

Program

	HS 95 AC	HS 85 MC	HS 91 CC	HS 30 IC	HS 45 OCI	HS 55 OCII	HS 80 PC	HS 60 PS	
9:30									
9:45	Opening Ceremony								
10:00	Delamarche (2), Werner Prize								
10:15	Fiebig (3), Gramaticakis Neumann Prize								
10:30	Wagenknecht (4), Gramaticakis Neumann Prize								
10:45	Coffee								
11:00	Members Assembly	Members Assembly	Members Assembly, Division of Chemical Research						
11:15		Tschopp (63)	Weber (98)	Parkin (128)	Pozzi (233)	Bandera(246)	Lang (345)	Janssen (416)	
11:30	Nilsson (5)	Feyen (64)			Rosenblade (234)	Herrmann (247)	Miloglydaov (346)		
11:45		Cecarelli (65)			Muster (235)	13	Maksytenko (347)		
12:00		Manley (66)			Sadler (129)	Falciola (236)	Hutin (249)	Wörner (348)	Geiger (417)
12:15	Bohni (6)	Raillard (67)	Neugebauer (99)		Fischer (237)	Kümin (250)	Kolano (349)	Vebert (418)	
12:30	Dayon (7)	Richter (68)	Vandevondele (100)	Poster Session			Short Poster Presentations		
12:45	Hueglin (8)	Stockmaier (69)	Plattner (101)					Zhang (419)	
13:00		Limbach (70)	Danielsson (102)						
13:15		Renaud (71)							
13:30	Poster Session								
13:45	Poster Session								
14:00	Poster Session								
14:15	Poster Session								
14:30	General Assembly of the Swiss Chemical Society HS 30							Velonia (420)	
14:45	Scheidegger (9)	Mattei (72)	Bollot (103)	Buryak (130)	d'Augustin (238)	Luedtke (251)	Bally (350)	Bornand (421)	
15:00	Grata (10)	Neumoin (73)	Horny (104)	Kuhni (131)	Mosse (239)	Bouamaied (252)	Albert (351)	Godt (422)	
15:15	Schmid (11)	Schwizer (74)	Baillod (105)	Freisinger (132)	Campagna (240)	Didier (253)	Willeke (352)		
15:30	Randon (12)	Lederer (75)	Cascella (106)	Filipuzzi (134)	Gorteau (241)	Velcicky (254)	Vliegen (353)	Tugulu (423)	
15:45		Schmid (76)	Tavernelli (107)	Medina-Molner (135)	Robert (136)	Schultz (242)	Coste (255)		Fouqueau (354)
16:00	Round Table Discussion	Simic (77)	Leoni (108)	Knobloch (136)	Seidel (243)	Kofoed (256)	Lutkouskaya (355)	Casari (424)	
16:15		Fiaux (78)	Guglielmi (109)	Heckenroth (138)	Noyes (244)	Zahn (257)	Bonalumi (356)		
16:30		Cutting (79)			Vallinayagam (245)	Gademann (258)			
16:45	Coffee								
17:00	Coffee								
17:15	Mettler Toledo Prizes for best oral presentations, SCS prizes for best poster contributions								
17:30	Mettler Toledo Prizes for best oral presentations, SCS prizes for best poster contributions								
17:45	Sir Jack Baldwin, Paracelsus Prize								
18:00	Sir Jack Baldwin, Paracelsus Prize								

Program of the Fall Meeting 2006

09.45–10.45 Opening Ceremony

University Zürich-Irchel, HS 30

Presentation of the Werner Prize 2006

Chair: *Georg Fráter*

Lecture of the Werner Prize Laureate 2006

Emmanuel Delamar

IBM Zürich Research Laboratory,
8803 Rüschlikon
'Microcontact Processing for Microtechnology
and Biology'
Abstract 2

Presentation of the Gramaticakis-Neumann Prize 2006

Chair: *Georg Fráter*

Lecture of the Gramaticakis-Neumann Prize Laureate 2006

Torsten Fiebig

Eugene F. Merkert Chemistry Center,
Boston College, USA
'DNA Photonics – Probing Light-Induced
Dynamics in DNA on the Femtosecond
Time Scale'
Abstract 3

Presentation of the Gramaticakis-Neumann Prize 2006

Chair: *Georg Fráter*

Lecture of the Gramaticakis-Neumann Prize Laureate 2006

Hans-Achim Wagenknecht

Universität Regensburg, 93053 Regensburg,
Germany
'Chromophore-Functionalized DNA:
From Photoinduced Electron Transfer to
Applications in Fluorescent DNA Analytics'
Abstract 4

10.45–11.00 Coffee Break

11.00–16.45 Analytical Chemistry

11.00–11.30 **General Assembly of the Members
of the Division**
University Zürich-Irchel, HS 95

11.30–13.00 **Lectures**
University Zürich-Irchel, HS 95
Abstracts 5–8

13.00–14.15 **Poster Session**
University Zürich-Irchel, Lichthof Area
Abstracts 13–62

14.15–14.45 **General Assembly of the
Swiss Chemical Society**
University Zürich-Irchel, HS 30

14.45–16.00 **Lectures**
University Zürich-Irchel, HS 95
Abstracts 9–12

16.00–16.45 **Round Table Discussion**
University Zürich-Irchel, HS 95

11.00–16.45 Medicinal Chemistry

11.00–11.15 **General Assembly of the Members
of the Division**
University Zürich-Irchel, HS 85

11.15–13.30 **Lectures**
University Zürich-Irchel, HS 85
Abstracts 63–71

13.30–14.15 **Poster Session**
University Zürich-Irchel, Lichthof Area
Abstracts 80–97

14.15–14.45 **General Assembly of the
Swiss Chemical Society**
University Zürich-Irchel, HS 30

14.45–16.45 **Lectures**
University Zürich-Irchel, HS 85
Abstracts 72–79

11.00–16.45 Chemical Research

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

11.15–16.30 Computational Chemistry

11.15–13.15 **Lectures**
University Zürich-Irchel, HS 91
Abstracts 98–102

13.15–14.15 **Poster Session**
University Zürich-Irchel, Lichthof Area
Abstracts 110–127, 457–459

14.15–14.45 **General Assembly of the
Swiss Chemical Society**
University Zürich-Irchel, HS 30

14.45–16.30 **Lectures**
University Zürich-Irchel, HS 91
Abstracts 103–109

11.15–16.30 Inorganic and Coordination Chemistry**11.15–12.45 Minisymposium***University Zürich-Irchel, HS 30*
Abstracts 128, 129**12.45–14.15 Poster Session***University Zürich-Irchel, Lichthof Area*
Abstracts 140–232**14.15–14.45 General Assembly of the Swiss Chemical Society***University Zürich-Irchel, HS 30***14.50–16.30 Lectures***University Zürich-Irchel, HS 30*
Abstracts 130–139**11.15–16.45 Organic Chemistry****Session 1 Synthesis and Synthetic Methodology I****11.15–12.30 Lectures***University Zürich-Irchel, HS 45*
Abstracts 233–237**12.30–14.15 Poster Session***University Zürich-Irchel, Lichthof Area*
Abstracts 259–344**14.15–14.45 General Assembly of the Swiss Chemical Society***University Zürich-Irchel, HS 30***14.45–16.45 Lectures***University Zürich-Irchel, HS 45*
Abstracts 238–245**Session 2 Organic Structure and Properties II****11.15–12.30 Lectures***University Zürich-Irchel, HS 55*
Abstracts 246–250**12.30–14.15 Poster Session***University Zürich-Irchel, Lichthof Area*
Abstracts 259–344**14.15–14.45 General Assembly of the Swiss Chemical Society***University Zürich-Irchel, HS 30***14.45–16.45 Lectures***University Zürich-Irchel, HS 55*
Abstracts 251–258**11.15–16.30 Physical Chemistry****11.15–12.30 Lectures***University Zürich-Irchel, HS 80*
Abstracts 345–349**12.30–14.15 Poster Session***University Zürich-Irchel, Lichthof Area*
Abstracts 357–415**14.15–14.45 General Assembly of the Swiss Chemical Society***University Zürich-Irchel, HS 30***14.45–16.30 Lectures***University Zürich-Irchel, HS 80*
Abstracts 350–356**11.15–16.30 Polymer Science****11.15–13.00 Lectures***University Zürich-Irchel, HS 60*
Abstracts 416–419**13.00–14.15 Poster Session***University Zürich-Irchel, Lichthof Area*
Abstracts 425–456**14.20–16.30 Lectures***University Zürich-Irchel, HS 80*
Abstracts 420–424**16.45–17.15 Coffee Break****17.15–17.30 Mettler Toledo Prizes for best oral presentations
SCS prizes for best poster contributions***University Zürich-Irchel, HS 30***Analytical Chemistry**2 poster and 1 oral presentations
Jury: R. Zenobi, J.-L. Veuthey**Medicinal Chemistry**1 poster and 2 oral presentations
Jury: W. Froestl, P. Mohr**Computational Chemistry**1 poster and 1 oral presentations
Jury: H.P. Lüthi, C.A. Daul**Inorganic and Coordination Chemistry**3 poster and 1 oral presentations
Jury: K. Severin, T.R. Ward, P.S. Pregosin**Organic Chemistry**2 poster and 2 oral presentations
Jury: M. Mayor, N. Finney, S. Bienz**Physical Chemistry**2 poster and 1 oral presentation
Jury: P. Hamm, V. Sandoghdar

Polymer Science
2 poster and 1 oral presentation
Jury: *R. Deschenaux, H.-A. Klok, A.D. Schlüter*

17.30–18.15 Presentation of the Paracelsus Prize 2006

University Zürich-Irchel, HS 30
Chair: *Georg Fráter*

Lecture of the Paracelsus Prize Laureate 2006

Professor Sir Jack E. Baldwin
University of Oxford, Oxford, UK
'Biomimetic Synthesis of Natural Products'
Abstract 1

DETAILED PROGRAM

Analytical Chemistry

11.00–11.30 General Assembly of the Members of the Division

University Zürich-Irchel, HS 95

11.30–13.00 Lectures

University Zürich-Irchel, HS 95
Abstracts 5–8
Chair: *J.-L. Veuthey*

11.30–12.15 *S. Nilson*

Applied Biochemistry, Lund Institute of Technology, Lund University, 221 00 Lund, Sweden
'Airborne Cell Chemistry & Nanoparticle based CEC'
Abstract 5

12.15–12.30

N. Bohni^a, V. Wennrich^b, B. Hattendorf^a, D. Günther^a
^aETH Zürich, Laboratory of Inorganic Chemistry, 8093 Zürich
^bUniversity of Leipzig, Institute for Geophysics and Geology, 04103 Leipzig, Germany
'The Use of Ostracod Shells as a Paleothermometer by Measuring Calcium Isotope Ratios and Trace Elements with ICPMS'
Abstract 6

12.30–12.45

L. Dayon^a, M. Prudent^a, M. Abonnenc^a, J. Josserand^a, C. Roussel^a, N. Lion^a, A. Brajter-Toth^b, H.H. Girault^a
^aLaboratoire d'Electrochimie Physique et Analytique, Ecole Polytechnique Fédérale de Lausanne, 1015 Lausanne
^bUniversity of Florida, Department of Chemistry, Gainesville, FL 32611, USA
'Microfabricated Electrospray Emitters for Peptide and Protein Tagging'
Abstract 7

12.45–13.00

C. Hueglin, A. Fischer, P. Graf, B. Schwarzenbach, B. Buchmann
Laboratory for Air Pollution and Environmental Technology, Empa, 8600 Dübendorf
'Determination of NH₃ in Ambient Air Using Photoacoustic Spectroscopy'
Abstract 8

13.00–14.15

Poster Session
University Zürich-Irchel, Lichthof Area
Abstracts 13–62

14.15–14.45

General Assembly of the Swiss Chemical Society
University Zürich-Irchel, HS 30

14.45–16.00

Lectures
University Zürich-Irchel, HS 95
Abstracts 9–12
Chair: *E. Vauthey*

14.45–15.00

A.M. Scheidegger, D. Grolimund, M. Harfouche, M. Willmann
Paul Scherrer Institute PSI, 5232 Villigen
'The Micro-XAS Beamline at the Swiss Light Source (SLS): A new Analytical Facility Dedicated to Micro-beam Applications'
Abstract 9

15.00–15.15

E. Grata^{a,b}, D. Guilleme^b, J. Boccard^{b,c}, G. Glauser^{a,b}, P. A. Carrupt^c, J.-L. Wolfender^a, S. Rudaz^b
^aLPP, University of Lausanne
^bLCAP, University of Lausanne
^cLCT – Pharmacochimie, School of Pharmaceutical Sciences, University of Geneva / University of Lausanne
'A Two-steps Strategy for the Efficient Detection and Localisation of Stress-induced Metabolites in *Arabidopsis Thaliana* by UPLC-TOF-MS'
Abstract 10

15.15–15.30

T. Schmid, J. Burkhard, R. Zenobi
Department of Chemistry and Applied Biosciences, ETH Zürich, 8093 Zürich
'Nanometer Scale Topographic and Chemical Imaging of Biofilms by Atomic Force Microscopy and Raman Spectroscopy'
Abstract 11

15.30–16.00

J. Randon
Laboratoire des Sciences Analytiques, Université Claude Bernard Lyon, 69622 Villeurbanne cedex, France
'Do we need a Master in Analytical Science? An Example in Lyon'
Abstract 12

16.00–16.45

Round Table Discussion, HS 95

16.45–17.15

Coffee Break

**17.15–17.30 Mettler Toledo Prizes
for best oral presentations
SCS prizes for
best poster ontributions**

**17.30–18.15 Presentation of the
Paracelsus Prize 2006**

Medicinal Chemistry

**11.00–11.15 General Assembly of the
Members of the Division**
University Zürich-Irchel, HS 85

11.15–13.30 Lectures
University Zürich-Irchel, HS 85
Abstracts 63–71
Chair: **H. P. Maerki**

11.15–11.30 **L. Tschopp^a, J.T. Patton Jr.^b, J.L. Magnani^b,
B. Ernst^a**
^aInstitute of Molecular Pharmacy, Pharmcenter
of the University of Basel, 4056 Basel
^bGlycomimetics Inc., Gaithersburg, MD, USA
'Exploring the Binding Site of E-Selectin'
Abstract 63

11.30–11.45 **F. Feyen, J. Gertsch, M. Wartmann,
K.-H. Altmann**
Department of Chemistry and Applied
Biosciences, ETH Zürich, 8093 Zürich
'Design and Synthesis of 12-Aza-Epothilones
(Azathilones)'
Abstract 64

11.45–12.00 **S.M. Ceccarelli, E. Pinard, H. Stalder,
D. Alberati**
F. Hoffmann-La Roche Ltd., Pharmaceutical
Division Basel, Discovery Chemistry,
4070 Basel
'Design, Synthesis and Structure-Activity
Relationship of N(1)-(2-phenyl-cylohexyl)-4-
amino-piperidine Derivatives as Potent and
Selective Glycine Reuptake Inhibitors'
Abstract 65

12.00–12.15 **P.W. Manley, W. Breitenstein, S. Cowan-Jacob,
M.R. Jensen, J. Mestan**
Novartis Institutes for BioMedical Research,
4002 Basel
'Nilotinib: A new Agent for the Treatment of
Imatinib-Resistant CML'
Abstract 66

12.15–12.30 **S. Raillard**
XenoPort, Inc., Santa Clara, CA 95051, USA
'XP13512, a Transported Prodrug of
Gabapentin, Overcomes the Saturable Oral
Absorption of Neurontin® in Humans'
Abstract 67

12.30–12.45 **H.G.F. Richter^a, D.R. Adams^b,
A. Benardeau^a, M.J. Bickerdike^b,
J.M. Bentley^b, T.J. Blench^b, I.A. Cliffe^b,
C. Dourish^b, P. Hebeisen^a, G.A. Kennett^b,
A.R. Knight^b, C.S. Malcolm^b, P. Mattei^a,
A. Misra^b, J. Mizrahi^a, N.J.T. Monck^b,
J.-M. Plancher^a, S. Roever^a, J.R.A. Roffey^b,
S. Taylor^a, S.P. Vickers^b**
^aF. Hoffmann-La Roche Ltd, 4070 Basel
^bVernalis Research Ltd, Wokingham,
RG41 5UA, UK
'Novel Hexahydropyrido[3',2':4,5]pyrrolo
[1,2- α]pyrazines as Potent and Selective Human
5-HT_{2C} Receptor Agonists'
Abstract 68

12.45–13.00 **D. Stokmaier, O. Khorev, K. Johansson,
D. Ricklin, B. Cutting, B. Ernst**
Institute of Molecular Pharmacy, Pharmcenter
of the University of Basel, 4056 Basel
'Targeting Hepatocytes via the
Asialoglycoprotein Receptor'
Abstract 69

13.00–13.15 **L.K. Limbach^a, T.J. Brunner^a, P. Wick^b,
R. N. Grass^a, P. Manser^b, P. Spohn^b,
A. Bruinink^b, W.J. Stark^a**
^aInstitute for Chemical and Bioengineering,
ETH Zürich
^bEmpa St. Gallen, Materials and Tissues
for Medicine
'In vitro Cytotoxicity Studies of Oxides
Nanoparticles and Comparison to Asbestos'
Abstract 70

13.15–13.30 **M. Koller, H. Allgeier, W. Froestl,
P. Floersheim, J. Kallen, K. Lingenhoehl,
S. Ofner, S. Urwyler, J. Renaud**
Novartis Institutes for BioMedical Research
Basel, Global Discovery Chemistry,
Neuroscience Department, 4002 Basel
'Discovery of a Novel Series of Quinazoline
Derivatives as Competitive AMPA Receptor
Antagonists: Design, Synthesis and SAR.'
Abstract 71

13.30–14.15 Poster Session
University Zürich-Irchel, Lichthof Area
Abstracts 80–97

**14.15–14.45 General Assembly of the
Swiss Chemical Society**
University Zürich-Irchel, HS 30

14.45–16.45 Lectures
University Zürich-Irchel, HS 85
Abstracts 72–79
Chair: **K. H. Altmann**

14.45–15.00 **P. Mattei**
F. Hoffmann-La Roche AG,
Discovery Chemistry, 4070 Basel
'Aminobenzoquinolizines: a New Class of
DPP-IV Inhibitors'
Abstract 72

- 15.00–15.15 **A. Neumoin, J. Mares, O. Zerbe**
Institute of Organic Chemistry,
University of Zürich, 8057 Zürich
'Structural Determinants of a Miniprotein:
The Importance of Individual Aminoacids in
Porcine Polypeptide YY (pPYY) for formation
of secondary and tertiary structure and
implications for folding'
Abstract 73
- 15.15–15.30 **D. Schwizer, A. Kato, M. Porro,
B. Cutting, B. Ernst**
Institute of Molecular Pharmacy, Pharmcenter
of the University of Basel, 4056 Basel
'Preorganization of E-Selectin Antagonists
in the Bioactive Conformation'
Abstract 74
- 15.30–15.45 **A. Lederer^a, B. Romagnoli^a, H. Henze^a,
R. Mukherjee^a, S.J. DeMarco^a,
J. Zumbunn^a, F.O. Gombert^a, S. Lociuoro^a,
C. Ludin^a, J.W. Vrijbloed^a, D. Obrecht^a,
F. Hamy^b, T. Klimkait^b, K. Moehle^c,
J.A. Robinson^c**
^aPolyphor AG, 4123 Allschwil
^bInPheno AG, 4051 Basel
^cUniversity of Zürich, 8057 Zürich
'Discovery of Highly Potent and Selective
CXCR4 Inhibitors Using Protein Epitope
Mimetics (PEM) Technology'
Abstract 75
- 15.45–16.00 **F.F.-F. Schmid, M. Meuwly**
Department of Chemistry, University of Basel,
4056 Basel
'Atomistic Study of Feedback Inhibition in
Guanylate Cyclase PLED'
Abstract 76
- 16.00–16.15 **Oliver Simić**
Expertise Program Proteases, Novartis Institute
for Biomedical Research, 4002 Basel
'Identification and Optimisation of Novel BACE
Inhibitors Based on the Hydroxyethylamine
Transition State Mimetic'
Abstract 77
- 16.15–16.30 **H. Fiaux^a, D. Kuntz^b, D. Rose^b,
S. Gerber-Lemaire^a, L. Juillerat Jeanneret^c**
^aLGSA, BCH, EPFL, 1015 Lausanne
^bOntario Cancer Institute, Toronto, Canada
^cUniversity Institute of Pathology, CHUV,
Lausanne
'Pyrrolidinone Based α -Mannosidase Inhibitors
act as Growth Inhibitors of Human
Glioblastoma Cells'
Abstract 78
- 16.30–16.45 **B. Cutting^a, D. Strasser^a, M. Porro^a,
S. Kelm^b, S. Shelke^a, G.-P. Gao^a, B. Ernst^a**
^aInstitute of Molecular Pharmacy, Pharmcenter
of the University of Basel, 4056 Basel
^bUniversity of Bremen, Fachbereich 2,
28334 Bremen, Germany
'Signal Enhancement and Pharmacophore
Characterization in NMR Saturation Transfer
Experiments'
Abstract 79

16.45–17.15 Coffee Break**17.15–17.30 Mettler Toledo Prizes
for best oral presentations
SCS prizes for
best poster contributions****17.30–18.15 Presentation of the
Paracelsus Prize 2006****Chemical Research****11.00–11.15 General Assembly of the
Members of the Division
University Zürich-Irchel, HS 30****Computational Chemistry**

- 11.15–13.15 Lectures**
University Zürich-Irchel, HS 91
Abstracts 98–102
Chair: **C. Daul**
- 11.15–12.15 **J. Weber**
Department of Physical Chemistry,
University of Geneva, 1211 Geneva 4
'The Emergence of Density Functional Theory
in Computational Quantum Chemistry'
Abstract 98
- 12.15–12.30 **J. Neugebauer**
Laboratorium für Physikalische Chemie,
ETH Zürich, 8093 Zürich
'Modeling Environmental Effects with Frozen
Density Embedding'
Abstract 99
- 12.30–12.45 **J. VandeVondele^{a,b}, M. Sulpizi^b, M. Sprik^b**
^aUniversity of Zürich, 8057 Zürich
^bUniversity of Cambridge, CB2 1EW,
Cambridge, UK
'From Solvent Fluctuations to Quantitative
Redox Properties of Quinones in Methanol and
Acetonitrile'
Abstract 100
- 12.45–13.00 **N. Plattner, M. Meuwly**
Department of Chemistry, University of Basel,
4056 Basel
'Distributed Multipole Potentials for Molecular
Dynamics Simulations'
Abstract 101
- 13.00–13.15 **J. Danielsson, S. Lutz, M. Meuwly**
Department of Chemistry, University of Basel,
4056 Basel
'Classical Dynamics on Multiple Potential
Energy Surfaces'
Abstract 102

- 13.15–14.15 Poster Session**
University Zürich-Irchel, Lichthof Area
Abstracts 110–127, 457–459
- 14.15–14.45 General Assembly of the Swiss Chemical Society**
University Zürich-Irchel, HS 30
- 14.45–16.30 Lectures**
University Zürich-Irchel, HS 91
Abstracts 103–109
Chair: **H. P. Lüthi**
- 14.45–15.00 **G. Bollot, S. Bhosale, N. Sakai, S. Matile, J. Mareda**
Department of Organic Chemistry, University of Geneva, 1211 Geneva 4
'Density Functional Studies of Naphthalenediimide Acceptors and Dialkoxynaphthalene Donors as Building Blocks in Supramolecular Architecture'
Abstract 103
- 15.00–15.15 **L. Horný^a, M. Quack^a, H.F. Schaefer^b, M. Willeke^a**
^aPhysical Chemistry, ETH Zürich, 8093 Zürich
^bCenter for Computational Chemistry, University of Georgia, Athens, Georgia 30602, USA
'The Isomers of Dimer (ClO)₂ Revisited'
Abstract 104
- 15.15–15.30 **P. Baillo, M.-C. Colombo, I. Tavernelli, U. Röthlisberger**
Laboratory of Computational Chemistry and Biochemistry, Federal Institute of Technology, Lausanne
'REMD Simulations of Prion Protein Misfolding: Towards the Scrapie Isoform'
Abstract 105
- 15.30–15.45 **M. Cascella^a, I. Tavernelli^a, A. Magistrato^b, P. Carloni^b, U. Röthlisberger^a**
^aLaboratory of Computational Chemistry and Biochemistry, Ecole Polytechnique Fédérale de Lausanne (EPFL)
^bInternational School for Advanced Studies (SISSA/ISAS) and INFN-Democritos center, Trieste, Italy
'Electron Transfer Properties of Azurin from Pseudomonas Aeruginosa by Hybrid QM/MM Molecular Dynamics Simulations'
Abstract 106
- 15.45–16.00 **I. Tavernelli**
Ecole Polytechnique Fédérale de Lausanne (EPFL), Laboratoire de Chimie et Biochimie Computationnelle, 1015 Lausanne
'Intramolecular Electron Transfer in Bis(methylene) Adamantyl Radical Cation: A Finite Temperature Study using SIC Corrected DFT'
Abstract 107

- 16.00–16.15 **S. Leoni**
Max-Planck-Institut für Chemische Physik fester Stoffe, 01187 Dresden, Germany
'Full-featured Simulation of Reconstructive Phase Transitions'
Abstract 108
- 16.15–16.30 **M. Guglielmi, I. Tavernelli, U. Röthlisberger**
Laboratoire de Chimie et Biochimie Computationnelle, Ecole Polytechnique Fédérale de Lausanne (EPFL), 1015 Lausanne
'Probing Combined Proton and Electron Transfer Along a Hydrogen-bonded Ammonia Wire Using Time Dependent Density Functional Theory'
Abstract 109
- 16.45–17.15 Coffee Break**
- 17.15–17.30 Mettler Toledo Prizes for best oral presentations SCS prizes for best poster contributions**
- 17.30–18.15 Presentation of the Paracelsus Prize 2006**

Inorganic and Coordination Chemistry

- 11.15–12.45 Minisymposium**
University Zürich-Irchel, HS 30
Chair: **P. S. Pregosin**
- 11.15–12.00 **G. Parkin**
Department of Chemistry, Columbia University, 10027 New York, USA
'Applications of Tris(mercaptoimidazolyl)hydroborato Ligands for Modeling Sulfur Rich Active Sites and for the Synthesis of Metallaboranes'
Abstract 128
- 12.00–12.45 **P.J. Sadler**
University of Edinburgh, EH9 3JJ, UK
'Coordination Chemistry for the Design of Therapeutic Metal Complexes'
Abstract 129
- 12.30–14.15 Poster Session**
University Zürich-Irchel, Lichthof Area
Abstracts 140–232
- 14.15–14.45 General Assembly of the Swiss Chemical Society**
University Zürich-Irchel, HS 30
- 14.50–16.30 Lectures**
University Zürich-Irchel, HS 30
Abstracts 130–139
Chair: **K. Severin, T. Ward**

- 14.50–15.00 **A. Buryak, K. Severin**
Institut des Sciences et Ingénierie Chimiques,
Ecole Polytechnique Fédérale de Lausanne
(EPFL), 1015 Lausanne
'Dynamic Combinatorial Libraries of dye
Complexes as Flexible Sensors for Peptides'
Abstract 130
- 15.00–15.10 **J. Kühni, P. Belser**
Department of Chemistry, University of
Fribourg, 1700 Fribourg
'Photochromic Dithienylethene Switches
Connected a Ruthenium(II) Center: Spacer,
the Key of Success?'
Abstract 131
- 15.10–15.20 **E. Peroza, E. Freisinger**
Institute of Inorganic Chemistry, University of
Zürich, 8057 Zürich
'The Cluster Structure of a Wheat
Metallothionein'
Abstract 132
- 15.20–15.30 **W.H. Ang^a, L. Juillerat-Jeanerath^b, P.J. Dyson^a**
^aEcole Polytechnique Fédérale de Lausanne
(EPFL), 1015 Lausanne
^bCentre Hospitalier Universitaire Vaudois
(CHUV), 1011 Lausanne
'Transition Metal Anticancer Drugs Designed to
Overcome Glutathione-S-Transferase Mediated
Drug Resistance'
Abstract 133
- 15.30–15.40 **S. Filipuzzi^a, P.S. Pregosin^a, S. Rizzato^b,
A. Albinati^b**
^aLaboratory of Inorganic Chemistry, ETH
Zürich, 8093 Zürich
^bDepartment of Structural Chemistry, University
of Milan, 20133 Milan, Italy
'Palladium-allyl Phosphoramidite Complexes.
Solid-state Structures and Solution Dynamics'
Abstract 134
- 15.40–15.50 **A. Medina-Molner, B. Spingler**
Institute of Inorganic Chemistry, University of
Zürich, 8057 Zürich
'Mononuclear and Dinuclear Metal Complexes
and Their Ability to Induce Z-DNA'
Abstract 135
- 15.50–16.00 **R. Robert, M. Aguirre, L. Bocher,
A. Weidenkaff**
EMPA, 8600 Dübendorf
'Synthesis and Characterization of
Perovskite-type Oxides for Geothermal and
Solar Thermoelectric Power Generation'
Abstract 136
- 16.00–16.10 **B. Knobloch, R.K.O. Sigel**
Institute of Inorganic Chemistry, University of
Zürich, 8057 Zürich
'Insights Into the Relationship Between
Cd²⁺ and RNA-Thiophosphate Derivatives'
Abstract 137

- 16.10–16.20 **M. Heckenroth, E. Kluser, M. Albrecht**
Department of Chemistry, University of
Fribourg, 1700 Fribourg
'Non-classically Bound Heterocyclic Carbene
Pd Complexes and Their Catalytic Application'
Abstract 138

- 16.20–16.30 **I. Krummenacher^{a,b}, F. Breher^b,**
^aDepartment of Chemistry and Applied
Biosciences, ETH Zürich, 8093 Zürich
^bInstitute of Inorganic Chemistry, University of
Karlsruhe (TH), 76131 Karlsruhe, Germany
'Group 14 Element Cages for Transition
Metal Coordination'
Abstract 139

16.45–17.15 Coffee Break

17.15–17.30 Mettler Toledo Prizes for best oral presentations SCS prizes for best poster contributions

17.30–18.15 Presentation of the Paracelsus Prize 2006

Organic Chemistry

Session 1 Synthesis and Synthetic Methodology I

- 11.15–12.30 **Lectures**
University Zürich-Irchel, HS 45
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Chair: **M. Mayor**
- 11.15–11.30 **D. Pozzi, P. Renaud**
Departement für Chemie und Biochemie,
Universität Bern, 3012 Bern
'Alcohols and Water as Reducing Agents in
Radical Reactions'
Abstract 233
- 11.30–11.45 **A. Pfaltz, S. Roseblade**
Institut für Organische Chemie, Universität
Basel, 4056 Basel
'Iridium Catalyzed Asymmetric Hydrogenation:
Synthetic and Mechanistic Studies'
Abstract 234
- 11.45–12.00 **L.S.A. Muster, T.A. Jenny**
Chemistry Department, University of Fribourg,
1700 Fribourg
'Polymerization and Dehydrogenation of
Acetylene with an Iron(0)/DIBAH Catalyst
on an Appropriated Template: Toward a Rational
Synthesis of Carbon Nanotubes'
Abstract 235
- 12.00–12.15 **C.A. Falcioia, A. Alexakis**
University of Geneva, 1211 Geneva 4
'Allylic Substrates for the Copper Catalyzed
Asymmetric S_N2' Reaction'
Abstract 236

- 12.15–12.30 **D.F. Fischer, M.E. Weiss, Z. Xin, S. Jautze, R. Peters**
Laboratorium für Organische Chemie,
ETH Zürich, 8093 Zürich
'FIP: a Practical Catalyst for Aza-Claisen
Rearrangements'
Abstract 237
- 12.30–14.15 **Poster Session**
University Zürich-Irchel, Lichthof Area
Abstracts 259–344
- 14.15–14.45 **General Assembly of the
Swiss Chemical Society**
University Zürich-Irchel, HS 30
- 14.45–16.45 **Lectures**
University Zürich-Irchel, HS 45
Abstracts 238–245
Chair: N.S. Finney
- 14.45–15.00 **M. d'Augustin, A. Alexakis**
Department of Organic Chemistry, University of
Geneva, 1211 Geneva 4
'Enantioselective Cu-catalyzed Conjugate
Addition to Trisubstituted Cyclohexenones.
Construction of Chiral Quaternary
Carbon Centers'
Abstract 238
- 15.00–15.15 **S. Mossé, A. Alexakis**
Department of Organic Chemistry, University of
Geneva, 1211 Geneva 4
'Organocatalyzed Asymmetric Michael Addition
Using 2,2'-Bipyrrrolidine Derivatives'
Abstract 239
- 15.15–15.30 **S. Bienz, M. Trzoss, L. Hristova, M. Campagna**
University of Zürich, 8057 Zürich
'A New Si-based Auxiliary for Stereospecific
Addition of Organometallics to
 α - and β -Hydroxy Carbonyl Compounds'
Abstract 240
- 15.30–15.45 **V. Gorteau, S. Matile**
University of Geneva, Department of Organic
Chemistry, 1211 Geneva
'Rigid Naphthalenediimides Rods as Anion- π
Slides in Lipid Bilayer Membranes'
Abstract 241
- 15.45–16.00 **D. Schultz, J.R. Nitschke**
Department of Organic Chemistry, University of
Geneva, 1211 Geneva 4
'Dynamic Assembly and Reassembly of
Metallo-organic Complexes from
Subcomponents'
Abstract 242
- 16.00–16.15 **T.M. Seidel, G. Bernardinelli, E.P. Kündig**
Department of Organic Chemistry, University of
Geneva, 1211 Geneva
'Chiral 2-(1-aminoalkyl)phenols as Building
Blocks for New Chiral Ligands'
Abstract 243
- 16.15–16.30 **J.R. Noyes, J.S. Siegel**
University of Zürich, 8057 Zürich
'Trioxatricornan Derivatives: Reactivity and
Building Blocks'
Abstract 244
- 16.30–16.45 **R. Vallinayagam^a, F. Schmitt,
L. Juillerat-Jeanneret^b, R. Neier^a**
^aUniversity of Neuchâtel, 2000 Neuchâtel
^bUniversity Institute of Pathology, CHUV,
1011 Lausanne
'Sugar ALA (5-Aminolevulinic acid)
derivatives - A Sweet Alternative for ALA in
PDT (Photodynamic therapy)?'
Abstract 245
- Session 2 **Organic Structure and Properties II**
- 11.15–12.30 **Lectures**
University Zürich-Irchel, HS 55
Abstracts 246–250
Chair: N.W. Luedtke
- 11.15–11.30 **D. Bandera^a, Y.-T. Wu^{a,b}, R. Maag^a, A. Linden^a,
J.S. Siegel^a**
^aUniversity of Zürich, 8057 Zürich
^bNational Cheng-Kung University, Tainan City,
Taiwan, R.O.C.
'Multiethynyl Substituted Corannulene
Derivatives: Synthesis and Properties'
Abstract 246
- 11.30–11.45 **A. Herrmann^a, B. Levranda^a, Y. Ruff^b,
J.-M. Lehn^b**
^aFirmenich SA, Division Recherche &
Développement, 1211 Genève 8
^bISIS, Université Louis Pasteur,
67083 Strasbourg, France
'Controlled Fragrance Release from Dynamic
Mixtures Obtained by Reversible Reaction of
Hydrazides With Volatile Aldehydes or Ketones'
Abstract 247
- 11.45–12.00 **F. Flachsmann, D. Anderson, G. Fráter,
M. Gautschi**
Givaudan Switzerland Ltd, Fragrance Research,
8600 Dübendorf
'Studies on o-Hydroxy Cinnamates as Traceless,
Light-Cleavable Precursors for
Perfumery Ingredients'
Abstract 248
- 12.00–12.15 **M. Hutin, G. Bernardinelli, J.R. Nitschke**
University of Geneva, 1211 Geneva 4
'Complex Architectures from Simple Building
Blocks Through Subcomponent Self- Assembly'
Abstract 249
- 12.15–12.30 **M. Kümin, H. Wennemers**
Department of Chemistry, University of Basel,
4056 Basel
'Functionalized Polyprolines – Switchable and
Conformationally Well-defined Molecular
Scaffolds'
Abstract 250

- 12.30–14.15 Poster Session**
University Zürich-Irchel, Lichthof Area
Abstracts 259–344
- 14.15–14.45 General Assembly of the Swiss Chemical Society**
University Zürich-Irchel, HS 30
- 14.45–16.45 Lectures**
University Zürich-Irchel, HS 55
Abstracts 251–258
Chair: **R. Dorta**
- 14.45–15.00 **N.W. Luedtke^a, D. Fried^b, R. Dexter^b, A. Schepartz^b**
^aOrganic Chemistry Institute, University of Zürich, 8057 Zürich
^bDepartment of Chemistry, Yale University, New Haven, USA
'Fluorogenic Detection and Capture of Well-Folded Proteins'
Abstract 251
- 15.00–15.15 **I. Bouamaied, E. Stulz**
University of Basel, 4056 Basel
'Porphyrin Substituted Oligonucleotides: Synthesis and Spectroscopy'
Abstract 252
- 15.15–15.30 **C. Didier, C. Craita, P. Vogel**
Ecole Polytechnique Fédérale de Lausanne, 1015 Lausanne
'Studies Towards the Total Asymmetric Synthesis of Apoptolidin and Analogues. Application of the Vogel's Cascade'
Abstract 253
- 15.30–15.45 **J. Velcicky^a, H. Ishikawa, G.I. Elliott, Y. Choi, Y. Li, M.M. Miller, D.L. Boger**
Department of Chemistry and Skaggs Institute for Chemical Biology, The Scripps Research Institute, La Jolla, CA 92037, USA
^aNovartis Pharma AG, 4056 Basel
'Total Synthesis of Vindoline and Vindorosine by Tandem [4+2]/[3+2]-Cycloaddition'
Abstract 254
- 15.45–16.00 **G. Coste, S. Gerber-Lemaire**
Institute of Chemical Sciences and Engineering, Ecole Polytechnique Fédérale de Lausanne (EPFL), 1015 Lausanne
'New Efficient Synthesis of Long Chain di- and Tri- Aminopolyols'
Abstract 255
- 16.00–16.15 **J. Kofoed, T. Darbre, J.-L. Reymond**
Department of Chemistry & Biochemistry, University of Berne, 3012 Bern
'Aldolase Peptide Dendrimers from Combinatorial Libraries'
Abstract 256
- 16.15–16.30 **A. Zahn, C. Leumann**
University of Bern, 3012 Bern
'Biphenylic DNA'
Abstract 257

- 16.30–16.45 **K. Gademann^a, S. Bonazzi^a, S. Güttinger^b, I. Zemp^b, U. Kutay^b**
^aLaboratorium für Organische Chemie, ETH Zürich, 8092 Zürich
^bInstitut für Biochemie, ETH Zürich, 8092 Zürich
'Controlling Cellular Pathways by Synthetic Natural Products'
Abstract 258

16.45–17.15 Coffee Break

- 17.15–17.30 Mettler Toledo Prizes for best oral presentations**
SCS prizes for best poster contributions

17.30–18.15 Presentation of the Paracelsus Prize 2006**Physical Chemistry**

- 11.15–12.30 Lectures**
University Zürich-Irchel, HS 80
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Chair: **M. Quack**
- 11.15–11.30 **B. Lang^a, N. Banerji^a, O. Mohammed^a, E. Nibbering^b, E. Vauthey^a**
^aUniversity of Geneva, 1211 Geneva 4
^bMax-Born-Institut, 12489 Berlin-Adlershof, Germany
'Ultrafast Time-resolved Infrared Studies on Photoinduced Bimolecular Electron Transfer'
Abstract 345
- 11.30–11.45 **V. Krylov, A. Kushnarenko, E. Miloglyadov, M. Quack, G. Seyfang**
Laboratorium für Physikalische Chemie, ETH Zürich, 8093 Zürich
'Fast Redistribution of Vibrational Energy in Methyl Iodides'
Abstract 346
- 11.45–12.00 **P. Maksyutenko, O.V. Boyarkin, T.R. Rizzo**
Ecole Polytechnique Fédérale de Lausanne, LCPM, ISIC, EPFL, 1015 Lausanne
'Direct Spectroscopic Measurement of Water Dissociation Energy'
Abstract 347
- 12.00–12.15 **H.J. Wörner, R. van der Veen, F. Merkt**
Laboratorium für Physikalische Chemie, ETH Zürich, 8093 Zürich
'The Jahn-Teller Effect in CH₄⁺ Characterized by High-resolution Photoelectron Spectroscopy'
Abstract 348

12.15–12.30 **C. Kolano^a, J. Helbing^a, M. Kozinski^a, W. Sander^b, P. Hamm^b**
^aPhysikalisch-Chemisches Institut, Universität Zürich, 8057 Zürich
^bLehrstuhl für Organische Chemie II, Ruhr-Universität Bochum, Germany
 'Towards a Molecular Movie: Real Time Observation of Hydrogen Bond Breaking by Transient 2D-IR Spectroscopy in a Cyclic Peptide'
 Abstract 349

12.30–14.15 **Poster Session**
 University Zürich-Irchel, Lichthof Area
 Abstracts 357–415

14.15–14.45 **General Assembly of the Swiss Chemical Society**
 University Zürich-Irchel, HS 30

14.45–16.30 **Lectures**
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 Abstracts 350–356
 Chair: **F. Merkt**

14.45–15.00 **K. Piech, A. Marcinek, T. Bally**
 Department of Chemistry, University of Fribourg, 1700 Fribourg
 'Radical Ions of N-Nitrosoamines and Their Fragmentation'
 Abstract 350

15.00–15.15 **S. Albert, M. Quack**
 Laboratorium für Physikalische Chemie, ETH Zürich, 8093 Zürich
 'The Highly Resolved FTIR Spectrum of Pyrimidine'
 Abstract 351

15.15–15.30 **S. Albert, H. Hollenstein, M. Quack, M. Willeke**
 Laboratorium für Physikalische Chemie, ETH Zürich, 8093 Zürich
 'Rovibrational Analysis of the High Resolution Infrared Spectrum of CH³⁵ClF₂ Involving the Vibrational Levels ν_4 , $2\nu_6$, $\nu_6 + \nu_9$ and $2\nu_6$: Experiment and Theory'
 Abstract 352

15.30–15.45 **E. Vliegen, F. Merkt**
 Laboratorium für Physikalische Chemie, ETH Zürich, 8093 Zürich
 'Rydberg Stark Deceleration of Atomic Hydrogen'
 Abstract 353

15.45–16.00 **A. Fouqueau, M. Meuwly**
 Department of Chemistry, University of Basel, 4056 Basel
 'Adsorption of Acridine Orange C₈/Water/Acetonitrile Interface'
 Abstract 354

16.00–16.15 **K. Lutkouskaya, G. Calzaferri**
 University of Bern, 3012 Bern
 'Dimensionality of Energy Transfer in Dye-loaded Zeolite L Host-guest Materials'
 Abstract 355

16.15–16.30 **N. Bonalumi, A. Vargas, D. Ferri, T. Mallat, A. Baiker**
 Institute for Chemical and Bioengineering, Department of Chemistry and Applied Biosciences, ETH Zürich, 8093 Zürich
 'Switch of Enantioselectivity on a Chirally Modified Metal Surface Induced by Conformational Changes'
 Abstract 356

16.45–17.15 Coffee Break

17.15–17.30 Mettler Toledo Prizes for best oral presentations
SCS prizes for best poster contributions

17.30–18.15 Presentation of the Paracelsus Prize 2006

Polymer Science

11.15–13.00 **Lectures**
 University Zürich-Irchel, HS 60
 Abstracts 416–419
 Chair: **R. Deschenaux**

11.15–12.00 **R. Janssen**
 Molecular Materials and Nanosystems, Eindhoven University of Technology, 5600 MB Eindhoven, The Netherlands
 'Bulk Heterojunction Polymer Solar Cells'
 Abstract 416

12.00–12.20 **T. Geiger, F. Nüesch**
 EMPA, Laboratory for Functional Polymers, 8600 Dübendorf
 'Polymeric Dyes'
 Abstract 417

12.20–12.40 **F. Teixeira, C. Vebert**
 University of Basel, 4056 Basel
 'Hierarchical and Functional Self-assembly of Polymers driven by Biochemical Interactions'
 Abstract 418

12.40–13.00 **A. Zhang, A. D. Schlüter**
 Department of Materials, ETH-Zürich, 8093 Zürich
 'Towards Helical Dendrinozed Polymers'
 Abstract 419

13.00–14.15 Poster Session
 University Zürich-Irchel, Lichthof Area
 Abstracts 425–456

14.20–16.30 Lectures
 University Zürich-Irchel, HS 60
 Abstracts 420–424
 Chair: **H.-A. Klok**

- 14.20–14.50 **K. Velonia**
Department of Organic Chemistry,
University of Geneva, 1211 Geneva 4
'Protein-polymer Amphiphiles:
Novel Approaches and Aggregation Studies'
Abstract 420
- 14.50–15.10 **M. Bornand, P. Chen**
Laboratorium für Organische Chemie der
ETH Zürich, 8093 Zürich
'Sequence Controlled Metathesis
Polymerization with Well-defined Catalysts'
Abstract 421
- 15.10–15.40 **A. Godt^a, G. Jeschke^b**
^aUniversität Bielefeld, 33615 Bielefeld,
Germany
^bMax-Planck-Institut für Polymerforschung,
55122 Mainz, Germany
'Spinning Around Rod-like and
Entwined Molecules'
Abstract 422
- 15.40–16.00 **S. Tugulu^a, M. Harms^b, M. Fricke^b,
D. Volkmer^b, H.-A. Klok^a**
^aÉcole Polytechnique Fédérale de Lausanne
(EPFL), Institut des Matériaux, Laboratoire des
Polymères, 1015 Lausanne
^bFaculty of Chemistry, University of Ulm,
89081 Ulm, Germany
'Polymer Brushes as Templates for Biomimetic
Materials Fabrication of Microstructured
Calcite Films'
Abstract 423
- 16.00–16.30 **W. Caseri**
Department of Materials, ETH Zürich,
8093 Zürich
'From Polymer-metal Nanocomposites to
Polymeric Metal Wires'
Abstract 424
- 16.45–17.15 Coffee Break**
- 17.15–17.30 Mettler Toledo Prizes
for best oral presentations
SCS prizes for
best poster contributions**
- 17.30–18.15 Presentation of the
Paracelsus Prize 2006**