CECE 2016

13th International Interdisciplinary Meeting on Bioanalysis

"… bringing people and ideas together …"

October 17 - 19, 2016
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Find the meeting history and more at www.ce-ce.org

Foreword

Welcome to CECE 2016, the 13th International Interdisciplinary Meeting on Bioanalysis. As in the previous years, it is our goal to: “bring together scientists from different disciplines who may not meet at other meetings”. CECE Junior will follow two days of linvited speaker’s lectures and poster sessions will be open during all three days. The organizers want to thank all invited speakers, sponsors and participants for their continuing support. Please, check our web at www.ce-ce.org for more information about the history, programs, photos and videos from the previouis years.

Brno, October 8, 2016

The Medal of Jaroslav Janák

The Medal of Jaroslav Janák for contributions to the development of analytical sciences was established by the Institute of Analytical Chemistry. Named after the inventor of the gas chromatograph (patented in 1952), founder of the institute (1956) and its long-term director, the medal is awarded to scientists who have significantly contributed to the development of separation sciences.

In 2016, the Medal of Jaroslav Janák goes to **Prof. Petr Boček**. In the early 1980' with the fresh university diploma, I started working in the group of electromigration methods headed by Petr Boček, a smiling friendly man commanding respect not only as a former sport wrestler but also as someone who knew practically everything about analytical separations and, especially, electrophoresis. There were fancy looking plexiglass instruments (often called chips in today's papers) powered by sparking high voltages. It was capillary isotachophoresis (ITP) and Petr's group was one of the world top laboratories in ITP. While ITP was the king of capillary separations in the early 1980's Petr was already interested in capillary zone electrophoresis and presented some of the early results at the Electrophorese Forum conferences organized by Prof. B. J. Radola in Munich, Germany. That time Prof. Radola also founded the journal Electrophoresis and invited Petr to become a member of the editorial board soon becoming an Associate Editor (1992-2000) and since 2001 serves as the Senior Deputy Editor. As an author and co-author of over 250 scientific papers and monographs on Chromatography and Electrophoresis, Petr had a major impact on the development of analytical separations and with over 7000 citations belongs to the most cited analytical chemists not only in the Czech Republic. He is regarded as one of the founders of the "Czech capillary electrophoresis school" highly prized especially for explanation and exact description of many electromigration related phenomena. Besides heading his department Petr was also the director of the Institute of Analytical Chemistry (1993-2001). It was my pleasure and privilege to know and work with Peter for many years. I wish to congratulate him to all his achievements and thank for all the work he has done for the Institute of Analytical Chemistry and science in general.

Franta Foret

Program of the CECE 2016

Hotel Continental, Brno, Czech Republic, October 17-19, 2016

8:00 – 15:00 **Registration (Monday, Tuesday)**

Monday, October 17

9:00 – 9:15 **CECE 2016 - Opening remarks**

9:15 – 9:45 **Jana Krenkova**
Institute of Analytial Chemistry of the CAS, v. v. i., Brno, Czech Republic
A NOVEL NANOSPRAY LIQUID JUNCTION INTERFACE FOR VERSATILE CE-MS

9:45 – 10:15 **Erdmann Rapp**
Max Planck Institute for Dynamics of Complex Technical Systems, Magdeburg, Germany
XCGE-LIF: A POWERFUL TOOL IN THE GLYCOANALYTICAL TOOLBOX

10:15 – 10:45 C**offee break**

10:45 – 11:15 **Guillaume Laurent Erny**
University of Porto, Porto, Portugal
UNLEASHING UNTARGETED HYPHENATED MS ANALYSIS WITH CHEMOMETRICS

11:15 – 11:45 **Andrew Ewing**
Chalmers Univ. and Univ. of Gothenburg, Göteborg, Sweden
ANALYTICAL MEASUREMENTS WITH CAPILLARY ELECTROPHORESIS, FROM ELECTROCHEMICAL CYTOMETRY TO ALZHEIMER'S PEPTIDE IN CSF

11:45 – 12:15 **Andras Guttman**
University of Veszprem, Veszprem, Hungary
GLYCOHISTOPATHOLOGY: MINING THE FFPE DEPOSITORIES BY CAPILLARY ELECTROPHORESIS

12:15 – 14:15 **Lunch break – poster session**

14:15 – 14:45 **Steven Wilson**
University of Oslo, Oslo, Norway
OPEN TUBULAR LIQUID CHROMATOGRAPHY-MASS SPECTROMETRY: A POWERFUL AND VERSATILE TOOL FOR BIOANALYSIS

14:45 – 15:15 **Radim Chmelik**
Brno University of Technology, Brno, Czech Republic
LIVE-CELL QUANTITATIVE PHASE IMAGING BY COHERENCE-CONTROLLED HOLOGRAPHIC MICROSCOPY

15:15 – 15:45 **Kareem Elsayad**
Vienna Biocenter Core Facilities, Vienna, Austria
UNRAVELLING AND UNDERSTANDING THE MECHANICAL PROPERTIES OF PLANTS USING BRILLOUIN LIGHT SCATTERING MICROSPECTROSCOPY

16:15 – 18:00 **City walk with invited speakers**

Tuesday, October 18

09:30 – 10:00 **Stavros Stavrakis**
ETH Zurich, Zurich, Switzerland
DROPLET-BASED MICROFLUIDICS: HIGH-THROUGHPUT EXPERIMENTATION ONE DROP AT A TIME

10:00 – 10:30 **Peter Ertl**
Vienna University of Technology, Vienna, Austria
ORGAN-ON-CHIP TECHNOLOGY: MONITORING DYNAMIC CELL RESPONSES UNDER CONTROLLED PHYSIOLOGICAL CONDITIONS

10:30 – 11:00 C**offee break**

11:00 – 11:30 **Blanca Lapizco-Encinas**
Rochester Institute of Technology, Rochester, USA
PARTICLE CAPTURE AND ENRICHMENT EMPLOYING NON-UNIFORM ELECTRIC FIELDS AND INSULATING STRUCTURES

11:30 – 12:00	**Zdeněk Hurák** *Czech Technical University, Prague, Czech Republic* SINGLE-PARTICLE HIGH-PRECISION MICRO-MANIPULATION USING DIELECTROPHORESIS
12:00 – 14:00	**Lunch break – poster session**
14:00 – 14:30	**Daniel Georgiev** *University of West Bohemia, Pilsen, Czech Republic* MANAGING CELL HETEROGENEITY IN MICROFLUIDIC DESIGN
14:30 – 15:00	**Michael V. Gorshkov** *Russian Academy of Sciences, Moscow, Russia* PROTEOGENOMICS AND SOME OF THE PITFALLS OF THE PROTEOMIC SIDE OF THIS COIN
15:00 – 15:30	**Jana Roithova** *Charles University, Prague, Czech Republic* HELIUM TAGGING INFRARED PHOTODISSOCIATION SPECTROSCOPY
15:30 – 16:00	**Renato Zenobi** *ETH Zurich, Zurich, Switzerland* ON-LINE ANALYSIS OF EXHALED BREATH VIA SECONDARY ELECTROSPRAY IONIZATION MASS SPECTROMETRY
16:00 – 16:05	**Invitation to CECE 2017, Veszprém, Hungary**
19:00	**Conference dinner with the traditional Moravian music**

Wednesday, October 19

9:00 – 9:15 **CECE Junior opening**

9:15 – 9:30 **Jasna Hradski**
Department of Analytical Chemistry, Faculty of Natural Sciences, Comenius University in Bratislava, Bratislava, Slovak Republic
DETERMINATION OF COUNTERION IN CANCER TREATMENT DRUG BY MICROCHIP ELECTROPHORESIS

9:30 – 9:45 **Renata Gerhardt**
Leipzig University, Leipzig, Germany
ON-CHIP HPLC WITH INTEGRATED DROPLET MICROFLUIDICS FOR FURTHER DOWNSTREAM PROCESSES

9:45 – 10:00 **Paweł Pomastowski**
Department of Environmental Chemistry and Bioanalytics, Faculty of Chemistry, Nicolaus Copernicus University, Torun, Poland; Interdisciplinary Centre of Modern Technology, Nicolaus Copernicus University, Torun, Poland
THE MALDI IONIZATION AS TOOLS OF MODERN BIOANALYTICS

10:00 – 10:15 **Lenka Portychová**
Department of Analytical Chemistry, Palacký University, Olomouc, Czech Republic; Research Institute for Organic Synthesis, Inc., Rybitví, Czech Republic
DETERMINATION OF URINARY INDICAN AND CREATININE USING AN UHPLC/ECD-DAD METHOD

10:15 – 10:30 **Viorica Railean-Plugaru**
Department of Environmental Chemistry and Bioanalytics, Faculty of Chemistry, Interdisciplinary Centre for Modern Technologies, Nicolaus Copernicus University, Toruń, Poland
BIO SILVER NANOPARTICLES AS A NEW OPPORTUNITY TO MEDICAL TRATMENT

10:30 – 11:00 C**offee break**

11:00 – 11:15 **Marton Szigeti**

MTA-PE Translational Glycomics Group, University of Pannonia, Veszprem, Hungary; Horvath Csaba Memorial Institute of Bioanalytical Research, University of Debrecen, Hungary

SINGLE RUN GLYCAN STRUCTURE IDENTIFICATION FOR CAPILLARY ELECTROPHORESIS

11:15 – 11:30 **Jan Vacek**

Department of Medical Chemistry and Biochemistry, Faculty of Medicine and Dentistry, Palacky University, Olomouc, Czech Republic

SWITCHING OF PROTEIN PROPERTIES UPON GLYCATION REVEALED BY ELECTROCATALYTIC APPROACH

11:30 – 11:45 **Adriana Arigò**

Department of "Scienze Chimiche, Biologiche, Farmaceutiche ed Ambientali", University of Messina, Messina, Italy

EXTRACTION, SEPARATION AND IDENTIFICATION OF BIOACTIVE COMPOUNDS IN "YOUNG BARLEY" THROUGH RP AND HILIC TECHNIQUES COUPLED TO MS/MS

11:45 – 12:00 **Jana Váňová**

Department of Analytical Chemistry, Faculty of Chemical Technology, University of Pardubice, Pardubice, Czech Republic

DETERMINATION OF DISTRIBUTION CONSTANTS OF ANTIOXIDANTS BETWEEN LIPOSOMES, ALKYLSULFATE MICELLES, OCTANOL AND WATER USING ELECTROKINETIC CHROMATOGRAPHY

12:00 – 13:30 **Lunch break – poster session – poster removal**

13:30 – 13:45 **Vratislav Peška**

Mendel Centre for Plant Genomics and Proteomics, Central European Institute of Technology, Masaryk University, Brno, Czech Republic

BAL31-NGS IN TELOMERE BIOLOGY

13:45 – 14:00 **Agnieszka Szmitkowska**

Central European Institute of Technology, Masaryk University, Brno, Czech Republic

ROLE OF IN VITRO PHOSPHORYLATION ASSAY IN UNDERSTADING MSP SIGNALING IN A. THALIANA

14:00 – 14:15 **Sona Valuchova**

Central European Institute of Technology, Masaryk University, Brno, Czech Republic

A NOVEL RAPID METHOD FOR DETECTING PROTEIN-NUCLEIC ACID INTERACTIONS

14:15 – 14:30 **Monika Skrutková Langmajerová**

Department of Biochemistry, Faculty of Science, Masaryk University, Brno, Czech Republic; Institute of Organic and Analytical Chemistry, University of Orleans and the French National Center for Scientific Research, Orleans, France

CAPILLARY ELECTROPHORESIS WITH ONLINE NANORAECTOR FOR CHARACTERISATION OF SKIN FIBROBLAST ELASTASE ACTIVITY FROM VARIOUS BIOLOGIC MATERIAL

14:30 **Closing remarks**

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Antonín Bednařík, Markéta Machálková, Kateřina Coufalíková, Pavel Houška, Eugene Moskovets, Jarmila Navrátilová, Jan Šmarda, Jan Preisler

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Tomas Vaclavek, Jana Krenkova, Frantisek Foret

P74 PREDICTION OF GRADIENT RETENTION DATA FOR HYDROPHILIC INTERACTION LIQUID CHROMATOGRAPHIC SEPARATION OF NATIVE AND FLUORESCENTLY LABELED OLIGOSACCHARIDES
Nikola Vaňková, Petr Česla

P75 COMBINED EFFECT OF TEMPERATURE AND CDO NANOPARTICLES TREATMENT ON PICEA ABIES
Kristýna Večeřová, Pavel Mikuška, Michal Oravec, Michaela Kozáčiková, Antonio Pompeiano, Pavel Coufalík, Otmar Urban

P76 IDENTIFICATION OF PROTEIN-PROTEIN BINDING INTERFACES BY USING PEPTIDE MICROARRAY TECHNIQUE
Pavlína Víšková, Lola Bajard-Ešner, Lukáš Trantírek, Silvie Trantírková, Jan Ryneš

P77 ANALYSIS OF INORGANIC POSPHORUS OXYANIONS BY CAPILLARY ZONE ELECTROPHORESIS
Sebastian Pallmann, Jana Šteflová

P78 DETERMINATION OF CRITICAL MICELLAR CONCENTRATION OF ACETONITRILE-WATER MIXTURES BY VARIOUS TECHNIQUES
Jana Steflova, Martin Stefl, Sarah Walz, Oliver Trapp

About the invited speakers

Jana Krenkova is a Staff Scientist at the Department of Bioanalytical Instrumentation, Institute of Analytical Chemistry of the Czech Academy of Sciences in Brno. She received her M.Sc. degree in Analysis of Biological Materials (2003) and Ph.D. degree in Analytical Chemistry (2007) at the University of Pardubice, Czech Republic. During years 2007-2010, she was as a postdoctoral fellow at the Lawrence Berkeley National Laboratory, Berkeley, CA, USA working on development of enzyme and nanoparticle-modified monolithic materials for bioanalytical applications. In 2010, she received a Marie Curie Fellowship and joined the group of Frantisek Foret at the Institute of Analytical Chemistry in Brno. Her research interests include monolithic materials, enzymatic reactors, nanoparticle synthesis, and separation/mass spectrometry coupling.

Erdmann Rapp studied chemistry at the universities of Konstanz and Tübingen in Germany. During his PhD, he was stipendiary of DFG graduate school for analytical chemistry at the Eberhard Karls University of Tübingen and did fundamental research and method development on miniaturized separation techniques coupled to MS and NMR. He was invited research fellow at the NMR Centre of Wageningen University (The Netherlands), studying fluid dynamics in miniaturized separation systems via NMR-imaging.

In 2001 he got research associate and head of the Laboratory for Miniaturized Separation Techniques at the Institute of Process Engineering of the Otto von Guericke University in Magdeburg (Germany). He continued his fundamental research on fluid dynamics in electrokinetically and hydrodynamically driven open tubular and packed capillaries and its impact on the analysis of biomolecules.

Since 2003 till present, he is head of Bio/Process Analytics at Max Planck Institute for Dynamics of Complex Technical Systems in Magdeburg (Germany). He and his team are working on the development and implementation of innovative cutting edge bio/process analytical tools for a deeper understanding of bio(techno)logical processes - in particular, on high-throughput tools for proteomics, glycoproteomics and glycomics to be able to handle large sample numbers arising along bioprocess development and biomarker discovery. With the invention of “glyXbox”, a high-performance glycoanalysis system, he got key founder of glyXera GmbH, providing glycoanalytical services to academia, clinics and industry.

Guillaume Erny is a principal researcher in the Laboratory for Process Engineering, Environment, Biotechnology and Energy, Faculty of Engineering of the University of Porto in Portugal. He received his PhD in Analytical Chemistry in 2003 from the University of York (UK). He was awarded the Ronal Belcher Award in 2002 (Royal Society of Chemistry, UK) for his work on the HVL function applied to capillary electrophoresis. He then held a postdoctoral position in the Laboratory of Biomolecular Science at UMIST, Manchester, UK; a postdoctoral position at the CSIC, Madrid, Spain; and a postdoctoral position at the University of Aveiro, Portugal. He developed a keen interest in chemometrics approaches applied to the analysis of hyphenated MS dataset and self-taught Matlab in order to test and develop the analysis algorithms. He lives in sunny and windy Aveiro, Portugal, with his wife and two daughters who keep him busy.

Andrew Ewing received a PhD from Indiana University. After 25 years at Penn State University, he is now Professor at Chalmers University and University of Gothenburg, Sweden. His group has pioneered small-volume chemical measurements at single cells, electrochemical detection for capillary electrophoresis, novel approaches for electrochemical imaging of single cells, and new electrochemical strategies to separate individual nanometer vesicles from cells and quantify their contents. His 300 publications have been cited over 16000 times with an H-index of 69. He has recently received the Charles N Reilley Award from the Society for Electroanalytical Chemistry (2013), the ACS Analytical Division Award in Electrochemistry (2013), the Norblad-Ekstrand Medal of the Swedish Chemical Society (2014), and the Pittsburgh Conference Award in Analytical Chemistry (2015). He is an Honorary Professor at both Nanjing University of Science and Technology and Beijing University of Science and Technology. He is a member of the Royal Swedish Academy of Sciences (2012) and the Gothenburg Academy of Arts and Sciences (2013).

András Guttman, MTA-PE Lendulet professor of Translational Glycomics, is the head of the Horváth Csaba Laboratory of Bioseparation Sciences and also leads the application efforts at Sciex. His work is focused on capillary electrophoresis and CESI-MS based glycomics and glycoproteomics analysis of biomedical and biopharmaceutical interests. Dr. Guttman has more than 290 scientific publications, wrote 35 book chapters, edited 4 textbooks and holds 23 patents. He is a member of the Hungarian Academy of Sciences, on the board of several international organizations, serves as editorial board member for a dozen scientific journals and has been recognized by numerous awards including the Analytical Chemistry Award of the Hungarian Chemical Society in 2000, named as Fulbright Scholar in 2012, received the CASSS CE Pharm Award in 2013, the Arany Janos medal of the Hungarian Academy of Sciences, the Pro Scientia award of the University of Pannonia and the Dennis Gabor Award of the Novofer Foundation in 2014.

During his PhD study, **Steven Ray Wilson** worked with the development of on-line 2D LC systems and the hyphenation of LC and NMR. After his PhD, he became involved in drug discovery efforts through the Cancer Stem Cell Innovation Center. Today, his focus is on applying miniaturized LC-MS systems in cancer diagnostics, working as an Associate Professor at the University of Oslo, collaborating with a number of medical environments.

Radim Chmelík

Education

1997, Ph.D., Faculty of Mechanical Engineering, BUT, Physical and Material Engineering

2002, Associate Professor, Faculty of Mechanical Engineering BUT, Applied Physics

2012, Professor, Faculty of Mechanical Engineering BUT, Applied Physics

Scientific activities

Coherence-controlled and correlation holographic microscopy, quantitative phase imaging, microscopy of three-dimensional objects, microscopy in turbid media, applications of holographic microscopy in living-cell biology, experimental biophotonics

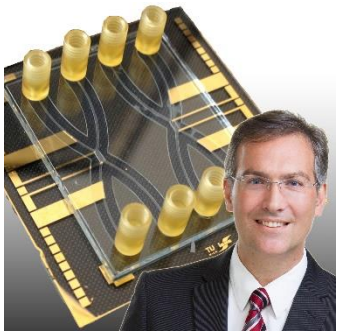
Industry cooperation
TESCAN ORSAY HOLDING, a. s., AREKO, s.r.o., Meopta - optika, s.r.o.
Prizing by scientific community
2013, Werner von Siemens Excellence Award 2013, in category: The most important result of development/innovation
2013, 1st place in Cooperation of the Year competition (AFI, AmCham, TACR)

Kareem Elsayad obtained his Masters Degree and PhD in the UK and the USA respectively in the field of condensed matter physics, before moving to Vienna to work on developing optical microscopy techniques for life science research applications as a postdoctoral researcher. Since the end of 2013 he heads the Advanced Microscopy division of the Vienna Biocenter Core Facilities (VBCF) in Vienna, where he oversees a team of optical physicsts and biophysicsts/biologists developing novel and cutting edge optical microscopy solutions for and in collaboration with life-science researchers primarily at the Vienna Biocenter.
Among other things he is inventor of a technique called Spectrally coded Optical Nanosectioning (SpecON) which utilizes the optical interaction of radiation from fluorophores with a nano-structured surface for axial superresolution imaging with a resolution <10nm. He has also developed and demonstrated the correlative microspectroscopy technique - Fluorescence Brillouin imaging (FBi), which can be used to in parallel map the biochemical constituents and mechanical properties within live cells and tissue.

As head of the Advanced microscopy facility his interests broadly cover all things optical microscopy related in particular microspectroscopy, time-resolved fluorescence techniques, light sheet microscopy and superresolution fluorescence microscopy. He is personally interested and engaged in the field of light-matter interactions and the mechanical and physical properties of biological matter in general, as well as designing & building novel optical microscopy setups that make use of the more unusual properties of light and its interaction with matter.

Stavros Stavrakis is currently a Senior Scientist in the deMello group in the Department of Chemistry and Applied Biosciences at ETH Zurich. He received his B.Sc. in Chemistry and Ph.D in Biophysical Chemistry from the University of Crete (Greece) in 2005. His research was focused on the application of time-resolved vibrational spectroscopies such as FTIR and Raman, applied to enzymatic systems (cytochrome c oxidase) involved in catalytic reactions accompanied with proton/charge

transfer reactions. In 2007 Dr. Stavrakis was awarded an Individual Outgoing Marie Curie Fellowship. As a Marie Curie fellow, he spent three years with Prof. Stephen Quake at Stanford University specializing in single molecule biophysics. The focus of his research was to develop new technologies to improve the throughput of current single molecule DNA sequencing platforms. This covered four broad areas: strategic surface deposition techniques, measuring DNA polymerase kinetics using single molecule FRET, single molecule colloidal lensing and novel surface chemistries for enhanced single molecule signals. The ability to achieve single molecule sensitivity with long working distance objectives enabled high temperature single molecule spectroscopy and the ability to measure the kinetics of a thermophilic DNA polymerase for the first time. As part of his fellowship he also worked as a postdoctoral fellow in Dr. David McGloin's lab at the University of Dundee, developing methods for optical trapping and rotation of single cells in microfluidic chips. His current research interests are focused on applications of single molecule fluorescence detection, and optofluidics in biology. Currently he has a team of postdocs and students developing new microfluidic/optofluidic platforms for single molecule enzymology, high-throughput imaging flow cytometry, fast enzyme kinetics, fluorescence lifetime combined with droplet microfluidics and high-throughput microfluidic single-cell screening platforms.



Peter Ertl holds an engineering degree in Biotechnology (BOKU, Austria), a PhD in Chemistry (Univ. Waterloo, Canada) and received his postdoctoral training as a biophysicist at University of California at Berkeley (US). Additionally, in 2003 Dr. Ertl co-founded a biotech start-up company where he served a number of years as Director of Product Development in Kitchener-Waterloo (CAD) developing benchtop-sized microbial analyzers. In 2005 Dr. Ertl moved to Austria where he worked as Senior Scientist in the Biosensor Technology unit at the AIT Austrian Institute of Technology. In 2016 he was appointed Professor for Lab-on-a-Chip Systems for Bioscience Technologies at Vienna University of Technology, where his research focuses on the development of advanced *in vivo* and *in vitro* diagnostic microsystems for biomedical research.

Blanca H. Lapizco-Encinas is an associate professor in the Department Biomedical Engineering at the Rochester Institute of Technology. Her current research efforts are focused on the development of microscale electrokinetic techniques for the manipulation of bioparticles, from macromolecules to cells. Her main research objective is to develop electrokinetic-based microdevices that would answer the needs of many different applications, such as: cell assessment for clinical/biomedical applications and

microorganism manipulation and detection for food safety and environmental monitoring. Her research work has been funded by the NSF and other funding agencies in the US and Mexico. Her research efforts have received awards from the Mexican Academy of Sciences and the L'OREAL for Women in Science program. The research findings obtained by her group have been presented in numerous international conferences. She serves as reviewer for various international Journals and has served as organizer and session chair for several conferences. She is a Deputy Editor for the Journal ELECTROPHORESIS and has served as Vice-President of the American Electrophoresis Society.

Zdeněk Hurák is a researcher and lecturer at the Department of Control Engineering, Faculty of Electrical Engineering, Czech Technical University in Prague. Web page of his research group is http://aa4cc.dce.fel.cvut.cz. He got his master's degree in aerospace electrical engineering (summa cum laude) at Military Academy, Brno, Czech Republic, in 1997. He was awarded Boeing Fellowship in 1999, which supported his 3-month research stay at Iowa State University, Ames, USA. In 2000 he started his Ph.D. study in control systems and robotics under supervision of Michael Šebek at Czech Technical University in Prague, Czech Republic, and defended it in 2004 with the thesis on l1 optimal control. He was a visiting researcher at TU Eindhoven, The Netherlands, May through December 2008. He was awarded Fulbright's scholarship for a visiting position at University of California, Santa Barbara, February through August 2014. These days he gives graduate lectures on optimal and robust control and undergraduate lectures on modeling and simulation of dynamic systems. He supervises graduate students, and manages research projects with academic and industrial partners. His research interests include algorithms for optimal, robust and distributed control, especially within the polynomial (algebraic) framework, and applications of advanced control schemes to electromechanical systems such as inertially stabilized camera platforms, piezoelectric micro-manipulators and non-contact micro-manipulation using dielectrophoresis. He is a Senior Member of IEEE and serves the community as a chair of Control Systems Chapter of Czech-Slovak Section of IEEE, and as a member of the editorial board of Automa journal (and Kybernetika journal in the past). He reviews for IEEE TAC, IEEE TCST, IFAC Automatica, IFAC Mechatronics, IFAC Control Engineering Practice and Asian Journal of Control. He (almost) regularly attends IEEE CDC and IFAC World Congress, and very often IEEE MSC, ACC, MTNS, IFAC ROCOND and a occasionally a few other conferences and workshops.

Daniel Georgiev received his Ph.D. from the University of Michigan, Ann Arbor, in 2007 in the area of Systems and control theory. His studies were funded by the National Science Foundation Graduate Research Fellowship and the University of New Mexico Presidential Scholarship. In 2007, he accepted a postdoctoral grant from the National Institute of Health for cross-training in biology. He completed his postdoctoral studies at the Klavins lab of synthetic biology, University of Washington, Seattle, WA. In 2010, Daniel Georgiev joined the Faculty of Applied Sciences, University of West Bohemia, where he founded the Synthetic biology laboratory (www.ccy.zcu.cz) within the NTIS research and the Department of cybernetics. Most recently, he cofounded XENO Cell Innovations, a startup company focused on commercialization of whole cell biosensor technologies.

Mikhail Gorshkov was graduated from Moscow Institute of Physics and Technology with PhD in Chemical Physics in 1987. His early research interests were in precise atomic mass measurements and mass spectrometry instrumentation. Since then he worked at The Ohio State University (Columbus, USA) and Pacific Northwest National Laboratory (Richland, USA) mainly focused on developing mass spectrometers and mass spectrometry based approaches for studying proteins. In 2002 he founded Laboratory of Physical and Chemical Methods for Structure Analysis at the Institute for Energy Problems of Chemical Physics, Russian Academy of Sciences. Currently, his laboratory's main areas of research are broadly within mass spectrometry instrumentation, liquid chromatography, and bioinformatics with applications in proteomics.

In 1998 **Jana Roithová** graduated in organic chemistry from the Faculty of Science of Charles University in Prague, she then continued with her PhD studies at the Faculty of Chemical Engineering of the Institute of Chemical Technology, Prague. Her PhD thesis was devoted to reaction dynamics and was completed under the supervision of Prof. Zdenek Herman (J. Heyrovsky Institute of Physical Chemistry). After obtaining the PhD title in 2003, she undertook a postdoctoral stay at the Technical University in Berlin in the group of Prof. Helmut Schwarz. From 2007 she is working at the Faculty of Science of the Charles University in Prague, where she presently holds a position of full professor and she is

also a head of the department of organic chemistry. She is author of more than 140 papers in peer-reviewed scientific journals.

The major research interests of J. R. involve development of new approaches for studying of reaction mechanisms and reactive intermediates by mass spectrometry. Typically several experimental approaches are combined with computational chemistry for obtaining of a detailed picture of chemical reactivity. She uses infrared predissociation spectroscopy for investigation of reactive ions/ionic intermediates in a cryogenic ion trap and various dedicated mass spectrometry experiments for uncovering of details of elementary reaction steps.

Renato Zenobi is Professor of Analytical Chemistry at the Organic Chemistry Laboratory of the Swiss Federal Institute of Technology (ETH) Zurich. Born in Zurich in 1961, he received a M.S. degree from the ETH Zurich in 1986, and a Ph.D. at Stanford University in the USA in 1990. This was followed by two postdoctoral appointments at the University of Pittsburgh (1990 - 1991) and at the University of Michigan (1991). Renato Zenobi returned to Switzerland in 1992 as a Werner Fellow at the EPFL, Lausanne, where he established his own research group. He became assistant professor at the ETH in 1995, was promoted to associate professor in 1997, and to full professor in 2000. He was chairman of the Organic Chemistry Laboratory in 2002-2003 and 2011-2012, served as the president of ETH's university assembly (Hochschulversammlung, HV) from 2006 – 2008, and of the lecturer's conference (Konferenz des Lehrkörpers, KdL) at ETH Zurich 2006 - 2010. Zenobi was a visiting professor at the Barnett Institute (Boston) in 2004/2005, and at the Institut Curie (Paris) in 2010. In 2010 he was appointed Associate Editor of Analytical Chemistry (American Chemical Society). He has chaired the 2014 International Mass Spectrometry Conference in Geneva, Switzerland.

Zenobi's research areas include laser-based analytical chemistry, electrospray and laser-assisted mass spectrometry, ambient mass spectrometry, and near-field optical microscopy and spectroscopy. He has made important contributions to the understanding of the ion formation mechanism in matrix-assisted laser desorption/ionization (MALDI) mass spectrometry, and to ambient ionization methods. He is well known for the development of analytical tools for the nanoscale, in particular TERS (tip-enhanced Raman spectroscopy), a spectroscopic methodology with ≈ 10 nm spatial resolution.

Renato Zenobi has received many awards for his scientific work, including the Thomas Hirschfeld Award (1989), an Andrew Mellon Fellowship (1990), the Ruzicka Prize (1993), the Heinrich Emanuel Merck-Prize (1998), the Redwood Lectureship from the Royal Society of Chemistry (2005), the Michael Widmer Award (2006), a honorary Professorship at East China Institute of Technology (2007), the Schulich Graduate Lectureship (2009), a honorary membership of the Israel Chemical Society

(2009), honorary professorships at the Chinese Academy of Sciences (Changchun), at Hunan University, and at Changchun University of Chinese Medicine (2010), the Mayent-Rothschild Fellowship (Institut Curie, Paris; 2010), the Fresenius Lectureship from the German Chemical Society (2012), the Thomson Medal (International Mass Spectrometry Foundation, 2014), the 2014 RUSNANO prize, and the 2015 Fresenius Award (German Chemical Society/GDCh).

Abstracts of oral presentations – Invited speakers

A NOVEL NANOSPRAY LIQUID JUNCTION INTERFACE FOR VERSATILE CE-MS

Jana Krenkova[1], Rob Haselberg[2], Govert W. Somsen[2], Frantisek Foret[1]

[1]Institute of Analytical Chemistry, v. v. i., Brno, Czech Republic
[2]Vrije Universiteit Amsterdam, Amsterdam, the Netherlands

Summary

Coupling of capillary electrophoresis (CE) with mass spectrometry (MS) represents a powerful combination to perform selective, efficient and sensitive analysis of a variety of compounds. Several interfaces to hyphenate CE and MS have been developed and most of them can be categorized into either the sheath-flow or sheathless arrangement.

In this work we present a new polyimide-based liquid junction nanospray interface, combining the advantages of sheath flow and sheathless designs. The liquid junction interface was prepared as a hybrid microfabricated plastic liquid junction sprayer allowing to perform analysis in standard (30-100 μm ID) separation capillaries. The interface incorporates a self-aligning port for coupling of the separation capillary as well as ports for automated flushing of both the liquid junction and the separation capillary. The interface permits performing CE both with and without electroosmotic flow. The use of large bore capillaries allows injection and preconcentration of larger sample volumes, favoring detection sensitivity. Different compositions of the spray liquid and BGE can be used when needed.

The performance of the interface is demonstrated for analysis of a broad range of analytes such as metabolites, peptides, glycans, and intact proteins, including monoclonal antibodies and their fragments. A comparison with a commercially available sheath-flow as well as sheathless (CESI) interface will be presented, discussing analytical parameters such as repeatability, linearity and sensitivity.

Acknowledgement

Financial support from the Grant Agency of the Czech Republic (16-09283Y, P206/12/G014), and the institutional research plan (RVO:68081715) is acknowledged.

XCGE-LIF: A POWERFUL TOOL IN THE GLYCOANALYTICAL TOOLBOX

Erdmann Rapp[1,2], René Hennig[1,2], Samanta Čajić[1], Thilo Muth[1,2], Robert Kottler[1], Udo Reichl[1,3]

[1]Max Planck Institute for Dynamics of Complex Technical Systems, Magdeburg, Germany
[2]glyXera GmbH, Magdeburg, Germany
[3]Otto-von-Guericke University, Chair of Bioprocess Engineering, Magdeburg, Germany

Summary

Glycomics is a rapidly emerging field that can be viewed as a complement to other „omics“ approaches. Hence, there is a dramatic increase in the demand for analytical tools and specific databases in glycobiology, respectively, glycobiotechnology. In order to enhance and improve the comparatively small existing glycoanalytical toolbox [1], fully automated, highly sensitive, reliable, high-throughput and high-resolution analysis methods including automated data evaluation are required.

Our glycoanalysis approach, based on multiplexed capillary gelelectrophoresis with laser induced fluorescence detection (xCGE-LIF) shows high potential for high-performance analysis of glycoconjugates. The development of this high-performance glycoanalysis system (method, software and database) and its application to different fields with respect to sample preparation, separation and automated data analysis is presented [2-6]. The smart applicability of the system is demonstrated for different types of glycosamples (biopharmaceuticals, vaccines, human milk and blood serum) [1-8]. This novel modular high-performance glycoanalysis system allows fully automated, highly sensitive, instrument-, lab- and operator-independent "real" high-throughput glycoanalysis. This is in contrast to the currently prevailing methods, where high-throughput is highly cost and lab-space intensive and ties up a lot of manpower.

References

[1] Huffman J.E., Pucic-Bakovic M., Klaric L., Hennig R., Selman M.H., Vuckovic F., Novokmet M., Kristic J., Borowiak M., Muth T, Polasek O., Razdorov G., Gornik O., Plomp R., Theodoratou E., Wright A.F., Rudan I., Hayward C., Campbell H., Deelder A.M., Reichl U., Aulchenko Y.S., Rapp E., Wuhrer M., Lauc G. (2014) Mol. Cell. Proteomics, 13, 1598-1610.

[2] Schwarzer J., Rapp E., Reichl U. (2008) Electrophoresis, 29, 4203-4214.

[3] Rapp E., Hennig R., Borowiak M., Kottler R., Reichl U. (2011) Glycoconjugate J., 28, 234-235.

[4] Ruhaak L., Hennig R., Huhn C., Borowiak M., Dolhain R., Deelder A., Rapp E., Wuhrer M. (2010) J. Proteome Res., 9, 6655-6664.

[5] Hennig R., Reichl U., Rapp E. (2011) Glycoconjugate J., 28, 331-332.

[6] Behne A., Muth T., Borowiak M., Reichl U., Rapp E. (2013) Electrophoresis, 34, 2311-2315.
[7] Kottler R., Mank M., Hennig R., Müller-Werner B., Stahl B., Reichl U., Rapp E. (2013) Electrophoresis, 34, 2323-2336.
[8] Hennig R., Cajic S., Borowiak M., Hoffmann M., Kottler R., Reichl U., Rapp E. (2016) Biochim Biophys Acta, 1860, 1728–1738.

UNLEASHING UNTARGETED HYPHENATED MS ANALYSIS WITH CHEMOMETRICS

Guillaume L. Erny, Arminda Alves

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Summary
The use of mass spectrometers (MS) as a detector has been a true game-changer in analytical separation techniques. Hyphenated MS techniques not only allow an easy identification of the main peaks, but, when used as the detector, MS has the unique ability to be simultaneously a near universal detector and extremely selective. Yet, while hyphenated MS techniques are unrivalled for targeted approaches, they do not easily allow a comprehensive analysis of unknown samples. This is mainly due to the large amount of noise that may hide relevant information, as well as the redundancy of signals generated by each compound entering the detector. This results from the ionisation mode: any chemicals entering the chamber will produce multiple ions and therefore will leave multiple footprints in the dataset that could be wrongly assigned to different compounds.

Chemometrics approaches can help in extracting, organising and visualising the information that is contained within a dataset. We recently developed such an approach, called clusters plot that allows a comprehensive analysis when using a separation technique hyphenated with high resolution mass spectrometry (X-HRMS). Briefly, after extracting all series of points (profiles) that are related to the transport and ionisation of a compound, a clustering analysis is used to classify all profiles based on their similarities. The aim is to group similar profiles in a cluster, where each cluster will regroup all the profiles related to one and only one compound.

The clusters plot is obtained after running a series of independent functions programmed using Matlab. All these functions are in open access and can be downloaded from https://finneeblog.wordpress.com/. This presentation aims at demonstrating the potential of this approach, as well as discuss its different assumptions and possible limitations. The presentation will be illustrated using deproteinized urine samples that were analysed using capillary electrophoresis hyphenated with time of flight mass spectrometry.

ANALYTICAL MEASUREMENTS WITH CAPILLARY ELECTROPHORESIS, FROM ELECTROCHEMICAL CYTOMETRY TO ALZHEIMER'S PEPTIDE IN CSF

Dimitri Brinet[1], Johan Dunevall[2], Yasmine Iacone[1], Jörg Hanrieder[1], Andrew Ewing[1,2]

[1]University of Gothenburg, Gothenburg, Sweden
[2]Chalmers University of Technology, Gothenburg, Sweden

Summary

Capillary electrophoresis with electrochemical detection (CEEC) has been used to develop methods to measure neurotransmitter storage in single cell vesicles with a method we called electrochemical cytometry and led to a new separationless method for electrochemical impact cytometry of nanometer vesicles. Additionally, we are using CEEC for analysis of the Alzheimer's-related Amyloid Beta (Aβ) peptide aimed at analysis in cerebral spinal fluid of patients. Here, CE is critically important to separate the different Aβ species and this has not been done before in cerebral spinal fluid samples.

Measuring the contents of individual nanometer transmitter vesicles is an analytical challenge and important to understand neurotransmission. We developed electrochemical cytometry to separate nanometer vesicles, lyse them on an electrode surface, and amperometrically detect the active contents of each vesicle in a high throughput manner. This led to a new method of electrochemical cytometry where the electrochemical response to single adrenal chromaffin vesicles filled with hormone transmitters as they impact a 33-um diameter disk-shaped carbon electrode can be meassured. This has been used to compare the amount in vesicles to the amount released and then to argue that the predominant mode of exocytosis is not all-or-none, but rather open and closed and the vesicles are reused.

Alzheimer's disease is a progressive disorder characterized, in part, by deposition of amyloid peptides made primarily of the Aβ peptide. These Aβ peptides are characterized by sequential cleavages of the amyloid precursor protein. These peptides can, however, assemble into possibly neurotoxic structures that might be the cause of the disease symptoms (1). A major difficulty in understanding the role of these structures is the challenge associated with isolating and monitoring these metastable species. We will present a label free CEEC method to separate, identify, and measure these species.

Reference

[1] Alzheimer's disease: the amyloid cascade hypothesis. Hardy, J.A., Higgins G.A., *Science* 1992.

GLYCOHISTOPATHOLOGY: MINING THE FFPE DEPOSITORIES BY CAPILLARY ELECTROPHORESIS

Andras Guttman[1,2], Boglarka Donczo[1], Marton Szigeti[1], Bryan Fonslow[2]

[1]Horvath Csaba Memorial Institute of Bioanalytical Research, University of Pannonia, Veszprem, Hungary
[2]Sciex, Brea, CA, USA

Summary

Glycohistopathology is a subset of the emerging field of molecular pathology to utilize the large number of tissue biopsy samples that are collected yearly for histology based diagnostics and archived in formalin-fixed and paraffin-embedded (FFPE) forms. Buffered formalin is the most commonly used fixative, which crosslinks the amino groups of proteins through methylene bridges, providing preservation to maintain the structural integrity of the specimens. Although FFPE samples have been used for molecular pathology studies before, such as for DNA analysis, little information is available on the effect of formalin-fixation on the sugar structures of the glycoproteins in these samples. In this presentation we report on the use of capillary electrophoresis with both laser induced fluorescence (LIF) and mass spectrometry (MS) detection methods to profile the released N-linked glycans from standard glycoproteins and tissue biopsy samples before and after the formalin-fixation and paraffin-embedding processes. The released carbohydrates were fluorophore labeled before analysis with a triple charged APTS tag. The resulting N-glycome patterns were very similar before and after formalin fixation and paraffin embedding. The low sample requirement of CE-LIF and CESI-MS was very useful to analyze miniscule sample amounts from the FFPE slides. To obtain detailed structural information, exoglycosidase based carbohydrate sequencing was also applied using. The sequencing results were verified by CESI-MS. Based on our preliminary results, FFPE samples represent a rich source for glycobiomarker discovery, especially with the associated clinical outcome information. In addition, this approach represents an unparalleled opportunity for retrospective and prospective studies in both biomedical and pharmaceutical interests.

OPEN TUBULAR LIQUID CHROMATOGRAPHY-MASS SPECTROMETRY: A POWERFUL AND VERSATILE TOOL FOR BIOANALYSIS

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Summary

For decades, open tubular liquid chromatography (OTLC) has promised excellent chromatographic performance. However, technical challenges obstructed its development, as well as the advances of other LC formats, making one ask "what do we need OTLC for anyway?"

However, in biomedical research, there is an increasing need for analyzing very limited biosamples, e.g. stem cells and disease-promoting extracellular vesicles such as tumor-derived exosomes. Here, OTLC may find a home, as it has in later years provided unprecedented sensitivity and is very well matched with nanospray-mass spectrometry (nESI-MS).

In our group, which focuses on e.g. stem cell-ness in cancer, OTLC-MS has recently been used for comprehensive and targeted proteomics, using an organic polymer layer on the inner walls of the columns as a stationary phase. However, we find that OTLC columns featuring a silica-based layer are highly versatile, allowing highly efficient separations for bottom-up proteomics as well as intact proteins. In addition, these columns allow for high resolution, attogram level detection of small molecules, such as breast cancer-related lipids. Coupled with on-line enzymatic reactors (also open tubular), OTLC can allow detection of trace analytes in just a few hundred cells.

OTLC systems are also being applied in other research areas, such as an analysis tool in counter-terrorism. In other words, OTLC is a tool that is beginning to show strong potential for practical use in several application areas.

LIVE-CELL QUANTITATIVE PHASE IMAGING BY COHERENCE-CONTROLLED HOLOGRAPHIC MICROSCOPY

Radim Chmelík[1,2], Jana Čolláková[1,2], Pavel Veselý[1]

[1]CEITEC - Central European Institute of Technology, Brno University of Technology, Brno, Czech Republic
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Summary

Quantitative phase imaging (QPI) is one of modern microscopical techniques that has emerged during last decades and substantially improved possibilities and quality of biomedical imaging. Image contrast in QPI originates from phase shifts of light introduced by an observed specimen. For this reason, high-contrast imaging of live cells is achieved non-invasively and without application of possibly phototoxic markers. The phase shifts measured by the QPI in individual image pixels are proportional to the dry-mass density in the corresponding points of observed cells [1]. Thus the distribution of mass in a cell and its changes over time can be observed and measured for hours and days. The advantage of coherence-controlled holographic microscopy (CCHM) equipped with incoherent-light source consists in one-shot imaging (similarly to wide-field) with clean background without any coherence artefacts, which provides a high accuracy of mass measurements. This is why CCHM suits ideally cell growth assessment as well as evaluation of their motility based on protrusion/ retraction measurement. In addition, the coherence-gate effect makes possible QPI of live-cell behavior in turbid or complex 3D milieu. We demonstrate the usage of the CCHM QPI qualities. The appraisal of cellular responses to the course of sub-toxic challenges even in turbid medium is substantially improved. The kind of cell death and modifications of cell behavior by pathological processes can be revealed.

Acknowledgement

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Reference

[1] H. G. Davies, H. G., and Wilkins, M. H. F., *Nature,* 1952, *169*, 541.

UNRAVELLING AND UNDERSTANDING THE MECHANICAL PROPERTIES OF PLANTS USING BRILLOUIN LIGHT SCATTERING MICROSPECTROSCOPY

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Summary

Brillouin Light Scattering (BLS) spectroscopy is an all-optical label-free technique which allows for the determination of the viscoelastic properties of a sample. BLS is generally a very weak process, based on the interaction of light with thermal density fluctuations, and thus challenging to implement for lifescience/biomedical applications. Recent advances in spectrometer and camera designs have however made it possible to perform BLS measurements on live cells, opening the door to a new means of studing the mechanical properties of biological systems. Here I will discuss the use of BLS Microspectroscopy and correlative Fluorescence – BLS Microspectrocopy to map the viscoelastic properties of cells and tissue in 3 dimensions, focusing on its use to understand the mechanical properties of plant cells. 3 dimensional mapping of the mechanical properties of plant cells is particularly interesting given the delicate balance between extracellular matrix (cell wall) mechanical properties and turgor pressure involved in defining cell shape, assuring "correct" development, for maintaining the structural integrity of the organism as a whole, and ultimately determining their survival subject to all types of environmental perturbations.

Firstly I will give an introduction to BLS including experimental setups and the physical principles it is based on. I will then discuss some details of the quantities that are and can be extracted from a BLS measurement and how and to what extent they may be compared to or compliment results obtained from alternative measurements of the mechanical properties of and within cells - such as those obtained using microrheology and perturbation-deformation techniques such as Atomic Force Microscopy (AFM). I then will present a series of studies on different live plant cells and tissue we have performed focusing on the physical and biological significance of the obtained results. Finally I will summarize the strengths of the technique, its limitations and some of the current challenges, along with an outlook of what we are working on, and some planned and potential future applications in biophysics research as well as medical diagnostics.

DROPLET-BASED MICROFLUIDICS: HIGH-THROUGHPUT EXPERIMENTATION ONE DROP AT A TIME

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Summary

The past 25 years have seen considerable progress in the development of microfabricated systems for use in the chemical and biological sciences. Interest in microfluidic technology has driven by concomitant advances in the areas of genomics, proteomics, drug discovery, high-throughput screening and diagnostics, with a clearly defined need to perform rapid measurements on small sample volumes. At a basic level, microfluidic activities have been stimulated by the fact that physical processes can be more easily controlled when instrumental dimensions are reduced to the micron scale [1]. The relevance of such technology is significant and characterized by a range of features that accompany system miniaturization. Such features include the ability to process small volumes of fluid, enhanced analytical performance, reduced instrumental footprints, low unit costs, facile integration of functional components within monolithic substrates and the capacity to exploit atypical fluid behaviour to control chemical and biological entities in both time and space.

My lecture will discuss recent studies that are focused on exploiting the spontaneous formation of droplets in microfluidic systems to perform a variety of analytical processes.

Droplet-based microfluidic systems allow the generation and manipulation of discrete droplets contained within an immiscible continuous phase [2]. They leverage immiscibility to create discrete volumes that reside and move within a continuous flow. Significantly, such segmented-flows allow for the production of monodisperse droplets at rates in excess of tens of KHz and independent control of each droplet in terms of size, position and chemical makeup. Moreover, the use of droplets in complex chemical and biological processing relies on the ability to perform a range of integrated, unit operations in high- throughput. Such operations include droplet generation, droplet merging/fusion, droplet sorting, droplet splitting, droplet dilution, droplet storage and droplet sampling [3, 4]. I will provide examples of how droplet-based microfluidic systems can be used to perform a range of experiments including nanomaterial synthesis [5], cell-based assays [6] and DNA amplification [7]. In addition, I will describe recent studies focused on the development of novel imaging flow cytometry platform that leverages the integration of inertial microfluidics with stroboscopic illumination [8] to allow for high-resolution imaging of cells at throughputs approaching 10^5 cells/second.

References

[1] A.J. deMello, *Nature*, 442 (2006) 394-402.

[2] X. Casadevall-i-Solvas & A.J. deMello, *Chemical Communications*, 47 (2011) 1936–1942.
[3] X. Niu, S. Gulati, J.B. Edel & A.J. deMello, *Lab Chip*, 8 (2008) 1837–1841.
[4] X.Niu, F. Gielen, J.B. Edel & A.J. deMello, *Nature Chemistry*, 3 (2011) 437-442.
[5] I. Lignos et al., *Nano Letters*, 16, (2016) 1869–1877.
[6] Soongwon Cho et al., *Analytical Chemistry*, 85 (2013) 8866–8872.
[7] Yolanda Schaerli et al., *Analytical Chemistry*, 81 (2009) 302-306.
[8] Hess et al., *Analytical Chemistry*, 87 (2015) 4965-4972.

ORGAN-ON-A-CHIP TECHNOLOGY: MONITORING DYNAMIC CELL RESPONSES UNDER CONTROLLED PHYSIOLOGICAL CONDITIONS

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Summary

Microfluidics is vital for cell analysis because it is the only technology capable of simulating the physiological environment of cells and cell assemblies to investigate cellular transport mechanisms and cell proliferation events in the presence of test reagents, temperature or shear force gradients. In light of the benefits of microfluidics, my research group at TUW is developing lab-on-a-chip systems containing integrated fluid handling, degassing and biosensing systems to non-invasively monitor dynamic cell population responses. We have successfully integrated different electro-analytical, magnetic and optical detection methods in microfluidic devices (a) to assess the behaviour of structured 3-dimensional Candida biofilms, (b) to monitor dynamic stress responses of mammalian cell populations and (c) to detect cell-to-cell and cell-to-matrix interactions. In course of the presentation various components including microvalves, micropumps, degassers and sensing systems for lab-on-a-chip will be presented as well as their potential for automated, miniaturized and integrated multilevel cell analysis will be discussed.

PARTICLE CAPTURE AND ENRICHMENT EMPLOYING NON-UNIFORM ELECTRIC FIELDS AND INSULATING STRUCTURES

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Summary

Microfluidics is a dynamic and rapidly growing field with potential applications in numerous areas, from food and water safety, to environmental monitoring and clinical analysis. Working on the microscale offers attractive advantages such as shorter processing times, low sample and reagent consumption and the possibility of portable systems with a high level of integration. Manipulation and analysis of biological particles is one of the fields that has been most benefited with the marriage of microfluidics and analytical sciences. Many of these applications require fast response methods able to handle/analyze high value biological products, in a gentle manner, without leading to cell damage or bioproduct denaturation.

Important research efforts are being devoted to the development of analytical techniques that can be used with microfluidic devices. Electrokinetics, electric field driven techniques, such as electrophoresis, electroosmosis and dielectrophoresis, are widely used in microfluidic devices, offering new ways to assess, manipulate and analyze bioparticles. Dielectrophoresis (DEP) is an electrokinetic transport mechanism driven by polarization effects when a dielectric particle is exposed to a spatially non-uniform electric field. DEP has great flexibility, since it can be used with charged and neutral particles employing AC or DC electric potentials. DEP offers more versatility than electrophoresis since it has the capability for significant particle enrichment, up to three orders of magnitude. DEP also offers means for effective continuous particle sorting.

This work is focused on insulator based DEP (iDEP), a dielectrophoretic mode that uses insulating structures between two external electrodes to create electric field gradients and generate dielectrophoretic forces on particles. This study includes experimental and mathematical modeling work. Particle mixtures, including biological cells, were separated and analyzed employing novel variations of iDEP. The results demonstrate that iDEP has great potential as a bioanalytical technique.

SINGLE-PARTICLE HIGH-PRECISION MICROMANIPULATION USING DIELECTROPHORESIS

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Summary

The talk will start by giving an overview of basic principles and state of the art in noncontact manipulation with one or several (micro)particles by shaping force fields of various physical origin. Typically, physical phenomena related to electricity and magnetism are exploited, in which case electric voltages applied to a regular array of (micro)electrodes or electric currents flowing through a regular array of coils are controlled. A promising physical phenomena for bioanalytical application is dielectrophoresis. The dielectrophoretic force derives from an electric field, thus the particle need not respond to a magnetic field. Neither does the particle have to be electrically charged. Although applicability of dielectrophoresis to sub-micron size particles has been demonstrated, dielectrophoresis seems particually suitable for particles of sizes around a micron and larger, hence a candidate for a biological cell manipulation technique. Indeed, use of dielectrophoresis for manipulation of cells has been documented many times in the literature, dating back to the pioneering work of Herbert Pohl in 1950s. The currently prevailing modes of use of dielectrophoresis are separation and characterization, in which cases a bulk of microparticles is manipulated at once. In this talk, however, we will focus on the use of dielectrophoresis for a high-precision manipulation of a single particle (single cell). After introducing the state of the art, we present our own results in this domain of single-particle manipulation using dielectrophoresis. Namely, we will show how a clever yet simple microelectrode layout in combination with a real-time optimization procedure can achive high-accuracy steering of a microparticle all over a flat surface, with the range of motion stretching up to a few milimeters. We will discuss the physical principles, fabrication issues and the control-algorithmic tricks upon which our solution rests. The functionality of the experimental platform developed by out team has been demonstrated in various scientific competitions: 4th and 5th place in IEEE RAS Mobile Microrobotics Challenge in 2012 and 2013, respectively, 1st place in Matlab and Simulink Student Design Challenge in 2013 (this one was based on magnetophoresis, though, but it is related). Numerous videos will accompany the talk. Our ultimate motivation for the presented research is to contribute to a development of a low-cost, fully automated and possibly disposable bioanalytical platform. We hope this talk might help recognize the potential of bridging the scientific domains of biology and chemistry and engineering domains of controls, automation and robotics.

MANAGING CELL HETEROGENEITY IN MICROFLUIDIC DESIGN

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Summary

Design of microfluidic devices and their integration in lab-on-chip concepts must consider phenotypic heterogeneity. Herein we take a look at heterogeneity in dielectrophoretic (DEP) response within an isogenic population. DEP is a highly sensitive method for non-invasive cell manipulation and monitoring. Cells exposed to non-uniform electric fields are acted on by DEP forces that are frequency-dependent and vary according to the cell internal state. Knowledge of a priori DEP heterogeneity attributed to sample preparation, spontaneous mutation, and non-uniform sample composition can be used to design cell screening applications (e.g., for blood typing or rare cell quantification). Knowledge of induced DEP heterogeneity attributed to cell-cell interaction, cell induction, and microfluidic environmental effects can be used to design integrated devices that characterize dynamic behaviors (e.g., multidrug resistance) that are otherwise difficult to measure. We've developed a method, called DEP cytometry, for quantifying both a priori and induced cell heterogeneity. Similar to flow cytometry that yields fluorescence histograms at given wavelengths, DEP cytometry yields DEP force histograms at given electrical field frequencies. Preliminary experimental data collected for wild type and mutant Saccharomyces cerevisiae populations illustrate the high throughput and sensitivity of the method. Differences between yeast strains can be detected with throughput of thousands of cells per minute in a PDMS based prototype device. The experimental method is complemented by developed in silico tools, whereby spatiotemporal distribution of cell states can be predicted for a rich set of microfluidic topologies. Jointly, the experimental and simulation tools enable design of microfluidic devices with inherent consideration for a priori and induced cell heterogeneity.

PROTEOGENOMICS AND SOME OF THE PITFALLS OF THE PROTEOMIC SIDE OF THIS COIN

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Summary

Shotgun proteomics results in identification of tryptic peptides by searching tandem mass spectra (MS/MS) against genome-centered protein database. In the search, a

reference database is typically employed that leaves coding genome variants behind. Thus, the proteins with single amino acid substitution may be left behind the search. In general, a use of one or more custom DNA and/or mRNA sequence databases for LC-MS/MS data search is becoming a growing trend in identifying the encoded variants of amino acid sequence originated from single amino acid polymorphism or alternative splicing. This area of research including the studies on genome re-annotations using proteomic data, is often referred to as proteogenomics. One of its objectives is extracting the biologically relevant information often hidden in the shotgun mass spectrometry data using the customized protein database containing proteins with residue substitutions due to gene mutations. Cancer proteogenomics is an important example because of a large amount of biologically relevant non-synonymous somatic mutations across the tumor genomes. These mutations can be revealed at the proteome level using the bottom-up LC-MS/MS analysis through identification of the so-called variant proteolytic peptides. These are the peptides which correspond to the part of the protein where the residue substitution event occurred due to the gene mutation. However, this approach aiming at identification of variant peptides using customized database searches of shotgun proteomic data is facing a number of challenges including a dilemma of selecting the most efficient database search strategy, sample preparation artifacts, false discovery rate estimation, and mutant protein quantification, among the others. In this talk we will highlight some of these issues using the results of our recent studies as well as the literature data.

The results considered in this talk were obtained with financial support from Russian Science Foundation, grant #14-14-00971 and in collaboration with Prof. Sergei Moshkovskii's lab from The Institute of Biomedical Chemistry, Russian Academy of Sciences.

HELIUM TAGGING INFRARED PHOTODISSOCIATION SPECTROSCOPY

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Summary

Infrared photodissociation spectroscopy became one of the standard tools in determination of the structure of the ions in the gas phase. Next to the often applied infrared multiphoton dissociation spectroscopy, many approaches based on the messenger technique have been developed. We are using helium tagging which permits investigation of highly reactive ions [1].

Helium tagging infrared photodissociation spectroscopy is performed with a tandem mass spectrometer containing a wire quadrupole trap cooled to 3 K. Mass-selected ions are trapped with helium buffer gas and form helium complexes.

Spectroscopy can be performed with tunable light sources in IR or VIS spectral range [2, 3].

I will show application of our approach for the investigation of hyper-valent metal-oxo complexes. We can routinely detect metal-oxo stretching vibrations (among others, I will show the first detection of copper(III)-oxo stretching mode). Recently, we have also demonstrated that we can spectroscopically distinguish triplet and quintet states of the iron(IV)-oxo complexes [4].

References

[1] J. Roithová, A. Gray, E. Andris, J. Jašík, D. Gerlich, Acc. Chem. Res. 2016, 49, 223–230.

[2] J. Jašík, D. Gerlich, J. Roithová, J. Am. Chem. Soc. 2014, 136, 2960 − 2962.

[3] J. Jašík, R. Navrátil, I. Němec, J. Roithová, J. Phys. Chem. , 2015, 119, 12648–12655.

[4] E. Andris, J. Jašík, L. Gómez, M. Costas, J. Roithová, Angew. Chem. Int. Ed. 2016, 55, 3637–3641.

ON-LINE ANALYSIS OF EXHALED BREATH VIA SECONDARY ELECTROSPRAY IONIZATION MASS SPECTROMETRY

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Summary

Exhaled breath contains relevant information on a person's health status. Our vision is to use real-time and completely non-invasive chemical analysis of exhaled breath for applications such as medical diagnosis, monitoring progress and treatment of diseases, drug compliance, pharmacokinetics, and others. The methodology we use to analyze breath in real time is based on secondary electrospray ionization coupled to high-resolution mass spectrometry (SESI-HRMS). It affords ppb-ppt limits of detection, and analysis of compounds with molecular weights up to 1000 Da.

A number of interesting questions can now be addressed via on-line mass spectrometric analysis of exhaled breath: is there a core pattern for individual phenotypes visible in mass spectrometric "breathprints"? Can diurnal changes be monitored via exhaled breath? Can diseases be diagnosed via exhaled breath, and if yes, which ones? Can proper drug use (or drug abuse) be detected via analysis of the chemical composition of exhaled breath? The presentation will focus on several examples in medical diagnosis, including the detection of novel biomarkers for diseases such as obstructive sleep apnea (OSA) and chronic obstructive pulmonary disease (COPD). Monitoring of drug compliance and pharmacokinetics via real-time SESI-MS will also be shown.

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