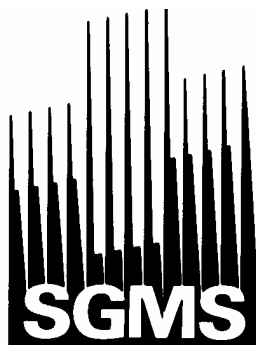


Swiss group for mass spectrometry  
Schweizerische Gruppe für Massenspektrometrie



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

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## Newsletter

We are very pleased to announce the

# SGMS Meeting 2006

**November 2 and 3, 2006**

**Mercure Hotel Beatenberg-Interlaken**

**the meeting starts at 11:15**

4 plenary lectures with **Rolf Rutishauser**, University of Zurich, Switzerland

**Thomas Laurell**, Lund University, Sweden

**Peter O'Connor**, University of Boston, USA

**Uwe Karst**, University of Munster, Germany

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## SGMS General Assembly 2006

**Mercure Hotel Beatenberg-Interlaken**

**Thursday November 02, 2006**

**~17:30**

We hope that many of our members will attend the General Assembly 2006 directly following the afternoon session.

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During the apéro as well as during the splendid "Italian Dinner Buffet" we will have plenty of time for discussions.

As usual latest news and updates will be served at the Muh-Bar.

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## ***News from the committee***

Following an initiative by Renato Zenobi and Marc Suter, both board members of the DAC (*Division of Analytical Chemistry of the Swiss Chemical Society*), the SGMS board has decided to submit for the International Mass Spectrometry Conference to be held in Switzerland in 2011 or 2012. The date will be definitively fixed at the IMSC in Prague 2006, when the IMSS board decides, if the IMSC changes from a triennial to a biennial cycle.

We are assisted in the submission process by FORSCHUNG LIVE, a professional event organizer at ETH Zurich. Deadline for submission is July 15<sup>th</sup>, 2006. Basel, Geneva, Lausanne, Lucerne, Montreux, Winterthur and Zurich have been evaluated as possible sites and we are currently negotiating with the top candidates.

The submission is backed by the Swiss Chemical Society and we already have commitment for some financial support. Academia, industry and two of our neighboring countries are represented on the organizing committee.

The members are:

Renato ZENOBI	ETH Zurich
Marc SUTER	Eawag, Dübendorf
Rudolf AEBERSOLD	ETH Zurich
Günter ALLMAIER	TU Wien, Austria
Laurent FAY	Nestlé Research Center, Lausanne
Detlef GÜNTHER	ETH Zurich
Gérard HOPFGARTNER	Univ. Geneva
Stefan SCHÜRCH	Univ. Bern
Giovanni SINDONA	Univ. Calabria, Italy
Andreas STÄMPFLI	F. Hoffmann-La Roche Ltd., Basel
Markus STÖCKLI	Novartis, Basel

The result of our submission will be known by the end of August, and the president of the SGMS will then inform the SGMS board members. The members will be fully briefed at the 2006 SGMS meeting in Beatenberg.

## ***The Eye and the Mind in modern plant morphology, exemplified by morphological "misfits" of tropical waterfalls***

***Rolf Rutishauser***

***Institut für Systematische Botanik  
Universität Zürich***

Biological morphology tries to elucidate body plans ("bauplans") of plants and animals. It is mainly comparative morphology (organography), dealing with concepts in order to compare the organs of different organisms. — There are various groups not fitting the bauplan of typical flowering plants. Such morphological "misfits" deviate considerably from the classical root-stem-leaf (or root-shoot) model known from most ferns and seed plants. The presentation will focus on river-weeds (family Podostemaceae) as morphological misfits among dicotyledonous flowering plants. They mainly occur in tropical waterfalls and river rapids, e.g. in Cameroon, Ghana, India and Mexico. Analyses of the genome (DNA) indicate that the river-weeds (podostemads) are closely related to St. John's wort (*Hypericum*) that also occurs in Europe! The podostemads are enigmatic for people interested in developmental genetics and evolution, for botanists studying their morphology and ecology: Which adaptations allow the river-weeds to survive in their extreme habitats? Most podostemads transformed their "roots" into green ribbons or disk-like crusts that are fixed to rocks inside the torrents. The example of the river-weeds exemplifies how botanists progress in their biodiversity research: (i) analysis of the plant forms; (ii) identification of the genera and species; (iii) listing the molecular and morphological characters into a data matrix; and (iv) phylogenetic reconstruction using computer programs. There are complementary views (perspectives) serving as heuristic devices for the elucidation of evolutionary and developmental aspects of plant forms, e.g. the holographic paradigm anticipated by AGNES ARBER (1879 – 1960), the continuum model and process morphology proposed by ROLF SATTLER. — The talk will finish with artificial life, i.e. virtual plants that only grow and flower inside computers.

## ***Microchip developments for sample preparation and MALDI-TOF MS interfacing***

***Thomas Laurell***

***Department of Electrical Measurements  
Lund University, Sweden***

Miniaturization strategies for protein sample preparation prior to mass spectrometry readout has clear benefits and is currently a focus area within the microchip and microfluidics field. The strategies along this line as pursued by the Lund Nanobiotechnology group will be reviewed. Piezodispensing as a means for precise sample deposition and on-spot enrichment as well as chip integrated solid phase extraction linked to MALDI-TOF MS readout will be discussed. A new approach to high capacity on-MALDI-target sample preparation - (ISET Integrated Sample Enrichment Target) - will also be presented.

## ***On the Role of Free Radical Reactions in Electron Capture Dissociation***

***Peter O'Connor***

***Boston University School of Medicine  
Department of Biochemistry***

The mechanism of electron capture dissociation is a matter of substantial debate at the moment. The original, non-ergodic mechanism implied one electron captured equals one backbone cleavage. This was clearly disproved in an experiment that performed ECD on doubly charged cyclic peptides, leading to the proposal that ECD initiates a free radical reaction cascade. Since then, a series of experiments have been performed to test this free radical cascade mechanism.

First, if the free radical cascade is true, then it implies that the radical can move through the molecule prior to cleavage. Since the best site for a radical in a peptide is on the alpha carbon of glycine, peptides were synthesized with deuteroglycine. ECD of these peptides showed that the deuterium atoms moved, which is observable as a mass shift. Clearly the radicals migrate during ECD.

Second, radical migration is presumed to occur on a  $>1$  microsecond timescale, suggesting that ECD proceeds through a long lived radical intermediate. A fairly simple, double resonant experiment can probe lifetimes on the  $>10$ - $100$  microsecond timescale, and this was applied to a series of peptides to see if some of the fragments observed were products of a long lived intermediate that exists for at least that long. New results will be presented to explore this, but in general, it appears that many or most (but not all) of the ECD fragments appear on a  $>1$  msec timescale. Clearly both

fast and slow mechanisms exist, but the fastest reactions that can currently be probed this way are slower than 10 microseconds.

Third, if radical propagation occurs on a slow timescale, then it can be modulated by adding groups to a peptide that contain large, distributed pi-bonded systems which should act as radical traps by resonantly stabilizing the radical. Coumarin can be easily tagged onto the molecule, providing such a system. ECD of a peptide with such a radical trap indicates that backbone fragments are suppressed, but side chain fragments are increased. Furthermore, double resonance shows that most of the side chain fragments are very slow, on the millisecond timescale.

Thus, the free radical cascade mechanism has withstood challenge by a series of experiments designed to test it. While the theory cannot be proven, it has not yet been disproved, and further experiments are planned to test it further.

## ***Strategies for the LC/MS analysis of non-polar compounds***

***Uwe Karst***

***Westfälische Wilhelms-Universität Münster  
Institut für Anorganische und Analytische Chemie***

In recent years, liquid chromatography/mass spectrometry (LC/MS) has become one of the most powerful analytical techniques for qualitative and quantitative analysis. This is mainly due to the invention of electrospray ionization (ESI) and atmospheric pressure chemical ionization (APCI). With these interfaces, polar compounds are typically detected by protonation in the positive ion mode and by deprotonation in the negative ion mode.

Non-polar analytes, however, which are particularly well separated in reversed-phase HPLC, are either detected with unsatisfactory results or not at all under these conditions. Therefore, strategies to improve the ionization for these compounds have to be developed. Some respective approaches are shown within this presentation.

One promising approach is the electrochemical conversion of the analytes to more polar or even charged products, which are then readily accessible by ESI or APCI. We have developed an on-line LC/electrochemistry/MS method with post-column oxidation of the analytes occurring in a commercial "coulometric" cell, which provides for up to quantitative conversion of the analytes prior to the mass spectrometer. Examples from different applications areas will be presented.

Another approach is based on an electron-capture effect, which is observed for selected nitroaromatic compounds when using the APCI interface as a source of low-energy electrons in the negative ion mode. Depending on the structure of the compound to be analyzed, either a dissociative or a non-

dissociative electron capture effect is observed. The electron capture effect competes with the classical deprotonation in LC/MS and provides for additional structural information on the analytes.

A third approach has been directed to the coordination of inorganic ions to analytes with limited polarity under formation of charged adducts. This has been explored with respect to the addition of  $\text{Ag}^+$  ions after separation of rubber vulcanization accelerators.

## ***President's Report 2005***

"It is a pleasure that in 2005 we could bring again more than 110 people up to the Beatenberg for the annual SGMS meeting.

In February the committee of the SGMS met at Hoffmann-La Roche in Basel. First discussion point was the positions of the two new committee members Stephan Brombacher and Laurent Bigler. Stephan got the job of the treasurer while Laurent Bigler got named the new contact person for the European Society of Mass Spectrometry.

But the main task of the day was to set up the annual SGMS Meeting at Beatenberg. It was amazing how fast we had established the topics and the persons who could give the talks. It is every year the same: Contact the preferred speakers and get a hopefully positive answer back as soon as possible. By the same time the first newsletter of the year should be ready to be printed and placed together with the registration form for the meeting on the SGMS homepage.

For the first time the committee decided to make the newsletter only available through the internet. Big troubles and a hot phone line! I got at least half a dozen phone calls explaining that the newsletter in printed form is an added value and so on and on. So the committee decided to ship in September by ordinary mail the first and second newsletter of the year 2005 together with a pink slip for the membership fees!

Anyway, the committee did a great job and managed to invite 4 outstanding scientists for giving lectures in various fields of modern analytical chemistry. Nano science was chosen as the non-mass spectrometric talk given by Marcel Mayor from the University of Basel. Eric Forest is giving us an insight into the use of mass spectrometry for studying the structure and interaction of proteins. Gary Glish is opening the second day teaching about the quadrupole

ion trap in proteomics and Thorsten Reemtsma is talking about fulvic acid molecules. Besides these 4 invited speakers the committee could again support 4 students, namely Ines Burkard, Jana Hüttig, Ingrid Langlois and Jan Tromp. It's a great pleasure to have these 4 students among us.

I should not forget to thank our sponsors for supporting the SGMS. Only this makes it possible to get outstanding scientists to the "Rigi" meeting and to have all the benefits of the Mercure Hotel Beatenberg-Interlaken at a reasonable price. My thanks go to Agilent (Schweiz) AG, Applied Biosystems, Brechbühler AG, Shimadzu Schweiz AG, Spectronex, Varian Incorporation and Waters Micromass MS Technologies.

Thanks also to my colleagues in the committee for helping me to run the SGMS and thank you for your attention."

## ***Minutes of the 2005 General Assembly of the Swiss Group for Mass Spectrometry***

**Mercure Hotel Beatenberg-Interlaken, 17:20**

### **Agenda**

#### **1. Nomination of the scrutineers**

Jürg Hau is nominated scrutineer for this year's general assembly.

#### **2. Approval of the minutes of the 2004 general assembly**

The minutes which were published in the SGMS newsletter Vol 23\_1 are approved unanimously by the members present.

#### **3. President's report and its approval**

Andreas Stämpfli reads his report (see Volume 24\_1). It is approved by all members present.

#### **4. Treasurer's report**

Our treasurer Stephan Brombacher informs us about the status of our finances:

##### Expenses in detail

<b>Account fees</b>	<b>90.55 CHF</b>
<b>Newsletter</b>	<b>1801.45 CHF</b>
<b>Rigi</b>	<b>6063.95 CHF</b>
<b>IMSS Fees</b>	<b>312.85 CHF</b>
<b>SGC Fees</b>	<b>655.00 CHF</b>
<b>Other</b>	<b>74.55 CHF</b>
<b>Total</b>	<b>8998.35 CHF</b>

##### Revenues in detail

<b>Sponsoring</b>	<b>5000.00 CHF</b>
<b>Member Fees</b>	<b>2601.00 CHF</b>
<b>Rigi Fees</b>	<b>2730.50 CHF</b>
<b>Interest</b>	<b>39.95 CHF</b>
<b>Total</b>	<b>10371.45 CHF</b>

##### Overall Balance

	Postal account	Banking account	Total
<b>Balance Oct. 1st, 2004</b>	27316.09	16305.78	<b>43621.87</b>
<b>Revenues</b>	3028.85	7342.60	<b>10371.45</b>
<b>Expenses</b>	6859.40	2138.95	<b>8998.35</b>
<b>Balance Sept. 30st, 2005</b>	23485.54	21509.43	<b>44994.97</b>
<b>Difference</b>	-3830.55	+5203.65	<b>+1373.10</b>

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

Peter Fischlewitz and Peter Oggenfuss confirm the correct bookkeeping of the SGMS accounts. The treasurer's report and the auditor's report are approved by all members present.

## 6. Decision of the 2005 membership fee

The member fee for 2006 remains at CHF 25.00 per year and member.

This is accepted by all members.

## 7. Admission of new members

The following new members are admitted to the SGMS:

Bourgogne	Mr.	Emmanuel	University of Geneva
Eichenberger	Mr.	Silvan	University of Zürich
Heinig	Dr.	Katja	F. Hoffmann-La Roche AG
Hofer	Mr.	Rainer	HR Instrument Services
Leuthold	Mr.	Luc Alexis	Université de Genève
Niedan	Mr.	Volker	Lonza AG
Reihnhardt	Dr.	Alain	ETH Hönggerberg
Waldt		Annick	Novartis Pharma AG

## 8. Election of the auditors

Peter Oggenfuss is available as auditor for another 2 years. Andreas Topp is the new auditor who replaces Peter Fischlewitz. The 2 auditors are elected by all members with great applause.

## 9. News from the SCS – HJ Walther

The next meeting of the SCS will be in April 2006. Info: Training Program of DAC (Division of Analytical Chemistry of the SCS) is now available on the SGMS Homepage. Please note that there is a reduced membership fee for all SGMS members, because the SGMS is a collective member of the SCS. Marc Suter is new treasurer of the DAC.

## 10. News from the EMS – L. Bigler

no news.

## 11. SGMS Homepage – M. Suter

- 22 job openings were posted since the last SGMS meeting
- Training courses in analytical chemistry are listed on the site
- Sponsors can post links to their training courses
- New links have been added (e.g. IUPAC Definition, etc.)

## 12. Individual proposals

No individual proposals

## 13. Miscellaneous

### a. Mailing the Newsletter: by email?

Sending by ordinary mail is highly preferred by all members. The SGMS decides to continue sending their newsletter by ordinary mail.

- ### b. **ms@romandie** is a new website for information exchange amongst the romandie MS people. Have a look at <http://www.ms.unige.ch> or through the "Links Page" on our site.

**The General Assembly closes at 18:20**

**Beatenberg, 27.10.05**

Thomas Läubli

A handwritten signature in black ink, appearing to read 'T. Läubli', with a stylized flourish above the first letter.

Secretary of the SGMS

## ***Rigi Meeting 2006, November 2 and 3***

### ***Mercure Hotel Beatenberg-Interlaken***

#### **Oral communications / Abstracts:**

Next to the plenary lectures there will be time for several oral communications from various participants. The time allotted will be 20 minutes. The abstract incl. author's name and address should be sent before **July 28, 2006** directly to the SGMS president, Andreas Staempfli, F. Hoffmann-La Roche Ltd, Basel by e-mail (andreas.staempfli@roche.com). The abstract should not exceed 2500 characters.

#### **Registration and Accommodation:**

Please, send your registration (only completely filled in forms!) to Andreas Staempfli not later than **September 28, 2006**.

There is absolutely no need to register personally at the Mercure Hotel Beatenberg-Interlaken! 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: phone-calls, mini-bar ... etc.).

We will again 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:

**CHF 250/ person** (single room occupancy)

**CHF 225/ person** (double room occupancy; please indicate roommate)

**CHF 175/ 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 15, 2006.

NOTE: to qualify for the regular rates payment **MUST** be received by September 15, 2006 - receipt of the registration form without payment will not qualify.

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

Please use the following bank information for your payment:

Credit-Suisse      BCL: 4094, 0094-919402-50  
                            IBAN: CH62 0409 4091 9402 5000 0  
                            SWIFT: CRESCHZZ30A

Schweizerische Gruppe für Massenspektrometrie  
c/o Dr. Andreas Stämpfli, CH-4102 Binningen

Make sure 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 payment form!

### **Cancellations**

Cancellation requests, received by e-mail before **September 28, 2006**, will qualify for a refund of the fees paid, less a handling charge of 25% of the total payment. After **September 28, 2006**, no refunds will be made; however, substitute participants can attend. Notification of all such changes must be sent to Andreas Staempfli by e-mail before October 31, 2006. 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:**

Details will be published together with the complete program and our official invitation, sent out in September and posted on our homepage ([www.sgms.ch](http://www.sgms.ch)).

**SGMS-Membership-Fee:**

Included is a pink payment form for the annual membership fee of 25 Fr. You are kindly asked to pay this fee as soon as possible. Please write your name in the comment field! The treasurer appreciates your cooperation. For those who have missed to pay the previous year, please pay a total of 50 Fr. for two consecutive years.

Only members from abroad may pay the membership fee directly to our treasurer Stephan Brombacher at the Meeting.

Please, use the following bank information for the payment of the annual membership fee:

Schweiz. Gruppe fuer Massenspektrometrie (SGMS)

UBS Switzerland BCL: 292, 10722181.0

IBAN: CH88 0029 2292 1072 2181 0

SWIFT: UBSWCHZH40M

## ***2006 General Assembly of the SGMS***

**Thursday November 02, 2006**

~ 17:30 h

Mercure Hotel Beatenberg-Interlaken

### **Agenda**

1. Nomination of the scrutineers.
2. Approval of the minutes of the 2005 general assembly.
3. President's report and its approval.
4. Treasurer's report.
5. Auditor's report and approval of treasurer's and auditor's report.
6. Decision on the 2006 membership fee.
7. Admission of new members.
8. Election of the President and the members of the committee.
9. News from the SCS - HJ. Walther.
10. News from ESMS - L. Bigler.
11. News from the IMSS – A. Staempfli
12. SGMS homepage - M. Suter.
13. Individual proposals.
14. Miscellaneous.

Individual proposals must be sent to [andreas.staempfli@roche.com](mailto:andreas.staempfli@roche.com) before October 19, 2006.

The President

Andreas A. Staempfli

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