast, Ireland Aminoarabinose ligands

Ian Wilson Scripps, USA Synthesis of bacterial mimetics of HIV gp120 glycan epitopes

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Cyril Aymonier

Institut de Chimie de la Matière Condensée de Bordeaux CNRS, France Synthesis and characterization of quantum dots for cellulose hybrid aerogels

Mikhail Balakshin

Aalto University, Espoo, Finland Lignin, chemistry, analysis and utilization, lignin structure, NMR spectroscopy of technical lignins

Gerhard Banik

State Academy of Art and Design, Stuttgart, Germany Conservational science, damage assessment of historic cellulosic objects

Wolfgang Bauer Technical University, Graz, Austria Pulp and paper science

Thomas Bechtold University of Innsbruck, Innsbruck, Austria Textile chemistry

Manuel Becker

LVWO Weinsberg, Referat Weinbau und Rebschutz, Germany Polysaccharide analysis

Eric Breitung

The Metropolitan Museum of Art, New York, USA Cellulose conservation science

Irene Brückle Ute Henniges

Staatliche Akademie der Bildenden Künste Stuttgart, Germany Loan traffic of cultural objects, aging of paper, analytics

Ewellyn Capanema ROSE Stockholm, Sweden Lignin chemistry, analysis and utilization, NMR spectroscopy of lignins

Vince Edwards

United States Department of Agriculture, USA Peptide-modified cellulosic aerogels for diagnostic protease sensing

Tomoki Erata Hokkaido University, Japan Solid state NMR spectroscopy, special CPMAS NMR techniques

Vincent Eijsink

Norwegian University of Life Sciences (NMBU), As, Norway Modification of celluloses by enzymes, cellulose analysis

Alfred French

USDA Agricultural Research Service, New Orleans, USA Solid state structure of cellulose and cellulose model compounds Computational carbohydrate chemistry

Lars Gille

University of Veterinary Medicine, Vienna, Austria EPR spectroscopy, spin trapping, testing of antioxidants in biological model systems, tocopherol and ubiquinone chemistry

Wolfgang Gindl-Altmutter, Ulrich Müller, Johannes Konnerth

Institute of Wood Technology and Renewable Materials, BOKU cooperation partner, Tulln Wood science

Yasuo Gotoh

Shinshu University, Ueda, Japan Cellulosic fibers, novel spinning technology, ionic liquids for cellulose spinning

Ulrike Hähner

Hochschule für angewandte Wissenschaft und Kunst Hildesheim, Holzminden, Göttingen Iron gall ink corrosion of paper

Merima Hasani

Chalmers University, Gothenburg Cellulose modification, cellulose oxidation, cellulose dissolution

Adriaan van Heiningen

University of Maine at Bangor, Chemical Engineering, USA Advanced pulping processes and modern biorefinery scenarios

Thomas Heinze

University of Jena, Germany Cellulose chemistry, derivatives of cellulose and other polysaccharides

Hendrikus W.G. van Herwijnen

Kplus, UFT Tulln, Austria Wood binders



Saida Ibragic University of Sarajevo, Bosnia and Herzegovina Analysis of plant extractives, medical plants

Akira Isogai University of Tokyo, Graduate School of Agricultural and Life Sciences, Japan Cellulose oxidation and analysis

Christian Jäger Bundesanstalt für Materialforschung Berlin (BAM), Germany Solid state NMR spectroscopy of celluloses and cellulose derivatives, special CPMAS NMR techniques

Myung-Joon Jeong Jeonbuk National University, Jeonju, South-Korea Cellulose conservation science

Kanji Kajiwara Shinshu University, Nagano, Japan Fiber technology, fiber modification

Toshinari Kawada Kyoto Prefectural University, Japan Synthesis of (isotopically labeled) cellulose model compounds

Ilkka Kilpelainen University of Helsinki, Finland Cellulose chemistry, NMR spectroscopy, novel ionic liquids

Alistair King University of Helsinki, Finland Cellulose chemistry, NMR spectroscopy of cellulose, ionic liquids

Mirjana Kostic University of Belgrade, Faculty of Technology and Metallurgy, Serbia Oxidative fiber modification

Marie-Pierre Laborie University of Freiburg, Germany Ionic liquids in cellulose and biomass processing

Wolfgang Lindner University of Vienna, Austria Chiral chromatography

Nilufar Mamadalieva

Leibniz Institute of Plant Biochemistry (IPB), Halle, Germany Analysis of plant extractives, traditional medical plants

Herman Mansur Federal University of Minas Gerais, Brazil Biobased nanomaterials

Petra Mischnick University of Braunschweig, Institute of Technology, Germany Analysis of polysaccharide building blocks

Hanna de la Motte RISE Stockholm, Sweden Textile chemistry

Fumiaki Nakatsubo Kyoto University, Japan Synthesis of (isotopically labelled) cellulose as well as cellulose and lignin model compounds

Jean-Marie Nedelec Institute of Chemistry, Clermont-Ferrand, France Cellulosic aerogels for tissue engineering applications

Christine Betty Nagawa Makerere University, Uganda Analysis of plant extractives, traditional medical plants

Thomas Netscher DSM Nutritional Products, Switzerland Chemistry of vitamin E and phenolic antioxidants

John Ralph University of Madison-Wisconsin Modification and characterisation of lignin

Kousaku Ohkawa Shinshu University, Department of Functional Polymer Science, Japan Intelligent fibers and functional textiles, fiber chemistry

José C. del Río Instituto de Recursos Naturales y Agrobiología de Sevilla (IRNAS-CSIC), Spain Lignins of annual plants, lignin analysis

Keita Sakakibara Kyoto University, Japan Biocompatible cellulosic aerogels with well-defined polymer brushes

Herbert Sixta

Aalto University, Helsinki, Finland / Lenzing AG, Austria Pulp and paper technology, biorefineries and biomass processing

Irina Smirnova

TU Hamburg-Harburg, Germany Development of lignin-based aerogels and carbon aerogels

Anna Sundberg

Åbo Akademi University, Turku, Finland Characterization of wood extractives by GC-MS, pulping and bleaching chemistry

Yasumitsu Uraki

Hokkaido University, Sapporo, Japan Chemistry of Biomaterials

Stina Grönqvist, Jenni Rahikainen

VTT Technical Research Centre of Finland Ltd, Espoo, Finland Pulp modification by enzymes, cellulose analysis

Tapani Vuorinen

Aalto University, Finland Characterisation of cellulosic pulps, reaction mechanisms in bleaching

Stefan Willför

Åbo Akademi University, Turku, Finland Characterization of wood extractives by GC-MS, novel pulping and spinning approaches, pulping and bleaching chemistry

Chunlin Xu

Åbo Akademi University, Turku, Finland Lignin characterization, fractionation and utilization



Appendix D Courses

Overview Teaching Portfolio 2020/2021

(Source: BOKUonline, Department site)

* semester hours = hours per week during the whole semester (approx. 14 weeks)

Abbreviations: engl, in English; PR, practical work; S, summer term; SE, seminar; VO, lecture; VS, lecture with seminar; UE, practical course; W, winter term;)

770 - Courses

770100	W	Allgemeine und anorganische Chemie (AW)	2	VO	
770102	W	Chemische Übungen (AW)	4	UE	
770113	W	Bachelorseminar	2	SE	
770150	W	Allgemeine Chemie	3	VO	
770151	W	Allgemeine Chemie (UBRM)	3	VO	
770152	W	Allgemeine Chemie	3	VO	
770101	S	Organische Chemie und Biochemie (AW)	3	VO	
770102	S	Chemische Übungen (AW)	4	UE	
770113	S	Bachelorseminar	2	SE	
770152	S	Allgemeine Chemie	3	VO	

• 7 different courses (20 semester hours*)

 \bullet Three courses in winter as well as in summer semester \rightarrow 29 semester hours

• In English: 0

771 - Courses

		I	<u> </u>	1	
771004	W	Dissertantenseminar aus Analytischer Chemie	2	SE	engl
771040	W	Masterseminar	2	SE	
771100	W	Einführung in die Chemie	3	VO	
771102	W	Einführung in die Chemie Übungen	2	UE	
771106	W	Instrumentelle Analytische und Physikalische Chemie Übungen	6	UE	
771109	W	Allgemeine und Physikalische Chemie	3	VO	
771118	W	Chemisches Rechnen I	1	VU	
771004	S	Dissertantenseminar aus Analytischer Chemie	2	SE	engl
771005	S	Advanced analytical methods in chemical oceanography	2	VO	engl
771040	S	Masterseminar	2	SE	
771100	S	Einführung in die Chemie	3	VO	
771105	S	Analytische Chemie Übungen	7	UE	
771108	S	Analytische Chemie	4	VO	
771303	S	Environmental and biotechnological analysis	2	VO	engl
771316	S	Chemisches Rechnen II	1	VU	

771317	S	Advanced instrumental analytical chemistry	3	VU	engl
771318	S	Project-based training on modern analytical techniques	4	UE	engl
771319	S	Determination of provenance and authenticity of food and food products	2	VS	engl
		by modern analytical methods			

• 15 different courses (44 semester hours*)

 \bullet Three courses in winter as well as in summer semester \rightarrow 51 semester hours

 \bullet Courses held several times: 771102 - 3 times, 771105 - 3 times, 771106 - 3 times \rightarrow 81 semester hours

• In English: 6 (17 semester hours)

772 - Courses

		1		
w	Masterseminar	2	SE	engl
W	Dissertantenseminar aus Biochemie	2	SE	engl
W	Grundlagen der Biochemie	3	VO	
W	Biochemische Übungen I	5	UE	
W	Practical course in biochemistry II	5	UE	engl
W	Biochemistry of trace elements	2	VO	engl
W	Glycobiology	2	VO	engl
W	Biochemie der Pflanzen	2	VO	
W	Biochemical seminar	2	SE	engl
W	Advanced practical course in biochemistry	3	PR	engl
W	Biochemical and biotechnological methods (analytics design)	3	VU	engl
W	Methods in protein characterization	4	VU	engl
W	Basic Course I - anylisis, design and engineering of proteins	2	VO	engl
S	Masterseminar	2	SE	engl
S	The molecular mechanisms of cancer immunotherapies	2	VO	engl
S	Dissertantenseminar aus Biochemie	2	SE	engl
S	Biochemische Übungen I	5	UE	
S	Biochemie des Stoffwechsels	3	VO	
S	Biophysical Chemistry	2	VU	engl
S	Protein chemistry and protein engineering	3	VU	engl
S	Practical course in biochemistry II	5	UE	engl
S	Proteomics	2	VU	engl
S	Kinetics of biochemical reactions	2	VU	engl
S	Advanced practical course in biochemistry	3	PR	engl
S	IC IA - spectroscopic and calorimetric analysis of proteins	2	UE	engl
S	Journal club BioTop II	1	SE	engl
	W W W W W W W W W W W W W S	WDissertantenseminar aus BiochemieWGrundlagen der BiochemieWBiochemische Übungen IWPractical course in biochemistry IIWBiochemistry of trace elementsWGlycobiologyWBiochemie der PflanzenWBiochemical seminarWAdvanced practical course in biochemistryWBiochemical and biotechnological methods (analytics design)WBiochemical and biotechnological methods (analytics design)WBasic Course I - anylisis, design and engineering of proteinsSMasterseminarSThe molecular mechanisms of cancer immunotherapiesSDissertantenseminar aus BiochemieSBiochemie des StoffwechselsSBiophysical ChemistrySProtein chemistry and protein engineeringSProteomicsSKinetics of biochemical reactionsSKinetics of biochemical reactionsSIC IA - spectroscopic and calorimetric analysis of proteins	WDissertantenseminar aus Biochemie2WGrundlagen der Biochemie3WBiochemische Übungen I5WPractical course in biochemistry II5WBiochemistry of trace elements2WGlycobiology2WBiochemie der Pflanzen2WBiochemical seminar2WBiochemical seminar3WBiochemical and biotechnological methods (analytics design)3WBiochemical and biotechnological methods (analytics design)3WBasic Course I - anylisis, design and engineering of proteins2SMasterseminar2SDissertantenseminar aus Biochemie2SBiochemische Übungen I5SBiochemische Übungen I5SBiochemistry and protein engineering3SProtein chemistry and protein engineering3SProtein chemistry and protein engineering3SProteomics2SKinetics of biochemical reactions2SKinetics of biochemical reactions2SAdvanced practical course in biochemistry3SIC IA - spectroscopic and calorimetric analysis of proteins2	WDissertantenseminar aus Biochemie2SEWGrundlagen der Biochemie3VOWBiochemische Übungen I5UEWPractical course in biochemistry II5UEWBiochemistry of trace elements2VOWGlycobiology2VOWBiochemie der Pflanzen2VOWBiochemical seminar2SEWAdvanced practical course in biochemistry3PRWBiochemical and biotechnological methods (analytics design)3VUWMethods in protein characterization4VUWBasic Course I - anylisis, design and engineering of proteins2SESThe molecular mechanisms of cancer immunotherapies2VOSBiochemische Übungen I5UESBiochemistry and protein engineering3VOSBiophysical Chemistry2VUSProtein chemistry and protein engineering3VUSProteomics2VUSProteomics2VUSKinetics of biochemistry II5UESKinetics of biochemical reactions2VUSAdvanced practical course in biochemistry3PRSIC IA - spectroscopic and calorimetric analysis of proteins2U

• 21 different courses (54 semester hours*)

 \bullet Five courses in winter as well as in summer semester \rightarrow 71 semester hours

- \bullet Courses held several times: 772112 10 times, 772305 6 times $\, \rightarrow \,$ 131 semester hours
- In English: 17 (53 semester hours)



773 - Courses

773108	W	Organische Chemie Übungen	3	UE	
773113	W	Organische Chemie für Lebensmittel- und Biotechnologen	3	vo	
773572	W	Masterseminar	2	SE	engl
773803	W	Dissertantenseminar aus Organischer Chemie	2	SE	engl
773010	S	Advances in protein crystallography	2	vo	engl
773108	S	Organische Chemie Übungen	3	UE	
773111	S	Chemische Übungen für Kulturtechniker	3	UE	
773114	S	Organische Chemie Übungen	3	UE	engl
773119	S	Chemische Übungen	4	UE	
773120	S	Organische Chemie	2	vo	
773310	S	Bioorganic chemistry	2	vo	engl
773311	S	Introduction into crystallography and NMR spectroscopy of proteins	2	vo	engl
773316	S	Modern methods in structural analyses	3	VU	engl
773572	S	Masterseminar	2	SE	engl
773803	S	Dissertantenseminar aus Organischer Chemie	2	SE	engl

• 12 different courses (31 semester hours*)

 \bullet Three courses in winter as well as in summer semester \rightarrow 38 semester hours

 \bullet Courses held several times: 773108/773114 - 10 times $\rightarrow\,$ 49 semester hours

• In English: 7 (20 semester hours)

774 - Courses

				,	
774110	w	Biomaterialchemie	2	VO	
774301	w	Chemie und Technologie nachwachsender Rohstoffe	2	VO	engl
774304	W	Masterseminar	2	SE	engl
774314	W	Biopolymers for sustainable utilization	2	VO	engl
774326	W	Chemikalien aus Biomasse	2	VO	
774327	W	Polymerchemie und Technologie	2	VO	
774402	W	Presenters club	1	SE	engl
774404	W	Dissertantenseminar Nachwachsende Rohstoffe	2	SE	engl
774405	W	Biorefinery I	2	VO	engl
774406	W	Scientific tools for ABC&M I	2	SE	engl
774109	S	Chemie NAWAROS	1	UE	
774125	S	Chemische Technologie NAWAROS	2	VO	
774304	S	Masterseminar	2	SE	engl
774305	S	Plant polysaccharde analysis	2	VO	engl
774322	S	Chemische Prozesse in Atmosphäre, Hydrosphäre und Geosphäre	2	VO	
774404	S	Dissertantenseminar Nachwachsende Rohstoffe	2	SE	engl
774408	S	Scientific retreat ABC&M I	3	SE	engl

• 15 different courses (29 semester hours*)

- \bullet Two courses in winter as well as in summer semester \rightarrow 33 semester hours
- In English: 9 (22 semester hours)

Courses of other departments with participation of lecturers from Chemistry

				-	
750405	W	Seminar to basic course / - analysis, design and engineering of proteins	1	SE	engl
740417	W	Journal club BioTop I	1	SE	engl
752347	W/S	Practical course in protein engineering and technology	5	PR	engl
790019	W/S	Contemporary science: international seminars at VIBT	1	SE	engl
802421	W	Doctoral Seminar BioTop I	1	SE	engl
891119	W	Utilisation of Renewable Materials	2	SE	engl
911332	W	Humus	2	VO	
930100	W	Einführung in die Agrarwissenschaften	2	VO	
930402	W	Seminar AgriGenomics I	0,5	SE	engl
940319	W	Cell and Molecular Biology I	3	VO	engl
940424	W	Seminar AgriGenomics III	0,5	SE	engl
970302	W	Naturstofftechnologien und Eigenschaften	3	PR	
970308	W	Bioraffinerie und Produkte aus nachwachsenden Rohstoffen	1	VO	
970403	W	Biorefinery journal club ABC&M	2	SE	engl
752345	S	Enzyme reactions: mechanisms and kinetics	2	VO	engl
790404	S	Lab rotation BioMatInt	1,5	UE	engl
891117	S	Bachelorseminar	2	SE	
891401	S	Biorefinery II	2	SE	engl
891402	S	Scientific tools for ABC&M II	2	SE	engl
891403	S	Scientific tools presenters club for ABC&M	1	SE	engl
891405	S	Scientific retreat ABC&M II	3	SE	engl
910402	S	Seminar AgriGenomics II	0,5	SE	engl
940402	S	Basic course II - biosynthesis, post-translational modifications and trafficking of recombinant proteins	2	VO	engl
940422	S	Doctoral Seminar BioTop II	1	SE	engl
950402	S	Seminar AgriGenomics IV	0,5	SE	engl
970402	S	Bio-Resources and Technologies	2	SE	engl
970406	S	Annual retreat AgroiGenomics	2	SE	engl

Summary

In total 770-771-772-773-774 (without participation in other departments):

- 70 different courses (178 semester hours*)
- Due to multiple runs $\rightarrow 323$ semester hours
- In English: 39 courses (112 semester hours)