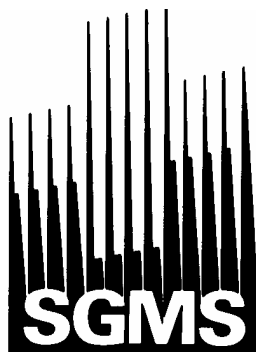


Swiss group for mass spectrometry
Schweizerische Gruppe für Massenspektrometrie



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

Newsletter

We are happy to announce our annual

Rigi Meeting 2001

We meet again at **Chaumont Hotel & Golf** above **Neuchâtel**. The meeting will take place on

October 25 and 26, 2001

and will start as usual at 1400. This year there will be 4 plenary lectures (abstracts within this volume). The final program will be published in detail end of September 2001 in the Newsletter Vol 19/2 together with exact travel information.

We are very pleased to invite you to the

SGMS General Assembly 2001

Chaumont Hotel & Golf above Neuchâtel
October 25, 2001
1815

following the afternoon session. We hope that many people will attend. Please see "Agenda for the General Assembly" later in this issue for more detailed information about it.

There will be plenty of time for discussions during Aperitif and Buffet-Dinner in the evening.

Latest news will be served at the bar.

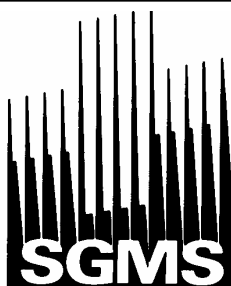
Contents see next side



In this Newsletter:

- Agenda for the General Assembly, 2001 3
- Abstracts of the plenary lectures given this year by
APCI-MS for Rapid and Dynamic Measurement of Flavour Release 4
by Prof. Dr. A.J. Taylor
The Effect of Nucleoside Proton Affinity 5
on the Formation of Zwitterionic Oligonucleotides
by Prof. Dr. Giovanni Sindona
- Mass Independent Single Molecule Detectors for Mass Spectrometry 7
by Dr. Gerber
- The Swiss Light Source 9
by Dr. Abela
- Annual "Rigi-Meeting", 2001: Registration/Accommodation... 10
- Copy of "Presidents Report 2000" 12
- Minutes of the General Assembly 2000 13
- Membership Application Form 17
- Actual list of the SGMS Committee Members 2001 19

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Schweizerische Gruppe für Massenspektrometrie



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Gruppo svizzero di spettrometria di massa

General Assembly of the SGMS 2001

Thursday, October 25, 2001
1815 h
Hotel Chaumont & Golf, NEUCHÂTEL

Agenda

1. Nomination of the scruteniens.
2. Approval of the minutes of the 2000 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 2002 membership fee.
7. Admission of new members.
8. Election of two auditors for 2002/2003.
9. News from the NSCG - HJ. Walther.
10. News form ESMS - R.Tabachi.
11. Individual proposals.
12. Miscellaneous:
 - RIGI Meeting 2002: where should we meet?
 - Organisation of International Mass Spectrometry Conference IMSC by SGMS in Switzerland ?

Individual proposals must be **sent by mail before October 4, 2001 to the president:** Dr. Laurent B. Fay, Nestlé Research Center, Vers-Chez-les-Blanc, CH-1000 Lausanne 26

for the committee

Andreas A. Staempfli



APCI-MS for Rapid and Dynamic Measurement of Flavour Release

Professor AJ Taylor
Division of Food Sciences, University of Nottingham
Sutton Bonington Campus
Loughborough LE12 5RD UK

Flavour analysis has been conventionally achieved by extraction of flavours from foods followed by GC-MS using EI and/or CI sources. These techniques have led to the identification of many of the flavour components in food, especially when coupled with GC-O odour Port Analysis. However, it has proved difficult to relate the flavour composition of a food with the perceived flavour characteristics.

One reason is that flavour release during eating of food affects the relative amounts of flavour (and their rate of delivery) to the olfactory and gustatory receptors. What is needed is a method for sampling air from the noses of people eating food to measure the release profile under in vivo conditions.

Of the methods available, Atmospheric Pressure Ionisation methods are particularly suitable as they tolerate water and make interfacing between humans and the MS simple. However, API needs close control to achieve quantitative, reproducible ionisation. In our lab we developed an API interface where the sample flow rate, water content and ionisation parameters were optimised to achieve reproducible results over a fairly wide range. Potential problems like ion suppression have been studied and some solutions found. Sensitivity is around 10 ppbv (nL volatile/L air) which allows many aroma compounds to be measured below, or close to their odour threshold. The limitations seem to be the ionisation efficiency of individual compounds and the amount of chemical noise in the system.

The MS issues will be presented and discussed along with examples of applications which show the potential of this technique for measuring flavour release in a variety of situations.

The Effect of Nucleoside Proton Affinity on the Formation of Zwitterionic Oligonucleotides

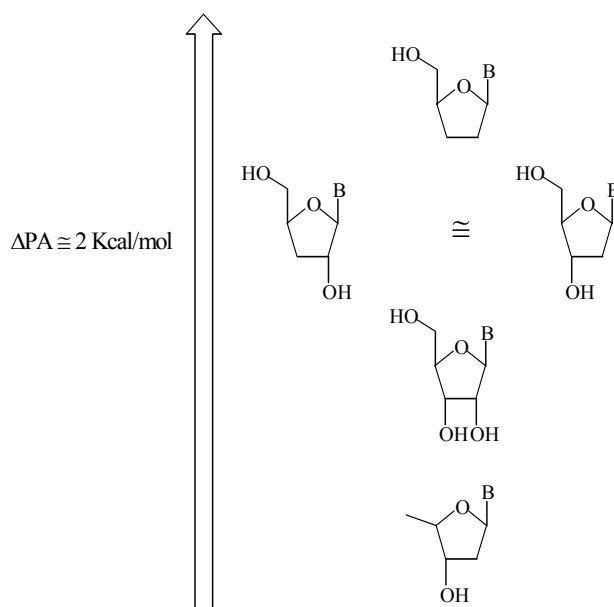
Prof. Dr. Giovanni Sindona
Dipartimento di Chimica, Università della Calabria
I-87030 Arcavacata di Rende (CS)

The existence of "zwitterionic" oligonucleotides was first proved in the early sixties from the crystallographic data obtained from an A_3 trimer. This structural motif accounts for the electroneutrality of an oligomer bearing basic and acidic sites. With the advent of desorption ionisation (DI) methods such as FAB and MALDI, it became clear that the formation of negative singly-charged gaseous species was not simply due to the neutralisation of (n-1) phosphodiester group of the oligomer backbone^{1, 2}.

The positively charged nucleobases, within gaseous zwitterionic oligonucleotides, could drive the fragmentation of the strands, through the formation of apurinic sites. The proton affinity (PA) of the nucleobases has been considered, therefore, an important parameter for the evaluation of the sequence of a given oligomer.

The PA of wild type and modified nucleosides and nucleobases have determined by Cooks kinetic method.³ with good accuracy and reproducibility. Unless otherwise suggested, it is now clear that the proton affinity of the same nucleobase can be substantially affected by minor modifications in the sugar structure (scheme).

The PA differences can be attributed to the stabilising/destabilising effects of the hydroxyl groups on the development of the positive charge on the nucleobase after protonation. It can not be excluded a PA change of the same nucleobase within a DNA strand, as a function of the environment.





However the PA differences between purine and pyrimidine nucleosides is higher than that due to sugar modification. It can be suggested that Guanosine should be the preferred protonation site and also the preferred oxidation site⁴ in DNA damaging processes.

1. G. Sindona et al., *J. Am. Chem. Soc.*, **1983**, *105*, 5607
2. M. L. Gross et al., *J. Am. Soc. Mass Spectrom.*, **2001**, *12*, 193
3. G. Sindona et al., *J. Mass Spectrom.*, **2000**, *35*, 139
4. G. Sindona et al., *J. Am. Soc. Mass Spectrom.* **2001**, *12*, 176

Mass Independent Single Molecule Detectors for Mass Spectrometry

Daniel Gerber^{1,3}, Dominique Gritti¹, Yvan Gonin¹, Alexandre Netuschill²,
Frédéric Rossel¹, Dominique Schenker¹, Jean-Luc Vuilleumier¹,
Damian Twerenbold^{1,3}

We have introduced a novel type of molecule detector - cryogenic particle detectors - in time-of-flight mass spectrometry as a solution to the well known decrease in quantum efficiency for molecules with increasing mass. Cryodetectors have been developed in the last two decades for x-ray astrophysics and dark matter search in cosmology. This type of particle detector operates at temperatures below 1 Kelvin. Cryodetectors measure the energy deposition of a single molecule with a large signal-to-noise ratio. In a time-of-flight mass spectrometer, the kinetic energy of a molecule is the product of the molecule charge and the acceleration voltage, and hence does not depend on molecule mass. Because cryodetectors measure the energy deposition of a single molecule, they show a mass independent detection sensitivity, which is 100% on impact.

Cryodetector time-of-flight mass spectrometers are operated in the single molecule counting mode. Standard time-of-flight spectra are obtained by creating histograms of the arrival times of the individual molecule events. A cryodetector signal, however, carries additional information: the pulse height is proportional to the total energy deposited by the detected molecule. This allows to select specific events when creating the time-of-flight spectra, e.g. by taking only molecules with a specific charged state. In addition, this pulse height information of the single molecule events allows to reduce the molecular background, e.g. by discarding events which do not have the required total kinetic energy owing to fragmentation or loss of charge during acceleration or free flight.



We have performed a variety of experiments using different cryodetectors. By direct comparison of identical samples in the same MALDI-TOF mass spectrometer with both ionizing detectors and cryodetectors, we verified the strong exponential decrease of ionizing detectors with increasing mass. For IgG molecules with a mass of 135 kDa accelerated at 16 kV, we infer an increase of intrinsic detection efficiency of cryodetectors of at least 3 orders of magnitude as compared to ionizing detectors. We performed experiments with equimolar polydispersive PEG samples with mean masses between 1000 Da and 35000 Da and obtained mass spectra with identical peak integrals.

¹ Institut de Physique, Université Neuchâtel, Rue A.-L.Breguet 1,
CH-2000 Neuchâtel, Switzerland

² Institut de Microtechnique, Université Neuchâtel, Rue Jaquet-Droz 1,
CH-2007 Neuchâtel, Switzerland

³ GenSpec SA, case postale 120, CH-2017 Boudry, Switzerland

The Swiss Light Source

Dr. Rafael Abela
Paul Scherrer Institut (PSI), 5232 Villigen

(abstract not yet received)



Rigi Meeting 2001, October 25 and 26, 2001

Chaumont Hotel & Golf above Neuchâtel

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 31, 2001** 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 before **September 14, 2001** ! Do not forget to specify, if you wish to occupy a single room. In case you will choose a double room, then indicate, with whom you will be sharing it.

There is no need to register personally at the Hotel Chaumont et Golf! 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.**

The **total costs for registration to the SGMS-meeting** are for

Hotel accomodation, including breakfast and dinner buffet:

230.-- SFr./person (single room occupancy)

210.-- SFr./person (double room occupancy)

Please, pay your fee with the enclosed pink payment form (marked "RIGI Meeting 2001") until **September 14, 2001.**

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.

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 October.

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".



2000 President's Report

This is the fourth year of activity of the present SGMS Committee and I would first like to acknowledge every member of this Committee for their continuous commitment and involvement in the management of the SGMS and also for the friendly atmosphere that we have created and kept during all of our Committee meetings and discussions.

I am very happy to see that our membership is increasing each year: Today we have 187 members. This size gives us a critical scientific mass in many different areas of mass spectrometry science. On the other hand being small permits us to keep the friendly and family atmosphere that has always been a characteristic of this scientific Society.

2000 was an exceptional year and many events were organised all over the world. For the SGMS, not taking into account the commemoration of the 10th birthday of the Society at Lausanne, this is the first time that the so-called "Rigi meeting" has been organised in a locality other than Rigi-Kaltbad. Given the number of people that are registered for this meeting here at Neuchâtel, I am very glad to see that a change in our tradition has been so well accepted. I hope that everybody will have fruitful discussions and an enjoyable time.

Last August, I went to Barcelona as representative of the SGMS to the International Scientific Committee of the 15th International Mass Spectrometry Conference. The meeting was very good and I was very proud to represent our Society. However, the SGMS is not a member of the International Mass Spectrometry Society. Considering the scientific audience of the SGMS members world-wide, I think we should change this situation to gain broader international recognition.

The SGMS Internet site is working well and has been used to publish open positions in our Companies, Institutes or Universities and also from outside Switzerland. This year 13 positions were published making this Web site a valuable source of information for people looking for a job.

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.

Signed the President

Minutes of the 2000 General Assembly of the Swiss Group for Mass Spectrometry

Hotel Chaumont & Golf: November 2nd, 2000

The assembly starts accordingly to the agenda at 18h10. Present are 55 regular members, including all 7 members from the SGMS committee. This year we are very proud to count again a new record participation to the conference (99 persons), although the "Rigi Meeting" was for the first time in a new area of Switzerland, in the hotel Chaumont & Golf above the lake of Neuchâtel.

The president, L. Fay opens the meeting, following the approved agenda, sent out previously within both Newsletters Vol. 18/1 and Vol. 18/2.

1. **Nomination of the scrutineers:**

Peter Kofel and Stefan Müller are nominated as scrutineers.

2. **Approval of the minutes of the 1999 General Assembly:**

The assembly approves the 1999 minutes without any further questions.

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

The president reads his 2000 report (see Newsletter 19.1).

He has information about the general situation of the SGMS, the IMSS Barcelona meeting in August 2000, the SGMS Internet site and some comments to the new conference place.

4. **Treasurer's report:**

Our treasurer HP. Moser informs the assembly about the normal expenses on our two accounts:

The **bank account** is stable and shows the usual movements, like e.g. travel expenses for guest speakers and Newsletter.

The **postal account** on the other side shows that the SGMS is a very healthy society, the balance is again higher than last year, which is partly due to the fact that not all bills have been paid yet.

The financial situation is over all well under control. Therefore HP. Moser does not see any reason to discuss a change of the regular membership fee (see also point 6) or any other changes.

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

P. Hirter reads the auditor's report and confirms the perfect bookkeeping of the SGMS. The treasurer's report and the auditor's report are both



accepted unanimously by the General Assembly without further comments and formal approval is given to the committee and both auditors.

P. Hirter and A. Staempfli are acknowledged for their auditor's work.

6. **Decision of 2001 membership fee:**

The assembly decides with no opposition that the annual fee for the regular membership remains unchanged at 25.-- SFr./individual member and 100.-- SFr./collective member.

7. **Admission of new members:**

22 new individual members are admitted to the SGMS (this year we lost for various reasons 9 members).

New admitted individual members:

| | | | |
|-----------------------|---------------------|-----------------------|-----------------------|
| <i>M. Bergmann</i> | <i>Y. Finck</i> | <i>P. Fischlewitz</i> | <i>K. Fluri</i> |
| <i>A. Fredenhagen</i> | <i>T. Goldmann</i> | <i>M. Heller</i> | <i>J. Hewel</i> |
| <i>J. Leu</i> | <i>M. Meier</i> | <i>A. Michel</i> | <i>S. Mohottolage</i> |
| <i>N. Mottier</i> | <i>J-M. Oberson</i> | <i>J. van Oostrum</i> | <i>C. Perret</i> |
| <i>C. Rolando</i> | <i>L. Spack</i> | <i>M. Stoeckli</i> | <i>R. Stoop</i> |
| <i>G. Tsoupras</i> | <i>R. Wicki.</i> | | |

8. **Election of the President and the Committee 2001/2002:**

President:

HP Moser asks the General Assembly to re-elect L.Fay as president for the SGMS for the next 2 years. All present members confirm this with no opposition.

Committee:

AM Weibel and U. Ranalder resign from the committee. Thomas Läubli and Andreas Stämpfli will replace the two leaving members. The General Assembly agrees to these changes.

K. Schellenberg replaces A. Staempfli as auditor (together with P. Hirter) for the next year.

9. **NSCS (New Swiss Chemical Society), present situation:**

HJ. Walther has a very short report, because there is not much to say due to the fact that the annual meeting of the NSCS will only take place later in November (more information about the NSCS can be found on their WEB-site).

10. **ESMS (European Society of Mass Spectrometry):**

R. Tabacchi informs about the present situation:

The ESMS had a meeting during the IMSS conference in Barcelona. He points out that Switzerland is one of the only countries, which has so far not officially joined the IMSS (see also point 11).

The ESMS will meet next time during the 16th IMSS conference in Edinburgh in 2003. (For more information see their WEB-site.)

11. **Individual Proposals:**

L. Fay proposes to join the IMSS as charter institutional member. This will cost as 200\$ per year. After a short discussion the General Assembly decides for image and representing reasons without any opposition to **join the IMSS.**

12. **Miscellaneous:**

Internet: Everything works well. Our site is pretty frequently visited. M. Suter also points out, that J. Hau assists him very generously.

As there are no further comments or questions, the General Assembly closes at 19:00 h.

AM. Weibel

(former secretary of the SGMS)

And once again a warm "Thank you" to AnneMarie Weibel and Urs Ranalder for all the time they gave over the past years to the SGMS.

A special "Thank you" to AnneMarie Weibel for writing the last "Minutes of the General Assembly".



**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:

Please fill in and send to the secretary of the SGMS:

Thomas Läubli / Brechbühler AG / Steinwiesenstrasse 3 / CH-8952 Schlieren
Fax: ++41 1 730 61 41 / Phone: ++41 1 732 31 31
email: thomaslaeubli@compuserve.com



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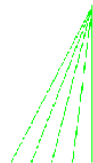
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