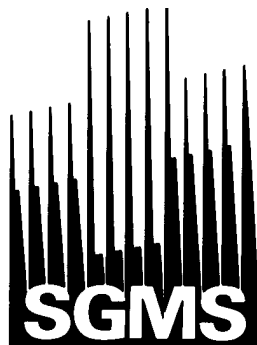


Swiss group for mass spectrometry  
Schweizerische Gruppe für Massenspektrometrie



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

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## Newsletter

It's a pleasure to announce our annual

# "Rigi Meeting" 2003

October 30 and 31, 2003

**Dorint Hotel Blüemlisalp Beatenberg**

**! 11:15 !**

Again with 4 plenary lectures! A business lunch will be included!

The final program of the meeting will be published in  
Newsletter Vol 21\_2 , September 2003

Also exact travel information will be given at that time.

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We are very pleased to invite you to the

## **SGMS General Assembly 2003**

Dorint Hotel Blüemlisalp Beatenberg

October 30, 2003

~17:00

We hope that many people will attend our General Assembly 2003 following the afternoon session. Please refer to "Invitation and Agenda for the General Assembly" later in this issue for more detailed information.

During the apero and the supreme "Blüemlisalp Schweizer Dinner Buffet" we will have plenty of time for discussions. As usual latest news will be served at the bars.

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Dear members, dear colleagues

I would like to thank you for electing me as the new President of the SGMS. It is a great honor for me and I will try to do my best for the SGMS.

In the past 6 years, Laurent Fay was heading our organization. He did an excellent job with his very charming and elegant French touch. Everyone loved him for his opening and closing words, especially when he demonstrated the facts and numbers of the Rigi Meeting registrations and payments and/or missing membership payments. He did a great job with a lot of engagement. Thank you very much Laurent! We all wish you a bright future and all the best for your "post president" mass spectrometry life.

Back in the eighties – I was a student at the University of Berne with Prof. Dr. U.P. Schlunegger – the Rigi Meeting used to be "the" conference to go. A meeting held at an outstanding historical place. Unfortunately the facility at the Rigi Kaltbad struggled and could no more be reanimated. With the Dorint Hotel Blüemlisalp, we had the chance to find an almost perfect facility located in the heart of Switzerland, in the very famous Bernese Oberland. During the "Rigi"-Meeting 2002, where we celebrated our 20th anniversary the Dorint Hotel Blüemlisalp managers and staff proved to be of extraordinary quality. The meeting was an exceptionally positive event. That's why most of you voted to stay also in 2003 at the Dorint Hotel Blüemlisalp.

I am looking forward seeing you there soon

Andreas Staempfli

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## ***BioAnalytical Applications of ICP-MS***

***Scott D. Tanner, Zoë A. Quinn, Vladimir I. Baranov  
and Dimitry R. Bandura,  
MDS-SCIEX, 71 Four Valley Drive, Concord,  
Ontario L4K 4V8 Canada***

The particular characteristics of Inductively Coupled Plasma Mass Spectrometry (ICP-MS) that address perceived shortcomings of other mass spectrometric approaches to bioanalysis will be discussed. These benefits include: exceptional sensitivity (to elements) that is independent of the chemical form in the sample, relative insensitivity (tolerance) of concomitant materials in the sample, large (9 orders of magnitude) linear dynamic range, capability for absolute quantification. The deficiency of ICP-MS for this application is that the ionization source totally destroys molecular (speciation) information, other than that which is gained through prior sample manipulation (such as chromatography or immunoassay). This deficiency, however, is turned to advantage for the determination of the state-of-phosphorylation of proteins through measurement of the total P concentration, especially when normalized to another element that can be taken as characteristic of the total protein content of the sample. In many instances, S is a convenient normalizing element, especially where homologous proteins or samples are assayed. Recent phosphorylation assays will be presented, including the discrimination of cancerous whole cell lysates. A novel application of ICP-MS is to multiplex immunoassays where the various protein complexes may be distinguished and quantified by the use of distinguishable elemental tags. In many instances, the presence of an elemental tag (or multiple copies thereof) does not affect the efficiency of the affinity binding; in fact, many commercial antibodies specifically employ lanthanides as fluorescence enhancers. In the instance that many copies of

an isotopic tag (for example, Nanogold™) are incorporated, the sensitivity and detection limit are directly enhanced. Because there are more than 50 elements that are suitable to the purpose, and more than a hundred isotopes of those elements that can be obtained in enriched form, the potential for multiplex analysis is evident. Data that demonstrates the advantages anticipated will be given, and the conditions that allow for multiplex analysis will be discussed. Current results for the simultaneous determination of multiple biomarkers are presented.

## ***MS and Structural Studies of Proteins and Protein Interactions***

***Kenneth B. Tomer, Christine Hager-Braun, Elisabeth O. Hochleitner,  
and Jenny M. Cutalo***

***National Institute of Environmental Health Sciences,  
National Institutes of Health,  
Department of Health and Human Services  
Research Triangle Park, NC, USA***

Mass spectrometry has long been known for its utility in peptide and protein identification, especially in the field of proteomics. The biological activity of molecules is dependent on its structure, on modifications, such as phosphorylation and glycosylation, and on its interactions with other biomolecules. The utility of mass spectrometry for characterization of these more complex structural interactions has been less recognized.

Over the past several years, we have been developing and applying mass spectrometry-based techniques to probe protein structural problems and protein:protein interactions. In these studies, we have used protection assays, differential chemical modification studies of surface-accessible amino acids of complexed and non-complexed proteins, and cross-linking agents to obtain information about the interacting surface of the proteins. A variety of separation techniques, such as nanoscale capillary LC and affinity chromatography, combined with mass spectrometry have been used to determine the results of these experiments. Molecular modeling based on these results has enabled us to determine structural parameters.

The major biological focus of these studies has been the structural characterization of HIV proteins and their interactions with other proteins that are relevant to HIV infection. Specifically, we have been characterizing glycan heterogeneity at glycosylation sites on HIV gp120, mapping epitopes on HIV proteins recognized by antibodies and have been probing interactions

between the HIV surface glycoprotein, gp120, and its cellular receptors. In this talk, our approaches to these problems will be outlined and several examples of their application will be presented.

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## ***A Time-Of-Flight mass spectrometer: a new horizon in GC separations***

***René J.J. Vreuls  
Vrije Universiteit  
Department of Analytical Chemistry and Applied Spectroscopy  
de Boelelaan 1083, 1081 HV Amsterdam, the Netherlands  
(e-mail: Vreuls@chem.vu.nl)***

Time-of-flight mass spectrometry (TOF-MS) is a very powerful technique with limits of detection in the low pg range. Furthermore, the spectrum storage rate can be as high as 500 spectra per second. Both advantages have been exploited using a faster GC mode than is commonly used in the GC laboratory. In this mode columns are short and narrow, while temperature gradients are steep (complete volatility range in 3–10 min). In combination with TOF-MS, detection limits in the low pg-range have been obtained, viz. 1–6 pg for organophosphorus pesticides, 4–60 pg for triazine herbicides and 0.3–6 pg for polycyclic aromatic hydrocarbons. Linearity of response (2 pg–10 ng range) and RSD values at adequate levels were good. Due to the high acquisition rate, automated spectral peak deconvolution could be used. This highly powerful software option enabled calculation of spectra from overlapping peaks. In actual practice this meant that peaks had to be separated only by 3 spectra (e.g. 0.15 s at a spectrum storage rate of 20 Hz). This was especially valuable in case of complex samples. GC–TOF-MS was applied to the determination of the above compound classes in various aqueous and solid extracts (by means of miniaturised extraction procedures). An aliquot was injected into the GC system using splitless or large-volume injection. The technique has meanwhile been accepted and applied to various analyte groups, e.g. doping in urine, VOCs in drinking water, explosives in waste water and many more.

Comprehensive GC (GCxGC) is a relatively new technique, which has proven to be very powerful for analysis of **very** complex samples. The compounds eluting from the first-dimension column are continuously trapped and reinjected into a very fast second-dimension column by means of a timed modulator. In the early stage of this technique, it has mainly been demonstrated in the field of oil industry, where various distillate fractions showed up containing thousands of ordered peaks. In the past few years many other applications have been described in the literature. Due to the narrow peaks in the second dimension, detection has to be in the 50–200 Hz range. Flame ionisation and electron capture detection have successfully been used. Identification is usually based on retention time determination in both dimensions using standards. Expertise knowledge and chemical intuition are also often used. The combination with TOF-MS resulted in a true three-dimensional separation technique. The high spectrum storage rate guaranteed full recording of the fast eluting peaks (150–250 ms at the base). Applications in the field of fruit (pesticides; volatile flavours), food (contaminants, flavours) and environmental analysis (pesticides; polycyclic aromatic hydrocarbons, PCBs and dioxins) will be demonstrated. Analytes of interest were isolated using newly developed miniaturised extraction procedures.

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## ***Quantitative and qualitative analysis of small molecules by mass spectrometry: with or without liquid chromatography ?***

***Gérard Hopfgartner  
University of Geneva, School of Pharmacy  
Life Sciences Mass Spectrometry  
20, Bd d'Yvoy, 1211 Geneva, Switzerland***

For the analysis of pharmaceutical compounds in biological fluids liquid chromatography combined with mass spectrometric detection is the method of choice either as a concentration, purification or/and a separation step in the analytical procedure. High throughput quantitative analysis is achieved with high-flow or parallel LC using generic sample preparation approaches, such as direct plasma injection.

Triple quadrupole mass analysers are largely used for the quantification of small molecules, while ion trap mass spectrometers are more suited for drug metabolism studies. Both mass spectrometers are complementary and ideally one would like to have all features of both instruments in one system. The situation becomes even more complex with hybrid instruments such as quadrupole time of flight mass spectrometer, where medium resolution and accurate mass of the precursor ions and the fragment ions can be obtained with high sensitivity. Accurate mass MS/MS spectra can also be recorded on triple quadrupoles with enhanced resolution. Recently, hybrid instruments using linear ion traps have become available opening completely new possibilities in qualitative and quantitative analysis.

Quantitative bioanalysis on an disposable ESI Chip has been demonstrated without chromatographic separation. With the high selectivity of mass spectrometric detection how much chromatography do we really need ?

A chromatographic peak elutes within 10 and 30 seconds. For quantitative analysis this is sufficient while for qualitative analysis several injections of the

same sample are required to perform all relevant experiments. Fraction collection prior MS detection and infusion of the relevant peaks by ESI Chip is one approach to overcome the time constrain. With off-line analysis various MS experiments can be performed for structure elucidation by minimising analysis time and sample consumption.

Selected examples in drug metabolism and quantitative analysis will be presented with the emphasis fish out needles in a haystack and quantify them.

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## ***2002 President's Report***

After 6 years of heading the SGMS Committee, it is time for me to retire from the position of President of the SGMS, but at the same time to leave the committee, enabling a new person to join it. I strongly believe that to avoid complacency or routine, new people need to join the Committee and bring new ideas to its organization. This is why I think that I should not stay on as President forever. I am sure that a change in Presidency will move the SGMS one step forward.

It is also the right time to draw up a balance sheet of the past six years. Running the SGMS was not the tremendous task one would imagine because of two main reasons. The first one is because the Society had been properly established by the previous Committees and Presidents. I would like to give them full credit for their work as several of them are with us today. The second reason is because I have had the chance to work with three very good Teams (the last three committees) and I would like to warmly thank all of them who have done their very best to keep the SGMS running. We have always managed the SGMS keeping in mind not only its strong tradition and its friendly atmosphere but also its scientific excellence. Moreover I am personally very happy that we have enrolled the SGMS in international scientific networks through its connection to the Web and its registration as a member of the International Mass Spectrometry Society. This gives more visibility to the SGMS and this is important if we want to keep the Society alive in the coming years.

As I have already written, being President of the SGMS has been a fantastic task not only from a scientific viewpoint but also on a more personal level. It gave me the opportunity to meet brilliant scientists and friendly people and I will hold many fond souvenirs of this experience.

To conclude, I wish every success to the new Committee and to the new President, and, it goes without saying, all the best to the SGMS.

Laurent Fay

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## ***Minutes of the 2002 General Assembly of the Swiss Group for Mass Spectrometry***

***Hotel Dorint Beatenberg – 14.11.2002***

The assembly starts at 14:20. It is the first time that the meeting takes place at the Hotel Dorint, Beatenberg. The president, L. Fay opens the meeting, following the approved agenda, sent out previously with the newsletter Vol 20\_2.

1. Nomination of the scrutineers:  
Jean Luc Wolfender and Fabrizio Sabini are nominated as the scrutineers.
  2. Approval of the minutes of the 2001 General Assembly:  
The assembly approves the 2001 minutes to 100% without any further questions.
  3. President's report and its approval:  
The president reads his 2002 report (see Newsletter 21\_1). The report is approved without any further questions.
  4. Treasurers report:  
Our Treasurer H.P. Moser informs the assembly about the normal expenses on our two accounts. The bank account has a balance of Fr. 13'417.00 per 30.9.02 and the Post Account has a balance of Fr. 22'181.00 per 1.10.02. The total balance is at + Fr. 3.5'598.00 compared to Fr. 36'777.00 (2001). The financial situation is very good and well under control.
  5. Auditors report and approval of the treasurer's report and auditor's report:  
Peter Hirter and Kurt Schellenberg confirm the perfect bookkeeping and ask for acceptance of the treasurer's report. Both, the treasurer's report and the Auditor's report are approved to 100% by the members.
  6. Decision of the 2003 membership fee:  
The assembly decides with no opposition that the annual fee for the regular membership remains unchanged at Fr. 25.-/Year for individual members and Fr. 100.-/Year for Collective members.
-

7. Admission of new members:  
15 new members are admitted to the SGMS:  
Figueiredo Joachim Neves, Schlichtherle-Cerny Dr. Hedwig, Göbel Anke, Tzouros Manuel, Hornberger Dr. Martin, Stolz Siegfried, Matter Urs, Kaufmann A., Knochenmuss Dr. Richard, Giger Mathias, Laue Grit, Schnider Christia, Tromp Jan, Niebel Jörg, Kölliker Stephan
8. Election of the President and the new SGMS committee  
100% agree to elect Andreas Stämpfli as the new president of the SGMS. Andreas accepts the election and thanks the members for the trust they have in him. 100% agree to the new committee including Jean Luc Wolfender as new member of the committee.
9. SCS (Swiss Chemical Society) – Information  
HJ. Walther has some points to mention:
  - Markus Straub becomes Head of the NSC
  - Promotion for young talents (Chemistry) will be supported
  - Promotion for contacts between potential students and universities
  - Support for recruiting activities
  - Contact with international organisations (FECS; IUPAC)
10. News from the ESMS  
R. Tabacchi has no news to report. For an update go to the homepage (Link on the SGMS Homepage). 6<sup>th</sup> IMSS Conference from 31.9.-5.10.03
11. Individual Proposals  
none
12. Miscellaneous:
  - Marc Suter: Internet Info: 22 job offerings last year: Site works fine.
  - The Assembly decides to stay in the DORINT for the next meeting in 2003.

Thomas Läubli

Secretary of SGMS

## ***Rigi Meeting 2003, October 30 and 31, 2003***

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 send before **August 18, 2003** directly to the SGMS president, Andreas Staempfli, F. Hoffmann-La Roche Ltd, Basel. The abstract should be not longer than 2500 characters. Please send your abstract only by e-mail to our president (andreas.staempfli@roche.com).

### **Registration and Accommodation:**

A **registration form** and a payment form are included with this mailing. Please, send your registration (completely filled in form!) to Andreas Staempfli not later than **September 30, 2003**.

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 be payed 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 (130 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 your roommate)

**Late Fee : An additional late fee of CHF 50** for registration will be applied to all payments received after September 30, 2003.

**NOTE:** to qualify for the regular rates **payment MUST** be received by **September 30, 2003** - receipt of the registration form without payment will not qualify.

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

Please, pay your registration fee with the enclosed pink payment form (marked "RIGI Meeting") or direct to the bank account:

Credit-Suisse BCL 4094, 0094-919402-50,  
Schweizerische Gruppe für Massenspektrometrie, CH-4102 Binningen

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

### **Cancellations**

Cancellation requests, received in writing before **September 30, 2003**, will qualify for a refund of the fees paid, less an administration handling charge of 25% of the total payment. After **September 30, 2003**, 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 shows:**

No refunds will be made.

### **Students support program:**

Students giving a talk (selection by the 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 we will be sent out in September and which will be 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 of the payment form! The cashier 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 H.P. Moser during the "Rigi Meeting".

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Swiss group for mass spectrometry  
Schweizerische Gruppe für Massenspektrometrie



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

Please join us for the

## ***General Assembly of the SGMS 2003***

Thursday, October 30, 2003

~1700 h

Dorint Hotel Blüemlisalp, Beatenberg

### **Agenda**

1. Nomination of the scrutineers.
2. Approval of the minutes of the 2002 general assembly.
3. Presidents 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 2003 membership fee.
7. Admission of new members.
8. Election of two Auditors
9. News from the NSCG - HJ. Walther.
10. News from ESMS - R.Tabacchi.
11. Individual proposals.
12. Miscellaneous.

Individual proposals must be **sent by (e)- mail before October 15, 2003** to the president: [andreas.staempfli@roche.com](mailto:andreas.staempfli@roche.com)

The President

Andreas A. Staempfli



### MEMBERSHIP APPLICATION

**Name:** \_\_\_\_\_

**First Name:** \_\_\_\_\_

**Title:** \_\_\_\_\_

**Prof. Address :**

\_\_\_\_\_

\_\_\_\_\_

\_\_\_\_\_

**Phone:** \_\_\_\_\_ **Fax:** \_\_\_\_\_

**E-Mail:** \_\_\_\_\_

**Instruments :** \_\_\_\_\_

**Fields of activities:** \_\_\_\_\_

**Are you already member of the New Swiss Chemical Society (NSCG)?** \_\_\_\_\_

**wishes to become member of the SGMS:**

**Date:** \_\_\_\_\_

**Signature:**

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