

University of Basel  
Department of Chemistry  
St. Johanns-Ring 19, Basel  
Big Lecture Hall



**SCS**

Swiss Chemical  
Society

**Division of  
Medicinal Chemistry &  
Chemical Biology**

Mini-Symposium

Thursday, May 22, 2014, 13.30h-17.45h

## Kinetics and Thermodynamics in Drug Discovery

Program

13.30h Introduction

13.35h **Gerhard Klebe**, University of Marburg  
Correlation of structure, thermodynamics and molecular  
dynamics to better understand drug binding

14.20h **David Swinney**, Institute for Rare and Neglected Diseases Drug  
Discovery  
Application of binding kinetics to drug discovery

15.05h Coffee Break

15.30h **Göran Dahl**, AstraZeneca  
Pharmacokinetics and the drug-target residence time concept

16.15h **David Sykes**, Novartis Institutes for Biomedical Research  
Exploring the relationship between  $\beta_2$ -adrenoceptor drug binding  
affinity/kinetic constants and physicochemical parameters

17.00h **Russel Petter**, Celgene  
Design and optimization of targeted covalent inhibitors

No registration – free admission  
[www.scg.ch/dmccb-minisymposium](http://www.scg.ch/dmccb-minisymposium)

Kindly sponsored by



Published by:  
Swiss Chemical Society  
Schwarztorstrasse 9  
CH-3007 Bern



**SCG**  
Schweizerische  
Chemische  
Gesellschaft

**SSC**  
Société  
Suisse  
de Chimie

**SCS**  
Swiss  
Chemical  
Society

[www.scg.ch](http://www.scg.ch)

Society News and Announcements

## KGF-SCS Industrial Science Awards

Dear CHIMIA readers,

On behalf of the KGF (Contact Group for Research Matters) it is my privilege to announce the prizewinners of the KGF-SCS Industrial Science Awards 2014. Together with the Swiss Chemical Society the KGF member companies honor outstanding achievements of industrial scientists working in Switzerland.

For more than 40 years KGF, a Swiss Industry Association, is supporting the promotion of scientific excellence and understanding in Switzerland and nearby regions.

In the name of the KGF I would like to congratulate all prizewinners for their outstanding scientific contributions.

Dr. Reto Naef  
KGF chair  
Novartis Pharma AG

Prof. E. Peter Kündig  
President  
Swiss Chemical Society

**KontaktGruppe für Forschungsfragen**  
Contact Group for Research Matters



## AWARD CEREMONIES AND AWARD LECTURES

The award ceremonies will take place on the occasion of the SCS Fall Meeting Dinner in Zurich on September 10, 2014. We are proud to announce the award lectures either in the plenary session or in one of the parallel sessions of the Fall Meeting at University of Zurich on September 11, 2014.

Thursday, September 11, 2014; SCS Fall Meeting Zurich

- *Dr. Hans-Ulrich Blaser*  
Winner of the Distinguished Industrial Investigator Award 2014. Plenary Session, 10:00h.
- *Dr. Werner Neidhart, F. Hoffmann La Roche Ltd*  
Winner of the Senior Industrial Investigator Award 2014. Invited lecture of the Session Medicinal Chemistry.
- *Dr. Andreas Natsch, Givaudan Schweiz AG*  
Winner of the Industrial Investigator Award 2014. Invited lecture of the Session Organic Chemistry.

- *Dr. Wolfgang Jahnke, Novartis Pharma AG*  
Winner of the Industrial Investigator Award 2014. Invited lecture of the Session Analytical Sciences.

For details please visit the SCS Fall Meeting website at <http://scg.ch/fallmeeting2014>

### KGF-SCS Distinguished Industrial Investigator Award 2014 Certificate and reward of CHF 15'000



The award is given to **Dr. Hans-Ulrich Blaser**, for his outstanding contributions to the development of highly selective and efficient catalysts for the industrial production of bioactive chiral compounds and for the leading role he played in asymmetric catalysis in both industry and academia.

#### Professional career

- 1971 PhD at ETH Zurich, Prof. A. Eschenmoser
- 1971–75 Postdoctoral studies at the University of Chicago (J. Halpern), Harvard University (J. A. Osborn) and Monsanto (Zurich)
- 1976–96 Central Research Laboratories, Ciba-Geigy
- 1996–99 Novartis
- 1999–12 Chief Technology Officer at Solvias
- 2004–12 Forschungsrat of the Swiss National Science Foundation whereof the last two years as president of the section II (natural sciences)

#### Scientific experience/contribution

Dr. Blaser has been one of the most impacting innovators, one of the most creative scholars, and an excellent entrepreneur creating sustainable value in Switzerland over the last thirty years.

As an *innovator*, Dr. Blaser is known throughout the world for his contributions – together with his team – to the development of an enantioselective process for the herbicide metolachlor, which remains as one of the largest industrial applications of asymmetric catalysis. In particular, the iridium catalyst used constitutes one of the most efficient systems disclosed so far, with turnover numbers exceeding one million. This fantastic potential could be only untapped through long, tedious and insightful experimental research of Dr. Blaser and his colleagues. It should be pointed out that this process to which Dr. Blaser contributed is currently presented to many undergraduate students all over the world as a leading example for the applications of catalysis.

As a *scholar*, Dr. Blaser contributed several fundamental insights into key catalytic processes. His pioneering work on the hydrogenation of ketoesters by platinum catalysts modified with cinchona alkaloids was conducted at a time, where this was often viewed as a laboratory curiosity. His insightful mechanistic studies led a fundamental understanding of the key steps involved, which led later to widespread use both in the scientific community and also on an industrial basis. In addition to many scientific peer-reviewed publications documenting his research, Dr. Blaser co-

edited a book on industrial catalysis, which quickly became the leading reference in the field.

As an *entrepreneur* and in his function as chief technology officer, Dr. Blaser significantly contributed to the development of Solvias as the key innovative company in the field of catalysis. His deep-rooted knowledge on catalysis paired with a realistic view of the feasibility of processes on an industrial scale led to many fruitful projects with industrial partners. This entrepreneurial spirit of Dr. Blaser helped to create and to sustain jobs and value in Switzerland and throughout the world.

The impact of Dr. Blaser's contributions definitely reach beyond Switzerland into the world, where many of the discoveries and developments of Dr. Blaser have changed the way chemical reactions are carried out.

*Prof. Karl Gademann (University of Basel)*

### KGF-SCS Senior Industrial Investigator Award 2014

Certificate and reward of CHF 10'000



The award is given to **Dr. Werner Neidhart**, F. Hoffmann La Roche, for his contributions to medicinal chemistry and the creation of multiple candidate drugs, particularly Endothelin antagonists Avosentan and Clazosentan and the marketed Bosentan/Tracleer.

#### Professional career

1980– PhD Thesis in synthetic organic chemistry, natural product synthesis, Prof. A. Gossauer, TU Berlin  
 1983– Post-doc studies, Prof. Sir A. R. Battersby, University of Cambridge (GB): Bio-organic chemistry  
 1985–... Preclinical Research Hoffmann-La Roche Basel  
 1991 Senior Scientist  
 1996 Scientific Specialist  
 2007 Expert Scientist  
 1995–... Lead chemist in area of cardiovascular, metabolic and infectious diseases

#### Scientific experience/contribution

Werner is one of the most creative and talented medicinal chemists I ever met. After joining Roche in the year 1985, Werner has worked most successfully on a number of different research projects; first as project member and since 1995 as lead chemist. The output of his contributions, reflected in the number of compounds advancing into late stage preclinical research, into clinical trials and ultimately on the market, is highly remarkable. Werner's hands convert almost any compound series into attractive drug candidates.

Werner has been an essential team member in the discovery of inhibitors of the aspartic protease Renin: Remikiren and Ciprokiren, which both advanced to clinical phase II trials in the early nineties. Later, he worked on Endothelin antagonists, since 1995 as lead chemist; thus, he contributed to the discovery of Bosentan, the first Endothelin antagonist on the market, which was launched as Tracleer by the Roche spin-out Biotech Actelion in 2001, to the discovery of Tezosentan, which was developed up to phase III (Actelion) and to the discovery of Clazosentan, which was out-licensed (Axovan / Actelion) and developed up to phase III. In 1998, Werner discovered Avosentan, a highly potent ETA selective Endothelin antagonist free of any liver liability. Unfortunately, Roche moved out of cardiovascular research soon thereafter and Avosentan was licensed to Speedel where it advanced to clinical phase III in diabetic nephropathy

as SPP301. In more recent times, two 11-beta Hydroxy-Steroid Dehydrogenase inhibitors were identified in the team led by Werner, one compound reached clinical phase II, one compound clinical phase I; and Werner and his team discovered the first non-covalent Hormone Sensitive Lipase inhibitors, which advanced into preclinical development.

Overall, Werner's work has led to an exceptionally high number of best quality clinical candidate compounds. Werner's success is based on the ideal mix of rational drug design and gut feeling combined with creative scientific curiosity allowing him to most rapidly identify druglike candidate compounds.

*Hans Peter Märki (Roche, Distinguished Scientist, Discovery Chemistry)*

### KGF-SCS Industrial Investigator Award 2014

Certificate and reward of CHF 7'000



The award is given to **Dr. Andreas Natsch**, Givaudan Schweiz AG, for his thorough investigation into the chemistry, biochemistry and microbiology of axilla malodor, culminating in the suppression of malodor causing processes and in the development of bacterial fragrance release from new families of odorant precursors.

#### Professional career

1993 Diploma in natural Sciences at ETH Zurich  
 1996 PhD at ETH Zurich  
 1997 Post doctoral studies at the Centro nacional de Biotecnologia, Madrid, Spain  
 1998 Scientist at Givaudan Schweiz AG, Zürich. Main focus biological activities of perfumery raw materials and essential oils (Antibacterial, antioxidant, anti-inflammatory)  
 2001 Senior Scientist at Givaudan Schweiz AG, Zürich. Main focus skin biochemistry (body odor formation) and new deodorant ingredients; bioactive fragrance formulations; development of alternative assays for skin sensitization.  
 2011 Research Fellow at Givaudan Schweiz AG. Main focus in vitro toxicology  
 2012 Senior Research Fellow at Givaudan Schweiz AG

#### Scientific experience/contribution

He has been leading the Givaudan efforts aiming at elucidating the biochemistry of the formation of human axilla malodor. This research led to the isolation and structure elucidation of several previously unknown key malodor precursors, the identification of the bacteria involved in the release of the mal-odorants and the isolation of novel key enzymes involved in the cleavage of the elucidated precursors. Consequently, he was able to develop potent enzyme inhibitors as well as alternative substrates, that upon enzyme action release a fragrance ingredient. These molecules represent a novel class of deo actives.

Fragrance ingredients have to be safe for consumers. The ban on animal testing for cosmetic ingredients, implemented this year, prompted Dr. Natsch to investigate alternative test assays. He further improved the DPRA assay proposed by P&G and he continued to investigate the chemical reactivity of skin allergens with peptides. This research combined with a smart idea led to the development of the KeratinoSens™ assay to predict the skin sensitization potential of chemicals without the need to animal tests. Thanks to the excellent results from a ring study with BASF,

Beiersdorf, P&G and IIVS, the assay is currently being evaluated by the OECD. This is an outstanding contribution to the safety testing of ingredients not only for the fragrances industry, but for the chemical industry as a whole.

*Dr. Markus Gautschi (Givaudan Fragrances S&T, Dübendorf)*

### KGF-SCS Industrial Investigator Award 2014

Certificate and reward of CHF 7'000



The award is given to **Dr. Wolfgang Jahnke**, Novartis Institutes for BioMedical Research, Basel, for his excellence in developing and applying biomolecular NMR spectroscopy and fragment-based lead discovery, resulting in crucial contributions to several drug discovery projects.

#### Professional career

- 1990 Diploma in Chemistry, University of Tübingen
- 1987/8 Visiting scholar at University of Arizona, Tucson
- 1994 PhD at Technical University of Munich on Structural Biology, group of Prof. Dr. Horst Kessler
- 1995 Post doctoral studies at Ciba-Geigy AG
- 1996–... Novartis Pharma AG, Basel, Structural Biology Lab head
- 2002 Novartis Leading Scientist Award
- 2005–... Senior Research Investigator II (Director)

#### Scientific experience/contribution

Wolfgang Jahnke has been running a laboratory for biomolecular NMR spectroscopy and other biophysical techniques such as Surface Plasmon Resonance (SPR) and Isothermal Titration Calorimetry (ITC) for 18 years within the Structural Biophysics group at Novartis. He supervises his lab associates and regularly also postdoctoral fellows, and personally conducts research as a bench scientist. He is an internationally recognized expert

in biomolecular NMR spectroscopy and fragment-based lead discovery (FBLD). He has developed novel methods in these fields and applied them with much success to a variety of drug discovery projects. It is for these outstanding achievements that Wolfgang Jahnke was nominated for the Industrial Science Award. His contributions are shown by an outstanding publication record, numerous invitations for plenary talks at high level scientific meetings such as the Gordon Conference, Keystone Conferences or important NMR or FBLD meetings, as an editor of the first book on fragment-based approaches in drug discovery, and by the invitation to co-organize fragment-based lead discovery conferences and the ENC conference. He recently got elected into the executive committee of the NMR section of the German Chemical Society. He is co-author of 80 scientific articles, book chapters or patents.

Wolfgang's contributions to internal projects that have not been published are significant. Beyond the specific expertise in NMR, Wolfgang Jahnke is experienced in drug discovery in all of its various aspects, including biology, chemistry, assays, and alternative lead finding approaches. He had the opportunity to initiate and lead two drug discovery projects very successfully, including seminal early contributions to a compound entering clinical trials. This experience allowed him to gain deeper insights and knowledge into the later stages of drug discovery, including pharmacokinetics, toxicology, chemical scale-up and the planning of proof-of-concept studies.

*Dr. Hans Widmer (Program Director, Industry-Academia Liaison)*

### A WARM WELCOME TO OUR NEW MEMBERS!

Period: 04.03.2014 – 25.03.2014

Victoria Custodis, Zurich – Veronika Ehmke, Basel – Nicolas Eichenberger, Boécourt – Maria Geormezi, Turgi – Justyna Lucja Kowal, Basel – Frederik Jürgen Malzner, WT-Tiengen – Diogo Filipe Mateus Rodrigues, Lausanne – Stephan Möller, Winterthur – Mathias Mosberger, Zurich – Ewa Pietrasiak, Zurich – Viktoria Reinmüller, Lausanne – Marleen Silbermann, Basel – Matthias Weiss, Baden.



## Die Welt ist voll von Halbwissen.

Wenn man sich in unbekannte Gefilde begibt, sollte man auf alles vorbereitet sein. Besonders im sensiblen beruflichen Umfeld der Chemie ist Halbwissen fehl am Platz. Deshalb arbeiten wir seit 1947 mit Leidenschaft und Akribie daran, dass evaluierte Daten und Fakten rund um das Themenfeld Chemie zur Verfügung stehen. Immer. Und ohne Ausnahme. So wurde „Der RÖMPP“ Synonym für inzwischen über 62.000 Stichwörter, auf die man sich verlassen kann. Das sollten Sie sich am besten selbst anschauen.

Nur 100% sind 100%.  
[www.roemp.com](http://www.roemp.com)

RÖMPP Online-Enzyklopädie für SCG-Mitglieder nur

CHF 175\* Regular Members  
CHF 75\* Studenten und PhD



SCS  
Schweizerische  
Chemische  
Gesellschaft

\*Pers. Jahreslizenzgebühr inkl. MwSt.

[www.scg.ch/roemp](http://www.scg.ch/roemp)

 Thieme

University of Zurich  
Department of Chemistry  
Winterthurerstrasse 190  
CH-8057 Zürich



**SCS**  
Swiss Chemical  
Society

Thu, 11 September 2014, 9:30 – 18:45

## Fall Meeting 2014

- Posters and short talks in 9 parallel sessions
- Lectures by invited speakers and award winners
- Poster and oral presentation awards
- Commercial exhibition

### Call for Contributions

Open from 10 February to 18 May

[www.scg.ch/fallmeeting](http://www.scg.ch/fallmeeting)

Published by:  
Swiss Chemical Society  
Schwarztorstrasse 9  
3007 Bern

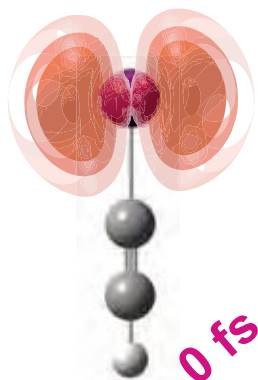
Hosted by:



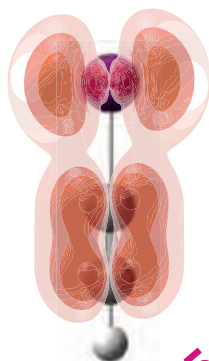
**Universität  
Zürich**<sup>UZH</sup>

**ETH**

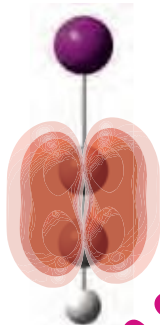
Eidgenössische Technische Hochschule Zürich  
Swiss Federal Institute of Technology Zurich



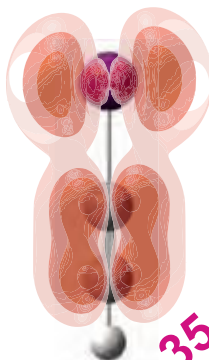
0 fs



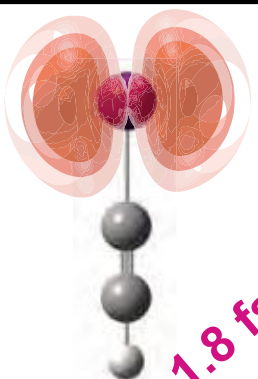
0.45 fs



0.9 fs



1.35 fs



1.8 fs



SCS

Division of  
Analytical Sciences

## Weiterbildung Analytik

Trenntechnik  
Analytische Anwendungen  
Methoden der Life Sciences  
Qualitätssicherung  
InCompany Trainings

Titel	Ort	Termin	Code
Validieren von Analysenverfahren I, Grundlagen	Dübendorf	06.05.2014	QS-8
Einführung in den ‚Inductively Coupled Plasma‘ (ICP) Massenspektrometrie	Zürich/ETH Hö	06.–07.05.2014	SP-4
Karl Fischer Titration	Zofingen	08.05.2014	AA-2
Interpretation von Massenspektren	Dübendorf	13.–14.05.2014	SP-8
Statistische Auswertung von Messwerten zur Qualitätssicherung	Basel	13.–15.05.2014	QS-3
Einführung in die Ionenchromatographie (IC)	Zofingen	15.05.2014	TR-8
Vergleich von Massenspektren mit Datenbanken: Tricks und Werkzeuge	Dübendorf	15.05.2014	SP-6
Oberflächen-gestützte Analytik und Sensorik mit der Schwingquarz-Mikrowaage	Dübendorf	16.05.2014	AA-7
Isolierung und Reinigung von Proteinen	Basel/Novartis	20.–21.05.2014	LS-3
Elektrochemische Titrationsmethoden: Einführung in die Praxis	Zofingen	22.05.2014	AA-1
Enantioselektive chromatographische Trennmethode	Dübendorf	26.05.2014	TR-14
Präparative Chromatographie	Freiburg	27.05.2014	TR-15
Einführung in die HPLC	Dübendorf	12.–13.06.2014	TR-9
Dünnschichtchromatographie: Einführung in die moderne Technik	Muttenz	16.–17.06.2014	TR-2
Grundlagen und Anwendungen in der Nah-Infrarot (NIR) Spektrometrie	Flawil	19.06.2014	SP-5
Referenzmaterialien zur Methodenvalidierung und Gerätequalifizierung	Dübendorf	25.06.2014	QS-14
Messunsicherheit in der Analytik	Dübendorf	26.06.2014	QS-5
Qualifizieren von Analysengeräten	Dübendorf	26.06.2014	QS-7
Validieren von Analysenverfahren II, Praktische Beispiele	Dübendorf	27.06.2014	QS-9
<b>Französisch</b>			
Principes de base en méthodologie – calculs statistiques	Genève	06.05.2014	AA-5f
Echantillonnage ou prélèvement représentatif en production, dans l’environnement et au laboratoire	Genève	07.–08.05.2014	AA-4f
Spéctrométrie d’absorption atomique avec four graphite (AAS-FG) et Spéctrométrie d’émission atomique à plasma inductif (ICP-OES)	Genève	09.05.2014	AA-1f
Préparation de l’échantillon liquide	Genève	13.05.2014	AA-2f
Analyse de matrices solides	Genève	14.05.2014	AA-3f
Analyse qualitative et quantitative en GC/MS	Genève	15.05.2014	MS-2f
Troubleshooting en GC/MS	Genève	16.05.2014	MS-3f
Les nouvelles tendances HPLC: comment améliorer sa productivité au laboratoire	Genève	20.–21.05.2014	LC-3f
Analytical Strategies for Volatile Compounds and Gases	Genève	23.05.2014	GC-4f

Es freut uns, Ihnen das Weiterbildungsprogramm 2014, das wir zusammen mit dem Centre de Compétence en Chimie et Toxicologie Analytiques (CCCTA) realisiert haben, vorzustellen.

**Einzelmitglieder der folgenden Fachverbände können unsere Kurse zum vorteilhaften Mitgliedertarif besuchen:**

Fachverband Laborberufe (FLB), Gesellschaft Deutscher Chemiker (GDCh), Schweizerische Arbeitsgemeinschaft für Spektrometrie und Elementaranalytik (SASP), Schweizerischer Chemikanten- und Chemisten-Verband (SCV), Schweizerische Gesellschaft für Lebensmittel- und Umweltchemie (SGLUC), Schweizerische Gruppe für Massenspektroskopie (SGMS) und Schweizerischer Verband Diplomierter Chemiker (SVC).

Falls Sie sich für unsere Veranstaltungen interessieren, erreichen Sie uns unter Telefon **058 765 52 00** oder Fax **058 765 58 01** oder mailen Sie an [verena.schmid@eawag.ch](mailto:verena.schmid@eawag.ch). Online-Anmeldung im Internet unter: [www.scg.ch/das](http://www.scg.ch/das)

### InCompany Training – Individuelle Beratung und Schulung

Im Rahmen des Weiterbildungsprogramms organisieren oder erarbeiten wir gemeinsam mit Ihnen InCompany-Schulungen und -Trainings nach Ihren Vorstellungen und Bedürfnissen. Profitieren Sie davon, dass wir für Sie

- Inhalte an firmenspezifische Anforderungen und Wünsche anpassen
- Frage- und Problemstellungen in Ihrem Einsatzgebiet gezielt behandeln
- praktische Übungen gegebenenfalls an Ihren Geräten durchführen
- Trainings bei Bedarf auch in französischer oder englischer Sprache durchführen

Ein weiterer Vorteil der InCompany-Trainings: für Ihre Mitarbeiterinnen und Mitarbeiter fallen keine Reise- und Übernachtungskosten an!

Experten stehen Ihnen für eine persönliche Bedarfsabklärung und Beratung gerne zur Verfügung.

Sie erreichen uns über  
Sekretariat Weiterbildung SCG/DAS  
Frau V. Schmid  
c/o EAWAG  
Überlandstrasse 133, 8600 Dübendorf  
Telefon 058 765 52 00  
E-Mail: [verena.schmid@eawag.ch](mailto:verena.schmid@eawag.ch)  
[www.scg.ch/das](http://www.scg.ch/das)