CHIMIA **2002**, *56*, No. 9

Detailed Program of the Congress

Focal Point: Analytical Chemistry

Organic Trace Analysis – Challenges – Unsolved Problems

Date/Time: Tuesday, October 15, 2002, 09.30–13.00
Rooms: Osaka + Samarkand

Description

Even in organic trace analysis, scientists are always looking for improvements which help to save time, increase the robustness of a method as well as enhance selectivity and sensitivity. In this session, leading experts in their fields will give a synopsis progress report of separation sciences including high-resolution liquid chromatography, electrochromatography and high-resolution gas chromatography. In addition, concepts and ideas will be presented on how to speed-up analysis and to increase selectivity.

Organized by

Prof. *Michael Oehme*, University of Basel

Chairperson

Prof. *Michael Oehme*, University of Basel

Program

09.30 **Dr. *Ronald E. Majors***, Agilent Technologies, Wilmington, DE 19808, USA
'New Directions in HPLC Column Technology for Rapid and Selective Separations'

10.10 **Prof. *Thomas Welsch***, Universität Ulm, Abteilung für Analytische Chemie, D-89069 Ulm, Germany
'The Potential of Electrochromatographic Separation Methods in Environmental Analysis'

10.50 Coffee break

11.20 **Prof. *Johan Roeraade***, Royal Institute of Technology, Analytical Chemistry Department, SE-100 44 Stockholm, Sweden
'New Concepts and Techniques for Trace Analysis by High Resolution GC'

12.00 **Prof. *Udo A.T. Brinkman***, Free University Amsterdam, The Netherlands
'Combining Forces: Rapid Sample Preparation and Sophisticated Detection/Identification'

12.40 Concluding remarks

Focal Point: Analytical Technology

Quality Assurance of Analytical Data: Measurement Uncertainty and Traceability in View of ISO 17025

Date/Time: Wednesday, October 16, 2002, 09.30–13.00
Room: Sydney

Description

Definition, determination and consequences of analytical measurement uncertainty are discussed. After a thorough explanation of current procedures to handle uncertainty, the focus is switched to practical applications in process control, the meaning of qualitative analysis near the limit of detection, a case study involving doping in sports events and the problems involved in setting legal limits (*e.g.* ILAC rules).
Five experts from academia, industry- and governmental organizations as well as from R&D-driven companies will give their interpretation from different points of view.

Organized by

Dr. *B. Schreiber* and Dr. *P. Radvila*, Division of Analytical Chemistry of the Swiss Chemical Society

Chairperson

Dr. *Bernhard Schreiber*, Division of Analytical Chemistry of the Swiss Chemical Society

Program

09.30 **Prof. *W. Wegscheider***, University of Leoben, Austria
'The Relationship between Traceability and Measurement Uncertainty'

10.00 **Dr. *M. Weber***, EMPA, St. Gallen
'Problems of Defining Uncertainty at the Detection Limit'

10.30 Coffee break

11.00 ***H.P. Ischi***, Schweizerische Akkreditierungsstelle, Bern
'Problems in Establishing Legal Limits Concerning Measurement Uncertainty'

11.30 **Dr. *B. Renger***, Baxter AG, Vienna, Austria
'Uncertainty in Process Control: The Limit of Setting Limits'

12.00 **Dr. *Jürg Rentsch***, SQTS-Swiss Quality Testing Services, Courtepin
'Measurement Uncertainty in the Validation of Quantitative PCR Methods in Food Analysis'

12.40 Concluding remarks

CHIMIA **2002**, *56*, No. 9

Focal Point: Biotechnology

Technologies for Genome Analysis: Applications in Biomedical Research

Date/Time: Wednesday, October 16, 2002, 13.00–17.15
Room: Sydney

Description

With the deciphering of whole genomes, a tremendous amount of data has been made available for research. In order to analyze all this information within a reasonable time frame and at reasonable cost, new technologies in DNA analysis as well as enzyme assays have been developed in the last few years in a symbiosis of biological, automation and miniaturization technologies. Examples are chip technologies for DNA analysis and microplate enzyme assays for high-throughput screening. Applications in biomedical research and in microbial diagnostics are presented here.

Organized by

Dr. *Beat Wipf*, F. Hoffmann-La Roche AG, Basel
Dr. *Ulrich Certa*, F. Hoffmann-La Roche AG, Basel

Chairperson

Dr. *Ulrich Certa*, F. Hoffmann-La Roche AG, Basel

Program

13.00 **Dr. *Philip Day***, ETH Zürich
'Neuroblastoma Aneuploidy and Transcriptome Profiling in Relation to the NMYC Oncogene'

13.45 **Dr. *Dorothe Foernzler,*** Roche Center for Medical Genomics, Basel
'SNP Discovery and Screening Technologies in Pharma Research and Development'

14.30 Coffee break

14.45 **Dr. *Ulrich Certa***, Roche Center for Medical Genomics, Basel
'Applications of DNA Microarrays in Functional Genomics'

15.30 **Dr. *Peter Nelboeck,*** Preclinical Development Roche AG, Basel
'From Gene to Screen'

16.15 **Dr. *Joachim Frey***, Institute for Veterinaire Bacteriology, University of Bern
'Analysis of Pathogenic Bacteria by Gene Chip Technology'

17.00 Concluding remarks

Focal Point: Environmental Analytical Chemistry

Emerging Environmental Contaminants

Date/Time: Tuesday, October 15, 2002, 09.30–13.00
Room: Sydney

Description
Sophisticated analytical techniques are necessary for the determination of trace contaminants in various environmental compartments. Qualitative identifications are followed by quality controlled quantitations and applications to a broad range of samples. The presented case studies cover several relatively bio-persistent chemicals and corresponding metabolites. The term 'emerging contaminants' refers to environmental pollutants which have been discovered and intensively studied during the past five years. Environmental field studies provide results which allow significant conclusions with regard to input sources and environmental behavior.

Organized by
Prof. *Walter Giger*, EAWAG, Dübendorf

Chairperson
Prof. *Jennifer Field*, Oregon State University, Corvallis, USA

Program

09.30	**Prof. *Jennifer Field***, Oregon State University, Corvallis, USA 'Perfluorinated Surfactants in Groundwater and Wastewater'
10.10	**Prof. *Jörg Metzger***, University of Stuttgart, Germany 'Flame Retardants in Wastewater Treatment Plants'
10.50	Coffee break
11.20	**Dr. *Thomas Polger***, Wädenswil, Swiss Federal Research Station (FAW) 'The Bactericide Triclosan and its Methyl Derivative in Surface Waters and in Wastewater'
12.00	**Dr. *Frank Sacher***, TZW Technologie Zentrum Wasser Karlsruhe, Germany 'Pharmaceuticals in Surface Waters and in Groundwaters'
12.40	Concluding remarks

Water Analysis

Date/Time: Tuesday, October 15, 2002, 13.30–17.00
Room: Sydney

Description
Improving the control of chemical water quality is a challenging task, for which the progress of analytical techniques is a significant base. Besides anthropogenically introduced contaminants, naturally derived water constituents must also be thoroughly investigated in different parts of the environment. A well-established exposure assessment is crucially important for the evaluation of environmental risks posed by various chemicals which occur in wastewaters and of which residual amounts can enter ambient waters and drinking water.

Organized by
Prof. *Walter Giger*, EAWAG, Dübendorf

Chairperson
Prof. *Martin Reinhard*, Stanford University, Stanford, USA

Program

13.30	**Prof. *Martin Reinhard***, Stanford University, Stanford, USA 'Emerging Contaminants in Tertiary Treated Water'
14.10	**Dr. *Urs von Gunten***, EAWAG, Dübendorf 'Ozonation By-products in Drinking Water'
15.40	Coffee break
15.20	**Dr. *Jorg Pietsch***, Technologiezentrum Wasser, Dresden, Germany 'Cyanobacterial Hepato- and Neurotoxins in Water'
16.00	**Prof. *Heinz Friedrich Schöler***, University of Heidelberg, Germany 'Naturally Produced Organochlorines in Terrestrial and Aquatic Environments'
16.40	Concluding remarks

Focal Point: Hyphenated Mass Spectrometry

Liquid Chromatography – Mass Spectrometry

Date/Time: Wednesday, October 16, 2002, 09.30–13.00
Room: Rio

Description

The identification of unknown compounds is essential in a wide variety of research areas and especially so in environmental analysis. Combining liquid chromatography with tandem mass spectrometry today allows the identification of substances that were not amenable to classical techniques. Environmental toxicologists and chemists increasingly focus on chemicals that can potentially cause adverse effects in organisms and humans. Since effect concentrations are often very low, but also because the matrix can affect sensitivity, selective enrichment has become a popular way for sample cleanup and lowering the limit of detection. Advances in environmental analysis, including techniques based on molecular recognition for selective enrichment or effect-oriented research, will be presented in this session.

Organized by

Prof. *Walter Giger*, EAWAG, Dübendorf

Chairperson

Dr. *Marc Suter*, EAWAG, Dübendorf

Program

09.30 **Prof. *Michael Oehme***, University of Basel
'Structure Elucidation Using LC/MS'

10.10 **Dr. *Lee Ferguson***, Pacific Northwest National Laboratory, Richland, WA, USA
'Advances in the Application of High-Performance Mass Spectrometry to Problems in Environmental Toxicology and Chemistry'

10.50 Coffee break

11.20 **Prof. *Marie Claire Hennion***, ESPCI, Paris, France
'Sample Pretreatment Based on Molecular Recognition for More Efficient LC/MS Environmental Analysis'

12.00 **Dr. *Martin Seifert,*** TU München, Germany
'Effect-oriented Analysis for the Determination of Estrogenic Compounds'

12.40 Concluding remarks

Isotope Ratio Gas Chromatography – Mass Spectrometry

Date/Time: Wednesday, October 16, 2002, 13.30–17.00
Room: Rio

Description

The highly precise measurement of isotope ratios has a long tradition in earth sciences. The elements of most interest are carbon, oxygen and hydrogen. More recently, the direct coupling of gas chromatography with the determination of isotope ratios for individual compounds was developed. This analytical method was first applied in organic geochemistry and yielded important results. Later, the same technique allowed the evaluation of sources and processes in food analyses and contaminated environments.

Organized by

Prof. *Walter Giger*, EAWAG, Dübendorf

Chairperson

Prof. *Walter Giger*, EAWAG, Dübendorf

Program

13.30 **Prof. *Pierre Albrecht***, University of Strasbourg, France
'Application in Organic Geochemistry'

14.10 **Prof. *Peter Schreier***, University of Würzburg, Germany
'Flavor Authenticity Studies'

14.50 Coffee break

15.20 **Dr. *Hélène Budzinski***, University of Bordeaux, France
'Source Identification of Oil Residues and Oiled Bird Feathers after an Oil Spill'

16.00 ***Luc Zwank***, EAWAG, Dübendorf
'Biotransformation of Volatile Chemicals in Groundwater'

16.40 Concluding remarks

CHIMIA **2002**, *56*, No. 9

Focal Point: Industrial Chemistry

Simulation Tools and Their Application in Chemical Manufacturing I

Date/Time: Wednesday, October 16, 2002, 10.00–12.30
Rooms: Osaka + Samarkand

Description

Simulation tools and models are becoming more and more important in the fields of process development and design, process parameter optimization or in the evaluation of process interactions and their dynamic simulation. Not only can they be instrumental in creating cost transparency and ultimately reducing costs or shortening time to market, they also significantly accelerate progress in process development or lead to the identification of optimization potential. The three lectures demonstrate the step by step use of a mass, energy and cost flow model, show the application of simulation tools with varying level of detail at different stages of process design, and further discuss the possibilities of using dynamic simulation within chemical production.

Organized by

Dr. *Rudolf Pfluger*, Syngenta Crop Protection, Münchwilen

Chairperson

Dr. *Hans Rudolf Dettwiler*, Lonza Ltd., Visp

Program

10.00 ***R. Gälli, G. Stucki,*** and ***D. Oehler,*** BMG Engineering Ltd., Schlieren
'Efficiency Engineering: Cost Reduction Through Modeling of Manufacturing Costs'

10.40 ***Andreas Heyl,*** Lonza Ltd., Visp
'Time to Market: The Use of Modern Simulation Tools for a Shorter Time to Market'

11.20 ***Michael Mayer,*** F. Hoffmann-La Roche AG, Basel
'Reaction Engineering: Application of a Dynamic Simulation for Optimization of Chemical Production Processes'

12.00 Concluding remarks

Simulation Tools and Their Application in Chemical Manufacturing II

Date/Time: Wednesday, October 16, 2002, 14.00–16.30
Rooms: Osaka + Samarkand

Description

Simulations aim at varying goals, such as avoiding costly experiments in reality, the prevention of large-scale pilot production procedures, or the analysis of cases where critical situations are not accessible experimentally. Besides, they are useful for the identification of possibly parametric sensitive processes, allow the prediction of hazardous situations, but also provide effective chemical process training for operators and experts in a safe environment. The three lectures shall explain which methods of simulation are most practically used during the development of a procedure, show the benefits of numeric simulation techniques in process safety, and highlight the potential of simulations in training skilled workers in chemical operations.

Organized by

Dr. *Rudolf Pfluger*, Syngenta Crop Protection, Münchwilen

Chairperson

Dr. *Hans Rudolf Dettwiler*, Lonza Ltd., Visp

Program

14.00 **Dr. *Bernhard Urwyler***, Syngenta Crop Protection, Münchwilen
'Process Technology: Simulation versus Experiment'

14.40 **Dr. *Francis Stoessel***, Swiss Institute for the Promotion of Safety & Security, Basel
'Safety: Benefits of Numeric Simulation Techniques in Process Safety'

15.20 ***Stefan Suter,*** Aprentas, Basel
'Training/Education: Simulation Training in Chemical Operations for Skilled Workers'

16.00 Concluding remarks

Focal Point: Industrial Chemistry

Production Today – Tomorrow: New Technologies in Modern Chemistry

Date/Time: Friday, October 18, 2002, 09.15–15.30
Rooms: Osaka + Samarkand

Description

During the session, the speakers will inform about the newest developments in the field of high-performance distillation, fractional layer crystallization and safe phosgenation. Moreover you will get an overview of the latest trends in UV and electron beam crosslinking and in the selection of silane blocking agents.

Organized by

Pedro Kaiser, Degussa, SVC, Basel

Chairperson

Pedro Kaiser, Degussa, SVC, Basel

Program

09.15 Welcome coffee

09.30 ***Christoph Jud***, Dow Europe, Horgen/President SVC
Introduction

09.45 **Dr. *Andrzey K. Kuszlik***, Sulzer Chemtech Ltd., Winterthur
'Fractional Layer Crystallization for Refining of Organics'

10.30 ***Ludger Fischer,*** Kühni AG, Allschwil
'High-performance Distillation Column Internals'

11.15 ***Daniel Hariri,*** Davy Process Technology, Pratteln
'Safe Phosgene Generation and Phosgenation'

12.00 Lunch break

13.00 **Prof. *Reiner Mehnert,*** Institut für Oberflächenmodifizierung, Universität Leipzig, Germany
'UV and Electron Beam Crosslinked Polyacrylate Nanocomposites and Their Applications'

13.45 **Dipl. Ing. *Marc Reifenscheid***, Linde-KCA, Dresden, Germany
'Front End Engineering for Pharmaceutical and Biotech Industry'

14.30 **Dr. *Markus Juza***, CarboGen Laboratories, Aarau
'Enantio Selective Chromatographic Separations in the Pharmaceutical Industry – Problems, Solutions and Surprises'

15.00 Concluding remarks, followed by an apéro

CHIMIA **2002**, *56*, No. 9

Focal Point: Inorganic Chemistry

Aqueous Organometallic Chemistry: From Life Sciences to Catalysis

Date/Time: Wednesday, October 16, 2002, 09.30–17.00
Room: Singapore

Description

The 'Minisymposium in Inorganic Chemistry' is dedicated to organometallic chemistry in water. The incentive for this recent topic is related to the widespread opinion that organometallics are generally unstable under aqueous and aerobic conditions. More recent research has focused on the use of water as a solvent for organic and organometallic reactions. Water would be a preferred solvent for industrial processes and is doubtless the solvent of life. The many favorable properties of organometallics have for a long time not been combined with the chemical potential of water. Thus, their role in catalysis or life science could be greatly extended. In just ten years fast growing research in this area has developed and a number of compounds have been shown to be versatile tools for many basic and practical purposes. Although still a relatively small community, some of the prominent researchers in the field will present their latest results from fundamental and applied research related to the use of organometallics in life science and catalysis.

Organized by

Prof. *Roger Alberto*, University of Zürich

Chairperson

Prof. *Roger Alberto*, University of Zürich

Program:

09.30 Welcome coffee

10.10 **Prof. *Georg Süss-Fink***, University of Neuchâtel
'Supramolecular Cluster Catalysis: A Case Study of Benzene Hydrogenation under Biphasic Conditions'

11.00 **Prof. *Seiji Ogo***, University of Nagoya, Japan
'pH-Dependent Activation of Small Molecules'

11.50 **Prof. *Michael Whittlesey***, Bath University, UK
'Structure, Property, and Reactivity Relationship in Organometallic Aqua Complexes of the Iron Triad'

12.40 Lunch break

14.00 **Prof. *Nils Metzler-Nolte***, Universität Heidelberg, Germany
'Labeling of Bioactive Peptides with Organometallics by Solid Phase Synthesis'

14.50 **Prof. *R.H. Fish***, Lawrence Berkeley National Laboratory, University of California, USA
'Synthesis and Structural Studies with $[Cp^*Rh(H_2O)_3](OTf)_2$ and Biomimetic NAD+ Models in Co-factor Regeneration and Chiral Synthesis'

15.40 **Prof. *G. Jaouen***, Université de Paris, France
'Targeting Organometallic Moieties onto the Oestradiol Receptor. Biochemical Applications'

16.30 Concluding remarks

Focal Point: Medicinal Chemistry

Ligand-Receptor-Interactions: From Understanding to Design

Date/Time: Wednesday, October 16, 2002, 09.30–13.00
Room: Montreal

Description
The ultimate step in drug action is its interaction with the biological target. This process, governed by physico-chemical forces, should be as specific as possible. High specificity paralleled by high affinity is one of the main pillars of a safe drug. Combination of biophysical techniques and computational chemistry approaches lead to a deeper understanding of this interaction and hence to the creation of sophisticated ligands adapted to the needs of the patient.

Organized by
Prof. *Gerd Folkers*, ETH Zürich

Chairperson
Prof. *Gerd Folkers*, ETH Zürich

Program:

09.30	***Hugo Kubinyi***, Weisenheim am Sand, Germany 'Understanding Ligand-Receptor Interactions'
10.10	***Osman Güner***, Accelrys, San Diego, USA 'Pharmacophores'
10.50	Coffee break
11.20	***Leonardo Scapozza***, D-ANBI, ETH Zürich 'Design of Genetic Switches'
12.00	***Wolfgang Jahnke***, Novartis Pharma AG 'NMR in Drug Discovery'
12.40	Concluding remarks

Structure-Properties Relationships and Kinetics

Date/Time: Wednesday, October 16, 2002, 13.30–17.00
Room: Montreal

Description
Controlled transport to the biological target, minimum side effects and a safe elimination is the second main pillar of drug activity. A detailed, context-dependent physico-chemical characterization of the ligand properties will help to understand transport and elimination processes. This may lead to the design of new compounds that bear pharmacophoric elements for optimal transport properties and minimizing distribution to unwanted tissues and targets.

Organized by
Dr. *Manfred Kansy*, F. Hoffmann-La Roche, Basel

Chairperson
Dr. *Manfred Kansy*, F. Hoffmann-La Roche, Basel

Program

13.30	***Pierre-Alain Carrupt***, Institut de Chimie thérapeutique, Section de Pharmacie Université de Lausanne, Lausanne-Dorigny 'Molecular Fields and Permeation'
14.10	***Alex Avdeef***, pION Inc. Boston USA 'Physico-chemical Profiling'
14.50	Coffee break
15.20	***Gerhard Klebe***, Pharmazie Universität Marburg, Germany 'Computational Approaches to Functional Similarity among Proteins'
15.50	***Luc Balant***, Department of Psychiatry, University of Geneva 'Pharmacokinetics'
16.30	Concluding remarks

CHIMIA **2002**, *56*, No. 9

Focal Point: Nanobiology Workshop

A Joint Session with BioValley Basel Life Science Week 2002

Date/Time: Wednesday, October 16, 2002, 17.15–19.00
Room: Sydney

Organized by
Prof. *Hans-Joachim Güntherodt*, University of Basel

Chairperson
Prof. *Hans-Joachim Güntherodt*, University of Basel

Program

17.15 **Prof. *Hans-Joachim Güntherodt***, Institute of Physics, University of Basel
Welcome

Prof. Dr. *Andreas Engel*, Biocenter, University of Basel
'Introduction to Nanobiology'

Prof. *Ueli Aebi*, Biocenter, University of Basel
'Nanotechnology in Medicine'

Prof. Dr. *Christoph Gerber*, IBM Research Laboratory and NCCR
'Biosensors Based on Nanomechanics'

19.00 Concluding remarks