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As Simple as *abc*: Speeding up Innovation

abc Technologies, Basel, January 26th–27th, 2005

Christof Brändli and Olaf Köhler*

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For the fifth time in a row, Chemspeed Technologies organized a meeting recognized as one of the first relevant scientific conferences in the new year. 100 participants from all over the world were gathering together to listen to high-end technology talks and cutting-edge scientific presentations. The city of Basel welcomed the participants, speakers, and exhibitors with a decent amount of snow – quite rare conditions in this part of Switzerland! *abc Technologies* (accelerated bio and chemical technologies) is becoming an important event within the field of high-output experimentation; a methodology that almost every synthetic and theoretical chemist applies in one way or another.

Prof. **Bruce Lipshutz** from the University of California Santa Barbara opened the conference with a spirited talk about organometallic reagents for heterogeneous catalysis. Entertaining episodes from his lab were mixed with his scientific approach of using cheap metals and supported reagents

for highly active and selective catalysts. He focuses on copper and nickel; two metals used already by the alchemists to turn into gold. Rapid cross-coupling reactions under microwave irradiation using nickel-on-charcoal, an even cheaper nickel-on-graphite catalyst for the reduction of phenols,



*Correspondence: Dr. O. Köhler
Chemspeed Technologies
Rheinstrasse 32
CH-4302 Augst
Tel.: +41 61 816 95 00
Fax: +41 61 816 95 09
E-Mail: chemspeed@chemspeed.com
www.chemspeed.com

or highly active copper-on-charcoal for asymmetric hydrosilylation were examples from his recent research activities. Prof. Lipshutz also pointed out the utilization of ultrasonication as a highly efficient and readily available method for mixing. In his talk, he demonstrated in an exciting way the feasibility and ease of this well-established method to improve heterogeneous reactions in his quest for reagents and methods at almost no costs.



Prof. Bruce Lipshutz

Resuming the subject of microwaves, Prof. **Ulrich Schubert** of Eindhoven's University of Technology and the Dutch Polymer Institute then completed the first session of presentations. In his inspiring talk, he presented the benefits of merging combinatorial and microwave-induced polymer synthesis with high-throughput analytics. High-tech macromolecular chemistry as depicted by Prof. Schubert serves as a powerful tool in both academia and industry: Basic research like the discovery of new polymers, optimization of reaction conditions as well as tailor-made synthesis and consequently polymer printing and characterization are all covered by automated platforms in his group. In association to the conference's title Prof. Schubert used examples of 'abc block copolymers'. In his very systematic approach, he combines instrumentation for the synthesis and analysis with highly advanced techniques like *e.g.* inkjet-printing of microdrops.

Dr. **Marc Oliver Kristen** from Basell Polyolefines impressed with a talk showing how high-throughput experimentation is very successfully applied in commercial research for polyolefin materials and polyolefin catalysts. High pressure and sophis-



Prof. Ulrich S. Schubert in discussion with Dr. Rolf Güller

ticated analytical techniques are only two of the challenges to face with polymer research targeting specific properties.



Dr. Marc O. Kristen

Dr. **Mathias Destarac** of Rhodia demonstrated how a single derivatization can ease the (polymer-)chemists' life: With the introduction of the xanthate group, Rhodia is capable of controlling radical polymerization in an automated way while still having access to a great variety of reagents. Thereby, Rhodia generates not only polymers with selected and desired properties but can also easily implement the customer's specific demands.

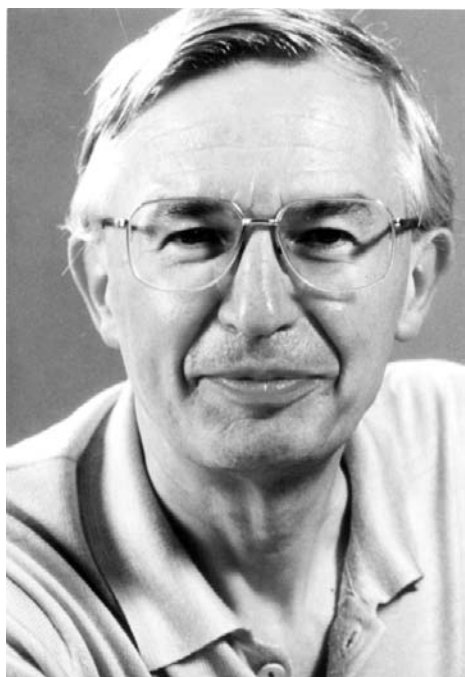
The afternoon of the first day included a *poster session* from a number of presenters and spotlight presentations from various companies exhibiting and sponsoring this event. Speakers from InsightFaraday Partnership (Dr. Maria Raimondi), Spotfire (Dr.

Philip J. Langley), Waters Informatics (Eric Groggnard), Solvias (Dr. Ralph Budnik), and Polymer Laboratories (Adrian Williams) gave an overview of how their companies deal with and/or integrate high-throughput experimentation and screening technologies. A tour to the fascinating world of music automatons and a wonderful dinner were part of the social event at the end of an interesting day.

The second day started with a firework of two excellent talks focusing both at least partly on 'virtual' approaches in chemistry making the bridge to the late-night talk of Chemspeed's CEO Rolf Güller who presented the vision of Chemspeed Technologies for the laboratory of the future by introducing new concepts.

Prof. **Jean-Marie Lehn** from University of Strasbourg, Nobel Price Laureate in Chemistry in 1987 for the invention of supramolecular chemistry, presented a 'dynamic' field in combinatorial chemistry. One of the key messages in his talk showed that selection within a system is only possible through the dynamic, constitutional diversity responding to the pressure of internal and – preferably – external factors. In reversible systems, this could lead to adaptation and eventually, one can make the link to evolution. The tools to study these reversible chemical systems enabled him to explain and prove his concepts and theories. During his presentation, he showed impressive examples of dynamic libraries of helical metal complexes, dynamic deconvolution methods for acetylcholinesterase inhibitors, and recent work on polymeric materials exhibiting reversible component exchange in covalent polymers.

Prof. **Jean-Louis Reymond** from the University of Bern divided his powerful presentation into three parts. With Cheminformatics, he picks interesting molecules



Prof. Jean-Marie Lehn

(below 160 Daltons) from virtual combinatorial libraries from the chemical universe with the help of mathematical graphs. He uses chemical intelligence to select sets of appropriate candidates and screen them for biological activity. His research on measure and visualization of enzyme activity brought him to the fascinating world of enzyme fingerprinting for different purposes like reactivity prediction, quality control, or drug diagnostics. Multidimensional measurements of enzyme activity with different probes are used to generate activity profiles. His last part focused on very recent work to synthesize and study artificial proteins. His



Prof. Jean-Louis Reymond

approach is based on peptide dendrimers, which eliminate the folding problem associated in conventional peptide research. The dendritic structure was assembled from a branching diamino building block. As a possible application, catalytic ester hydrolysis of histidine-containing dendrimers was shown. Prof. Reymond presented split-and-mix approaches and on-bead screening results which allow single-bead sequencing by quantitative amino acid analysis.

An overview of the hit-to-lead process at Schering's medicinal chemistry department was presented using a kinase inhibitor library by Dr. **Knut Eis**. An integrated workflow including scaffold selection, chemistry optimization, library design, library production by automation equipment and post synthetic selection produced a very promising 10,000 compound library. In his talk, Dr. **Janak Padia** of Avalon Pharmaceuticals demonstrated the fascinating interaction between biology and chemistry in the area of genomics: With the identification of gene expression information, drug candidates can be easily identified and optimized corresponding to the active site(s) of a target molecule. Schering's Dr. **Christoph Huwe** rounded up the second session by presenting the optimization process of a real drug candidate. By scanning different ligands under various reaction conditions at one time, Dr. Huwe showed the tremendous activity gains of a progressing amine library. In an automated three-step optimization, Schering increased the activity of the corresponding library by a factor of 100. The use of automated reactor systems in the development of asymmetric hydroxylation catalyst was explained by Dr. **Albert L. Casalnuovo** from DuPont Agricultural Products. The differences between process research in agricultural and pharma research were well pointed out and explained during the very fascinating talk. A success story par excellence for the development of a zirconium catalyst was presented. In the optimization of chemical processes for the production of active pharmaceutical ingredients at Siegfried Ltd., the use of lab automation and high throughput synthesis equipment was demonstrated by Dr. **Michael K. Levis**. Special attention was turned to the demanding precision and repeatability requirements in process optimization. During this presentation it was shown how Siegfried managed to successfully integrate the right equipment for a specific problem.

The final speaker of the conference, Prof. **Thomas R. Ward** from the University of Neuchâtel, gave an impressive overview of his recent work in second-sphere enantioselective catalysis. Usually, the catalysts are designed in such a way that the substrate

binds directly to the chiral centre resulting in a chirality transfer from catalyst to substrate. In enzymatic systems, the first coordination sphere supplies the catalytic activity for a reaction, while selectivity derives from the second coordination sphere. He now integrates successfully organometallic catalysis in enzymes by anchoring known chiral metal complexes into a coenzyme. Using random and site-directed mutagenesis, he alters the second-sphere coordination site and applies it in rhodium-catalyzed enantioselective hydrogenations. With this genetic optimization approach, he reached very high enantioselectivity. As one of the highlights, he then showed one of his most recent results from transfer hydrogenation reactions using chiral ruthenium complexes which are stable and highly active systems.



Prof. Thomas R. Ward

The conference showed again very clearly the variety and diversity of applying automation in chemistry and biology. The focus of all the speakers lay in the quality of results generated from instruments that accelerate the synthesis and sample handling process. An electronic copy of all presentations in the pdf format is available online on www.abctechnologies.ch.

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