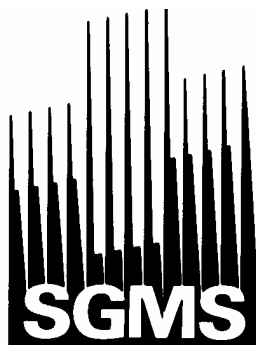


Swiss group for mass spectrometry
Schweizerische Gruppe für Massenspektrometrie



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

Newsletter

We are very pleased to invite you to the

SGMS Rigi Meeting 2005

October 27 and 28, 2005

Dorint Hotel Blüemlisalp, CH-3803 Beatenberg

11:15

4 plenary lectures with **Eric Forest**, Institute for Structural Biology Grenoble

Gary Glish, University of North Carolina

Marcel Mayor, University of Basel

Thorsten Reemtsma, Technical University of Berlin

SGMS General Assembly 2005

Dorint Hotel Blüemlisalp, CH-3803 Beatenberg

Thursday October 27, 2005

~17:30

We hope that many of our members will attend our General Assembly 2005 following the afternoon session. Please refer to "Invitation and preliminary Agenda for the General Assembly" later in this issue for more detailed information.

During the apéro as well as during this year's new and first time "Blüemlisalp Italian Dinner Buffet" we will have plenty of time for discussions.

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

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Dear members and sponsors

It is indeed a pleasure to announce the SGMS Rigi Meeting 2005. Again we could organize 4 exciting plenary lectures, with three covering very interesting mass spectrometric areas, while the special topic this year is nano-technology.

Please feel free to submit an abstract for an oral presentation about new developments in the field of mass spectrometry and allied topics. The abstracts will be reviewed by the committee, which will strongly favor academia related talks.

The schedule for submitting abstracts has changed: Abstracts should be sent to "andreas.staempfli@roche.com" not later than July 17, 2005. This early date is due to the fact that we would like to publish the overall program of the SGMS Rigi Meeting 2005 before the closing time for registrations. I hope we will get many abstracts for an oral presentation so that we can again compile a very interesting program.

The SGMS would like to encourage students to present their work at the SGMS Rigi Meeting. Students giving a talk will be sponsored and will be hosted free of charge. Please include a proof of "student" status with your abstract submission.

A maximum of 110 participants only can register for the meeting due to the limited space available in the conference room. Admission will be according to the date of registration. Thank you very much for your understanding!

I look forward to meeting you in Beatenberg.

Andreas Stämpfli

Molecular Electronics: Devices of Tomorrow?

Marcel Mayor

***University of Basel, Department of Chemistry
St. Johannisring 19, CH-4056 Basel, Switzerland
marcel.mayor@unibas.ch***

Silicon-based integrated circuits have continuously reduced the feature sizes of devices and therewith the cost per functional unit also. However, further decrease in feature size is nowadays becoming increasingly difficult (and expensive) due to physical limitations. Molecular electronics, understood as the integration of molecular structures to supplement specific functionalities on a semiconductor chip, is a promising alternative concept to further reduce both, the feature size and the costs per functional unit. However, currently this remains speculation as the technology to integrate and to address molecules and their assemblies on a chip has not been developed yet. But the strongly increased research activity has already led to some experimental breakthroughs.

Supramolecular chemistry plays a leading role in molecular electronics. Tailor-made molecular devices as potential functional units have already proven to perform specific functions like switching between two configurations triggered by external stimuli. In addition, the integration of molecular structures in electronic circuits crucially depends on the molecules' supramolecular assembly properties.

An introduction will present the historical background and worldwide current research activities in the field of molecular electronics. Subsequent, own contributions to molecular electronics will be discussed. In particular, investigations to integrate single molecules in electronic circuits and the resulting correlations between molecular structures and electronic transport

properties will be presented. The thereby gathered molecular structure *vs.* electronic conductivity information further allows designing molecular architectures with tailor-made properties, as will be shown by an example of a single molecule rectifier. Further research activities are geared towards molecules with electronic transport properties leading to particular physical properties, like persistent currents or hysteretic switching.

The lecture is focused on the amazing potential of molecular structures to be designed and synthesized to perform particular electronic functions, perhaps even in electronic circuits of tomorrow. However, the fact that this research is still in its infancy and that many innovative ideas and new concepts are still required for the parallel integration of large numbers of molecules or their assemblies will not be hidden.

The Quadrupole Ion Trap and Proteomics: New Developments in Top-Down and Bottom-Up Analysis

Gary L. Glish

***University of North Carolina, Department of Chemistry
CB# 3290
Chapel Hill, NC 27599***

While the quadrupole ion trap is already a very powerful and commonly used tool for bottom-up proteomics analysis, performance improvements can be made to increase the information available in these experiments. New methods for CID in the quadrupole ion trap that provide increased sequence coverage, and, in some cases, generate immonium product ions will be presented. Also, a method to increase throughput by analyzing multiple peptide ions simultaneously will be discussed. As a complement to the bottom-up approach, the analysis of intact proteins (top-down) using infrared multiphoton photodissociation will be presented.

Use of mass spectrometry to study the structure and the interactions of proteins.

Eric Forest (eric.forest@ibs.fr)

***Institut de Biologie Structurale (CEA-CNRS-UJF)
Laboratoire de spectrométrie de masse des protéines
41 rue Jules Horowitz
38027 Grenoble Cedex 1 France.***

In the post-genomic era, the interest of proteins appears again as they execute and control the majority of cellular activities. Through their interactions they play a critical role in cell function or dysfunction.

Characterizing the structure of a protein and the interaction with its partners is a key step in the knowledge of its function and in the use of this protein either as a drug or as a drug target.

Beside the well known role of mass spectrometry (MS) in proteomics, MS can provide useful information in structural biology when associated with other techniques.

For more than ten years the combination of hydrogen exchange and MS has been widely used, providing views on protein structure and protein dynamics. Associating proteolysis with proteases working at low temperature and low pH, local information can be obtained. It enables the identification of the solvent accessible regions of a protein, the location of conformational changes induced by the binding of a partner and the following of the folding or unfolding of proteins. With the help of directed mutagenesis, it is also possible to finely define the interaction regions with ligands or other proteins. This method gives structure information in complement to the classical techniques such as NMR or X-ray crystallography. Compared to them, MS offers the advantage of requiring small amounts of sample in conditions close to the physiological ones. Furthermore MS can work much easier on large proteins or complexes.

Several examples illustrating the power of this approach will be given.

Insight into fulvic acid molecules by electrospray mass spectrometry

Thorsten Reemtsma

***Technical University of Berlin
Department of Water Quality Control
10623 Berlin, Germany***

Decades of research on humic material seemed to confirm that this kind of natural organic matter was chemically ill-defined and consisted of a seemingly infinite number of unique molecules. It is the merit of electrospray ionization-mass spectrometry that this picture has changed so rapidly in the past years, at least for the very polar fulvic acid fraction of humic material. High resolution mass spectrometry provided the first information on single intact molecules of fulvic acids and offered the potential to investigate these molecules further. Meanwhile molecular formulas of hundreds to thousands of fulvic acid molecules could be determined.

The investigation of fulvic acid isolates by ESI-MS revealed an astonishing degree of regularity at very different levels: (a) periodic intensity distributions were visible in scan spectra recorded by quadrupole MS, (b) the oligomeric character of fulvic acids of higher molecular weight was detected by size-exclusion chromatography (SEC) -MS analyses and (c) regularities were determined also on the level of elemental composition of fulvic acid molecules by TOF- and FTICR-MS. And finally (d) Q-TOF-MS investigations suggest that also the structure of fulvic acid molecules is very regular. Based on the results obtained by these mass spectrometric methods structure proposals have been developed for low molecular weight fulvic acids.

With SEC coupled to high resolution MS it is now possible to compare NOM isolates of different origin, to study the reactivity of these molecules and to take up the question of their source materials and formation processes, again. Mass spectrometry may finally enable us to replace the yet only operational definition of fulvic acids by a well defined chemical definition, based on elemental composition and molecular structures.

President's Report 2004

Despite the late date in the year it is a pleasure that 111 persons registered to the traditionally called SGMS "Rigi-Meeting". I am proud that many of the 183 members of our society are actively participating at our annually meeting what really proves that the committee again did a very good job in the organization and in the selection of the invited speaker.

Thanks to all the committee members for their continuous commitment and involvement in the management of the SGMS. All people who have had the opportunity to hear our starting session by Kurt Paulus might have remembered that in earlier days we always had a non-mass spectrometric talk in the program. Earlier this year in February the committee decided to re-lance this idea and from now on we will include a non-mass spectrometric topic at every upcoming "Rigi"-meeting.

On the other hand we would like to focus strongly on state-of-the-art mass spectrometric science and try to get top notch scientists like Alain van Dorsselaar, Peter Schoenmakers and Ron Heeren up to the Beatenberg. Of course we could never invite great scientists without our 7 sponsors. Agilent Schweiz AG, Applied Biosystems, Brechbühler AG, Micromass MS Technologies, Shimadzu Europe, Spectronex AG and since 2 months also Varian Schweiz AG. These 7 companies are financially supporting our society. Due to them we are in a very good financial situation and could again invite 4 students from different universities in Switzerland and from abroad. Please enjoy the presentations given by Christian Emmenegger, Kornél Nagy, Fernando Romero and Roland Staack.

Early this year the steering committee of the University of Basel decided to cancel the two analytical chairs at the Department of Chemistry. The SGMS

committee has written a letter to the Dean Professor Tanner expressing the absolute need of an analytical education for chemists. Especially in Basel home of different pharmaceutical companies the university has the duty to assure a complete chemical education. It was the first time that the SGMS committee got politically active and I hope that you all support our intentions. Regarding the job opportunities we face a difficult economy and this is also reflected in the fact that we could only upload 9 job offers during the year on our homepage. On the other hand we had 3 unsolicited applications, unfortunately with a very limited response. This might be due to the fact that we did not publish this extensively. Please visit our homepage more often. You will find there many interesting topics. First we offer to our active members the possibility to have a link to their homepages. We have active links to our sponsors' homepages. In addition we provide for suppliers - for just SFr 100 - the possibility of a link. As a new feature our sponsors have the possibility of posting their courses in mass spectrometry and related topics. This is also open for universities.

At the end I have the duty to address special thanks to our two leaving committee members: Hanspeter Moser and Raffaele Tabacchi. Both of them were members of the committee for many years. Hanspeter was treasurer for 10 years. He did a very good job. Our finances are better than ever. The same is true for Raffaele Tabacchi. Many years he represented our society in the European society of mass spectrometry. Hanspeter and Raffaele contributed very much to the SGMS.

Minutes of the 2004 General Assembly of the Swiss Group for Mass Spectrometry

Beatenberg, Hotel Dorint – 25.November 2004 -17:20

Agenda

1. **Nomination of the scrutinizers**

Peter Kofel and Jens Donath are nominated as the scrutinizers

2. **Approval of the minutes of the 2003 general assembly**

The notes are approved by 100% of the members.

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

Andreas Stämpfli, our president reads his 2004 report (see Vol 23_1). The report is approved by all members.

4. **Treasurer's report**

Hanspeter Moser, our treasurer informs us about the current status of the accounts:

- Banking Account Balance: **CHF 16'305.78** per 30.9.2004.

- Postal Account Balance: **CHF 27'316.09** per 30.9.2004.

- **Total Balance:** **CHF 43'621.87** per 30.9.2004

- Balance per 1.10.2003 was CHF 29'890.02

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

Peter Oggenfuss and Peter Fischlewitz confirm the perfect bookkeeping of the SGMS Accounts

6. **Decision of the 2005 membership fee**

The member fee for 2004 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:

- | | |
|------------------------|---------------------------|
| - Gertraud Hayn | COMET AG |
| - Paul Gerhard Lassahn | Spectronex AG |
| - Oliver Scheidegger | ETH Höggerberg |
| - Rene Brunisholz | ETH Höggerberg |
| - Heinrich Müller | Covanis GmbH |
| - Joachim Figueredo | Mepha AG |
| - Manuel Tharin | Philip Morris Products SA |
| - Stephane Roudier | Philip Morris Products SA |
| - Julia Rebstein-Mutti | Philip Morris Products SA |

8. **Election of the President**

Andreas Stämpfli is confirmed as president of the SGMS for another 2 years by the general assembly with great applause.

9. **Election of new members and members of the SGMS committee.**

Hanspeter Moser and **Raphaelle Tabacchi** are leaving the committee and their work for the committee is acknowledged by Andreas Stämpfli and also with great applause from the whole general assembly.

New committee members are **Laurent Bigler** from the University of Zurich and **Stephan Brombacher** from Novartis Pharma Basel. Both new committee members are approved with great applause by 100% of the members.

10. **Statutes**

Andreas informs about the proposal for changing the statutes: The committee proposes to dismiss the term collective members but have active sponsors instead of that. During the last years 7 companies (manufacturers or suppliers of MS equipment) were established as sponsors.

For further details see newsletter 22_2 (November 2004)

Mr. Gassmann proposes to change the term active members to the term members. The committee will do that when reviewing the statutes next time and this is agreed by the members.

11. **News from the SCG – HJ Walther.**

The SCG moved their headquarters to the house of sciences in Berne.

7 collective members were present at their general assembly.

Ilmac 2005 will take place in Basel (24-27 May 2005). Next meeting of the SCG is in October 2005.

12. **News from the ESMS – R.Tabacchi**

No news, due to no meetings!

13. SGMS Homepage

- Since 2003: only 11 members have used link possibilities.
- Since 2004: 3 unsolicited job applications
- Since 2004: Suppliers have a link to their homepage. Only 9 jobs were posted last year.
- Please visit the sponsors link

14. Individual Proposals

no individual proposals

15. Miscellaneous

nothing

The General Assembly closes at 18:25

Beatenberg, 25.11.04

Thomas Läubli

A handwritten signature in black ink, appearing to read 'Läubli' with a stylized flourish above the first letter.

Secretary of SGMS

Rigi Meeting 2005, October 27 and 28

Dorint Hotel Blüemlisalp, Beatenberg

Oral communications / Abstracts:

The meeting will be supplemented by 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 17, 2005** directly to the SGMS president, Andreas Staempfli, F. Hoffmann-La Roche Ltd, Basel. The abstract should be not exceeding 2500 characters.

Please send your abstract by e-mail to andreas.staempfli@roche.com

Registration and Accommodation:

Please, send your registration (completely filled in form!) to

Andreas Staempfli not later than **September 30, 2005**.

There is absolutely no need to register personally at the Hotel Dorint, Beatenberg! The SGMS committee will again manage the hotel reservation and payment.

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

We will again strictly follow the order of registration for the distribution of the hotel rooms (~100 rooms available!).

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

CHF 250/ person (single room occupancy)

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

CHF 160/ person (accompanying person; double room occupancy;

please indicate roommate)

Late Fee: An additional late fee of CHF 50 for registration will be applied to all payments received after September 30, 2005.

NOTE: to qualify for the regular rates **payment MUST** be received by **September 30, 2005** - receipt of the registration form without payment will not qualify.

There is **no** possibility of attending the meeting only, without Hotel accommodation. Thanks for your understanding!

Please, pay your registration fee to the bank account:

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

Don't forget to **mark your name and address on the payment form.**

Cancellations

Cancellation requests, received in by email before **September 30, 2005**, will qualify for a refund of the fees paid, less an administration handling charge of 25% of the total payment. After **September 30, 2005**, no refunds will be made; however, substitute participants can be nominated to attend. **All such changes must be notified to Andreas Staempfli, in writing, before the meeting. Changes will not be accepted at the meeting.**

No show: No refund will be made.

Students support program:

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

Travel Information:

Details will be published together with the complete program and our official invitation, which will be sent out in October and which will be posted on our homepage (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 St. Brombacher during the "Rigi Meeting".

Please, pay your annual membership fee to the bank account:

UBS Switzerland BCL: 292, 10722181.0

IBAN: CH88 0029 2292 1072 2181 0

SWIFT: UBSWCHZH40M

Schweiz. Gruppe fuer Massenspektrometrie
(SGMS)

Please join us for the
General Assembly of the SGMS 2005

Thursday, October 27, 2005

~17:30 h

Dorint Hotel Blüemlisalp, Beatenberg

Agenda

1. Nomination of the scrutinizers.
2. Approval of the minutes of the 2004 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 Auditors.
9. News from the SCS - HJ. Walther.
10. News from ESMS - L. Bigler.
11. SGMS homepage - M. Suter.
12. Individual proposals.
13. Miscellaneous.

Individual proposals must be **sent by email before October 12, 2005**
to andreas.staempfli@roche.com.

The President
Andreas A. Staempfli

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Newsletter [Andreas A. Stämpfli](#)

Thanks to our sponsors

