Vol 20_1 July 2002

Swiss group for mass spectrometry
Schweizerische Gruppe für Massenspektrometrie

SGMS

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

Newsletter

We are happy to announce our annual

Rigi Meeting 2002

November 14 and 15, 2002

Dorint Hotel Blüemlisalp Beatenberg

! 10:00 !

4 pleanary lectures! A business lunch will be included!

The final program of our anniversary meeting will be published in in Newsletter Vol 20_2 end of September 2002. Also exact travel information will be given at that time.

We are very pleased to invite you to the

SGMS General Assembly 2002

Dorint Hotel Blüemlisalp Beatenberg

November 14 , 2002

13:30

We hope that many people will attend our General Assembly 2002 following the afternoon session. Please refere to "Invitation and Agenda for the General Assembly" later in this issue for more detailed information.

During the apero (special event) and the supreme "Blüemlisalp Schweizer dinner buffet" (incl. a special event) we will have plenty of time for discussions. As usual latest news will be served at the bar.

Contents see next side

In this Newsletter you will find:

Rigi Meeting 2002 on Beatenberg! Why?

For 17 years the Rigi Kaltbad was the location for the famous Rigi meeting of the Swiss group for mass spectrometry. Only once, namely for the 10th anniversary the meeting took place at the EPFL in Lausanne. In the years 1997, 1998 and 1999 when the Rigi meeting was still at the Rigi, hotel accomodation for all of the participants was difficult to organize. In 1999 the situation was really bad and the organizers decided to look for another location. The Hotel & Golf Chaumont in Neuchâtel was a chance. The accomodation was almost perfect. Travelling distances equali for almost all of the participants. Only the meeting room was not that great. The screen could not be seen from all the places and also the accustics of the room was very poor. Air conditioning is something we better not talk about! Due to these reasons the committee of the SGMS decided to look for another location. Finding a hotel with more than 120 rooms and with a meeting room what can hold up to 120 people - and this for an affordable price - is not that easy. Going back to the Rigi Kaltbad is not possible due to the unchanged hotel situation up there. Bad news for all who beloved that marvellous scenery.

But what do you think about Eiger, Mönch and Jungfrau?

Opposite of these three famous Swiss mountains is Beatenberg, situated on a platform above the Lake of Thun. AND there is the Dorint Hotel Blüemlisalp. Up to 130 rooms and a rectangular shaped meeting room holding up to 120 people. Travelling distances aren't too bad. The highway leads directly to Interlaken and from there it's a perfect mountain drive up to Beatenberg. Travelling gets even more exiting by train and with the still yellow "Postauto". Exact travel information will be given in the second Newsletter.

DO not forget: It's our 20st anniversary!

ans

Can we cover the metabolome only by means of mass spectrometry?

***Fiehn O., #Costisella, B. & *Tolstikov VV**
***Max-Planck-Institute of Molecular Plant Physiology, 14424 Potsdam (Germany)**
 # University of Dortmund, Dept. of Chemistry, Dortmund (Germany)
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Analogous to the transcriptome and the proteome, an organism's metabolome is defined as the complete set of its metabolites present in a certain tissue under defined conditions. Plant metabolomes are comprised by thousands of individual compounds. Is it possible to identify and quantitate all metabolites in a biological system by means of mass spectrometry?

Currently, the answer is a clear 'no'. However, in the context of functional genomics, there is the need to analyse as detailed as possible the response of an organism to genetic, environmental or developmental perturbation. We have therefore started to analyse parts of the metabolome in an unbiased way by combining GC-TOF with mass spectral deconvolution, and RP and HILIC-ion trap-MS^3 at positive and negative ESI for assessing the relative abundance of all detectable peaks, with currently some 1,000 peaks to be found in a plant sample. This strategy leads to a high number of unidentified compounds, and *de novo* identification is an essential part of truly metabolomic approaches. Using the example of a novel amino-callose found in cucurbit phloem we demonstrate how ion trap mass spectrometry alone may be misleading in structural elucidation, and that accurate mass MS is required by necessity. We compared the use of GC-Quadrupole MS (!), QTOF and FT-MS for that purpose, and concluded that without the additional help of 2D µNMR, metabolites cannot be elucidated, even with the help of software like MassFrontier or databases like KEGG and Beilstein. After *de*

novo identification of several metabolites we later found to be already published, we concluded that it would be a great help to have a comprehensive biological LC/MS library, despite the fact that standardisation between different instruments is hardly possible.

As a biological application example, the comparison of a silent SuSy antisense potato line and its corresponding Desirée cultivar is shown. Using the peak areas of identified and unidentified compounds, we normalized each individual plant sample to the total metabolome content. Metabolic distances as well as shifts in biochemical networks could be computed. Network generation was performed by correlation analysis and 3D visualization. By investigating these networks, novel hypotheses on hexose transformations and sugar alcohol metabolism could be generated.

IRM-GC-MS techniques to characterise sources and sinks of organic contaminants in ground water

Hans H. Richnow
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In the past decade, stable isotope chemistry has received increasing attention in environmental science. The stable isotope signature of organic substances yields useful information to decipher source, distribution, and fate of organic substances in the ground water. The isotopic composition (D/H, $^{13}C/^{12}C$, $^{15}N/^{14}N$, $^{37}Cl/^{37}Cl$) of organic contaminant can used as fingerprints to trace their origin (Smallwood et al., 2002; Drenzek et al., 2002) which may have some potential in forensic approaches with respect to separate pollution sources. Isotope fractionation processes can be used to characterised *in situ* biodegradation.

Monitoring of ground water contamination has gained importance in the context of risk assessment, plume management strategies, and in the evaluation of remediation measures, in particular where natural attenuation concepts are applied. Thus, innovative approaches are needed to monitor processes governing the concentration of contaminants in the aquifer. A decrease of pollutants concentration in a contamination plume could have many reasons like dilution, sorption or biological degradation, but only the latter leads to sustainable contaminant reduction. Thus, the assessment and quantification of *in situ* biodegradation is essential to evaluate the risk of contaminated aquifers and is essential prove the success of monitored natural attenuation (MNA) or any other remedy.

To characterise *in situ* biodegradation, a concept based on the isotope fractionation of organic contaminants during biodegradation had been developed (Richnow and Meckenstock, 1999; Meckenstock et al., 1999; Richnow et al., 2002). Biodegradation of pollutants such as aromatic hydrocarbons and chlorinated ethenes leads to an enrichment of ^{13}C and ^{2}H in the residual fraction (Meckenstock et al., 1999; Hunkeler et al.,1999; Bloom et al., 2000; Ward et. al., 2000; Morasch et al., 2001). This fractionation process can be described by the Rayleigh-Equation. The relation between concentration and isotopic composition of a compound is described

by the kinetic isotope fractionation factor (α). In laboratory degradation experiments with batch cultures, the isotope fractionation factors have been determined for some typical BTEX, mineral oil and chlorinated groundwater contaminants. These factors were applied to quantify the biodegradation in several field studies and to evaluate the validity of the isotope fractionation concept.

Various test sites with distinct geochemical and hydrological characteristics were examined for isotopic fractionation to assess the *in-situ* biodegradation. Laboratory derived isotope fractionation factors were applied to calculate the extent of biodegradation (Vieth et al., 2002). Test site comprises variety of contaminants, such as (i) tar oils (BTEX and naphthalene), (ii) landfill leachate with BTEX, mineral oils (diesel fuel) and (iii) chlorinated solvents. Isotope fractionation may be well used to evaluate the biodegradation in contaminated aquifers independent of other concentration diminishing processes such as sorption and dilution. In the context of Natural Attenuation, this concept has a large potential to improve ground water monitoring and risk assessment strategies.

Modern IRM-GC-MS systems can be used in routine analysis and enable the exploitation of the large potential of isotope chemistry in ground water research. This paper discusses various aspects of IRM-GC-MS approaches in ground water analysis chemistry from a technical and scientific perspective.

References

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Vieth A., Kästner M., Morasch B., Meckenstock R. U., Richnow H. H.(2001): TerraTech 5, 37-41.

Ward JA, Ahad JME, Lacrampe-Couloume G, Slater GF, Edwards EA, Sherwood Lollar B (2000): Environ. Sci. Technol. 34, 4577-4581.

The Development of Quadrupole Field Mass Spectrometers

M. S. Story

While the principles were thoroughly published in the early 50's, widespread availability of mass spectrometers utilizing these principles was not given until 20 years later. Linear and three dimensional quadrupole (ion trap) mass spectrometers represent the overwhelming majority of instruments operating in laboratories today.

As with any technology, there needed to be a driving force for the commercial development. Individuals and companies often do initiate this development, but without a significant market need to direct the technical development to a unique solution, there is most often failure. The success of quadrupole and ion trap mass spectrometry has relied on the environmental and biotechnology markets to provide the problems and support for academic, industrial, and commercial use and development.

This will be a retrospective description of these technical developments and the inter-play of instrumentation development, academia, and market needs.

MALDI MS Imaging of Biological Tissue: A Powerful Tool in the Drug Discovery Process

Markus Stoeckli, Analytical and Imaging Sciences, Novartis Pharama AG,Basel

The detailed analysis of biological tissues for their molecular contents is a key element in the search for cures for diseases. A wide variety of techniques is available for this challenging task, but there is a continuous need for tools that enable the collection of large amounts of data with higher spatial resolution in a short time.

Expression profiling by mass spectrometry is a powerful technique that can quickly provide information on a wide range of molecular contents in tissues, but its spatial resolution is only as good as the tissue portion used for the experiment. The goal of our work was to identify molecular entities in tissues and to localize them within small, defined cell populations.

A method is presented for direct spatial analysis of biological tissue sections for their molecular distribution. The technique takes advantage of the very sensitive matrix-assisted laser desorption/ionization mass spectrometry technology and employs a commercial instrument with modifications only to a few components and the software. With this setup, hundreds of molecular images can be generated simultaneously and within just a few minutes. The current features are a spatial resolution of 50 µm and a sensitivity in the attomol range.

In this presentation, the basic principle of this technology is demonstrated, covering the complete process from tissue preparation to image analysis. Improvements developed in our lab will be shown, which allow fast data acquisition and processing. The potential of this method for the drug development process is shown in examples of protein and drug imaging.

Reference

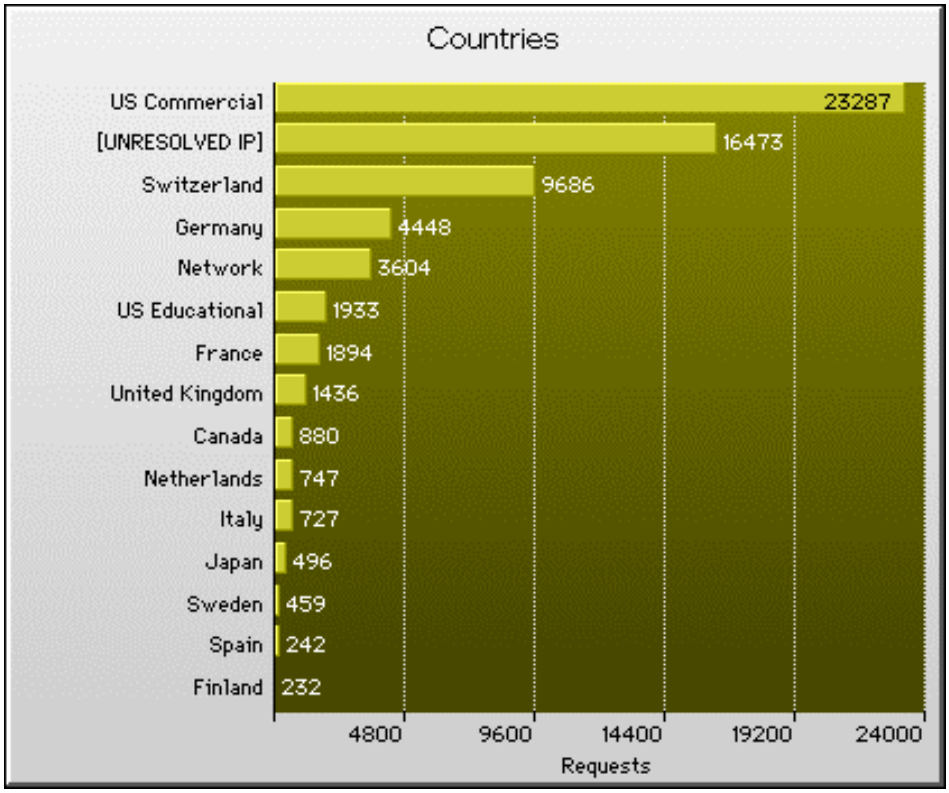
Stoeckli et al., A new technology for the analysis of protein expression in mammalian tissues. Nat. Med., 2001 7(4), 493-496

2001 President's Report

24.10.2001

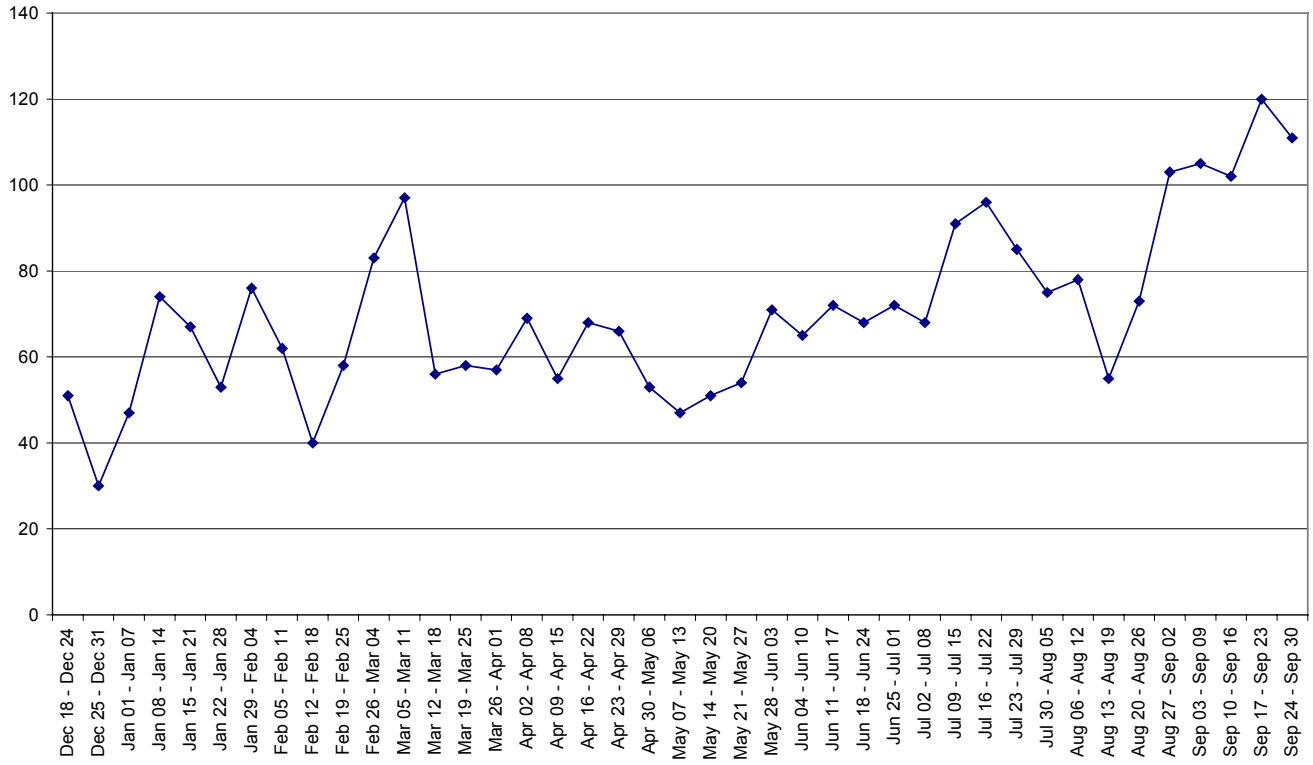
This is the first year of activity for the present SGMS Committee and I would first like to acknowledge every member of this Team for their continuous commitment and involvement in the management of the SGMS. We have a friendly atmosphere that makes every Committee meeting enjoyable. Because being the secretary is a time-consuming function, we decided to split this activity and today Andreas is our Newsletter Editor and Thomas is our Secretary *per se* and responsible for keeping our files in order.

Our Society is in good shape with 188 members (+ 9%). Our sponsorship revenues are increasing and three private companies are financially committed towards the SGMS, namely Agilent, Brechbühler and Shimadzu. I would like to acknowledge their contributions. A warm thank you also to Dr. Walter Vetter for the donation of 250 sFr.



Country Access Statistics for 758 Day Period:
Jun 04 1999 13:58:03 to Jun 30 2001 23:29:36 (Statistics from our Server)

The SGMS Internet site is active and has been used to publish open positions in our Companies, Institutes or Universities and also for outside Switzerland. This year 19 positions were published (CH 8, Europe 6, US/Canada 5) making this Web site useful for the mass spectrometry community.



Fastcounter Statistics (the little counter on our site)

To promote active participation of students during the Rigi Meeting, the SGMS committee has decided that those giving talks will be invited by the SGMS. I am very pleased to say that Stephan Brombacher, University of Basel-will be our invited student. Congratulation to him.

Finally, I would like to thank all those who have helped me to keep the SGMS running, especially the other members of the Committee. On behalf of the Committee I wish you all the best for the coming year.

Minutes of the 2001 General Assembly of the Swiss Group for Mass Spectrometry

Hotel Chaumont & Golf: October 25th, 2001

The assembly starts with a slight delay to the agenda at 18:30. According to the participants list there are 69 regular members including all 7 member from the SGMS committee present. It is the second time that the meeting takes place at the Hotel Chaumont & Golf above the Lake of Neuchâtel. The president, L. Fay opens the Geberal Assembly, following the approved agenda, sent out previously with the newsletter Vol 19.2.

1. Nomination of the scrutineers:
   Ludovica Verzegnassi and Jörg Hau are nominated as the scrutineers.
2. Approval of the minutes of the 2000 General Assembly:
   The assembly aproves the 2000 minutes without any further questions.
3. President's report and it's approval:
   The president reads his 2001 report (see Newsletter 20.1). This year's invited student is Stefan Brombacher from the University of Basel.
   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. 23'346.94 per 1.10.01 and the Post Account has a balance of Fr. 13'430.55 per 1.10.01. The total balance is at + Fr. 36'777.49 per 1.10.01 compared to Fr. 37'775.89 (2000). The financial situation is very good an 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 treasurerer's report. Both, the treasurer's report and the Auditor's report are approved to 100% by the members.

6. Decision of the 2002 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:

   13 new members are admitted to the SGMS

   New members are:

   Klaus Wuchner, Fabrizio Sabini, Jens Donath, Walther Mühlecker, Peter Wipfli, Andreas Topp, Raymond Villemet, Holger Kurth, Winfried Fiedler, Iris Barmé, Stephane Roudier, Michael Affolter, Francesca Giuffrida

8. Election of two auditors for 2002/2003

   Urs Beat Ranalder and Peter Oggenfuss are elected as auditors for the next 2 years. Thank you both for your engagement.

9. NSCS (New Swiss Chemical Society) – Inormation

   HJ. Walther has some points to mention.

   The society has a new name: SCG(SCS)-

   Schweizerische Chemische Gesellschaft.

   They have new statutes

   A new web site is in progress

   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)

11. Individual Proposals:

    - Rigi Meeting 2002: Where should we meet?

      The General Assembly agrees that the SGMS Comittee is looking for a location to hold the 20th anniverary meeting in 2002.

    - Organisation of one of the next International MS Conference by SGMS?

      With 8 against 7 votes (the rest of the general assy has not given a vote here) the general assembly decides not to organise an international MS Conference

12. Miscellaneous:

    Marc Suter: Internet Info; no news

    Laurent Fay: More than 30% of the participants in 2001 have registred after the deadline. The participants are reminded that everyone should try to register prior to the deadline because the organisational issues become very difficult with last minute reservations.

As there are no further comments or questions, the General Assembly closes at 19:05h

Thomas Läubli

Secretary of SGMS

Rigi Meeting 2002, November 14 and 15, 2002

Dorint Hotel Bluemlisalp, Beatenberg

Oral communications / Abstracts:

The meeting will be supplemented by oral communications from various participants. The time allotted will be 20 minutes. Abstract with author's name and address should be send before **August 25, 2002** directly to the SGMS president, Laurent Fay, Nestlé. Please send your abstracts only by e-mail to our president (laurent-bernard.fay@rdls.nestle.com)

Registration (Payment) and Accommodation:

A **registration form,** as well as the corresponding payment form are included with this mailing. Please, send your registration (completely filled in form!) to Laurent Fay not later than **September 30, 2002**. Due to organisational reasons **no late nor ad hoc registration** will be **accepted.**
There is no need to register personnally 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 hope that there should be enough rooms available for all members, who wish to participate this year at our "Rigi-meeting". However, we also would nevertheless like to notify you, that **we will again strictly follow the order of registration for the distribution of the hotel rooms** (**130** rooms available!).

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.

The **total costs for registration to the SGMS-meeting** for Hotel accomodation, including business lunch, dinner buffet, breakfast and of course special events are:

255 SFr./person (single room occupancy)

235 SFr./person (double room occupancy; please indicate your roommate.)

There is no possibility of attending only to the meeting without Hotel accomodation. Thanks for understanding!

Please, pay your fee with the enclosed pink payment form (marked "RIGI Meeting 2002") until **end of September.**
Don't forget to **mark clearly name(s) and address on your payment form(s)**. We are spending every year more time tracking the payment sent to the SGMS without ANY name! Our president will appreciate very much your help.

Travel Information:

Details will be published together with the complete program and our official invitation, which we 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.- SFr.** You are kindly asked to pay this fee as soon as possible. Please write your name(s) 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.-- SFr. for two consecutive years.

Only members from abroad may pay the membership fee directly to our treasurer H.P. Moser during the "Rigi Meeting".

Swiss group for mass spectrometry
Schweizerische Gruppe für Massenspektrometrie

SGMS

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

Please join us for the

General Assembly of the SGMS 2002

Thursday, November 14, 2002

1330 h

Dorint Hotel Blüemlisalp, Beatenberg

Agenda

1. Nomination of the scrutineers.
2. Approval of the minutes of the 2001 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 the President and the SGMS committee.
9. News from the NSCG - HJ. Walther.
10. News form ESMS - R.Tabachi.
11. Individual proposals.
12. Miscellaneous

Individual proposals must be **sent by (e)- mail before October 31, 2002 to the president**: Dr. Laurent B. Fay, Nestlé Research Center, Vers-Chez-les-Blanc, CH-1000 Lausanne 26

for the committee

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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