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SOCIETE SUISSE DE CHIMIE SSC

SWISS CHEMICAL SOCIETY SCS

DIVISIONS
ANALYTICAL CHEMISTRY
CHEMICAL RESEARCH
MEDICINAL CHEMISTRY

DIVISIONEN
ANALYTISCHE CHEMIE
CHEMISCHE FORSCHUNG
MEDIZINISCHE CHEMIE

DIVISIONS
CHIMIE ANALYTIQUE
RECHERCHE CHIMIQUE
CHIMIE THERAPEUTIQUE

Fall Meeting 2005 Herbstversammlung 2005 Assemblée d'automne 2005

Thursday, October 13th, 2005
Donnerstag, 13. Oktober 2005
Jeudi, 13 octobre 2005

Lausanne

**Ecole Polytechnique Fédérale de Lausanne
Centre Est**

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 Ecole polytechnique fédérale de Lausanne, EPFL-ISIC, Station 6, 1015 Lausanne
 Tel.: +41 21 693 3611, E-Mail: scs.fallmeeting@epfl.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, as this will be required at the entrance of the buildings and will have to be worn as a name tag during the meeting.

Non-members of the SCS will be asked to pay a CHF 50.– 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 a round-trip train ticket to Lausanne/Renens (2nd class, ½ fare) by sending a filled-in reimbursement form to the SCS central office along with their used train ticket. The form will be available at the registration desk of the meeting and can be downloaded from the SCS website (<http://www.swiss-chem-soc.ch/young/reimbursement.html>). For members traveling from abroad, only travel expenses within Switzerland will be covered (2nd class, ½ 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 next to the meeting venues.

Coffee breaks: Coffee and drinks will be available until 10.00 in the morning and a coffee break will be organized between 16.30 and 17.00, before the Grammaticakis-Neumann Prize presentation.

Transportation

By train: Only a number of limited parking spaces will be available on the campus of the Ecole polytechnique fédérale de Lausanne. Hence, travel by train is recommended. The EPFL campus can be easily reached by tram, either from Lausanne or Renens train stations. Travelers arriving at Lausanne can continue their journey with the InterRegio train to Renens (1 stop, 4 min). From Renens station, the trip by tram (TSOL) to EPFL (tram stop *UNIL-Sorge*) takes 7 min. Alternatively, travelers arriving in Lausanne can take the metro (metro station is across the square from the train station) to *Place du Flon*, and then the tram (TSOL, 13 min.) to *UNIL-Sorge*. The map shows the way from the tram stop (*UNIL-Sorge*) to the entrance of the meeting. More information on how to get to EPFL campus, timetables and interactive maps are available on the webpage at <http://map.epfl.ch/>.

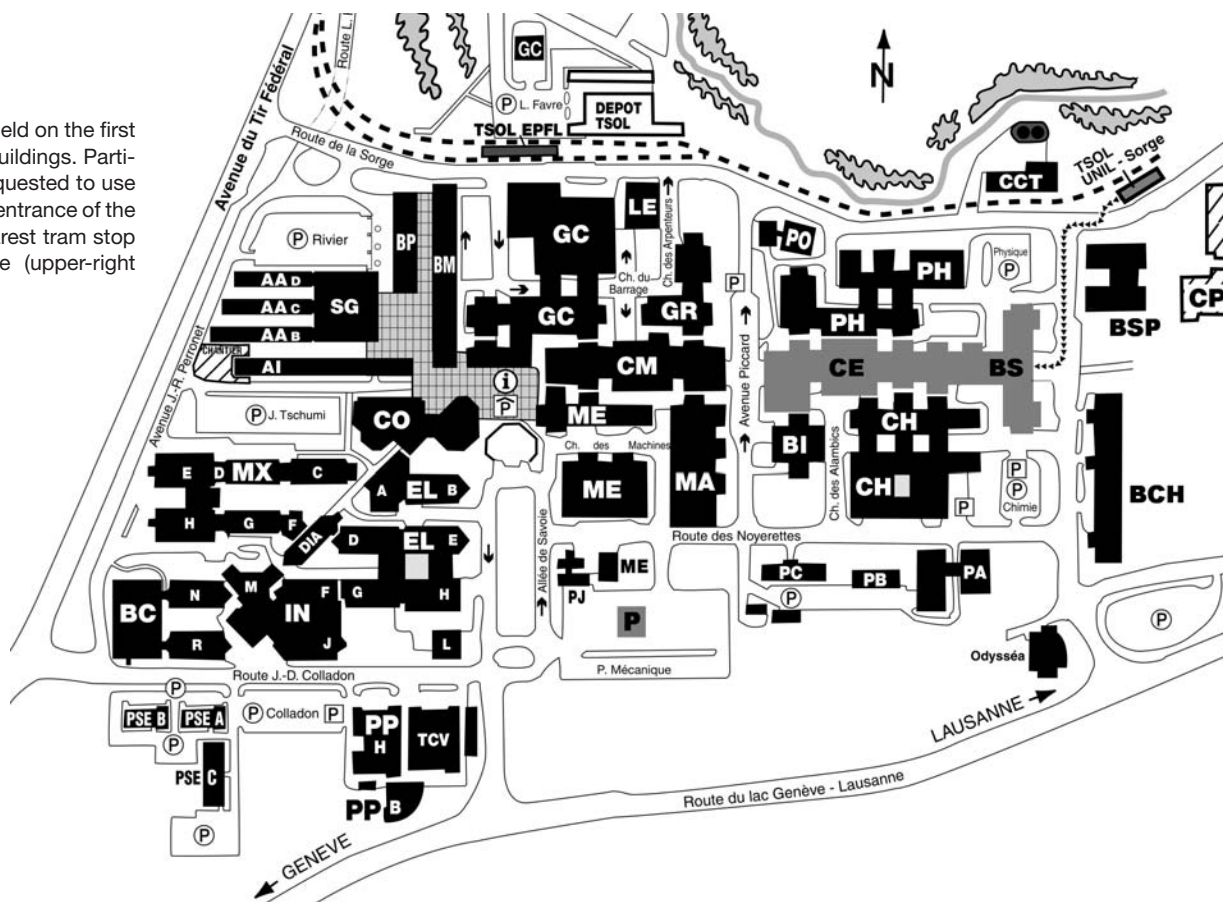
By car: On the freeway, follow Lausanne-Sud, exit at UNIL-EPFL and then turn right at the sign EPFL/UNIL. Limited space will be available at the parking lot 'Mécanique' (see map). One-day parking permits will be sold at the registration desk for CHF 5.–.

Train Timetable

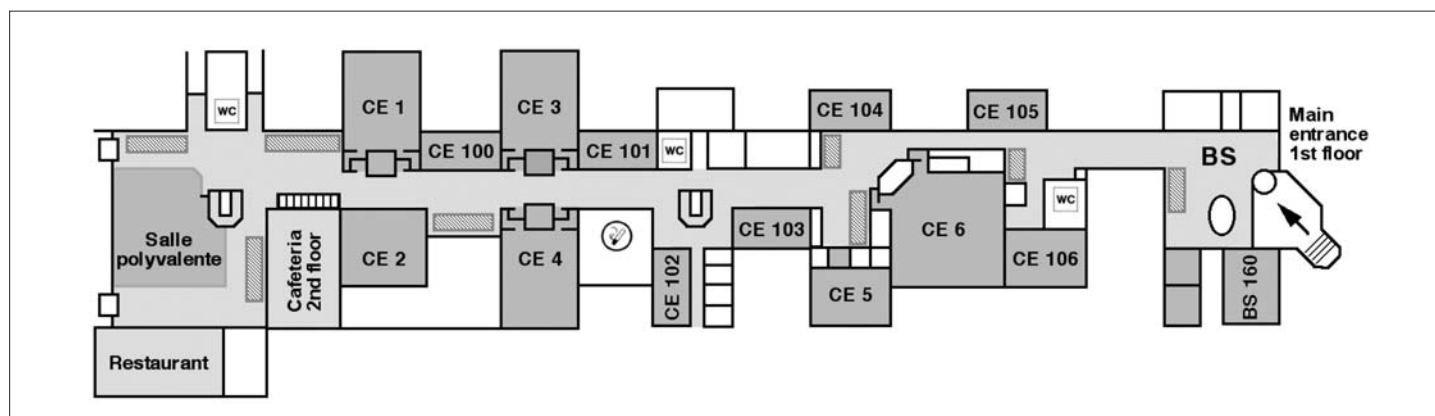
Morning				Evening			
Train from	Departure	Arrival Lausanne	Arrival Renens	Departure Renens	Departure Lausanne	Arrival	Train to
Basel	07.05	09.15	09.24	18.34	18.45	20.53	Basel
Bern	08.04	09.15	09.24	18.34	18.45	19.56	Bern
Fribourg	08.26	09.15	09.24	18.34	18.45	19.33	Fribourg
Genève	08.36	09.15	09.24	18.31	18.42	19.15	Genève
Neuchâtel	08.34	09.15	09.24	18.34	18.45	19.25	Neuchâtel
Zürich	07.04	09.15	09.24	18.34	18.45	20.56	Zürich

EPFL Campus

The meeting will be held on the first floor of BS and CE buildings. Participants are kindly requested to use exclusively the main entrance of the BS building. The nearest tram stop is TSOL UNIL-Sorge (upper-right corner on the map).



Detailed Map of Lecture Rooms



CE 6: Opening Ceremony, 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

Salle Polyvalente, Main Hall, CE 100, CE 101, CE 102, CE 103, CE 105: Poster sessions

Sponsors

The organization of the meeting gratefully acknowledges the generous support of the following fine companies (see the meeting website <http://scs-fallmeeting.epfl.ch> for an updated list of sponsors):

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Program of the Fall Meeting 2005

10.00–10.50 Opening Ceremony

EPFL, CE 6

Presentation of the Werner Prize 2005

Chair: Georg Fráter

Lecture of the Werner Prize Laureate 2005

Ruth Signorell

University of British Columbia, Vancouver,
BC V6T 1Z1, Canada

'Physical Chemistry of Dust: From
Atmospheric Aerosols to Drug Nanoparticles'
Abstract 1

11.00–16.30 Analytical Chemistry

11.00–11.30 General Assembly of the Members of the Division

EPFL, CE 2

11.30–12.50 Lectures

EPFL, CE 2

Abstracts 3, 7, 8

12.50–14.30 Poster Session

EPFL, CE 100

Abstracts 13–48

14.30–16.30 Lectures

EPFL, CE 2

Abstracts 4, 9–12

11.00–16.30 Medicinal Chemistry

11.00–11.10 General Assembly of the Members of the Division

EPFL, CE 5

11.15–13.15 Lectures

EPFL, CE 5

Abstracts 49–56

13.15–14.15 Poster Session

EPFL, CE 103

Abstracts 66–81

14.15–16.30 Lectures

EPFL, CE 5

Abstracts 57–65

11.00–16.30 Chemical Research

11.00–11.15 General Assembly of the Members of the Division

EPFL, CE 6

11.15–16.30 Computational Chemistry

11.15–12.45 Lectures

EPFL, CE 106

Abstracts 82–87

12.45–14.30 Poster Session

EPFL, CE 105

Abstracts 96–106

14.30–16.30 Lectures

EPFL, CE 106

Abstracts 88–95

11.15–16.30 Inorganic and Coordination Chemistry

11.15–12.45 Minisymposium

EPFL, CE 6

Abstracts 5, 6

12.45–14.30 Poster Session

EPFL, CE Salle Polyvalente

Abstracts 117–206

14.30–16.30 Lectures

EPFL, CE 6

Abstracts 107–116

11.15–16.30 Organic Chemistry

Session A1 Synthesis and Synthetic Methodology I

11.15–12.45 Lectures

EPFL, CE 1

Abstracts 207–212

12.45–13.00 Poster Talks

EPFL, CE 1

Abstracts 213–215

Session B1 Organic Structure and Properties I

11.15–12.45 Lectures

EPFL, CE 3

Abstracts 216–221

12.45–13.00 Poster Talks

EPFL, CE 3

Abstracts 222–224

Sessions A & B

13.00–14.30 Poster Session

EPFL, CE Salle Polyvalente

Abstracts 239–299

Session A2 Synthesis and Synthetic Methodology II

14.30–16.30 Lectures

EPFL, CE 1

Abstracts 225–231

Session B2 Organic Structure and Properties II

14.30–16.30 Lectures

EPFL, CE 3

Abstracts 232–238

11.15–16.30 Physical Chemistry

11.15–12.45 Lectures

EPFL, CE 4

Abstracts 300–305

12.45–13.00 Poster Talks

EPFL, CE 4

Abstracts 306–310

- 13.00–14.30** **Poster Session**
EPFL, CE 101
Abstracts 313, 320–363
- 14.30–16.30** **Lectures**
EPFL, CE 4
Abstracts 311, 312, 314–319
- 16.30–17.00** **Coffee Break**
- 17.00–17.15** **Presentation of the Awards for the Best Oral and Poster Presentations**
EPFL, CE 6

Analytical Chemistry

2 poster and 1 oral presentations
Jury: *R. Zenobi, H.H. Girault*

Medicinal Chemistry

1 poster and 2 oral presentations
Jury: *W. Froestl, P. Mohr*

Computational Chemistry

1 poster and 1 oral presentations
Jury: *U. Röthlisberger, C.A. Daul*

Inorganic and Coordination Chemistry

3 poster and 1 oral presentations
Jury: *K. Severin, T.R. Ward, P.S. Pregosin, E. Constable*

Organic Chemistry

2 poster and 2 oral presentations
Jury: *J. Siegel, N. Finney, K. Gademann, J. Nitschke, C. Bochet, H. Wennemers, T. Darbre*

Physical Chemistry

2 poster and 1 oral presentation
Jury: *F. Merkt, E. Vauthey, M. Rossi*

17.15–18.00 **Presentation of the Grammaticakis-Neumann Prize 2005***EPFL, CE 6*Chair: *Georg Fráter***Lecture of the Grammaticakis-Neumann Prize Laureate 2005***Dario M. Bassani*

Université de Bordeaux I, Talence, France
'Exciting Supramolecular Assemblies'
Abstract 2

DETAILED PROGRAM**Analytical Chemistry**

- 11.00–11.30** **General Assembly of the Members**
EPFL, CE 2
- 11.30–12.10** **Invited lecture**
Reginald M. Penner
University of California, Irvine, CA 92697, USA
'Chemical Sensing Using Metal Nanowire Arrays'
Abstract 3
- 12.10–12.50** **Lectures**
EPFL, CE 2
Abstracts 7, 8
Chair: *R. Zenobi*
- 12.10–12.30 *V. Chaurin*^a, G. Bianké^b, E.C. Constable^a, M. Egorov^c, R. Häner^b, C. Housecroft^a, J. Lebreton^c
^aUniversity of Basel, CH-4056 Basel
^bUniversity of Bern, CH-3012 Bern
^cLaboratoire de Synthèse Organique, F-44322 Nantes
'Oligonucleotide-Arrays: Use of Oligonucleotide-Metal Conjugates for the Detection of DNA'
Abstract 7
- 12.30–12.50 *M. Prudent*, T.C. Rohner, C. Roussel, H.H. Girault
Ecole polytechnique fédérale de Lausanne, CH-1015 Lausanne
'Metal Ions-Peptides Complexes Study by Micro-Chip ESI-MS'
Abstract 8
- 12.50–14.30** **Poster Session**
EPFL, CE 100
Abstracts 13–48
- 14.30–15.10** **Invited lecture**
Emmanuel Delamar, D. Juncker, H. Schmid
IBM Zürich Research Laboratory, CH-8803 Rüschlikon
'Microfluidics for Bioanalytical Applications'
Abstract 4
- 15.10–16.30** **Lectures**
EPFL, CE 2
Abstracts 9–12
Chair: *H.H. Girault*
- 15.10–15.30 *C. Frei*, D. Günther
ETH Zürich, CH-8093 Zürich
'Comparison of Various Powder Preparation Techniques for LA-ICP-MS Analysis'
Abstract 9

- 15.30–15.50 **R.J. Wenzel**, A. Nazabal, R. Zenobi
ETH Zürich, CH-8093 Zürich
'Measurement of Intact, High Mass Protein Complexes by MALDI Mass Spectrometry'
Abstract 10
- 15.50–16.10 **Y. Henchoz**^{a,b}, L. Geiser^a, P.-A. Carrupt^b, J.-L. Veuthey^a
^aUniversity of Geneva, CH-1211 Geneva 4
^bEcole de Pharmacie Genève-Lausanne, CH-1211 Genève 4
'Rapid Determination of pKa Values by Capillary Zone Electrophoresis'
Abstract 11
- 16.10–16.30 **L.A. Leuthold**, J.-F. Mandscheff, E. Varesio, G. Hopfgartner
University of Geneva, CH-1211 Geneva 4
'Desorption Electrospray Ionization Mass Spectrometry (DESI-MS): Direct Drug Tablets Analysis'
Abstract 12
- 16.30–17.00 Coffee Break**
- 17.00–17.15 Presentation of the Awards for Best Oral and Poster Presentations**
- 17.15–18.00 Presentation of the Grammaticakis-Neumann Prize**
- 12.00–12.15 **D. Strasser**^a, S. Shelke^a, B. Cutting^a, M. Porro^a, G.-P. Gao^a, T. Viseruna^a, O. Schwardt^a, S. Rabbani^a, H. Gächje^b, S. Kelm^b, B. Ernst^a
^aUniversity of Basel, CH-4056 Basel
^bUniversity of Bremen, D-28334 Bremen
'Exploring the Binding Mode of Sialic Acid Derivatives as Myelin-associated Glycoprotein (MAG) Ligands'
Abstract 52
- 12.15–12.30 **U. Grether**, A. Bénardeau, J. Benz, A. Binggeli, B. Bittner, M. Böhringer, A. Flament, H. Hilpert, G. Hirth, H. Isel, B. Kuhn, H.P. Märki, M. Meyer, P. Mohr, K. Püntener, S. Raab, F. Ricklin, A. Ruf, U. Sprecher, P. Verry, N. Wyttenbach
F. Hoffmann-La Roche Ltd., CH-4070 Basel
'PPAR α/γ Co-Agonists: Combining Antidiabetic and Hypolipidemic Activity'
Abstract 53
- 12.30–12.45 **H. Fiaux**^a, D. Kuntz^b, P. Vogel^a, D. Rose^b, S. Gerber-Lemaire^a, L. Juillerat Jeanneret^c
^aEcole polytechnique fédérale de Lausanne, CH-1015 Lausanne
^bOntario Cancer Institute, Toronto, Canada
^cUniversity Institute of Pathology, CHUV, CH-1000 Lausanne
'Pyrrolidine Derivatives as New Inhibitors of α -Mannosidases and Growth Inhibitors of Human Cancer Cells'
Abstract 54

Medicinal Chemistry

- 11.00–11.10 **General Assembly of the Members**
EPFL, CE 5
- 11.15–13.15 **Lectures**
EPFL, CE 5
Abstracts 49–56
Chair: **W. Froestl**
- 11.15–11.30 **H. Fretz**, O. Houille, K. Hilpert, M. Singer, S. Brand, O. Peter, V. Breu, T. Giller, O. Valdenaire, M. Riederer
Actelion Pharmaceuticals Ltd., CH-4123 Allschwil
'Novel Pyrazolidine-3,5-Dione Derivatives are P2Y₁₂ Receptor Antagonists and Inhibit ADP-Triggered Blood Platelet Aggregation'
Abstract 49
- 11.30–11.45 **A. Vaupel**
Novartis Institutes of Biomedical Research, CH-4002 Basel
'VEGFR2 Kinase Inhibitors for Antiangiogenic Therapy in Cancer'
Abstract 50
- 11.45–12.00 **E. Schweizer**, J. Olsen, K. Schärer, A. Hoffmann-Röder, F. Diederich
ETH Zürich, CH-8093 Zürich
'Molecular Recognition Studies in the Active Site of Thrombin'
Abstract 51
- 12.45–13.00 **S. Veenstra**, P. Felber, T. Hauri
Novartis Pharma AG, CH-4057 Basel
'Novel Highly Stereoselective Synthesis of (\pm)-(2R*,4S*,5S*)-Hydroxyethylene Transition State Mimetics'
Abstract 55
- 13.00–13.15 **C. Fuhrer**^a, S. Ruetz^b, E. Grüter^a, R. Häner^a
^aUniversity of Bern, CH-3012 Bern
^bNovartis Institutes of Biomedical Research, CH-4002 Basel
'Synthesis and Further Derivatization of Furo[3,4-c]pyranones with Antiproliferative and Apoptotic Activity'
Abstract 56
- 13.15–14.15 Poster Session**
EPFL, CE 103
Abstracts 66–81
- 14.15–16.30 Lectures**
EPFL, CE 5
Abstracts 57–65
Chair: **P. Mohr**
- 14.15–14.30 **R.M. Rodríguez Sarmiento**, A. Alanine, A. Cesura, A.W. Thomas, R. Wyler
F. Hoffmann-La Roche Ltd., CH-4070 Basel
'Discovery of Novel, Potent and Fully Selective MAO-B Inhibitors Using an Elegant Hit to Lead Paradigm'
Abstract 57

- 14.30–14.45 **C. Starckenmann**, Y. Niclass, M. Troccaz, A.J. Clark
Firmenich SA, CH-1211 Genève 8
'Identification of the Precursor of (S)-3-Methyl-3-Sulfanylhexan-1-ol, the Sulfury Malodour of Human Axilla-Sweat'
Abstract 58
- 14.45–15.00 **K. Johansson**, R. Born, D. Stokmaier, D. Ricklin, S. Rabbani, B. Ernst
University of Basel, CH-4056 Basel
'Cloning and Characterization of Cysteine Mutants of the Asialoglycoprotein Receptor H1-CRD'
Abstract 59
- 15.00–15.15 **A. Zumbuehl**, D.G. Anderson, R. Langer
MIT, Cambridge, MA 02139, USA
'Gene Therapy Using Degradable Poly (β -Amino Esters)'
Abstract 60
- 15.15–15.30 **O. Zerbe^a**, J. Mares^a, J. Müller^b, A. Skirgailiene^a, R.R. Schmidt^b
^aUniversity of Zürich, CH-8057 Zürich
^bUniversität Konstanz, D-78457 Konstanz
'A Model for Cell Surface Exposed Carbohydrate Units'
Abstract 61
- 15.30–15.45 **M. Rogers–Evans**, L. Alig, A. Alanine, M. Andjelkovic, A. Benardeau, K. Bleicher, A. Bourson-Sleight, P. David-Pierson, W. Guba, J. Higelin, D. Kube, T. Lübbers, S. Mohr, W. Neidhart, J.-M. Plancher, C. Rocha, S. Röver, G. Schneider, J. Smit, S. Taylor
F. Hoffmann-La Roche Ltd., CH-4070 Basel
'CB-1 Antagonists: From Knowledge Based Design to Lead Optimization'
Abstract 62
- 15.45–16.00 **J. Maibaum**
Novartis Pharma AG, CH-4002 Basel
'Aliskiren: A Structurally Unique Oral Renin Inhibitor'
Abstract 63
- 16.00–16.15 **O. Khorev**, D. Stokmaier, O. Schwardt, B. Ernst
University of Basel, CH-4056 Basel
'Fluorescent Trivalent Gal/GalNAc-Terminated Ligands for the Asialoglycoprotein Receptor (ASGP-R)'
Abstract 64
- 16.15–16.30 **P. Furet**, K.-H. Altmann, G. Bold, P. Manley, T. Meyer, J. Mestan, W. Stark
Novartis Institutes for Biomedical Research, CH-4002 Basel
'Discovery of a New Class of Angiogenesis Inhibitors by Molecular Modeling'
Abstract 65

16.30–17.00 Coffee Break**17.00–17.15 Presentation of the Awards for Best Oral and Poster Presentations****17.15–18.00 Presentation of the Grammaticakis-Neumann Prize****Chemical Research****11.00–11.15 General Assembly of the Members**
EPFL, CE 6**Computational Chemistry****11.15–12.45 Lectures**
EPFL, CE 106
Abstracts 82–87
Chair: **U. Röthlisberger**

11.15–11.30 **O.V. Yazyev**, L. Helm
Ecole polytechnique fédérale de Lausanne, CH-1015 Lausanne
'Magnetization of Metallic Carbon Nanotubes by Paramagnetic Centers'
Abstract 82

11.30–11.45 **F.F.-F. Schmid**, M. Meuwly
University of Basel, CH-4056 Basel
'Molecular Dynamics Approach to Characterize the Guanylate Cyclase PleD'
Abstract 83

11.45–12.00 **O. Naef^a**, J.-N. Aebischer^a, M. Amrhein^b, G. Corminboeuf^a, S. Crelier^c, E. Vanoli^a, P. Voirin^a
^aEcole d'ingénieurs de Fribourg, CH-1705 Fribourg
^bEcole polytechnique fédérale de Lausanne, CH-1015 Lausanne
^cHaute école valaisanne, CH-1950 Sion
'Information Extraction from the Evolving Factor Analysis'
Abstract 84

12.00–12.15 **M.A. Lill**, M. Dobler, A. Vedani
Biographics Laboratory 3R, CH-4056 Basel
University of Basel, CH-4056 Basel
'Impact of Induced Fit for Ligand Binding to Proteins: Development of Multidimensional QSAR Technologies'
Abstract 85

12.15–12.30 **M. Dulak**, T.A. Wesolowski
University of Geneva, CH-1211 Geneva 4
'Intermolecular Complexes from van der Waals to Hydrogen Bonds: Benchmark Calculations Using Subsystem Formulation of Density Functional Theory'
Abstract 86

12.30–12.45 **P. Banushkina**, M. Meuwly
University of Basel, CH-4056 Basel
'Ligand Migration in Complex Environments'
Abstract 87

12.45–14.30 Poster Session
EPFL, CE 105
Abstracts 96–106

- 14.30–16.30 Lectures**
EPFL, CE 106
Abstracts 88–95
Chair: **C. Daul**
- 14.30–14.45 **S. Lammers**, J. Danielsson, M. Meuwly
University of Basel, CH-4056 Basel
'Reactive Molecular Dynamics Simulation of Proton Transfer in Proteins'
Abstract 88
- 14.45–15.00 **A. Daina**, S. Rey, L. Novaroli, M. Reist, P.-A. Carrupt
Ecole de Pharmacie Genève-Lausanne, CH-1211 Genève 4
'Pre- and Post-processing Molecular Interaction Fields Tools in Receptor-Based Drug Design Strategy towards Neurodegenerative Diseases'
Abstract 89
- 15.00–15.15 **F. Bajor**^a, F. Bourasset^b, S. Cisternino^b, J.-M. Scherrmann^b, P.-A. Carrupt^a
^aEcole de Pharmacie Genève-Lausanne, CH-1211 Genève 4
^bUniversité Paris 5 & 7, Hôpital Fernand Vidal, F-75475 Paris
'A 3D Solvatochromic Model of Blood-brain Barrier Permeation Based on Molecular Interaction Fields Descriptors'
Abstract 90
- 15.15–15.30 **I. Lin**, O.A. von Lilienfeld, M.D. Coutinho-Neto, I. Tavernelli, U. Röthlisberger
Ecole polytechnique fédérale de Lausanne, CH-1015 Lausanne
'Atom Centered Potentials for London Dispersion Forces in Density Functional Theory'
Abstract 91
- 15.30–15.45 **I. Tavernelli**, U. Röthlisberger
Ecole polytechnique fédérale de Lausanne, CH-1015 Lausanne
'Response Properties of Liquid Water using Time Dependent Density Functional Theory'
Abstract 92
- 15.45–16.00 **E. Tapavicza**, I. Tavernelli, U. Röthlisberger
Ecole polytechnique fédérale de Lausanne, CH-1015 Lausanne
'Computation of Non-Adiabatic Coupling Using Time-Dependent DFT'
Abstract 93
- 16.00–16.15 **M.C. Colombo**, P. Baillod, I. Tavernelli, U. Röthlisberger
Ecole polytechnique fédérale de Lausanne, CH-1015 Lausanne
'A Study of the Structural Stability of the C-terminal Domain of the Mouse Prion Protein'
Abstract 94

- 16.15–16.30 **M. Atanasov**^{a,b,c}, C. Daul^a, P. Comba^c
^aUniversity of Fribourg, CH-1700 Fribourg
^bBulgarian Academy of Sciences, 1113 Sofia, Bulgaria
^cRuprecht-Karls-Universität Heidelberg, D-69120 Heidelberg
'Theoretical Studies on the Electronic Properties and the Chemical Bonding of Transition Metal Complexes using DFT and Ligand Field Theory'
Abstract 95

16.30–17.00 Coffee Break**17.00–17.15 Presentation of the Awards for Best Oral and Poster Presentations****17.15–18.00 Presentation of the Grammaticakis-Neumann Prize****Inorganic and Coordination Chemistry**

- 11.15–12.45 Minisymposium**
EPFL, CE 6
Chair: **P.S. Pregosin**
- 11.15–12.00 **Richard Winpenny**
University of Manchester, Manchester M13 9PL, UK
'Studies of Heterometallic Wheels and Chains'
Abstract 5
- 12.00–12.45 **Brian F.G. Johnson**
University of Cambridge, Cambridge CB2 1TN, UK
'Clusters and Nanoparticles – Their Use in Catalysis'
Abstract 6
- 12.45–14.30 Poster Session**
EPFL, CE Salle Polyvalente
Abstracts 117–206
- 14.30–16.30 Lectures**
EPFL, CE 6
Abstracts 107–116
Chair: **K. Severin, T.R. Ward**
- 14.30–14.40 **M.C. Erat**, R.K.O. Sigel
University of Zürich, CH-8057 Zürich
'The Influence of Divalent Metal Ions on the Solution Structure of a Group II Intron Branch-Point Domain'
Abstract 107
- 14.40–14.50 **M. Cantuel**^a, D. Imbert^b, J.-C. Bünzli^b, C. Piguet^a
^aUniversity of Geneva, CH-1211 Geneva
^bEcole polytechnique fédérale de Lausanne, CH-1015 Lausanne
'Self-Assembled Heterotrimetallic d-f-d Triple Helicates'
Abstract 108

- 14.50–15.00 **S. Constant**, R. Frantz, G. Bernardinelli, J. Lacour
University of Geneva, CH-1211 Geneva
'Effective Stereocontrol of Chiral Piano-Stool Metal Complex Geometry by a Coordinating Enantiopure Counterion'
Abstract 109
- 15.00–15.10 **S. Gallo**, R.K.O. Sigel
University of Zürich, CH-8057 Zürich
'Synthesis of Coenzyme B₁₂ Analogs and Investigations on their Interactions with the B₁₂ Responsive Riboswitch RNA'
Abstract 110
- 15.10–15.20 **E. Burri**, K. Severin
Ecole polytechnique fédérale de Lausanne, CH-1015 Lausanne
'Site-Isolated Porphyrin Catalysts in Imprinted Polymers'
Abstract 111
- 15.30–15.40 **V.M. Iyer**, P. Belser
University of Fribourg, CH-1700 Fribourg
'Thioacetate Functionalised Metal Complexes and Optical Molecular Switches: Precursors for Self Assembled Monolayers (SAMs) on Gold'
Abstract 112
- 15.40–15.50 **M.-L. Lehaire**^a, P. Grundler^b, A.E. Merbach^b, R. Schibli^a
^aPaul Scherrer Institute, CH-5232 Villigen
^bEcole Polytechnique Fédérale de Lausanne, CH-1015 Lausanne
'Reactivity of the Novel Organometallic Aqua-Ion [(CO)₂(NO)Re(H₂O)₃]²⁺: Kinetics of H₂O Substitution and ¹⁷O Exchange of CO Ligands'
Abstract 113
- 15.50–16.00 **M. Lama**, O. Mamula
Ecole polytechnique fédérale de Lausanne, CH-1015 Lausanne
'Polynuclear Ln(III) Complexes: Self-Assembled Helix formed by a Chiral Bipyridine-Carboxylate Ligand'
Abstract 114
- 16.10–16.20 **Z. Grote**, R. Scopelliti, K. Severin
Ecole polytechnique fédérale de Lausanne, CH-1015 Lausanne
'Organometallic Receptors for Lithium Ions in Water'
Abstract 115
- 16.20–16.30 **C. Malan**, M. Skander, T. Ward
Université de Neuchâtel, CH-2007 Neuchâtel
'Artificial Metalloenzymes: (Strept)Avidin as Host for Enantioselective Hydrogenation'
Abstract 116
- 16.30–17.00 Coffee Break**
- 17.00–17.15 Presentation of the Awards for Best Oral and Poster Presentations**

17.15–18.00 Presentation of the Grammaticakis-Neumann Prize

Organic Chemistry

- Session A1
11.15–12.45 Lectures
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Abstracts 207–212
Chair: **J. Siegel**
- 11.15–11.30 **K. Gademann**, Y. Bethuel, D. Wäckerlin, B. Malisova, S. Tosatti, S. Zürcher, M. Textor
ETH Zürich, CH-8093 Zürich
'The Cyanobacterial Iron Chelator Anachelin – From Fe(III) Binding to Surface Binding'
Abstract 207
- 11.30–11.45 **A. Schlatter**, W.-D. Woggon
University of Basel, CH-4056 Basel
'Enantioselective Hydrogen Transfer Reactions Catalyzed by Ruthenium(II) Amino Alcohol Complexes Attached to β-Cyclodextrin'
Abstract 208
- 11.45–12.00 **D. Josien-Lefebvre**, C. Le Drian
Ecole nationale supérieure de chimie de Mulhouse, F-68093 Mulhouse
'Total Synthesis of the Cyanoglucoside Isolated from *Ilex Warburgii*'
Abstract 209
- 12.00–12.15 **G. Coste**, S. Gerber-Lemaire
Ecole polytechnique fédérale de Lausanne, CH-1015 Lausanne
'New Route towards Functionalized Polyamines and Polyhydroxymacrolactones'
Abstract 210
- 12.15–12.30 **S. Gerber-Lemaire**, A.T. Carmona Asenjo, P. Vogel
Ecole Polytechnique fédérale de Lausanne, CH-1015 Lausanne
'New Asymmetric Synthesis of Polyketides and Functionalized Spiroketal'
Abstract 211
- 12.30–12.45 **L. Hristova**, M. Trzoss, S. Bienz
University of Zürich, CH-8057 Zürich
'A New Si-based Chiral Auxiliary for the Stereoselective Addition of Organometallics to α and β-Silyloxy Carbonyl Compounds'
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- 12.45–13.00 Poster Talks**
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- V. Gorteau**, Abstract 213
J. Waser, Abstract 214
A.W. Buss, Abstract 215

- Session B1**
11.15–12.45 *Organic Structure and Properties I*
Lectures
EPFL, CE 3
Abstracts 216–221
Chair: **N. Finney**
- 11.15–11.30 **I. Trkulja**, R. Häner
University of Bern, CH-3012 Bern
'Stabilization of an Intrastrand Nucleic Acid Triplex by Replacing the Loop Sequence with Phenanthrene Building Blocks'
Abstract 216
- 11.30–11.45 **C. Perazzolo**, J. Wist, G. Bodenhausen
Ecole polytechnique fédérale de Lausanne, CH-1015 Lausanne
'Effects of Protein-Pheromone Complexation on Correlated Chemical Shift Modulations'
Abstract 217
- 11.45–12.00 **L. Saucède**, S. Dos Santos, A. Chandravarkar, B. Mandal, R. Mimna, K. Murat, M. Camus, G. Tuchscherer, M. Mutter
Ecole polytechnique fédérale de Lausanne, CH-1015 Lausanne
'Switch on Amyloid β Peptide Self-Assembly by Enzyme-Triggered Acyl Migration'
Abstract 218
- 12.00–12.15 **S. Litvinchuk**, D. Pasini, T. Miyatake, H. Tanaka, S. Matile
University of Geneva, CH-1211 Geneva
'Synthetic Pores for Sugar Sensing in Soft Drinks and More'
Abstract 219
- 12.15–12.30 **J. Vachon**, G. Bernardinelli, J. Lacour
University of Geneva, CH-1211 Geneva
'Synthesis and Resolution of the First Non Racemic Diquats'
Abstract 220
- 12.30–12.45 **N. Amiot**, K. Heintz, B. Giese
University of Basel, CH-4056 Basel
'Analog Synthesis towards Target Fishing for C-Di-GMP'
Abstract 221
- 12.45–13.00** **Poster Talks**
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- A. Sisson**, Abstract 222
G. Bianké, Abstract 223
O.F. Aebischer, Abstract 224
- Sessions A & B**
13.00–14.30 **Poster Session**
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- Session A2**
14.30–16.30 *Synthesis and Synthetic Methodology II*
Lectures
EPFL, CE 1
Abstracts 225–231
Chair: **K. Gademann**
- 14.30–14.45 **M. Lovchik**^a, G. Fráter^{a,b}, A. Goetze^b
^aUniversity of Zürich, CH-8057 Zürich
^bGivaudan Schweiz AG, CH-8600 Dübendorf
'Total Synthesis of *Junione* by the S_Ni' Reaction'
Abstract 225
- 14.45–15.00 **Y. Bethuel**^a, J.F. Blom^b, K. Gademann^a
^aETH Zürich, CH-8093 Zürich
^bUniversity of Zürich, CH-8802 Zürich
'Diversity-Oriented Synthesis of Anachelin as a Tool to Study the Biological Function'
Abstract 226
- 15.00–15.15 **M. Turks**, P. Vogel
Ecole polytechnique fédérale de Lausanne, CH-1015 Lausanne
'New Methodology towards *anti,syn* and *anti,anti* Stereotriads and its Application to the Synthesis of Naturally Occurring Polypropionates'
Abstract 227
- 15.15–15.30 **J.D. Revell**, D. Gantenbein, R. Kovasy, H. Wennemers
University of Basel, CH-4056 Basel
'Tripeptides as Efficient and Selective Aldol Catalysts'
Abstract 228
- 15.45–16.00 **P. Schär**, P. Renaud
University of Bern, CH-3012 Bern
'The Total Synthesis of (–)-Lepadiformine'
Abstract 229
- 16.00–16.15 **S. Gille**, N. Cabello, J.-C. Kizirian, A. Alexakis
University of Geneva, CH-1211 Geneva
'Simple 1,2-Diamine Ligands for Asymmetric Addition of Aryllithium Reagents to Imines'
Abstract 230
- 16.15–16.30 **C. Mazet**, V. Köhler, A. Pfaltz
University of Basel, CH-4056 Basel
'Synthesis of Sterically and Electronically Tunable Anionic C₂-symmetric Bisoxazoline Analogues and their Application in Asymmetric Catalysis'
Abstract 231
- Session B2**
14.30–16.30 *Organic Structure and Properties II*
Lectures
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Abstracts 232–238
Chair: **J. Nitschke**
- 14.30–14.45 **A. Enriquez**, E.P. Kündig, T. Lomberget
University of Geneva, CH-1211 Geneva 4
'[Cr(CO)₃(⁶-5,8-Naphthoquinone)]: A New Entry into Highly Enantioenriched Planar Chiral Complexes'
Abstract 232
- 14.45–15.00 **A. Clouet**, T. Darbre, J.-L. Reymond
University of Bern, CH-3012 Bern
'Discovery of New Functional Peptide Dendrimers, as Enantioselective Catalysts, and Host for Vitamin B12'
Abstract 233

- 15.00–15.15 **V. Malinovskii**, J.S. Lindsey
North Carolina State University,
Raleigh NC 27695, USA
'Porphyrin Based Systems for Molecular
Information Storage'
Abstract 234
- 15.15–15.30 **A. Herrmann**
Firmenich SA, CH-1211 Genève 8
'Photochemical Release of Bioactive Substances.
Concepts and Applications for Controlled
Fragrance Delivery'
Abstract 235
- 15.45–16.00 **D. Schultz**, J.R. Nitschke
University of Geneva, CH-1211 Geneva 4
'Selection Rules for Helicate Ligand-
Component Self-Assembly: Steric, pH, Charge,
and Solvent Effects'
Abstract 236
- 16.00–16.15 **M. Nagel**^a, T. Lippert^b
^aEMPA, CH-8600 Dübendorf
^bPaul Scherrer Institute, CH-5232 Villigen
'Photodecomposable Materials Designed for
Laser Applications: Triazene-Based Polymers
as Photodynamic Release Layers'
Abstract 237
- 16.15–16.30 **A. Karim**, K.K. Baldrige, A. Linden,
J.S. Siegel
University of Zürich, CH-8057 Zürich
'Frictionless Cyclophanes from 2,6-Diaryltolan
Derivatives'
Abstract 238
- 16.30–17.00 Coffee Break**
- 17.00–17.15 Presentation of the Awards for Best
Oral and Poster Presentations**
- 17.15–18.00 Presentation of the Grammaticakis-
Neumann Prize**

Physical Chemistry

- 11.15–12.45 **Lectures**
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Abstracts 300–305
Chair: **M. Rossi**
- 11.15–11.30 **C. Manca**^a, C. Tanner^b, M. Thut^b,
S. Leutwyler^b
^aETH Zürich, CH-8093 Zürich,
^bUniversity of Bern, CH-3000 Bern
'Understanding the Solvent Effect in Transfer
along a Hydrogen Bonded Wire'
Abstract 300
- 11.30–11.45 **A. Kamariotis**, S. Mercier, O. Boyarkin,
R. Beck, M. Bush, E.R. Williams, T.R. Rizzo
Ecole polytechnique fédérale de Lausanne,
CH-1015 Lausanne
'Infrared Spectroscopic Study of Gas-Phase
Zwitterion Formation: Hydrated Valine-Li⁺ and
Valine-H⁺'
Abstract 301
- 11.45–12.00 **P. Pratte**, M.J. Rossi
Ecole polytechnique fédérale de Lausanne,
CH-1015 Lausanne
'The Heterogeneous Chemical Reaction of HO-
Cl and HOBr with Sea Salt and Model Aerosols
in an Atmospheric Flow Tube Reactor at 300K
in the Range 40 to 93% Relative Humidity'
Abstract 302
- 12.00–12.15 **A. Fouqueau**, M. Meuwly
University of Basel, CH-4056 Basel,
'Structures and Dynamics of Protonated Water
Clusters'
Abstract 303
- 12.15–12.30 **A. Fürstenberg**^a, M. Julliard^a,
T. G. Deligeorgiev^b, E. Vauthey^a
^aUniversity of Geneva, CH-1205 Genève
^bUniversity of Sofia, 1126 Sofia, Bulgaria
'Ultrafast Dynamics of Fluorescent DNA
Intercalators'
Abstract 304
- 12.30–12.45 **W. Gawelda**^{a,b}, V.T. Pham^a, M. Kaiser^a,
Y. Zaushitsyn^{a,b}, R. Abela^b, M. Chergui^a,
C. Bressler^a
^aEcole polytechnique fédérale de Lausanne,
CH-1015 Lausanne
^bSwiss Light Source, Paul Scherrer Institut,
CH-5232 Villigen
'Transient Electronic and Molecular Structure
of Photoexcited Coordination Chemistry
Compounds'
Abstract 305
- 12.45–13.00 Poster Talks**
EPFL, CE 4
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- 12.45–12.48 **V.T. Pham**, Abstract 306
12.48–12.51 **T.A. Paul**, Abstract 307
12.51–12.54 **V.R. Reddy**, Abstract 308
12.54–12.57 **S.M. Zakeeruddin**, Abstract 309
12.57–13.00 **K. Wojciechowski**, Abstract 310
- 13.00–14.30 Poster Session**
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- 14.30–16.30 Lectures**
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Chair: **F. Merkt**

- 14.30–14.45 **C. Klein**, M.K. Nazeeruddin, P. Liska, P. Comte, M. Grätzel
Ecole polytechnique fédérale de Lausanne, CH-1015 Lausanne
'A New Paradigm in Molecular Engineering of Sensitizers for Solar Cell Applications'
Abstract 311
- 14.45–15.00 **J.-D. Grunwaldt**, M. Caravati, A. Baiker
ETH Zürich, CH-8093 Zürich
'In situ Spectroscopic Studies in Supercritical Carbon Dioxide: Selective Oxidation of Benzyl Alcohol on Pd/Al₂O₃ as Model Reaction'
Abstract 312
- 15.00–15.15 **O. Bossart**, G. Calzaferri
University of Bern, CH-3012 Berne
'Dye-Loaded Zeolite L Antenna Materials for Organic Light Emitting Diodes'
Abstract 314
- 15.15–15.30 **S. Cavadini**^a, J. Dittmer^b, S. Antonijevic^a, G. Bodenhausen^{a,c}
^aEcole polytechnique fédérale de Lausanne, CH-1015 Lausanne
^bAarhus University, DK-8000 Aarhus
^cEcole Normale Supérieure, F-75231 Paris
'Slow Diffusion by Singlet State NMR'
Abstract 315
- 15.30–15.45 **R.D. Beck**, P. Maroni, D.C. Papageorgopoulos, M. Sacchi, T.T. Dang, T.R. Rizzo
Ecole polytechnique fédérale de Lausanne, CH-1015 Lausanne
'State-Resolved Gas/Surface Reactivity of Methane in the Symmetric C-H Stretch Vibration on Ni(100)'
Abstract 316
- 15.45–16.00 **E. Portuondo-Campa**^a, A. Tortschanoff^a, F. van Mourik, J.-E. Moser^a, A. Kornherr^c, M. Chergui^a
^aEcole polytechnique fédérale de Lausanne, CH-1015 Lausanne
^bUniversität Wien, A-1090 Wien
'Ultrafast Solvation at Water/ZrO₂ Interfaces'
Abstract 317
- 16.00–16.15 **E. Loginov**, M. Drabbels
Ecole polytechnique fédérale de Lausanne, CH-1015 Lausanne
'Photoelectron Spectroscopy of Aromatic Molecules Embedded in Liquid Helium Nanodroplets'
Abstract 318
- 16.15–16.30 **M. Benmelouka**, A. Borel, L. Helm, A.E. Merbach
Ecole polytechnique fédérale de Lausanne, CH-1015 Lausanne
'Electronic Spin Relaxation Mechanism Study of Acyclic and Macrocyclic Gd(III) Complexes Based MRI Contrast Agents: Multi-Frequency and Multi-Temperature EPR Approach'
Abstract 319
- 16.30–17.00 Coffee Break**
- 17.00–17.15 Presentation of the Awards for Best Oral and Poster Presentations**
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