

Award Lectures Overview

- 09:55 **Hans-Ulrich Blaser**, St. Gallen (formerly Ciba-Geigy, Novartis and Solvias) is awarded the KGF-SCS Distinguished Industrial Investigator Award 2014 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.

«Looking Back on 35 Years of Industrial Catalysis» [PS-002] ; Lecture hall G30.

- 10:30 **Harald Walter**, Hans Tobler, Camilla Corsi and Denis V. Gribov, Syngenta Crop Protection Mönchwil AG are awarded the Sandmeyer Award 2014 for their successful and innovative efforts in discovering, developing, and producing new broad-spectrum agrochemical fungicides.

«Sedaxane, isopyrazam and solatenol: Novel broad-spectrum fungicides inhibiting succinate dehydrogenase (SDH) – synthesis challenges and biological aspects» [PS-003] ; Lecture hall G30.

- 11:15 **Andreas Natsch**, Givaudan Schweiz AG is awarded the KGF-SCS Industrial Investigator Award 2014 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.

«The human scent: Chemicals, enzymes and genes and our 'olfactive self'» [OC-001] ; Lecture hall G45.

- 11:15 **Erwin Reisner**, University of Cambridge, UK is awarded the Grammaticakis-Neumann Award 2014 for his research combining synthesis, photochemistry, photophysics, and molecular photobiology to develop artificial photosynthesis.

«Protein film photoelectrochemistry of the water oxidation enzyme Photosystem II» [CE-001]; Lecture hall G20.

- 16:15 **Werner Neidhart**, F. Hoffmann-La Roche AG is awarded the KGF-SCS Senior Industrial Investigator Award 2014 for his contributions to medicinal chemistry and the creation of multiple candidate drugs, particularly Endothelin antagonists Avosentan and Clazosentan and the marketed Bosentan/Tracleer.

«Challenges & Rewards in Medicinal Chemistry Targeting Cardiovascular & Metabolic Diseases» [MC-003] ; Lecture hall G19.

- 16:35 **Wolfgang Jahnke**, Novartis Institutes for Biomedical Research is awarded the KGF-SCS Industrial Investigator Award 2014 for his excellence in developing and applying biomolecular NMR spectroscopy and fragment-based lead discovery, resulting in crucial contributions to many drug discovery projects.

«Contributions of biomolecular NMR to drug discovery» [MC-004] ; Lecture hall G19.

- 17:00 **Richard R. Schrock**, Massachusetts Institute of Technology is awarded the Paracelsus Award 2014 for his seminal work in synthetic and mechanistic organo-transition metal chemistry.

«The Olefin Metathesis Reaction - Approaching Fifty Years of Age» [PS-004] ; Lecture hall G30.

Plenary Sessions – G30



Chair: Prof. E. Peter Kündig

Session Endowment: Givaudan Suisse SA

- 09:55 **KGF-SCS Distinguished Industrial Investigator Award Lecture 2014: Looking Back on 35 Years of Industrial Catalysis [PS-002]**
Hans-Ulrich Blaser, St. Gallen (formerly Ciba-Geigy, Novartis and Solvias)
- 10:30 **Sandmeyer Award Lecture 2014: Sedaxane, isopyrazam and solatenol: Novel broad-spectrum fungicides inhibiting succinate dehydrogenase (SDH) – synthesis challenges and biological aspects [PS-003]**
Harald Walter, Syngenta Crop Protection Mönchwil AG
- 17:00 **Paracelsus Award Lecture 2014: The Olefin Metathesis Reaction - Approaching Fifty Years of Age [PS-004]**
Richard R. Schrock, Massachusetts Institute of Technology

Abstract codes

[XY-001]...[XY-009]	Award or invited lecture
[XY-011]...[XY-019]	Morning session lecture
[XY-021]...[XY-029]	Afternoon session lecture
[XY-031]...[XY-039]	Short poster presentations
[XY-101]...[XY-199]	Poster

AS	Analytical Sciences
CC	Computational Chemistry
CE	Catalysis Sciences & Engineering
IC	Inorganic Chemistry
MC	Medicinal Chemistry & Chemical Biology
OC	Organic Chemistry
PC	Physical Chemistry
PI	Polymers Colloids & Interfaces
PS	Plenary Session

Name = Presenting Author

Name = Research Leader

PARALLEL SESSIONS

Analytical Sciences [AS]

Morning Session – G95

Chair: Dr. Stefan Schürch

Session Endowment:

- 11:15 **Chemical Analysis by Mass Spectrometry in Space - Initial Results from the Comet Churyumov-Gerasimenko [AS-001]**
Kathrin Altweg, University of Berne
- 12:00 **Microscale probing and patterning of biological surfaces using nested hydrodynamic flow confinement and recirculation of sub-microliter volumes of liquid [AS-014]**
Govind Kaigala, IBM Research GmbH
- 12:15 **A Droplet Microfluidic ICP-MS Sample Introduction System [AS-015]**
Pascal Emilio Verboket, *Petra Dittrich*, ETH Zurich
- 12:30 **Electrostatic Spray Ionization Mass Spectrometry for Biochemical Analysis and Imaging [AS-016]**
Liang Qiao, *Hubert Girault*, EPFL Lausanne

Afternoon Session – G95

Chair: Dr. Marc Suter

- 15:00 **2D-algal arrays on-chip as a tool for environmental biosensing [AS-021]**
Coralie Sussillon, *Vera Slaveykova*, University of Geneva
- 15:15 **Quantification of ghrelin and des-acyl ghrelin in human plasma by using cubic selected reaction monitoring LC-MS [AS-022]**
Jonathan Sidibé, *Gérard Hopfgartner*, University of Geneva
- 15:30 **Laser based N₂O isotopomer analysis bridges the gap between pure culture studies and field applications [AS-023]**
Ellen Gute, EMPA Dübendorf
- 15:45 **Direct voltammetric As(III) sensing in natural waters on a gel integrated renewable gold nanoparticle microelectrode [AS-024]**
Romain Touilloux, *Eric Bakker*, University of Geneva
- 16:00 **Native ESI-MS: Buffer Concentration Effect on Protein-Ligand Binding Affinities [AS-025]**
Agni Faviola Mika Gavriilidou, *Renato Zenobi*, ETH Zurich
- 16:15 **Instrumentino: An open-source modular Python framework for controlling Arduino based experimental instruments [AS-026]**
Joel Koenka, *Peter Hauser*, University of Basel
- 16:30 **Capillary zone electrophoresis as a capable tool in endotoxin and carbohydrate analysis [AS-027]**
Blanka Bucsella, *Franka Kálmán*, University of Applied Sciences and Arts Northwestern Switzerland, FHNW

Computational Chemistry [CC]



Morning Session – G85

Chair: Prof. Jürg Hutter

Session Endowment: IBM Research GmbH

- 11:15 **Light Matter Interaction: The role of quantum coherence in energy transfer [CC-001]**
Sabre Kais, Qatar Environment and Energy Research Institute, Doha, Qatar
- 11:45 **Reviving geminal wavefunction theory: Accurate description of strong electron correlation at mean-field computational cost [CC-013]**
Peter Limacher, Paul W. Ayers, McMaster University
- 12:00 **Four-Component Density Matrix Renormalization Group [CC-014]**
Stefan Knecht, Markus Reiher, ETH Zurich
- 12:15 **Implementation of exact and approximate methods for nonadiabatic quantum molecular dynamics induced by the interaction with the electromagnetic field [CC-015]**
Aurélien Patoz, Jiri Vanicek, EPFL Lausanne
- 12:30 **Towards Intramolecular SAPT [CC-016]**
Antonio Prlj, Clemence Corminboeuf, EPFL Lausanne

Afternoon Session – G85

Chair: Prof. Markus Reiher

- 15:00 **Full-dimensional quantum dynamics and spectroscopy of ammonia isotopomers [CC-021]**
Csaba Fábri, *Martin Quack*, ETH Zurich
- 15:15 **Learning the error: Augmenting legacy quantum chemistry with machine learning [CC-022]**
Raghunathan Ramakrishnan, *O. Anatole von Lilienfeld*, University of Basel
- 15:30 **Unravelling the stabilization mechanism of Al-doped Li-ion conducting Garnets by first-principle simulations. [CC-023]**
Teodoro Laino, IBM Research GmbH
- 15:45 **Ab-initio Simulation of two-dimensional Networks on the Surface of Water [CC-024]**
Ralph Koitz, *Jürg Hutter*, University of Zurich
- 16:00 **Re-Engineering the B1 Domain of Streptococcal Protein G (GB1): Teaching an Old Dog New Tricks [CC-025]**
Esra Bozkurt, *Ursula Röthlisberger*, EPFL Lausanne
- 16:15 **Reactive Processes onto the Multidimensional Potential Energy Surface: Molecular Dynamics of the MbNO system [CC-026]**
Maksym Soloviov, *Markus Meuwly*, University of Basel
- 16:30 **Anion- π and cation- π interactions on the same aromatic surface [CC-027]**
Marie Humbert-Droz, *Stefan Matile*, University of Geneva

Catalysis Sciences & Engineering [CE] Morning Session – G20

Chair: Dr. Davide Ferri

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Session Endowment: Clariant International Ltd

- 11:15 **Grammaticakis-Neumann Award Lecture 2014: Protein film photoelectrochemistry of the water oxidation enzyme Photosystem II [CE-001]**
Erwin Reisner, University of Cambridge, UK
- 11:45 **Interplay between complexity and universality in industrial catalysts [CE-002]**
Pascal Raybaud, IFP Energies nouvelles
- 12:15 **C-H Activation on Tri-Coordinated Cr(III) Silica Surface Sites Initiates Ethylene Polymerization [CE-015]**
Murielle F. Delley, *Christophe Copéret*, ETH Zurich
- 12:30 **Transient studies of methane steam reforming over ceria-promoted Rh/Al₂O₃ [CE-016]**
Renata Duarte, *Jeroen A. van Bokhoven*, ETH Zurich

Afternoon Session – G20

Chair: Dr. Jeremy Luterbacher

- 15:00 **Investigation of factors affecting the crystallisation of zeotype Sn-Beta with elemental mapping [CE-003]**
Esben Taarning, Haldor Topsoe A/S
- 15:30 **Mesopore quality determines the lifetime of hierarchically-structured zeolite catalysts [CE-023]**
Maria Milina, *Javier Pérez-Ramírez*, ETH Zurich
- 15:45 **1D and 2D Tuning of Cobalt-based Water Oxidation Catalysts [CE-024]**
Fabio Evangelisti, *Greta Ricarda Patzke*, University of Zurich
- 16:00 **Structured Fe₂O₃–based Catalyst for Reduction of Nitroarenes under Mild Conditions [CE-025]**
Oliver Beswick, *Liubov Kiwi-Minsker*, EPFL Lausanne
- 16:15 **NH₃ promoted formic acid decomposition over monolithic Au/TiO₂ catalyst: Rate enhancement without NH₃ oxidation [CE-026]**
Manasa Sridhar, *Oliver Kröcher*, *Paul Scherrer Institute*, *Villigen and EPFL Lausanne*
- 16:30 **Lactic acid production from biomass: a new chemocatalytic process compared to fermentation by LCA analysis [CE-027]**
Pierre Dapsens, *Javier Pérez-Ramírez*, ETH Zurich

Inorganic & Coordination Chemistry [IC] Morning Session – G30

Chair: Prof. Thomas Ward



Session Endowment: Contact Group for Research Matters (KGF)

- 11:15 **Nitrogenase: Mechanism and Applications [IC-001]**
Markus W. Ribbe, University of California, Irvine (US)
- 12:00 **Functionalised Clathrochelate Complexes – New Building Blocks for New Supramolecular Structures [IC-014]**
Matthew Wise, *Kay Severin*, EPFL Lausanne
- 12:15 **Iron Catalysts for Hydrogenation of Aldehydes: an Alternative to Precious Noble Metals [IC-015]**
Simona Mazza, *Xile Hu*, EPFL Lausanne
- 12:30 **Synthesis, Structure and Reactivity of a Ruthenium Complex with an Unusual P₄Cl₂ Ligand [IC-016]**
Mark Bispinghoff, *Hansjörg Grützmacher*, ETH Zurich

Afternoon Session – G30

Chair: Prof. Kay Severin

- 15:00 **Supported alkene metathesis catalysts: from reaction intermediates to structure activity relationship [IC-021]**
Victor Mougel, *Christophe Copéret*, ETH Zurich
- 15:15 **Performance and in situ characterization of ceria-based non-stoichiometric oxides for the conversion of solar energy using two-step thermochemical cycles [IC-022]**
Matthäus Rothensteiner, *Paul Scherrer Institute*, *Villigen*, *Jeroen A. van Bokhoven*, *ETH Zurich and Paul Scherrer Institute*, *Villigen*
- 15:30 **The surprising lability of homoleptic and heteroleptic bis-(2,2':6',2''-terpyridine) chromium(III) complexes [IC-023]**
Jonas Schönlé, *Catherine E. Housecroft*, University of Basel
- 15:45 **Peptide Conjugates of Dinuclear Arene Ruthenium Trithiolato Complexes [IC-024]**
Federico Giannini, University of Berne, *Georg Süss-Fink*, *University of Neuchâtel*
- 16:00 **Antimicrobial metal-containing Schiff base complexes [IC-025]**
Sonja Kracht, *Katharina Fromm*, University of Fribourg
- 16:15 **Aspects of the vibrational optical activity (VOA) of tetranuclear Cobalt transition metal complexes [IC-026]**
Patric Oulevey, *Thomas Bürgi*, University of Geneva
- 16:30 **X-ray structures of an octameric RNA duplex in the presence of six different divalent and trivalent metal ions reveal a particular innersphere binding to O4 of uracil [IC-027]**
Michelle F. Schaffer, *Roland K.O. Sigel*, University of Zurich

Medicinal Chemistry & Chemical Biology [MC]**Morning Session – G19**

Chair: Prof. Jean-Louis Reymond



Session Endowment: Actelion Ltd

- 11:15 **Engineering of high affinity probes for the visualization and analysis of bivalent epigenetic marks in living cells [MC-011]**
Aurore Delachat, *Beat Fierz*, EPFL Lausanne
- 11:30 **Sphingosine-1-Phosphate Lyase Inhibitors as an Alternative Therapeutic Strategy to S1P-Receptor Agonists for the Treatment of Multiple Sclerosis [MC-012]**
Berndt Oberhauser, Novartis Pharma AG
- 11:45 **Disulfide-based prodrugs for improving the oral bioavailability of poorly water soluble drugs [MC-013]**
Tao Sun, *Jean-Christophe Leroux*, ETH Zurich
- 12:00 **Selective Aldosterone Synthase Inhibitors (ASI) - Design of an Orally Active Proof of Concept Compound [MC-014]**
Johannes Aebi, *Kurt Amrein*, F. Hoffmann-La Roche AG
- 12:15 **Ru(II) Complexes and Photodynamic Therapy: a Win-Win Combination [MC-015]**
Cristina Mari, *Gilles Gasser*, University of Zurich
- 12:30 **Discovery of novel and highly selective allosteric inhibitors of PAK1 [MC-001]**
Alexei Karpov, Novartis Pharma AG

Afternoon Session – G19

Chair: Dr. Heinz Fretz

- 15:00 **Discovery of a potent P2Y₁₂ receptor antagonist with an improved efficacy/safety profile [MC-021]**
Eva Caroff, Actelion Pharmaceuticals Ltd, Allschwil
- 15:15 **Transannular cyclization of the sesquiterpene lactone nobilin into cadinanolide derivatives [MC-022]**
Maria De Mieri, *Matthias Hamburger*, University of Basel
- 15:30 **From Synthesis in Flow to Integrated Dose-Response Screening in Flow [MC-002]**
Rainer E. Martin, F. Hoffmann-La Roche AG
- 15:45 **Designed Cell Penetrating Peptide Dendrimers Efficiently Internalize Cargo into Cells [MC-024]**
Emilyne Blattes, *Jean-Louis Reymond*, University of Berne
- 16:00 **Synthesis and fungicidal activity of quinolin-6-yloxyacetamides, a novel class of tubulin polymerization inhibitors [MC-025]**
Laura Quaranta, Syngenta Crop Protection AG
- 16:15 **KGF-SCS Senior Industrial Investigator Award Lecture 2014: «Challenges & Rewards in Medicinal Chemistry Targeting Cardiovascular & Metabolic Diseases» [MC-003]**
Werner Neidhart, F. Hoffmann-La Roche AG
- 16:35 **KGF-SCS Industrial Investigator Award Lecture 2014: «Contributions of biomolecular NMR to drug discovery» [MC-004]**
Wolfgang Jahnke, Novartis Institutes for Biomedical Research

Organic Chemistry [OC]**Morning Session – G45**

Chair: Prof. Andreas Pfaltz

Session Endowment: Syngenta Crop Protection AG

- 11:15 **KGF-SCS Industrial Investigator Award 2014: The human scent: Chemicals, enzymes and genes and our 'olfactive self' [OC-001]**
Andreas Natsch, Givaudan Schweiz AG
- 11:45 **Highly Enantioselective Rh(I)-Catalyzed Activation of Cyclobutanones Enantiotopic C-C Bond. [OC-013]**
Laetitia Souillart, *Nicolai Cramer*, EPFL Lausanne
- 12:00 **Pd-catalyzed selective arylations of aldehydes [OC-014]**
Ivan Franzoni, *Clément Mazet*, University of Geneva
- 12:15 **New Synthetic Applications of Nitrous Oxide [OC-015]**
Gregor Kiefer, *Kay Severin*, EPFL Lausanne
- 12:30 **Pyridine Dearomatization Through Double Ru-Metal Carbene Insertions [OC-016]**
Florian Medina, *Jérôme Lacour*, University of Geneva

Afternoon Session – G45

Chair: Dr. Henning Jessen

- 15:00 **Sterol C(14)-demethylase inhibitors as fungicides for use in crop protection [OC-002]**
Sebastian Wendeborn, Syngenta Crop Protection AG
- 15:30 **Difunctionalization of Activated Alkenes via Radical Addition/Desulfonylation/1,4-Aryl Migration Cascade Reaction [OC-023]**
Wangqing Kong, *Cristina Nevado*, University of Zurich
- 15:45 **Total Synthesis of Aspidosperma Family Monoterpene Indole Alkaloids [OC-024]**
Olivier Wagnières, *Jieping Zhu*, EPFL Lausanne
- 16:00 **Syntheses and Applications of Acylboronates in Chemoselective Amide Formations [OC-025]**
Hidetoshi Noda, *Jeffrey W. Bode*, ETH Zurich
- 16:15 **Setting the Hook for Specific Single Walled Carbon Nanotubes (SWCNT) [OC-026]**
Ina Bodoky, *Marcel Mayor*, University of Basel
- 16:30 **Rational Design of a Gold Carbene Precursor Complex for a Catalytic Cyclopropanation Reaction [OC-027]**
David Ringger, *Peter Chen*, ETH Zurich

Physical Chemistry [PC]**Morning Session – G40**

Chair: Prof. Stefan Willitsch

Session Endowment: Bruker BioSpin

- 11:15 **Bruker: Session Endowment Talk [PC-001]**
Guest speaker from Bruker Physik GmbH
- 11:45 **Attosecond photoelectron spectroscopy [PC-013]**
Martin Huppert, *Hans Jakob Wörner*, ETH Zurich
- 12:00 **Submm wave spectroscopy in the range 72 to 100 GHz of meta- and ortho-D-phenol: Probing tunneling switching dynamics [PC-014]**
Ziqiu Chen, *Martin Quack*, ETH Zurich
- 12:15 **Control of chemical reactivity through spatial separation of molecular conformations [PC-015]**
Daniel Rösch, *Stefan Willitsch*, University of Basel
- 12:30 **Rydberg Spectroscopy of Zeeman-Decelerated Beams of Metastable Helium Molecules [PC-016]**
Paul Jansen, *Frédéric Merkt*, ETH Zurich

Afternoon Session – G40

Chair: Prof. Peter Hamm

- 15:00 **Probing a Conformational Change of a Photoswitchable Allosteric Protein with Ultrafast IR Spectroscopy [PC-021]**
Brigitte Stucki-Buchli, *Peter Hamm*, University of Zurich
- 15:15 **Light-induced charge transfer in the cytochrome bc₁ at high quantum yield [PC-022]**
Adrien Chauvet, *Majed Chergui*, EPFL Lausanne
- 15:30 **Orientation and excited-state dynamics of DNA probes at liquid/water interfaces [PC-023]**
Giuseppe Leonardo Licari, *Eric Vauthey*, University of Geneva
- 15:45 **Photoelectric conversion based on light induced proton pumps and proton-coupled electron transfer reactions [PC-024]**
Xiaojiang Xie, *Eric Bakker*, University of Geneva
- 16:00 **Long-lived Charged Carriers in Oligothiophene Nanowires [PC-025]**
Damien Rolland, *Holger Frauenrath*, EPFL Lausanne
- 16:15 **Charge-transfer dissociation at organic donor-acceptor interfaces probed with time-resolved electroabsorption [PC-026]**
Jelissa De Jonghe, *Jacques-E. Moser*, EPFL Lausanne
- 16:30 **Particle size and shape dependence of the ionic diffusivity in LiMnPO₄ cathode for lithium ion batteries [PC-027]**
Nam Hee Kwon, *Katharina Fromm*, University of Fribourg

Polymers, Colloids & Interfaces [PI]**Morning Session – G55**

Chair: Prof. Christian Hinderling

Session Endowment: Dow Europe GmbH

- 11:15 **Observation of single-molecules at interfaces: fundamentals and applications [PI-001]**
Andrei Honciuc, Zurich University of Applied Sciences, ZHAW
- 11:45 **Stimuli-Responsive (Bio)Hybrid Coiled Coil Peptide-Polymer Microgels [PI-013]**
Vitaliy Kolesov, *Harm-Anton Klok*, EPFL Lausanne
- 12:00 **Organic-Inorganic Nanocomposite Scintillators: HfO₂:Eu Luminescent Nanoparticles Embedded into Polymer Films [PI-014]**
Alessandro Lauria, *Walter Caseri*, ETH Zurich
- 12:15 **Modeling multiradicals in bulk crosslinking copolymerization [PI-015]**
Stefano Lazzari, ETH Zurich
- 12:30 **Short Poster Presentations: Polymers, Colloids & Interfaces [PI-016]**
Chaired by Christian Hinderling, Zurich University of Applied Sciences, ZHAW

Afternoon Session – G55

Chair: Prof. Dieter Schlüter

- 15:00 **Generating anisotropic microstructures in colloidal gels [PI-002]**
Jan Vermant, ETH Zurich
- 15:30 **Tunable aggregation of sterically demanding peryleneimides induced by the conjugation with rigid oligoproline scaffolds. [PI-023]**
Urszula Lewandowska, *Helma Wennemers*, ETH Zurich
- 15:45 **Effect of hydrophobicity on nanoparticle formation: a case of ABC asymmetric triblock copolymers [PI-024]**
Evgeniia Konishcheva, *Wolfgang Meier*, University of Basel
- 16:00 **Tandem Ring Opening-Ring Closing Metathesis for Synthesis of Functional Metathesis Catalysts [PI-025]**
Amit Nagarkar, *Andreas Kilbinger*, University of Fribourg
- 16:15 **The role of peptides in the formation of silver nanoparticles [PI-026]**
Matthias Messerer, *Katharina Fromm*, University of Fribourg
- 16:30 **Particle Aggregation in Ionic Liquids [PI-027]**
Gregor Trefalt, *Michal Borkovec*, University of Geneva