Swiss Group for Mass Spectrometry
Schweizerische Gruppe für Massenspektrometrie
Groupe suisse de spectrométrie de masse
Gruppo svizzero di spettrometria di massa

2015 SGMS Meeting

[Plenary Lectures | Registration | Abstract Submission | Short Communications | Posters]

The 33rd meeting of the SGMS will be held at the Dorint Resort Blüemlisalp Beatenberg, October 29-30, 2015 high above Lake Thun in the Bernese Oberland, with a scenic view of the Swiss Alps!

Registration and Abstract Submission NOW AVAILABLE

DEADLINE abstract submission is now September 15th 2015 !

Preliminary Program

Thursday 29-10-2015

Session 1
Chair: Bertran Gerrits, Novartis Institute for Biomedical Research, Basel

11:25 - 11:30 **Welcome**

11:30 - 12:15 **Plenary 1**

12:30 - 14:00 **Lunch**

Session 2
Chair:

14:00 - 14:45 **Plenary 2**

14:45 - 15:45 Short Communications 1
15:45 - 16:15 **Coffee Break**
Session 3
Chair:
16:15 - 16:55 Short Communications 2
17:00 - 18:00

18:00 - 20:00 **Poster Session**
19:00 - 20:00 **Apéro**
20:00 **Blüemlisalp Dinner Buffet**

Friday 30-10-2014

Session 4
Chair:
08:30 - 09:15 Plenary 3
09:15 - 10:45 Short Communications 3
10:15 - 10:45 **Coffee Break**
Session 5
Chair:
10:45 - 11:30 Plenary 4
11:30 - 12:30 Short Communications 4
12:30 **Closing Remarks**

Registration

The registration form is available in WORD or PDF
Please send your registration to registration(at)sgms(dot)ch not later than **October 1st, 2015**. There is absolutely no need to register personally at the Dorint Hotel Blüemlisalp, Beatenberg! The SGMS committee will manage all hotel reservations and payments. We will strictly follow a first come first serve policy for the hotel room assignment.

See the registration form for prices.
There will be an additional fee of CHF 25.- for late registration (after August 31st, 2015).

All PhD students attending the annual SGMS meeting pay a reduced fee of CHF 100.-, but will have to share rooms.

Submission of Abstracts

Next to the plenary lectures there will be time for several **oral presentations** from various participants as well as **poster presentations**. The time allotted will be 20 minutes. The deadline for abstract submission for both talks and posters is **September 1st 2015**. Please submit your abstract including author's name and

address directly to the president of the SGMS, Bertran Gerrits (abstract(at)sgms(dot)ch). The abstract should not exceed 2500 characters.

Guidelines for the submission of abstracts:

- Include the name of the contact person (spell out first name) as well as the complete address and e-mail.
- Do not use any logos (company, institute, ...) on the abstracts.
- We can read most of the common word processing formats.
- If you include figures, copy/paste them as figures, not as a link.
- Do not use halftoning or colour: We publish in pure b/w.
- Include your e-mail address.

Plenary Lectures

Rosina, one year at comet Churymov -Gerasimenko

Kathrin Altwegg

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and the ROSINA team

In situ mass spectrometry in space has its own challenges. Not only has the mass spectrometer to be lightweight and energy efficient, but it also has to withstand a broad temperature range, high vibration levels during launch and a wide variety of pressures. Autonomous operation over long times, immunity to cosmic rays and high compression of data are other prerequisites for successful instruments on board spacecraft. The probably most advanced instrument currently flying aboard a spacecraft is the ROSINA (Rosetta Sensor for Ion and Neutral Analysis) instrument on board the ESA Rosetta spacecraft encountering comet 67P/Churyumov-Gerasimenko. Rosetta is following the comet from almost 4 AU through its perihelion at 1.3 AU and out again for more than 1 ½ years. The closest distances of just a few kilometers to the comet has been reached during the delivery of the lander Philae in November. The cometary atmosphere consists mostly of water and CO/CO2. However, it is known that comets have quite a diversified organic part in their coma, both as volatiles and as dust. Furthermore, isotopic ratios in water and other molecules can give very strong indications on the formation process of cometary, and therefore solar system material.

In this talk I will give a short overview on the ROSINA instruments and some of the discoveries made so far in the cometary coma, which give us valuable information on the origin and evolution of our solar system.

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The great paradox of the 21st century:

We are unable to identify 70-90% of small molecules in biological samples and rivers on Earth, while humans have endeavored to analyze the soil on Mars, the atmosphere on Jupiter and the sea on Titan.

Robert Mistrik

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Mass spectrometers coupled with high- or ultra-performance chromatographic techniques allow the detection of thousands of small molecules in a complex sample; however their efficient and reliable identification is still a major bottleneck that is hindering progress in various scientific fields. The majority of the unidentified compounds are not entirely unknown to the chemical world, however their true identity remains elusive since their reference spectra are not available. There is also a growing concern that even those compounds reported as positively identified are in fact incorrect annotations confused either with structural isomers displaying similar fragmentation patterns or even with structurally unrelated isobaric compounds sharing common elemental composition. Some emerging “de novo” identification computer programs are likely to contribute to the inaccuracies, since they often apply proteomic-like fragmentation principles or use purely combinatorial bond-breaking logic, although small molecules definitively do not fragment in a uniform manner and often undergo non-trivial electron displacements or complex rearrangements.

Even though many reported “automated” structure annotation methods did not hold the promise they might have hoped for, there are functional ways that can assists in identification of vast number of unknowns, which will be presented. Those methods are based on heuristic and quantum chemical methods rather than relying on combinatorial methods or molecular formula calculations. In addition, a whole array of methodological challenges the mass spectrometrists are facing when aiming to overcome the identification bottleneck will be discussed.

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Myxobacterial secondary metabolomics: Towards a comprehensive survey of a promising natural products resource

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Natural products with their unique structural diversity are of exceptional importance for drug discovery. Among natural product-based drugs approved by the FDA, those originating from microbial sources make up 30% [1]. Myxobacteria represent an important source of novel natural products exhibiting a wide range of biological activities, and a number of secondary metabolites from myxobacteria are currently investigated as potential leads for novel drugs [2]. Together with activity-guided screening and genome mining, metabolomics-based approaches using modern mass spectrometry techniques can help to bridge the gap between genome-encoded potential and the usually contradictory low numbers of secondary metabolites known from a specific producer [3]. While it would be desirable to obtain a fully unbiased picture of the secondary metabolome using a single instrumental setup, this is usually prohibited by the high structural complexity of secondary metabolites. In this contribution, an effort is made to create a comprehensive overview of myxobacterial secondary metabolomes using mass spectrometric data from ~2500 complex myxobacterial extracts, representing a diversity-oriented subset of our strain repository. The crucial prerequisites enabling our study are: i) access to an extensive myxobacteria collection sampled at locations worldwide, including isolates from rare and under-exploited habitats, ii) a sensitive analytical platform using high-resolution TOF-MS (and recently also FT-ICR MS) for both targeted and untargeted secondary metabolome analysis, and iii) a database-assisted bioinformatics platform allowing us to conduct data evaluation across large numbers of secondary metabolomes and at the same time to dig deep into individual secondary metabolite profiles. I will present results of a statistical survey covering our entire reference extracts collection and taking into account most known myxobacterial secondary metabolites. Furthermore, we exemplify how metabolomics-and statistics-based approaches can contribute to reveal novel metabolite candidates and demonstrate how these methods underpin our efforts to isolate seizable quantities of newly discovered natural products, through the identification of alternative sources featuring improved production of target compounds.

1. E. Patridge, P. Gareiss, M. S. Kinch, and D. Hoyer, An analysis of FDA-approved drugs: natural products and their derivatives, Drug Discov. Today, pp. 8–11, 2015.
2. R. Müller, J. Wink, Future potential for anti-infectives from bacteria – How to exploit biodiversity and genomic potential Int. J. Med. Microbiol., pp. 3-13, 2014.
3. D. Krug and R. Müller, Secondary metabolomics: the impact of mass spectrometry-based approaches on the discovery and characterization of microbial natural products, Nat. Prod. Rep., pp. 768–83, 2014.

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Challenge and success of mass spectrometry based quantitative proteomics on clinical body fluid cohorts

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In the last couple of years we have applied mass spectrometry based proteomics to clinically oriented research projects with access to patient cohorts trying to get insight into how well the body responds to a treatment for a disease or to monitor a medical condition progress. The different clinical divisions have carefully collected patient samples over years with the goal to find biological molecules that are a sign of normal or abnormal processes in a disease or suggesting new ways of diagnosis. We have analyzed these body fluid samples of patients and identified unique signatures of proteins responsible for the diagnosis, prognosis and therapeutic prediction of a disease such as neurodegenerative disorders, atopic eczema and rheumatoid arthritis.

Proteomics analysis of patient cohort samples requires high technical reproducibility, stable and accurate quantitation in a high throughput manner. We have successfully applied single shot label free analysis on latest generation high resolution mass spectrometry instrumentation in order to extract quantitative information. Simultaneously to the detection of protein abundance changes we were also identifying and quantifying “silent” posttranslational modifications, such as isoAsp as well as IgG glycosylation by employing multiple dissociation techniques.

The largest mass spectrometric data set we have acquired on plasma samples from different Alzheimer’s cohorts and we have found regulated proteins viable for diagnosis as well as protein based classification models for disease prediction and progression.

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High Resolution Mass Spectrometry for in Depth Understanding of Complex OMICS Challenges and Comprehensive Characterization of Large Molecular Weight Assemblies

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Quadrupole Time-Of-Flight mass spectrometry (QTOF) has evolved into a versatile high performance technology during recent years. Today, they can achieve mass accuracies of < 1 ppm and resolving powers up to 80,000; opening a wealth of analytical options. QTOF technology accommodates large ion populations per scan thus providing a unique statistical base for the measurement of isotope patterns and an unusually high intra-spectra dynamic range of up to > 5 orders of magnitude.

These instrument characteristics allow reliable molecular formula determination based on accurate mass and isotopic pattern matching for small molecules. Thus enabling the identification of statistically relevant molecular features in complex mixtures.

QTOFs are further applied in large scale OMICS applications, particularly in metabolomics and proteomics as they can provide scan speeds of up to ~100 spectra/sec. High mass accuracy and resolution independent of scan speed and peak abundance with accurate isotope representation translates into sensitive and accurate quantification capabilities.

For large molecules such as antibody subunits in the 25 kDa range, correct isotope pattern representations allow validation of subunit composition and even sensitive detection and quantification of subtle modifications such as protein deamidation, which can only be detected by quantifying a slight distortion of the isotopic pattern. Such assessments may permit the determination of critical quality attributes of biopharmaceuticals.

A wide variation of technology extensions such as ETD fragmentation, ion mobility separation, scan modes such as SWATH, MSE or HR-XICs further broaden the application range of QTOFs, e.g., to further structure elucidation, targeted screening and quantification applications.

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Short Communications

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Posters

(Size: 146 cm high x 118 cm wide)