

SCHWEIZERISCHE CHEMISCHE GESELLSCHAFT

SOCIÉTÉ SUISSE DE CHIMIE

SWISS CHEMICAL SOCIETY

DIVISIONS
ANALYTICAL CHEMISTRY
CHEMICAL RESEARCH
MEDICINAL CHEMISTRY

DIVISIONEN
ANALYTISCHE CHEMIE
CHEMISCHE FORSCHUNG
MEDIZINISCHE CHEMIE

DIVISIONS
CHIMIE ANALYTIQUE
RECHERCHE CHIMIQUE
CHIMIE THÉRAPEUTIQUE

Fall Meeting 2004 Herbstversammlung 2004 Assemblée d'automne 2004

Thursday, October 7th, 2004
Donnerstag, 7. Oktober 2004
Jeudi, 7 Octobre 2004

Zürich

University of Zürich
Irchel Campus

Organizing Committee

Prof. Heinz Berke (Chairman) – University of Zürich
 Dr. Wolfgang Froestl – Novartis Pharma AG, Basel
 Prof. Paul Pregosin – ETH Zürich
 Prof. Jay Siegel – University of Zürich
 Prof. Walter Giger – EAWAG Dübendorf
 Frau Bea Spichtig – University of Zürich

Prof. Claude Daul – University of Fribourg
 Prof. Roger Alberto – University of Zürich
 Prof. Martin Quack – ETH Zürich
 Dr. Ferdinand Wild – University of Zürich
 Dr. Roland Wenger – Wenger Chemtech, Riehen

Secretary

Frau Bea Spichtig, Anorganisch-chemisches Institut der Universität Zürich
 Winterthurerstrasse 190, CH-8057 Zürich
 Tel: +41 44 635 46 80, Fax: +41 44 635 68 02, E-Mail: spichtig@aci.unizh.ch

Information

No registration for SCS members is required to participate in the meeting, coffee breaks and snacks, all of which are free of charge. Please do not forget to carry your membership card, which will be required at the entrance of to meeting.

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

Students who are members of the SCS can request reimbursement of their travel expenses on the basis of the return train ticket to Zürich (2nd class, 1/2 fare) by sending a filled-in reimbursement form to the SCS central office along with their train ticket. The form will available at the registration desk of the meeting. For members coming from abroad only the travel expenses within Switzerland will be reimbursed (2nd class, 1/2 fare).

Lunch: Drinks and coffee will be offered by the SCS in the vicinity of the poster session. A cafeteria and a restaurant are located in the vicinity of the conference rooms.

Coffee Breaks: Coffee and drinks will be available until 10.00 and a coffee break is organized from 16.30 to 17.00 before the award presentations.

Transportation

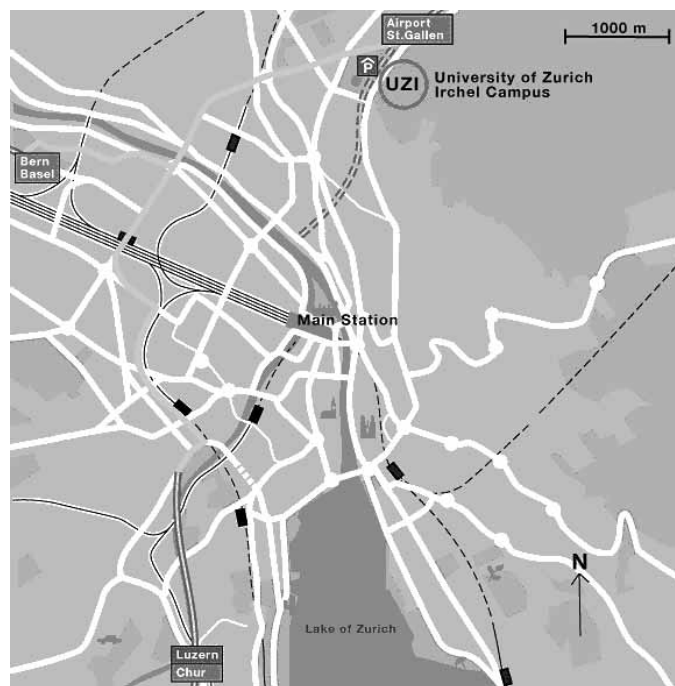
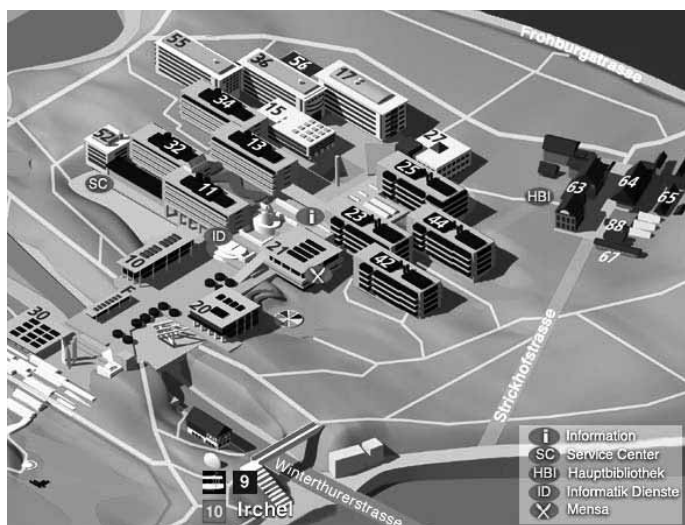
By train: Although the University of Zürich-Irchel does have parking facilities, travel by train is recommended. From Zürich main station, the University of Zürich-Irchel can be reached by tram no. 10 (tramstop Irchel, 15 min) or by trams 7 or 14 (tramstop Milchbuck, 10 min). From both stops a five-minute walk takes you to the campus.

More information regarding travel by train can be found under www.sbb.ch. For a schedule of the tram, see www.vbz.ch. For those traveling by car, a map which outlines the way to the Irchel Campus is available (PDF format) on our homepage www.scs-fallmeeting.unizh.ch.

Train Timetable

| Morning | | | Evening | | |
|------------|-----------|----------------|------------------|---------|-----------|
| Train from | Departure | Arrival Zürich | Departure Zürich | Arrival | Train to |
| Basel | 08.20 | 09.20 | 18.02 | 18.52 | Basel |
| Bern | 08.17 | 09.26 | 18.04 | 19.13 | Bern |
| Fribourg | 07.51 | 09.26 | 18.04 | 19.34 | Fribourg |
| Genève | 06.30 | 09.26 | 18.07 | 21.16 | Genève |
| Lausanne | 07.06 | 09.26 | 18.07 | 20.33 | Lausanne |
| Neuchâtel | 07.08 | 08.53 | 18.07 | 20.51 | Neuchâtel |

University of Zurich, Irchel Campus



Detailed Map of the Lecture Rooms

HS 30 General Assembly and Inorganic and Coordination Chemistry

HS 45 and HS 55 Organic Chemistry

HS 85 Medicinal Chemistry

HS 91 Computational Chemistry

HS 95 Analytical Chemistry

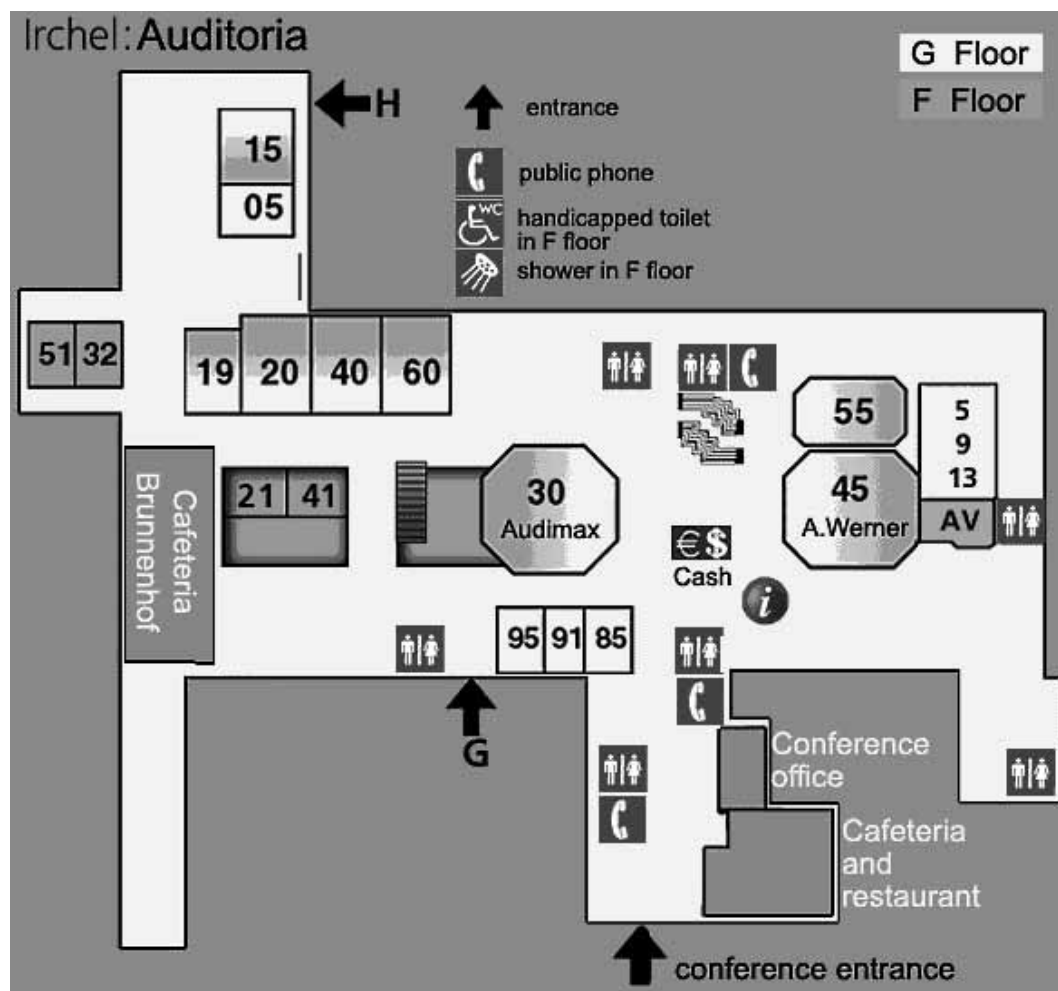
HS 60 Physical Chemistry

Main Hall (Lichthof) and area around **HS 30**: Poster Sessions

Main Hall (Lichthof):

Contact Chemists

Information Desk



Program of the Fall Meeting 2004

- 10.00–10.50 Opening Ceremony**
University of Zürich, Irchel, HS 30
- Presentation of the Werner Prize for 2004**
Chair: **Prof. André Merbach**
- Lecture of the Werner Prize Laureate 2004**
Prof. Paul J. Dyson
Ecole polytechnique fédérale de Lausanne,
Institut des sciences et ingénierie chimiques,
Lausanne
'Biphasic Chemistry Utilizing Ionic Liquids'
Abstract 2
- 11.00–16.30 Analytical Chemistry**
- 11.00–11.30 General Assembly of Members**
University of Zürich, Irchel, HS 95
- 11.30–12.40 Lectures**
University of Zürich, Irchel, HS 95
Abstracts 5–7
- 12.40–14.30 Poster Session**
Main Hall, University of Zürich, Irchel
Abstracts 14–59, 410
- 14.30–16.30 Lectures**
University of Zürich, Irchel, HS 95
Abstracts 8–13
- 11.00–16.45 Medicinal Chemistry**
- 11.00–11.15 General Assembly of Members**
University of Zürich, Irchel, HS 85
- 11.15–13.00 Lectures**
University of Zürich, Irchel, HS 85
Abstracts 60–66
- 13.00–14.00 Poster Session**
Main Hall, University of Zürich, Irchel
Abstracts 76–86
- 14.00–16.15 Lectures**
University of Zürich, Irchel, HS 85
Abstracts 67–75
- 11.00–16.30 Chemical Research**
- 11.00–11.15 General Assembly of Members**
University of Zürich, Irchel, HS 30
- 11.15–16.30 Computational Chemistry**
- 11.15–12.30 Lectures**
University of Zürich, Irchel, HS 91
Abstracts 87–91
- 12.30–14.30 Poster Session**
Main Hall, University of Zürich, Irchel
Abstracts 99–126
- 14.30–16.30 Lectures**
University of Zürich, Irchel, HS 91
Abstracts 92–98
- 11.15–16.30 Inorganic and Coordination Chemistry**
- 11.15–12.45 Minisymposium**
University of Zürich, Irchel, HS 30
Abstracts 3, 4
- 12.45–14.30 Poster Session**
Main Hall, University of Zürich, Irchel
Abstracts 137–232
- 14.30–16.30 Lectures**
University of Zürich, Irchel, HS 30
Abstracts 127–136
- 11.15–16.30 Organic Chemistry**
- Session One*
11.15–12.30 Lectures
University of Zürich, Irchel, HS 45
Abstracts 233–237
- Session Two*
11.15–12.30 Lectures
University of Zürich, Irchel, HS 55
Abstracts 245–249
- 12.30–13.03 Short Poster Presentations**
University of Zürich, Irchel, HS 45
Abstracts 257–267
- 13.05–14.30 Poster Session**
Main Hall, University of Zürich, Irchel
Abstracts 268–359
- Session One*
14.30–16.30 Lectures
University of Zürich, Irchel, HS 45
Abstracts 238–244
- Session Two*
14.30–16.30 Lectures
University of Zürich, Irchel, HS 55
Abstracts 250–256
- 11.15–16.30 Physical Chemistry**
- 11.15–12.30 Lectures**
University of Zürich, Irchel, HS 60
Abstracts 364–368
- 12.30–12.45 Short Poster Presentations**
University of Zürich, Irchel, HS 60
Abstracts 376–380

- 12.45–14.30 **Poster Session**
Main Hall, University of Zürich, Irchel
Abstracts 381–409
- 14.30–16.30 **Lectures**
University of Zürich, Irchel, HS 60
Abstracts 369–375
- 10.00–16.00 Swiss Young Chemists' Committee**
Information desk
University of Zürich, Irchel, Lichthof
- 16.30–17.00 Coffee Break**
- 17.00–17.15 Presentation of the**
Mettler Toledo Awards for the Best
Oral and Poster Presentations
University of Zürich, Irchel, HS 30
- Analytical Chemistry:**
2 poster and 1 oral presentations
Jury: *W. Giger, R. Zenobi*
- Medicinal Chemistry:**
1 poster and 2 oral presentations
Jury: *P. Floersheim, W. Froestl, H.P. Märki*
- Computational Chemistry:**
1 poster and 1 oral presentation
Jury: *C.A. Daul, J. Hutter*
- Inorganic and Coordination Chemistry:**
3 poster and 1 oral presentations
Jury: *P.S. Pregosin, R. Alberto, A. Togni*
- Organic Chemistry:**
2 poster and 2 oral presentations
Jury: *S. Bienz, J.S. Siegel, J.A. Robinson, A. Alexakis, D. Hilvert*
- Physical Chemistry:**
2 poster and 1 oral presentations
Jury: *M. Chergui, P. Hamm*
- 17.15–18.00 Presentation of the**
Paracelsus Prize 2004
University of Zürich, Irchel, HS 30
Presented by Prof. *G. Fráter*
- Lecture of the Paracelsus Laureate**
George M. Whitesides
Harvard University, Cambridge, MA 02138, USA
'Dynamic Self-Assembly, Complexity, and Emergence'

DETAILED PROGRAM**Analytical Chemistry**

- 11.00–11.30 General Assembly of Members**
University of Zürich, Irchel, HS 95
- 11.30–12.40 Lectures**
University of Zürich, Irchel, HS 95
Abstracts 5–7
Chairperson: *W. Giger*
- 11.30–12.10 Plenary Lecture**
W.S. Hancock
Barnett Institute of Chemical and Biological Analysis, Northeastern University, Boston, MA 02115, USA
'The Characterization of the Plasma/Serum Proteome'
Abstract 5
- 12.10–12.25 *M. Reth, A. Ciric, Z. Zencak, M. Oehme*
University of Basel, CH-4057 Basel
'Chlorinated Paraffins – Less Regarded Contaminants in Fishes From the Baltic Sea and the European Arctic'
Abstract 6
- 12.25–12.40 *P. Kovarik^a, C. Grivel^b, E. Bourgogne^b, G. Hopfgartner^b*
^aMDS-Sciex, Concord, ON Canada
^bUniversity of Geneva, CH-1211 Geneva
'Quantitative Analysis of Talinolol in Human Plasma Using MALDI on a Triple Quadrupole Mass Spectrometer'
Abstract 7
- 12.40–14.30 Poster Session**
Main Hall, University of Zürich, Irchel
Abstracts 14–59, 410
- 14.30–16.30 Lectures**
University of Zürich, Irchel, HS 95
Abstracts 8–13
Chairperson: *R. Zenobi*
- 14.30–14.45 *P. Babiak, J.-L. Reymond*
University of Bern, CH-3012 Bern
'High-Throughput Fluorescence Enzyme Assays on Solid Support'
Abstract 8
- 14.45–15.00 *J. Boccard^c, E. Grata^{ab}, A. Thiocone, M. Muller^c, S. Rudaz^b, J.-L. Wolfender^a*
^aLaboratoire de Pharmacognosie Phytochimie,
^bLaboratoire de Chimie Pharmaceutique, Université Genève, CH-1211 Genève, ^cSIB, CMU, CH-1211 Genève
'Statistic Comparisons of LC-MS Ion Maps in Metabolomic Studies'
Abstract 9

- 15.00–15.15 **M. Tanner, D. Günther**
ETH-Hönggerberg, CH-8093 Zürich
'Direct Laser Ablation Sample Introduction for Inductively Coupled Plasma Mass Spectrometry'
Abstract 10
- 15.20–15.35 **N. Lion, L. Dayon, C. Roussel, H.H. Girault**
EPFL, CH-1015 Lausanne
'Microfluidic Front-End Technologies for Electrospray Mass Spectrometry'
Abstract 11
- 15.35–15.50 **A. Nazabal^a, S. Hornemann^b, A. Aguzzi^c, R. Zenobi^a**
^aDepartment of Chemistry, ^bInstitute of Molecular Biology and Biophysics, ETH-Hönggerberg, CH-8093 Zurich
^cInstitute of Neuropathology, University Hospital of Zürich, CH-8091 Zürich
'Probing Prion Conformations by Hydrogen/Deuterium Exchange Analyzed by MALDI ToF MS and Ion Trap MS'
Abstract 12
- 15.50–16.30 Plenary Lecture**
A. Manz, M. Heule, C.X. Zhang, Y. Xu
Institute for Analytical Sciences,
D-44139 Dortmund, Germany
'Continuous-Flow Chips for Bioassays and Isoelectric Focusing'
Abstract 13
- 16.30–17.00 Coffee Break**
- 17.00–17.15 Presentation of the Mettler Toledo Awards for the Best Oral and Poster Presentations**
- 17.15–18.00 Presentation of the Paracelsus Prize**
- Medicinal Chemistry**
- 11.00–11.15 **General Assembly of Members**
University of Zürich, Irchel, HS 85
Report of the President and the Treasurer on the year 2003
- 11.15–13.00 **Lectures**
University of Zürich, Irchel, HS 85
Abstracts 60–66
Chairperson: *W. Froestl*
- 11.15–11.30 **E. Altmann, R. Lattmann, C. Betschart, S. Jacob, N. Teno, M. Missbach**
Novartis Institutes for BioMedical Research, CH-4002 Basel
'Novel 2-Cyano-Purine Derived Inhibitors of the Cysteine Protease Cathepsin K'
Abstract 60
- 11.30–11.45 **C. García-Echeverría, M.A. Pearson, A. Marti, T. Meyer, J. Mestan, J. Brueggen, H.-G. Capraro, R. Cozens, D.B. Evans, D. Fabbro, P. Furet, D. Graus Porta, J. Liebetanz, G. Martiny-Baron, F. Hofmann**
Novartis Institutes for Biomedical Research, CH-4002 Basel
'The Discovery of Insulin-Like Growth Factor I Receptor Kinase Inhibitors'
Abstract 61
- 11.45–12.00 **H. Dehmlow, J. Ackermann, J. Aebi, D. Blum, P. Coassolo, P. Hartman, M. Kansy, H.P. Märki, O. Morand, E. Von der Mark, N. Panday, A. Ruf, R. Thoma, T. Schulz-Gasch**
F. Hoffmann-La Roche Ltd, CH-4070 Basel
'Oxidosqualene Cyclase (OSC) Inhibitors'
Abstract 62
- 12.00–12.15 **G. Jaeschke, A. Alanine, A. Bourson Sleight, B. Büttelmann, H. Fischer, R. Gill, M.-P. Heitz Neidhart, J. Huwylar, J.A. Kemp, M. Kansy, V. Mutel, E. Pinard, G. Trube, R. Wyler**
F. Hoffmann-La Roche Ltd, CH-4070 Basel
'Synthesis and Biological Evaluation of **b**-Aminosulfones as Novel NMDA-NR1/2B Subtype Selective Antagonists'
Abstract 63
- 12.15–12.30 **L. Awad, J. Riedner, P. Vogel**
EPFL, CH-1015 Lausanne
'Synthesis of a C-Linked Disaccharide Analog of the Thomsen Friedenreich (T)-Epitope **a**-O-Conjugated to L-Serine and Formation a Cluster as Potential Anticancer Vaccine'
Abstract 64
- 12.30–12.45 **J. Becaud, T.J. Ryan, C. Leumann**
University of Bern, CH-3012 Bern
'Oligonucleotide Based Artificial Nucleases'
Abstract 65
- 12.45–13.00 **O. Schwardt^a, G.-P. Gao^a, S. Shelke^a, J. von Orelli^a, H. Gähje^a, S. Kelm^a, B. Ernst^a**
^aUniversity of Basel, CH-4056 Basel
^bUniversity of Bremen, D-28334 Bremen, Germany
'The Biological Role of Neuraminic Acid in Gangliosides Binding to MAG'
Abstract 66
- 13.00–14.00 Poster Session**
Main Hall, University of Zürich, Irchel
Abstracts 76–86
- 14.00–16.15 Lectures**
University of Zürich, Irchel, HS 85
Abstracts 67–75
Chairperson: *H.P. Märki*
- 14.00–14.15 **D. Ricklin, B. Ernst**
University of Basel, CH-4056 Basel
'Improving Biosensor Activity and Data Quality by Site-Directed Immobilization Strategies'
Abstract 67

- 14.15–14.30 **S. Rabbani, F. Corona, B. Ernst**
University of Basel, CH-4056 Basel
'*Helicobacter Pylori* $\alpha(1,4)$ -Fucosyltransferase:
A Novel Transferase for the Chemoenzymatic
Synthesis of Oligosaccharide Mimetics'
Abstract 68
- 14.30–14.45 **R. Born, H.-J. Gober, G. de Libero,**
M. Pyrzybylski, B. Ernst
University of Basel, CH-4056 Basel
'Asialoglycoprotein Receptor, a Therapeutic
Target: Monoclonal Antibodies and their
Characterization'
Abstract 69
- 14.45–15.00 **P. Furet, P. Imbach, M. Noorani, J. Koepler,**
K. Laumen, M. Lang, V. Guagnano, P. Fuerst,
J. Roessel, J. Zimmermann,
C. Garcia-Echeverria
Novartis Institutes for Biomedical Research,
CH-4002 Basel
'Structure-Based Design of a New Class of
Proteasome Inhibitors'
Abstract 70
- 15.00–15.15 **C. Beerli, M. Bigaud, V. Brinkmann, C. Bruns,**
P. Bühlmayer, D. Guerini, K. Hinterding,
K. Menninger, C. Pally, B. Nüsslein-Hildesheim,
M. Streiff, G. Weckbecker, K. Welzenbach,
F. Zecri, C. Spanka
Novartis Institutes for BioMedical Research,
CH-4002 Basel
NIBR713: A New FTY720 Derived
Immunomodulator
Abstract 71
- 15.15–15.30 **H. Thorsteinsdottir, V. Zoete, T. Schwede,**
M. Meuwly
University of Basel, CH-4056 Basel
'Evaluating the Applicability of Homology
Models to Structure-Based Drug Development'
Abstract 72
- 15.30–15.45 **G. Thoma**
Novartis Institutes for Biomedical Research,
CH-4056 Basel
'Orally Bioavailable Antagonists for Human
and Primate CCR5'
Abstract 73
- 15.45–16.00 **L. Alig, M. Andjelkovic, K. Bleicher,**
A. Bourson, P. David-Pierson, T. Lübbbers,
W. Neidhart, J.-M. Plancher, M. Rogers-Evans,
G. Schneider, S. Taylor, S. Röver
F. Hoffmann-La Roche Ltd, 4070 Basel
'CB1 Antagonists – From Knowledge Based
Design to Lead Optimisation'
Abstract 74
- 16.00–16.15 **R. Lysek, P. Vogel**
EPFL, CH-1015 Lausanne
'Total Asymmetric Synthesis of Conduramines
and Analogues and their Glycosidase
Inhibitory Activities'
Abstract 75
- 16.30–17.00 Coffee Break**

**17.00–17.15 Presentation of the
Mettler Toledo Awards for the
Best Oral and Poster Presentations**

17.15–18.00 Presentation of the Paracelsus Prize

Chemical Research

- 11.00–11.15 General Assembly of Members**
University of Zürich, Irchel, HS 30

Computational Chemistry

- 11.15–12.30 Lectures**
University of Zürich, Irchel, HS 91
Abstracts 87–91
Chairperson: *J. Hutter*
- 11.15–11.30 **B. Kirchner^a, A.P. Seitsonen^b, J. Hutter^b**
^aUniversity of Bonn, D-53115 Bonn, Germany
^bUniversity of Zurich, CH-8057 Zürich
'Green Chemistry: Properties of Ionic Liquid
AlCl₃ via Car-Parrinello Molecular Dynamics'
Abstract 87
- 11.30–11.45 **J.-N. Aebischer^a, M. Amrhein^b, E. Vanoli^a,**
G. Corminboeuf^a, O. Naef^a
^aUniversity of Applied Sciences of West
Switzerland (HES-SO), CH-1700 Fribourg
^bOnline Control SARL, CH-1003 Lausanne
'Chemometric Optimization of Chemical
Reactions With Spectroscopic Measurements'
Abstract 88
- 11.45–12.00 **W. Sudholt, K.K. Baldrige**
University of Zurich, CH-8057 Zurich
'Continuum Electrostatics Calculations on
Protein-Ligand Complexes: Application to
Catalytic Antibodies and Approach to
Automation'
Abstract 89
- 12.00–12.15 **I. Tavernelli, E. Tapavicza, U. Röthlisberger**
EPFL, CH-1015 Lausanne
'Excited State Molecular Dynamics Using
Time-Dependent DFT Including Non-Adiabatic
Effects'
Abstract 90
- 12.15–12.30 **A. Vargas, T. Bürgi, A. Baiker**
ETH-Hönggerberg, CH-8093 Zürich
'Enantioselective Hydrogenation of Ketones on
Cinchona Alkaloid Modified Platinum: Towards
Tailored Chiral Catalysts'
Abstract 91
- 12.30–14.30 Poster Session**
Main Hall, University of Zürich, Irchel
Abstracts: 99–126
- 14.30–16.30 Lectures**
University of Zürich, Irchel, HS 91
Abstracts 92–98
Chairperson: *C.A. Daul*

- 14.30–14.45 **O. Yazyev^a, L. Helm^a, I. Tavernelli^a, V.G. Malkin^b**
^aEPFL, CH-1015 Lausanne
^bSlovak Academy of Sciences, SK-84536 Bratislava, Slovak Republic
 ‘Predicting Hyperfine Coupling Constants With Density Functional Theory’
 Abstract 92
- 14.45–15.00 **A. Stirling^a, M. Iannuzzi^a, M. Parrinello^a, F. Molnar^b, V. Bernhart^b, G. A. Luinstra^b**
^aETHZ, USI-Campus, CH-6900 Lugano
^bBASF AG, Ludwigshafen, Germany
 ‘Modeling Homogeneous Catalysis: **b**-Lactone Synthesis From Epoxide and CO’
 Abstract 93
- 15.00–15.15 **V. Weber**
 University of Fribourg, CH-1700 Fribourg
 ‘The Linear Scaling Self-Consistent Perturbed Projection Method for High Order Response’
 Abstract 94
- 15.15–15.30 **C. Rauzy^a, M. Wille^b, T.F. Naegler^b, C.A. Daul^a**
^aUniversity of Fribourg, CH-1700 Fribourg
^bUniversity of Bern, CH-3012 Bern
 ‘DFT Study of Equilibrium Mo-Isotope Fractionations From Vibrational Spectroscopy’
 Abstract 95
- 15.45–16.00 **D.R. Nutt, M. Meuwly**
 University of Basel, CH-4056 Basel
 ‘Binding of NO to Fe(II) and Fe(III): A Comparative Study’
 Abstract 96
- 16.00–16.15 **C. Gossens, I. Tavernelli, U. Rothlisberger**
 EPFL, CH-1015 Lausanne
 ‘Rational Design of Organo-Ruthenium Anticancer Compounds’
 Abstract 97
- 16.15–16.30 **M. Sulpizi^a, A. Laio^b, U. Rothlisberger^a**
^aEPFL, CH-1015 Lausanne
^bETHZ, USI Campus, CH-6900 Lugano
 ‘Electron Transfer induced Dissociation of Chloro-Cyano-Benzene Radical Anion: Driving Chemical Reactions *via* Charge Restraints’
 Abstract 98
- 16.30–17.00 Coffee Break**
- 17.00–17.15 Presentation of the Mettler Toledo Awards for the Best Oral and Poster Presentations**
- 17.15–18.00 Presentation of the Paracelsus Prize**
- Inorganic and Coordination Chemistry**
- 11.15–12.45 **Minisymposium**
 University of Zürich, Irchel, HS 30
 Chairperson: P.S. Pregosin
- 11.15–12.00 **André E. Merbach**
 EPFL, CH-1015 Lausanne
 ‘Perspectives in Inorganic Structural Genomics’
 Abstract 3
- 12.00–12.45 **Stephen Mann**
 School of Chemistry, University of Bristol, Bristol BS8 1TS, United Kingdom
 ‘Synthesis and Self-assembly of Nanoparticle Arrays and Nanostructured Material’
 Abstract 4
- 12.45–14.30 Poster Session**
 Main Hall, University of Zürich, Irchel
 Abstracts 137–232
- 14.30–16.30 Lectures**
 University of Zürich, Irchel, HS 30
 Abstracts 127–136
 Chairperson: A. Togni
- 14.30–14.40 **F. Boccini, A. Domazou, S. Herold**
 ETH-Hönggerberg, CH-8093 Zürich
 ‘Mechanistic Studies of the Reaction Between Peroxynitrite and Oxyhemoglobin in the Presence of Carbon Dioxide’
 Abstract 127
- 14.40–14.50 **F. Breher, H. Rüegger**
 ETH-Hönggerberg, CH-8093 Zürich
 ‘Towards a Potential Application of Organometallic Main Group Element Compounds as Molecular-Based Memory Devices’
 Abstract 128
- 14.50–15.00 **M.C. Erat, M. Wächter, R.K. O. Sigel**
 University of Zürich, CH-8057 Zürich
 ‘Structural and Functional Insights into the Mechanism of Inhibition of a Group II Selfsplicing Intron by Ca²⁺’
 Abstract 129
- 15.10–15.20 **I. Fernandez Nieves, F. Breher, E. Martinez Viviente, P.S. Pregosin**
 ETH-Hönggerberg, CH-8093 Zurich
 ‘PGSE NMR Diffusion Measurements: Ion Pairing and Aggregation States in Classical Lithiated Species’
 Abstract 130
- 15.20–15.30 **V. Mahadevan Iyer, P. Belser**
 University of Fribourg, CH-1700 Fribourg
 ‘Optimizing Oligo Thiols for Self-Assembled Monolayers on Gold Surfaces’
 Abstract 131
- 15.30–15.40 **L. Québatte, R. Scopelliti, K. Severin**
 EPFL, CH-1015 Lausanne
 ‘Combinatorial Catalysis With Bimetallic Complexes: Robust and Efficient Catalysts for Atom-Transfer Radical Additions’
 Abstract 132

- 15.50–16.00 **A.D. Sadow, A. Togni**
ETH-Hönggerberg, CH-8093 Zürich
'Enantioselective Catalytic Hydrophosphination'
Abstract 133
- 16.00–16.10 **B. Spingler**
University of Zürich, CH-8057 Zürich
'Weakly Coordinating Anions: The Underestimated Supporting Actors in DNA Chemistry'
Abstract 134
- 16.10–16.20 **E. Terazzi^a, G. Bernardinelli^a, J.-P. Rivera^a, B. Donnio^b, D. Guillon^b, D. Imbert^c, J.-C. Bünzli^c, C. Piquet^a**
^aUniversity of Geneva, CH-1211 Geneva
^bInstitut de Physique et de Chimie des Matériaux de Strasbourg, 67037 Strasbourg, France
^cEPFL, CH-1015 Lausanne
'Lanthanide-Containing Metallomesogens. Mesomorphism Tuned by the Size of the Lanthanide Metal Ions'
Abstract 135
- 16.20–16.30 **O.S. Wenger, B.S. Leigh, J.R. Winkler, H.B. Gray**
California Institute of Technology, Pasadena, CA 91125, USA
'Tuning the Rates of Distant Separation in Frozen Solutions'
Abstract 136
- 16.30–17.00 Coffee Break**
- 17.00–17.15 Presentation of the Mettler Toledo Awards for the Best Oral and Poster Presentations**
- 17.15–18.00 Presentation of the Paracelsus Prize**
- Organic Chemistry**
- Session One*
- 11.15–12.30 **Lectures**
University of Zürich, Irchel, HS 45
Abstracts 233–237
Chairperson: J.S. Siegel
- 11.15–11.30 **E. Delort, T. Darbre, J.-L. Reymond**
University of Bern, CH-3012 Bern
'Synthesis of a Fourth Generation Catalytic Peptide Dendrimer With Very High Esterolytic Activity'
Abstract 233
- 11.30–11.45 **J.K. Klostermann, Y. Yasui, M. Loepfe, E. Zysman-Coleman, D. Rheingold, A. Linden, J.S. Siegel**
University of Zürich, CH-8057 Zürich
'Chemical Topology of Interlocking Rings'
Abstract 234
- 11.45–12.00 **S. Kaiser, S.P. Smidt, A. Pfaltz**
University of Basel, CH-4056 Basel
'Quinoline Derived P,N-Ligands and their Use in Asymmetric Catalysis'
Abstract 235
- 12.00–12.15 **M. Lochner, S.J. Atkinson, M.E. Di Francesco, T. Kühn, I. Paterson**
University of Cambridge, CB2 1EW Cambridge, United Kingdom
'Studies Towards the Total Synthesis of (–)-Peloruside A'
Abstract 236
- 12.15–12.30 **L.C. Bouchez, P. Vogel**
EPFL, CH-1015 Lausanne
'Sulfur Dioxide-Mediated Syntheses of Polyene-Containing Natural Products'
Abstract 237
- 12.30–13.03 Short Poster Presentations**
University of Zürich, Irchel, HS 45
V.A. Asov; M. Fontana; G. Corminbœuf; V. Gorteau; B. Jolivet; Y. Bethuel; M.-L. Goddard, M. Nishihara, R. Mimna, P. Schär; L.-S. Sonntag
Abstracts 257–267
- 13.05–14.30 Poster Session**
Main Hall, University of Zürich, Irchel
Abstracts 257–363
- 14.30–16.30 Lectures**
University of Zürich, Irchel, HS 45
Abstracts 238–244
Chairperson: A. Alexakis
- 14.30–14.45 **G. Fráter^{ab}, A. Goeke^b, M. Lovchik^a**
^aUniversity of Zürich, CH-8047 Zürich
^bGivaudan Schweiz AG, 8600 Dübendorf
'Novel, Stereoselective Synthesis of Cyclobutanones'
Abstract 238
- 14.45–15.00 **P. Holzer, T.R. Chan, V.V. Fokin, K.B. Sharpless**
The Scripps Research Institute, La Jolla, CA 92037, USA
'Polytriazoles-Copper(I) Complexes as Efficient Catalysts in the 1,3-Dipolar Cycloaddition'
Abstract 239
- 15.00–15.15 **M. Oberli, G. Rüedi, H.-J. Hansen**
University of Zürich, CH-8057 Zürich
'Diradical-Promoted (n+2–1) Ring Expansion: A New Reaction for the Preparation of Specifically Substituted Macrocycles'
Abstract 240
- 15.15–15.30 **A. Mezzetti, C. Becker, C. Bonaccorsi, C. Schärer, A. Togni**
ETH-Hönggerberg, CH-8093 Zürich
'Ruthenium-Catalyzed Asymmetric Atom-Transfer Reactions'
Abstract 241

15.45–16.00 **R. Árvai, H. Ratni, A.D. William, E.P. Kündig**
University of Geneva, CH-1211 Geneva
'Chromium-Mediated Approach Towards the
Synthesis of the Lythraceae Alkaloid
(+)-Vertine'
Abstract 242

16.00–16.15 **B. Laleu, C. Herse, P. Mobian, C. Nicolas,
G. Bernardinelli, J. Lacour**
University of Geneva, CH-1211 Geneva
'[4]Heterohelicenium Cations as Novel Chiral
Scaffolds'
Abstract 243

16.15–16.30 **F. Denes, F. Beaufils, P. Renaud**
University of Bern, CH-3012 Bern
'Thiophenol and Diethylphosphite:
New Reagents for Efficient 1,5-Hydrogen
Abstraction-Cyclization Cascade Processes'
Abstract 244

16.30–17.00 Coffee Break

17.00–17.15 **Presentation of the
Mettler Toledo Awards for the
Best Oral and Poster Presentations**

17.15–18.00 **Presentation of the Paracelsus Prize**

Session Two

11.15–12.30 **Lectures**
University of Zürich, Irchel, HS 55
Abstracts 245–249
Chairperson: *J.A. Robinson*

11.15–11.30 **L. Reymond, X. Wu, S. Pitsch**
EPFL, CH-1015 Lausanne
'Modified Oligoribonucleotides Containing
Polar 2'-O-Substituents: Synthesis and
Properties'
Abstract 245

11.30–11.45 **P. Krattiger, R. Kovasy, H. Wennemers**
University of Basel, CH-4056 Basel
'Peptides as Asymmetric Catalysts for Aldol
Reactions'
Abstract 246

11.45–12.00 **K. Gademann, Y. Bethuel**
ETH-Hönggerberg, CH-8093 Zürich
'Unraveling the Mystery of Cyanobacterial Iron
Acquisition'
Abstract 247

12.00–12.15 **Y. Baudry, D. Ronan, S. Matile**
University of Geneva, CH-1211 Geneva
'Synthesis of {242}- and {323}-Rigid-Rod
b-Barrels'
Abstract 248

12.15–12.30 **C. Brotschi, C. J. Leumann**
University of Bern, CH-3012 Bern
'Bipyridyl and Biphenyl-Residues as
Hydrophobic Non-Hydrogen-Bonding Base
Substitutes in DNA'
Abstract 249

12.30–13.03 **Short Poster Presentations**
University of Zürich, Irchel, HS 45
*V.A. Asov; M. Fontana; G. Corminbœuf;
V. Gorteau; B. Jolivet; Y. Bethuel;
M.-L. Goddard, M. Nishihara, R. Mimna,
P. Schär; L.-S. Sonntag*
Abstracts 257–267

13.05–14.30 **Poster Session**
Main Hall, University of Zürich, Irchel
Abstracts 257–363

14.30–16.30 **Lectures**
University of Zürich, Irchel, HS 55
Abstracts 250–256
Chairperson: *D. Hilvert*

14.30–14.45 **S.M. Langenegger, R. Häner**
University of Bern, CH-3012 Bern
'Excimer Formation Induced by Interstrand
Stacking'
Abstract 250

14.45–15.00 **A. Chandravarkar, B. Mandal, S. Dos Santos,
L. Patiny, G. Tuchscherer, M. Mutter**
EPFL, CH-1015 Lausanne
'Switch-Peptides: *ISN*-Induction of
Conformational Transitions Relevant in
Degenerative Diseases'
Abstract 251

15.00–15.15 **D. Meyer, W.-D. Woggon**
University of Basel, CH-4056 Basel
'Synthesis and Characterisation of a New
Family of Iron Porphyrins'
Abstract 252

15.15–15.30 **R. Manetsch^a, A. Krasiński^a, J. Raushel^a,
Z. Radic^b, P. Taylor^b, H.C. Kolb^a,
K.B. Sharpless^a**
^aThe Scripps Research Institute, La Jolla,
CA 92037, USA ^bUniversity of California
San Diego, La Jolla, CA 92093, USA
'*In situ* Click Chemistry: Optimization Leads
to the Discovery of Novel Highly Potent
Acetylcholinesterase inhibitors'
Abstract 253

15.45–16.00 **I. Sietlaff, A. Arnold, K. Johnsson**
EPFL, CH-1015 Lausanne
'A Protein Microarray Using AGT Fusion
Proteins'
Abstract 254

16.00–16.15 **K. Vamvaca, B. Vögeli, P. Kast, K. Pervushin,
D. Hilvert**
ETH-Hönggerberg, CH-8093 Zurich
'An Efficient Enzyme Lacking Structural
Preorganization'
Abstract 255

16.15–16.30 **L. Hintermann**
RWTH Aachen, D-52074 Aachen, Germany
'Asymmetric Organocatalysis: Oxa-Michael
Reactions'
Abstract 256

16.30–17.00 **Coffee Break**

**17.00–17.15 Presentation of the
Mettler Toledo Awards for the
Best Oral and Poster Presentations**

17.15–18.00 Presentation of the Paracelsus Prize

Physical Chemistry

- 11.15–12.30 Lectures**
University of Zürich, Irchel, HS 60
Abstracts 364–368
Chairperson: *P. Hamm*
- 11.15–11.30 *M. Allan***
University of Fribourg, CH-1700 Fribourg
‘Excitation of the Electronic Fine Structure Transitions in NO by Impact of Low-Energy Electrons’
Abstract 364
- 11.30–11.45 *R. Schanz, V. Botan***
University of Zürich, CH-8057 Zürich
‘Femtosecond Studies in the Ground State: the IR-Driven *cis-trans* Isomerization of Nitrous Acid (HONO)’
Abstract 365
- 11.45–12.00 *S. Albert, S. Bauerecker, M. Quack, A. Steinlin***
ETH-Hönggerberg, CH-8093 Zürich
‘Rovibrational Overtone Spectroscopy at 150 K: The CF-Stretching Polyads ($n = 1, 2, 3$) of CHCl_2F ’
Abstract 366
- 12.00–12.15 *S. Lammers, M. Meuwly***
University of Basel, CH-4056 Basel
‘Dissociable and Polarizable Force Fields for Double Proton Transfer Reactions’
Abstract 367
- 12.15–12.30 *C. Minkowski, G. Calzaferri***
University of Bern, CH-3012 Bern
‘One-Dimensional Förster Energy Transfer in Dye Loaded Zeolite L’
Abstract 368
- 12.30–12.45 Short Poster Presentations**
University of Zürich, Irchel, HS 60
A. Fürstenberg; A. Abraham; A. Currao;
C. Leiggenger; M. Willeke
Abstracts 376–380
- 12.45–14.30 Poster Session**
Main Hall, University of Zürich, Irchel
Abstracts 376–409
- 14.30–16.30 Lectures**
University of Zürich, Irchel, HS 60
Abstracts 369–375
Chairperson: *M. Chergui*
- 14.30–14.45 *P. Maroni, T.T. Dang, D.C. Papageorgopoulos, R.D. Beck, T.R. Rizzo***
EPFL, CH-1015 Lausanne
‘State Resolved Gas/Surface Reactivity of Methane Prepared by Stimulated Raman Pumping’
Abstract 369

- 14.45–15.00 *N. Bonalumi, T. Bürgi, A. Baiker***
ETH-Hönggerberg, CH-8093 Zürich
‘Enantioselective Hydrogenation on Chirally Modified Platinum Studied by Concentration Modulation Attenuated Total Reflection IR Spectroscopy’
Abstract 370
- 15.00–15.15 *M. Quack^a, J. Stohner^b***
^a*ETH-Hönggerberg, CH-8093 Zürich*
^b*Zürich University for Applied Sciences ZHW, CH-8401 Winterthur*
‘Parity Violation in CDBrClF: The Role of Anharmonicity and Anharmonic Couplings’
Abstract 371
- 15.15–15.30 *J. Bredenbeck, J. Helbing, P. Hamm***
University of Zürich, CH-8057 Zürich
‘Ultrafast IR Spectroscopy Reveals Conformational Dynamics of Photo-Switchable Peptides’
Abstract 372
- 15.45–16.00 *C. Keresszegi, D. Ferri, T. Mallat, A. Baiker***
ETH-Hönggerberg, CH-8093 Zürich
‘*in Situ* ATR-IR Study of the Liquid-Phase Alcohol Oxidation on $\text{Pd}/\text{Al}_2\text{O}_3$ ’
Abstract 373
- 16.00–16.15 *L. Frunz, G. Pirngruber, R. Prins***
ETH-Hönggerberg, CH-8093 Zürich
‘Synthesis of Microporous/Mesoporous Aluminosilicates’
Abstract 374
- 16.15–16.30 *C. Bauer, J.-P. Abid, H.H. Girault***
EPFL, CH-1015 Lausanne
‘Role of Adsorbates on Hot Electron Thermalization in Small Metal Nanoparticles’
Abstract 375

16.30–17.00 Coffee Break

Presentations of the Mettler Toledo Awards for the Best Oral and Poster Presentations

- 17.00–17.15** *University of Zürich, Irchel, HS 30*
Chairperson: *H. Berke, Mettler Toledo AG*

Presentations of the Paracelsus Prize 2004

- 17.15–18.00 Presentation of the Paracelsus Prize 2004**
University of Zürich, Irchel, HS 30
Presented by **Prof. G. Fráter**
- Lecture of the Paracelsus Laureate**
George M. Whitesides
Harvard University, Cambridge, MA 02138, USA
‘Dynamic Self-Assembly, Complexity, and Emergence’