#### SCS FALL MEETING 2015, POSTER SESSIONS

Name (regular font) = Presenting Author Name (italic font) = Main Research Leader

#### **Analytical Sciences [AS] Poster Session**

Jury members: Stefan Schürch, University of Bern, Hanspeter Andres, METAS

Investigating the binding sites of RAPTA-C and RAPTA-EA to a 50 amino acid peptide using ETD fragmentation and ChemInfo algorithms [AS-101]

Laure Menin, Paul Dyson, EPF Lausanne,

Nano-SIMS to study the distribution of metal based anti-cancer compounds in vitro [AS-102]

Ronald FS Lee, Paul Dyson, EPF Lausanne

A Universal Low-Flow Secondary ElectroSpray Ionizer: High Sensitivity Volatile Analysis on Pre-existing MS Instruments [AS-103]

César Barrios, Pablo Martinez-Lozano Sinues, ETH Zurich

Characterization of a 2D Polymer Monolayer with Tip-**Enhanced Raman Spectroscopy [AS-104]** 

Feng Shao, Renato Zenobi, ETH Zurich

Target plate material resistivity influences LDI efficiency [AS-105]

Guido Paul Zeegers, Renato Zenobi, ETH Zurich

Sr isotope ratios and Rb-Sr ages by LA-ICPMS with isobar separation by on-line electrothermal vaporization [AS-106] Hale Ceren Yilmaz, Bodo Hattendorf, ETH Zurich

Full-metal AFM probes for tip-enhanced Raman spectroscopy [AS-107]

Jacek Szczerbiński, Renato Zenobi, ETH Zurich

MALDI-MS for Population Profiling with Single-Cell Resolution [AS-108]

Jasmin Krismer, Renato Zenobi, ETH Zurich

Observing gas-phase proton transfer reactions inside the MALDI plume [AS-109]

Mario Francesco Mirabelli, Renato Zenobi, ETH Zurich

Quantification of Trace Elements in Brass and Silicate Glasses by Portable Laser Ablation Sampling and Subsequent ICPMS [AS-110]

Peter Velicsanyi, Detlef Günther, ETH Zurich

Nucleoside phosphate monitoring in cell cultures using MALDI **TOF MS [AS-111]** 

Robert Steinhoff, Renato Zenobi, ETH Zurich

Gap-mode TERS spectra of small organic amides and small peptides: is the amide I mode present? [AS-112] Üzeyir Dogan, ETH Zürich

Novel fluorescence assays for monitoring recombinant proteins during biotechnological production and purification [AS-

Enrico Antonino Condemi, Jean-Manuel Segura, HES-SO Valais

Defensin Levels in Spider Hemolymph [AS-114]

Alena Krüger, Stefan Schürch, University of Bern

Binding of Metallocenes to Short Oligonucleotides [AS-115] Rahel Eberle, Stefan Schürch, University of Bern

Elucidation of the gas-phase structure of a sugar-modified DNA analogue [AS-116]

Yvonne Hari, Stefan Schürch, University of Bern

Carbonate-Selective Potentiometric Solid Contact Electrode [AS-118]

Dajing J Yuan, Eric Bakker, University of Geneva

Efficient normal phase MS directed purification of natural products at the preparative scale [AS-119]

Davide Righi, Jean-Luc Wolfender, University of Geneva

Ion-selective Nanospheres as Heterogeneous Indicator Reagents in Complexometric Titrations [AS-120]

Jingying Zhai, Eric Bakker, University of Geneva

Charged Solvatochromic Dyes as Signal Transducers in Fluorescent and Colorimetric Ion Selective Nanosensors

Xiaojiang Xie, University of Geneva

Quantifying the detection capabilities of LA-ICPMS [AS-122] Alex Ulianov, François Bussy, University of Lausanne

The ICPMS signal as a doubly stochastic Poisson process [AS-

Alex Ulianov, University of Lausanne

Online analysis of mass spectra of hydrocarbons [AS-124] Luc Patiny, EPF Lausanne

Lipid droplets and large unilamellar lipid vesicles investigated by asymmetric-flow field-flow fractionation in combination with multi-angle light-scattering [AS-125]

Valerija Vezočnik, University of Ljubljana, Ema Žagar, National Institute of Chemistry Slovenia

Native nano-ESI-MS Applied to Fragment Based Drug Discovery. [AS-126]

Agni Gavriilidou, Renato Zanobi, ETH Zurich

Unraveling the requirements for immortality - Phenotype characterization of the  $\Delta tlc1$  Type II ALT survivors. [AS-127]

Alfredo J. Ibanez, ETH Zurich

UV-fs-LA-ICPMS of La<sub>0.4</sub>Ca<sub>0.6</sub>MnO<sub>3</sub> PLD thin Films [AS-128] Kevin Guex, Detlef Günther, ETH Zurich

Dopant-induced conformational changes of proteins in the gas phase evaluated by Transversal Modulation Ion Mobility Spectrometry [AS-129]

Nicole Andrea Meyer, Renato Zenobi, ETH Zurich

Comprehensive detection of obstructive sleep apnea in humans and drug monitoring in mice by real-time breath analysis [AS-130]

Pablo Martinez-Lozano Sinues, ETH Zurich

Studying the 3-(2-Furoyl)quinoline-2-Carboxaldehyde (FQ) protein labelling reaction to improve accuracy of quantification in capillary electrophoresis-sodium dodecyl sulfate with laser induced fluorescence detection (CE-SDS-LIF) [AS-131]

Miriam Arrell, HES-SO Valais

Thin Layer Chemical Modulations by a Combined Selective Proton Pump and pH Probe for Direct Alkalinity Detection

Majid Ghahraman Afshar, Eric Bakker, University of Geneva

Ion-exchange nanosphere doped hydro-gel as buffer for electrochemical AS(III) detection in weakly buffered environmental media [AS-133]

Romain Touilloux, Eric Bakker, University of Geneva

Ion-selective fluorescent and pH independent nanosensors based on functionalized polyether macrocycles [AS-134]

Zdenka Jarolímová, Eric Bakker, University of Geneva

Solve complex and challenging mass spectrometry problems directly from the browser [AS-135]

Luc Patiny, EPF Lausanne

#### Chemical Composition and Biological Activities of Essential Oils Extracted from Pittosporum Mannii Hook (Pittosporaceae) [AS-136]

Souaibou Yaouba, University of Nairobi

#### Computational Chemistry [CC] Poster Session

Jury members: Tomasz Wesolowski, University of Geneva, Jiri Vanicek, EPF Lausanne, Matthew Wodrich, EPF Lausanne

#### Averaged Molecular Dynamics Trajectories in Frozen-Density Embedding Theory [CC-101]

Andrey Laktionov, EPF Lausanne, Tomasz Adam Wesolowski, University of Geneva

#### Effect of Mixed Organic Cations on the Phase Stability of Hybrid Organic/Inorganic Lead Perovskites for Solar Cell Applications [CC-102]

Ariadni Boziki, Ursula Röthlisberger, EPF Lausanne

### Computational Investigations of a β-Class Carbonic Anhydrase from *Desulfovibrio vulgaris* [CC-103]

Esra Bozkurt, Ursula Röthlisberger, EPF Lausanne

## Intramolecular symmetry-adapted perturbation theory - a tool for elucidating the weak intramolecular interactions [CC-104]

Ewa Pastorczak, Jérôme Gonthier, EPF Lausanne

#### Visualizing and quantifying molecular excited state interactions with scalar fields. [CC-105]

Laurent Vannay, Clemence Corminboeuf, EPF Lausanne

### Empirical valence bond simulations of the hydride transfer step in the monoamine oxidase B [CC-106]

Matej Repic, EPF Lausanne

#### A TD-DFT-based Approach to Describe Electron Dynamics of Molecules in Intense Laser Fields [CC-107]

Pablo Lopez Tarifa, Ursula Röthlisberger, EPF Lausanne

# Computational Rationalization of the selectivity of Ru(II) and Os(II) anticancer agents in HIS/HER binding to the histone components of the Nucleosome Core Particle [CC-108] Thibaud von Erlach, *Ursula Röthlisberger*, EPF Lausanne

## Investigation of the Posttranslational Modifications Expressed in Polyteonamide B by Molecular Dynamics Simulations [CC-109]

Annick Renevey, Sereina Riniker, ETH Zurich

# Mechanistic Study of Denitrification in Truncated Hemoglobin using Adiabatic Reactive Molecular Dynamics [CC-110] Akshaya Kumar Das, University of Basel, Markus Meuwly, University of Basel

#### Assembly of a diverse 10M GDB Fragment Set [CC-111] Ricardo Visini, *Jean-Louis Reymond*, University of Bern

## DFT study of the influence of guest-host interactions on the high-spin/low-spin energy difference in Co(bpy)<sub>3</sub><sup>2+</sup>@Y [CC-112]

Andrea Missana, Andreas Hauser, University of Geneva

#### Accounting for electronic polarization in subsystem DFT calculations [CC-113]

Emilie Chalaye-Chemineau, *Tomasz Adam Wesolowski*, University of Geneva

### Study of Excited State Geometries of Organic Chromophores [CC-114]

Marie Humbert-Droz, University of Geneva

#### Pyrphyrin Adsorption on Au(111) Surface: Influence of Herringbone Reconstruction [CC-115]

Yeliz Gurdal, University of Zurich

#### Exploiting dispersion-driven aggregators as a route to new onedimensional organic nanowires [CC-116]

Adrien Nicolai, Clemence Corminboeuf, EPF Lausanne

### Statistical Averaging over Molecular Dynamics Ensembles in Frozen-Density Embedding Theory [CC-117]

Andrey Laktionov, EPF Lausanne, Tomasz Adam Wesolowski, University of Geneva

## Molecular binding mechanism of a potent ruthenium-arene anticancer agent to the nucleosome core particle (NCP) [CC-118]

Giulia Palermo, Ursula Röthlisberger, EPF Lausanne

#### EVOLVE: a new genetic algorithm toolbox for protein engineering [CC-119]

Marta A. S. Perez, Ursula Röthlisberger, EPF Lausanne

#### The role of dispersion-correction in the description of metalligand bonds in density functional theory [CC-120] Martin Peter Bircher, *Ursula Röthlisberger*, EPF Lausanne

Wattin Feter Briefler, Orsula Romitsberger, EFF Lausan

The role of Mg<sup>2+</sup> ions in adenylate cyclase [CC-121] Siri Van Keulen, *Ursula Röthlisberger*, EPF Lausanne

### The reactivity of hypervalent $\lambda^{3,4}$ -iodanes explored using ab initio (meta-)dynamics [CC-122]

Oliver Sala, ETH Zurich

### The new second-generation ETH DMRG program for quantum chemical applications [CC-123]

Stefan Knecht, Markus Reiher, ETH Zurich

#### Bohmian Mechanics with virtual particles [CC-124]

Oliver Thorsten Unke, Markus Meuwly, University of Basel

### A Force Field Approach to Reproduce Grotthuss Mechanism in Reactive Systems [CC-125]

Zhen-Hao Xu, Markus Meuwly, University of Basel

#### New computational approaches for liquids and energy-related compounds [CC-126]

Sandra Luber, Jürg Hutter, University of Zurich

#### Physical Organic Characterisation of the Molecule-Electrode Contact in Single Molecule Junctions [CC-127]

Ganna Grynova, Clemence Corminboeuf, EPF Lausanne

## Multicenter Bonding in Hypervalent λ<sup>3</sup>-Iodanes: New Insight from the Analysis of Domain Averaged Fermi Holes [CC-128]

Halua Magalhães, ETH Zurich

#### Processing Data from Quantum Chemical Calculations using Turbomole-XML-eXist [CC-129]

Stefan Heinen, Hans Peter Lüthi, ETH Zurich

### Thermal stability predictions as a tool for inherently safer process design [CC-130]

Nadia Baati, Thierry Meyer, EPF Lausanne

#### Catalysis Sciences & Engineering [CE] Poster Session

Jury members: S. David Tilley, University of Zürich, Jeremy Luterbacher, EPF Lausanne, Martin Albrect, University of Bern

## Effect of the Pd-state in perovskite-type $A(B,Pd)O_{3\pm\delta}$ (A=La,Y;B=Mn,Fe,Co) oxidation catalysts in terms of $CH_{4}$ -oxidation activity [CE-101]

Arnim Eyssler, EMPA Dübendorf

#### Hydrogen Storage in Formic Acid/Carbon Dioxide Systems -Solvent Effects: Heat of Mixing and pH of the Reaction Media [CE-102]

Cornel Fink, Gábor Laurenczy, EPF Lausanne

### Insights into the Ionic Liquid-Promoted Electrochemical Reduction of $CO_2$ [CE-103]

Genevieve Lau, EPF Lausanne

Ni<sub>2</sub>P nanoparticles as Janus catalyst for electrochemical water splitting [CE-104]

Lucas-Alexandre Stern, Xile Hu, EPF Lausanne

#### Aerogels for CO<sub>2</sub> Capture [CE-105]

Marco Roman Holzer, Andreas Züttel, EPFL Valais/Wallis

Selective dehydrogenation of formic acid over sub-nanometric gold particles supported on silica [CE-106]

Amaia Beloqui-Redondo, ETH Zürich

Esterification of 2-Methoxyphenol and Octanoic Acid over modified MCM-41 for Biomass Conversion [CE-107] Bahir Duraki, ETH Zurich

#### Simple One-Pot Synthesis of Iridium-Titanium Oxide Composites [CE-108]

Emma Oakton, Christophe Copéret, ETH Zurich

Silver-indium catalysts for the electrochemical reduction of carbon dioxide [CE-109]

Gastón Larrazábal, Javier Pérez-Ramírez, ETH Zurich

Electrocatalysts for carbon dioxide recycling based on silverindium materials [CE-110]

Gastón O. Larrazábal, Javier Pérez-Ramírez, ETH Zurich

Highly selective basic zeolites for the dehydrogenation of ethanol to acetaldehyde [CE-111]

Giacomo Marco Lari, Javier Pérez-Ramírez, ETH Zurich

Stability of tin-containing zeolites in continuous biomass conversions [CE-112]

Giacomo Marco Lari, Javier Pérez-Ramírez, ETH Zurich

Structure-performance relationships of hybrid nanocatalysts for selective hydrogenation [CE-113]

Gianvito Vilé, Javier Pérez-Ramírez, ETH Zurich

CO activation on Ruthenium Nanoparticles: *Ab Initio* calculations under reaction conditions. [CE-114] Lucas Foppa, *Aleix Comas-Vives*, ETH Zurich

Impact of defect chemistry in zeolite desilication [CE-115] Marilyne Boltz, *Javier Pérez-Ramírez*, ETH Zurich

Improving the Oxygen Evolution Kinetics of a Nanostructured Composite Hematite Photoanode [CE-116]

Mario Bärtsch, ETH Zurich, Jan Augustyński, University of

Dehydrogenation and Polymerization on Cr(III) Silicates Are Rate-Determined by an Analoguous Mechanistic Step [CE-117]

Murielle F. Delley, Christophe Copéret, ETH Zurich

Improved Solution Finding in Industrial Waste Incineration Scheduling Through Implementation of Multi-Objective Strategies [CE-118]

Oliver Weder, Konrad Hungerbühler, ETH Zurich

Handling forecast uncertainty in industrial waste incineration scheduling [CE-119]

Ralph Bannerman, Konrad Hungerbühler, ETH Zurich

Towards a general pore connectivity index in hierarchicallyorganized zeolites by positron annihilation spectroscopy [CE-120]

Robbie Warringham, Javier Pérez-Ramírez, ETH Zurich

Integration of Hierarchical Waste Incineration Scheduling Levels for Improved Industrial Performance [CE-121] Samuel Perren, *Konrad Hungerbühler*, ETH Zurich Cu Particle Size and Support Effect on CO<sub>2</sub> Hydrogenation to MeOH over Supported Cu Catalysts [CE-122]

Shohei Tada, Christophe Copéret, ETH Zurich

Why does the addition of Fe increase the activity and stability of Ni-based dry reforming catalysts: An in-situ XRD and XAS study. [CE-123]

Sung Min Kim, Christophe Copéret, ETH Zurich

Atomistic Description of Silica Supported (SiO)W(NAr)(=CHtBu)(OR) Catalysts Through DNP-SENS [CE-124]

Ta-Chung Ong, Christophe Copéret, ETH Zurich

Design of mild base catalysts for the deoxygenation of bio-oil by aldol condensation [CE-125]

Tobias Keller, Javier Pérez-Ramírez, ETH Zurich

Fast pyrolysis of lignin: Relating the Structure with Product selectivity [CE-126]

Victoria Custodis, *Jeroen A. van Bokhoven* ETH Zurich/PSI Villigen

Novel catalysts for the oxybromination of methane [CE-127] Vladimir Paunovic, *Javier Pérez-Ramírez*. ETH Zurich

Encapsulated Polarizing Agents for Application in Dynamic Nuclear Polarization Surface Enhanced NMR Spectroscopy [CE-128]

Wei-Chih Liao, Christophe Copéret, ETH Zurich

Opportunities of catalysis for tuning selectivity during lignin catalytic fast pyrolysis [CE-129]

Zhiqiang Ma, Jeroen A. van Bokhoven ETH Zurich/PSI Villigen

Electrocatalytic water oxidation with  $\text{Co}_{1\text{-x}}\text{M}_x\text{NCN}$  metal carbodiimides [CE-130]

Rafael Müller, Greta Ricarda Patzke, University of Zurich

Approaches towards heterogenization of Ru(II) half-sandwich catalysts for asymmetric hydrogenation [CE-131]
Beáta Vilhanová, Institute of Chemical Technology, Prague,

Czech Republic, Jeroen A. van Bokhoven, ETH Zurich/PSI Villigen

Hierarchical Pd/ZSM-5 catalysts for methane oxidation in the presence of steam [CE-132]

Andrey W. Petrov, Jeroen A. van Bokhoven, PSI Villigen

Structural analysis of individual Fluid Catalytic Cracking catalyst particle studied by synchrotron-based ptychographic X ray-computed tomography [CE-133] Julio C. da Silva, PSI Villigen, Jeroen A. van Bokhoven, ETH Zurich/PSI Villigen

Exploring the self-regenerating function of perovskit-type oxides on catalytically active nickel [CE-134]

Patrick Steiger, PSI Villigen

Time-resolved measurements of the terahertz conductivity in noble metal-on-TiO<sub>2</sub> nanoparticles for photocatalytic applications [CE-135]

Arno Schneider, PSI Villigen, Jacques-E. Moser, EPF Lausanne

Dual-phase Zn-modified ceria nanocrystals: establishing a correlation between the structural characteristics, oxygen storage capacities and catalytic activities [CE-136] Fangjian Lin, PSI Villigen

From mechanism to catalyst design: Highly active formic acid decomposition catalysts under SCR-relevant conditions [CE-

Manasa Sridhar, PSI Villigen, Oliver Kröcher, PSI Villigen and EPF Lausanne

In situ X-ray Absorption Spectroscopy of Ce<sub>0.5</sub>Zr<sub>0.5</sub>O<sub>2-d</sub> at 1773 K [CE-138]

Matthäus Rothensteiner, PSI Villigen, Jeroen A. van Bokhoven, ETH Zurich/PSI Villigen

Investigating the influence of CO and ceria on  $CH_4$  abatement on Pd-based TWC using modulation excitation spectroscopy [CE-139]

Valentina Marchionni, PSI Villigen

Tuning reactant selectivity in the direct aldol-Tishchenko reaction using space constraints in multifunctional MOFs [CE-140]

Xiaoying Xu, PSI Villigen, Jeroen A. van Bokhoven, ETH Zurich/PSI Villigen

Synthesis of hollow ZSM-5 nano-reactors containing coppermetal oxide nanoparticles [CE-141]

Jin Hee Lee, PSI, Jeroen A. van Bokhoven, ETH Zurich/PSI Villigen

Engineering Streptavidin as Scaffold for the Design of Artificial Metalloenzymes [CE-142]

Hendrik Mallin, Thomas R. Ward, University of Basel

Towards cheap and sustainable energy sources by exploiting self-organized catalyst micro- and nano structures [CE-143] Roche Marcel Walliser, *Edwin C. Constable*, University of Basel

**Dynamic kinetic resolution of allylic acetates [CE-144]** Valentin Köhler, University of Basel

Heterogenization of chiral Ru(II) catalysts on mesoporous silica *via* the arene ligand [CE-145]

Jaroslav Aubrecht, University of chemistry and technology, *Petr Kačer, Institute of Chemical Technology, Prague, Czech Republic* 

Synthesis of highly active ruthenium catalyst for transfer hydrogenation of ketones [CE-146]

Leoš Kořený, University of Chemistry and Technology, Prague, *Petr Kačer, Institute of Chemical Technology, Prague*, *Czech Republic* 

 $TiO_2$  and Ag-doped  $TiO_2$  nanocontainers as photocatalysts for  $CO_2$  reduction [CE-147]

Nelly Hérault, Katharina Fromm, University of Fribourg

Metal Center Tuning of Layered Double Hydroxides for Electrochemical Water Oxidation [CE-148]

Fabio Evangelisti, Greta Ricarda Patzke, University of Zurich

Doped Manganese Oxides as Water Oxidation Catalysts [CE-149]

Michael Olah, Greta R. Patzke, University of Zurich

Optimization of Ceria-Based Materials for Solar Thermochemical Two-Step CO<sub>2</sub>-Splitting [CE-150] Roger Jacot, University of Zurich, *Aldo Steinfeld, ETH Zurich* 

Screening of Lewis Acidic Chlorometallate Ionic Liquids Combined with Nanoparticle Catalysts for Aromatic Hydrogenation Activity [CE-151]

Alena Karakulina, Paul Joseph Dyson, EPF Lausanne

Continuous flow synthesis of metal-organic frameworks utilizing microwave irradiation [CE-152]

Daniel Antti Steitz, ETH Zürich, Jeroen A. van Bokhoven, ETH Zurich/PSI Villigen

Cationic co-doped  $TiO_2$  nanoparticles as efficient visible-light active photocatalyst: experimental and theoretical study [CE-153]

Darinka Primc, ETH Zürich

Design and technical development of iron zeolite catalysts for the gas phase oxidation of glycerol to dihydroxyacetone [CE-154]

Giacomo Marco Lari, Javier Pérez-Ramírez, ETH Zurich

Zinc-rich copper catalysts promoted by gold for methanol synthesis [CE-155]

Oliver Martin, Javier Pérez-Ramírez, ETH Zurich

Evidence on the direct formation of methane from H<sub>2</sub>O and CO<sub>2</sub> by thermochemical cycles using Ni- and Rh-doped ceria [CE-156]

Fangjian Lin, PSI Villigen

Towards stabilization of active methanation catalysts: Effect of boron promotion [CE-157]

Anastasios Kampolis, Oliver Kröcher, PSI Villigen

Superior durability of flame-made WO<sub>3</sub>/CeO<sub>x</sub>-TiO<sub>2</sub> DeNO<sub>x</sub> catalysts [CE-158]

Katarzyna Anna Michalow-Mauke, Oliver Kröcher, PSI Villigen

Photo-catalytic evolution of dihydrogen from water by Ni@MOF: a nickel catalyst encapsulated inside MIL-125-NH<sub>2</sub> (Ti) [CE-159]

Kim Meyer, PSI Villigen, Jeroen A. van Bokhoven, ETH Zurich/PSI Villigen

Metal-support interaction of platinum nanoparticles supported on yttria stabilized zirconia catalysts for environmentally important reaction systems [CE-160]

Rima J Isaifan, Qatar Environment and Energy Research Institute (QEERI), Elena A Baranova, University of Ottawa

#### Inorganic Chemistry [IC] Poster Session

Jury members: Albert Ruggi, University of Fribourg, Gábor Laurenczy, EPF Lausanne, Anne-Sophie Chauvin, EPF Lausanne

Homogeneous Catalytic Hydrogen Storage and Release in the Formic Acid-Carbon Dioxide Couple using Ruthenium Pre-Catalysts. [IC-101]

Antoine van Muyden, Gábor Laurenczy, EPF Lausanne

Self-sorting of Pd-based coordination cages: the importance of subtle steric effects [IC-102]

Giacomo Cecot, Kay Severin, EPF Lausanne

Small Molecule Activation at siloxide "ate" complexes of f elements [IC-103]

Julie Andrez, EPF Lausanne

A viable hydrogen storage and release system based on formate and bicarbonate salts: mechanistic insights into the hydrogen release step. [IC-104]

Katerina Sordakis, Gábor Laurenczy, EPF Lausanne

Multi-Electron Redox Reactions Promoted by f-Elements Complexes [IC-105]

Marta Falcone, Marinella Mazzanti, EPF Lausanne

Carboxylic acid-functionalized clathrochelate complexes as scaffolds for supramolecular metalloligands [IC-106] Mathieu Marmier, *Kay Severin*, EPF Lausanne

**Selective Hydrogen Production from Formic** 

Acid: Development of Homogeneous Iron Catalysts in Aqueous Solution [IC-107]

Mickael Montandon-Clerc, Gábor Laurenczy, EPF Lausanne

Supramolecular cages from clathrochelates and stabilized imines [IC-108]

Suzanne Maria Jansze, Kay Severin, EPF Lausanne

Nickel Complexes as Catalysts for Silane Dehydrogenation and Hydrogenative Cleavage Reactions of Oligosilanes. [IC-109] Bruno Pribanic, *Hansjörg Grützmacher*, ETH Zurich

Synthesis of New Polarization Matrices for Dynamic Nuclear Polarization [IC-110]

Daniel L Silverio, Christophe Copéret, ETH Zurich

The Mechanism of C-H activation by Transition Metal Siloxides [IC-111]

Deven Paul Estes, Christophe Copéret, ETH Zurich

Catalytic Dehydrogenation of Amino Boranes – Formation of Condensed Borazine Compounds [IC-112]

Fabian Müller, Hansjörg Grützmacher, ETH Zurich

Cycloaddition Reactions of Diazoalkane Ruthenium Complexes with Chiral PNNP Ligands [IC-113]

Joël Egloff, Antonio Mezzetti, ETH Zurich

Synthesis and Application of N-Trifluoromethyl N-Heterocyclic Carbene Ligands and Their Complexes [IC-114] Pascal Engl, *Antonio Togni*, ETH Zurich

Iron(II) Catalysts with a P-Stereogenic NPPN Ligand for the Enantioselective Strecker Reaction of Azomethine Imines [IC-115]

Raffael Huber, Antonio Mezzetti, ETH Zurich

Low temperature synthesis of nickel silicide: from preparing colloidal nanoparticles to coating silicon [IC-116]
Tsung-Han Lin, Christophe Copéret, ETH Zurich

Quantitatively Analyzing Metathesis Catalyst Activity and Structural Features in Silica-Supported Tungsten Imido– Alkylidene Complexes [IC-117]

Victor Mougel, Christophe Copéret, ETH Zurich

Amorphous Cobalt Silicate Nanobelts@Carbon Composites as Stable Anode Material for Lithium Ion Batteries [IC-118] Wei Cheng, ETH Zurich

High Resolution Powder X-ray Diffraction on Functional Metal-Organic Frameworks with UiO-66 Topology [IC-119] Marco Taddei, PSI Villigen, Jeroen Anton van Bokhoven, ETH

Synthesizing Functionalized [M(η<sup>6</sup>-arene)<sub>2</sub>]<sup>+</sup> (Re, <sup>99(m)</sup>Tc)
Complexes for Receptor Targeting [IC-120]
Giuseppe Meola, Roger Alberto, University of Zurich

Zurich

Target Specific Multimodality Nanoparticles for (Nano)Medical Applications [IC-121]

Michel Wuillemin, Henrik Braband, University of Zurich

Structural and magnetic investigations of a mononuclear 4f polyoxometalate family with single molecule magnet behaviour [IC-122]

Robin Güttinger, Pierre-Emmanuel Car, University of Zurich

Exceptionally long-lived light-emitting electrochemical cells: multiple intra-cation  $\pi$ -stacking interactions in [Ir(C^N)<sub>2</sub>(N^N)][PF<sub>6</sub>] emitters [1] [IC-123] Andreas M. M. Bünzli, University of Basel

Porphyrin-decorated polypyridines for dye sensitized solar cells [IC-124]

Angelo Lanzilotto, Edwin C. Constable, University of Basel

Asymmetric copper(I)-based dyes to combine with sterically demanding anchoring ligands for dye-sensitized solar cells. [IC-125]0

Annika Büttner, Edwin C. Constable, University of Basel

Going to Extremes: From Fluorine-Free Blue to Stable Red Emitting Iridium Complexes for LEECs [IC-126] Cathrin D. Ertl, *Edwin C. Constable*, University of Basel

Anionic Ir(III) Complexes for Light-Emitting Electrochemical Cells [IC-127]

Collin D. Morris, Catherine E. Housecroft, University of Basel

Influence of a co-adsorbent on the performance of copper(I)based dye-sensitized solar cells [IC-128]

Frederik J. Malzner, Edwin C. Constable, University of Basel

Rhodium-catalyzed Olefin Cyclopropanation by Engineered Streptavidin [IC-129]

Jingming Zhao, Thomas R. Ward, University of Basel

Strong, Chemically Robust Photoreductants [IC-130] Laura A. Büldt, University of Basel, *Oliver S. Wenger, Basel* 

Modifying spacers and anchoring groups for heteroleptic Cu(I) - 6,6'-dimethyl-2,2'-bipyridine based DSSCs [IC-131]

Maximilian Klein, Edwin C. Constable, University of Basel

Heteroleptic light-emitting copper(I) complexes for possible applications in LECs and OLEDs [IC-132]

Sarah Keller, Catherine E. Housecroft, University of Basel

The Performance of a Series of Copper(I) Phenanthroline Dyes in DSCs [IC-133]

Sebastian Olivier Fürer, Catherine E. Housecroft, University of Basel

Tuning the in vitro cell cytotoxicity of dinuclear arene ruthenium trithiolato complexes: Influence of the arene ligand [IC-134]

Lennart Geiser, University of Bern

Synthesis, reactivity and cytotoxicity of dithiolato diruthenium complexes  $[(\eta^6\text{-}p\text{-}cymene)_2Ru_2(\mu_2\text{-}SR)_2X_2]$ , X = Cl, I [IC-135] Lennart Geiser, University of Bern

Did the presence of a guest in the cavity of an arene ruthenium metallaprism modify its reactivity towards biomolecules? [IC-136]

Lydia Paul, Julien Furrer, University of Bern

Synthesis of metal oxide precursors for the generation of oxides or similar nanomaterials for Na-ion battery cathode production [IC-137]

Benoît Baichette, Katharina Fromm, University of Fribourg

Stimuli responsive cavitands for triggered release of antimicrobial drugs [IC-138]

Noémie Voutier, Katharina Fromm, University of Fribourg

Sn/C composite anode material for lithium ion batteries [IC-139] Sivarajakumar Maharajan, *Katharina Fromm*, University of Fribourg

Pyridine versus pyrazine in asymmetric didentate ligands: unexpected behaviour in  ${\rm Fe^{II}}$  spin crossover complexes [IC-140]

Timothée Lathion, Claude Piguet, University of Geneva

Synthesis of heteroaryl *meso* substituted porphyrins, and their coordination with ruthenium complexes [IC-141]

Balazs Brem, University of Neuchâtel, Luminita Silaghi-Dumitrescu, Babes-Bolyai University

Anti-Cancer Activities of Zwitterion-Bridged Arene Ruthenium Metalla-Assemblies [IC-142]

Minghui Yuan, Bruno Therrien, University of Neuchatel

Poly versus Mono-Disperse Rodlike Lipophilic

Fluoroacetylacetonate Eu(III) Complexes: Mesomorphic and Thermodynamic Consequences [IC-143]

Sebastiano Guerra, University of Neuchatel, Claude Piguet, University of Geneva

Water-soluble organometallic assemblies containing photoswitchable ligands [IC-144]

Thomas Cheminel, Bruno Therrien, University of Neuchatel

Efficient Triplet Blue Emitters Based on Neutral Gold(III) Complexes [IC-145]

Alexander Szentkuti, Koushik Venkatesan, University of Zurich

Investigating the structure of the metallothionein 2 protein from the plant *Cicer arietinum* [IC-146]

Alma Salim, Eva Freisinger, University of Zurich

- Highly Homoperfluorinated Ionic Liquids for NMR Field Probes for Magnetic Field Monitoring in MRI [IC-147] Anna Christina Looser, *Roger Alberto*, University of Zurich
- Photocatalytic Proton Reduction with Molecular Ru and Co Complexes Immobilized on Hydrophobic Silica [IC-148] Cyril Bachmann, *Roger Alberto*, University of Zurich
- Unique histidine-rich metallothioneins "cracking the code" [IC-149]

Jelena Habjanic, Eva Freisinger, University of Zurich

Tackling the structure of the metal binding domains of a plant metallothionein 3 [IC-150]

Jovana Jakovleska, Eva Freisinger, University of Zurich

Characterization of Mg<sup>2+</sup> binding sites in the CPEB3 ribozyme studied by NMR spectroscopy. [IC-151]
Kenneth Adea, *Roland K.O. Sigel*, University of Zurich

- **Polyoxometalate catalysts for artificial photosynthesis [IC-152]** Kim Dimuth von Allmen, *Greta R. Patzke*, University of Zurich
- B<sub>12</sub> derivatives with a modified corrin structure [IC-153] Lucas Prieto, *Felix Zelder*, University of Zurich
- Influence of hetero-biaryl-ligands on the photophysical properties of  $[Re^INCS(CO)_3 diimine]$ -type photosensitizers. [IC-154]

Mathias Lukas Mosberger, Roger Alberto, University of Zurich

- Covalently labeling of the *btuB* riboswitch with fluorophores for the studies at the single molecule level [IC-155] Meng Zhao, *Roland K.O. Sigel*, University of Zurich
- N-Heterocyclic Carbenes Stabilizing Ligands for Various Oxidation States of Rhenium and Technetium [IC-156] Michael Benz, *Henrik Braband*, University of Zurich
- Pyrphyrin and Phenphyrin Scaffold Revisited: Physico-Chemical Properties and Photocatalysis [IC-157] Stephan Schnidrig, , Roger Alberto, University of Zurich
- A General Approach of Reduced Graphene Oxide Nanocomposite Aerogels with Multifunctional Electrode Materials towards Advanced Lithium-ion Batteries [IC-158] Guobo Zeng, Markus Niederberger, ETH Zurich
- Phosphine oxidation catalyzed by zerovalent cobalt complexes using nitrous oxide as oxidant [IC-159]

  Thomas Lucien Gianetti, *Hansjörg Grützmacher*, ETH Zurich

Multitopic precursors for oxide materials' synthesis [IC-160] Alba Finelli, *Katharina M. Fromm*, University of Fribourg

Stability and reactivity of dinuclear thiolato-bridged arene ruthenium complexes and their interactions with biological ligands [IC-161]

David Stibal, Georg Süss-Fink, University of Neuchatel

Using Oxidative Quenching of a Copper Photosensitizer for Light-Driven Hydrogen Production [IC-162]
Johannes Windisch, Roger Alberto, University of Zurich

Peptide Backbone Vitamin B<sub>12</sub> Derivative: a Biomimetic Model IIC-1631

Marjorie Sonnay, Felix Zelder, University of Zurich

#### Medicinal Chemistry & Chemical Biology [MC] Poster Session

Jury members: Leonardo Scapozza, University of Geneva, Cornelia Zumbrunn, Actelion, Christian Heinis, EPF Lausanne, Georg Jaeschke, F. Hoffman-La Roche

Siglec-8 – A Novel Target For Asthma [MC-101]

Blijke Suzanne Kroezen, Basel, Beat Ernst, University of Basel

Chemically defined chromatin and protein engineering via EPL to study histone ubiquitination on the single molecule level [MC-102]

Andreas Linus Bachmann, EPF Lausanne

- Engineering of a specific probe for the visualization and analysis of bivalent epigenetic marks in living cells [MC-103]

  Aurore Delachat, *Beat Fierz*, EPF Lausanne
- The Power of the 'SCS': Improving the Pharmacological Properties of Peptide Therapeutics [MC-104] Christopher Kourra, *Nicolai Cramer*, EPF Lausanne
- An "in vivo" temperature dependence study of the protoporphyrine IX delayed fluorescence lifetime while measuring the oxygen partial pressure. [MC-105]
  Emmanuel Louis Arthur Gerelli, Georges Wagnières, EPF Lausanne
- $HP1\alpha \ dynamic \ binding \ to \ different \ compaction \ states \ of \ chromatin \ [MC-106]$

Louise Bryan, Beat Fierz, EPF Lausanne

- Tackling Malaria by Inhibiting the SHMT Enzyme [MC-107] Geoffrey Schwertz, François Diederich, ETH Zurich
- Investigation of an engineered AaLS-13 capsid and Identification of the encapsulation pathway for GFP (+36) by high mass MALDI MS analysis [MC-108] Katharina Root, *Renato Zenobi*, ETH Zurich
- Fluorine Scan at the Active Sites of Rhodesain and Human Cathepsin L: Enhanced Binding Affinity by Stacking of Fluorinated Phenyl Rings on Flat Dipeptide Fragments [MC-109]

Maude Giroud, Franois Diederich, ETH Zurich

 $O^6$ -Alkylguanine Post-lesion DNA synthesis by Y-family DNA polymerase  $\zeta$  characterized with synthetic nucleosides [MC-110]

Michael Heinrich Räz, Shana Sturla, ETH Zurich

- Structural Characterization of Oligoproline [MC-111]
  Patrick Wilhelm, *Helma Wennemers*, ETH Zurich
- Cell Penetrating Peptides Based on an Oligoproline Scaffold [MC-112]

Philipp Raschle, Helma Wennemers, ETH Zurich

Oligoprolines as Scaffolds for Tumor Targeting with Hybrid Bombesin Analogues [MC-113]

Stefanie Dobitz, Helma Wennemers, ETH Zurich

Impact of minor groove alkylation on transcription by RNA polymerase II [MC-114]

Stefano Malvezzi, Shana Sturla, ETH Zurich

Novel azobenzene-derived visible light photoswitches for biological applications [MC-115]

Zbigniew Pianowski, Karlsruher Institut für Technologie (KIT)

Bacterial Resistance to Silver: The Role of SilE Protein [MC-116]

Valentin Chabert, Katharina Fromm, University of Fribourg

The use of phosphorylated peptides to explore the folding properties of the protein tau required for AT8 antibody recognition [MC-117]

Yves Jacquot, Université Pierre et Marie Curie, Paris, Guy Lippens, University of Lille 1

Pollen induced asthma - could small molecules in pollen exacerbate the protein-mediated allergic response? [MC-118]

Alen Bozicevic, Matthias Hamburger, University of Basel

Search for alternatives to copper in organic farming: Fungicidal activity of a *Juncus effusus* medulla extract and its active constituent, dehydroeffusol, against downy mildew and apple scab [MC-119]

Justine Ramseyer, Matthias Hamburger, University of Basel

Natural and semisynthetic antitrypanosomal sesquiterpene lactones from *Anthemis nobilis* [MC-120]

Maria De Mieri, Matthias Hamburger, University of Basel

Antagonizing Bacterial Adhesion – Hit Identification by a Dynamic Combinatorial Chemistry Approach [MC-121] Priska Frei, Beat Ernst, University of Basel

It's better to bend than to break [MC-122]

Said Rabbani, Beat Ernst, University of Basel

Development of small molecular tools for the cellular study of adenosine  $A_1$  receptors [MC-123]

Jennifer Hemmings, Martin Lochner, University of Bern

Fluorescent probes for the cellular study of the 5-HT<sub>3</sub>A receptor – synthesis and evaluation of near-infrared probes [MC-124] Jonathan Simonin, *Martin Lochner*, University of Bern

Peptide dendrimer as SiRNA transfection reagent [MC-125] Marc Heitz, *Tamis Darbre*, University of Bern

Excess Electron Transfer in DNA Containing a Pyrenyl Donor and Multiple Stable Phenanthrenyl Base-Surrogates [MC-126]

Pascal Röthlisberger, Christian Leumann, University of Bern

Antimicrobial Cyclic Peptides with L,D- architecture Targeting Pseudomonas aeruginosa [MC-127]

Runze He, Jean-Louis Reymond, University of Bern

Synthesis of a Geminal Difluorinated Tricyclic Nucleoside Analog [MC-128]

Sibylle Frei, Christian Leumann, University of Bern

Synthesis of photo-crosslinking probes and their application for the site-selective chemical modification of the 5-HT<sub>3</sub> receptor [MC-129]

Thomas Jack, Martin Lochner, University of Bern

Design of 3D Protein Fingerprint and its Application to Map the Protein Data Bank [MC-130]

Xian Jin, Jean-Louis Reymond, University of Bern

QPD-BA, A Precipating Dye For Monitoring Hydrogen Peroxide In Living Cells [MC-131]

Eric Lindberg, Nicolas Winssinger, University of Geneva

Protein Glycoconjugation by bioorthogonal click chemistry [MC-132]

Takuya Machida, Nicolas Winssinger, University of Geneva

Platinum-Porphyrin Conjugates as Highly Phototoxic Agents against Human Cancer Cells [MC-133]

Bernhard Spingler, University of Zurich

RNA internal loop: suitable binding site for metallointercalators? [MC-134]

Elena Alberti, Daniela Donghi, University of Zurich

Secrets of *in vitro* RNA folding and splicing revealed by fluorescent PNA labels [MC-135]

Ilija Vukadin, Roland K.O. Sigel, University of Zurich

RNA and Oxaliplatin: Investigation of Possible Platinum Binding Sites [MC-136]

Marianthi Zampakou, Daniela Donghi, University of Zurich

Studies on the mode of action of cationic  $\beta$ -hairpin antibiotics [MC-137]

Matthias Urfer, John A. Robinson, University of Zurich

Towards *in vivo* splicing of group II intron ai5γ [MC-138] Maya Gulotti-Georgieva, *Roland K.O. Sigel*, University of Zurich

Characterization of group II introns retrohoming site at the single molecule level. [MC-139]

Mokrane Khier, Roland K.O. Sigel, University of Zurich

Correlation between structure and antimicrobial activity of chitosan-alkyl thiomers – a biological study [MC-140] Simona Conti, *Greta Ricarda Patzke*, University of Zurich

Peptide Shuttle System to Deliver PNAs to their Place of Action [MC-141]

Susann Zelger-Paulus, Roland K.O. Sigel, University of Zurich

Roles of the continuous internal water pathway in G-proteincoupled receptors activations [MC-142]

Shuguang Yuan, Actelion Pharmaceuticals Ltd., Horst Vogel, EPF Lausanne

Molecular Mechanism of Ruthenium and Gold Anticancer Agents in the Allosteric Regulation of the Nucleosome Core Particle (NCP) [MC-143]

Giulia Palermo, Ursula Röthlisberger, EPF Lausanne

Bicyclic peptide that selectively inhibits MMP-2 [MC-144] Maola Khan, *Christian Heinis*, EPF Lausanne

Long-Lived States of Pairs of Fluorine-19 Nuclei: a new Tool for Ligand-Protein Screening [MC-145]

Roberto Buratto, Geoffrey Bodenhausen, EPF Lausanne

Comparison of <sup>18</sup>F-labeled alpha and gamma-conjugated folate derivatives for tumor imaging using positron emission tomography (PET) [MC-146]

Silvan David Boss, Simon Mensah Ametamey, ETH Zurich

Human Biomonitoring Bridging Gaps between Medicine and Environment [MC-147]

Basem Shomar, Qatar Environment and Energy Research Institute (QEERI)

Palladium-mediated Suzuki-Miyaura coupling: an efficient method for the formation of therapeutically relevant protein conjugates [MC-148]

Anaëlle Dumas, Université Paris-Sud

Enzyme catalyzed sulfur-carbon bond formation by ergothioneine biosynthetic sulfoxide synthase [MC-149] Kristina Goncharenko, *Florian Seebeck*, University of Basel

Electrostatic Effect Of Halogenation On The Thermodynamic Stability Of Rapid Insulin Analogs [MC-150]

Krystel El Hage, Markus Meuwly, University of Basel

Preventing aggregation of porphyrinic photosensitizers using a biodegradable triblock copolymer [MC-151]
Ilche Gjuroski, *Julien Furrer*, University of Bern

Why are Vesicles of the Artificial 1,3-Diamidophosholipid Pad-PC-Pad Mechanosensitive? [MC-152]

Dennis Müller, Andreas Zumbühl, University of Fribourg

Addressing the tempormandibular joint disorder [MC-153] Etienne Stalder, *Andreas Zumbühl*, University of Fribourg

Computer-aided drug design unveils the structural requisites for selective GPBAR1 activation [MC-154]

Francesco Saverio Di Leva, University of Naples Federico II

### NMR investigation of the human RNA BCL2 G-quadruplex: restricting folding dynamics [MC-155]

Alicia Dominguez-Martin, Roland K. O. Sigel, University of Zurich

Metal ion dependency and multimerization behavior of biologically relevant human RNA G-quadruplexes [MC-156] Helena Guiset-Miserachs, *Roland K.O. Sigel*, University of Zurich

### Structure - antimicrobial activity relationships of chitosan-alkyl thiomers [MC-157]

Matteo Croce, Greta Ricarda Patzke, University of Zurich

### Real-time Characterisation of a Large, Catalytic and Dynamic RNA by Single Molecule Microscopy. [MC-158]

Mélodie C.A.S. Hadzic, Roland K.O. Sigel, University of Zurich

### Pore size matters - A crowding study of ribozyme folding and activity [MC-159]

Richard Börner, Roland K.O. Sigel, University of Zurich

#### The binding mechanism between a $B_{12}$ -specific RNA and its ligand coenzyme $B_{12}$ [MC-160]

Sofia Gallo, Roland K.O. Sigel, University of Zurich

#### Organic Chemistry [OC] Poster Session

Jury members: Martin Lochner, University of Bern, Amalia Poblador Bahamonde, University of Geneva, Jieping Zhu, EPF Lausanne, Jérôme Waser, EPF Lausanne

### 1-Alkynyltriazenes as Functional Analogues of Ynamides [OC-101]

Florian Gérald Perrin, Kay Severin, EPF Lausanne

#### Convergent Synthesis of Glycopeptide Dendrimer Biofilm Inhibitors based on the Chloroacetyl-Thioether-Cysteine (ClAc) Ligation [OC-102]

Gaëlle Michaud, Jean-Louis Reymond, University of Bern

#### Mechanism, Optimization and Scope studies of Rh(II) Catalyzed One-Step Multi-Component Macrocyclization Reactions [OC-103]

Daniele Poggiali, Jérôme Lacour, University of Geneva

### Synthesis and application of tetrafluoroethylation reagents based on hypervalent iodine [OC-104]

Jiri Vaclavik, Antonio Togni, ETH Zurich

### Synthesis of a Hydrogen-Bonded Quaterthiophene and its Use in Organic Field-Effect Transistors [OC-105]

Bilal Özen, Holger Frauenrath, EPF Lausanne

#### [4+2]-Annulations of Aminocyclobutanes [OC-106] Daniele Perrotta, *Jérôme Waser*, EPF Lausanne

Synthesis of chiral Ruthenium-cyclopentadienyl complexes and application to formal [4+2] cyclizations of yne-enones [OC-107]

David Kossler, Nicolai Cramer, EPF Lausanne

#### Synthesis, Characterization and Application of Styrene-Functionalized Imidazolium Salts [OC-108]

Felix D. Bobbink, Paul Dyson, EPF Lausanne

### Rhodium(III)-Catalyzed C-H Activation Rapid Access to Versatile Organic Molecules [OC-109]

Manh Van Pham, Nicolai Cramer, EPF Lausanne

## Chiral Cyclopentadienyl-Iridium Complexes as Catalysts for Cycloisomerizations of N-tethered 1,6-Enynes [OC-110] Michael Christian Dieckmann, Nicolai Cramer, EPF Lausanne

### Annulation of strained Rings, a Usefull Tool for the Synthesis of Nucleoside Analogues [OC-111]

Sophie Racine, Jérôme Waser, EPF Lausanne

#### Vicinal Amino Alcohols Synthesis from Allyl Amines via in Situ Tether Formation and Pd-Catalyzed Carboetherification [OC-112]

Ugo Orcel, Jérôme Waser, EPF Lausanne

#### Total Synthesis of (±)-Aspidophylline A [OC-113]

Weiwu Ren, Jieping Zhu, EPF Lausanne

#### Synthesis and Properties of Quinone-Type Push-Pull Chromophores [OC-114]

Cagatay Dengiz, François Diederich, ETH Zurich

### Stereoselective Organocatalytic Synthesis of Oxindoles with Adjacent Tetrasubstituted Stereocenters [OC-115]

Oliver Dieter Engl, Helma Wennemers, ETH Zurich

#### Synthesis of Tröger's Base Analogues via a Phase-Transfer-Catalyzed Double Aza-Michael Reaction Under Base-Free Conditions [OC-116]

Takuya Kamiyama, Jan Cvengros, ETH Zurich

#### Towards a Short Synthesis of (*R*,*R*,*R*)-α-Tocopherol [OC-117] Thomas Netscher, F. Hoffmann-La Roche AG

### Chiral verdazyl radicals for metal-organic functional assemblies [OC-118]

Mattia Poretti, *Olimpia Mamula-Steiner*, Haute Ecole d'Ingénierie et d'Architecture Fribourg

#### Hyaluronic Acid-Based Hydrogels for Drug Delivery [OC-119]

Roger Marti, School of Engineering and Architecture of Fribourg

## Efficient Access to Functionalized Cyclobutanone Derivatives Using Cyclobuteniminium Salts as Highly Reactive Michael Acceptors and Dienophiles [OC-120]

Alexandre Lumbroso, *Alain De Mesmaeker*, Syngenta Crop Protection AG

### Strigolactam: New potent strigolactone analogues for the germination of Orobanche Cumana [OC-121]

Alexandre Lumbroso, *Alain De Mesmaeker*, Syngenta Crop Protection AG

#### $6\pi/10\pi$ -electrocyclization of ketene-iminium salts for the synthesis of substituted naphthylamines [OC-122]

Amandine Kolleth-Krieger, *Alain De Mesmaeker*, Syngenta Crop Protection AG

## Asymmetric synthesis of (+)-GR-24 and the four stereoisomers of (+)-5-deoxystrigol using [2+2]-cycloadditions of keteneiminiums to olefins [OC-123]

Pierre-Yves Dakas, *Alain De Mesmaeker*, Syngenta Crop Protection AG

#### Organocatalytic Atroposelective Aldol Condensation [OC-124]

Achim Link, Christof Sparr, University of Basel

#### Total Synthesis of Fidaxomicin [OC-125]

Elias Kaufmann, Karl Gademann, University of Basel

#### Preparation of Fidaxomicin Analogs via Total Synthesis [OC-126]

Hiromu Hattori, Karl Gademann, University of Basel

### Setting the Hook for Specific Single Walled Carbon Nanotubes [OC-127]

Ina Bodoky, Marcel Mayor, University of Basel

#### Direct preparation of pyrrolizidines using imines and isonitriles [OC-128]

Isabel Patrizia Kerschgens, Karl Gademann, University of Basel

Chemical modification of peptide and proteins for UV postionization and quantum interference experiments [OC-129]

jonas schaetti, Valentin Köhler, University of Basel

Towards a Perylene-Based Cyclophane with Charge-Transfer Capability [OC-130]

Kevin Weiland, Marcel Mayor, University of Basel

Synthesis of a Diacetylene-Bridged Geländer-Type Oligomer [OC-131]

Linda Maria Bannwart, Marcel Mayor, University of Basel

Synthesis of an Unknown Tetracyclic Derivative of Norbornane [OC-132]

Lorenzo Delarue Bizzini, Marcel Mayor, University of Basel

Molecules in Gasphase: Synthesis of Multi-Porphyrin-Systems for Quantum Interference Experiments [OC-133]
Lukas Felix, *Marcel Mayor*, University of Basel

Rotational restricted and functionalized CBP derivatives for blue emitting OLEDs [OC-134]

Manuel Hellstern, Marcel Mayor, University of Basel

Total synthesis of Aeruginosin 828A [OC-135]

Manuel Scherer, Karl Gademann, University of Basel

Radical Cyclizations involving Aryl Azides as Radical Traps [OC-136]

Benjamin Wyler, Philippe Renaud, University of Bern

Lipid Linked Oligosaccharide (LLO) Analogues as Bacterial Oligosaccharyltransferase (OST) PgLB Substrates [OC-137] Jérémy Boilevin, *Jean-Louis Reymond*, University of Bern

Synthesis of Nitrogen-Containing Macrocycles via  $\alpha$ -Imino Diazo Intermediates [OC-138]

Alejandro Guarnieri Ibáñez, Jérôme Lacour, University of Geneva

Enantiospecific C-H Azidation and ensuing functionalization of Tröger Bases [OC-139]

Alessandro Bosmani, Jérôme Lacour, University of Geneva

A Series of Novel Redox Gradient Fullerenes in Triple-Channel Photosystems [OC-140]

Altan Bolag, Stefan Matile, University of Geneva

The Anion-π Interaction: A Tuneable Non-Covalent Interaction for Catalysis [OC-141]

Franois Nicolas Miros, Stefan Matile, University of Geneva

Twisted Push-Pull Fluorophores as Mechanosensitive Probes [OC-142]

Saeideh Soleimanpour, Stefan Matile, University of Geneva

Arylamine Tribenzopentaphenes: Versatile Synthesis and study of their Hole Mobility [OC-143]

Andrew H. Rice, University of Washington, Seattle, USA

Route to the controlled formation of prostaglandin double bonds [OC-144]

Katalin Molnár, BME Szerves Kemia es Technologia Tanszek

Towards a Total Synthesis of Fijiolide A [OC-145] Christoph Heinz, *Nicolai Cramer*, EPF Lausanne

Molecular and Polymeric Nanostructures Based on a Novel AAA-DDD Triple Hydrogen Bonding Motif [OC-146] Marcus Papmeyer, *Kay Severin*, EPF Lausanne

Revisiting the Suzuki Coupling Based on Volcano Plots and Linear Scaling Relations [OC-147]

Michael Busch, Clemence Corminboeuf, EPF Lausanne

Suzuki-Miyaura Cross-Coupling Reactions of Unactivated Alkyl Halides Catalyzed by a Nickel Pincer Complex [OC-148] Thomas Di Franco, *Xile Hu*, EPF Lausanne

Towards the Total Synthesis of the 3-Acyltetramic Acid Antibiotics Bu-2313A/B [OC-149]

Claudio Bomio, Karl-Heinz Altmann, ETH Zurich

KAT ligation for 3D control in hydrogels using 2-photon microscopy [OC-150]

Dmitry Mazunin, Marcy Zenobi-Wong, ETH Zurich

Towards the Total Synthesis of Acalycixeniolide F [OC-151] Leo Betschart, *Karl-Heinz Altmann*, ETH Zurich

Functional Cumulene-Based Molecular Materials [OC-152] Przemyslaw Gawel, François Diederich, ETH Zurich

Synthesis, Characterization and Application of an Ethano-Tröger's Base Derived Electrophilic Fluorinating Reagent [OC-153]

Raul Pereira, ETH Zurich, Veronique Gouverneur, University of Oxford

Cyanomethylation of aryl halides by domino Suzuki/fragmentation reaction [OC-154] Juraj Velcicky, Novartis Pharma AG

Stabilization of Non-Kekulé Triangulene [OC-156]

Michal Juricek, University of Basel

Multi-Catalyst Screening for the Asymmetric Morita-Baylis-Hillman Reaction by Mass Spectrometric Monitoring of the Back Reaction [OC-157]

Patrick Isenegger, Andreas Pfaltz, University of Basel

Helically Chiral Biradicaloid Polycyclic Aromatic Hydrocarbon [OC-158]

Prince Ravat, University of Basel

Concentration Controlled Synthesis of Molecular Daisy Chains

- Towards [c2]Daisy Chains as Functional Materials [OC159]

Sylvie Drayss-Orth, Marcel Mayor, University of Basel

Modular Synthesis, Functionalization and resolution of Cationic [6]HELICENES [OC-160]

Geraldine Labrador, Jérôme Lacour, University of Geneva

Online swiss army knife for organic chemists [OC-161] Luc Patiny, EPF Lausanne

Structure Refinement of a \( \beta\)-Heptapeptide Using RDCs

Measured in a Stretched PVA Gel in Methanol [OC-162]

Carla Rigling, \( Marc-Olivier Ebert, \) ETH Zurich

Peptide-Catalyzed Stereoselective Conjugate Addition Reactions of Aldehydes to Maleimides [OC-163]

Claudio Grünenfelder, Helma Wennemers, ETH Zurich

Enantioselective Aldol Reactions with Fluoromalonyl Halfthioesters as Masked Fluoroacetates [OC-164] Jakub Saadi, *Helma Wennemers*, ETH Zurich

Physical Chemistry [PC]

**Poster Session**Jury members: Hans Jakob Wörner, ETH Zürich, Marcel Drabbels, EPF Lausanne, Samuel Leutwyler, University of Bern

A dive into the Cytochrome  $b_6 f$  complex via ultrafast spectroscopy. [PC-101]

Adrien Chauvet, Majed Chergui, EPF Lausanne

Revealing conformers of protonated tryptophan by IR-IR-UV triple resonance spectroscopy of cold ions. [PC-102]
Aleksandr Y Pereverzev, EPF Lausanne

Bond-selective chemisorption of methane isotopologues on Pt(111) [PC-103]

Ana Gutiérrez-González, *Rainer Beck*, EPF Lausanne

**Ultrafast Electro-modulated Differential Absorption** Spectroscopy of Methylammonium Lead Iodide Perovskite Thin Films: Evidence for Carriers Trapping and Accumulation at the Surface [PC-104] Arun Aby Paraecattil, Jacques-E. Moser, EPF Lausanne

Cold ion spectroscopy reveals the exact structure of protonated helical peptides in the gas-phase. [PC-105]

Chiara Masellis, Thomas R Rizzo, EPF Lausanne

Femtosecond transient absorption spectroscopy of CsPbX<sub>3</sub> perovskite nanoparticles [PC-106]

F. G. Santomauro, Majed Chergui, EPF Lausanne

Photoinduced charge transfer mechanism in Diketopyrrolopyrrole(DPP) dye-sensitiezed solar cell [PC-

Heewon Bahng, EPF Lausanne

Spectroscopic studies of kinetically trapped conformations in the gas phase: the case of triply protonated bradykinin [PC-

Liudmila Voronina, Thomas R Rizzo, EPF Lausanne

State-to-state scattering of CH<sub>4</sub>(v<sub>3</sub>) from Ni(111) and LiF(100) surfaces. [PC-109]

Maarten van Reijzen, Rainer Beck, EPF Lausanne

Infrared spectroscopy of mobility-selected H<sup>+</sup>-Gly-Pro-Gly-Gly (GPGG) [PC-110]

Michael Z Kamrath, Thomas R Rizzo, EPF Lausanne

Electronic energy transfer in model peptides [PC-111] Valeriu Scutelnic, Thomas R. Rizzo, EPF Lausanne

Pushing the limits of cold ion spectroscopy: structural characterization of protonated ubiquitin in the gas phase [PC-112]

Vladimir Kopysov, Oleg V Boyarkin, EPF Lausanne

Photoassociation of cesium atoms upon Rydberg excitation in a dense ultracold gas [PC-113]

Heiner Saßmannshausen, Frédéric Merkt, ETH Zurich

Precision Spectroscopy in Cold Molecules: The First Rotational Intervals of He<sup>+</sup><sub>2</sub> by High-Resolution Spectroscopy and Rydberg-Series Extrapolation [PC-114] Luca Semeria, Frédéric Merkt, ETH Zurich

Continuous trap loading of Rydberg-Stark decelerated metastable helium using overlaid electric and magnetic traps [PC-115]

Matija Zesko, Frédéric Merkt, ETH Zurich

MQDT-assisted high-resolution spectroscopy of the Rydberg states of H2 - ionization energy of H2 and rovibrational structure of H<sub>2</sub>+ [PC-116]

Maximilian Beyer, Frédéric Merkt, ETH Zurich

High-Resolution VUV-Absorption Spectroscopy using Phase Modulation [PC-117]

U. Hollenstein, Frédéric Merkt, ETH Zürich

Mapping the electronic states of small transition metal clusters by nonlinear spectroscopy [PC-118]

Martin Beck, Peter Pal Radi, PSI Villigen

Dissociation dynamics of dissolved CH<sub>3</sub>I studied with timeresolved resonant inelastic X-ray scattering [PC-119] Rok Bohinc, PSI Villigen

Femtosecond Time-resolved Spectroscopy in the Extreme **Ultraviolet Spectral Range [PC-120]** 

Jakob Grilj, Stanford University School of Medicine, Majed Chergui, EPF Lausanne

Quantum-Logic Spectroscopy for Single Trapped Molecular Ions [PC-121]

Gregor Hegi, Stefan Willitsch, University of Basel

Towards hybrid trapping of cold molecules and cold molecular ions [PC-122]

Dominik Haas, Stefan Willitsch, University of Basel

**Cold Ion-Neutral Reactions in Next-Generation Ion-Atom Hybrid Traps [PC-123]** 

Pascal Eberle, Stefan Willitsch, University of Basel

Ionic Liquids based on crown ether as electrolytes for batteries [PC-124]

Hervé YAO, Katharina M. Fromm, University of Fribourg

Electrons and ionic liquids - a novel approach to study electron scattering from nonvolatile compounds [PC-125]

Khrystyna Regeta, Michael Allan, University of Fribourg

Ligand exchange reactions with Palladium, Platinum doped Au25(SR)18 clusters [PC-126]

Annelies Sels, Thomas Bürgi, University of Geneva

**Tracking Solvent Controlled Photoinduced Electron Transfer** Using Broadband Fluorescence Up-Conversion [PC-127] Arnulf Rosspeintner, Eric Vauthey University of Geneva

Ligand exchange reaction of chiral Pd<sub>2</sub>Au<sub>36</sub>(SR)<sub>24</sub> cluster [PC-128]

Bei Zhang, Thomas Bürgi, University of Geneva

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Christoph Nançoz, Eric Vauthey, University of Geneva

Excited-state dynamics of radical ions [PC-130]

Joseph Samuel Beckwith, Eric Vauthey, University of Geneva

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Marta Brucka, Damien Jeannerat, University of Geneva

Ultrafast Intersystem-crossing Dynamics and Breakdown of the Kasha-Vavilov's Rule of Naphthalenediimides [PC-132] Oleksandr Yushchenko, Eric Vauthey, University of Geneva

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Qinchao Sun, Andreas Hauser, University of Geneva

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Teresa Delgado, Andreas Hauser, University of Geneva

Marangoni flow driven maze solving [PC-135] Rita Toth, EMPA

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Shuyu Liang, EMPA, Hansjörg Grützmacher, ETH Zurich

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Aurélien Patoz, Jiri Vanicek, EPF Lausanne

Hyperpolarized para-ethanol [PC-138]

Daniele Mammoli, Geoffrey Bodenhausen, EPF Lausanne

**Excitonic Effects and Optical Spectra of Single Walled Carbon** Nanotubes for Biosensor Applications in Life Sciences and Medicine [PC-139]

Dejan M Djokic, Ardemis A. Boghossian, EPF Lausanne

Studying Xe Migration in Truncated Hemoglobin with **Molecular Dynamics Simulations [PC-140]** 

Polydefkis Diamantis, EPF Lausanne, Markus Meuwly, University of Basel

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Katrin Dulitz, Frédéric Merkt, ETH Zurich

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Ondřej Tkáč, Frédéric Merkt, ETH Zurich

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Urs Hartfelder, Jeroen Anton van Bokhoven, ETH Zurich

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Brahim Aïssa, Qatar Environment and Energy Research Institute (QEERI)

### **Gas-phase Microsolvation of an Adenine Analogue [PC-145]**Luca Siffert, *Samuel Leutwyler*, University of Bern

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Maria A. Trachsel, Samuel Leutwyler, University of Bern

### Unusually long-lived transient negative ion of c- $C_4F_8O$ formed by electron impact ionisation [PC-147]

Radmila Janeckova, University of Fribourg

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Elia Previtera, University of Geneva

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Harekrishna Ghosh, Thomas Bürgi, University of Geneva

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Jakob Bierwagen, Hans Hagemann, University of Geneva

#### Gold nanowire fabrication with lipid nanotubes [PC-151]

Kristina Jajcevic, Kaori Sugihara, University of Geneva

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Martin Magg, University of Geneva, Bruce R. Weisman, Rice University

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Roberto Diego Ortuso, Kaori Sugihara, University of Geneva

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Margherita Orazietti, Peter Hamm, University of Zurich

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Jury members: Stephen Schrettl, EPF Lausanne, Dorina Opris, EMPA, Samuel Jones, EPF Lausanne

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Mihai Lomora, Cornelia Gabriela Palivan, University of Basel

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Bjoern Schulte, Holger Frauenrath, EPF Lausanne

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Francois Noverraz, Sandrine Gerber, EPF Lausanne

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Nicolas Luisier, Kay Severin, EPF Lausanne

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Solène Passemard, Sandrine Gerber, EPF Lausanne

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Andreas Herrmann, Firmenich SA

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Shirin Shokoohi, Research Institute of Petroleum Industry

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Rachel Louise Alexander, Swansea University UK

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Yves Jacquot, Université Pierre et Marie Curie, Paris

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Guojun Ke, Marcel Mayor, University of Basel

## Synthetic biocompartments with selective membrane permeability towards protons and monovalent cations [PCI-111]

Mihai Lomora, Cornelia Gabriela Palivan, University of Basel

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Tomaz Einfalt, Cornelia Gabriela Palivan, University of Basel

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Caroline D. Bösch, Robert Häner, University of Bern

### The formation of large assemblies through single, non-covalently attached pyrene phosphates [PCI-114]

Markus Probst, Robert Häner, University of Bern

### Hierarchical self-assembly of the DNA-grafted supramolecular polymers [PCI-115]

Yuliia Vyborna, Robert Häner, University of Bern

#### Pt<sup>(0)</sup> containing metallosupramolecular polymers [PCI-116] Luis Miguel Olaechea, *Christoph Weder*, University of Fribourg

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Marc Karman, Christoph Weder, University of Fribourg

#### Side reactions in polycondensation of aromatic amino acids [PCI-118]

Michael Badoux, Andreas Kilbinger, University of Fribourg

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Milene Tan, Katharina Fromm, University of Fribourg

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Sarah-Luise Abram, Katharina Fromm, University of Fribourg

#### DNA complexation effect on a cyanine probe studied at liquid/water interfaces by SSHG [PCI-121]

Giuseppe Leonardo Licari, Eric Vauthey, University of Geneva

#### Large-scale self-assembled gold nanoparticle arrays and plasmonic-enhanced fluorescence [PCI-122]

Mahshid Chekini, Thomas Bürgi, University of Geneva

### Dispersion stability of layered double hydroxide particles in the presence of polyelectrolytes [PCI-123]

Marko Pavlovic, University of Geneva

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Tianchi Cao, Michal Borkovec, University of Geneva

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Fabian Deuber, Christian Adlhart, Zurich University of Applied Sciences, ZHAW

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Nicola Zucchetto, *Dominik Brühwiler*, Zurich University of Applied Sciences, ZHAW

Surface Activity of Nanoparticle Suspensions at Interfaces [PCI-127]

Yong Zen Tan, Andrei Honciuc, Zurich University of Applied Sciences, ZHAW

Ellipsoid-Shaped Superparamagnetic Nanoclusters through Emulsion Electrospinning [PCI-128]

Markus B. Bannwarth, EMPA

Long-lived charge carriers in organic Nanowires [PCI-129] Regina Judith Hafner, *Holger Frauenrath*, EPF Lausanne

Porous nitrogen-doped carbon materials generated from fractal gels for  $CO_2$  capture [PCI-130]

Anna Beltzung, Massimo Morbidelli, ETH Zurich

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Leon F. Scherz, A. Dieter Schlüter, ETH Zurich

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Loredana Protesescu, Maksym Kovalenko, ETH Zurich

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Mario Lenz, Petra Dittrich, ETH Zurich

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Sandra Luginbühl, *Peter Walde*, ETH Zurich

Stability of radiation grafted polymer electrolyte membranes for water electrolysis cells [PCI-135]

Albert Albert, PSI Villigen

Chemical functionalization of nanocelluloses: a route to functional materials [PCI-136]

Philippe Tingaut, EMPA

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Almudena Gallego, University of Basel, Markus Arndt, University of Vienna

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Dalin Wu, University of Basel, Andrei Honciuc, Zurich
University of Applied Sciences, ZHAW

Janus Dumbbells: A flexible template for colloidal chemistry [PCI-139]

Florian Guignard, Marco Lattuada, University of Fribourg

Stimuli-responsive azo-containing polymeric materials [PCI-140]

Mathieu André Ayer, Christoph Weder, University of Fribourg

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Nico Bruns, University of Fribourg

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Radu Tanasescu, Andreas Zumbühl, University of Fribourg

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Simonetta Rima, Marco Lattuada, University of Fribourg

Development of cell membrane mechanosensor for quantitative force detection of peptides [PCI-144]

Jiri Kulhavy, Kaori Sugihara, University of Geneva

Characterization of voltage sensitive dyes with free-standing lipid bilayers [PCI-145]

Maria Tsemperouli, Kaori Sugihara, University of Geneva

Ionic liquids and ion-specific effects in particle aggregation: an experimental study beyond the Hofmeister series [PCI-146] Tamas Oncsik, *Michal Borkovec*, University of Geneva

Tuning the nanostructure and the properties of silica surfaces by heat treatment [PCI-147]

Valentina Valmacco, Michal Borkovec, University of Geneva

Enhancing the Rheological Properties of a Sulfobetaine using a Cationic Surfactant [PCI-148]

Shirin Shokoohi, Research Institute of Petroleum Industry

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