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Paracelsus Prize 2008 **1**

From Molecules to Molecular Systems

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Systems chemistry indicates a new frontier of research in molecular sciences, moving beyond the borders of traditional reductionist approaches and studies of single molecular entities to multi-component (multi-)-functional chemical systems. The challenge is to create new functions from an ensemble of molecular components at different hierarchical levels or via molecular networks with emerging properties. These approaches might allow, for instance, the development of entirely novel molecular computing and information storage systems, nano-scale machinery, sustainable catalytic processes and smart materials. The systems chemistry approach will provide fundamental insight in how molecular processes are interconnected.
Inspired by Nature we design molecular systems in which the control of molecular dynamics is coupled to specific functions. This will be illustrated in the control of function and organization at different hierarchical levels. Following a brief overview on the developments of molecular switches and light-driven unidirectional molecular motors, the focus will be on the control of dynamic functions in complex systems and autonomous motion. Furthermore the motion of a large collection of motors on a surface and molecular transmission phenomena are presented. Besides rotary motion induced by light, molecular motors that run on chemical fuels will be reported. Finally, progress in our attempts to achieve autonomous motion is discussed.

Werner Prize 2008 **2**

Absorbing X-rays to Understand Catalysis

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It is an old dream of scientists in the field of heterogeneous catalysis to discover the structure of the catalytically active sites and to understand structure – performance relations. This would enable the engineering of better catalysts and processes. More often than not, however, the structure of the catalytically active sites is unknown.
Spectroscopic methods and instrumentation have been developed that aid the unraveling of the structure of catalysts during a reaction. X-ray absorption spectroscopy is a particularly valuable tool to determine the geometric and electronic structure of solid catalysts, as measurements can be performed in situ. The combination of in situ measurements with the synthesis of extremely well-defined catalytic systems and detailed kinetic measurements provides insight into structure – performance relations, which open the door to design of better catalysts.
Catalysis by gold is a very active field. Many new reactions have been proposed, although the origin of its peculiarly high catalytic activity and selectivity remains barely understood. This lecture will focus on the progress made in understanding the origin of the catalytic properties of supported nano-sized gold particles.

[1] Bus, E., Prins, E., van Bokhoven, J.A. *Catal. Commun.* **2007**, *8*, 1397
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Grammaticakis-Neumann Prize 2008 **3**

Shedding Light on Nucleic Acids

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Most of the processes in living organisms are exquisitely spatiotemporally regulated. If we want to understand this well-choreographed interplay or the problems and diseases resulting from perturbations thereof, the tools we use for studying nature must allow us to test the living systems in an equally spatiotemporally well-defined manner. This spatiotemporal control requires a combination of an addressing mechanism with which to choose ideally arbitrarily selectable regions of interest and a strategy of coupling this signal to biologically active molecules. One such addressing mechanism is the irradiation with light. Light can be easily created and manipulated with readily-available technologies like the laser technology in combination with microscopes and it is an orthogonal trigger signal because the majority of cells and tissues do not respond to this input signal. One such coupling of trigger and effect is the strategy of attaching photolabile groups to strategic positions in biologically active molecules.
We are interested in the synthesis and application of such light-activatable ("caged") DNA and RNA because nucleic acids are the base for powerful techniques such as for example RNA interference for the regulation of genes and aptamers for the regulation of the function of proteins. In each realm we have already shown that we can put the respective effect under the control of light – which will provide a very precise new tool for example for developmental biology.

Dr. Max Lüthi Prize **4**

Metabolic profiling of sugar phosphates by HPLC-MS using mixed-mode stationary phases

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This paper reports the possible use of novel mixed-mode stationary phases for the separation and detection by high performance liquid chromatography-tandem mass spectrometry of sugar phosphates, which are notoriously difficult to separate using reversed-phase materials.
Target sugar phosphates were glucose 6-phosphate, fructose 6-phosphate, ribose 5-phosphate, dihydroxyacetone phosphate, phosphoglyceric acid, fructose 1,6-bisphosphate and ribulose 1,5-bisphosphate. This compounds were best separated on a Primesep SB® column by gradient elution using aqueous ammonium formate and acetonitrile as mobile phases. Analytes were identified by their precursor/product ions and retention times. Standard curves of neat authentic standards were generated for concentrations in the low picomole to nanomole range, with correlation coefficients of $R2 > 0.99$.
The developed method was tested on a tobacco leaf extract. Due to important matrix effect, it was decided not to attempt quantification as long as the extraction procedure would not be improved. Nevertheless, this method will be potentially faster, more sensitive and less expensive than the current techniques for quantification of sugar phosphates from plant samples such as enzymatic techniques [1] or thin layer chromatography requiring radioactive labeling. It will also help the profiling of the Calvin cycle intermediates.

[1] Madhusudana R. Norman T., *Plant Physiol.* **1989**, 90, 814-819.

Dr. Max Lüthi Prize **5**

Remodelling, Optimization and Characterisation of Absorption Columns to Precipitate Hydrogen Chloride and Sulphur Dioxide

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The aim of the first part of this thesis is to create an extensive safety documentation for the operation of two absorption columns and a reactor, i.e. the drawing up of checklists, the revision of operating instructions as well as designing a reactions-, resistance- and a HAZOP-list. Besides, a comprehensive substance-data-collection for HCl and SO_2 has been made for the planned use in absorption.
A further aspect deals with the rebuilding of glass-raschig-ring-columns to modern high-capacity random and structured packed columns. For the description of these packings an overview of the applied measuring technique and analyses will be given.
The last part of this dissertation explores mass-transfer and hydraulics of the new baffles. For the mass transfer the investigation of the number of mass transfer units that the new packings provide for the system HCl/H_2O is of immediate importance.

Dr. Max Lüthi Prize **6**

Deposition of Fragrance Precursors on Fabrics

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The purpose of this work was to consider the influence on deposition during a laundering. The deposition on cotton was measured under different washing conditions. A broad variety of molecules was investigated. An HPLC analytical method was developed to quantify the interesting substances in a washing emulsion. Adsorption of these substances to the vessel surfaces distorted the detection rate. Due to the addition of liquid detergents the problem could get overcome and adsorption was avoided. As a result, the recovery rate was between 90 to 100 % allowing for a reliable analysis. Since there are no interdependencies between the different substances, the deposition could be analyzed for several substances in the same experiment.
The following interrelations were found: An increasing deposition comes along with an increased substance concentration in the washing liquid. This was observed in the case of liquid detergent as well as with a fabric softener. If the liquid detergent concentration was increased, the deposition decreased. This behavior is caused by the formation of micelles, being formed if the liquid detergent concentration is high enough to allow for. The micelles are able to include the substances.
The ratio of the washing liquid to textile mass influences the deposition also. Using more liquid lowered the deposition. The influence of the molecular structure is not clear. Two different mechanisms have been determined. The first refers on solubility in the washing liquid, taking in account the polarity of the substances. The second refers on interaction between substance and substrate by conjugated pi-bond systems.

Analytical Chemistry **7**

Current Position of GC-MS and LC-MS in Clinical and Forensic Toxicology

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Reliable analytical data are a prerequisite for competent expertises in clinical and forensic toxicology. Nowadays, hyphenated mass spectrometric techniques, particularly gas chromatography/mass spectrometry (GC-MS) and liquid chromatography/mass spectrometry (LC-MS), are indispensable tools in clinical and forensic toxicology due to their high sensitivity and specificity. They are used for screening, library-assisted identification, and quantification of drugs, poisons and their metabolites, prerequisites for competent expertises in these fields. In addition, they allow studying metabolism of new drugs or poisons as a basis for developing screening procedures in biological matrices, most notably in urine, or toxicological risk assessment. Concepts and procedures using GC-MS and LC-MS techniques in these areas with special focus on multi-analyte procedures will be presented and discussed [1-7]. The presentation will close with a short discussion of the future position of GC-MS and LC-MS in these fields.

1. H.H. Maurer. Position of chromatographic techniques in screening for detection of drugs or poisons in clinical and forensic toxicology and/or doping control [review]. *Clin. Chem. Lab. Med.* 42, 1310-1324 (2004).
2. H.H. Maurer and F.T. Peters. Towards High-throughput Drug Screening Using Mass Spectrometry. *Ther. Drug Monit.* 27, 686-688 (2005).
3. H.H. Maurer. Advances in analytical toxicology: Current role of liquid chromatography-mass spectrometry for drug quantification in blood and oral fluid [review]. *Anal. Bioanal. Chem.* 381, 110-118 (2005).
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5. T. Kraemer and L.D. Paul. Bioanalytical procedures for determination of drugs of abuse in blood [review]. *Anal. Bioanal. Chem.* 388, 1415-1435 (2007).
6. H.H. Maurer. Current role of liquid chromatography-mass spectrometry in clinical and forensic toxicology [review]. *Anal. Bioanal. Chem.* 388, 1315-1325 (2007).
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Analytical Chemistry **8**

Analytical Forum "SHARE and BENEFIT"
Exchange of Teaching and Teachers in Analyical Sciences

Urban Frey, Detlef Günther, Gerard Hopfgartner

Division of Analytical Chemistry, SCS, www.sach.ch

Analytical Chemistry is a field of research which is continuously expanding into a wide variety of interdisciplinary fields of science. The state of the art use of analytical instrumentation is a prerequisite for supporting other fields of research or further development of instrumentation. However, education of students is dominantly hosted in Chemistry and depends significantly on the existing infrastructure. In addition, research in this field becomes highly specialised and is so diverse that lab courses for students are lacking adequate instrumentation which makes "first-hand" education difficult to maintain excellence in education of Analytical Chemistry.
Reviewing the different Universities and Universities of applied sciences within Switzerland indicate however, that we have a large pool of resources for improving the teaching by sharing our expertise, but the interactions are missing. Based on this lack of interaction and the potential for improving the teaching, Division of Analytical Chemistry supports the formation of a platform where lectures for students can be "offered and booked". The lecture topics should be focused on techniques and instrumentation and should be combined with some "educational supportive" examples. Further details how to enter this platform, the benefit from participation will be presented.