



Vorwort

Die Österreichische Gesellschaft für Analytische Chemie (ASAC) lädt gemeinsam mit der Fachgruppe Analytische Chemie in der Gesellschaft Deutscher Chemiker und der Division Analytische Wissenschaften der Schweizerischen Chemischen Gesellschaft (SCS) zur ANAKON 2023 ein, die an der Technischen Universität Wien veranstaltet wird.



Ein herzliches Willkommen zur ANAKON 2023 !

Als wichtigste gemeinsame Konferenz und zugleich Aushängeschild der deutschen, österreichischen und schweizerischen Analytischen Chemie bietet die ANAKON 2023 die Möglichkeit zu einem persönlichen wissenschaftlichen Austausch zwischen Analytikerinnen und Analytikern aus dem deutschsprachigen Raum – aber natürlich auch darüber hinaus. Der starken Internationalisierung der Forschung wollen wir dadurch Rechnung tragen, dass die wissenschaftlichen Beiträge auf Englisch präsentiert werden sollen.

Die rasante Entwicklung, die wir in den letzten Jahren in allen wichtigen Bereichen unseres Lebens beobachtet haben, wäre ohne die Beiträge und Leistungen der Analytischen Chemie undenkbar, wenn nicht sogar unmöglich gewesen: Die Analytische Chemie mit ihrer immer größer werdenden Vielfalt an innovativen und leistungsstarken Methoden ist wesentliches Element in den Materialwissenschaften, sie unterstützt pharmazeutische Entwicklungen und ermöglicht Diagnostik im medizinischen und therapeutischen Umfeld. Sie wird bei der Herstellung und Kontrolle der Sicherheit von Lebensmitteln eingesetzt, im Umweltschutz und in der Prozessüberwachung. Analytische Chemie trägt nicht nur zum grundlegenden Erkenntnisgewinn bei, sondern auch zur Erhöhung der Qualität und Wertschöpfung unserer Produkte und zum Schutz der menschlichen Gesundheit. Gerade dieser Aspekt wurde durch die Corona-Pandemie der breiten Öffentlichkeit eindrucksvoll vor Augen geführt.

Die ANAKON 2023 hat sich zum Ziel gesetzt, gerade dieser Vielfalt und Innovation im Bereich der Analytischen Chemie den passenden Rahmen zur Präsentation zu bieten.

Wir freuen uns daher ganz besonders, dass die ANAKON 2023 nach einer pandemiebedingten Unterbrechung nun wieder in Präsenz stattfinden kann, und hoffen, Sie bei der ANAKON 2023 in Wien begrüßen zu dürfen!

Foreword

The Austrian Society for Analytical Chemistry (ASAC), together with the Analytical Chemistry section of the Society of German Chemists and the Analytical Sciences Division of the Swiss Chemical Society (SCS), invite you to ANAKON 2023 which is being held at the TU Wien.

A warm welcome to ANAKON 2023!

As the most important joint conference and at the same time the flagship event for German, Austrian and Swiss analytical chemistry, ANAKON 2023 offers the opportunity for a personal scientific exchange between analysts from German-speaking countries - and of course also beyond. We would like to take account of the strong internationalization of research by inviting the scientific contributions in English.

The rapid development that we have witnessed in recent years in all areas of our daily lives would have been unthinkable, if not impossible without the contributions and achievements of analytical chemistry: with its ever-increasing variety of innovative and powerful methods, analytical chemistry is an essential driver in materials science, it supports pharmaceutical developments and enables diagnostics in the medical and therapeutic environment. It is used in the production and control of food safety, in environmental protection and in process monitoring. Analytical chemistry not only contributes to gaining fundamental knowledge, but also to increasing the quality and added value of our products and protecting human health. This aspect in particular was brought to the attention of the general public by the Corona pandemic.

Without doubt, ANAKON 2023 will offer the right setting for the presentation of this diversity and innovation in the field of analytical chemistry.

We are therefore delighted that ANAKON 2023 can now take place again in person after a pandemic-related interruption, and we sincerely hope to be able to welcome you to ANAKON 2023 in Vienna!



Martina Marchetti-Deschmann



Erwin Rosenberg



Victor U. Weiss

Conference Chairs ANAKON 2023

Conference Committees

Conference Chairs

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Erwin Rosenberg	TU Wien	Austria
Victor U. Weiss	TU Wien	Austria

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Peter Lieberzeit	Universität Wien	Austria
Andreas Limbeck	TU Wien	Austria
Hanno Stutz	Paris-Lodron-Universität Salzburg	Austria
Renato Zenobi	ETH Zurich	Switzerland

Conference Venue TU Wien

In 2023, ANAKON will take place right in the center of Vienna, at TU Wien. Under the motto "Technology for people" research, teaching and learning have been carried out at TU Wien for more than 200 years. TU Wien is Austria's largest research and educational institution in the field of technology and natural sciences. More than 5.400 scientists conduct research in five research areas at eight faculties. The content of the studies offered is derived from excellent research. Around 30.000 students in 55 courses benefit from it. About 1.500 students are enrolled in Technical Chemistry.

TU Wien is one of the few university locations in Austria where Analytical Chemistry is represented by three professorships. The research topics that are dealt with here together with cooperation partners from academia and industry are diverse and make Analytical Chemistry a sought-after course content, especially for students.

ANAKON 2023 will be organized in the so-called "Freihaus" of TU Wien, right in the center of Vienna. The conference venue is in the immediate vicinity of the central local transport hub "Karlsplatz", which is connected by underground lines U1, U2, and U4, tram lines 1, 2 and 65 and bus lines 4A and 59A.



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For the lectures, the conference venue offers spacious and modern lecture halls, which are equipped with up-to-date AV technology. The posters are co-located in the wide corridors between the lecture halls, where the company exhibition and coffee breaks take place, and provide ample opportunities for lively discussions and interactions.

An on-site restaurant is available, but as the venue is just a few minutes' walk from the very popular Naschmarkt (food market), there are plenty of welcoming restaurants, bars and cafes where you can enjoy a hearty lunch, a cool drink, or savor a delicious cup of coffee.

Welcome Event

The ANAKON 2023 welcome event will take place on Tuesday, April 11th, 2023 at the conference site. From 18h00 onwards, directly after the final session of this day, you can meet with friends, enjoy some snacks and discuss science with your colleagues.

Conference Dinner

We are delighted to announce that the conference dinner of ANAKON 2023 will take place in the festive hall of the Vienna City Hall ("Rathaus") on Thursday, April 13th, 2023. The location can be easily reached from the conference site either after a scenic 25 min walk along Ringstraße or via public transport (approx. 15 min transfer time). Please contact the ANAKON 2023 crew in case you have questions how to get there.



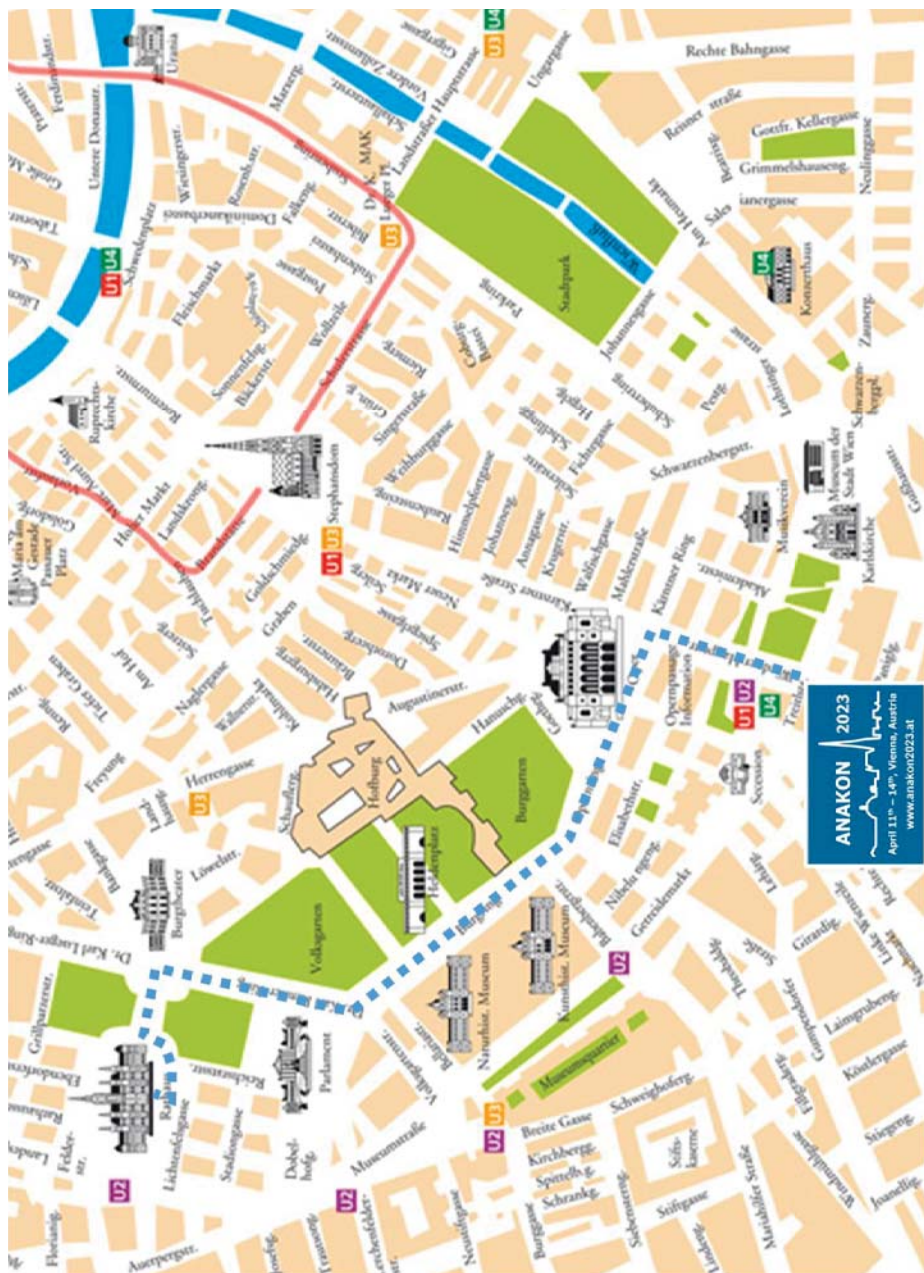
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The Vienna City Hall was built from 1872 -1883 on Ringstraße in Neo-Gothic style. It houses a great festive hall of 71 meters length and 20 meters width which provides the perfect setting for our conference dinner. The 18.5-meter-high hall is lined on three sides by a gallery, the fourth side opens onto the town hall square via a loggia. We are looking forward to meeting you there, at the ANAKON 2023 conference dinner! Please do not forget to register for this event – an extra registration is mandatory!

Vienna City Map



Program Overview

11.04.2023							
Room 1		Room 2		Room 3		Room 4	
Main Lecture Hall		Lecture Hall 5		Lecture Hall 6		Nöbauer Lecture Hall (Lecture Hall 8)	
		10h00 - 12h00 Hochschullehrtreffen					
12h30 - 12h40 ORGANIZERS							
12h40 - 12h50 M. MIHOVILOVIC							
12h50 - 13h05 R. KRŠKA							
13h05 - 13h15 ASAC Honorary Membership - C. HUHN							
13h15 - 14h00 Freseniuspreis - M. THEVIS							
14h00 - 14h45 Plenary Lecture - K. GERWERT							
14h45 - 16h00 Coffee Break, Exhibition, Poster Setup ANAKON for 13.04.2023							
Session A 16h00 - 18h00 "Omics"		Session B 16h00 - 18h00 "Miniaturization"		Session C 16h00 - 18h00 "Process Analysis"		Session D 16h00 - 18h00 "Biosensing"	
18h00 - 21h30 Welcome Reception							
12.04.2023							
Room 1		Room 2		Room 3		Room 4	
Main Lecture Hall		Lecture Hall 5		Lecture Hall 6		Nöbauer Lecture Hall (Lecture Hall 8)	
08h15 - 08h20 Session Opening							
08h20 - 08h55 Fachgruppenpreis - N. STRITTMATTER							
08h55 - 09h30 H. Malissa Award - G. KÖLLENSPERGER							
09h30 - 10h15 Plenary Lecture - K. STERFLINGER							
10h15 - 11h15 Coffee Break, Exhibition							
Session E 11h15 - 13h15 "Clinical Analysis"		Session F 11h15 - 13h15 "Cultural Heritage"		Session G 11h15 - 13h15 "Separation Sciences"		Session H 11h15 - 13h15 "Spectroscopic Applications"	
13h15 - 14h15 Lunch Break, Exhibition							
13h30 - 14h15 Lunchtime seminar SHIMADZU		13h30 - 14h15 Lunchtime seminar S.T. JAPAN-EUROPE GmbH		13h30 - 14h15 Lunchtime seminar BRUKER		13h30 - 14h15 Lunchtime seminar CAREER IN INDUSTRY	
14h15 - 15h45 Poster Session							
Session I 15h45 - 17h45 "Imaging"		Session J 15h45 - 17h45 "Foodomics"		Session K 15h45 - 17h45 "Lipidomics"		Session L 15h45 - 17h45 "Micro-/Nanoplastics"	
17h45 - 18h45 Exhibition, Poster Exchange for 13.04.2023							
18h00 - 19h00 Meeting Mitgliederversammlung / Wahl		19h00 - 20h30 Meeting AK Chemometrie und Qualitätssicherung (Beleites)		19h00 - 20h00 Meeting DAAS (Engelhard)			
19h00 - 20h30 Meeting AK Separation Sciences (Vogel)		20h00 - Open-end Meeting (external location) Junganalytiker:innen Treffen (Viehoff)					

13.04.2023							
Room 1		Room 2		Room 3		Room 4	
Main Lecture Hall		Lecture Hall 5		Lecture Hall 6		Nöbauer Lecture Hall (Lecture Hall 8)	
08h55 - 09h00 Session Opening							
09h00 - 09h30 DAAS Preis Award - C. KIRSCHBAUM							
09h30 - 10h15 Plenary Lecture and Fritz Pregl Medal Award - B. MIZAIKOFF							
10h15 - 11h15 Coffee Break, Exhibition							
Session M 11h15 - 13h45 "Session honouring the 80th birthday of the Fritz-Pregl-Medal (ASAC) awardee W. Lindner"		Session N 11h15 - 13h15 "Spectroscopy"		Session O 11h15 - 13h15 "Environmental Analysis"		Session P 11h15 - 13h15 "Industrial Analysis"	
13h15 - 14h15 Lunch Break, Exhibition							
13h30 - 14h15 Lunchtime seminar AGILENT	13h30 - 14h15 Lunchtime seminar AB SCIEX	13h30 - 14h15 Lunchtime seminar BRUKER		13h30 - 14h15 Lunchtime seminar CAREER IN ACADEMIA			
14h15 - 15h45 Poster Session							
Session Q 15h45 - 17h45 "Elemental Analysis"		Session R 15h45 - 17h45 "Chemometrics"		Session S 15h45 - 17h45 "Ion Mobility"		Session T 15h45 - 17h45 "Separation Science"	
18h45 - 00h00 Conference Dinner - Vienna City Hall							
14.04.2023							
Room 1		Room 2		Room 3		Room 4	
Main Lecture Hall		Lecture Hall 5		Lecture Hall 6		MassSpec Forum Vienna 2023	
						Poster Setup MassSpec Forum	
Session U 09h00 - 11h00 "Food Authenticity and Safety"		Session V 09h00 - 11h00 "Material Analysis"		Session W 09h00 - 11h00 "Nanoscopy"		Session X 09h00 - 11h00 "Mass Spectrometry"	
11h00 - 11h30 Coffee Break, Exhibition							
11h30 - 13h30 Science Slam for Selected Posters for Poster Prize						Session Y 11h30 - 13h30 "Mass Spectrometry"	
13h30 - 14h30 Lunch Break, Exhibition							
14h30 - 15h15 Plenary Lecture - D. GÜNTHER						Session Z 15h00 - 16h20 "Mass Spectrometry"	
15h15 - 15h30 Poster Prizes Awarded							
15h30 - 15h45 EuroAnalysis 2023							
15h45 - 16h00 ANAKON 2025							
16h00 - 16h15 Closing, Farewell						16h20 - 16h35 Closing, Farewell	
Poster Removal ANAKON						Poster Removal MassSpec Forum	

Session Overview

Session A – “Omics”

Tuesday, April 11th 2023, 16h00 – 18h00

Main Lecture Hall (Lecture Hall 1)

Chair: G. Köllensperger

Co-Chair: tba

KN01	16h00 - 16h40	<i>R. Schumacher</i>	“Stable isotope-assisted metabolomics of plants and fungi”
O01	16h40 - 17h00	<i>R. Schmid</i>	“Enriching Molecular Networks by repository-scale MS searches in microbe monocultures and plant and food extracts”
O02	17h00 - 17h20	<i>A. Vadakkechira</i>	“Comparison of on-line breath analysis using SESI-MS with exhaled breath condensate”
O03	17h20 - 17h40	<i>F. Herzog</i>	“Quantitative crosslinking and mass spectrometry indicates kinetochore complex stabilization”
O04	17h40 - 18h00	<i>K. Böttinger</i>	“HPLC-MS aided quantification of minor abundant glycosylation species of monoclonal antibodies”

Session B – “Miniaturization”

Tuesday, April 11th 2023, 16h00 – 18h00

Lecture Hall 5

Chair: D. Belder

Co-Chair: tba

KN02	16h00 - 16h40	<i>S. Eeltink</i>	“Novel microchip designs for establishing the next generation of multi-dimensional LC”
O05	16h40 - 17h00	<i>M. van der Loh</i>	“Analysis of double emulsion droplets with ESI-MS”
O06	17h00 - 17h20	<i>A. Hohensee</i>	“Developing a multiplex PCR for the highly parallel detection of respiratory pathogens on a Lab-on-a-Chip Platform”
O07	17h20 - 17h40	<i>T. Mayr</i>	“Determination of respiration and acidification rates in dynamic cell cultures and organ-on-chips”
O08	17h40 - 18h00	<i>M. Breitfeld</i>	“High-throughput droplet-printing of concentration gradients for multimodal fluorescence and MALDI-MS analysis”

Session C – “Process Analysis”

Tuesday, April 11th 2023, 16h00 – 18h00

Lecture Hall 6

Chair: B. Lendl

Co-Chair: K. Wieland

KN03	16h00 - 16h40	<i>M. Maiwald</i>	“Quantitative NMR Spectroscopy (qNMR) as an Indispensable Instrumental Analytical Method and its Metrological Application”
O09	16h40 - 17h00	<i>B. Gruber</i>	“Comprehensive analytics for screening waste streams”
O10	17h00 - 17h20	<i>C. Herwig</i>	“On-line coupling of HPLC – Potentials for real time control of product quality and process performance”
O11	17h20 - 17h40	<i>A. Schwaighofer</i>	“Laser-based IR Spectroscopy for In-Line Monitoring of Proteins in Preparative Chromatography”
O12	17h40 - 18h00	<i>D. Friebe</i>	“Process-accompanying analysis of phosphorus species by ETV-ICP-OES”

Session D – “Biosensing”

Tuesday, April 11th 2023, 16h00 – 18h00

Nöbauer Lecture Hall (Lecture Hall 8)

Chair: P. Lieberzeit

Co-Chair: tba

KN04	16h00 - 16h40	<i>N. Nakatsuka</i>	“Bioanalytical Nanotools to Quantify Neurotransmitters in the Brain”
O13	16h40 - 17h00	<i>J. Brandmeier</i>	“Digital and analog upconversion-linked immunosorbent assay for the detection of SARS-CoV-2”
O14	17h00 - 17h20	<i>S. Passreiter</i>	“Automated detection of neutralizing SARS-CoV-2 antibodies using a competitive chemiluminescence immunoassay”
O15	17h20 - 17h40	<i>F. Thier</i>	“Towards rapid and cost-effective sensing for thrombocyte viability monitoring using QCM”
O16	17h40 - 18h00	<i>G. Morlock</i>	“2LabsToGo system with disruptive analytical strategy”

Session E – “Clinical Analysis”

Wednesday, April 12th 2023, 11h15 – 13h15

Main Lecture Hall (Lecture Hall 1)

Chair: *R. Birner-Grünberger*

Co-Chair: *I. Burger*

KN05	11h15 - 11h55	<i>A. Sickmann</i>	“Quantification of therapeutic proteins with focus on TDM”
O17	11h55 - 12h15	<i>C. Huber</i>	“Tackling extreme proteoform complexity by means of chromatography and mass spectrometry”
O18	12h15 - 12h35	<i>S. Hold</i>	“Novel orphan disease diagnostic environment – advances in mass spectrometry for clinical analysis”
O19	12h35 - 12h55	<i>A. Kabir</i>	“Biofluid Sampler: A New Arsenal for Clinical Studies using Whole Blood”
O20	12h55 - 13h15	<i>X. Fu</i>	“Advanced unified monophasic lipid extraction protocol with wide coverage on the polarity scale optimized for large-scale untargeted clinical lipidomics analysis of platelets”

Session F – “Cultural Heritage”

Wednesday, April 12th 2023, 11h15 – 13h15

Lecture Hall 5

Chair: *M. Schreiner*

Co-Chair: *tba*

KN06	11h15 - 11h55	<i>K. Janssens</i>	“Non-invasive (chemical) imaging of works of art – some case studies illustrating current possibilities and limitations”
O21	11h55 - 12h15	<i>S. Caterino</i>	“New insight in the chemistry of iron-gall inks through the use of an innovative methodological approach”
O22	12h15 - 12h35	<i>A. Malissa</i>	“Spectroscopy-Driven Characterization of Degradation-Induced Changes in Sheep Parchment for Early Damage Assessment”
O23	12h35 - 12h55	<i>H. Khaliliyan</i>	“Hemicelluloses in Rag Paper”
O24	12h55 - 13h15	<i>R. Haubner</i>	“Material studies of Roman bronze parts from the archaeological site of Burg, Burgenland”

Session G – “Separation Sciences”

Wednesday, April 12th 2023, 11h15 – 13h15

Lecture Hall 6

Chair: *C. Huhn*

Co-Chair: *tba*

KN07	11h15 - 11h55	<i>N. Pamme</i>	“Analytical chemistry in continuous flow – from pathogen pre-concentration and separation to integrated bioassays”
O25	11h55 - 12h15	<i>S. Jaag</i>	“Comparison of reversed-phase columns by gradient kinetic plots for the separation of proteins”
O26	12h15 - 12h35	<i>L. Schwalb</i>	“A new approach for the comprehensive chemical description of complex pharmaceutical products”
O27	12h35 - 12h55	<i>M. Jensen</i>	“PROTACs - Tackling related challenges in determination of physicochemical properties”
O28	12h55 - 13h15	<i>S. Kochmann</i>	“Reshaping the analytical perspective on molecular stream separation”

Session H – “Spectroscopic Applications”

Wednesday, April 12th 2023, 11h15 – 13h15

Nöbauer Lecture Hall (Lecture Hall 8)

Chair: *R. Nießner*

Co-Chair: *tba*

KN08	11h15 - 11h55	<i>L. Emmenegger</i>	“Quantum cascade laser spectroscopy for high-precision measurements of trace-gases and their isotopes”
O29	11h55 - 12h15	<i>J. Wacławek</i>	“Highly Compact Laser-Based Trace Gas Detection”
O30	12h15 - 12h35	<i>M. Schmitt</i>	“Raman spectroscopic characterization of smart polymers and photocatalytic systems”
O31	12h35 - 12h55	<i>J. Thissen</i>	“Online coupling of size exclusion chromatography to Raman spectroscopy for protein analysis”
O32	12h55 - 13h15	<i>G. Quintás</i>	“Digital image analysis and lipidomics as references for quantification of liver steatosis by IR spectroscopy”

Session I – “Imaging”

Wednesday, April 12th 2023, 15h45 – 17h45

Main Lecture Hall (Lecture Hall 1)

Chair: *J. Popp*

Co-Chair: *tba*

KN09	15h45 - 16h25	<i>R. Heeren</i>	“Translational molecular imaging in SpatialOMX: single cells and the future of imaging MS”
O33	16h25 - 16h45	<i>M. Calvarese</i>	“Rigid endomicroscopic system for cancer diagnosis and tissue removal”
O34	16h45 - 17h05	<i>C. Wolf</i>	“Complementary Imaging Methods for Tattoo Pigment Analysis in Human Skin Tissue with Adverse Reaction”
O35	17h05 - 17h25	<i>M. Schaier</i>	“LA-ICP-TOFMS as a tool for exploring the mechanisms of chemoresistance in OxPt-treated HCT116 tumors”
O36	17h25 - 17h45	<i>I. Beer</i>	“Using imaging techniques for a deeper understanding of electricity production in microbial biofilms growing on brewery waste”

Session J – “Foodomics”

Wednesday, April 12th 2023, 15h45 – 17h45

Lecture Hall 5

Chair: *E. Leitner*

Co-Chair: *tba*

KN10	15h45 - 16h25	<i>A. Cifuentes</i>	“Neuroprotective activity of orange juice by-products investigated in an in vivo Alzheimer’s model by Foodomics”
O37	16h25 - 16h45	<i>B. Moser</i>	“Exploration and identification of volatile spoilage markers in freshwater fish using DHS-GC-TOFMS”
O38	16h45 - 17h05	<i>M. Sulyok</i>	“Performance of an LC-MS/MS Method Covering 1000 Analytes in Processed Grain-Based Foodstuffs”
O39	17h05 - 17h25	<i>F. Stappert</i>	“Multi 2D comprehensive liquid chromatography for the separation of highly chemically complex samples”
O40	17h25 - 17h45	<i>B. Horstkotte</i>	“Automated centrifugation-less sample deproteinization and homogeneous liquid-liquid extraction for complex sample analysis coupled online to HPLC”

Session K – “Lipidomics”

Wednesday, April 12th 2023, 15h45 – 17h45

Lecture Hall 6

Chair: *G. Hopfgartner*

Co-Chair: *tba*

KN11	15h45 - 16h25	<i>E. Rampler</i>	“Glycolipids – New Challenges in Lipidomics”
O41	16h25 - 16h45	<i>J. Kuligowski</i>	“The lipidome of extracellular vesicles derived from human milk”
O42	16h45 - 17h05	<i>E. Hayen</i>	“Deciphering the structural diversity of cardiolipins and their oxidation products by multidimensional analysis techniques”
O43	17h05 - 17h25	<i>E. Pittenauer</i>	“Structural elucidation of archaeal diether phospholipids by MALDI high-energy CID/tandem TOF-MS”
O44	17h25 - 17h45	<i>S. Giannoukos</i>	“Characterization of the diurnal pattern of breath short-chain fatty acids and enteric methane emissions in dairy cows”

Session L – “Micro-/Nanoplastics”

Wednesday, April 12th 2023, 15h45 – 17h45

Nöbauer Lecture Hall (Lecture Hall 8)

Chair: *C. Engelhard*

Co-Chair: *tba*

KN12	15h45 - 16h25	<i>N. Ivleva</i>	“Raman Microspectroscopy for Analysis of Micro- and Nanoplastics”
O45	16h25 - 16h45	<i>L. Brunnbauer</i>	“Spatially resolved investigations of the elemental composition of aged microplastics using LA-ICP-MS and LIBS”
O46	16h45 - 17h05	<i>M. Huber</i>	“Stimulated Raman Scattering: A new approach to detect nanoplastics in flow”
O47	17h05 - 17h25	<i>D. Materic</i>	“Nanoplastics in the Dutch Wadden Sea – the missing plastic paradox”
O48	17h25 - 17h45	<i>U. Karst</i>	“Multimodal imaging to study the uptake of nanoparticles and their biological effects in tissues”

Session M – “Session Honoring the 80th birthday of the Fritz-Pregl-Medal (ASAC) awardee W. Lindner”

Thursday, April 13th 2023, 11h15 – 13h15

Main Lecture Hall (Lecture Hall 1)

Chair: *M. Lämmerhofer*

KN13	11h15 - 11h45	<i>K. Schug</i>	“Method Development Strategies for On-Line Supercritical Fluid Extraction – Supercritical Fluid Chromatography – Mass Spectrometry”
KN14	11h45 - 12h15	<i>G. Hopfgartner</i>	“Enhanced Molecular Information in Complex Samples by Mass Spectrometry using Multimodal Ionisation and Fragmentation”
KN15	12h15 - 12h45	<i>P. Schoenmakers</i>	“Manipulating liquid-chromatographic selectivity without changing the column”
KN16	12h45 - 13h15	<i>R. Krska</i>	“Emerging global food safety challenges and related analytical solutions”

Session N – “Spectroscopy”

Thursday, April 13th 2023, 11h15 – 13h15

Lecture Hall 5

Chair: *C. Huck*

Co-Chair: *tba*

KN17	11h15 - 11h55	<i>G. Ramer</i>	“Chemical Characterization at the Nanoscale Using AFM-IR”
O49	11h55 - 12h15	<i>T. Mayerhöfer</i>	“Quantitative evaluation of IR and corresponding VCD spectra”
O50	12h15 - 12h35	<i>A. Schroter</i>	“NIR-to-VIS Spectral Shifters: Revisiting the Upconversion Nanoparticle Composition and Surface Functionalization for Bioanalytical Applications”
O51	12h35 - 12h55	<i>M. Selakovic</i>	“Analysis of Breath-related Volatile Organic Compounds by Laser Absorption Spectroscopy”
O52	12h55 - 13h15	<i>R. Luo</i>	“Deep Learning based 3D Raman Spectral Data Analysis for Colorectal Tissue Diagnosis”

Session O – “Environmental Analysis”

Thursday, April 13th 2023, 11h15 – 13h15

Lecture Hall 6

Chair: *A. Kasper-Giebl*

Co-Chair: *tba*

KN18	11h15 - 11h55	<i>J. Hollender</i>	“High-resolution mass spectrometry has boosted non-target screening of persistent organic pollutants in environmental samples”
O53	11h55 - 12h15	<i>R. Zimmermann</i>	“A new single particle aerosol mass spectrometer for the simultaneous detection of health-relevant polycyclic aromatic hydrocarbons, soot and inorganic components from individual airborne particles”
O54	12h15 - 12h35	<i>R. Marks</i>	“LC with simultaneous IRMS and HRMS detection: A powerful new tool for process investigations”
O55	12h35 - 12h55	<i>E. Jennings</i>	“Molecular Insights into Biodegradability of Ozonation Products from Effluent Organic Matter”
O56	12h55 - 13h15	<i>H. Czech</i>	“Photochemical aging increases toxicity of EURO 6 gasoline vehicle exhaust in lung epithelial cells”

Session P – “Industrial Analysis”

Thursday, April 13th 2023, 11h15 – 13h15

Nöbauer Lecture Hall (Lecture Hall 8)

Chair: *M. Arlt*

Co-Chair: *tba*

KN19	11h15 - 11h55	<i>M. Wende</i>	“First Steps Towards an Autonomous Research Lab for Elemental Analysis”
O57	11h55 - 12h15	<i>J. H. Gross</i>	“Analysis of anionic surfactants in commercial detergents by atmospheric pressure field desorption”
O58	12h15 - 12h35	<i>J. Pichler</i>	“Mass Spectrometry Advances for Lubricant Characterization”
O59	12h35 - 12h55	<i>C. Zanetti</i>	“The potential of Intact Cell Mass Spectrometry and Proteomics as monitoring tool for E. coli fermentations”
O60	12h55 - 13h15	<i>A. Bruchmann</i>	“Lab automation as module for data integrity in the analytic lab”

Session Q – “Elemental Analysis”

Thursday, April 13th 2023, 15h45 – 17h45

Main Lecture Hall (Lecture Hall 1)

Chair: *J. Irrgeher*

Co-Chair: *tba*

KN20	15h45 - 16h25	<i>C. Vogt</i>	“New developments in X-ray spectroscopy for spatially resolved and speciation analysis”
O61	16h25 - 16h45	<i>F. Simon</i>	“An improved method for the determination of PFASs using HR-CS-GFMAS via GaF detection”
O62	16h45 - 17h05	<i>K. Leopold</i>	“2-D μ XRF investigation of soft matter photocatalytic active materials”
O63	17h05 - 17h25	<i>H. S. Till</i>	“Exploring the boundaries of double excitation in TXRF”
O64	17h25 - 17h45	<i>M. Weiss</i>	“Multimodal characterization for proton conducting oxide-based electrochemical nitrogen fixation cells”

Session R – “Chemometrics”

Thursday, April 13th 2023, 15h45 – 17h45

Lecture Hall 5

Chair: *G. Gauglitz*

Co-Chair: *tba*

KN21	15h45 - 16h25	<i>A. de Juan</i>	“Chemometrics and hyperspectral images: unraveling information from the chemical pictures of our samples”
O65	16h25 - 16h45	<i>C. Beleites</i>	“Uncovering many Nested Sources of Variance”
O66	16h45 - 17h05	<i>I. Sumerskii</i>	“Comprehensive Lignin Analysis by IR Spectroscopy and Chemometry”
O67	17h05 - 17h25	<i>J. Zuber</i>	“Characterization of soluble and insoluble lignin oligomers by means of FT-ICR-MS”
O68	17h25 - 17h45	<i>P. Filzmoser</i>	“Robust statistical methods applied to high-dimensional data from tribology”

Session S – “Ion Mobility”

Thursday, April 13th 2023, 15h45 – 17h45

Lecture Hall 6

Chair: **S. Hann**

Co-Chair: **tba**

KN22	15h45 - 16h25	<i>T. Causon</i>	“IM-MS: key measurands and physical insights for gas-phase ions”
O69	16h25 - 16h45	<i>R. Zenobi</i>	“Gas-Phase Structures of Biomolecular Ions”
O70	16h45 - 17h05	<i>C. Lenth</i>	“On-site detection method for sulphur mustard for safe underwater work”
O71	17h05 - 17h25	<i>C. Brungs</i>	“10k Compounds in 3 Days: From Data Acquisition to the Automatic Generation of an open MSn Library”
O72	17h25 - 17h45	<i>C. Erbacher</i>	“Online Digestion for a Rapid Screening of Protein-Metallodrug-Interactions via Trapped Ion Mobility Spectrometry-Mass Spectrometry (TIMS-MS)”

Session T – “Separation Sciences”

Thursday, April 13th 2023, 15h45 – 17h45

Nöbauer Lecture Hall (Lecture Hall 8)

Chair: **C. Klampfl**

Co-Chair: **K. Böttinger**

KN23	15h45 - 16h25	<i>G. Gmeiner</i>	“Forensic and Doping Analysis: Similarities, Dissimilarities, Case Reports”
O73	16h25 - 16h45	<i>S. Bräuer</i>	“Vanadium in fly agaric mushrooms: Accumulation, speciation and distribution”
O74	16h45 - 17h05	<i>A. Höchsmann</i>	“Flow Rate determination of the Nanoflow Sheath Liquid CE-MS-coupling applying the nanoCEasy Interface”
O75	17h05 - 17h25	<i>S. Buckenmaier</i>	“Dealing with the “Moving 1D-Target” Issue in Two-Dimensional Chromatography Separations”
O76	17h25 - 17h45	<i>P. Boeker</i>	“Advances and applications of flow-field thermal gradient GC”

Session U – “Food Authenticity and Safety”

Friday, April 14th 2023, 09h00 – 11h00

Main Lecture Hall (Lecture Hall 1)

Chair: *W. Goessler*

Co-Chair: *S. Bräuer*

KN24	09h00 - 09h40	<i>C. Elliott</i>	“How untargeted analysis has become a weapon in the fight against food fraud”
O77	09h40 - 10h00	<i>H. Emons</i>	“Analytical Science for the Design of EU Legislation: The Case of Food Allergens”
O78	10h00 - 10h20	<i>A. Hochegger</i>	“Mineral Oils in Food: Outcome of an Interdisciplinary Project”
O79	10h20 - 10h40	<i>N. Manousi</i>	“Utilization of polar fabric phase sorptive extraction membranes to monitor the salivary levels of vitamin B12 following the administration of sublingual tablets and oral sprays”
O80	10h40 - 11h00	<i>S. Pieczonka</i>	“Archeochemistry reveals the first steps into modern industrial brewing”

Session V – “Material Analysis”

Friday, April 14th 2023, 09h00 – 11h00

Lecture Hall 5

Chair: *A. Limbeck*

Co-Chair: *tba*

KN25	09h00 - 09h40	<i>T. Prohaska</i>	“The analytical challenge in materials science – novel approaches for in situ measurements”
O81	09h40 - 10h00	<i>D. Kau</i>	“Thermal-optical analysis of water insoluble carbon – how to handle interferences caused by mineral dust”
O82	10h00 - 10h20	<i>D. Bleiner</i>	“Combined Elemental and Chemical Information by means of Laser Induced XUV Spectrometry (LIXS)”
O83	10h20 - 10h40	<i>B. Meermann</i>	“New Quantification strategies for short transient signals based on Microdroplet Generators”
O84	10h40 - 11h00	<i>V. Göldner</i>	“Laser Desorption/Ionization-Mass Spectrometry for the Analysis of Electrode Interphases in Lithium Ion Batteries”

Session W – “Nanoscopy”

Friday, April 14th 2023, 09h00 – 11h00

Lecture Hall 6

Chair: tba

Co-Chair: tba

KN26	09h00 - 09h40	<i>N. Kumar</i>	“Label-free Biomolecular Analysis at the Nanoscale using Tip enhanced Raman Spectroscopy”
O85	09h40 - 10h00	<i>U. Yilmaz</i>	“Introducing flat, silicon ATR for bottom illuminated AFM-IR measurements”
O86	10h00 - 10h20	<i>C. Krafft</i>	“Classification of single cells and identification of infections by optical photothermal infrared spectroscopy and imaging”
O87	10h20 - 10h40	<i>K. Kronenberg</i>	“Combining elemental and molecular bioimaging techniques to investigate pathological tissue types”
O88	10h40 - 11h00	<i>Y. Pandey</i>	“Nanoscale investigation of phase-separated ternary lipid monolayer using tip-enhanced Raman spectroscopy (TERS)”

Session X – “Mass Spectrometry”

Friday, April 14th 2023, 09h00 – 11h00

Nöbauer Lecture Hall (Lecture Hall 8)

Chair: *C. Huber*

Co-Chair: *M. Lebede*

KN27	09h00 - 09h40	<i>E. Cappellini</i>	“Tandem mass spectrometry-based analysis of ancient protein for palaeontology, archaeology and art”
O89	09h40 - 10h00	<i>Q. Liu</i>	“Mass Spectrometry Reveals High Levels of Hydrogen Peroxide in Pancreatic Cancer Cells”
O90	10h00 - 10h20	<i>T. Letzel</i>	“Non-target screening workflow of plant metabolomes to reveal changes caused by an inflammatory drug incubation”
O91	10h20 - 10h40	<i>S. Berlanda</i>	“High-throughput MALDI-MS screening of an integral membrane monooxygenase mutant library to enhance bioprocess space-time yield and titer”
O92	10h40 - 11h00	<i>S. Bock</i>	“Intense characterization of a complex fusion protein via electrophoresis: combining chemical cleavage and prefractionation”

Session Y – “MassSpec Forum”

Friday, April 14th 2023, 11h30 – 13h30

Nöbauer Lecture Hall (Lecture Hall 8)

Chair: *R. Ahrends*

Co-Chair: *tba*

	11h30 - 11h40	<i>A. Rizzi</i>	“Obituary Erich Schmid”
MSF01	11h40 - 12h10	<i>S. Razzazi-Fazeli</i>	“History of Biological Mass Spectrometry: From Isotopes to Proteomics”
MSF02	12h10 - 12h30	<i>M. Cziferszky</i>	“Molecular interactions of metallodrugs with biomolecules: top-down and energy-resolved mass spectrometry studies”
MSF03	12h30 - 12h50	<i>D. Wolrab</i>	“Human plasma bioanalysis using UHPSFC/MS”
MSF04	12h50 - 13h10	<i>I. Aissa</i>	“Structural characterization of isomeric lipid A species by NACE-ESI-MS/MS method”
MSF05	13h10 - 13h30	<i>A. D. Zamfir</i>	“Ion mobility mass spectrometry of chondroitin sulfate in human decorin”

Session Z – “MassSpec Forum”

Thursday, April 13th 2023, 15h00 – 16h20

Nöbauer Lecture Hall (Lecture Hall 8)

Chair: *C. Gerner*

Co-Chair: *tba*

MSF06	15h00 - 15h20	<i>M. Zumstein</i>	“Biotransformation of Antimicrobial Peptides in Wastewater”
MSF07	15h20 - 15h40	<i>A.-S. Egger</i>	“Proteo-Metabo-Flux – Linking Acetyl-CoA and acetylation dynamics for accurate determination of histone acetylation rates”
MSF08	15h40 - 16h00	<i>M. Pristner</i>	“Untargeted and targeted metabolomics of plasma and fecal samples from a cohort of extremely premature infants”
MSF09	16h00 - 16h20	<i>T. Kipura</i>	“Development of an IC-FAIMS-MS method for targeted metabolomics”