Fall Meeting 2011
Herbstversammlung 2011
Assemblée d’automne 2011

Friday, September 9, 2011
Freitag, 9. September 2011
Vendredi, 9 septembre 2011

Ecole Polytechnique Fédérale de Lausanne
Centre Est
Organizing Committee

MER Dr Sandrine Gerber (Chair) – EPF Lausanne
Prof. Karl-Heinz Altmann – ETH Zurich
Prof. Clémence Corminboeuf – EPF Lausanne
Prof. Frédéric Merkt – ETH Zurich
Prof. Jacques-Edouard Moser – EPF Lausanne
Prof. Frank Scheffold – University of Fribourg
Prof. Kay Severin – EPF Lausanne
Prof. Jieping Zhu – EPF Lausanne

Prof. Paul Dyson (Co-chair) – EPF Lausanne
Prof. Christian Bochet – EPF Lausanne
Prof. Harm-Anton Klok – EPF Lausanne
Prof. Markus Meuwly – University of Basel
Prof. Philippe Renaud – University of Bern
PD Dr. Stefan Schürch – University of Bern
Prof. Thomas Ward – University of Basel

Secretariat

Ms. Sandra Jeanneret, Ms. Madeleine Steffen,
Institute of Chemical Sciences and Engineering, Ecole Polytechnique Fédérale de Lausanne,
SB ISIC-GE, Station 6, CH-1015 Lausanne
Tel. +41 21 693 3611, +41 21 693 55 29, E-mail: scs.fallmeeting@epfl.ch

Information

No registration for SCS members is required to participate in the meeting, coffee breaks and lunch, all of which are free of charge.

Non-members of the SCS will be asked to pay a 50 CHF entrance fee, which will provide access to the conferences, poster sessions, coffee breaks and lunch.

Lunch: Sandwiches, pastries and drinks will be offered by the SCS in the vicinity of the poster session. A cafeteria and a restaurant are located next to the meeting venues.

Coffee breaks: Coffee and drinks will be available until 11.30 in the morning and a coffee break will be organized between 17.00 and 17.15, before the SCS – DSM and SCS – Metrohm Awards presentation.

Transportation

By train: Only limited parking space will be available on the campus of the Ecole Polytechnique Fédérale de Lausanne. Hence, traveling by train is recommended. EPFL campus can be easily reached by metro (tramway), either from Lausanne or Renens train stations. Travelers arriving at Lausanne can continue their journey with the metro (m2 line from the train station to Flon, m1 line from Flon to UNIL-Sorge). From Renens station, the trip by metro (m1 line) to UNIL-Sorge stop is 7 min. More information on how to get to EPFL campus, timetables and interactive maps are available on the webpage at http://map.epfl.ch/.

By car: On the motorway, follow Lausanne-Sud, exit at UNIL-EPFL, drive West for 1.7 km and then turn right at the sign EPFL. Limited space will be available at the parking of the building Odyssea (see EPFL campus map here below). One-day parking permits will be sold on the parking lot and at the registration desk for CHF 5.–.

Train Timetable

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<th>Morning</th>
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<td>Basel</td>
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The meeting will be held on the first floor of BS and CE buildings. Participants are kindly requested to use exclusively the East entrance on the first floor of BS building. The nearest tramway station is UNIL-Sorge (upper-right corner on the map). The way from the tramway station and from the parking lot to the entrance of the conference premises will be marked out with yellow signs.

Detailed Map of Lecture Halls

CE 6: Opening Ceremony, Awards presentations, Plenary lectures, and Inorganic and Coordination Chemistry
CE 1 and CE 3: Organic Chemistry
CE 4: Physical Chemistry
CE 2: Analytical Chemistry
CE 5: Medicinal Chemistry
CE 106: Computational Chemistry
BS 160: Polymer Sciences

Main Hall, SPO, CE 100, CE 101, CE 102, CE 103, CE 104, CE 105, BS 170: Posters
Sponsors

The organization of the meeting gratefully acknowledges the generous support of the following companies and institutions.

Commercial Exhibition

A number of exhibitors will be presenting products and services of direct interest to the scientists attending the Fall Meeting. The following companies have already confirmed their participation. See the meeting website (www.scg.ch/fallmeeting) for an updated list of commercial booths.
<table>
<thead>
<tr>
<th>Time</th>
<th>Session</th>
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<td>09.45–11.00</td>
<td>PLENARY SESSION</td>
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<td>09.45–11.00</td>
<td>Opening Ceremony</td>
<td>EPFL, CE 6</td>
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<td>11.00–17.00</td>
<td>PARALLEL SESSIONS</td>
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<td>11.00–17.00</td>
<td>Division of Analytical Chemistry</td>
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<td>11.00–11.30</td>
<td>General Assembly of the Members</td>
<td>EPFL, CE 2</td>
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<td>11.30–12.15</td>
<td>Invited lecture</td>
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<td>12.15–13.00</td>
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<td>Abstracts AC1–AC3</td>
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<td>13.00–14.30</td>
<td>Poster Session</td>
<td>EPFL, CE 100</td>
<td>Abstracts AC10–AC56</td>
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<td>14.30–15.00</td>
<td>General Assembly of the Members of the Swiss Chemical Society</td>
<td>EPFL, CE 6</td>
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<td>15.00–15.30</td>
<td>Brechbühler lectures</td>
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<td>15.30–17.00</td>
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<td>Abstracts AC4–AC9</td>
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<td>11.00–17.00</td>
<td>Division of Medicinal Chemistry</td>
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<td>11.00–11.15</td>
<td>General Assembly of the Members</td>
<td>EPFL, CE 5</td>
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11.15–11.45 | Actelion lecture                           | EPFL, CE 5  |
11.45–13.00 | Lectures                                   | EPFL, CE 5  |
|           |                                            |             | Abstracts MC1–MC5                                                      |
| 13.00–14.30 | Poster Session                             | EPFL, CE 103| Abstracts MC14–MC65                                                   |
| 14.30–15.00 | General Assembly of the Members of the Swiss Chemical Society | EPFL, CE 6 |                                                                        |
| 15.00–17.00 | Lectures                                   | EPFL, CE 5  |
|           |                                            |             | Abstracts MC6–MC13                                                    |

11.00–17.00 | Division of Chemical Research              |             |                                                                        |

11.30–17.00 | Computational Chemistry                    |             |                                                                        |
| 11.30–13.00 | Lectures                                   | EPFL, CE 106| Abstracts CC1–CC6                                                     |
| 13.00–14.30 | Poster Session                             | EPFL, CE 105| Abstracts CC14–CC48                                                  |
| 14.30–15.00 | General Assembly of the Members of the Swiss Chemical Society | EPFL, CE 6 |                                                                        |
| 15.00–15.30 | Invited lecture                            | EPFL, CE 106| Abstract CC7                                                          |
| 15.30–17.00 | Lectures                                   | EPFL, CE 106| Abstract CC8–CC13                                                    |

11.30–17.00 | Inorganic and Coordination Chemistry       |             |                                                                        |
| 11.30–13.00 | Minisymposium                              | EPFL, CE 6  |
|           |                                            |             | Abstracts IC1–IC3                                                     |
| 13.00–14.30 | Poster Session                             | EPFL, CE SPO| Abstracts IC14–IC89                                                  |
| 14.30–15.00 | General Assembly of the Members of the Swiss Chemical Society | EPFL, CE 6 |                                                                        |
| 15.00–17.00 | Lectures                                   | EPFL, CE 6  |
|           |                                            |             | Abstracts IC4–IC13                                                    |
11.30–17.30  Organic Chemistry
Session A1  11.30–11.45  Synthesis and Catalysis
Lecture of the Max-Lüthi Award Laureate 2011
EPFL, CE 1
Abstract OC1

11.45–13.15  Lectures
EPFL, CE 1
Abstracts OC2–OC6, OC 35

Session B1  11.30–13.00  Techniques, Properties and Mechanisms
Lectures
EPFL, CE 3
Abstracts OC15–OC20

Sessions A & B  13.00–14.30  Poster Session
EPFL, CE SPO
Abstracts OC29–OC123

14.30–15.00  General Assembly of the Members of the Swiss Chemical Society
EPFL, CE 6

Session A2  15.00–15.15  Synthesis and Catalysis
Firmenich lecture
EPFL, CE 1
Abstract OC7

15.15–17.00  Lectures
EPFL, CE 1
Abstracts OC8–OC14

17.00–17.15  Coffee Break

11.30–17.00  Physical Chemistry
11.30–12.45  Lectures
EPFL, CE 4
Abstracts PC1–PC5

12.45–13.00  Poster talks
EPFL, CE 4
Abstracts PC14–PC18

13.00–14.30  Poster Session
EPFL, CE 101
Abstracts PC19–PC80

14.30–15.00  General Assembly of the Members of the Swiss Chemical Society
EPFL, CE 6

15.00–17.00  Lectures
EPFL, CE 4
Abstracts PC6–PC13

11.00–17.00  Division of Polymers and Colloids
11.00–11.15  General Assembly of the Members of the Division
EPFL, BS 160

11.15–11.45  Invited lecture
EPFL, BS 160
Abstract PO1

11.45–12.00  Dow lecture
EPFL, BS 160

12.00–13.15  Lectures
EPFL, BS 160
Abstracts PO2–PO6

13.15–14.30  Poster Session
EPFL, BS 170
Abstracts PO14–PO52

14.30–15.00  General Assembly of the Members of the Swiss Chemical Society
EPFL, CE 6

15.00–15.30  Invited lecture
EPFL, BS 160
Abstract PO7

PLENARY SESSION

17.15–17.45  Presentation of the Awards for the Best Poster and Oral Presentations, Sponsored by DSM and the Metrohm Foundation
EPFL, CE 6

Analytical Chemistry
3 posters and 2 oral presentations
Jury: S. Schürch, C. Staub

Medicinal Chemistry
3 posters and 2 oral presentations

Computational Chemistry
2 posters and 2 oral presentations
Jury: C. Corminboeuf, M. Meuwly

Inorganic and Coordination Chemistry
4 posters and 2 oral presentations

Organic Chemistry
6 posters and 4 oral presentations

Physical Chemistry
3 posters and 2 oral presentations
Jury: T. Bally, R. Beck

Polymers and Colloids
3 posters and 2 oral presentations
DETAILED PROGRAM

Analytical Chemistry
Sponsored by Brechbühler

11.00–11.30 General Assembly of the Members
EPFL, CE 2
Chair: Gérard Hopfgartner

11.30–12.15 Invited lecture
EPFL, CE 2
Chair: Stefan Schürch
Maria Perla Colombini
University of Pisa, Pisa, Italy
‘Analytical Chemistry in Art’

12.15–13.00 Lectures
EPFL, CE 2
Abstracts AC1–AC3
Chair: Stefan Schürch

12.15–12.30 Hao Wang, D. Gromilund, D. Günther, L. Van Loon, C. N. Borca
Swiss Light Source, PSI, CH-5232 Villigen
ETH Zurich, CH-8093 Zurich
Laboratory of Waste Management, PSI, CH-5232 Villigen
‘Quantitative Microscopic Studies with High Spatial Resolution of Contaminant Diffusion into Opalinus Clay Rock’
Abstract AC1

12.30–12.45 Alfredo J. Ibáñez, S. Fagerer, R. Zenobi
ETH Zurich, CH-8093 Zurich
Abstract AC2

12.45–13.00 Michel Wagner, E. Varesio, G. Hopfgartner
School of Pharmaceutical Sciences, University of Geneva, University of Lausanne, CH-1211 Genève 4
‘A novel non-card based format for dried blood spots analysis for µsLLE liquid chromatography mass spectrometric analysis’
Abstract AC3

13.00–14.30 Poster Session
EPFL, CE 100
Abstracts AC10–AC56

14.30–15.00 General Assembly of the Members of the Swiss Chemical Society
EPFL, CE 6

15.00–15.30 Brechbühler lectures
EPFL, CE 2
Chair: Christian Staub

15.00–15.15 Philippe Mottay, U. Hofstetter, P. Pichler, R. Estebananz
Brechbühler AG, CH-8952 Schlieren
‘Latest development in LC-GC instrumentation’

15.15–15.30 Lizzy van den Heuvel, S. Fagerer, R. Zenobi
ETH Zurich, CH-8093 Zurich
‘Rapid Large Volume Penetration of Crude Contaminant into Opalinus Clay Rock’
Abstract AC4

15.30–17.00 Lectures
EPFL, CE 2
Chair: Christian Staub

15.30–15.45 Tatiana Egorova, R. Dietiker, B. Hattendorf, D. Günther
ETH Zurich, CH-8093 Zurich
‘Ion Funnel as a New Interface for ICPMS’
Abstract AC4

15.45–16.00 Silvan R. Stucki, A. Nyakas, S. Schürch
University of Bern, CH-3012 Bern
‘Tandem Mass Spectrometry of Platinated DNA Quadruplexes’
Abstract AC5

16.00–16.15 Zhongshu Li, X. Zhang
ETH Zurich, CH-8093 Zurich
‘A Straightforward Approach to Study the Intrinsic Properties of Host-Guest Cyclodextrin Complexes in the Gas Phase’
Abstract AC6

16.15–16.30 Sebastian Cap, L. L. Simon, K. Hungerbühler
ETH Zurich, CH-8093 Zurich
‘Calibration Free Reactive Dissolution Kinetic Modeling with in situ FBRM, ATR-IR, and Calorimetry’
Abstract AC7

ETH Zurich, CH-8093 Zurich
‘Nanoscale Chemical Imaging of Segregated Lipid Domains using Tip-Enhanced Raman Spectroscopy’
Abstract AC8

16.45–17.00 David Tonoli, E. Varesio, G. Hopfgartner
School of Pharmaceutical Sciences, University of Geneva, University of Lausanne, CH-1211 Genève 4
‘Acetaminophen toxicity: QUAL/QUAN liquid chromatography high resolution mass spectrometric approaches for drug metabolism and metabolomic investigations’
Abstract AC9

17.00–17.15 Coffee Break

17.15–17.45 Presentation of the Awards for the Best Poster and Oral Presentations, sponsored by DSM and the Metrohm Foundation

Medicinal Chemistry
Sponsored by Actelion

11.00–11.15 General Assembly of the Members
EPFL, CE 5
Chair: Karl-Heinz Altmann
11.15–11.45 Actelion lecture
EPFL, CE 5
Chair: Hans Peter Märki

Bibiana Heidmann-Benacer, Ralf Brunner
Actelion Pharmaceuticals Ltd, CH-4123 Allschwil
‘Characterization of a novel antimalarial chemotype’

11.45–13.00 Lectures
EPFL, CE 5
Abstracts MC1–MC5
Chair: Hans Peter Märki

11.45–12.00
G. M. Benson,*, K. H. Bleicher,*, D. Blum,*,
E. Chaput,*, N. Clemann,*, S. Feng,*, C. Gardes,*,
U. Grether,*, P. Hartmann,*, B. Kühn,*, R. E. Mariani,*, J.-M. Plancher,*, Hans G. F. Richter,*,
M. G. Rudolphi,*, F. Schuler,*, S. Taylor*
*F. Hoffmann-La Roche Ltd, CH-4070 Basel
Roche R&D Center (China) Ltd, Shanghai 201203, China
‘Identification of a novel class of potent and selective small molecule FXR agonists based on the benzimidazolyl-acetamide scaffold’
Abstract MC1

12.00–12.15 Raphael Schiess, E. Perrino, D. Neri, K.-H. Altmann
ETH Zurich, CH-8093 Zurich
‘A New Synthetic Approach to Side Chain-Modified Analogues of Cyclopropyl-Epothilone B’
Abstract MC2

12.15–12.30 Gebhard Thoma
Novartis Institutes for BioMedical Research, CH-4002 Basel
‘A potent Jak3 inhibitor with high selectivity within the Janus kinase family – On the roles of Jak1 and Jak3 in signal transduction’
Abstract MC3

*School of Pharmaceutical Sciences, University of Geneva, University of Lausanne,
CH-1211 Genève 4
*University of Bern, CH-3012 Bern
‘Adenosine kinase overexpression leads to a trypanostatic effect in Trypanosoma brucei’
Abstract MC4

*ETH Zurich, CH-8093 Zurich
*University of Freiburg, 79104 Freiburg, Germany
‘Actelion Pharmaceuticals Ltd, CH-4123 Allschwil
‘Structure-Based Design and Synthesis of Non-peptidic Novel Inhibitors for the Malarial Target Plasmepsins’
Abstract MC5

13.00–14.30 Poster Session
EPFL, CE 103
Abstracts MC14–MC65

14.30–15.00 General Assembly of the Members of the Swiss Chemical Society
EPFL, CE 6

15.00–17.00 Lectures
EPFL, CE 5
Abstracts MC6–MC13
Chair: Yves Auberson

15.00–15.15 Harald Mauser
F. Hoffmann-La Roche Ltd., CH-4070 Basel
‘Design of Small Molecule Protein-Protein Inhibitors’
Abstract MC6

15.15–15.30 Trixi Brandl
Novartis Institutes for BioMedical Research, CH-4002 Basel
‘Trypsin inhibitors for the treatment of pancreatitis: A long way from the prime site into the S3/4 pocket’
Abstract MC7

15.30–15.45 Cindy Fellay, C. Chidley, K. Johnsson
EPF Lausanne, CH-1015 Lausanne
‘Discovering Protein Targets of Drugs Using Yeast-Based Screen’
Abstract MC8

15.45–16.00 Olivier Schwardt, S. Rabbani, M. Wittwer, A. Zalewski, B. Cutting, B. Ernst
University of Basel, CH-4056 Basel
‘Design, Synthesis and Biological Evaluation of Mannosyl Triazoles as FimH Antagonists’
Abstract MC9

16.00–16.15 Daniela Abgottspon, O. Schwardt, S. Kleeb, M. Scharenberg, S. Rabbani, B. Ernst
University of Basel, CH-4056 Basel
‘In Vitro and In Vivo evaluation of Squaric Acid Derivatives as FimH Antagonists’
Abstract MC10

16.15–16.30 Selena Milicevic Septon, P. Dennler, S. D. Krämer, R. Schibli, S. M. Ametamey
ETH Zurich, CH-8093 Zurich
‘In A Search of Fluorinated PET Tracers for Imaging of mGluR5’
Abstract MC11

Novartis Research Foundation, San Diego, CA-92121, USA
Novartis Institutes for BioMedical Research, CH-4002 Basel
‘The Scripps Research Institute, La Jolla, CA-92037, USA
‘Modulators of Human Stem Cell Fate in the Context of Regenerative Medicine’
Abstract MC12

13.00–14.30 Poster Session EPFL, CE 105 Abstracts CC14–CC48

14.30–15.00 General Assembly of the Members of the Swiss Chemical Society EPFL, CE 6

15.00–15.30 Invited lecture EPFL, CE 106 Chair: Markus Meuwly Hans Jörg Limbach Nestlé Research Center, Vers-chez-les-Blanc, CH-1000 Lausanne ‘How to thermostat coupled heat and mass transport in MD simulations and other challenges from the world of foods’ Abstract CC7

15.30–17.00 Lectures EPFL, CE 106 Abstracts CC8–CC13 Chair: Markus Meuwly

11.00–11.30 General Assembly of the Members EPFL, CE 6

Chemical Research

11.30–11.45 Tomáš Zimmermann, J. Vaniček EPFL Lausanne, CH-1015 Lausanne ‘Evaluation of the non(a)diabaticity of the quantum molecular dynamics using the dephasing representation of quantum fidelity’ Abstract CC1

11.45–12.00 Pierre-André Cazade, M. Meuwly University of Basel, CH-4056 Basel ‘Oxygen Dynamics and Energetics of Migration Pathways in Truncated Hemoglobin’ Abstract CC2

12.00–12.15 Basile F. E. Curchod, I. Tavernelli, U. Röthlisberger EPFL Lausanne, CH-1015 Lausanne ‘Trajectory-based solution of the nonadiabatic quantum dynamics equations: an on-the-fly approach for molecular dynamics simulations’ Abstract CC3

12.15–12.30 Martin Smiesko University of Basel, CH-4056 Basel ‘Alignator – a computer program for induced-fit docking: Validation on the nuclear receptors’ Abstract CC4

12.30–12.45 Andreas Glöss, M. P. Brandle, H.-P. Lüthi ETH Zurich, CH-8093 Zurich ‘A quantum chemical data base approach for method development and data processing’ Abstract CC5

12.45–13.00 Allessandra Nurissio, P.-A. Carrupt, A. Daina School of Pharmaceutical Sciences, University of Geneva, University of Lausanne, CH-1211 Genève 4 ‘Molecular docking using the Molecular Lipophilicity Potential as hydrophobic descriptor: impact on the GOLD docking performance’ Abstract CC6


15.45–16.00 Laura Zoppi, A. Ferretti, L. Martin-Samos, K. K. Baldridge Universidad de Zaragoza, 50009 Zaragoza, Spain ²Istituto Nanoscience, 41100 Modena, Italy ³CNR-IOM DEMOCRITOS and SISSA, 34136 Trieste, Italy ‘Electron transport across a corannulene-SWCNT junction’ Abstract CC9

16.00–16.15 Steven M. A. Donald, M. Reiher ETH Zurich, CH-8093 Zurich ‘Computational methods for finding the ideal nitrogen fixation catalyst’ Abstract CC10

16.15–16.30 Tanya K. Todorova, L. Roch, C. Corminboeuf EPFL Lausanne, CH-1015 Lausanne ‘Oxygen and Proton Reduction by Metallocenes in Non-Aqueous Media’ Abstract CC11

16.30–16.45 Piotr de Silva, J. Korchowiec University of Geneva, CH-1211 Geneva ³Jagiellonian University, 30-060 Cracow, Poland ‘Multiregional Localized Molecular Orbitals’ Abstract CC12
16.45–17.00  **Marco Stenta, C. Bovigny, M. Dal Peraro**  
EPF Lausanne, CH-1015 Lausanne  
‘LpxC: insights into substrate binding and selectivity’  
Abstract CC13

17.00–17.15  **Coffee Break**

17.15–17.45  **Presentation of the Awards for the Best Poster and Oral Presentations, sponsored by DSM and the Metrohm Foundation**

Inorganic and Coordination Chemistry  
Sponsored by KGF (Kontaktgruppe für Forschungsfragen)

11.30–13.00  **Minisymposium**  
**EPFL, CE 6**  
Abstract IC1–IC3  
Chair: **Thomas R. Ward**

11.30–12.00  **Richard A. Andersen**  
University of California, Berkeley, CA-94720, USA  
‘Reactions of Cp₂CeH: Breaking C–H and C–O Bonds and Making C–C Bonds’  
Abstract IC1

12.00–12.30  **Olivier Maury**  
ENS Lyon, UMR CNRS 5182, 69007 Lyon, France  
‘Two-photon sensitized lanthanides luminescence: Bio-imaging applications from the green to the infra-red’  
Abstract IC2

12.30–13.00  **Christophe Copéret**  
ETH Zurich, CH-8093 Zurich  
‘What is alumina? A molecular point of view’  
Abstract IC3

13.00–14.30  **Poster Session**  
**EPFL, CE SPO**  
Abstracts IC14–IC89

14.30–15.00  **General Assembly of the Members of the Swiss Chemical Society**  
**EPFL, CE 6**

15.00–17.00  **Lectures**  
**EPFL, CE 6**  
Abstracts IC4–IC13  
Chair: **Kay Severin, Thomas R. Ward**

15.00–15.12  **A. Togni, Esteban Mejía**  
ETH Zurich, CH-8093 Zurich  
‘Rhenium-Catalyzed Trifluoromethylation of Arenes and Heteroarenes by Hypervalent Iodine Reagents’  
Abstract IC4

15.12–15.24  **Dominique F. Schreiber, A. D. Phillips**  
University College Dublin, Ireland  
‘β-Diketiminato Ruthenium(II)-arene Complexes in Homogeneous Lewis-acid Catalysis of the Diels-Alder Reaction’  
Abstract IC5

15.24–15.36  **Miguel Guttentag, A. Rodenberg, P. Hamm, R. Alberto**  
University of Zurich, CH-8057 Zurich  
‘Homogenous Photocatalytic Hydrogen Evolution from Water under Acidic Conditions’  
Abstract IC6

15.36–15.48  **Georg Geisberger, G. R. Patzke**  
University of Zurich, CH-8057 Zurich  
‘Development of Biopolymeric Drug Carriers for Targeted Delivery of Polyoxometalates’  
Abstract IC7

15.48–16.00  **Erin Sheepwash, K. Severin**  
EPF Lausanne, CH-1015 Lausanne  
‘Dative B–N bonds in Supramolecular Chemistry’  
Abstract IC8

16.00–16.12  **Mona A. Furrer, B. Therrien**  
University of Neuchâtel, CH-2000 Neuchâtel  
‘New functionalized π–arene ruthenium complexes for biological applications’  
Abstract IC9

University of Basel, CH-4056 Basel  
‘Mechanistic Investigations on a Highly Selective Artificial Transfer Hydrogenase for the Reduction of Cyclic Imines’  
Abstract IC10

16.24–16.36  **Fabio Zobi, O. Blacque, R. A. Jacobs, M. C. Schaub, A. Y. Bogdanova**  
University of Zurich, CH-8057 Zurich  
‘17 e– Rhenium CO-Releasing Molecules on a Cobalamin Scaffold’  
Abstract IC11

16.36–16.48  **Kai Zhou, H. Brandl, W. Buckel, F. Zelder**  
University of Zurich, CH-8057 Zurich  
‘Coordination chemistry and biological activity of vitamin B12 derivatives with a peptide backbone’  
Abstract IC12

The University of Edinburgh, Edinburgh, EH9 3JJ, UK  
‘A Molecular Pentafoil Knot’  
Abstract IC13

17.00–17.15  **Coffee Break**

17.15–17.45  **Presentation of the Awards for the Best Poster and Oral Presentations, sponsored by DSM and the Metrohm Foundation**

Organic Chemistry  
Sponsored by Firmenich

Session A1  
**Synthesis and Catalysis**

11.30–11.45  **Lecture of the Max-Lüthi Award Laureate 2011**
11.45–12.00  Thomas Nauser\textsuperscript{a}, C. Schöneich\textsuperscript{b},
W. H. Koppenol\textsuperscript{b}
\textsuperscript{a}ETH Zurich, CH-8093 Zurich
\textsuperscript{b}The University of Kansas, Lawrence, USA
‘Intramolecular H-Shift Reactions in Cysteiny1 Radicals’
Abstract OC16

12.00–12.15  Christof Spar\textsuperscript{a}, R. Gilmour
ETH Zurich, CH-8093 Zurich
‘Fluoro-Organocatalysts: Conformer Equivalents as a Tool for Mechanistic Studies’
Abstract OC17

12.15–12.30  F. Moradi-Afropoli\textsuperscript{a}, Samad Nejad Ebrahim\textsuperscript{a},
S. Zimmermann\textsuperscript{b}, M. Quitschau\textsuperscript{c}, M. Smiesko\textsuperscript{b},
M. Hamburger\textsuperscript{b}
\textsuperscript{a}Tehran University of Medical Sciences, Tehran, Iran
\textsuperscript{b}University of Basel, CH-4056 Basel
‘Antiplasmodial Bisabolene Oxide Derivatives from Artemisia persica – Absolute Configuration by Density Functional Theory Calculation of ECD Spectra’
Abstract OC18

12.30–12.45  Roman S. Erdmann, H. Wennemers
University of Basel, CH-4056 Basel
‘Functionalized Collagen Model Peptides’
Abstract OC19

12.45–13.00  Jens P. Hermes, F. Sander, M. Mayor
University of Basel, CH-4056 Basel
‘Formation, functionalization and assembly of dendrimer stabilized gold nanoparticles’
Abstract OC20

Session A2
15.00–15.15  Firmenich lecture
EPFL, CE 1
Chair: Jérôme Waser
J. Kuhne, Olivier Knopff
Firmenich SA, CH-1211 Geneva 8
‘New Approches to the Synthesis of the Musk Odorants (R)-Muscone and (R,Z)-5-Muscenone’
Abstract OC7

15.15–17.00  Lectures
EPFL, CE 1
Abstracts OC8–OC14
Chair: Jérôme Waser

15.15–15.30  Elangovan Elamparuthi\textsuperscript{a}, C. Fellay\textsuperscript{b},
M. Neuburger\textsuperscript{c}, K. Gademann\textsuperscript{a}
\textsuperscript{a}University of Basel, CH-4056 Basel
\textsuperscript{b}EPF Lausanne, CH-1015 Lausanne
\textsuperscript{c}University of Basel, CH-4056 Basel
‘Towards the Total Synthesis of Cyrneine A,”
Abstracts OC29–OC123
15.30–15.45 Adnan Ganić, A. Pfaltz
University of Basel, CH-4056 Basel
‘Iridium Catalyzed Hydrogenation of Alkyl Boronic Esters’
Abstract OC8

15.45–16.00 Simon N. Kessler, H. A. Wegner
University of Basel, CH-4056 Basel
‘Bidentate Lewis Acids as Efficient Catalysts for the Inverse Electron Demanding Diels-Alder Reaction’
Abstract OC10

16.00–16.15 Pierre Mateo, P. Renaud
University of Bern, CH-3012 Bern
‘Addition of Mono-organocopper Reagents to Thioiminium Ions’
Abstract OC11

16.15–16.30 Aurélien Bigot, A. E. Williamson, M. J. Gaunt
University of Cambridge, Cambridge, CB2 1EW, UK
‘Copper Catalysed Enantioselective α-Arylation of Silyl Ketenimides’
Abstract OC12

16.30–16.45 Ludovic Gremaud, A. Alexakis
University of Geneva, CH-1211 Genève 4
‘Enantioselective Copper Catalyzed 1,4 addition to challenging Michael acceptors and synthesis of relevant target molecules’
Abstract OC13

16.45–17.00 Sirinporn Thamapipol, E. P. Kündig
University of Geneva, CH-1211 Genève 4
‘Synthesis of ent-Ledol by Application of Chiral Ru Lewis acid Catalyzed Asymmetric Intramolecular Diels-Alder Reactions’
Abstract OC14

Session B2 Techniques, Properties and Mechanisms
15.00–17.00 Lectures
EPFL, CE 3
Abstracts OC21–OC28
Chair: Jieping Zhu

15.00–15.15 Florian P. Seebeck
University of Basel, CH-4056 Basel
‘Oxidative sulfur transfers’
Abstract OC21

15.15–15.30 Tanguy Saget, N. Cramer
EPF Lausanne, CH-1015 Lausanne
‘Accessing Functionalized Allene Intermediates By C-C Fragmentation’
Abstract OC22

15.30–15.45 M. Pröller, Milan Kivala
University of Erlangen-Nürnberg, 91054 Erlangen, Germany
‘Functional π-Conjugated Materials Based on Bridged Triphenylamines’
Abstract OC23

15.45–16.00 Ankit Sharma, L. Guénée, J.-V. Naubron, J. Lacour
University of Geneva, CH-1211 Genève 4
‘One-step Catalytic Asymmetric Synthesis of Configurationally Stable Tröger Bases’
Abstract OC24

16.00–16.15 Jetsuda Areephong, M. Lista, N. Sakai, S. Maille
University of Geneva, CH-1211 Genève 4
‘Self-Organizing Surface-Initiated Polymerization (SOSIP): A New Approach to Organic Solar Cells’
Abstract OC25

16.15–16.30 Rahul S. Kathayat, N. S. Finney
University of Zurich, CH-8057 Zurich
‘Fluorescence-based Metal ion detection: Binding induced conformational restriction mechanism’
Abstract OC26

16.30–16.45 Derik F. Frantz, K. K. Baldridge, J. S. Siegel
University of Zurich, CH-8057 Zurich
‘Molecular Spur Gears’
Abstract OC27

16.45–17.00 X. Huang, Nuno Maulide
Max-Planck Institut für Kohlenforschung, 45470 Mülheim, Germany
‘Novel Transformations Mediated by Sulfur Reagents: From Ylide Transfer to Direct Arylation of Carbonyl Compounds’
Abstract OC28

17.00–17.15 Coffee Break

17.15–17.45 Presentation of the Awards for the Best Poster and Oral Presentations, sponsored by DSM and the Metrohm Foundation

Physical Chemistry
11.30–12.45 Lectures
EPFL, CE 4
Abstracts PC1–PC5
Chair: Jacques-Edouard Moser

11.30–11.45 Nicola Salvi a, S. Ulzega a, F. Ferrage b, G. Bodenhausen b
a EPF Lausanne, CH-1015 Lausanne
b ENS, CNRS UMR 7203, 75231 Paris Cedex 05, France
‘Correlated motions in biomolecules by HDR NMR spectroscopy’
Abstract PC1

11.45–12.00 Marina Fedoseeva, P. Fita, E. Vauthey
University of Geneva, CH-1211 Genève 4
‘Xanthene dyes as a dynamic probe for hydrogen-bonding properties at liquid interfaces: time-resolved second harmonic generation study’
Abstract PC2
12.00–12.15  
**Frederico A. Lima**, C. Milne*, M. Benfatto*, M. Chergui*  
*EPF Lausanne, CH-1015 Lausanne  
*LNFE, INFN CP13, 00044 Frascati, Italy  
‘Multiple-scattering analysis of the time-resolved XAS spectra of ligated Myoglobin in physiological media’  
Abstract PC3

12.15–12.30  
**Leo-Philipp Heiniger**, N. Tétreault, F. Sauvage, M. Grätzel  
EPF Lausanne, CH-1015 Lausanne  
‘Light management in dye-sensitized solar cells’  
Abstract PC4

12.30–12.45  
**Felix H. J. Hall**, S. Willitsch  
University of Basel, CH-4056 Basel  
‘Chemical reactions at ultralow temperatures: charge transfer and radiative processes in the Ca++Rb system’  
Abstract PC5

12.45–13.00  
**Poster talks**  
EPFL, CE 4  
Abstracts PC14–PC18

**Jakob Grilj**, Abstract PC14  
**Robert J. Nieckarz**, Abstract PC15  
**Fivos Perakis**, Abstract PC16  
**Giulia Di Domenicantonio**, Abstract PC17  
**Nuttapol Pootrakulchote**, Abstract PC18

13.00–14.30  
**Poster Session**  
EPFL, CE 101  
Abstracts PC19–PC80

14.30–15.00  
**General Assembly of the Members of the Swiss Chemical Society**  
EPFL, CE 6

15.00–17.00  
**Lectures**  
EPFL, CE 4  
Abstracts PC6–PC13  
Chair: Frédéric Merkt

15.00–15.15  
**Christian Seiler**, S. D. Hogan, F. Merkt  
ETH Zurich, CH-8093 Zurich  
‘Dynamical processes in Rydberg stark deceleration and trapping’  
Abstract PC6

15.15–15.30  
**Carine Manca Tanner**, V. Zelenková-Horká, S. Albert, M. Quack  
ETH Zurich, CH-8093 Zurich  
‘High-resolution spectroscopy and intramolecular vibrational energy redistribution (IVR) in methylidide isotopomers’  
Abstract PC7

15.30–15.45  
**Georgios Papadopoulos**, A. Svenden, O. V. Boyarkin, T. R. Rizzo  
EPF Lausanne, CH-1015 Lausanne  
‘Cold ion spectroscopy of FAIMS-selected conformations of biomolecules’  
Abstract PC8

15.45–16.00  
**Mateusz L. Donten**, J. Van de Vondele, P. Hamm  
University of Zurich, CH-8057 Zurich  
‘Laser induced pH jumps and pH equilibration’  
Abstract PC9

16.00–16.15  
**Jan C. Brauer**, J.-E. Moser  
EPF Lausanne, CH-1015 Lausanne  
‘Probing the Influence of Electrolyte on the Charge Carrier Generation Dynamics in DSSC using THz Time-Domain Spectroscopy’  
Abstract PC10

16.15–16.30  
**Phil Morten Hundt**, H. Ueta, R. D. Beck  
EPF Lausanne, CH-1015 Lausanne  
‘Quantum-state Resolved Studies of the Physiosorption and Chemiosorption of Water’  
Abstract PC11

16.30–16.45  
**Christiane Kartusch**, M. Makosch, J. Sá, K. Hungerbuehler, J. A. van Bokhoven  
ETH Zurich, CH-8093 Zurich  
‘Dynamic structure of supported gold in liquid phase hydrogenation’  
Abstract PC12

16.45–17.00  
**Heron Vrubel**, D. Merki, X. Hu  
EPF Lausanne, CH-1015 Lausanne  
‘Amorphous Molybdenum Sulfide as Catalyst for Electrochemical Hydrogen Production in Water’  
Abstract PC13

17.00–17.15  
Coffee Break

17.15–17.45  
Presentation of the Awards for the Best Poster and Oral Presentations, sponsored by DSM and the Metrohm Foundation

**Polymers and Colloids**  
Sponsored by Dow

11.00–11.15  
**General Assembly of the Members**  
EPFL, BS 160  
Chair: Bettina Steinmann

11.15–11.45  
**Invited lecture**  
EPFL, BS 160  
Chair: Harm-Anton Klok

Leiden University,2333CC Leiden, The Netherlands  
‘The coiled-coil connection; from self-assembly to membrane fusion’  
Abstract PO1

11.45–12.00  
**Dow lecture**  
EPFL, BS 160  
Chair: Harm-Anton Klok
Rudy Koopmans  
Dow Europe GmbH, CH-8810 Horgen  
‘Self-assembling polymers – Making a Difference’

12.00–13.15 Lectures  
EPFL, BS 160  
Abstracts PO2–PO6  
Chair: Harm-Anton Klok

12.00–12.15 Javier Reguera, M. Ye, I. Pons-Siepermann, S. C. Glotzer, F. Stellacci  
EPF Lausanne, CH-1015 Lausanne  
‘One-step synthesis of Janus Nanoparticles by self-assembly monolayers’  
Abstract PO2

12.15–12.30 Renata Negrini, R. Mezzenga  
ETH Zurich, CH-8093 Zurich  
‘pH-Responsive Lyotropic Liquid Crystals for Controlled Drug Delivery’  
Abstract PO3

EPF Lausanne, CH-1015 Lausanne  
‘Design of Water Soluble Initiators for the Modification of Alumina Surfaces by SI-ATRP’  
Abstract PO4

12.45–13.00 Prashant Sinha, M. Finessi, I. Szilagyi, P. Maroni, M. Borkovec  
University of Geneva, CH-1211 Geneva 4  
‘Transition from repulsive double layer forces to attractive van der Waals forces observed between model latex particles using colloidal probe technique’  
Abstract PO5

13.00–13.15 Margaret Holme, B. Müller, A. Zumbuehl, T. Saxer  
University of Geneva, CH-1211 Geneva 4  
‘Shear Stress Sensitive Nanocontainers for Targeted Drug Delivery’  
Abstract PO6

13.15–14.30 Poster Session  
EPFL, BS 170  
Abstracts PO14–PO52

14.30–15.00 General Assembly of the Members of the Swiss Chemical Society  
EPFL, CE 6

15.00–15.30 Invited lecture  
EPFL, BS 160  
Chair: Frank Scheffold

Hans M. Wyss  
Eindhoven University of Technology, Eindhoven, the Netherlands  
‘Relaxation and flow of soft colloids’  
Abstract PO7

15.30–17.00 Lectures  
EPFL, BS 160  
Abstracts PO8–PO13  
Chair: Frank Scheffold

15.30–15.45 Frédéric Cardinaux, T. G. Mason, F. Scheffold  
University of Fribourg, CH-1700 Fribourg  
University of California Los Angeles, CA 90095, USA  
‘Heterogeneous dynamics in dense monodisperse emulsions’  
Abstract PO8

15.45–16.00 Gergely Kali, K. Renggli, N. Bruns  
University of Basel, CH-4056 Basel  
‘Protein Based Catalysts for Atom Transfer Radical Polymerization’  
Abstract PO9

16.00–16.15 Tolga Goren, K. J. Rosenberg, R. Crockett, N. D. Spencer  
ETH Zurich, CH-8093 Zurich  
EMPA, CH-8600 Dübendorf  
‘Interrelationship between Structure, Hydration and Lubricity of the Biomimetic Graft Copolymer Poly(L-lysine)-graft-Dextran’  
Abstract PO10

16.15–16.30 Maren Schulze, A. F. M. Kilbinger  
University of Fribourg, CH-1700 Fribourg  
‘Tubular helices based on substituted oligo(p-benzamido)s’  
Abstract PO11

EPF Lausanne, CH-1015 Lausanne  
‘A Wet Chemical Approach towards Functional Carbon Nanostructures’  
Abstract PO12

16.45–17.00 G. Trubitsyn, C. Di Tommaso, R. Gurny, Michael Möller  
School of Pharmaceutical Sciences, University of Geneva, University of Lausanne, CH-1211 Genève 4  
‘Novel PEG-hexPLA micellar drug carriers with a covalently labeled Nile Red fluorescence marker’  
Abstract PO13

17.00–17.15 Coffee Break

17.15–17.45 Presentation of the Awards for the Best Poster and Oral Presentations, sponsored by DSM and the Metrohm Foundation