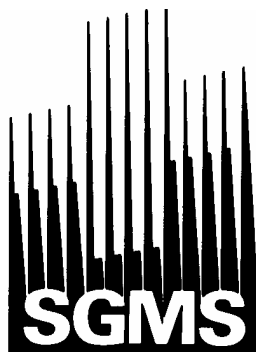


Swiss group for mass spectrometry  
Schweizerische Gruppe für Massenspektrometrie



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

## *Newsletter*

# ***Rigi Meeting 2001***

***and***

## ***General Assembly***

*Chaumont Hotel & Golf, Neuchâtel.*

***October 25 and 26, 2001***

### **In this Newsletter:**

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## PROGRAM OF THE 2001 "RIGI" MEETING I

THURSDAY AFTERNOON

**14:00 – 15:10      Opening**

Session 1:	<b>Chairman: Raffaele Tabacchi</b>
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**14:10 – 15:10      Daniel Gerber, University of Neuchatel, Neuchatel.**  
Mass independent single molecule detectors for mass spectrometry.

**15:10 – 15:30      Martin Resch, Shimadzu Schweiz GmbH, Reinach.**  
Fundamental design principles of a MALDI-TOF for high throughput sample analysis.

**15:30 – 15:50      Gérard Bondoux, Waters European Headquarter, S<sup>t</sup> Quentin Yvelines, France.**  
Using the mass spectrometer for triggering a fraction collector. Various aspects of MS directed autopurification.

**15:50 – 16:10      Ludovica Verzegnassi, Nestlé Research Centre, Lausanne**  
Challenges in food trace analysis by LC-MS/MS: sulfonamides in honey.

**16:10 – 16.30      Coffee Break**

Session 2:	<b>Chairman: Marc Suter</b>
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**Agilent Technologies**

**16:30 – 17:30      Prof. Giovanni Sindona, Universita della Calabria, Arcavacata di Rende, Italy.**

The effect of Nucleoside Proton Affinities on the Formation of Zwitterionic Oligonucleotides

**17:30 – 17.50      Stephan Schürch, University of Bern, Bern.**

Gas-Phase dissociation of Mixed-Sequence RNA/DNA Oligonucleotides.

**17:50 – 18:10      Christian Guenat, Novartis Pharma AG, Basel.**

The Fourier Transform Mass Spectrometer (FTMS). Is this powerful analytical tool ripe for chemists and biochemists in the pharmaceutical industry?

**18:10– 18:15      Pause****18:15 – 19:15      General Assembly 2001****19:15 – 20:30      Aperitif sponsored by****20:30 - ...      Dinner**

## PROGRAM OF THE 2001 "RIGI" MEETING II

FRIDAY MORNING

Session 3:	<b>Chairman: Laurent Fay</b>
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- 09:00 – 10:00**      **Prof Andy J. Taylor, University of Nottingham, UK.**  
APCI-MS for rapid and dynamic measurement of flavour release.
- 10:00 – 10:20**      **Vittorio Raverdino, Agilent Technologies, Geneva.**  
Atmospheric pressure photoionization (APPI):  
Selective or complementary ionization technique for LC/MS?
- 10:20 – 10.40**      **Stephan Brombacher, University of Basel, Basel.**  
Advantages and problems of the analysis of di-carbonyl-DNPH derivatives with HPLC-MS<sup>n</sup> using APCI(-).
- 10:40 – 11:00**      **Coffee Break**

Session 4:	<b>Chairman: Andreas Staempfli</b>
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- 11:00 – 12:00**      **Dr. Rafael Abela, Paul Scherrer Institut, Villigen.**  
The Swiss Light Source.
- 12:00 – 12:20**      **M. Kohler, Swiss Federal Laboratories for Materials Testing and Research, Dübendorf.**  
Characterization of ageing products of ester based synthetic lubricants by LC/ESI-MS, ESI-MS/MS and HR-EI-MS.
- 12:20 – 12:40**      **G. Laue, Syngenta Crop Protection, Basel.**  
Metabolic profiling as a diagnostic tool for mode-of-action identification (MoA) in herbicide research
- 12:40 – 13:00**      **F. Friedli, MSP-Friedli, Koeniz.**  
Important additions to computer assisted spectra evaluation.
- 13:00**                **Closing remarks**



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Session 1: 14:10 – 15:10

## ***Mass Independent Single Molecule Detectors for Mass Spectrometry***

Daniel Gerber<sup>1,3</sup>, Dominique Gritti<sup>1</sup>, Yvan Gonin<sup>1</sup>, Alexandre Netuschil<sup>2</sup>,  
Frédéric Rossel<sup>1</sup>, Dominique Schenker<sup>1</sup>, Jean-Luc Vuilleumier<sup>1</sup>,  
Damian Twerenbold<sup>1,3</sup>

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.

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CH-2000 Neuchâtel, Switzerland

<sup>2</sup> Institut de Microtechnique, Université Neuchâtel, Rue Jaquet-Droz 1,  
CH-2007 Neuchâtel, Switzerland

<sup>3</sup> GenSpec SA, case postale 120, CH-2017 Boudry, Switzerland

Session 1: 15:10 - 15:30

## ***Fundamental Design Principles of a MALDI QIT ToF for High Throughput Sample Analysis***

Martin Resch<sup>+</sup> , Gerd Paulus<sup>+</sup> , Neil Loftus<sup>\*</sup> , Emmanuel Raptakis<sup>\*</sup> ,  
Rachel Martin<sup>\*</sup>

In high throughput sample analysis three criteria are typically applied sample analysis time, sample capacity and confidence in data assignment. The rate limiting factor is often data processing. To significantly enhance confidence and certainty of data a MALDI Quadrupole Ion Trap Time of Flight mass spectrometer has been developed. This instrument is designed to provide unprecedented levels of structural information through MS<sup>n</sup> analysis and sequencing with a high degree of confidence derived from the inherent mass accuracy and resolution of the ToF mass analyser.

The AXIMA-QIT-ToF mass spectrometer (Kratos Analytical, UK) configuration incorporates radically new technology in trapping ions, rather than an analogue rf generator for creating the sinusoidal quadrupole electric field a digital ion trap has been developed. The Digital Ion Trap<sup>TM</sup> technology results in high mass resolution across MS and MS<sup>n</sup> analysis, constant mass accuracy (10 ppm) across MS and MS<sup>n</sup> and works with a wide mass range of ions trapped - to 50 kDa.

This paper will focus on certain key design elements and provide an insight into the results generated by a MALDI QIT ToF instrument.

<sup>+</sup> Shimadzu Schweiz GmbH, Römerstrasse 3, CH-4153 Reinach BL

<sup>\*</sup> Shimadzu Biotech, Wharfside, Trafford Wharf Road, Manchester, M17 1GP. UK.

Session 1: 15:50 – 16:10

***Using the Mass Spectrometer  
for Triggering a Fraction Collector  
Various Aspects of MS Directed Autopurification***

Gerard Bondoux<sup>1</sup>, Jing Lin  
Waters European Headquarter, BP 608  
78056 St Quentin Yvelines, France

It's only a few years ago that the first papers were presented on the use of a mass spectrometer for the automated purification of compounds libraries.

With the increasing use of combinatorial chemistry in the drug development process, researchers were faced with new challenges: verify the synthesis of the large number of molecules generated by combinatorial chemistry, and purify hundreds of samples per week.

Mass spectrometry was naturally the technique of choice for the characterisation of the combinatorial chemistry libraries. The information provided was mainly the verification of the molecular weight. UV or ELSD detection was used to provide the purity information.

When the molecular weight of the molecule is known, using MS as a detector for the purification is very attractive. The expected benefit is the reduction of the number of collection tubes and fractions to handle, since it is possible to collect only peaks with the expected molecular weight. Large pharmaceutical companies (Pfizer, Abbott, Dupont...), combinatorial chemistry libraries suppliers and instrument manufacturers were involved in the developments. First papers were published in 1998, demonstrating automation possibilities.

Today, MS is widely accepted in the purification/isolation work. The main application domain is still in the early drug discovery stage (leads discovery, leads optimization), but new applications are appearing. One of them is the purification of multi-charged molecules (peptides, oligonucleodites). Another one is the isolation of small chromatographic peaks (impurities, metabolites) for further characterization.

In that paper, we will discuss and illustrate the various advantages and aspects of MS directed autopurification. We will present various application examples, and show how to optimise the mass load and throughput by careful selection of the instrument configuration and separation conditions. Software aspects and implementation into the laboratory environment will be also presented.

<sup>1</sup> gerard\_c\_bondoux@waters.com

Session 1: 16:10 – 16:30

***Challenges in Food Trace Analysis by LC-MS/MS:******Sulfonamides in Honey***

L.Verzegnassi

Nestlé Research Centre, Nestec Ltd, Vers-chez-les-Blanc  
P.O. Box 44, 1000 Lausanne 26.

Residues of antibiotics such as sulfonamides can be found in honey due to their prophylactic and often illegal use to combat diseases in bees. These residues are of great concern because of the potential allergenic reactions they may illicit in certain individuals and their potential contribution to the increase of antibiotic resistance via the food chain.

Trace analyses of antimicrobials in complex matrices such as food require detection methods that can achieve part-per-billion (ppb) levels. Liquid chromatography coupled to electrospray ionization tandem mass spectrometry (LC-ESI-MS/MS) is indeed the technique of choice, yielding conclusive evidence on the analyte identity at such low concentrations.

However, simultaneous quantitation of multiple sulfonamides in honey extracts by LC-ESI-MS/MS becomes challenging because of the considerable matrix effect. The impact of the honey matrix on the ionization efficiency varies from one honey to other, making matrix-matched quantitation without an internal standard for each analyte difficult. Thus, the use of a  $^{13}\text{C}_6$  sulfonamide standard in such a selective multiresidue method does not allow to compensate for matrix effects and can only be used to assess the ruggedness of the technique.



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Agilent Technologies (Schweiz) AG presents

Session 2: 16:30 – 17:30

## ***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)

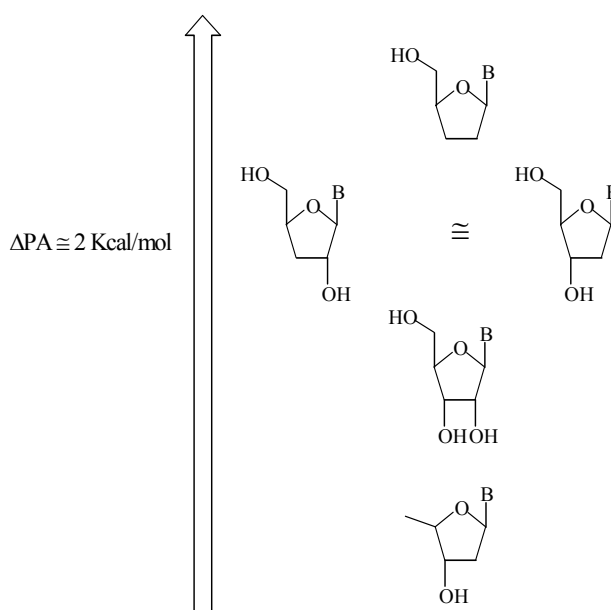
The existence of "zwitterionic" oligonucleotides was first proved in the early sixties from the crystallographic data obtained from an  $A_3$  trimer. This structural motif accounts for the electroneutrality of an oligomer bearing basic and acidic sites. With the advent of desorption ionisation (DI) 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<sup>1, 2</sup>.

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 been determined by Cooks kinetic method.<sup>3</sup> 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 site<sup>4</sup> 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

Session 2: 17:30 – 17:50

## ***Gas-phase Dissociation of Mixed-Sequence RNA/DNA Oligonucleotides***

Stefan Schürch  
Department of Chemistry and Biochemistry  
University of Bern, Freiestrasse 3, CH-3012 Bern

The fragmentation of mixed ribo- and deoxyribo-oligonucleotides upon low-energy collision-induced dissociation in a hybrid quadrupole time-of-flight mass spectrometer was investigated. The preferences for base loss and backbone fragmentation of a number of mixed-sequence pentanucleotides were studied. Product ion spectra revealed a site- and base-specific dissociation behavior, which is strongly influenced by the presence of the ribose 2'-substituent. Mechanistic aspects of base loss and backbone cleavage of oligoribonucleotides and mixed RNA/DNA sequences are discussed. Additional results obtained from CID of dodecanucleotides demonstrate the potential of tandem mass spectrometry for sequence elucidation of unnatural oligonucleotides.

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Session 2: 17:50 – 18:10

## ***The Fourier Transform Mass Spectrometer (FTMS)***

### ***Is this Powerful Analytical Tool Ripe for Chemists and Biochemists in the Pharmaceutical Industry?***

Christian Guenat  
Novartis Pharma AG, Basel  
Research Department

Although Fourier transform mass spectrometry (FTMS) has been introduced about thirty years ago, the chemical industry, and in particular the pharmaceutical industry, recognized its potential only in the past decade after new external ionization sources were adapted to those instruments. FTMS is certainly the most powerful tool in mass spectrometry, and with its unique features FTMS opens up a whole range of new possibilities to the mass spectroscopist dealing with a variety of chemical and biochemical problems. It can solve several analytical problems not amenable to any other mass spectrometer, or it can perform many tasks better, faster or more efficiently than other instruments. The field of applications is very broad across the drug discovery process, including natural/synthetic product structural analysis, combinatorial library development/confirmation, non-covalent interactions, proteomics and genomics, and oligonucleotides.

With this in mind we have completed an evaluation based on potential applications encountered in the drug discovery process. This presentation will show several results obtained during this evaluation and give some insights about the FTMS technology.

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Session 3: 9:00 – 10:00

## ***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.

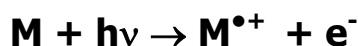
***Atmospheric Pressure Photoionization (APPI):  
Selective or Complementary Ionization Technique  
for LC-MS ?***

Vittorio Raverdino  
Agilent Technologies Schweiz AG  
39, rue de Veyrot  
1217 Meyrin , Switzerland

Although the photoionization technique is applied in some gas-chromatographic detectors (PID) to specifically detect compounds in different matrices, the development of a photoionization source for a mass spectrometer coupled with a liquid chromatograph is relatively new.

GC photoionization detectors are generally used to achieve more selectivity for aromatic compounds and organic compounds containing heteroatoms. They are considered as non-destructive detectors where an ultraviolet light lamp is a means of ionizing the analytes from a GC column. Only a very small fraction of the analyte molecules are actually ionized in this way.

For an APPI source, the ionization of compounds eluting from HPLC needs to be performed in the gas phase, and sufficient energy must be brought from the light source to the molecules (M) to produce radical-ions or promote proton exchange with the surrounding ionized mobile phase (SH) :



and/or



Therefore, in a first step is a heated nebulizer brings the mobile phase plus the substance to the vapor phase. A krypton lamp emits photons at an energy level sufficient to selectively ionize compounds eluting from HPLC in

most cases, whereas the common solvents used for reverse phase separation are not efficiently ionized.

The addition of a dopant to the mobile phase is sometimes useful to promote the proton exchange in order to induce the formation of ions for the mass spectrometer.

Although all possible fields of application of APPI have not yet been completely explored, most of non-polar and medium polarity analytes in the molecular weight range roughly between 70 and 1000 can be analyzed successfully, except those that exhibit too high primary ionization potentials.

Between the most important parameters that can influence ionization efficiency of an APPI source can be mentioned: thermal degradation during the vaporization step, molecular structure, mobile phase composition, temperature, others.

The comparison of APPI with « classical » API-ES and APCI sources for LC-MS applications leads to several considerations:

- (1) possibility of APPI to ionize substances that normally cannot be ionized by the classical sources
- (2) obtain better detection limits for specific compounds
- (3) obtain complementary information from different sources

APPI can be applied in different application areas as for example: « small » molecules for combinatorial libraries, steroids, aromatics, drug discovery, toxicology, molecules of interest in the food and beverages areas and others, vitamins and others.

Session 3: 10:20 – 10:40

***Advantages and Problems of the Analysis of di-Carbonyl-DNPH Derivatives with HPLC-MS<sup>n</sup> using APCI(-) Ionization.***

Stephan Brombacher, Michael Oehme and Basil Boesch  
Organische Analytische Chemie  
Universität Basel, Switzerland

Air sampling combined with transformation to 2,4-dinitrophenylhydrazone derivatives (carbonyl-DNPHs) under acidic conditions and determination with HPLC/UV has become one of the standard methods for carbonyl monitoring. Traditional up to C5 carbonyls are determined in this way. In recent publications long chained carbonyls (up to C12) are measured and mass spectrometers are used as alternative detectors. In our workgroup a Finnigan LCQ ion trap mass spectrometer operated with an atmospheric pressure chemical ionization (APCI) ion source in the negative ion mode is used for the determination of carbonyl-DNPHs.

During real air sample measurements several unknown compounds were detected which are assumed to be dicarbonyls. To gain more information about this molecule class, especially about fragmentation behavior and ionization properties, six dicarbonyl-DNPHs (glyoxal, methylglyoxal, 2,3-butandione, 2,3-pentandione, 2,4-pentandione and 1,5-pentandial) were synthesized and investigated with LC/MSn.

In the first part of the presentation the fragmentation behavior of some dicarbonyl-DNPHs in the ion trap is shown. The MS2-spectra of 2,4-butandione and 1,5-pentandial are compared and several of the fragments and fragmentation pathways are explained.

In the second part the influence of the ion source geometry on the ionization behavior of dicarbonyl-DNPHs is shown for glyoxal-DNPH and methylglyoxal - DNPH. The examples demonstrate that the linearity of the detector as well as the limits of detection (LOD) are strongly linked to the position of the corona needle in the APCI ion source. In contrary to the dicarbonyl-DNPHs the

carbonyl-DNPHs like formaldehyde-DNPH are only affected in their LODs but not in their linear behavior in the MS-detector.



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Session 4: 11:00 – 12:00

## ***The Swiss Light Source***

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

The design of the Swiss Light Source has to fulfill a variety of requirements. It need to provide hard X-Rays for the large community of materials sciences and crystallography researches, while also serving the broad community of surface scientists with soft x-rays and ultraviolet photons.

After a construction period of only three years, the first beamlines are in the commisioning phase and pilot experiments have been performed. The outstanding parameters of the facility and new developments on the accelerator, the beamlines and the related experimental infrastructure will be presented.

A short description on the present research possibilities will be given. The last part of the presentation will be focussed on future research areas.

Session 4: 12:00 – 12:20

***Characterization of Ageing Products  
of Ester Based Synthetic Lubricants  
by LC/ESI-MS, ESI-MS/MS and HR-EI-MS***

Martin Kohler and Norbert V. Heeb

Swiss Federal Laboratories for Materials Testing and Research  
Überlandstrasse 129, CH-8600 Dübendorf, Switzerland

Ester based synthetic lubricants such as phthalates, adipates, sebacates, neopentylpolyol esters and pentaerythritol tetraesters are widely used due to their excellent tribological properties. The key to improve the long-term stability of these products is to understand the chemical and physical processes induced by tribological stress (friction, wear, heat, water, and oxygen).

Ageing products of a commercial jet engine oil based on pentaerythritol tetraesters which were formed upon operation in an aviation turbine were detected by electrospray ionization mass spectrometry (ESI-MS) and characterized by LC/ESI-MS [1]. The fatty acid composition of these ageing products was investigated by ESI-MS/MS analysis. The ammonium adducts of the newly formed pentaerythritol tetraester degradation products were found to be suitable MS/MS parent ions to investigate the fatty acid composition of such esters. The tetraesters formed during tribological stress upon jet engine operation were found to have a different fatty acid composition, containing in parts, longer fatty acid chains. These findings were consistent with increased chromatographic retention times of these newly formed compounds on a reversed phase column. Exact mass measurements using high resolution direct-inlet electron impact ionization mass spectrometry (HR-EI-MS) gave additional insight on the processes involved in ageing of pentaerythritol tetraesters upon tribological stress.

ESI-MS, LC/ESI-MS, ESI-MS/MS and HR-EI-MS proved to be versatile tools to study the chemical composition (distribution of homologues) as well as the mechanism of ageing of ester based lubricants on a molecular level. Due to its high sensitivity, ESI-MS can also be used to characterize and identify trace levels of ester-based lubricants in other matrices such as mineral oils.

[1] M. Kohler, N. V. Heeb, J. Chromatogr. A, 2001, 926, 161-165

Session 4: 12:20 – 12:40

## ***Metabolic Profiling as a Diagnostic Tool for Mode-of-Action (MoA) Identification in Herbicide Research***

G. Laue, J. Blanz, T. Brodmeier, E. Gassmann, and K. Kreuz  
Syngenta Crop Protection AG, P.O. Box, CH-4002 Basel

Among the 'omics' technologies "metabonomics" or "metabolic profiling" has received relatively little attention so far. Whereas genomics and proteomics are in the center of the scientific interest the screening of endogenous metabolites just began to emerge.

Besides NMR, FTMS, and LC/MS approaches, GC/MS appears to be the most promising technology. It allows a relatively convenient and sensitive compound identification at the expense of a time-consuming sample preparation and derivatization.

Herbicides are widely used for controlling weeds in crops. They can be classified according to their mode of action (MoA) or target site. About 20 different MoAs are currently known to be covered by commercial herbicides. For some herbicides the exact MoA still remains unknown, for others more than one MoA is discussed. For a variety of reasons extensive efforts are currently made to discover novel MoAs.

We present the exploitation of Metabolic Profiling to MoA research. The application of herbicides causes specific changes in the metabolic profiles. Using GC/MS, these changes are extracted based on the quantitative analysis of a large number of biochemical pathway intermediates and products yielding typical patterns. The comparisons of untreated and treated plants allow the classification of known MoA and, at least as important, may give clues to tackle novel MoAs.

Session 4: 12:40 – 13:00

## ***Important Additions to Computer Assisted Spectra Evaluation***

F. Friedli and P.Kofel  
MSP  
CH-3098 Köniz

One year ago we reported on the same occasion an overview of the spectra evaluation package MassLib. The point was the large diversity of requirements brought into play by users with very different needs shaping this longlife product to become more and more comprehensive whilst remaining most advanced technologically and algorithmically. Quite frequently the real performance originally intended, -structure elucidation in the case of MassLib-, turned out not to be the decisive point for regular use. Therefore a number of new possibilities were added to MassLib during the last year. Not all of them are easily recognized to be important but as a matter of fact they are:

To run MassLib on a Windows/CITRIX based server for the intranet is now a proven solution. Special care was taken to prevent the easy duplication of the precious user libraries by program internal access control hindering list output of spectra of sensitive libraries and a modification of the standard file open box disabling the direct access to and hence the possibility for duplication of the library files themselves.

MassLib now treats GC/MS runs with retention indices automatically. This provides true identification based on the two independent variables: spectrum and chromatographic retention.

MassLib now stores postscript graphics as intermediate output to the disk and starts a batch process e.g. the conversion into the .pdf format and automatic mail to the chemist or simply a clear print.

Masslib now offers the automatic comparison of an analysis file against a reference file. The last year version was just able to compare individual spectra of two analyses.

MassLib now offers a quick visual structure check showing possible substructures interactively for any masspeak in mass spectra having a (hypothetical) structure assigned to.

## **TRAVEL INFORMATION:**

### **Public Transport:**

All trains will arrive at Neuchâtel between 12:51 and 13: 07. Take the north exit of the station (underway) and the bus No. 7 (departure every 10 min. ) until La Coudre. There, the cogwheel train will lead you up the hill directly to the Hotel Chaumont.

For informations: [raphael.tabacchi@unine.ch](mailto:raphael.tabacchi@unine.ch)

### **By Car: From Lausanne, Bern, Zürich or Basel:**

Take highway **EXIT Neuchâtel-Maladière**. Follow the road until you reach a turn-a-round (two from Lausanne!). Go straight, then on next intersection (traffic lights) turn right (in front of building "L'Express"), continue straight following the sign "H" (Hospital) Les Cadolles .... and up to Chaumont.

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## **SPONSORSHIPS:**

- SGMS is again very much pleased to thank **Agilent Technologies (Schweiz) AG** for their generous sponsorship:

This year we are proud to present **Prof. Giovanni Sindona, Università della Calabria, Arcavacata di Rende, Italy** in the name of **Agilent Technologies (Schweiz) AG**.

- And in addition: **Brechbühler AG** has again volunteered to sponsor this year our SGMS-meeting as well.

They **will invite us to the Aperitif**, which will take place as usual just after the General Assembly.

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## **MISSING PAYMENTS:**

Those members who failed to pay so far their annual membership fee will be reminded with a short notice from our treasurer HP. Moser.

Thanks to our sponsors

## Who's coming

Aebi Beat	IRM Bern
Aerni Hans-Rudolf	EAWAG, Dübendorf
Albrecht Daniel	Shimadzu
Amrein Walter	ETH Zürich
Aydin Nebahat	Université Genève
Bigler Laurent	OCI, Zürich
Blaser Armin	Sissach
Bondoux Gerard	Waters France
Brombacher Stephan	Universität Basel
Chesnoy Sergiy	Universität Zürich
Daher Sawsan	Université Genève
Dietemann Patrick	ETH Zürich
Doll Martin	Bruker Daltronix
Dollt Heribert	F. Hoffmann-La Roche, Basel
Erny Johannes	Applied Biosystems, Rotkreuz
Fay Laurent B.	Nestlé Research Center, Vers-Chez-les-Blancs
Filot Marc	Universität Bern
Fink Yvan	Université Genève
Fischlewitz Peter	F. Hoffmann-La Roche, Basel
Friedli Felix	MSP-Friedli, Koeniz
Gassmann Ernst	Syngenta, Basel
Gäumann Tino	EPFL Ecublens
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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

## ***General Assembly of the SGMS 2001***

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

### **Agenda**

1. Nomination of the scruteners.
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.Tabacchi.
11. Individual proposals:
  - RIGI Meeting 2002: where should we meet?
  - Organisation of International Mass Spectrometry Conference IMSC by SGMS in Switzerland ?
12. Miscellaneous:
  - no subject at printing date.

for the committee

Andreas A. Staempfli

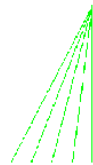
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