# 2026 Winter Conference on Plasma Spectrochemistry

Short Courses
Professional Development Courses
Friday – Tuesday
January 9 – 13, 2026

# **Course Descriptions**



Friday 9, Sat 10, Sun 11, Mon 12, Tu 13

# **Course Hours:**

8 am - 12 noon 1 pm - 5 pm 7 pm - 11 pm

Latest Version 102425

# 2026 Winter Conference Short Courses Friday, January 09 – Tuesday, January 13, 2026 Schedule

### **Analysis by Plasma Spectrochemistry**

SA-01 LA-ICP-MS: Elemental Analysis of Incremental Tissues as an Indicator of Past Pollution Events and Micronutrient Status, Friday, January 9, 7 pm, Dula Amarasiriwardena, daNS@hampshire.edu, Hampshire College, School of Natural Science, Amherst. MA 01002-3359

**SA-02** Environmental Isotope Geochemistry: Plasma Spectrochemistry as an Essential Tool, Saturday, January 10, 8 am, Michael E. Ketterer, michael.ketterer@nau.edu, Department of Chemistry and Biochemistry, Northern Arizona University, Box 5698, Flagstaff, AZ 86011-5698

SA-03 Short Course on Fluorine Detection with ICPMS and ESIMS and Applications Including PFAS, Sunday, January 11, 7 pm, Jörg Feldmann, Joerg.feldmann@uni-graz.at, j.feldmann@abdn.ac.uk, and Viktora Müller, TESLA - Analytical Chemistry Institute of Chemistry, University of Graz, Universitätsplatz 1, 8010 Graz, Austria

SA-04 Implementing Clinical ICP-MS for Clinical Diagnosis, Biomonitoring and Emergency Response. Sunday,

January 11, 8 am, Cynthia D. Ward, CWard@cdc.gov, and Deanna Jones, DMJones1@cdc.gov, Centers for

Centers for Disease Control and Prevention (CDC), 4770 Buford Hwy, Mailstop S110-5, Atlanta, GA 30341-3717

SA-05 Unrivaled Reactions and How They Apply to Single Particle and Single Cell ICP-MS Applications, Sunday, January 11, 7 pm, Ruth Merrifield, ruth.merrifield@perkinelmer.com, Chady Stephan, <a href="mailto:chady.stephan@perkinelmer.com">chady.stephan@perkinelmer.com</a>, and Aaron Hineman, Aaron.Hineman@perkinelmer.com, PerkinElmer, 501 Rowntree Dairy Rd, Woodbridge, ON L4L 8H1, Canada

SA-06 Elemental Imaging at Micro- and Nanometer Scale for Applications in Biology, Nutrition, Toxicology, and Geology. Saturday, January 10, 1 pm, Dirk Schaumlöffel, dirk.schaumloeffel@univ-pau.fr, IPREM CNRS UMR 5254, Heloparc, 2 Avenue du President Angot, 64053 Pau, France

SA-07 Sample Classification Using Elemental Analysis, Monday, January 12, 7 pm, Lukas Brunnbauer and Andreas Limbeck Univ. andreas.limbeck@tuwien.ac.at, and <a href="mailto:lukas.brunnbauer@tuwien.ac.at">lukas.brunnbauer@tuwien.ac.at</a>, TU Wien, Institute of Chemical Technologies and Analytics, Getreidemarkt 9/164, A-1060 Vienna, Austria

SA-08 GC-ICP-MS Analysis, January, Saturday, 10, 8:00 am, Bill Geiger, bill@consci.com, 1416 Southmore, Pasadena, TX 77502 SA-09 Some Statistics Applied to Analytical Chemistry Using R and Microsoft Excel, Tuesday, January 13, 7 pm, George L. Donati, george.donati@health.ny.gov, Wadsworth Center, Biggs Laboratory, New York State Department of Health. Empire State Plaza, Albany, NY 12237

**SA-10 Nanomaterials Characterization By ICP-MS In Single Particle Mode And Related Techniques,** Saturday, January 10, 8:00 am, **Carsten Engelhard** <sup>1.2</sup>, carsten.engelhard@bam; deengelhard@chemie.uni-siegen.de, <sup>1</sup> BAM, Bundesanstalt für Materialforschung und -prüfung, Richard-Willstätter-Straße 11, 12489 Berlin <sup>2</sup>University of Siegen, Department of Chemistry and Biology, Adolf-Reichwein-Str. 2, D-57076 Siegen, Germany.

### **Sample Introduction Approaches**

SS-01 A Practical Guide to Nebulizers and the Role They Play In Modern Sample Introduction Systems

\*(how to get from sample to the correct analytical result)", Saturday, January 10, 7 pm, Steve Mangum, steve.mangum@icpms.com, Senior Field Application Scientist, 23308 S. 132nd Street, Chandler AZ 85249

SS-03 Latest Advances in Laser Ablation-Based Chemical Analysis and Emerging Applications: LIBS, LA-ICP-(OES/MS), and Tandem LA – LIBS, Monday, January 12, 7 pm, Jhanis Gonzalez, <a href="mailto:jhanis@appliedspectra.com">jhanis@appliedspectra.com</a>, <a href="mailto:jhanis@appliedspectra.com">jhanis@appliedspectra.com</a>, <a href="mailto:jhanis@appliedspectra.com">jhanis@appliedspectra.com</a>, <a href="mailto:jhanis@appliedspectra.com">jjgonzalez@lbl.gov</a>, <a href="mailto:Appliedspectra.com">Applied Spectra</a>, <a href="mailto:jhanis@appliedspectra.com">jhanis@appliedspectra.com</a>, <a href="mailto:jjgonzalez@lbl.gov">jjgonzalez@lbl.gov</a>, <a href="mailto:Appliedspectra.com">Applied Spectra</a>, <a href="mailto:jhanis@appliedspectra.com">jjgonzalez@lbl.gov</a>, <a href="mailto:Appliedspectra.com">Applied Spectra</a>, <a href="mailto:jhanis@appliedspectra.com">jjgonzalez@lbl.gov</a>, <a href="mailto:Appliedspectra.com">Appliedspectra.com</a>, <a href="mailto:jjgonzalez@lbl.gov">jjgonzalez@lbl.gov</a>, <a href="mailto:appliedspectra.com">jjgonzalez@lbl.gov</a>, <a href="mailto:appliedspectra.com">jjgonzalez@lbl.gov</a>, <a href="mailto:appliedspectra.com">jjgonzalez@lbl.gov</a>, <a href="mailto:appliedspectra.com">jjgonzalez@lbl.gov</a>, <a href="mailto:appliedspectra.com">jjgonzalez@lbl.gov</a>,

SS-06 Artificial Intelligence (e.g., via Artificial Neural Networks, Machine Learning, Deep Learning) with Applications to ICP and to Microplasma Spectrochemistry, Sunday, January 11, 1 pm, Vassili Karanassios, vkaranassios@uwaterloo.ca, University of Waterloo, Department of Chemistry and Waterloo Institute for Nanotechnology, Waterloo, ON N2L 3G1, Canada

SS-07 Microwave-Assisted Sample Preparation for Trace Elemental Analysis: Think Blank & Go Green, Sunday, January 11, 8 am. Joaquim A. Nóbrega, djan@terra.com.br OR djan@ufscar.br, Department of Chemistry, Federal University of São Carlos, São Carlos, SP, Brazil

#### **Plasma Spectrochemical Techniques**

ST-01 Accurate and Precise Isotopic Analysis by MC-ICPMS, Sunday, January 11, 1 pm, Lu Yang, lu.yang@nrc-cnrc.gc.ca, National Research Council Canada, 1200 Montreal Rd, Ottawa, ON, K1A 0R6, Canada

ST-02 Building or Modifying Your Laboratory for Trace and Ultra-trace Analyses, Sunday, January 11, 8 am, Ela Bakowska, ela@bakowska.com, bakowskae@corning.com, Elba Elemental Consulting, PO Box 1053, Corning, NY 14830

ST-03 Single Particle ICP-MS, ETV-ICP-MS, GC-ICP-MS, HPLC-ICP-MS, ICP-MS: Method Development, Problem Solving, Troubleshooting and Optimization, Saturday, January 10, 1 pm, Mark Fresquez, mwf6@cdc.gov, Centers for Disease Control and Prevention, 4770 Buford Hwy NE, MS S110-4, Atlanta, GA 30341-3717

ST-04 Analysis Of Nano- And Micromaterials Using Laser Ablation Single Particle-ICP-MS, Sunday, January 11, 7 pm, Andreas Limbeck, andreas.limbeck@tuwien.ac.at, and Lukas Brunnbauer, lukas.brunnbauer@tuwien.ac.at, TU Wien, Institute of Chemical Technologies and Analytics, Getreidemarkt 9/164, A-1060 Vienna, Austria

ST-05 Introduction to Chemometrics for Spectral Analysis, Sunday, January 11, 8 am, Neal B. Gallagher, nealg@eigenvector.com, Eigenvector Research Inc., 300 Bella Strada Lane, Manson, WA 98831 USA

ST-06 SP ICP-MS Data Processing with SPCal. From Zero to Hero. David Clases, Sunday, January 11, 1 pm,

<u>David.Clases@uni-graz.at</u>, Universitätsplatz 1, 8010, Graz, Austria, **and Thomas Lockwood**, Thomas.Lockwood@uts.edu.au,

NanoMicroLab at the University of Graz, Graz, Austria, and University of Technology Sydney, Sydney, Australia

ST-07 Metrology for Particle Characterisation: From Nanomaterials to Microplastics, Tuesday, January 13, 8 pm Heidi Goenaga Infante, Heidi.Goenaga-Infante@lgcgroup.com & Guillermo Redondo Fernandez,

guillermo.fernandez@lgcgroup.com, UK National Measurement Laboratory, LGC, The Priestley Building, 10 Priestley Road Guildford, GU2 7XY, United Kingdom

### **Spectrochemical Instrumentation**

SI-01 ICP-MS I: Introduction, Saturday, January 10, 1 pm, John Olesik,olesik.2@osu.edu, 125 S. Oval Mall, 275 Mendenhall Laboratory, School of Earth Sciences, Ohio State University, Columbus, OH 43210

SI-02 ICP-MS II: Advanced, Sunday, January 11, 1 pm, John Olesik ,olesik.2@osu.edu, 125 S. Oval Mall, 275 Mendenhall Laboratory, School of Earth Sciences, Ohio State University, Columbus, OH 43210

SI-03 The Rise of Microwave Induced Plasmas: Fundamentals and Applications, Saturday, January 10, 7 pm, Guillermo Grindlay Lledó, guillermo grindlay@ua.es, University of Alicante, Faculty of Science, Crta\ San Vicente s/n, San Vicente del Raspeig, Alicante, Spain

SI-04 Agilent ICP-Expert and Masshunter ICP-MS Software Workshop, Tuesday, January 13, 7 pm, Bert Woods, bert\_woods@agilent.com, Agilent Technologies, 2850 Centerville Rd, Wilmington, DE 19808

SI-05 Theory and Practical Use of Reaction Cells and Collision Cells for ICP-MS, Sunday, January 11, 1 pm, Patrick Gray, patrick gray@fda.hhs.gov, Deanna M Jones, (CDC) hii4@cdc.gov, Center for Food Safety and Applied Nutrition, Office of Regulatory Science, 5001 Campus Drive, College Park, U.S. Food and Drug Administration, College Park, MD 20740 and 4770 Buford Hwy NE MS S110-5, Atlanta, GA 30341-3717

# 2026 Winter Conference Short Courses Short Course Schedule by Date

# Friday, January 9, 7 pm

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# Saturday, January 10, 7 pm

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### Sunday, January 11, 7 pm

**SA-03** Short Course on Fluorine Detection with ICPMS and ESIMS and Applications Including PFAS, Sunday, January 11, 7 pm, Jörg Feldmann, joerg.feldmann@uni-graz.at, j.feldmann@abdn.ac.uk, and Viktora Müller, TESLA - Analytical Chemistry Institute of Chemistry, University of Graz, Universitätsplatz 1, 8010 Graz, Austria

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# Monday, January 12, 7 pm

**SA-07 Sample Classification Using Elemental Analysis,** Monday, January 12, 7 pm, Lukas Brunnbauer and Andreas Limbeck Univ. andreas.limbeck@tuwien.ac.at, and <a href="mailto:lukas.brunnbauer@tuwien.ac.at">lukas.brunnbauer@tuwien.ac.at</a>, TU Wien, Institute of Chemical Technologies and Analytics, Getreidemarkt 9/164, A-1060 Vienna, Austria

SS-02 Laser Ablation Mass Spectrometry, Monday, January 12, at 7:00, Detlef Günther, guenther@inorg.chem.ethz.ch, Department of Chemistry and Applied Biosciences, ETH Zurich, Vladimir-Prelog- Weg 1, 8093 Zurich, Switzerland

SS-03 Latest Advances in Laser Ablation-Based Chemical Analysis and Emerging Applications: LIBS, LA-ICP-(OES/MS), and Tandem LA – LIBS, Monday, January 12, 7 pm, Jhanis Gonzalez, <a href="mailto:jhanis@appliedspectra.com">jhanis@appliedspectra.com</a>, <a href="mailto:jjgonzalez@lbl.gov">jjgonzalez@lbl.gov</a>, Applied Spectra, Inc., 950 Riverside Pkwy, Suite 90, West Sacramento, CA 95605-15071

SA-09 Some Statistics Applied to Analytical Chemistry Using R and Microsoft Excel, Tuesday, January 13, 7 pm, George L. Donati, george.donati@health.ny.gov, Wadsworth Center, Biggs Laboratory, New York State Department of Health. Empire State Plaza, Albany, NY 12237

SI-04 Agilent ICP-Expert and Masshunter ICP-MS Software Workshop, Tuesday, January 13, 7 pm, Bert Woods, bert woods@agilent.com, Agilent Technologies, 2850 Centerville Rd, Wilmington, DE 19808

ST-07 Metrology for Particle Characterisation: From Nanomaterials to Microplastics, Tuesday, January 13, 8 pm

Heidi Goenaga Infante, Heidi Goenaga-Infante@Igcgroup.com & Guillermo Redondo Fernandez,

guillermo.fernandez@lgcgroup.com, UK National Measurement Laboratory, LGC, The Priestley Building, 10 Priestley Road Guildford, GU2 7XY, United Kingdom

# 2026 Winter Conference Short Courses Friday, January 09 – Tuesday, January 13, 2026

# **Course Descriptions**

Analysis by Plasma Spectrochemistry

SA-01 LA-ICP-MS: Elemental Analysis of Incremental Tissues as an Indicator of Past Pollution Events and Micronutrient Status, Friday, January 9, 7 pm, Dula Amarasiriwardena, daNS@hampshire.edu, Hampshire College, School of Natural Science, Amherst, MA 01002-3359

Human teeth, hair, shells, tree rings, and fish otoliths are examples of incrementally deposited tissues with a defined time axis. These tissues are repositories of trace metals and excellent materials for detecting past pollution episodes. We will introduce how microprobe techniques like LA-ICP-MS methods can be used for analysis of these incremental tissues. We will present LA-ICP-MS instrumentation, theory, practice, troubleshooting hints, sample preparation, and instrument calibration strategies for LA-ICP-MS. Unique applications in biology, environmental sciences, archeology, anthropology, and forensic science will be presented. Analytical advantages and limitations of each method will be discussed.

#### **Key Learning Objectives:**

□ We will learn about the theory and fundamentals of LA-ICP-MS □ What are the incremental tissues, and their biology and chemistry □ Analytical advantages and limitations and troubleshooting skills. □ We will introduce how microprobe techniques, such as LA-ICP-MS methods, can be used for the analysis of these incremental tissues to gain valuable archived elemental information for interdisciplinary applications.

#### Course outline:

□ LA-ICP-MS principles and instrumentation. □ Analytical advantages, limitations, and troubleshooting skills

□ What are incremental biological tissues? □ What is the archived elemental information in hard tissues (teeth, bones, tree rings, hair, etc.)? □ Sample preparation and calibration strategies □ . Data analysis □ . Elemental bioimaging □ . Applications in biology, environmental sciences, anthropology, and archaeology.



**Dula Amarasiriwardena**, Emeritus Professor of Chemistry at Hampshire College, Amherst, Massachusetts, received his Ph.D. in Analytical Chemistry from North Carolina State University, Raleigh, NC. Dula teaches analytical chemistry, environmental chemistry, and general chemistry. His research focuses on the transport properties and fate of trace metals and metal nanoparticles in soil and aquatic environments. Dula is also interested in applying laser ablation (LA)-ICP-MS to investigate trace metal nutrition and exposure to toxic metal pollutants using hard tissues such as human teeth and hair. Professor Amarasiriwardena served as a *Fulbright Specialist* in Chile. He serves on the editorial boards of *Environmental Pollution and Applied Spectroscopy Practica*.

Instructor's Web site: http://helios.hampshire.edu/~daNS/index.html

**SA-02** Environmental Isotope Geochemistry: Plasma Spectrochemistry as an Essential Tool, Saturday, January 10 8 am, Michael E. Ketterer, michael.ketterer@nau.edu, Department of Chemistry and Biochemistry, Northern Arizona University, Box 5698, Flagstaff, AZ 86011-5698.

The majority of the chemical elements possess multiple isotopes. Natural or synthetic variation of isotope compositions is widely used in geochemistry and the environmental sciences for gaining insight into the sources, transport and fate of these elements in the natural and human-affected environment. This course provides a broad overview of the isotope geosciences, with emphasis on sources of these variations and the use of plasma spectrochemistry to generate the requisite data. Applications to environmental/geochemical studies of important elements such as Pb, Sr, Nd, U, and Pu will be discussed, using examples from the literature. **Keywords:** Isotopes, environmental sciences, geochemistry, ICPMS, source/transport/fate processes

Michael E. Ketterer obtained his primary and secondary education in Buffalo, NY, and received a B.S. in Chemistry from the University of Notre Dame in 1980. He pursued graduate studies in electron transfer and interfacial chemistry at the University of Colorado under the direction of Prof. Carl A. Koval, receiving a Ph.D. in 1985. After brief employment as an industrial electrochemist, he worked from 1987-1993 at the US Environmental Protection Agency's forensic laboratory and was Assistant Professor at John Carroll University from 1993-1998. Mike has since taught at Northern Arizona University (1998-2013) and Metropolitan State University of Denver (2013-2018) and is presently Professor Emeritus at Northern Arizona University. His research interests include plasma spectrochemistry, an interest that began when he first used an Elan 250 in 1988, and applications of isotope measurements in environmental geosciences. Mike has published ~100 peer-reviewed papers in his career, is a prolific collaborator, and has traveled and lectured worldwide in pursuit of his scientific interests. As an Emeritus, Mike is pursuing consulting and *pro bono* work, focusing on assistance to communities affected by legacy Cold War-era nuclear contamination.

**SA-03** Short Course on Fluorine Detection with ICPMS and ESIMS and Applications Including PFAS, Sunday, January 11, 7 pm, Jörg Feldmann, .feldmann@uni-graz.at, j.feldmann@abdn.ac.uk, and Viktoria Müller, TESLA - Analytical Chemistry Institute of Chemistry, University of Graz, Universitätsplatz 1, 8010 Graz, Austria

Fluorine is one of the elements which cannot directly be detected by conventional ICPMS. How fluorine is forming a detectable ion will be explained. This course will give also some background, how environmental analysis for organofluorines such as F-containing pesticides and F- containing pharmaceuticals and PFAS (Per and polyfluorinated alkylated substances) is routinely analysed by target LC-MS/MS. Furthermore, will be demonstrated how ICPMS can be used for non-target HR-ESIMS. Applications about PFAS in food contact materials, ski wax, accumulation in wildlife as well as fluorinated compounds in sewage water. Additionally, we will feature how LA-ICPMS can be conducted for fluorine.

Jörg Feldmann received his PhD at the University of Essen (Germany) in 1995; he studied volatile metals and metalloids in the environment by using GC-ICP-MS. He was a Feodor Lynen Postdoc (Alexander von Humboldt) at the University of British Columbia, Canada, in 1995-1997, when he investigated the complementary use of GC-MS and GC-ICP-MS for volatile tin, antimony, and bismuth compounds. Since 1997, he has been a Lecturer at the University of Aberdeen, Scotland, and became a full Professor in 2003. Recently, he moved to the University of Graz in Graz, Austria. He has published over 100 papers in peer-reviewed journals, mainly about arsenic speciation. His focus is on the determination of the arsenosugar metabolism by seaweed-eating sheep and the transport and biotransformation of arsenic in plants, and the pros and cons of ES-MS and ICP-MS, and the online combination of both MS techniques

**SA-04** Implementing Clinical ICP-MS for Clinical Diagnosis, Biomonitoring and Emergency Response. Sunday, January 11, 8 am, Cynthia D. Ward, CWard@cdc.gov, and Deanna Jones, DMJones1@cdc.gov, Centers for Centers for Disease Control and Prevention (CDC), 4770 Buford Hwy, Mailstop S110-5, Atlanta, GA 30341-3717

The successful application of inductively coupled plasma mass spectrometry (ICP-MS) in a clinical laboratory depends on addressing several key issues, such as method validation, contamination control, CLIA regulations, quality control, and method troubleshooting. We will discuss these issues in detail as well as the key requirements for a clean-room type of laboratory environment. Laboratory infrastructure and methodological considerations to provide analytical support for biomonitoring studies, epidemiological assists, and emergency response will be covered. This course is of interest to scientists involved with or responsible for the testing of clinical samples in research, public health, or diagnostic labs. **Keywords:** Clinical ICP-MS, method validation, biomonitoring, clinical diagnosis, quality control, emergency response, metals, inorganic analysis, speciation, clean-room

Cynthia Ward is the Deputy Branch Chief of the Inorganic and Radiation Analytical Toxicology (IRAT) Branch. She has over 28 years of experience, 20 at the CDC, in the analysis of inorganic elements in various matrices using spectroscopy (ICP-OES and ICP-MS), atomic absorption, chromatography and other techniques. Her current responsibilities include assisting with the planning, implementation, oversight, and execution of laboratory programs focused on research and development of analytical methods and the analysis of trace, toxic, and essential elements (e.g., mercury (total and organic), arsenic (total and speciated), cadmium, lead, and uranium) and radionuclides in biological matrices.

**Deanna Jones** is the Chief of the Speciation and Lot Screening Laboratories in the IRAT Branch. She has over 17 years of experience at the CDC developing methods for measuring trace elements in biological samples using chromatography and ICP-MS. Her laboratory performs arsenic and mercury speciation methods and provides technical support to state and local public health labs. She is proficient in qualitative and quantitative statistical data analysis, method validation and evaluating analytical figures of merit, Clinical Laboratory Improvement Amendments (CLIA) regulations including Proficiency Testing (PT) requirements, and Quality Assurance/Quality Control (QA/QC) review.

**SA-10 Nanomaterials Characterization By ICP-MS In Single Particle Mode And Related Techniques,** Saturday, January 10, 8 am, **Carsten Engelhard** <sup>1.2</sup>, carsten.engelhard@bam.de; engelhard@chemie.uni-siegen.de, <sup>1</sup> BAM, Bundesanstalt für Materialforschung und -prüfung, Richard-Willstätter-Straße 11, 12489 Berlin<sup>-2</sup>University of Siegen, Department of Chemistry and Biology, Adolf-Reichwein-Str. 2, D-57076 Siegen, Germany.

Single particle inductively coupled plasma mass spectrometry (spICP-MS) is a powerful technique that can provide unique information on the elemental composition of nanoparticles (NPs). In this short course, fundamental principles of spICP-MS, instrumentation, and selected applications will be discussed. This course will begin with a tutorial on spICP-MS basics including sampling, sample preparation, microsecond time-resolved detection, data processing, and data evaluation. A particular emphasis will be placed on measurement artifacts that may lead to errors in results and particle size histograms. In the second part, selected applications will be highlighted including the detection of NPs in complex matrices and environmental samples. This course is intended for those with a background in ICP-MS, but beginners are also very welcome to attend. Keywords: ICP-MS, spICP-MS, Nano, Particle Characterization



Dr. Carsten Engelhard is an Associate Professor of Analytical Chemistry and the Department Chair of the Department of Chemistry and Biology at the University of Siegen. He received his Dr. rer. nat. degree in 2007 from the University of Muenster, Germany, and was a post-doctoral fellow at Indiana University from 2008 to 2010 under the guidance of Prof. G.M. Hieftje. Carsten has 15 years of experience in ultra trace elemental analysis, mass spectrometry, instrumentation, surface analysis, and nanoparticle detection. He has published more than 80 peer-reviewed articles and two book chapters in this field. Since 2023, he is chairman of the board of the German Working Group for Analytical Spectroscopy (DAAS) in the Analytical

Division of the German Chemical Society (GDCh), and he is head of the Department 1 Analytical Chemistry; Reference Materials at the Federal Institute for Materials Research and Testing (BAM), Berlin, Germany.

SA-05 Unrivaled reactions and how they apply to Single Particle and Single Cell ICP-MS applications, Sunday, January 11, 7 pm, Ruth Merrifield, ruth.merrifield@perkinelmer.com, Chady Stephan, <a href="mailto:chady.stephan@perkinelmer.com">chady.stephan@perkinelmer.com</a>, and Aaron Hineman, Aaron.Hineman@perkinelmer.com, PerkinElmer, 501 Rowntree Dairy Rd, Woodbridge, ON L4L 8H1, Canada. This course will briefly review the theory of SP-ICP-MS focusing on the state-of-the-art innovations in hardware and software to control interferences and clustering to achieve the lowest nanoparticle detection limits in complex matrices, in relation to the latest applications in environmental, forensic, semiconductor and microplastic sciences.

We will introduce the concept of single cell-ICP-MS and discuss the challenges faced when analyzing cells suspensions, with an indepth focus on the necessary hardware and software requirements to quantify accurately the number of particles and/or metal content in individual unicellular organisms, with a focus on various human and environmental health applications.



**Ruth Merrifield** is the Atomic Spectroscopy Technical Product Manager at PerkinElmer, with over 20 years of experience in both analytical chemistry and physics and has a strong background in atomic spectroscopic technologies. Ruth earned her PhD in nanoscale physics from the University of Birmingham, UK and was an Assistant Professor in the Center for Environmental Nanoscience & Risk at the University of South Carolina before joining PerkinElmer in 2017. Ruth has expertise in single particle and single cell analysis as well as coupling new techniques to the ICP-MS platform.



**Chady Stephan** holds a Ph.D. in Analytical Chemistry from Université de Montréal. He joined PerkinElmer as an atomic spectroscopy application scientist. He has since then occupied various roles within the organization. He currently directs a team of market managers focusing on core capabilities and value proposition within focused end markets. He is a thought leader in elemental analysis with over 30 peer-reviewed papers and book chapters.



Aaron Hineman is the Inorganic Product Line Leader at PerkinElmer, with over 25 years of expertise in analytical chemistry and atomic spectroscopy. With a deep understanding of atomic spectroscopic technologies, hyphenated speciation workflows, and sample preparation techniques, Aaron is passionate about delivering impactful solutions and sharing knowledge through training, customer engagements, and industry events. Previously, Aaron served as a Senior Field Application Scientist, mastering ICP-MS and ICP-OES instrumentation, and spent a decade developing analytical methodologies in environmental and geochemical labs. Outside of work, he enjoys snowboarding, skiing, obstacle races, and biking.

SA-06 Elemental Imaging at Micro- and Nanometer Scale for Applications in Biology, Nutrition, Toxicology, and Geology. Saturday, January 10, 1 pm, Dirk Schaumlöffel, dirk.schaumloeffel@univ-pau.fr, IPREM CNRS UMR 5254. Heloparc. 2 avenue du president Angot, 64053 Pau, France.

This course provides in the first part an overview of different element specific imaging techniques such as Laser Ablation ICP-MS, TEM-X/EDS, synchrotron radiation XRF, and secondary ion mass spectrometry. Specifications and limitations regarding spatial resolution and sensitivity will be discussed. The second part will focus on the technique and challenges of nanoscale secondary ion mass spectrometry (NanoSIMS) for elemental and isotopic imaging at the submicrometer level. The third part of this course will highlight different applications including sample preparation techniques for NanoSIMS. Applications from our work on plant and animal tissue, cell cultures as well as geological samples will be presented and discussed. Finally, in the last part, solutions for the treatment of imaging data and their limitations will be presented. **Keywords**: Elemental imaging, SIMS, nm resolution, sample preparation, plant and animal tissue, subcellular

Dirk Schaumlöffel obtained his doctorate in analytical chemistry in 1995 at the Philipps University in Marburg, Germany, and then carried out research at the GKSS research center in Geesthacht. After a stay in the USA, he went to the University of Pau, France where he obtained his habilitation in analytical chemistry in 2008. Since 2011 he has been a research professor at the French National Center for Scientific Research (CNRS) and he teaches at the University of Pau. His research includes analytical-chemical developments for the determination of essential and toxic trace elements in biological organisms. Main research activities are imaging methods for the localization of trace elements in tissue and cells in the nanometer level using secondary ion mass spectrometry (NanoSIMS) with applications in the environment, biomedicine and toxicology. Dirk Schaumlöffel is director of the public-private joint laboratory SPECIMAN, editor-in-chief of the Journal of Trace Elements in Medicine and Biology, General Secretary of the Federation of European Societies on Trace Elements and Minerals (FESTEM), and president of the German Society for Minerals and Trace Elements (GMS).

**SA-07 Sample Classification Using Elemental Analysis,** Monday, January 12, 7 pm, Lukas Brunnbauer and Andreas Limbeck Univ. andreas.limbeck@tuwien.ac.at, and <a href="mailto:lukas.brunnbauer@tuwien.ac.at">lukas.brunnbauer@tuwien.ac.at</a>, TU Wien, Institute of Chemical Technologies and Analytics, Getreidemarkt 9/164, A-1060 Vienna, Austria.

In recent years, much progress has been made in sample classification/discrimination based on elemental fingerprinting techniques. To achieve this, elemental analysis is combined with multivariate statistics to gain information about differences or variations within the investigated samples and build classification models. In this short course, we will briefly present the concepts and approaches used for assessing elemental contents and provide an intuitive overview of common supervised and unsupervised chemometric methods and their potential for sample classification. Additionally, an interactive Python-based example is discussed to demonstrate the practical workflow. **Keywords:** multi-element analysis, elemental fingerprint, chemometrics, statistical analysis, machine learning, sample authentication, product adulteration, forensic analysis.

**Lukas Brunnbauer** received his PhD in Technical Chemistry from the TU Wien. Currently, he is working as a Postdoctoral Researcher at TU Wien in the research group "Surface Analytics, Trace Analytics, and Chemometry." His research is mainly focused on spatially resolved polymer characterization using LIBS and LA-ICP-MS.

**Andreas Limbeck** is an expert in the field of atomic spectroscopy with over 20 years of research experience. In recent years, he has developed advanced expertise in the application of LA-ICP-MS and LIBS for the chemical analysis of solid materials, particularly for the quantitative determination of element distributions in various sample types. Since 2021, he has been a full professor for "Analytical Chemistry of Materials" at the Faculty of Technical Chemistry at TU Wien.

# SA-08 GC-ICP-MS Analysis, January, Saturday, 10, 8:00 am, Bill Geiger, bill@consci.com, 1416 Southmore, Pasadena, TX 77502

The course provides practical information based on experienced knowledge using gas chromatography coupled with ICP-MS detection. Topics include interfacing, hardware options and modification, chromatographic fittings, sample presentation, use of gas and liquid sampling valves, column issues and selection, tuning, software issues, standard generation, and applications. The course will provide tips and tricks that will be helpful to those beginning the use of this hyphenated technology, hopefully avoiding possible pitfalls. **Keywords:** ICP-MS, Gas Chromatography, GC-ICP-MS, Semiconductor Precursors, Petrochemical, Sulfur Speciation, Element Specific Detection.

**Bill Geiger** is currently a partner at CONSCI, Ltd., a commercial lab providing services to the specialty, electronic, aerospace, and petrochemical industries. Bill has been doing chromatography for over 30 years and GC-ICP-MS for over 25 years. He has presented numerous papers and posters at PittCon as well as the Winter Plasma Conference. He has authored or edited book chapters on the use of chromatography using many different detectors, including ICP-MS.

SA-09 Some Statistics Applied to Analytical Chemistry Using R and Microsoft Excel, Tuesday, January 13, 7 pm, George L. Donati, george.donati@health.ny.gov, Wadsworth Center, Biggs Laboratory, New York State Department of Health. Empire State Plaza, Albany, NY 12237

In this short course, we will use the R programming language and Microsoft Excel to explore fundamental statistical concepts applied to analytical chemistry. Topics such as population and sample; normal and t distribution; outlier, *F*- and *t*-tests; least-squares regression and traditional calibration methods; and limit of decision, limit of detection and limit of quantification will be discussed. This is a hands-on course, so attendees are required to bring their laptop with R, RStudio, and MS Excel installed. R is a free (open source) software environment for statistical computing and graphics. Its most recent version can be downloaded at https://cran.r-project.org/bin/windows/base/. RStudio is an integrated development environment (IDE) used to run R. The latest version of RStudio for desktop can be downloaded free at <a href="https://www.rstudio.com/products/rstudio/download/">https://www.rstudio.com/products/rstudio/download/</a>. **Keywords:** R; MS Excel; Statistical tests; Uncertainty; Normality evaluation; Least-squares regression; Traditional calibration methods; Limit of detection; Limit of decision; Limit of quantification. **Who should take this course:** Any spectroscopist interested in easily applying statistical tools available in R and MS Excel to their analytical chemistry work.

IMPORTANT: Due to limited time for computer troubleshooting, it is recommended that attendees bring a PC (rather than a Mac) to this course, as R, RStudio, and MS Excel work best with Windows.



George L. Donati received his M.Sc. in Analytical Chemistry from the Federal University of São Carlos (UFSCar, Brazil, 2006), and his Ph.D. in Chemistry from Wake Forest University (WFU, USA, 2010). He has contributed to the development of several calibration strategies, such as the interference standard method (IFS), multi-energy calibration (MEC), standard dilution analysis (SDA), multi-isotope calibration (MICal), multispecies calibration (MSC), multi-internal standard calibration (MISC), etc., which improve the accuracy and sample throughput of different spectrochemical methods. George is the Deputy Director of the Laboratory of Inorganic and Nuclear Chemistry at the Wadsworth Center (New York State Department of Health), where he oversees the trace element analysis of samples of public health interest for the State of New York. He also directs a research program focused on the development of new calibration strategies, and the application of advanced statistical and machine learning tools, along with trace element data, to

study a broad range of issues, from matrix effects in plasma-based spectrochemical methods to anemia of inflammation and diabetes mellitus. George is a member of the advisory boards of the Journal of Analytical Atomic Spectrometry and the Brazilian Journal of Analytical Chemistry, and the editorial board of Atomic Spectroscopy. He has published more than 115 peer-review papers and four book chapters on several topics associated with spectrochemical and trace element analysis and was awarded with the 2020 JAAS Emerging Investigator Lectureship.

#### Sample Introduction Approaches

SS-01 A Practical Guide to Nebulizers and the Role They Play In Modern Sample Introduction Systems\* \*(how to get from sample to the correct analytical result), Saturday, January 10, 7 pm, Steve Mangum, steve.mangum@icpms.com, Senior Field Application Scientist, 23308 S. 132nd Street, Chandler, AZ 85249

This course will discuss the variety of nebulizer options, their uses, and proper selection, in conjunction with the complete sample introduction system. This will provide analysts with information and options to choose the proper configuration of sample introduction systems to best utilize their ICP and ICP-MS instrumentation.



**Steve Mangum** has over 30 years of experience in atomic spectroscopy, spending his first 10 years working in a certified environmental laboratory running flame/furnace, ICP, and ICP-MS. Steve then spent the next 20 years as a spectroscopy Product Specialist for one of the large instrument manufacturers, helping laboratories implement new instrumentation and developing analytical methods. This experience has given Steve a strong background in methods and instrumentation, especially in environmental, nutritional supplement, and semiconductor applications. Steve holds a Master's degree from the University of Utah and is currently working as a Field Application Scientist for Elemental Scientific, helping customers improve their analytical capabilities.

SS-02 Laser Ablation Mass Spectrometry, Monday, January 12, at 7:00, Detlef Günther, guenther@inorg.chem.ethz.ch, Department of Chemistry and Applied Biosciences, ETH Zurich, Vladimir-Prelog- Weg 1, 8093 Zurich, Switzerland

Laser Ablation inductively coupled plasma mass spectrometry has become the major technique for trace element analysis and isotope ratio determinations. Especially, imaging and quantification strategies have been improved, which makes the method widely applicable. Modern instrumentation, such as low UV lasers as well as time of flight mass spectrometers, is available and applied, and some of the pros and cons of the technique, as well as currently available equipment, will be discussed.

**Detlef Günther** is a full professor for Trace Element and Micro Analysis at the Department for Chemistry and Applied Biosciences (D-CHAB) at ETH Zurich. His research in the field of Analytical Chemistry is focused on instrument and method development for trace and ultra-trace element analysis and isotope ratio determinations using high spatial resolution laser ablation and inductively coupled plasma mass spectrometry. His group contributed publications to fundamental and applied research in Analytical Chemistry. He received the Lester Strock Award, the European Award for Plasma Mass Spectrometry, and the Widmer Award. In 2014, he became a member of the German National Academy of Science, Leopoldina. From 2015 until 2022, he served as Vice President for Research and Corporate Relations at ETH Zurich.

SS-03 Latest Advances in Laser Ablation-Based Chemical Analysis and Emerging Applications: LIBS, LA-ICP-(OES/MS), and Tandem LA – LIBS, Monday, January 12, 7 pm, Jhanis Gonzalez, <u>jhanis@appliedspectra.com</u>, jjgonzalez@lbl.gov, Applied Spectra, Inc., 950 Riverside Pkwy, Suite 90, West Sacramento, CA 95605-15071

Over the past 50 years, laser ablation has evolved into a cutting-edge technology that plays a pivotal role in a wide array of chemical analysis applications. Significant breakthroughs in our understanding of the ablation process, coupled with advancements in laser and detector technology, have transformed it into a highly reliable method for analytical measurements. This course is designed to equip you with a comprehensive understanding of the fundamental mechanisms behind the ablation process that are essential for achieving precise and accurate results using LIBS and ICP-MS. Participants will explore state-of-the-art systems, examine compelling application examples, and uncover the exciting directions for future developments in this dynamic field. **Keywords:** Laser ablation, ICP-MS, LIBS, chemical analysis, elemental isotopic and molecular analysis, microanalysis, Imaging.



**Dr. Jhanis J. Gonzalez C**. is a distinguished scientist in Chemistry (Physics-Chemistry). He earned his Ph.D. from Universidad Central de Venezuela in 2002. Dr. Gonzalez serves as the Technical Director of Product R&D and Management at Applied Spectra, Inc., and is a Principal Scientific Engineering Associate at Lawrence Berkeley National Laboratory, demonstrating his expertise and leadership in the field.

SS-06 Artificial Intelligence (e.g., via Artificial Neural Networks, Machine Learning, Deep Learning) with Applications to ICP and to Microplasma Spectrochemistry, Sunday, January 11, 1 pm, Vassili Karanassios, vkaranassios@uwaterloo.ca, University of Waterloo, Department of Chemistry and Waterloo Institute for Nanotechnology, Waterloo, ON N2L 3G1, Canada

Artificial Intelligence (and its variants) are receiving significant attention in the scientific journals [2, 2] and won the Nobel in Physics (2024) and in Chemistry (2024) (with expected significant future increases in market size). This short course is divided into two unequal parts. Part 1 deals with an introduction and fundamentals of AI, and Part 2 with applications of AI in plasma spectrometry. [1] V. Karanassios et al., "Artificial Neural Networks (ANNs) for spectral interference correction using a large-size spectrometer and ANN-based deep learning for a miniature one", invited **open access** book chapter, InTech Publishing, Chapter 12, Pages 227-249, InTech Publishing, Dec. 20, **2017**, DOI: 10.5772/intechopen.71039

[2] C. Tat and V. Karanassios, "Artificial intelligence (and related topics, e.g., Machine Learning, Deep Learning, artificial Neural Networks) as applied to the teaching and to the practice of analytical spectrochemistry, SPIE Proc., Volume 13026, Next-Generation Spectroscopic Technologies XVI; 130260H (2024); DOI: 10.1117/12.3013600



Vassili Karanassios is a Professor of Chemistry at the University of Waterloo (Ontario, Canada) and a co-founder of a degree-program in nano-technology engineering at the same University. Professor Karanassios received his Ph. D. from the University of Alberta (Edmonton, Canada) and was a Post Doctoral Fellow at McGill University (Montreal, Canada). In 2009, he held a Leverhulme award in the UK where he was a visiting Professor in Chemistry (Sheffield University), an Overseas Fellow of Churchill College (Cambridge University, UK), and a visiting Professor of Engineering (Cambridge University, UK) in the Center for Advanced Photonics and Electronics (CAPE). Professor Karanassios and his group published (among others) on 3D printing, on microfluidics and nanofluidics, on and on rapid prototyping, on spectral interference correction using Artificial Neural Networks (ANNs) and Deep Learning,

and on smartphone-enabled data acquisition and signal-processing from a variety of sensors for *on-site* chemical analysis and (potentially) for IoT applications and on microplasmas for elemental analysis.

SS-07 Microwave-Assisted Sample Preparation for Trace Elemental Analysis: Think Blank & Go Green, Sunday, January 11, 8 am. Joaquim A. Nóbrega, djan@terra.com.br OR djan@ufscar.br, Department of Chemistry, Federal University of São Carlos, São Carlos, SP, Brazil

This short course will present both theory and selected applications for sample preparation, featuring microwave-assisted digestion for trace elemental analysis. Sample preparation procedures for ICP-MS and ICP-OES, including microwave power, reagent temperature, pressure, matrices, and chemical compatibility, will be presented. Trace analysis will be discussed considering analytical blanks and contamination control. Benefits resulting from closed vessels digestion and special procedures, such as digestions using dilute nitric acid solutions with emphasis on green procedures using the minimum amount of reagents and generating a minimum amount of residues, will be presented. Applications for different types of samples, such as biological and botanical tissues, medicines (USP 232 and 233), and foods, will be highlighted. Green chemistry aspects related to microwave-assisted digestion will be discussed. **Keywords**: microwave-assisted digestion, analytical blank, green procedures, dilute nitric acid, reagent purification, reagent recovery.



Joaquim A. Nóbrega received his Ph.D. from the State University of Campinas (1992) and completed his postdoctoral training with Ramon Barnes (University of Massachusetts, Amherst, MA, 1996) and with Bradley Jones (Wake Forest University, Winston-Salem, NC, 2003). He is Full Professor in the Department of Chemistry, Federal University of São Carlos (São Carlos, São Paulo State, Brazil). His research interests are sample preparation for inorganic analysis, atomic absorption spectrometry, atomic emission spectrometry, and inductively coupled plasma mass spectrometry. He co-authored a chapter in 2011, updated in 2024, on "Microwave-Assisted Sample Preparation for Spectrochemistry" published in the online Encyclopedia of

Analytical Chemistry (John Wiley & Sons). He is a member of the Brazilian Society of Chemistry, Brazilian Society for the Advancement of Science, American Chemical Society, and Fellow Member of The Royal Society of Chemistry.

### Plasma Spectrochemical Techniques

ST-01 Accurate and precise isotopic analysis by MC-ICPMS, Sunday, January 11, 1 pm, Lu Yang, lu.yang@nrc-cnrc.gc.ca, National Research Council Canada, 1200 Montreal Rd, Ottawa, ON, K1A 0R6, Canada

This short course focuses on recent developments in isotopic fractionation (mass bias) and its correction models for achieving accurate and precise determinations of both absolute isotope ratios and delta isotope ratios using MC-ICP-MS. While mass-dependent fractionation (MDF) has traditionally been the accepted phenomenon, the recognition and reporting of mass-independent fractionation (MIF) within MC-ICP-MS has significantly increased over the past two decades. MIF plays a critical role in the selection of isotopic fractionation correction models, as applying mass-dependent models to isotopes exhibiting mass-independent fractionation can lead to biased isotope ratio measurements. This course will explore the implications of MIF on several widely used mass bias correction models, examining the core concepts, assumptions, advantages, limitations, and practical considerations for isotope ratio determinations in detail. **Keywords:** Delta isotope ratio, absolute isotope ratio, MC-ICP-MS, isotopic fractionation, mass-independent fractionation

Lu Yang is a Senior Research Officer at the National Research Council of Canada (NRC, Ottawa, Canada) and a Fellow of the Royal Society of Chemistry, leading research in applications of ICP-MS and MC-ICP-MS. She has published over 140 research papers. The isotopic measurements for mercury, germanium, indium, iridium, osmium, hafnium, and lead from her lab have been adopted by IUPAC as the best available isotopic composition measurements, and the standard atomic weights of Hg, Ge, Ir, and Hf are based on her lab's results. She is a NRC's representative at the Isotope Ratio Working Group of CCQM (Consultative Committee for Amount of Substance) of the BIPM (International Bureau of Weights and Measures), and services as an Associate Editor of Frontiers in Chemistry (Analytical Chemistry) and Editorial Board member of Spectroscopy and the Advisory board member of JAAS.

ST-02 Building or Modifying Your Laboratory for Trace and Ultra-trace Analyses, Sunday, January 11, 8 am, Ela Bakowska, ela@bakowska.com, bakowskae@corning.com, Elba Elemental Consulting, PO Box 1053, Corning, NY 14830

Reducing and eliminating sources of elemental contamination and optimizing the laboratory layout can achieve improvements in trace or ultra-trace capabilities. Based on my experience in building two new labs and modifying several others, I will share best practices for minimizing contamination and optimizing workflow, as well as guidelines for procuring new instrumentation. Cost-saving alternatives for lab design and operation will be presented. Sample preparation considerations for different applications will be discussed. **Keywords:** Laboratory design/upgrade, contamination prevention, supplies, instrumentation, sample preparation, automation, ICP-MS

Ela Bakowska is Principal Scientist and Manager at Corning RDC and Technical Director at Elba Elemental Consulting. She has



more than 30 years of experience in ICP-MS. Ela holds an M.S. in Physical Chemistry from the Warsaw University (Poland) and a Ph.D. in Analytical Chemistry from the University of Massachusetts, Amherst. During her career, Ela established the first application ICP-MS lab at HP and expanded and modernized several other labs. For eight years, she was an ICP-MS application chemist for HP/Agillent, and in this role, she assisted multiple new users in modernizing and upgrading their labs. Since 2001 (again becoming a user), she has purchased multiple ICP-MS systems from different vendors. Ela's experience includes the development of methods for the preparation and analysis of various types of glass, ceramics, raw materials, plastics, semiconductor, clinical, forensic, environmental, nuclear, and pharmaceutical samples. Since 2010, Ela has continuously upgraded and automated sample preparation labs and instrumental labs (including Clean Rooms) at Corning RDC, especially sample preparation areas dedicated to ultra-trace levels testing. In 2022, the new Center of Excellence was completed, and all ICP-MS labs were relocated

to areas custom-designed for contamination control. Her research focus is testing of glass, raw materials, Extractables and Leachables (E&L), and surface contamination. During 15 years at Corning RDC, Ela purchased two HR-ICP-MS systems, four Q-ICP-MS, and one ICP-QQQ-MS.

ST-03 Single Particle ICP-MS, ETV-ICP-MS, GC-ICP-MS, HPLC-ICP-MS, ICP-MS: Method Development, Problem Solving, Troubleshooting and Optimization, Saturday, January 10, 1 pm, Mark Fresquez, mwf6@cdc.gov, Centers for Disease Control and Prevention, 4770 Buford Hwy NE, MS S110-4, Atlanta, GA 30341-3717

This short course will cover hyphenated techniques related to ICP-MS, enabling ultra-trace elemental analysis with minimal interferences. The course will discuss selectivity, optimization, troubleshooting, problem-solving, and method development of these specific techniques, as well as the issues involved in analyzing difficult matrices, with an emphasis on especially troublesome blank contaminations. Discussion on isotope dilution, Single Particle-ICP-MS, desolvating sample introduction systems, sample preparation, and troubleshooting of ICP-MS hyphenated systems and ICP-MS instrumentation in general. **Keywords:** ICP-MS, Single Particle-ICP-MS, desolvating sample introduction, interferences, hyphenated, troubleshooting, method, ultra- trace, maintenance



Mark Fresquez earned his B.S. in Chemistry in 1988 and subsequently his M.S. in Analytical Chemistry at New Mexico State University. Mark began his career in commercial environmental trace metal analysis laboratories and the New Mexico Department of Health Scientific Laboratory Division (NMDOH-SLD) working with a wide variety of matrices and instrumentation including ETV-AAS, CV-AAS, ICP-OES and ICP-MS for 13 years. Afterwards, he was employed at the Centers for Disease Control and Prevention (CDC), working with arsenic speciation in urine utilizing HPLC-ICP-MS and mercury speciation in blood using GC-ICP-MS. Subsequently at CDC in the Tobacco and Volatiles Branch (TVB) he was responsible for development of methods for analysis of tobacco and smoke for toxic metals. Most recently while working in the IRAT Branch at CDC he was responsible for developing an acidic method for analysis of urine mercury by ICP-MS amongst other methods of analysis as a Research Chemist. He has over 30 years of inorganic trace metals analysis experience with a wide range of instrumentation, including ETV-AAS,

ICP-OES/AES, ICP-MS, HPLC-ICP-MS, GC-ICP-MS, Single Particle ICP-MS, and ETV-ICP-MS.

ST-04 Analysis Of Nano- And Micromaterials Using Laser Ablation Single Particle-ICP-MS, Sunday, January 11, 7 pm, Andreas Limbeck, andreas.limbeck@tuwien.ac.at, and Lukas Brunnbauer, lukas.brunnbauer@tuwien.ac.at, TU Wien, Institute of Chemical Technologies and Analytics, Getreidemarkt 9/164, A-1060 Vienna, Austria

Single-particle inductively coupled plasma mass spectrometry (sp-ICP-MS) has become a powerful tool for the analysis of nanomaterials. Even though conventional sp-ICP-MS provides valuable information about particle composition, size, and number concentrations, sample introduction of nano- and micromaterials in liquid suspension is related to challenges such as stability of the particle suspension or spectral interferences caused by the suspension medium. In this short course, the use of laser ablation as a sampling method for sp-ICP-MS analysis of nanoparticles and microplastics will be presented. The benefits and drawbacks of this approach will be discussed and illustrated with the help of suitable application examples. **Keywords:** Single particle analysis, laser ablation, nanoparticles, microplastics, statistical analysis, material science, environmental analysis.

**Andreas Limbeck** is an expert in the field of atomic spectroscopy with more than 20 years of research experience. Over the last few years, he has developed advanced expertise in the application of LA-ICP-MS and LIBS for the chemical analysis of solid materials, particularly for the quantitative determination of element distributions in various sample types. Since 2021 he is full professor for "Analytical Chemistry of Materials" at the Faculty of Technical Chemistry at TU Wien.

**Lukas Brunnbauer** received his PhD in Technical Chemistry from TU Wien. Currently, he is working as a Postdoctoral Researcher at TU Wien in the research group "Surface Analytics, Trace Analytics, and Chemometry." His research is mainly focused on spatially resolved polymer characterization using LIBS and LA-ICP-MS.

ST-05 Introduction to Chemometrics for Spectral Analysis, Sunday, January 11, 8 am, Neal B. Gallagher, nealg@eigenvector.com, Eigenvector Research Inc., 300 Bella Strada Lane, Manson, WA 98831 USA.

Chemometrics tools enable information extraction from complex multivariate data sets such as those created by ICP-MS, GC-MS, OES and TOF-SIMS. This course will cover principal components analysis for exploratory analysis and anomaly detection, partial least squares for quantification and classification, shift invariant tri-linearity for parallel factor analysis of GC/LC-MS data, and iterative target detection in hyperspectral imaging for surface analysis. Preprocessing can make the critical difference for successful information extraction, and this course will discuss centering and scaling, smoothing and differentiation, and clutter suppression to account for the often-present interference signal. **Keywords**: mass spectrometry, multivariate data analysis, GC-MS, hyperspectral imaging, PCA, PLS.

Neal Gallagher earned a Ph.D. in Chemical Engineering with a mathematics minor from the University of Arizona in 1992, an M.S. in



Chemical Engineering from the University of Washington in 1987 and B.S. degrees in Chemical Engineering and Engineering Physics from the University of Colorado in 1985. Recent research includes novel algorithms for iterative target detection in hyperspectral imaging and shift-invariant tri-linearity (SIT) for modeling hyphenated chromatography data. Since founding Eigenvector in January 1995, Neal has been intimately involved in chemometrics consulting, teaching short courses and software development including algorithms for detection, classification and quantification. Specific interests include hyperspectral imaging, process modeling, multi-variate curve resolution and classical least squares modeling.

ST-06 SP ICP-MS Data Processing with SPCal. From Zero to Hero. David Clases, Sunday, January 11, 1 pm, <a href="David.Clases@uni-graz.at">David.Clases@uni-graz.at</a>, Universitätsplatz 1, 8010, Graz, Austria, and Thomas Lockwood, Thomas.Lockwood@uts.edu.au, NanoMicroLab at the University of Graz, Graz, Austria & University of Technology Sydney, Sydney, Australia

This workshop is designed for the processing of raw SP ICP-MS data using SPCal\*, a data analysis tool developed by our group and now applied in labs worldwide. It is suitable for both beginners and experienced users and is vendor-independent. The workshop consists of two parts: first, we will introduce the theoretical and statistical background of SP ICP-MS, explain key algorithms in SPCal, and demonstrate its application to data from both quadrupole and TOF instruments. The second part is a hands-on session. Participants can bring their own data or use example datasets provided to explore processing, calibration, and visualization.

Keywords: single particle, ICP-QMS, ICP-TOFMS, nanoparticle, transport efficiency, statistics, calibration, automation, visualization

\* The software program central to this workshop was conceptualized through close collaboration between Thomas and David and has been continuously improved since its first release in 2021 (SPCal on GitHub). It is designed to enable transparent, harmonized, rapid, and accurate data processing, shaped by feedback from the scientific community.

### IMPORTANT: To participate in the hands-on session, we ask attendees to bring their own (Windows-operated) laptop.



**David Clases** completed his PhD at the University of Münster in 2017 and received a postdoctoral fellowship at the University of Technology Sydney. Following a lectureship there, he returned to Europe in 2021 and founded the NanoMicroLab at the University of Graz, initially serving as Assistant Professor. He is now Associate Professor and leads a group of seven researchers. His work focuses on advancing atomic spectroscopy for nano- and microanalysis, addressing key challenges in environmental and biomedical science.



**Thomas Lockwood** studied and completed his PhD at the University of Technology Sydney in 2022. He then worked as a technical officer and later as a postdoctoral researcher. He has an extensive background in data science and programming and has developed software solutions for a range of instrumental platforms and experimental setups. He is currently relocating to Austria to join the NanoMicroLab.

### Spectrochemical Instrumentation

SI-01 ICP-MS I: Introduction, Saturday, January 10, 1 pm, John Olesik,olesik.2@osu.edu, 125 S. Oval Mall, 275 Mendenhall Laboratory, School of Earth Sciences, Ohio State University, Columbus, OH 43210

ICP characteristics as an ion source, ion extraction, operating principles of ion optics, ion focusing, quadrupole and sector mass analysis, and detectors will be described. The general analytical capabilities, applications survey, and an introduction to matrix effects will be presented. **Keywords:** ICP-MS characteristics, instrumentation, interferences, applications.

John Olesik is a Research Scientist, Adjunct Associate Professor, and Director of the Trace Element Research Laboratory in the School of Earth Sciences at The Ohio State University. He received his PhD from the University of Wisconsin-Madison working on spark emission spectroscopy and was a postdoc at Indiana University in Gary Hieftje's group. For more than 35 years his research has been on the fundamental processes in plasma spectrochemistry (including sample introduction, ICP-OES, ICP-MS, and single particle ICP-MS), as well as practical considerations and applications in a huge variety of environmental, biological, biomedical, geological, and materials disciplines. This includes time-resolved measurement of ions produced from individual monodisperse and polydisperse droplets, nanoparticles, and microparticles. Among the awards he has received are the Lester Strock Award from the Society for Applied Spectroscopy and the Spectrochemical Analysis Award from the American Chemical Society.

SI-02 ICP-MS II: Advanced, Sunday, January 11, 1 pm, John Olesik, olesik. 2@osu.edu, 125 S. Oval Mall, 275 Mendenhall Laboratory, School of Earth Sciences, Ohio State University, Columbus, OH 43210

Detailed consideration will be given to basic cases of matrix effects, the removal of polyatomic ion interferences (including solvent removal, collisional dissociation, high-resolution, and cool plasma), alternative mass analyzers, analysis of limited solution volumes, and the removal of interferences. **Keywords:** ICP-MS characteristics, operation, instrumentation, interferences, applications

John Olesik is a Research Scientist, Adjunct Associate Professor, and Director of the Trace Element Research Laboratory in the School of Earth Sciences at The Ohio State University. He received his PhD from the University of Wisconsin-Madison working on spark emission spectroscopy and was a postdoc at Indiana University in Gary Hieftje's group. For more than 35 years his research has been on the fundamental processes in plasma spectrochemistry (including sample introduction, ICP-OES, ICP-MS, LA-ICP-MS, and single particle ICP-MS), as well as practical considerations and applications in a huge variety of environmental, biological, biomedical, geological, and materials disciplines. This includes time-resolved measurement of ions produced from individual monodisperse and polydisperse droplets, nanoparticles, and microparticles. Among the awards he has received are the Lester Strock Award from the Society for Applied Spectroscopy and the Spectrochemical Analysis Award from the American Chemical Society.

SI-03 The Rise of Microwave Induced Plasmas: Fundamentals and Applications, Saturday, January 10, 7 pm, Guillermo Grindlay Lledó, guillermo.grindlay@ua.es, University of Alicante, Faculty of Science, Crta. \ San Vicente s/n, San Vicente del Raspeig, Alicante, Spain

Microwave-induced plasma (MIP) technology has significantly evolved in recent years, and thereby, analytical figures of merit by such discharges for many elements are on par with those afforded by inductively coupled plasma (ICP) in optical emission and mass spectrometry. Moreover, this technology offers some unique analytical capabilities for the analysis of complex matrices and direct air analysis. This course is designed to review the state of the art of MIP technology with special emphasis on instrument optimization, figures of merit, and current applications. Finally, the session will be concluded with a discussion of the strengths and weaknesses of MIPs regarding ICPs. **Keywords:** Microwave plasma, inductively coupled plasma, optical emission spectrometry, mass spectrometry, matrix effects, calibration strategies, instrument optimization



**Guillermo Grindlay** earned his B.S in Chemistry and his PhD in Analytical Chemistry at the University of Alicante. After postdoctoral stays at Delft University of Technology (Netherlands) and Ghent University (Belgium), he returned to his alma mater as a lecturer in 2008, and he became a senior lecturer in 2019. His research interests are focused on developing novel analytical instrumentation and methodologies for metals, nanomaterials, and organics determination in complex samples using ICP- and MIP-based techniques as well as gaining insight into the origin of non-spectral interferences for such type of plasmas.

SI-04 Agilent ICP-Expert and Masshunter ICP-MS Software Workshop, Tuesday, January 13, 7 pm, Bert Woods, bert woods@agilent.com, Agilent Technologies, 2850 Centerville Rd, Wilmington, DE 19808

Come hone your skills with our software bootcamps. Learn about the latest in software solutions for spectroscopy, and discuss the entire analytical process from method development to data analysis with our experts. PCs are provided with the latest software loaded. Half the course will cover the ICP Expert software, followed by a session on MassHunter software for ICP-MS. ICP Expert is for ICP-OES systems, and MassHunter is for ICP-MS and ICP-QQQ systems. Current and prospective users of Agilent atomic spectroscopy equipment are encouraged to take this course. **Keywords:** software, Agilent, ICP-OES, ICP-MS, Masshunter.

SI-05 Theory and Practical Use of Reaction Cells and Collision Cells for ICP-MS, Sunday, January 11, 1 pm, Patrick Gray, patrick.gray@fda.hhs.gov, Deanna M Jones, (CDC) hii4@cdc.gov, Center for Food Safety and Applied Nutrition, Office of Regulatory Science, 5001 Campus Drive, College Park, U.S. Food and Drug Administration, Centers for Disease Control and Prevention, College Park, MD 20740 and 4770 Buford Hwy NE MS S110-5, Atlanta, GA 30341-3717

The design and operation of reaction cells and collision cells used for isobaric interference removal in ICP-MS will be discussed. The course begins with an introduction to the principles and kinetics of ion-molecule reactions and the operation of the rf devices (quadrupoles, hexapoles, octapoles, etc.). The various efficiencies of the ion chemistry (primarily ion reactivity, production of the ions within the cell) will be evaluated, concluding that where high efficiency of the primary chemistry is obtained, reaction of the analyte ion with impurities and the formation of new interferences within the cell becomes essential. Various means of suppressing these effects, including kinetic energy discrimination and band pass operation of the cell, will be contrasted and compared, and effects related to the order of the multipole device will be considered. Examples of the application of reaction cell and collision cell methods in the semiconductor, environmental, clinical, geochemical, and isotopic analysis will be presented. **Keywords:** Collision cell, reaction cell, spectral interference, chemical resolution, pressurized multipole, chemistry, ion dynamics, ion-molecule chemistry, in-cell produced interferences, multipole operating point, energy discrimination



**Patrick Gray** is a Chemist at U.S. Food & Drug Administration based in Silver Spring, Maryland. Previously, Patrick was a Research Chemist at the U.S. Department of Defense.

**Deanna Jones** is the Chief of the Speciation and Lot Screening Laboratories in the IRAT Branch. She has over 17 years of experience at the CDC developing methods for measuring trace elements in biological samples using chromatography and ICP-MS. Her laboratory performs arsenic and mercury speciation methods and provides technical support to state and local public health labs. She is proficient in qualitative and quantitative statistical data analysis, method validation, and evaluating analytical figures of merit, Clinical Laboratory Improvement Amendments (CLIA) regulations, including Proficiency Testing (PT) requirements, and Quality Assurance/Quality Control (QA/QC) review.

ST-07 Metrology for Particle Characterisation: From Nanomaterials to Microplastics, Tuesday, January 13, 8 pm Heidi Goenaga Infante, Heidi.Goenaga-Infante@lgcgroup.com & Guillermo Redondo Fernandez, guillermo.fernandez@lgcgroup.com, UK National Measurement Laboratory, LGC, The Priestley Building, 10 Priestley Road Guildford, GU2 7XY, United Kingdom

This short course will illustrate how some of the analytical challenges related to the characterization of *i*) nanomaterials, including those used in drug delivery systems/nanomedicines and *ii*) microplastics in food-related samples have been overcome through a variety of practical examples in which platforms including the combination of asymmetrical field-flow-fractionation (AF4) with light scattering/ICP-MS, Optical Particle Imaging Analysis, LD-IR and spICP-MS play a key role. It will also highlight remaining analytical challenges driven by legislation, existing reference materials as well as the importance of interlaboratory comparisons to assess the state-of-the-art of measurements performed by expert laboratories.

**Keywords:** nanomedicines; reference materials; particle characterization; microplastics; particle metrology; single particle ICP-MS; emerging regulations; interlaboratory comparisons



Heidi Goenaga Infante's scientific career of over twenty-five years of experience on elemental and speciation analysis started with the award of a PhD from Oviedo University, Spain. This was followed up by a Postdoctoral Research fellowship at the University of Antwerp, Belgium. Currently, she is a Science Fellow of LGC where she has worked since 2003. She is also the Chief Scientist and Director of Chemical Metrology of the National Measurement Laboratory hosted by LGC. Heidi is chair of the Editorial Board of the RSC Journal of Analytical Atomic Spectrometry. Her Metrology research interests mainly lye in trace element speciation analysis, metalomics/protein research, the characterisation of nanomaterials, quantitative bio-imaging and the characterisation of reference materials and standards. Heidi Goenaga-Infante is the UK representative at the Inorganic Analysis

Working Group of the international Consultative Committee for Metrology in Chemistry (CCQM). She is the LGC representative at ISO TC 24 (Particle characterisation). She is the EURAMET representative for inorganic analysis at the CCQM Key Comparison Working Group and the LGC representative at the EURMET TC MC Strategy group. She is the leading author of over a 185 scientific research papers and 8 book chapters. Heidi was awarded the 2020 Lester W. Strock Award from SAS and the 2023 European Award for Plasma Spectrochemistry. Heidi is a visiting Professor at Strathclyde University, UK and Honorary Senior Research Fellow of the University of Liverpool, UK.



**Guillermo Redondo Fernandez** completed his PhD in Chemical, Biochemical and Structural Analysis and Computational Modelling, in 2024 at the University of Oviedo (Spain). Then, he joined the UK National Measurement Laboratory (NML) at LGC as a Researcher, where he is developing analytical methods with ICP-MS and hyphenated techniques (i.e. AF4-MALS-UV-RI) to study nanomedicines. He is specialized in the design, synthesis and characterization of nanomaterials and their application in food, cosmetics and/or medicine. Guillermo is also a British Standards Institution (BSI) LBI/37 committee member, participating in the development of standards related to particle characterization and contributing with world-wide experts to ISO/TC 24.

Last Updated: 10/24/25