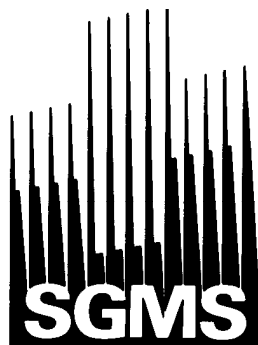


Swiss group for mass spectrometry
Schweizerische Gruppe für Massenspektrometrie



Groupe suisse de spectrométrie de masse
Gruppo svizzero di spettrometria di massa

Newsletter

2011 SGMS Meeting

October 27 and 28

Dorint Resort Blüemlisalp

Beatenberg

Featuring...

Paola Picotti	Inst Molecular Systems Biology, ETHZ
Philippe Schmitt-Kopplin	Inst for Ecological Chemistry, Munich
Helmut Segner	Inst of Animal Pathology, Univ Bern
Ian Wilson	Astra Zeneca, Macclesfield, Cheshire, UK

SGMS General Assembly 2011

Dorint Resort Blüemlisalp

Thursday October 27

Please attend our General Assembly following the afternoon session. Later we will join for the Apéro and the famous "Dinner Buffet".

There will be plenty of time for discussions. Latest news will be served at the bars.

NEW

abstract to be sent to abstract@sgms.ch

registration to be sent to registration@sgms.ch

In this Newsletter:

- Message from the President 3
- Abstracts of the plenary lectures

Ian Wilson

- LC-MS-based profiling for metabonomics/metabolomics –
the current challenges 5

Paola Picotti

- Selected reaction monitoring in targeted proteomics:
from cellular networks to complete proteome maps 6

Philippe Schmitt-Kopplin

- Ultrahigh resolution mass spectrometry approaches and new data
evaluation strategies for complex environmental mixtures 8

Helmut Segner

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Message from the President

The 28th SGMS annual meeting took place November 4–5 at the Hotel Dorint Beatenberg. A record breaking 130 participants enjoyed a high quality scientific program, with four plenary lectures and 12 additional contributions (see www.sgms.ch > MS Meetings > 2010). Prof Jyotsna Sharma (Texas Tech University, Lubbock, TX, USA) opened the conference with a talk on “Orchids: models of biological complexity”, in which she illustrated the elaborate deception ploys used by orchids for attracting pollinators. She also explained how orchids obtain essential nutrients through the specialized interaction with mycorrhizal fungi, using plant hormones to guide the fungal hyphae to grow together with their roots. Prof Cathy Costello (Boston University School of Medicine, Boston, MA, USA) showed why it was important to not only focus on proteins, but also look at N- and O-linked glycans when addressing biomedical questions. This is true because the glycosylation status of cell surface proteins and lipids influences interactions of individual cells and even whole organisms, with one another and with the environment. Prof Andrej Shevchenko (MPI, Dresden, GER) then presented tips and tricks for lipid profiling in metabolic diseases research, and Prof Jean-Luc Veuthey (University of Geneva and Lausanne, EPGL, Geneva, CH) discussed how to down-scale to ultrafast, high-throughput, and high resolution UHPLC for pharmaceutical analysis. Prof Veuthey also talked about the use of a high-throughput in-capillary CYP450 bioreactor with subsequent UHPLC separation for the analysis of drug metabolites.

The SGMS again waived registration fees for student presenters at the meeting and for the first time honored the best student presentation with the SGMS Student Award. Aurélien Thomas (Geneva University Hospital) was the winner who received an Amazone gift certificate of € 400 for his presentation.

The Thursday afternoon session was followed by the 2010 General Assembly of the SGMS. During this occasion the president and the whole board was confirmed for another period of 2 years. Eight new members were admitted by acclamation and Advion was welcomed as the newest sponsor of the SGMS. It was also announced that the 20th International Mass Spectrometry Conference to be held in Geneva in 2014 and co-organized by the SGMS has received seed money in the amount of € 10'000 from the International MS Foundation. After the general assembly, the participants met for an aperitif, followed by a delicious dinner buffet, and long discussions in the Muh Bar.

Dr Marc J-F Suter, President SGMS



Aurélien Thomas

Recipient of the SGMS Student Award

(Picture by St Müller)

LC-MS-based profiling for metabonomics/metabolomics – the current challenges



Ian Wilson

Drug Metabolism and Pharmacokinetics IM
Mereside
Alderley Park
Macclesfield
Cheshire SK10 4TG
United Kingdom

The discovery of valid biomarkers, present in biofluids and tissues as a means of studying the metabolic response of organisms to normal physiological changes, toxins or disease progression is a major analytical challenge for metabonomics/metabolomics. Whilst the application of powerful analytical methods in an untargeted fashion provides a hypothesis free approach to biomarker discovery there are many pitfalls awaiting the unwary. However, when performed properly these global metabolite profiling methods for the detection of new biomarkers should also be hypothesis generating. Here the use of LC-MS will be described for metabolic profiling investigations that illustrate the great potential of this type of study, as well as some of the more obvious sources of error. These applications will describe studies covering metabolic profiling in animal models, including those dealing with ethanol toxicity and obesity, humans and novel humanised mouse liver models. The many practical challenges faced in the application of LC-MS for the detection of biomarkers in this role will be considered together with some pragmatic solutions. The current challenges, ways of tackling them and the future evolution of metabolic profiling techniques will be considered by references to these applications.

***Selected reaction monitoring in targeted proteomics:
from cellular networks to complete proteome maps***



Paola Picotti

Institute of Molecular Systems Biology, ETHZ
Zürich
Switzerland

To study and model the properties of cellular networks –e.g. metabolic or signaling networks– it is crucial to measure all the elements that constitute them, which are often associated to a wide range of molecular properties and cellular abundances. However, comprehensive measurements are still technically difficult, even in a simple organism such as yeast and especially at the proteome level. To overcome the limitations of classical approaches we applied a targeted proteomic workflow based on selected reaction monitoring (SRM) to the analysis of yeast cellular networks. First, we tested the depth and sensitivity of the SRM-based approach. We demonstrated that proteins spanning the whole range of abundance, between $1.3E6$ copies/cell and <50 copies/cell could be detected by SRM in yeast proteome digests. Then we applied the approach to the analysis of a yeast metabolic network. Proteins in the network were quantified by SRM in yeast grown under a series of conditions inducing radically different metabolic setups and in a growth time-course of yeast cells transiting through a series of metabolic phases. The quantitative dataset generated highlighted how yeast metabolism adapts to changing conditions of supply and demand of nutrients. It indicated that *S. cerevisiae* expresses superfluous proteins, not necessarily used in a particular

metabolic condition and allowed to suggest differential functionality for several metabolic isoenzymes. All the SRM assays developed were deposited to the web-accessible SRMATlas database, which supports the collection and dissemination of the assays. Finally, to overcome the bottlenecks of SRM assay development, we introduced a method based on unpurified synthetic peptide libraries, that allows for the high-throughput and low-cost optimization and validation of SRM assays for any set of proteins or proteome of interest. The approach was used to develop a complete set of SRM assays for the ~6,000 proteins that constitute the proteome of *S cerevisiae*. Similarly, the approach was expanded to the generation of SRM assays for >90% of the human proteome, using a set of 170,000 peptides and the corresponding public human SRM assay library is currently under construction. The power and the bottlenecks of this approach will be discussed.

Ultrahigh resolution mass spectrometry approaches and new data evaluation strategies for complex environmental mixtures



Philippe Schmitt-Kopplin

Institute for Ecological Chemistry
HelmholtzZentrum Munich
Neuherberg
Germany

Natural organic matters (NOM) are ubiquitous in terrestrial and aquatic ecosystems and play a fundamental role in the environment. NOM are complex biogeochemical mixtures of non repetitive materials existing in such a vast amount, that their quantity easily exceeds the amount of functional biomolecules. During diagenesis, they continuously undergo degradation and chemical reformation, governed by the fundamental restrains of thermodynamics and kinetics, resulting the extreme intricacy. The natural diversity of these complex organic materials denotes high variability and density of binding sites, which enable them to behave as natural buffer against environmental and chemical extremes. Furthermore natural organic matter defines the bioavailability and cycling of organic and inorganic nutrients and pollutants. Therefore an improved understanding of its composition and the characterization and structural analysis of geopolymers, which feature a substantial extent of both polydispersity and molecular heterogeneity, is most demanding with respect to methodology and concepts. Ultrahigh resolution mass spectrometry is one possible approach among others based on separation and spectroscopy and is shown here in the

analysis of such complex mixtures. Besides classical tools developed in house for the analysis of these materials based on exact mass differences, new approaches in visualizing the vast amount of data and structure information will be presented. The non-targeted way in investigating NOM was the basis of development of non-targeted metabolomics, approaches and data evaluation tools to unravel the metabolite diversity and interconnectivity using network and graph theory approaches.

The Lake Thun “Mystery”: high prevalence of coregonids with malformed gonads in Lake Thun



Helmut Segner

Centre for Fish and Wildlife Health
Vetsuisse Faculty
University of Bern
Bern
Switzerland

Most morphological traits show some degree of quantitative and/or qualitative variation. The question of how to differentiate between ‘normal’ and ‘abnormal’ states of a given trait, and whether an abnormal phenotype is induced genetically, environmentally or by gene-environment interaction, is not trivial to answer. This is particularly true for wildlife species, with an often rather limited knowledge on their biological traits. Whitefish, *Coregonus lavaretus*, from the pre-alpine, oligotrophic Lake Thun, Switzerland, show a remarkable variation of gonad morphology. The variations occur at high prevalence and can be classified into distinguishable morphological categories. As Lake Thun serves as drinking water reservoir for nearly half a million people, and as fish serve as sentinels of environmental quality, the observation of malformed gonads gives rise to the questions if these alterations represent normal or abnormal morphological variations, and what the cause(s) of the alterations are. To answer the first question, an extensive monitoring program was initiated, covering not only Lake Thun, but also two neighboring lakes, i.e. Lake Biel and Lake Brienz. The results were analyzed at three hierarchical levels, i.e. (i) among lakes, (ii) among the ecoforms of whitefish within the lakes, and (iii) among spawning sites within ecoforms. The results revealed that gonad alterations are not restricted to Lake Thun,

but that Lake Thun is unique with respect to frequency and type of malformations. Among the four whitefish forms present in Lake Thun, the so-called “Brienzig” showed the highest frequency of gonad alterations, and males were generally more affected than females. In searching for possible malformation-inducing factors in the Lake Thun ecosystem, we tested a variety of factors that are known to be able to influence gonad morphology of fish, including genetic factors, parasite infections and environmental chemicals. Particular emphasis has been given to endocrine-disrupting compounds, i.e. substances that interfere with the endogenous hormone system. In a series of long-term rearing and exposure experiments, we could provide evidence that (i) the gonad deformations are environmentally, not genetically induced (what does not yet exclude a gene-environment interaction), and (ii) among environmental factors, neither parasites nor endocrine disrupting compounds are responsible for the induction of the gonad malformations, but that the inducing factor is contained in Lake Thun plankton which is the natural food of whitefish. Current research aims to identify the plankton-borne factor(s) being responsible for the induction of the gonad malformations.

Minutes of the 2010 General Assembly of the Swiss Group for Mass Spectrometry

Dorint Hotel Beatenberg– 04.November 2010 – 18:00

Agenda

1. Nomination of the scrutineers

Hans-Peter Moser and Peter Oggenfuss were elected by all members present.

2. Approval of the minutes of the 2009 general assembly

The minutes were approved unanimously.

3. President's report and its approval

After the 2009 SGMS Meeting, which has been covered in the president's report 2009 published in the June 2010 Newsletter (Vol 28/1), the board met to reevaluate the technical aspects of the meeting.

Board Member Meeting October 31, Beatenberg

Payment of the membership and registration fees were slow to come in. For this reason we decided to send printed payment slips together with the Newsletter Vol 28/1.

We also decided to provide hardcopies of the Newsletter 2, which includes the conference program, at the meeting, after several people had criticized that no Newsletter hardcopies had been sent out prior to the 2009 meeting. This year the Newsletter was announced by e-mail prior to the meeting.

It was also decided that a separate account should be opened for the IMSC2014 in order to clearly separate SGMS business from the conference organization. Eventually this will be incorporated into the overall IMSC2014 accounting.

The board members also agreed to continue the practice of providing student travel awards to up to 5 students presenting at the SGMS meeting. It was also decided to honor the best student presentation with a SGMS student award.

Board Member Meeting January 27, Olten

This meeting was primarily for deciding on the plenary speakers.

Jyotsna Sharma was chosen for a special topic and Cathy Costello, Andrej Schevchenko and Jean-Luc Veuthey for the MS topics,

Minor changes to the SGMS site were decided, as well as who from the board would be SCS delegate

IMSC2014

Renato Zenobi and myself went to Geneva to select a PCO (see under point 9) and a designer for the Logo and site template.

European MS History Book (Keith Jennings)

Lots of e-mail traffic generated by a request from Alison Ashcroft regarding a book on European MS History edited by Keith Jennings.

Lots of people contributed:

Olaf Boernsen, Martin Schär, Renato Zenobi, Yury Tsybin and Laurent Bigler

I had also contacted Martin Suter and Hans Balsiger

As a result of all these discussions, we started thinking about adding

- i) a Swiss MS History page to our site and*
- ii) an Alumni page with people who contributed greatly to MS instrumentation and methods in Switzerland*

All of this is clearly under construction, but we already got contributions to the Alumni page. Anybody who is interested is most welcome to help in doing this.

Sponsors and Members

Since 2005 we have a very stable number of members, ranging between 176 and 187. Currently 183 are paying members, not including the once that applied just now.

This year we are very happy to announce that Advion has also become our newest sponsor of SGMS. We have now a total of 12 sponsors, up by 5 since 2005.

Finally we record the number of 131 participants, 106 or 60% of these are members of the SGMS.

I would like to thank all board members for their great support during the year, especially Andreas for doing a perfect job in organizing accommodation and other aspects of this meeting and also in putting together the newsletter, and Stephan and Matthias for keeping track of addresses and payments. Also Steph Müller for taking 1st class pictures under less than ideal conditions ...

and finally the Dorinth staff for all their help and troubleshooting when needed.

The Presidents report 2010 was approved by all members.

4. Treasurer's report

	<i>Postal Account</i>	<i>Banking Account</i>	<i>IMSC2014 Account</i>	<i>Savings Account</i>	<i>Total</i>
Assets per Oct. 1 st ,2009	26'764.24	27349.71	0.00	0.00	59'099.45
Revenues	43.75	50'075.48	0.00	0.00	50'119.23
Expenses	15.90	32'503.10	0.00	0.00	32'519.00
Internal transfer	-26'792.09	-10'000.00	20'000.00	16792.09	0.00
Assets per Sept.30 st ,2010	0.00	42'052.62	20'000.00	16792.09	78'844.71
Surplus revenue	-26'764.24	7'130.52	20'000.00	16792.09	17'600.23

*Major changes compared to 2009 are the consolidation to one bank.
The postal account was not needed for 2 years in a row.
Opening of a savings account and an IMSC2014 account, and
transfer of 20 kCHF to this account as decided by the SGMS
committee and accepted by the general assembly.*

5. Auditor's report and approval of treasurer's and auditor's report

Andreas Topp and Peter Oggenfuss have checked the treasurer report. Andreas Topp reads the auditor's report.

*The treasurer's report was accepted and approved by all members.
Andreas Topp and Peter Oggenfuss have both accepted to act as auditors again.*

6. Decision on the 2010 membership fee

The membership fee for 2010 remains at CHF 25.00 per year and member.

This is accepted by all members present.

7. Admission of new members

The following new members were admitted to the SGMS:

Dr. Hannelore Kaspar, Thermo Fisher Scientific (Schweiz) AG

Dr. Ben C. Reynolds, ETH Zurich

Dr. Michael Scherer, AB SCIEX (Switzerland) GmbH

Dr. Goetz Schlotterbeck, FHNW Basel

Hans-Rudolf Schmutz, Raurica Consulting

Silvan Stucki, University of Bern

Dr. Michal Svoboda, Tecan Schweiz AG

Dr. Daniel Vetter, ERC

Dr. Xiangyang Zhang, ETH Zürich

8. Election of the president and committee members

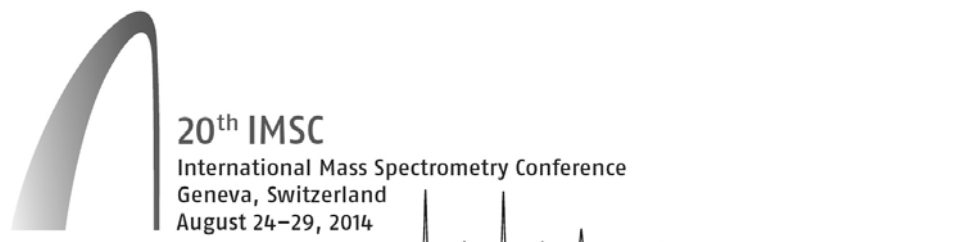
Marc Suter, Yury Tsybin, Jean-Luc Wolfender, Stephan Brombacher, Laurent Bigler, Andreas Stämpfli and Matthias Herzog are re-elected by all members present.

9. IMSC2014

The IMSC committee has selected SYMPORG SA as professional congress organizer.

The IMSC2014 committee got commitment not only from the SGMS (20'000.-), but also from the IMSF (CHF 10'000.- seed money)

The logo of the IMSC2014 will be:



10. News from the IMSF and EMS

The Italian Chemical Society Division of Mass Spectrometry presented a project for an IMSF international MS school

11. The SGMS homepage

Marc Suter presented some infos on the SGMS homepage traffic.

The most visitors are coming from Switzerland, Germany and the United States. The "job page" is still the most visited page.

There are new infos in the Membership section about the benefits of a SGMS Sponsorship.

12. News from the SCS

No news

13. Individual proposals

No proposals

14. Miscellaneous

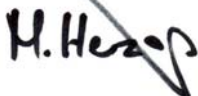
Events in 2011

- *8th Uppsala Conference and School – 6.-10.2.2011 in Villars (CH)*
- *ANAKON2011 - 22.-25.3.2011 in Zürich*
- *ICCE 2011 – 11.-15.09.2011 in Zürich*
- *SGMS 2011 – 27./28.10.2011 in Beatenberg*

The General Assembly closed at 19:03

Beatenberg, 04.11.2010

Matthias Herzog



Secretary of the SGMS

SGMS Meeting 2011, October 27 and 28

Dorint Resort Blüemlisalp, Beatenberg

Next to the plenary lectures there will be time for several oral communications from various participants. The time allotted will be 20 minutes. Please allow some minutes for discussion. The abstract incl. author's name and address should be sent **latest by August 10, 2011** directly to the SGMS by e-mail (**abstract@sgms.ch**). The abstract should not exceed 2500 characters.

Please note that the lecture hall is equipped with PC projection facilities only. To avoid technical problems everybody will be using the PC provided by the organizers (no personal laptops or MACs allowed). Only presentations prepared or saved as Microsoft Office Power Point 2003/2007/2010 will be accepted.

In preparing your presentation, please consider that your presentation has to be formatted horizontally and remember the dictum "less is more". To obtain clear slides, consider the differences between the size of your office and that of an auditorium for 120 people. The attendants sitting in the last row also have the right to read the contents of your slides without any problem. Please test your slides on readability.

Registration and Accommodation:

Please, send your registration (only completely filled in forms!) to **registration@sgms.ch** not later than **October 1, 2011**. Either PDF by e-mail or filled in printed form by ordinary mail will be accepted (mail address on registration form).

There is absolutely no need to register personally at the Dorint Resort Blüemlisalp! The SGMS committee will again manage the hotel reservation

and payments. Only the "extras" will have to be paid directly at the hotel-reception (like: extra nights, phone-calls, muh-bar, mini-bar ...).

We will strictly follow a first come first serve policy for the distribution of the hotel rooms (~110 rooms available!).

Registration fees including Hotel accommodation, business lunch, dinner buffet and breakfast and social event:

CHF 300/ person (single room occupancy)

CHF 270/ person (double room occupancy; please indicate roommate)

CHF 230/ person (accompanying person; double room occupancy; please indicate roommate)

Late fee: An additional late fee of CHF 50 will be enforced for all payments received after September 1, 2011. NOTE: to qualify for the regular rates payment MUST be received by September 1, 2010 - receipt of the registration form without payment will not qualify.

There is absolutely no possibility of attending the meeting without Hotel accommodation. Thank you for your understanding!

Please make your payment to

Schweiz. Gruppe fuer Massenspektrometrie (SGMS)
UBS Switzerland BCL: 292, 10722181.0
IBAN: CH88 0029 2292 1072 2181 0
SWIFT: UBSWCHZH40M

Make sure that we can track your payment by ensuring that your name is clearly stated on the payment form. Every year we receive unidentifiable payments due to misleading information on the incoming payments!

Cancellations

Cancellation requests, received by e-mail before October 1st, 2011, will qualify for a refund of the fees paid, less a handling charge of 25% of the total payment. After October 1st, 2011, no refunds will be made; however, substitute participants can attend.

Notification of all such changes must be **sent to registration@sgms.ch** by e-mail **before October 16, 2011**.

Changes will not be accepted at the meeting.

No show: No refund will be made.

Students support program:

Students giving a talk (selection by SGMS Board) will be hosted free of charge. For more information, please call any of the SGMS committee members.

Travel Information:

Travel details together with the complete program will be published on our homepage (www.sgms.ch).

SGMS Membership Fee:

Included in the mail is a pink payment form for the annual membership fee of 25 Fr. Please write your name in the comment field!

UBS Switzerland BCL: 292, 10722181.0

IBAN: CH88 0029 2292 1072 2181 0

SWIFT: UBSWCHZH40M

You are kindly asked to pay this fee as soon as possible.

2011 General Assembly of the SGMS

Thursday October 27, 2011

time to be announced

Dorint Resort Blüemlisalp, Beatenberg

Agenda

1. Nomination of the scrutineers
2. Approval of the minutes of the 2010 general assembly
3. President's report
4. Treasurer's report
5. Auditor's report
6. Decision on the 2011 membership fee
7. Changes of the statutes
8. Election of one new member of the board
9. Election of the auditors
10. Admission of new members
11. IMSC2014
12. News from the IMSF, EMS and SCS
13. The SGMS homepage
14. Individual proposals
15. Miscellaneous

Individual proposals must be sent to **marc.suter@eawag.ch** before
October 21, 2011.

The President, Marc Suter

Changes of statutes: 2011 GA (proposal)

During the past years the committee of the SGMS has been composed of up to 7 members. At the moment only 2 of the current committee members represent the French part of Switzerland. By far too low a number, considering the high number of mass spectrometers in companies and institutes located in the Romandie. Of course more people in the committee would help keeping pace with the fast spread and use of mass spectrometry in nutritional and pharmacological sciences.

The committee of the SGMS proposes therefore the following changes of the statutes (changes in ***bold/italic***):

5.1 Composition of the committee

5.1.1 The committee consists of five to ***nine*** members:

- the president
- the vice president
- the treasurer
- the secretary
- ***one to five members-at-large***

Complete section of the current statutes to be replaced:

5.1 Composition of the committee

5.1.1 The committee consists of five to seven members:

- the president
- the vice president
- the treasurer
- the secretary
- one to three assessors

President	<i>Marc J-F Suter</i> Eawag Ueberlandstr. 133 CH-8600 Dübendorf marc.suter@eawag.ch Phone +41-58-765 5479
SCS representative Internet	
Vice President	<i>Jean-Luc Wolfender</i> Ecole de Pharmacie Genève-Lausanne Université de Genève Quai Ansermet 30 CH-1211 Genève 4 jean-luc.wolfender@pharm.unige.ch Phone +41-22-379 3385
Secretary	<i>Matthias Herzog</i> AB Sciex Steinbruchstrasse 11 CH-5200 Brugg matthias.herzog@absciex.com Phone +41-800 835 044
Treasurer	<i>Stephan Brombacher</i> Novartis Pharma AG WSJ-145.8.15 CH-4002 Basel stephan.brombacher@novartis.com Phone +41-61-324 6808
EMS representative	<i>Laurent Bigler</i> OCI, Universität Zürich Winterthurerstr. 190 CH-8057 Zürich lbigler@oci.uzh.ch Phone +41-44-635 4286
SGMS Meeting Newsletter	<i>Andreas A Stämpfli</i> F. Hoffmann-La Roche AG Bau 65 / 109A CH-4070 Basel andreas.staempfli@roche.com Phone +41-61-688 3131
Member at Large	<i>Yury O Tsybin</i> Laboratory of Biomolecular Mass Spectrometry EPFL SB ISIC LSMB BCH 4307 CH-1015 Lausanne yury.tsybin@epfl.ch Phone+41-21-693 9751

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