INFORMATION

News

Fourth Solvias Science Day

Hans-Ulrich Blaser
Solvias AG, P.O. Box, CH 4002 Basel
E-Mail: hans-ulrich.blaser@solvias.com

The major goal of the Solvias Science Day is the presentation and discussion of new strategies, concepts, and solutions in the field of synthetic and analytical chemistry by leading experts from universities, the life science industry as well as by Solvias' scientists. The fourth Science Day took place on January 28, 2005 under the motto 'New Strategies, Technologies, and Concepts in Research and Development' and encompassed the areas of synthesis, catalysis, and analytical methodology. About 160 colleagues from research, development, and production in the life science and fine chemicals industry attended the four sessions with eight presentations. This occasion was also a suitable setting for honoring the winners of the 'Solvias Ligand Contest 2004'. Looking back, the event was clearly a success: All comments from customers and colleagues showed us that the fourth Solvias Science Day achieved its goals concerning science, information and – yes – also marketing the Solvias services.

The presentations can be grouped into the three categories: 'Synthetic and Analytical Methodologies', 'Industrial Collaborations', and 'Award Lectures'.

Synthetic and Analytical Methodologies

Prof. *Erick M. Carreira* (ETH Zürich) presented a lecture on 'Studies in asymmetric synthesis' discussing the following ongoing projects in the area of catalytic asymmetric synthesis: The enantioselective reduction of β,β-disubstituted nitroalkenes catalyzed by Josiphos Cu(I) complexes, giving optically active β,β-disubstituted nitroalkanes in very good yields and selectivities; the development of chiral [2.2.2]-bicyclooctadienes as a new family of ligands for several enantioselective reactions involving late transition-metals and finally, a modular atropisomeric P,N-ligand family, PINAP, which is conveniently prepared and resolved and is very effective for the Cu-catalyzed coupling of acetylenes and imines, affording products with the highest enantioselectivity reported for this transformation to date.

Dr. *Franka Kálmán* (Solvias AG) gave an overview on the use of capillary electrophoresis (CE) as an analytical tool in the pharmaceutical/biopharmaceutical industry. Several examples of efficient analytical method development, method validation and QC batch release were presented and validation parameters, criteria and results of CE methods used for release testing of (bio)pharmaceutical compounds were described. Finally, the application of CE was discussed for long term stability studies according to ICH guidelines, and for dissolution rate testing, where a huge number of samples have to be analyzed in a short period of time with high reproducibility.

Industrial Collaborations

The next three presentations described collaboration projects of Solvias with industrial partners.

Dr. *Barbara Monse* (SiRENADE Pharmaceuticals, Martinsried) talked about 'Design and synthesis of unusual indolocarbazole derivatives as disease-modifying treatment in Alzheimer's disease'. She described how, starting from an in-licensed early lead analogue of a natural compound, a focused compound library

of 578 compounds was generated in house. Based on the complete profile of compound properties studied in a series of *in vitro* and *in vivo* experiments, compound SRN-003-556 was chosen as SiRENADE's most promising preclinical candidate. The syntheses leading to SRN-003-556 starting from a medicinal chemistry program was presented as well as the development of a scalable synthesis, pharmacological evaluation and the structure-activity relationships.

Frédéric Naud (Solvias AG) and *Carsten Rüggeberg* (Rohner AG, Pratteln) gave a joint lecture entitled 'Ru-(phosphino-oxazoline) complexes as effective, industrially viable catalysts for the enantioselective hydrogenation of aryl ketones'. Naud described how a known catalytic system with little industrial potential was transformed into a highly efficient catalyst for the asymmetric hydrogenation of aryl ketones with very good enantioselectivities as well as high turnover numbers. Rüggeberg reviewed the different steps which were necessary to transfer the laboratory process to the manufacturing plant and described how 300 kg of a specific chiral alcohol were produced at Rohner AG after a development time of only two months.

Joseph D. Armstrong, III (Merck & Co, Rahway) described in his lecture 'DPP-IV inhibitor MK-0431, the search for the ultimate synthesis' how in the course of development of synthetic routes to DPP-IV inhibitor MK-0431, two highly efficient asymmetric syntheses of a β-amino acid moiety were developed. One was the heterogeneous diastereoselective reduction of enamino amide using phenyl glycinamide as the chiral auxiliary, and the other one an unprecedented Rh-Josiphos catalyzed enantioselective reduction of an unprotected enamino amide as described below in the award lecture by *Yi Hsiao*. The asymmetric hydrogenation route was finally chosen as the manufacturing route and several tons of MK-0431 has already been produced *via* this newly discovered method.

Solvias Ligand Contest Award Lectures

The Solvias Ligand Contest invites researchers to submit accounts describing new or improved applications for Solvias ligands. For the year 2004, the jury has awarded the first prize *ex aequo* to three winners in recognition of their significant contributions in the area of chiral catalysis utilizing Solvias' proprietary chiral ligands:

- To Dr. *Yi Hsiao* and the *Merck Process Research Team* (Merck & Co, Rahway) in recognition of "the very high potential for synthetic and industrial application of an unprecedented new methodology for the synthesis of β-amino acid esters and amides with no need to use protecting groups".
- To Prof. *Ben L. Feringa* (University of Groningen) in recognition of "the high synthetic potential of the first practical, generally applicable catalytic method for the enantioselective conjugate addition to cyclic and acyclic enones using Grignard rather than organozinc reagents".
- To Prof. *John F. Hartwig* (Yale University) in recognition of "the very high potential for synthetic and industrial application of the Palladium Josiphos catalysts with extraordinarily high turnover numbers for the amination of aryl and heteroaryl chlorides – a significant improvement over previously reported catalysts".

Dr. *Yi Hsiao* entitled his award lecture 'Highly efficient synthesis of β-amino acid derivatives *via* asymmetric hydrogenation of unprotected enamines'. He explained the importance of β-amino acids as components of biologically active peptides and small molecule pharmaceuticals and pointed out that current methods for β-amino acids synthesis are not general, practical, efficient, or environmentally benign. In the course of the project described by Dr. Armstrong, Dr. Hsiao discovered an unprecedented enantioselective hydrogenation of unprotected enamino esters and amides using commercially available Josiphos ligands. Contrary to accepted thinking, these results clearly show that the N-acyl group is not a prerequisite for such transformations to be effective. The new method gives high enantioselectivity (93–97% ee), high reactivity and has wide applicability.

Prof. *Ben L. Feringa* lectured on 'Copper-catalyzed asymmetric conjugate addition of Grignard reagents to cyclic and acyclic enones'. While asymmetric conjugate addition of dialkylzinc reagents is well developed, the high reactivity associated with Grignard reagents has hampered their application for catalytic 1,4-additions with useful levels of selectivity. In this lecture Feringa described the first highly enantioselective conjugate addition of Grignard reagents to enones catalyzed by copper complexes based on Taniaphos and Josiphos ligands. The new methodology is very efficient and achieves high enantioselectivities for the conjugate addition to both cyclic and acyclic enones.

Prof. *John F. Hartwig* presented a lecture on 'Highly-reactive, long-lived catalysts for new palladium-catalyzed coupling reactions'. He gave some background information on the importance of the palladium-catalyzed formation of aromatic carbon–nitrogen and carbon–oxygen bonds from aryl halides and triflates and described how basic studies led to the discovery that Josiphos ligands are uniquely suited for this chemistry. With the new palladium Josiphos catalysts a variety of amines can be coupled to both aryl and heteroaryl chlorides with catalyst loadings a low as 0.005 mol%, making the technology very interesting for technical applications.

From the many comments both during and after the symposium we can conclude that also the fourth Solvias Science Day was an unqualified success and we have every intention to continue the series.

Hochschule Wädenswil (HSW): Neue Dozierende für Umwelt und Natürliche Ressourcen

28. Februar 2005. Für die Abteilung Umwelt und Natürliche Ressourcen an der Hochschule Wädenswil konnten drei neue Dozierende verpflichtet werden:

Dr. *Peter Schumacher*, dipl. Ing.-Agr. ETH, studierte Agronomie mit der Vertiefung Pflanzenproduktion an der ETH Zürich. Die Spezialisierung im Weinbau erfolgte bereits im Studium mit Semester- und Diplomarbeiten und während diverser Praktika, unter anderem auf Weingütern in Chile und Argentinien. Im Anschluss an sein Studium forschte er in einer befristeten Anstellung an der Agroscope Wädenswil im Bereich der Rebenphysiologie. Es folgte das Doktorat an der ETH am Institut für angewandte Entomologie. 1998 wurde er an der damaligen Ingenieurschule Wädenswil als Lehrbeauftragter für Weinbau angestellt. Zwei Jahre später folgte die Wahl zum Hauptlehrer. Seit Herbst 2004 leitet er die Fachstelle Weinbau, unterrichtet im Studienbereich Hortikultur und ist neu Dozent für Weinbau.

Dr. *Frank Hartmann* ist promovierter Umweltingenieur und diplomierter Mittelschullehrer. Im Anschluss an sein Umweltingenieurstudium an der ETH Zürich doktorierte Frank Hartmann an der Abteilung Stoffhaushalt und Entsorgungstechnik an der EAWAG (Eidgenössische Anstalt für Wasserversorgung, Abwasserreinigung und Gewässerschutz) Dübendorf bzw. der ETH Zürich. Parallel zu seiner Dissertation (Themenbereich Modellierung der Wasserbewegung in Müllschlackendeponien) war er als Universitätsassistent im Bereich regionaler Stoffhaushalt tätig. Im Anschluss an seine Dissertation arbeitete er als Projektmanager und wissenschaftlicher Mitarbeiter in einem interdisziplinären Forschungsteam an der EMPA (Eidgenössische Materialprüfungs- und Forschungsanstalt) St. Gallen, wo er sich inhaltlich mit nachhaltiger Ressourcenbewirtschaftung befasst hat.

Danach war er als Dozent an der Fachhochschule Konstanz tätig. Seit Februar 2005 forscht und lehrt Frank Hartmann an der HSW im Rahmen des Studienbereichs Naturmanagement.

Roland Beer, lic.rer.pol., studierte Volks- und Betriebswirtschaft an der Universität Bern. Seine Marketingerfahrung erwarb er sich in leitenden Positionen in nationalen und internationalen Unternehmen in den Branchen Finanzen, Telekommunikation, Energie und Logistik. Roland Beer hat umfassende Praxiskenntnis mit vernetzten Kommunikationsprogrammen für Firmen, Privathaushalte, Handel, Institutionen und Medien. Seit Mitte Februar ist Roland Beer als Marketingdozent für Studierende des Studiengangs „Umwelt und Natürliche Ressourcen" an der Hochschule Wädenswil tätig.

Medienrückfragen beantwortet:
Hochschule Wädenswil, Corporate Communications
Birgit Camenisch
Tel.: 044 789 99 54, E-Mail: b.camenisch@hsw.ch

Latest News from COST: Launch of Three Chemistry Actions

COST (Cooperation in the field of Scientific and Technical research) is launching a series of new COST Actions in the chemistry domain. The basic principles of COST are a 'bottom up' mechanism, à la carte participation of COST member states, Brussels 'COST Office' financing of coordination and national financing of research projects

General information about COST in Switzerland is available from the homepage of the SER (State Secretariat of Education and Research; http://www.sbf.admin.ch) and from the National COST coordinator PD Dr. Eva M. Klaper (eva.klaper@sbf.admin.ch).

Information from the COST Office in Brussels, as well about the new COST Chemistry Actions that are described below, are available from the contacts given with each Action description and at http://cost.cordis.lu or http://costchemsitry.epfl.ch.

COST Action D33: 'Nanoscale Electrochemical and Bio-Processes at Solid-Aqueous Interfaces of Industrial Materials'

The main objective of the Action is to develop the understanding of biochemical processes at solid-aqueous interfaces leading to a universal approach to all biofouling related issues. To reach the main objective the following three secondary objectives have to be fulfilled:

– Development, adaptation and coupling of surface science methods for an improved analysis of the chemical processes occurring at the interfaces between materials and (micro) organisms,
– Analyses of chemical and biological processes causing adhesion of macromolecules, (microbial) cells, consortia *etc.* to materials surfaces,
– Understanding of the elementary steps leading to biocorrosion, biofouling, biofilms (also in health-related environments or food industry), bioleaching *etc.* in order to inhibit or improve the respective processes.

Duration: 04.05.2005–03.05.2009

Contact in Switzerland: Dr Rudolf Morach, Ciba Spezialitätenchemie AG, Werkstofftechnik, K-105.1, CH-4002 Basel, Tel.: +41 (0)61 636 19 05, Fax: +41 (0)61 636 20 69 rudolf.morach@cibasc.com

COST Action D34: 'Molecular Targeting and Drug Design in Neurological and Bacterial Diseases'

The main objective of the Action is to build on existing knowledge at the chemistry/biology interface, with a view to developing new target-oriented molecules and classes of molecules with therapeutic applications in the area of bacterial and neurological diseases. In order to fulfil this objective the following subtopics will be considered:

– The use of multivalent ligands, such as glycoclusters
– Targeting of drug delivery
– Inhibitors of target enzymes
– Molecules targeting diseases (mostly neurological) characterised by protein misfolding and aggregation

Duration: 22.02.2005–21.02.2009

Contact in Switzerland: Prof. Pierre Vogel, EPFL SB ISIC LGSA, BCH 5307, CH-1015 Lausanne, Tel. : +41 (0)21 693 93 71, Fax: +41 (0)21 693 93 75, pierre.vogel@epfl.ch

COST Action D35: 'From Molecules to Molecular Devices: Control of Electronic, Photonic, Magnetic and Spintronic Behaviour'

The main objective is to increase the knowledge and understanding of molecular electronic, photonic, magnetic and spintronic behaviour and to design new active chemical systems and processes that could find use in molecular devices. Secondary objectives are:

– To find and mechanistically understand new types of photo- and electro-induced processes and reveal ways how to control them at a molecular level.
– To design, synthesise and investigate selected molecular building blocks, molecule-based systems, nanomolecular materials, molecule-surface interfaces, molecular conductors, *etc.*, and to understand their cooperativity and emergence of new collective electronic, photonic, magnetic and spintronic phenomena.
– To develop and apply quantum mechanical methods to describe spectroscopic, magnetic and time-dependent phenomena accurately and to simulate environmental effects in condensed media.
– To demonstrate operational principles of selected types of molecular devices and to develop their prototypes (*e.g.* in the field of light-energy conversion and integrated optics).

The collaborative research carried out within this COST Action will provide knowledge enabling the development of new functional molecules and molecular electronic, photonic or magnetic devices as well as devices based on molecular recognition and motion. The international scientific community will be the main benefactor of this research. Selected scientific results could provide grounds and stimulus for device-development in high-tech small-medium enterprises active in the fields of light-energy conversion, photonics, electronics or sensors.

A scientific kick-off workshop for this Action will take place at the University of Zurich, November 25–27, 2005.

http://www.COSTD35.unizh.ch

Duration: 21.01.2005 – 10.02.2010

Contact in Switzerland: Prof. Heinz Berke, Universität Zürich, Anorganisch-Chemisches Institut, Winterthurerstr 190, CH-8057 Zürich, Tel.: +41 (0)44 635 46 81, Fax: +41 (0)44 635 68 02, hberke@aci.unizh.ch

Lectures

Basler Chemische Gesellschaft

17.30 Uhr
Institut für Organische Chemie, St. Johanns-Ring 19, Kleiner Hörsaal

18. Mai 2005 Mittwoch	Prof. Dr. *Lia Addadi* The Weizmann Institute of Science, Rehovot, Israel Title to be announced

Berner Chemische Gesellschaft

Mittwoch, 16.30 Uhr
Hörsaal EG 16, Departement für Chemie und Biochemie, Freiestr. 3
(Kaffee um 16.10 Uhr vor dem Hörsaal)

11. Mai 2005	Prof. *Wolfgang Baumeister* Director, Max-Planck-Institute of Biochemistry, Martinsried 'Mapping Molecular Landscapes inside Cells by Cryoelectron Tomography'
25. Mai 2005	Prof. *Reinhold Tacke* Institut für Anorganische Chemie, Lehrstuhl I, Würzburg 'Silicon-Based Drugs: The 'Rocky' Path from Basic Research to the Practical Application'

Sociéte Fribourgoise de Chimie (SFC) Freiburger Chemische Gesellschaft (FCG)

Tuesday, 17.15h
Grand Auditorium, Chemistry Department, Pérolles
Coffee, tea, and croissants will be served in front of the auditoire about 30 min before the lectures.

10. Mai 2005	Dr. *Albert Kuonen* F. Hoffmann-La Roche Ltd, Pharmaceuticals Division 'Evolution of Niotechnically Derived Pharmaceuticals (Biologics) at Roche'
24. Mai 2005	Prof. *Samuel Leutwyler* Departement für Chemie und Biochemie, Universität Bern 'Hydrogen-Atom and Proton Transfer Through Molecular Wires'

Institut für Physikalische Chemie der Universität Basel

Mittwoch, 16.30 Uhr
Kleiner Hörsaal Raum 404, 2. Stock, Klingelbergstrasse 80

Mittwoch 11. Mai 2005 16.30 Uhr	Prof. *Dr. I. Sims* Astronomie Expérimentale, Université de Rennes 1, France 'Astrochemistry – Laboratory Studies of Molecular Processes of Relevance to Astronomy'
Montag 23. Mai 2005 16.30 Uhr	Prof. Dr. *R. Whetten* Schools of Chemistry and Physics, Georgia Institute of Technology, Atlanta, USA Title to be announced

Département de Chimie minérale, analytique et appliqué, Université de Genève

Sciences, Salle A-150, les mercredis à 16h30
30, quai Ernest Ansermet, Genève

4 mai 2005	Dr. *Jean Susini* X-Ray Microscopy and X-Ray Micro-Analysis, European Synchrotron Radiation Facility, Grenoble, France 'Synchrotron Based X-Ray Imaging Techniques'
11 mai 2005	Prof. *Talal Mallah* Université Paris Sud, Laboratoire de Chimie Inorganique, Orsay, France 'Coordination Chemistry at the Nanoscale: Towards Molecular Magnetic Nanoobjects'
18 mai 2005	Dr. *Giuseppe Foffi* Institut Romand de Recherche Numérique en Physique des Matériaux, Ecole Polytechnique Fédérale de Lausanne 'Dynamical and Thermodynamical Properties in Short Ranged Attractive Colloidal Systems: Glass and Gel Formation'
25 mai 2005	Prof. *Ursula E. Spichiger-Keller* Center for Chemical Sensors and Chemical Information Technology (CCS), Swiss Federal Institute of Technology, Zurich 'Chemical Sensors = Molecular Recognition + Material Science + Information Technology'

Département de Chimie Organique, Université de Genève

Sciences II, Auditoire A-100, 16h30
30, quai Ernest Ansermet, Genève
http://www.unige.ch/sciences/chiorg/seminars.html

Jeudi 12 mai 2005	Prof. *Lutz Hans Gade* Ruprecht-Larls-Universität, Heidelberg, Heidelberg, D TBA
Jeudi 19 mai 2005	Prof. *Kurt Faber* Department of Chemistry, University of Graz, Graz, A 'Biocatalytic Enantio-Convergent Cascade-Reactions for Natural Product Synthesis'
Lundi 30 mai 2005	Prof. *David Milstein* The Weizmann Institute of Science, Israel TBA

Institut de Chimie, Université de Neuchâtel

Petit Auditoire, 10h30

Mercredi 11 mai 2005	Prof. *Helmut Alt* Universität Bayreuth, Allemagne 'How to Commercialise a Metallocene Catalyst? From the Bench to the Plant'
Jeudi 12 mai 2005	Prof. *Helmut Alt* Universität Bayreuth, Allemagne 'The Fine Tuning of Catalysts for Ethylene Oligomerisation and Polymerisation'
Lu.-Ma.-Me 23-25 mai 2005	Prof. *Robert Whetten* Georgia Techn, USA à définir

Laboratorium für Organische Chemie der ETH Zürich

Montag, 16.30 Uhr
Hörsaal HCI J3
ETH Hönggerberg, 8093 Zürich

2. Mai 2005	Prof. Dr. *Herman S. Overkleeft* Universität Leiden, Leiden, NL 'Chemical Proteomics Profiling of Functional Biomolecules'
9. Mai 2005	Prof. Dr. *Ilan Marek* Technion – Israel Institute of Technology, Haifa, Israel 'Metal-Mediated Multicomponent Reactions'
30. Mai 2005	Prof. Dr. *Goverdhan Mehta* Indian Institute of Science, Bangalore, India 'Total Synthesis of Biologically Active Natural Products'

Anorganisch Chemisches Institut der Universität Zürich

Friday, 17.00
Room 34 F 48
Winterthurerstrasse 190, Zürich-Irchel

13. May 2005	Dr. *Peter Faller* University Paul Sabatier (Toulouse III) 'Interactions of Metal Ions and Peptides/Proteines Linked to Alzheimer's Disease'
20 May 2005	Dr. *Zdeněk Havlas* Czech Academy of Sciences, Prag Title to be announced
27. May 2005	Prof. *David J. Cole-Hamilton* University of St. Andrews, UK 'Continuous Flow Homogeneous Catalysis Using Supercritical Fluids'

Organisch-chemisches Institut der Universität Zürich

Dienstag, 17.15 Uhr
Hörsaal 91
Winterthurerstrasse 190, Zürich-Irchel
(siehe auch www.oci.unizh.ch)

3. Mai 2005	Prof. Dr. *Christian G. Bochet* Department of Chemistry, University of Fribourg (CH) 'Chromatic Orthogonality: A New Form of Selectivity in Organic Synthesis'
10. Mai 2005	Prof. Dr. *Ronald G. Brisbois* Department of Chemistry, Macalester College, St. Paul (USA) 'A Decade of Undergraduate Research Focused on the Cylopentadienyl-Co-Cyclobutadienyl (CpCoCb) Metallocene Scaffold'
17. Mai 2005	Prof. Dr. *Michael Orfanopoulos* Department of Chemistry, University of Crete (Greece) 'Photocycloadditions to [60]Fullerene: Mechanisms and Synthetic Applications'
24. Mai 2005	Prof. Dr. *Philip E. Dawson* The Scripps Research Institute (USA) 'Synthetic Protein Chemistry'
31. Mai 2005	Prof. Dr. *Paul G. Wenthold* Department of Chemistry, Purdue University (USA) 'Reactivity and Structure of Open-Shell Organic Ions'

Zürcher Hochschule Winterthur

Abteilung Chemie und Biologische Chemie, Chemiegebäude C402
Donnerstag, 17.00 Uhr

19. Mai 2005	Dr. *Marianne Wilmer* Pentapharm AG, Basel 'Entwicklung von Analyseverfahren zur Diagnostik erworbener oder angeborener Störungen der Blutgerinnung'

Novartis Chemistry Lectureship 2004/2005

Location:	Novartis Pharma AG, Auditorium Horburg, WKL-430.3.20 Müllheimerstrasse 195, CH-4057 Basel
Time:	10.30 am ('Get Together': 10.00 am)
May 18, 2005	Prof. *Matthew D. Shair* Harvard University, Cambridge, USA To be announced