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Mass Spectrometry:
Applications to the Clinical Lab

MSACL 2017 EU

4th Annual EU Congress & Exhibits

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Changing the Paradigm of Molecular Diagnosis

Isabelle Fournier
University Lille 1

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The Association for
Mass Spectrometry:
Applications to the Clinical Lab

MSACL 2017 EU

The 4th Annual European Congress
of
The Association for

Mass Spectrometry:
Applications to the Clinical Lab

Salzburg, AUSTRIA

September 10 - 14, 2017

Salzburg Congress Center

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Please take a moment to acknowledge the members of the Scientific Committee who are pivotal in development of the Scientific Program.

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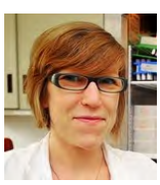
:: TDM / Small Molecules



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:: TDM / Small Molecules

Elizabeth Want, PhD
Imperial College London
:: Metabolomics

Michael Wright
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Stefan Zimmerman, MD
University Hospital Heidelberg, Germany
:: Microbiology

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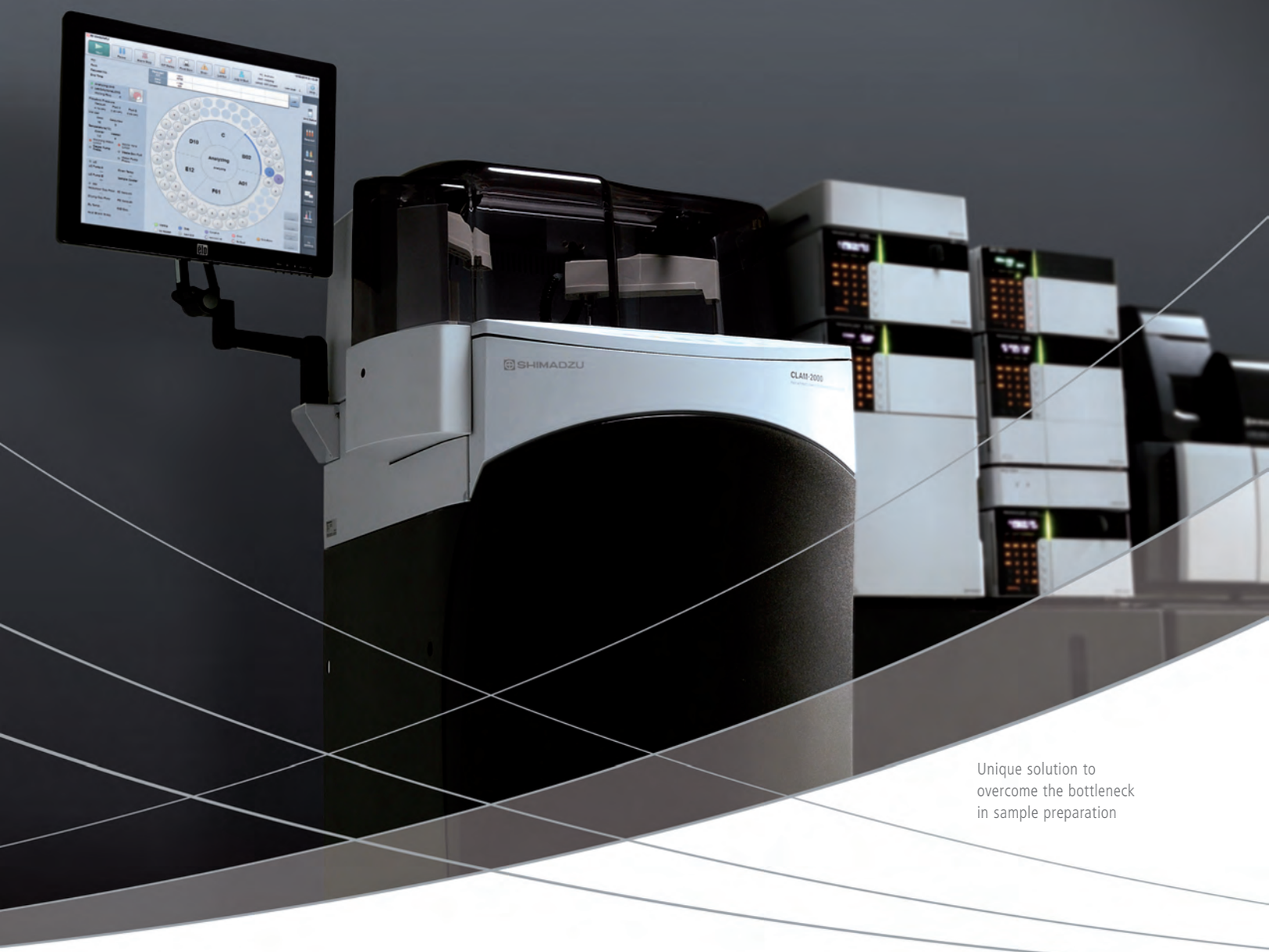

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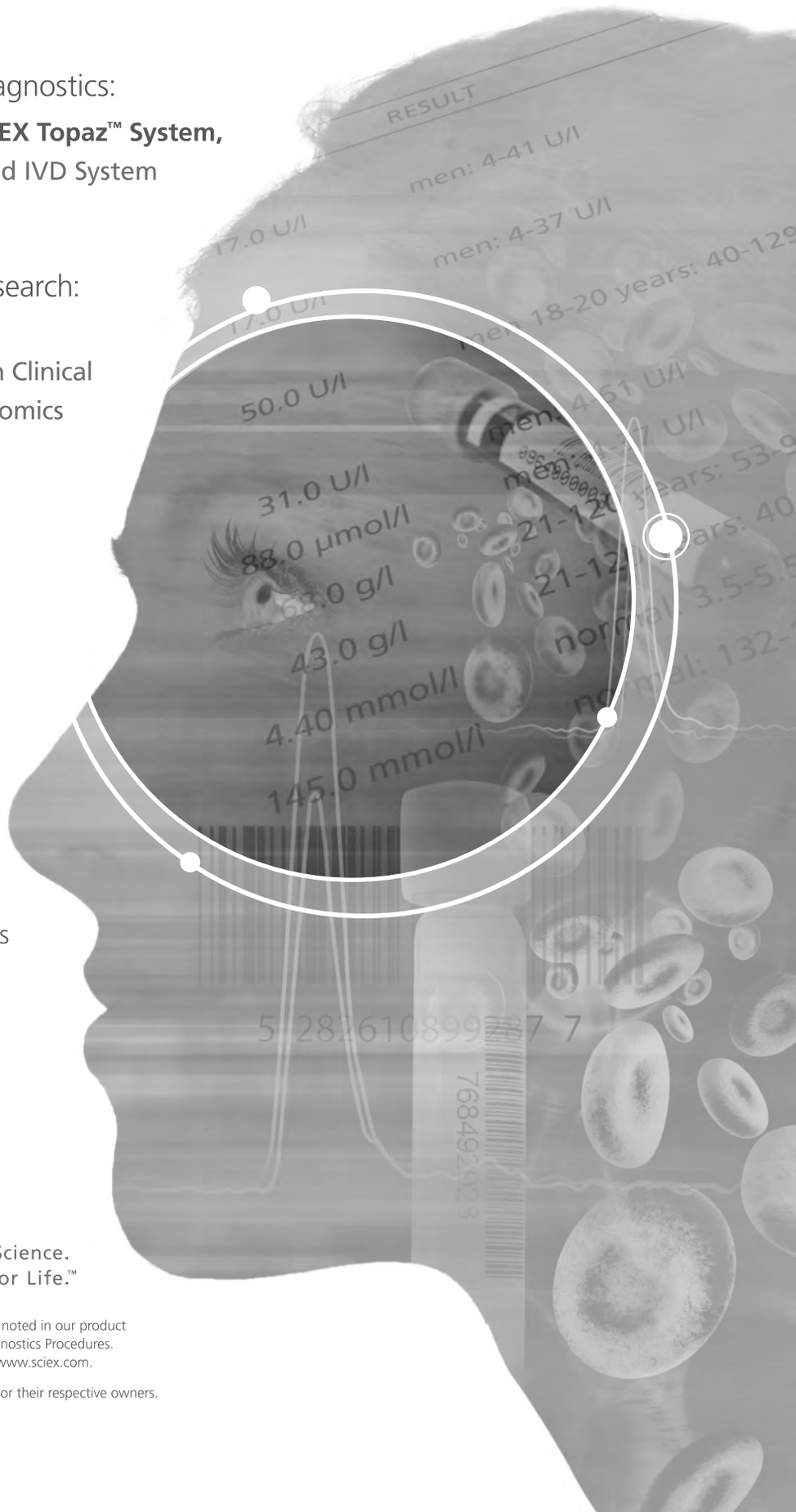
Wednesday (14:00 - 14:30)

For people interested in clinical research:

Workshop SWATH®Acquisition-MS
for Quantitation and Identification in Clinical Proteomics, Lipidomics, and Metabolomics
Wednesday (08:15 - 08:45)

Workshop New advances and technologies in Mass Spectrometry for Clinical Research
Thursday (08:15 - 08:45)



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Smoking is **prohibited** within the conference facility. If smoking outside the congress center please refrain smoke within 15m of any doorway.

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Your badge constitutes your admission pass to the Congress Center. Please display your badge prominently while attending the congress and all associated functions. If you have not registered you will be escorted to the registration desk to get one, or off the premises. If you determined to be sharing badges, your badge will be confiscated and you will be escorted off the premises.

Parking
Sheraton Garage - entrance via Auerspergstraße with direct access to Salzburg Congress.
Mirabell-Kongress-Garage - entrance via Mirabellplatz, 2-3 minutes walk to Salzburg Congress.

Breakfast
It is recommended that you take breakfast before arriving at the Congress Center, although each morning we will have a welcome coffee with a limited selection of light baked goods.

Dinner Receptions
Evening Exhibit Hall Receptions provide a buffet style meal and drinks while allowing you the time to commune with exhibitors and fellow colleagues.

Tape Recording/Video Recording Policy
Please observe the MSACL policy which prohibits operation of tape recorders, video recorders, cameras, or camera phones, except for official association equipment, at all congress sessions, committee meetings, in the Exhibit Hall, and during the plenary sessions. If you want to see a copy of a poster, check to see if it is already uploaded online.

Note: Throughout Conferences MSACL may be videotaping and taking photographs to be used for promotional or educational purposes by MSACL. If you do not wish to appear on camera, please notify the videographer or photographer and your request will be honored.

Presenter Info and Guidelines

Podium Presentations

Locations: *Mozart Hall, Papageno, Paracelsus, Trakl, Doppler*

- If an individual is unable to present or does not show, the presentation time slot will be left open. ***IT WILL NOT BE FILLED BY THE NEXT SPEAKER***. The next speaker will begin presenting at his/her scheduled time.
    - **Back-Up Presenters**: If a presenter does not show a back-up presenter may be called to fill in the open spot. *Session Chairs, please contact registration immediately on determining that a speaker may not show so that efforts may be put in place to locate a back-up speaker*
- Speakers: Please make an effort to repeat any questions from the audience before answering.
- Podium presentations are ***20 minutes*** including Q&A.
- PC Laptops running Windows 7 Enterprise & Office 2010 will be provided.
- Presenters should check-in 15-20 minutes prior to their Session (NOT their talk) with either the Session Chair or AV Support on-hand to upload their presentation files to the primary presentation lap-top computer.
- Presenters should bring their presentations on thumb (USB) drives for placement on a single presentation computer from which all presenters will access their PowerPoint presentations.
- Laser pointers will be provided.

Poster Presentations

Location: *1st Floor/ Exhibit Hall*

Posters will be placed for the entire conference starting on Tuesday at 17:30. Posters will be up for the duration of the congress. Please see poster abstract information for attendance details.

- Poster dimensions should be A0 (841 x 1189 mm) in PORTRAIT format.
- Poster Boards are plastic.
- Adhesive velcro to place your poster WILL BE provided.

Schedule Overview: Sunday

Time	Event
11:00 19:00	**BADGE PICKUP** *Location:* Registration Foyer
11:00 14:00	**LUNCH ON OWN** *Location:* Salzburg Old City Enjoy Lunch in the Old Town of Salzburg.
14:00 18:00	**SHORT COURSES** *Location:* Various Coffee Breaks every 0:50 for 10 minutes.
Every 0:50 for 10 min	**COFFEE BREAKS** *Location:* Registration Foyer Take a quick coffee break.
18:00 18:30	**WINE & CHEESE RECEPTION** *Location:* Registration Foyer
18:00 Your Decision	**DINNER ON OWN** *Location:* Salzburg Old City Enjoy Dinner in the Old Town of Salzburg.
18:30 20:00	**PRIVATE: SHORT COURSE INSTRUCTOR DINNER & DISCUSSION** *Location:* Salon Mozart. In hallway from Congress Center to Sheraton.

Schedule Overview: Monday

Time	Event
8:00 9:00	**WELCOME COFFEE** *Location:* Registration Foyer Enjoy coffee, a pastry and a chat with colleagues before the day starts.
9:00 13:00	**SHORT COURSES** *Location:* Mozart, Papageno, Paracelsus, Trakl, Doppler Coffee Breaks every 0:50 for 10 minutes. Lunch from 13:00-14:00 in Registration Foyer.
Every 0:50 for 10 min	**COFFEE BREAKS** *Location:* Registration Foyer
13:00 14:00	**LUNCH** *Location:* Registration Foyer Sandwiches provided in Registration Foyer.
14:00 18:00	**SHORT COURSES** *Location:* Mozart, Papageno, Paracelsus, Trakl, Doppler Coffee Breaks every 0:50 for 10 minutes.
18:00 18:30	**WINE & CHEESE RECEPTION** *Location:* Registration Foyer
18:00 Your Decision	**DINNER ON OWN** *Location:* Salzburg Old City Take Dinner in the Old Town of Salzburg.

Schedule Overview: Tuesday

Time	Event
8:00 16:00	**PLACE POSTERS** *Location:* Exhibit Hall on 1st Floor ALL posters should be placed by 16:00.
8:00 9:00	**WELCOME COFFEE** *Location:* Registration Foyer Enjoy coffee, a pastry and a chat with colleagues before the day starts.
9:00 12:30	**SHORT COURSES** *Location:* Mozart, Papageno, Paracelsus, Trakl, Doppler, Trapp
Every 0:50 for 10 min	**COFFEE BREAKS** *Location:* Registration Foyer
12:30 14:00	**OPENING LUNCH IN RECOGNITION OF TRAVEL GRANTEES** *Location:* Europa Hall
13:30 13:45	**WELCOME, INTRODUCTION & ORIENTATION** *Location:* Europa Hall
13:45 14:00	**CMS JOURNAL UPDATE** *Location:* Europa Hall
14:00 14:45	**PLENARY LECTURE SERIES : OPENING : Prof. Dr. R.P.H. (Rainer) Bischoff** *Location:* Europa Hall
14:45 15:00	**COFFEE BREAK** *Location:* Registration Foyer
15:00 16:00	**SCIENTIFIC SESSION 1** *Location:* Mozart 1-3, 4-5, Papageno, Paracelsus
16:00 16:15	**COFFEE BREAK** *Location:* Europa Foyer
16:15 16:45	**POSTER LIGHTNING TALKS** *Location:* Europa Poster presenters present their posters from the podium within 90 seconds and 1-3 slides.
16:45 17:30	**EXHIBITOR LIGHTNING TALKS** *Location:* Europa Exhibitors present their from the podium within 90 seconds and 1-3 slides.
17:30	**EXHIBITS OPEN** *Location:* Exhibit Hall on 1st Floor
17:30 20:00	**EXHIBITOR RECEPTION** *Location:* Exhibit Hall on 1st Floor with a buffet dinner served in the Exhibit Hall.
18:00 19:00	**MEET-THE-EXPERTS: Booth Tours** *Location:* Exhibit Hall on 1st Floor Join an booth tour and learn more about what experienced practioners are looking for during the exchange, and how they interact with the booth vendors
19:00 20:00	**TROUBLESHOOTING POSTER ROUNDS Part I** *Location:* Exhibit Hall on 1st Floor
20:00 21:00	**DISCUSSION GROUP: The Future of MS in the Clinic** *Location:* Various ... with a touch of wine and cheese, and other beverages.
21:00 Your Decision	**ENJOY THE CITY** *Location:* Salzburg Old City Explore the Old Town of Salzburg.

Schedule Overview: Wednesday

Time	Event
8:00 8:30	**WELCOME COFFEE** *Location:* Registration Foyer
8:15 8:45	**CORPORATE WORKSHOPS** *Location:* Mozart 4-5, Papageno, Paracelsus, Trakl
8:30 9:00	**COFFEE BREAK** *Location:* Europa Foyer
9:00 9:45	**PLENARY LECTURE SERIES: Prof. Ian Wilson, PhD** *Location:* Europa Hall
9:45 10:45	**POSTERS ATTENDED** *Location:* Exhibit Hall on 1st Floor Selected posters to be attended for 1 hour. Refer to program for posters attended during this period.
10:45 11:45	**SCIENTIFIC SESSION 2** *Location:* Mozart 1-3, 4-5, Papageno, Paracelsus
11:45 12:00	**COFFEE BREAK** *Location:* Europa Hall Foyer
12:00 12:45	**DISTINGUISHED CONTRIBUTION AWARD: PLENARY LECTURE SERIES** **Prof. Isabelle Fournier, PhD** *Location:* Europa Hall
12:45 14:00	**LUNCH** *Location:* Exhibit Hall on 1st Floor
14:00 14:30	**CORPORATE WORKSHOPS** *Location:* Mozart 4-5, Papageno, Paracelsus
14:30 14:45	**COFFEE BREAK** *Location:* Registration Foyer and Exhibit Hall
14:45 15:45	**SCIENTIFIC SESSION 3** *Location:* Mozart 1-3, 4-5, Papageno and Paracelsus
15:45 16:00	**COFFEE BREAK** *Location:* Registration Foyer and Exhibit Hall
16:00 16:30	**CORPORATE WORKSHOPS** *Location:* Mozart 4-5, Papageno
16:30 16:45	**COFFEE BREAK** *Location:* Registration Foyer and Exhibit Hall
16:45 17:45	**SCIENTIFIC SESSION 4** *Location:* Mozart 1-3, 4-5, Papageno, Paracelsus
17:45 19:30	**RECEPTION** *Location:* Exhibit Hall on 1st Floor
18:30 19:30	**POSTERS ATTENDED** *Location:* Exhibit Hall on 1st Floor Selected posters to be attended for 1 hour. Refer to program for posters attended during this period.
18:30 19:30	**MEET-THE-EXPERTS: Poster Tours** *Location:* Exhibit Hall on 1st Floor Join a poster tour and participate in a dynamic discussion.
19:30 20:30	**DISCUSSION GROUPS** *Location:* Various
20:30 Your Decision	**ENJOY THE CITY** *Location:* Salzburg Old City

Schedule Overview: Thursday

Time	Event
8:00 9:00	**WELCOME COFFEE** *Location:* Registration Foyer Enjoy coffee and a pastry before joining a corporate workshop.
8:15 8:45	**CORPORATE WORKSHOPS** *Location:* Papageno
9:00 10:00	**SCIENTIFIC SESSION 5** *Location:* Mozart 1-3, 4-5, Papageno, Paracelsus
9:00 10:00	**EXHIBITOR FEEDBACK SESSION** *Location:* 1st Floor - Lower Cafe
10:00 11:00	**POSTERS ATTENDED** *Location:* Exhibit Hall on 1st Floor
10:00 11:00	**COFFEE BREAK** *Location:* Exhibit Hall
11:00 12:00	**SCIENTIFIC SESSION 6** *Location:* Mozart 1-3, 4-5, Papageno, Paracelsus
12:00 14:00	**LUNCH RECEPTION** *Location:* Exhibit Hall on 1st Floor with foosball tournament.
12:30 13:30	**MEET-THE-EXPERTS: OFFICE HOURS FORUM** *Location:* Cafe: Lower Level Have a question from the congress that you have been itching to ask? Or a problem from work that you want to get feedback on? Or feedback on the congress? Sign up at the registration desk for 10-min blocks to share time and ideas with domain experts in a relaxed setting.
13:00 14:00	**TROUBLESHOOTING POSTER ROUNDS Part II** *Location:* Exhibit Hall on 1st Floor Review the Troubleshooting Posters with an expert docent as they explore and investigate troubleshooting issues in clinical mass spectrometry.
14:00	**EXHIBITS CLOSED** *Location:* Exhibit Hall on 1st Floor
14:00 14:15	**POSTER AWARD PRESENTATION** *Location:* Mozart
14:15 15:00	**PLENARY LECTURE SERIES : Christa Cobbaert** *Location:* Mozart
15:00 16:30	**CLOSING RECEPTION with Winning Posters on Display** *Location:* Registration Foyer Wine & Cheese, Beer & Nuts. Kaiserschmarrn
16:30	**CONGRESS CLOSED** *Location:* Congress Center

clinical mass spectrometry

cms

an international journal

Subject areas include:

- Imaging
- Toxicology
- Metrology
- Microbiology
- Endocrinology
- Neonatal screening
- Protein quantification
- On-site technologies
- Therapeutic drug monitoring
- Cross technology investigations
- New technologies including automation
- Mass spectrometry based clinical studies
- Regulatory aspects in diagnostics
- Clinical metabolomics and analyses
- Error & risk assessment and patient safety
- Validation, standardization and QC
- Data analysis and informatics

Types of papers:

- reviews
- tutorials
- full papers
- invited editorials
- guidelines and best practice documents
- letters, case studies, protocols, application notes

MSACL

Clinical Mass Spectrometry

m/z

Official Journal of MSACL

https://www.journals.elsevier.com/clinical-mass-spectrometry

Plenary Speaker Series

Day	Time	Speaker(s)
Tuesday	14:00	Rainer Bischoff
Wednesday	9:00	Ian Wilson
Wednesday	***12:00***	***Isabelle Fournier***
Thursday	14:15	Christa Cobbaert

Tuesday @ 14:00 in Europa Hall

Quantification of Proteins in Complex Biological Samples by LC-MS

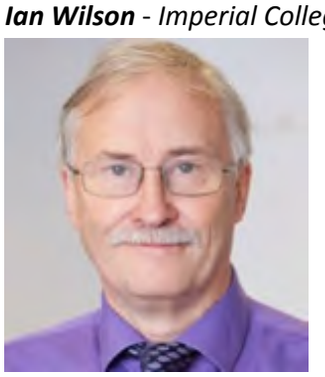
Rainer Bischoff - *University of Groningen* (r.p.h.bischoff@rug.nl)

‣ The quantification of proteins in complex biological samples is central to many areas of research, as well as to industrial and clinical applications. Especially the clinical chemistry laboratory uses quantitative protein assays on a daily basis to assist in medical decision making, for example, in defining the best therapy for a given disease or in disease diagnosis. While quantitative protein assays have relied and rely to a major part on ligand binding assays (LBAs) and in particular on immunoassays, we experience the advent of liquid chromatography – mass spectrometry (LC-MS) assays as an alternative or complement to LBAs. In this lecture I will delineate the advantages and shortcomings of LBAs and LC-MS assays with the goal of showing that there is no single approach that can answer all questions. I will notably address the point that proteins do not exist as single molecular entities in vivo and that we must therefore refer to proteins as families.

Wednesday @ 9:00 in Europa Hall

Smaller, Better, Faster Metabolic Phenotyping Using LC-MS and LC-IMS-MS

Ian Wilson - *Imperial College London* (i.wilson@imperial.ac.uk)



‣ For the discovery of biomarkers via MS and LC/MS-based metabolic phenotyping (metabotyping) studies employing untargeted metabonomic/metabolomic methods there is always a tension between maximising throughput and obtaining the most comprehensive metabolic profiles possible. In particular, rapid profiling methods can suffer from ion suppression, leading to analytes being missed, whilst “deep” profiling is time consuming. The introduction of ultra (high) performance LC provided a significant improvement in efficiency and enabled many more metabolites to be detected per unit time compared to conventional HPLC. This presentation will explore further advances resulting from the use of miniaturisation and the combination of U(H)PLC-MS with ion mobility spectrometry (IMS) to enhance the efficiency of metabotyping for both rapid and comprehensive profiling approaches.

Distinguished Contribution Awardee

Wednesday @ 12:00 in Europa Hall

Laser-based Mass Spectrometry in Clinics: Changing the Paradigm of Molecular Diagnosis

Isabelle Fournier - *Laboratoire PRISM U1192, INSERM* (isabelle.fournier@univ-lille1.fr)

‣ By bridging surface analysis with access to biomolecules of various molecular weight and polarity including higher molecular weight polar compounds such as proteins, Matrix Assisted Laser Desorption Ionization (MALDI) reseals a unique ability for clinical applications. This was clearly demonstrated by the introduction and development of MALDI MS Imaging (MALDI MSI) which after 15 years has now acquired its letters of nobility. Indeed deploying dedicated strategy MALDI MSI can be used to image the distribution of both endogenous and endogenous molecules within biological tissues to access a vast variety of applications in the field of basic sciences as well as clinics. In clinics, MALDI MSI starts to be employed as a molecular histology tool allowing to perform retrospective and prospective studies on patient's cohorts for biomarkers hunting, as a new diagnosis and prognosis tool as well as for patient's classification or stratification in the objective to get personalized medicine. However, such laser based technology can also be translated to the in-vivo context for developing MS as a tool for guided surgery in the surgery room.

Thursday @ 14:15 in Mozart Hall

Prospects of Apolipoprotein Profiling for Precision Cardiovascular Diagnostics

Christa Cobbaert - *Department of Clinical Chemistry and Laboratory Medicine, Leiden University Medical Centre, Leiden, the Netherlands* (C.M.Cobbaert@lumc.nl)

‣ Lipid abnormalities account for more than 60% of the population attributable risk for myocardial infarction and are the most important single target for prevention, together with smoking cessation and blood pressure lowering. Although statin therapy is the cornerstone of dyslipidemia management, LDLc lowering with statins reduces major coronary events by only one quarter, with 75% of events still occurring. Dyslipidemic patients remain at high Residual vascular Risk despite treatment for high LDLc in accordance with current standards of care. Atherogenic dyslipidemia is a key factor associated with Residual vascular Risk. So far, atherogenic dyslipidemia is largely under-diagnosed and under-treated in clinical practice as only overall lipid classes are measured rather than detailed molecular entities with specific functionalities. Comprehensive protein biomarkers are needed to obtain a better understanding of incident cardiovascular disease, but also for improved patient selection for evaluating treatment efficacy and safety. Recent mass spectrometry advances enable deep apolipoprotein proteomics to uncover mechanisms of coronary disease risk.

Young Investigator Grants

Travel Grants were provided to support 46 Young Ivnstigators (MD/residents/fellows and PhD - students / post-docs) and young faculty members (less than 4 years since appointment) who submitted abstracts that have been accepted for presentation at the conference.

Ioana Abbas *School of Analytical Sciences Adlershof*
Mina Adam *Imperial College Londonm*
Ida Bøgh Andersen *Vejle Hospital*
Valeria Avataneo *University of Turin*
Forough Bahadory *Prince of Wales Hospital, Sydney, Australia*
Timur Baygildiev *Moscow State University*
Marianne Bergmann *Lillebaelt Hospital*
Annachiara D'Urso *Fondazione IRCCS Istituto Neurologico Carlo Besta*
Lisa Delahaye *University of Ghent*
Meritxell Deulofeu Figueras *University of Masaryk*
Julia Dittrich *University Hospital Leipzig*
Finnur Eiriksson *University of Iceland*
Neus Fabregat-Cabello *University of Liège*
Tanja Farrokh-Eslamlou *Imperial College London*
Giovanna Fatiguso *University of Turin*
Fabio Favata *University of Turin*
Claudia Fredolini *Royal Institute of Technology, Stockholm, Sweden*
Björn Fröhlich *UVic Genome BC Proteomics Centre*
Hector Gallart-Ayala *University of Lausanne*
Alexander Gaudl *Leipzig University*
Krzysztof Gorynski *Nicolaus Copernicus University Collegium Medicum*
James Hawley *University Hospital South Manchester*
Lennart Huizing *M4I division of IMS, Maastricht Unviversity*
Kyoung-Soon Jang *Korea Basic Science Institute*
Mira Kim *University of Yonsei*
Mikael Lindström *HUSLAB*
David Marshall *University Hospital of South Manchester*
Wojciech Michno *University of Gothenburg*
Amanda Moreno *Universidad Nacional Autonoma de Mexico*
Anna Mroz *Imperial College London*
Antonis Myridakis *Imperial College London*
Shabarinath Nambiar *Murdoch University, Western Australia*
Charles Nichols *Vanderbilt University*
Pranav Patel *Imperial College London*
Stéphanie Peeters *University of Liège*
Ivan Plyushchenko *Lomonosov Moscow State University*
Natalja Pustovalova Nørskov *Aarhus Univerity*
Andrijana Ščavničar *University Hospital Centre Zagreb*
Madlen Sander *Leipzig University*
Marta Sans *The University of Texas*
Andraz Smon *University Medical Centre Ljubljana*
Zdenek Spacil *Masaryk University*
Menelaos Tzafetas *Imperial College London*
Anna van der Veen *University Medical Center Groningen*
Naomi Vos *M4I division of IMS, Maastricht University*
Vincen Wu *Imperial College London*

Lab Director Grants

Travel Grants were provided to 8 individuals leading clinical labs who have minimal exposure and are interested in gaining more understanding of its clinical applications.

Artuela Çaku *Centre Hospitalier de l'Université de Sherbrooke*
Matteo Conti *Metropolitan Laboratory of Bologna*
France Debaugnies *Laboratoire National de Santé, Luxembourg*
Sophie Hepburn *The Ipswich Hospital NHS Trust*
Caroline Le Goff *University Hospital of Liège, University of Liège, Belgium*
Ruben Musson *University Medical Center Utrecht*
Igor Rodin *Moscow State University, Analytical Research Centre*
Michel Salzet *U1192 Inserm, PRISM Laboratory*

Lab Director & Trainee Travel Grants supported in part by:

ThermoFisher SCIENTIFIC

CIL Cambridge Isotope Laboratories, Inc. isotope.com

Trainee Grants

Trainee Grants were provided to 8 individuals training to lead clinical labs. These individuals have had minimal exposure to mass spectrometry and are interested in gaining more understanding of its clinical applications.

Dennis Bernieh *De Montfort University - UK*
Hong Bui *Atalmedial Medical Diagnostic Centers*
Aleysha Cross *University Hospitals of Leicester NHS Trust*
Joanna Flatt *Cardiff and Vale UHB, National Health Service*
claude hercend *Necker Universitary Hospital*
Helen Jerina *University Hospitals of Leicester*
Marina Pijanovic *Medical laboratory Medilab*
Alessia Tommasini *University of Bologna*

Short Course Overview

The Short Course Program provides a rapid introduction to topics, issues and techniques. Each course is led by one or more distinguished instructors with expertise in the respective course areas.

Data Science 101
Breaking up with Excel: A Newbie's Introduction to the R Statistical Programming Language
Duration: *Sunday 14:00 → Tuesday 12:30*
Location: *Mozart 5*
Level: *1-2 (Beginner - Intermediate)*
Instructor(s): **Daniel Holmes, MD & Stephen Master, MD, PhD**

Have you ever tried to do Deming regression in Excel only to discover that it is not available? Have you had your figure rejected by a journal because the resolution was not good enough? Have you wished that you could figure out a way to stop manually transcribing your LC-MS/MS results into the LIS?

Well, your wait is over because this year at MSACL we will be offering a course for complete programming newbies that will help you get going analyzing real data related to LC-MS/MS assay development, validation, implementation and publication. The only background expected is the ability to use a spreadsheet program. The skills that you will acquire will allow you to take advantage of the many tools already available in the R language and thereafter, when you see that your spreadsheet program does not have the capabilities to do what you need, you will no longer have to burst into tears. You will be empowe-R-ed.

The course will be run over two days and time will be evenly split between didactic sessions and hands on problem solving with real data sets. Drs Holmes and Master will adopt a “no student left behind policy”. Students will be given ample time to solve mini problems taken from real life laboratory work and focused on common laboratory tasks. All attendees will need to bring a laptop with the R language installed R Studio interface installed. Students may use Windows, Mac OSX or Linux environments. Both R and R studio are free and open-source. No cash required.

Students should be prepared for learning what computer programming is really like. This may involve some personal frustration but it will be worth it.

Obtaining the Software
Instructions for installing the R language are here: http://cran.r-project.org/
Instructions for installing R Studio are here: http://www.rstudio.com/

Course Description

The course will cover:

- The major types of R variables: vectors (numerical, character, logical), matrices, data frames and lists.
- The important classes: numeric, character, list and changing between them
- Importing data from Excel
- Dealing with non-numeric instrument data: the “<10”s and “>1000”s.
- Manipulating your data: sub-setting, which, match, sort, unique, cut
- Simple statistical tests: mean, median, quantiles (normal ranges), t-tests, ANOVA, Wilcoxon.
- Data merges: matching rows between sets
- Exporting data to Excel-like format.
- Regressions: Ordinary Least Squares,Passing Bablok, Deming, weighted regressions.
- Non-linear regressions
- Looping: Doing things repeatedly
- Writing your own functions
- Making highly customized graphs: scatter plots, regression lines, histograms, box plots, qq-plots
- Putting it all together projects:
    - Preparing method comparison regression and Bland Altman plots
    - Preparing mass spectrometry data for upload to LIS.

Lab Medicine 101
Basics of Laboratory Medicine
Duration: *Monday 14:00 → Tuesday 12:30*
Location: *Mozart 2*
Level: *1 (Beginner)*
Instructor(s): **Prof. Dr. med. Michael Vogeser**

This 8-hour course aims to make scientists familiar with the basic concepts of clinical pathology and laboratory medicine. Typical processes and workflows in the various categories of clinical laboratories are described and discussed. Topics that are addressed include in particular:

1. Basic technologies (photometry, immunoassays, electrochemical methods, cytometry, immuno-fluorescence, etc.)
2. Automation and working characteristics of analyzer configurations including total laboratory automation
3. -Concept of total testing process including pre- and post-analytical processes
4. Performance characteristics
5. Quality management
6. Regulatory background
7. Sample materials
8. Clinical decision making, reference ranges, decision levels, diagnostic and clinical algorithms
9. Logistics, sample transport
10. Economic considerations
11. Characteristics of IVD industry

LC-MSMS 101
Getting Started with Quantitative LC-MS/MS in the Diagnostic Laboratory
Duration: *Sunday 14:00 → Tuesday 12:30*
Location: *Mozart 4*
Level: *1-2 (Beginner - Intermediate)*
Instructor(s): **Judy Stone, PhD & Grace van der Gugten**

Is your laboratory under pressure to purchase an LC-tandem MS or is the ROI you wrote last year haunting you now? This short course is designed for attendees implementing quantitative LC-tandem MS for patient testing who have laboratory medicine experience but no mass spectrometry training - CLS bench analysts, supervisors, R&D scientists, and laboratory directors. Theoretical concepts necessary for a robust implementation of clinical mass spectrometry will be presented – but the emphasis is on practical recommendations for:

- LC-MS/MS system purchasing
- site preparation and installation
- defining preliminary MSMS and LC parameters for your first method
- selecting and optimizing sample preparation for your first method
- choosing internal standards, solvents, and water, making reagents and calibrators
- adjusting sample preparation, LC and MSMS parameters to achieve the desired assay performance
- establishing data analysis & review criteria and an interface to the LIS
- pre-validation stress testing and method validation
- preventative maintenance and troubleshooting
- maintaining quality in production.

Our goal is to present just enough theory so you can report high quality results, while opening a window to the depth and complexity of clinical mass spectrometry such that your appetite is whetted to learn more.

Previous exposure to the principles of clinical method validation, either didactic or practical, is assumed. A glossary of common LC-MSMS terms/acronyms, and diagrams delineating basic LC and MSMS instrument components and functions will be emailed to attendees a week prior to the beginning of the course. This material will also be addressed at the beginning of the course, but the initial learning curve can be steep and review prior to the course will be beneficial if you have absolutely no previous exposure with LC-MSMS.

LC-MSMS 202
Practical LC-MS Maintenance and Troubleshooting
Duration: *Sunday 14:00 → Tuesday 12:30*
Location: *Paracelsus*
Level: *2 (Intermediate)*
Instructor(s): **Erik J. Soderblom, PhD & Chris Shuford, PhD**

The general goal of the course is to enable practitioners of LC-MS/MS in the clinical laboratory to quickly recognize and diagnose specific problems with instrumentation, in order to decrease downtime and cost of repairs. The course includes 'best practices' for instrumentation installation, upkeep and maintenance, practical troubleshooting workflows for LC and MS, and will use problem sessions to reinforce skillsets. Although the course uses examples from specific instrumentation for demonstration, the content is geared to be vendor-neutral and applicable to all LC-MS systems. Additionally, we will provide an opportunity to have instrumentation troubleshooting questions from your laboratory addressed by the facilitators.

Brief outline of course content:

- **General "Best Practices" for Successful LC/MS Operation**
    1. Best Practices; Getting Started on the Right Foot
    2. Breaking the System Down
    3. System Suitability! What is it, and how do I properly implement?
- **Focus on Liquid Chromatography**
    1. Diagnostics using the "heartbeat" of your Chromatographic system
    2. Key System components and where things go wrong
    3. LC troubleshooting workflow
    4. Maintenance Intervals; service contract or do-it-yourself?
    5. Problem sets
- **Focus on Mass Spectrometry**
    1. Discussion of Source, Transfer Optics, Vacuum and how each is critical to your system
    2. MS Troubleshooting workflow
    3. Ion optics cleaning and upkeep; what is 'charging'?
    4. Problem sets
- **Integrated System**
    1. Ionization
    2. System Communications
    3. Multi-vendor configurations
    4. Strategies to simplify
    5. Integrated real-lab problem scenarios and team exercises

While some basics of instrument component operation will be covered, it will be most beneficial to scientists with experience actively using LC-MS/MS as an analysis tool. While an in-depth discussion of how to operate each individual instrument is surely outside the scope of any short course, specific system setups will be used as examples and attendees will be encouraged to ask questions about specific systems in their own laboratories.

LC-MSMS 301
Development and Validation of Quantitative LC-MS/MS Assays for Use in Clinical Diagnostics
Duration: *Sunday 14:00 → Tuesday 12:30*
Location: *Papageno*
Level: *3 (Advanced)*
Instructor(s): **Russell Grant, PhD & Brian Rappold**

This16-hour course will briefly introduce the key aspects of the LC-MS/MS experimental workflow and then focus on processes and experimental designs for assay development and analytical validation of assays to be employed within clinical diagnostics.

The first day will describe method development in detail, including how-to guides for initial optimization of mass spectrometry systems, chromatographic development and sample preparation schemes. Techniques and technologies for streamlining analytical performance will also be described. Transitional experiments from development to validation will be discussed in detail to stress test methodologies prior to analytical validation.

Day two will cover all details pertinent in validation of LC-MS/MS analytical workflows. Experimental designs for all aspects of validation, putative acceptance criteria and analytical solutions will be shown. Key validation criteria of selectivity, carry-over, matrix effect, accuracy, precision, linearity, stability and inter-assay correlation will be described using multiple case studies.

Metabolomics 202
Metabolomics: Approaches, Applications and Challenges
Duration: *Sunday 14:00 → Tuesday 12:30*
Location: *Doppler*
Level: *1-2 (Beginner to Intermediate)*
Instructor(s): **Julijana Ivanisevic, PhD & Elizabeth Want, PhD**

Metabolome: Downstream of Genome

- Central Dogma of Molecular Biology – From Genotype to Metabotype
- Historical Perspective of Metabolomics
- Technological platforms (NMR, GC/MS, LC/MS) and Applications
- OmicChallenge – Metabolite Diversity

Approaches in Metabolomics

- Targeted versus Untargeted (work on the front end vs. work on the back end, instrumentation, etc.)
- Experimental Design and Sample Preparation (depending on the approach)
- Choice of Analytical Platform (depending on the approach and metabolites of interest)
- OmicChallenge – « Big » Data Reduction

Data (Pre)Processing in Untargeted Experiments

- Step by step from peak picking to peak grouping and annotation
- Open-access platforms
- Hands-on XCMS Online
- Omic Challenge – Metabolite Identification

Statistical Analysis, Metabolite Identification and Mapping onto Pathways

- Univariateversus Multivariate Statistics (SIMCA, MetaboAnalyst)
- Metabolite Matching against Metabolite Databases (METLIN, HMDB, LIPIDMAPS, MassBank)
- Metabolite Set Enrichement Analysis and Network Modeling (MetaboAnalyst, KEGG, BioCyc, Mummichog, Ingenuity)
- Omic Challenge – Integration with other Omic Technologies in a Biologically Relevant Context

Proteomic Microbiology 201
Bottom-Up and Top-Down Proteomic Approaches for Bacterial Identification and Characterization, a Focus on MALDI-TOF and Advanced Technologies
Duration: *Monday 14:00 → Tuesday 12:30*
Location: *Mozart 3*
Level: *1-2 (Beginner - Intermediate)*
Instructor(s): **Jean Armengaud, PhD, Stefan Zimmermann, MD**

This course will present an overview of bottom-up and top-down techniques for microbial identification using mass spectrometry-based technologies as well as their use in determination of microbial characteristics such as antibiotic resistance profiles. Topics to be discussed include:

- Comparison of bottom-up versus top-down proteomic approaches,
- Why top down proteomics is well-suited for microbial identification and characterization,
- Discrimination of closely related strains by top-down proteomics approaches.,
- Collection and interpretation of MALDI-TOF data,

- Proteogenomics as a means for improving annotations based on genomic sequence analysis and its use in identification of key protein markers in MALDI-TOF spectra.
- The concept of proteoforms as a means of categorizing the PTM states of proteins.
- The application of these techniques and technologies to antibiotic resistance determination,
- Novel methodologies that are currently emerging for the analysis of difficult samples, such as mixtures of pathogens and spores present within complex matrices.
- Recent advances for pathogen quantitation by tandem mass spectrometry.
- Use of MALDI-TOF for identification of viruses, molds and parasites.

Proteomics 201
Clinical Proteomics
Duration: *Sunday 14:00 → Tuesday 12:30*
Location: *Trakl*
Level: *2-3 (Intermediate - Advanced)*
Instructor(s): **Andy Hoofnagle, MD, PhD & Cory Bystrom, PhD**

This course will explore the background of clinical proteomics and approaches to method development and validation. We will provide the motivation for using mass spectrometry to quantify proteins in clinical research and in clinical care. The promise of mass spectrometry to improve the accuracy and precision of results is only realized with robust methods. In order to prepare participants to begin to develop their own robust methods for quantification we will focus on the following topics:

- Why mass spec for peptides and proteins
- Optimization of digestion and other aspects of the method
- Internal standards
- Calibration
- Immunoaffinity enrichment
- Validation
- Quality control
- Case studies

MEET THE 3XP3RT5*

* THE TERM ‘EXPERT’ IS AMBIGUOUS, BUT WE’RE GOOD AT SOME THINGS RELATED TO CHROMATOGRAPHY AND MASS SPECTROMETRY IN LABORATORY MEDICINE

Discussion Groups

Tuesday from 20:00 to 21:00

The Future of MS in the Clinical Lab
Mozart 4-5
Lead(s): Brian Keevil , Michael Vogeser & Randy Julian

Fully-Automated Plug and Play: High-performance precision tests that are available for more patients is a definitive benefit, but is full automation really feasible for demanding analytes, and, even if it is, will there will be a (dangerous) trade-off between convenience and analytical performance? Also, will these plug and play developments impact the perceived need for trained mass spectrometrist and might there be an impact on the continued implementation of mass spectrometry in the lab as a result?
Regulation: Is the safety of LDTs a problem? What types of regulation should we be advocating for in order to increase the overall benefit for the patient?

Wednesday from 19:30 to 20:30

Design of Experiments - Get it right from the beginning
Mozart 4-5
Lead(s): Margrét Thorsteinsdóttir

We will demonstrate how method development can become much more efficient by utilizing design of experiments (DoE) approach. DoE offers many advantages including performing experiments in accordance to predefined plan, modelling by empirical functions and graphical visualization. Example from optimization of a LC-MS/MS clinical diagnostic method will show that DoE is very cost-effective, allowing the effect of variables to be assessed with only a fraction of the experiments that would be required by changing one-separate-factor-at-time (COST) approach and spots critical setting early on.

Mass Spectrometry Data Standards Discussion
Papageno
Lead(s): Patrick Mathias

Defining data standards for mass spectrometry that are specific to clinical laboratory operations will speed adoption of mass spectrometry into the clinical laboratory by facilitating ease of data transfer (from instrument to laboratory information system and vice versa). While mass spectrometry offers superior analytic performance, the ease of data transfer between instruments and clinical laboratory information systems is inferior to conventional high volume analyzers. This is due in large part to the lack of standardized data formats (file formats, specifications for file exports, etc.) and limited availability of interfaces to common laboratory information systems or middleware. These barriers increase the effort required for adoption and scaling of clinical mass spectrometry and require individual clinical laboratories to "reinvent the wheel" in developing interface solutions (if the resources to do so are even available). Our Mass Spectrometry Data Standards workgroup aims to lower these barriers to integrating mass spectrometry into the clinical laboratory by defining data standards that are specific to clinical laboratory applications. We are gathering stakeholder input from a broad spectrum including end users, mass spectrometry vendors, liquid handlers, and laboratory information system/middleware vendors to characterize current practices. In this discussion we will summarize the current issues the workgroup is aware of, solicit input from stakeholders, and identify key issues for our workgroup to address in developing these standards.

Scientific Committee Review
Paracelsus
Lead(s): David Herold

Scientific Committee meeting to review and plan.

Thursday from 9:00 to 10:00

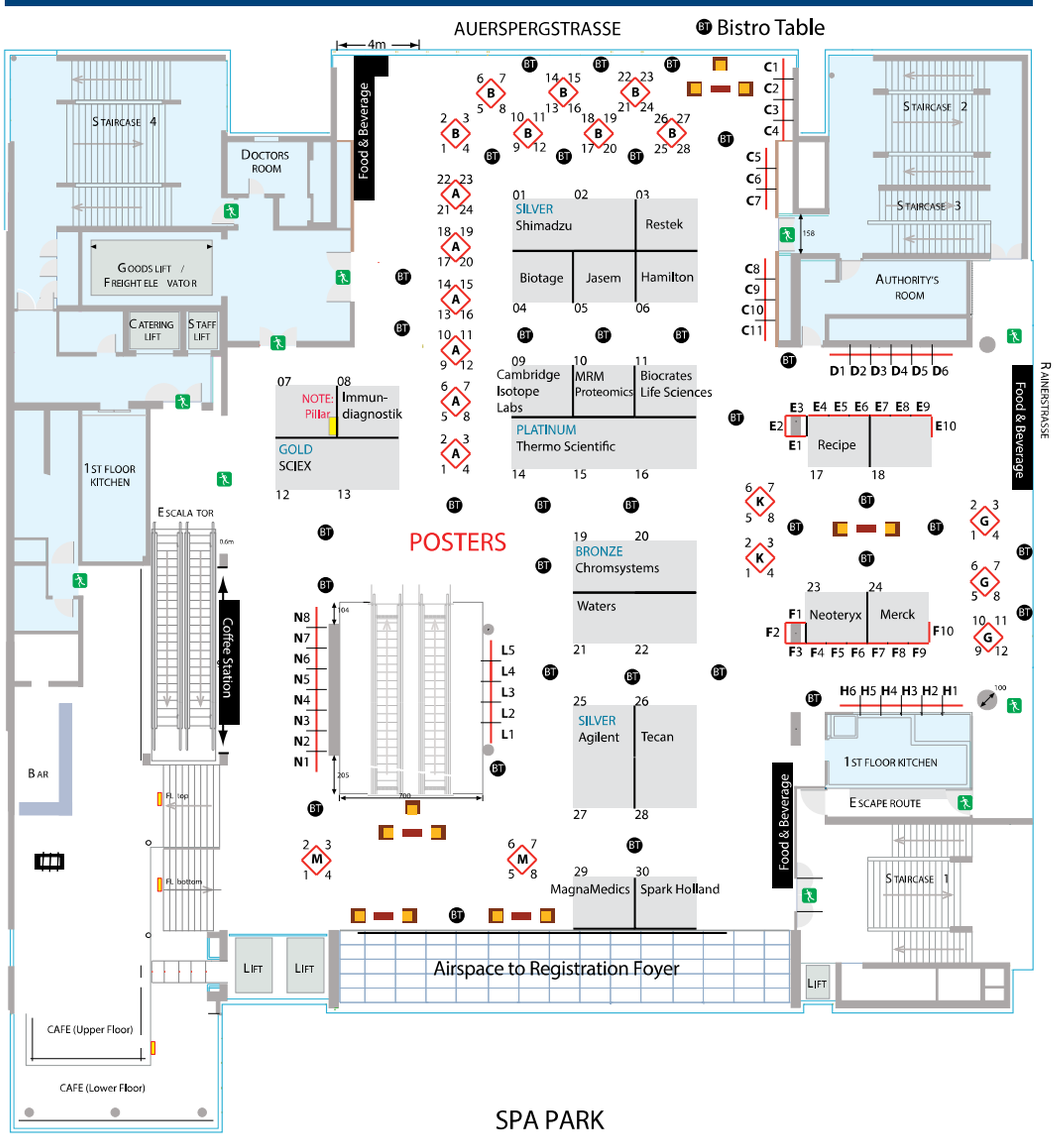
Exhibitor Feedback Meeting
@ 1st Floor Lower Level Cafe
Lead(s): Chris Herold

Exhibitors, let MSACL know your thoughts on the how the congress is working for you and what we can do to make the experience better.

Exhibits Summary

Tuesday	
8:00 – 16:30	Exhibitor Set-Up (EXHIBITS CLOSED) – Poster Placement for Presenters Permitted.
17:30 – 20:00	**Opening Reception** in Exhibit Hall
Wednesday	
9:45 - 10:45	**Coffee Break** in Exhibit Hall
12:45 – 14:00	**Lunch** provided in Exhibit Hall .
14:30 – 14:45	**Coffee Break** in Exhibit Hall
15:45 - 16:00	**Coffee Break** in Exhibit Hall
16:30 - 16:45	**Coffee Break** in Exhibit Hall
17:45 – 19:30	**Reception** in Exhibit Hall
Thursday	
9:00 – 10:00	**Exhibitor Feedback Session** in LowerCafe, 1st Floor
10:00 - 11:00	**Coffee Break** in Exhibit Hall
12:00 – 14:00	**Closing Lunch** in the Exhibit Hall.
14:00	**EXHIBITS CLOSED**
14:00 – 17:40	***Exhibitor Breakdown and Packing in Exhibit Hall Only***
17:40	***Package Pickup from Loading Bay Allowed to Begin***
21:00	***Deadline for removal of Exhibits from Exhibit Hall***

Exhibit Hall / 1st Floor



SPA PARK

Exhibitors

Agilent Technologies Booth #25,27
http://www.agilent.com/chem
With an industry leading portfolio of analytical products for your clinical research laboratory, Agilent Technologies delivers everything your laboratory needs from sample preparation to final answers. From automation and sample preparation technologies, columns and consumables, laboratory informatics, to liquid and gas chromatography systems, and mass spectrometry systems such as ICP-MS, GC/MS, and LC/MS, Agilent provides premiere analytical solutions that will ensure confident identification and quantitation of both endogenous and exogenous substances in complex biological matrices with the utmost accuracy, productivity and reliability.

Biocrates Life Sciences Booth #11
http://www.biocrates.com
Biocrates provides the fast track to metabolic biomarker signatures, with standardized and highly reproducible solutions for the quantitative analysis of hundreds of endogenous metabolites. Biocrates' metabolic phenotyping technology is among the most widely used approaches in metabolomics. It has contributed to more than 800 scientific publications in a large variety of applications. Targeted Metabolomics kits build the cornerstone of Biocrates' portfolio. These allow for metabolomics analyses in your own laboratory, eliminating the need to invest resources into method development. A new kit for broad lipid and metabolic profiling with HRAM mass spectrometers has recently been introduced. Biocrates' targeted metabolomics kits have proven excellent analytical performance in international ring trials, as well as in proficiency tests organized by national clinical chemistry societies. Biocrates also operates an analytical services laboratory, which can provide quantitative analysis of more than 700 metabolites.

Biotage AB, Sweden Booth #04
http://www.biotage.com
Biotage AB, Sweden is a global leader in life science technology. With a broad scope of tools for synthesis, work-up, purification, evaporation and analysis, the company provides knowledge and expertise in the areas of analytical chemistry and medicinal chemistry.

Cambridge Isotope Labs Booth #09
http://www.isotope.com
Cambridge Isotope Laboratories, Inc. is the world leader in the manufacture and separation of stable isotopes and isotope-labeled compounds. CIL and Euriso-Top (a European subsidiary of CIL) offer highly pure compounds that are uniformly or selectively enriched in ^{13}C, ^{15}N, D, ^{18}O or ^{17}O. CIL's labeled reagents are used in proteomics, metabolomics, metabolism, and environmental applications for quantitative mass spectrometry. Our products include MRM PeptiQuantTM assay kits, SILAC protein quantitation kits, media and reagents, 99% enriched amino acids, Mouse Express® Lys $^{13}C_6$ and ^{15}N mouse feed and tissue, ^{15}N spirulina, intact labeled proteins, growth media for protein expression, cell-free protein synthesis products, environmental contaminants standards for ultra-trace analysis, steroids, acylcarnitines, drug metabolites, nucleic acids, lipids and carbohydrates. CIL has cGMP capabilities; a majority of substrates can be manufactured to Q7A compliance.

Chromsystems Booth #19,20
http://www.chromsystems.com/en-gb
Chromsystems is a leading global company providing ready-to-use kits, multilevel calibrators and quality controls for routine clinical diagnostics by LC-MS/MS and HPLC. Our parameter menu covers a range of areas such as newborn screening, therapeutic drug monitoring, steroid analysis, vitamin profiling and more. We continuously expand our portfolio with additional tests all ensuring a highly accurate and cost-effective analysis. We enable laboratories to add new parameters into their diagnostic routine and expand their testing menu without prior technical expertise. They can immediately start the analysis with a minimum of time for the sample preparation. The products are comprehensively validated, and in particular LC-MS/MS methods with all widely used tandem mass spectrometers. They are CE-IVD compliant, satisfying regulatory requirements in the laboratory. We combine these high quality products with an excellent support programme and service for our customers.

Hamilton Robotics Booth #06
http://www.hamilton.ch
Solutions for automated Assays. Fully automated processing of clinical assays requires single-source solutions that are tailor-made for each particular application. Customers benefit from HAMILTON's state-of-the-art technology, the knowledge of a highly qualified team of specialists and solid experience in planning and implementing total solutions for LC-MS sample preparation and a wide range of other applications. Based on the innovative MICROLAB® liquid handling platforms, HAMILTON also offers ready-to-use standard solutions for a wide range of toxicology applications: (1) Protein precipitation, (2) Solid phase extraction, (3) Automated QC and calibration curve preparation, (4) Direct sample injection, (5) Sample dilution, and (6) Reformatting.

Immundiagnostik Booth #08
http://www.immundiagnostik.com

Jasem Booth #05
http://www.jasem.com.tr
We are adapting diagnostics for chromatography coupled mass spectrometry. Jasem serves customers ready-to-use diagnostic kits for clinical analysis based on HPLC and mass spectrometry. Our core mission is to provide innovative trustworthy and accurate results. Hence, our straightforward and economic solutions are being used extensively in clinical and food laboratories. Our foundational purpose is clinical and food analysis kit development that provides: (1) simple and practical sample preparation, (2) short analysis time, (3) reliable and sensitive analysis, (4) low analysis cost (without derivatization, SPE or concentration), and (5) longer column life-time.

MagnaMedics Booth #29
http://www.magnamedics.com
MagnaMedics offers the innovative, magnetic bead-based MagSiMUS method, for the clean-up of clinical biological samples prior to their injection and analysis on LC-MS/MS and (U)HPLC instruments. MagSiMUS is a quick, flexible and cost-effective method, and especially very easy to automate with e.g. the PAL-RTC autosampler or the MagSiMUS-DX liquid handling robot. MagSiMUS solutions can be used with any LC and/or MS system and also offered as reagent rental solutions.

Merck Booth #24
http://www.sigmaaldrich.com
The life science business of Merck combines strong innovative R&D teams with a global network spanning more than 60 countries and 70 manufacturing sites. Innovations include BioSPME for rapid extraction from biological matrices for LC/MS or direct MS, in-line SPE cartridges for effective extraction and phospholipid removal and in HPLC and LC/MS, the latest developments in monolith and fused core column technologies, all of which can be seen on booth 24. The company provides a product portfolio of 300,000 products, including over 20,000 reference materials, along with Cerilliant Certified Reference Materials, all with easy access to comprehensive data through one of the most advanced web platforms.

MRM Proteomics Booth #10
http://www.mrmproteomics.com
MRM Proteomics Inc. is at the leading edge of proteomics technology. We offer a wide range of proteomics services and easy-to-use kits for do-it-yourself protein quantitation. We are also currently involved in developing clinical diagnostics. Our technologies include: MRM-MS with paired heavy/light peptide standards for high-precision highly-multiplexed quantitation of hundreds of proteins from low-volume samples; Patented iMALDI-MS technology for robust high-throughput clinical proteomics; HDX structural characterization of proteins and biosimilars, approaching single-residue resolution; and Tissue imaging of peptides and >500 lipids using innovative matrices and techniques (patent pending). Our mission is to offer the highest quality of proteomics technologies on the market today. Although our services fit with many diverse applications, we recognize that research projects are not "one-size-fits-all." Our expertise allows us to offer custom-tailored solutions for your specific research needs.

Neoteryx Booth #23
http://www.neoteryx.com
Neoteryx delivers on the promise of microsampling technology, enabling biological specimen collection anytime, anywhere, by anyone, while reducing costs and improving the clinical experience. Benefits of Volumetric Absorbtive Microsampling (VAMS™) technology include improved comfort (particularly for children and the elderly), reduced animal usage, and a more economical specimen collection method for low-resourced regions.

RECIPE Chemicals + Instruments Booth #17
http://www.recipe.de/en/index.html
Starting business in 1982, RECIPE is one of the leading companies in HPLC and LC-MS/MS diagnostics today. For mass spectrometry, RECIPE offers CE/IVD labelled ClinMass® LC-MS/MS Complete Kits. Furthermore, several reagents such as ClinMass® Optimisation Mixes and Internal Standards, ClinCal® Calibrators and ClinChek® Controls are available for a reliable and standardised LC-MS/MS analysis. All products are developed and produced in our state-of-the-art production plant in Munich. RECIPE is recognised worldwide as a reliable partner for clinical laboratories and is certified by the quality management standards EN ISO 9001 and 13485.

Restek Booth #03
http://www.restek.com
A leading innovator of chromatography solutions for both LC and GC, Restek has been developing and manufacturing columns, reference standards, sample preparation materials, accessories, and more since 1985. We provide analysts around the world with products and services to monitor the quality of air, water, soil, food, pharmaceuticals, chemicals, and petroleum products. Our experts have diverse areas of specialization in chemistry, chromatography, engineering, and related fields as well as close relationships with government agencies, international regulators, academia, and instrument manufacturers. www.restek.com

SCIEX Booth #12,13
http://www.sciex.com
SCIEX's global leadership and world-class service and support in the capillary electrophoresis and liquid chromatography-mass spectrometry industry have made it a trusted partner to thousands of the scientists and lab analysts worldwide who are focused on basic research, drug discovery and development, food and environmental testing, forensics and clinical research. As part of AB SCIEX, SCIEX Diagnostics brings the power, flexibility, reliability, and accuracy of mass spectrometry technology to clinical testing laboratories. Offering an expanding portfolio of mass spectrometry based solutions and assays for in vitro diagnostic use, SCIEX Diagnostics enables customers to deliver high quality diagnostic information to clinicians who make decisions affecting patient care.

Shimadzu Booth #01,02
https://www.shimadzu.eu
Shimadzu is one of the worldwide leading manufacturers of analytical instrumentation. Its equipment and systems are used as essential tools in all areas of clinical research. Since more than 140 years, Shimadzu is at the service of science ensuring precise and reliable analyses. Among the leaders in GCMS as well as in LCMS, Shimadzu is offering a full range of LC-MS/MS systems to fit all needs depending on the application, and will introduce new solutions for screening and quantitation in toxicology field. In addition, the unique and flexible fully automated sample preparation system seamlessly integrated with our LC-MS/MS range will be shown: CLAM-2000. Take the opportunity to visit our booth “1 & 2”.

Spark Holland Booth #30
http://www.sparkholland.com/
Spark Holland is a specialist in front-end HPLC and UHPLC instrumentation for LC/MS. We are an independent company owned privately by Spark personnel. Our business model is largely based on OEM and in that arena we are best known for our prominent position in autosamplers for HPLC, UHPLC, and micro LC. We are also well recognized for our advanced online solid phase extraction (SPE) technology. Recently, we added automated Dried Blood Spot extraction to the palette of front-end instruments using our patented Flow-Through Desorption (FTDTM) technology. We aim to provide best in class instrumentation through continuous innovation, ensuring our commitment by spending more than 12% of our revenues on R&D. Plus, we have mastered the demanding art of OEM partnering! Spark Holland is ISO 13485 certified.

Tecan Booth #26,28
http://www.tecan.com
Tecan (www.tecan.com) is a leading global provider of laboratory instruments and solutions in biopharmaceuticals, forensics and clinical diagnostics. The company specializes in the development, production and distribution of automated workflow solutions for laboratories in the life sciences sector. Its clients include pharmaceutical and biotechnology companies, university research departments, forensic and diagnostic laboratories. As an original equipment manufacturer (OEM), Tecan is also a leader in developing and manufacturing OEM instruments and components that are then distributed by partner companies. Founded in Switzerland in 1980, the company has manufacturing, research and development sites in both Europe and North America and maintains a sales and service network in 52 countries. In 2016, Tecan generated sales of CHF 506 million (USD 511 million; EUR 464 million). Registered shares of Tecan Group are traded on the SIX Swiss Exchange (TECN; ISIN CH0012100191).

Thermo Scientific Booth #14-16
http://www.thermoscientific.com/msacleu
Thermo Fisher Scientific Inc. is the world leader in serving science, with revenues of $17 billion and approximately 50,000 employees in 50 countries. Our mission is to enable our customers to make the world healthier, cleaner and safer. We help our customers accelerate life sciences research, solve complex analytical challenges, improve patient diagnostics and increase laboratory productivity. Through our premier brands – Thermo Scientific, Applied Biosystems, Invitrogen, Fisher Scientific and Unity Lab Services – we offer an unmatched combination of innovative technologies, purchasing convenience and comprehensive support. For more information, please visit www.thermofisher.com.

Waters Booth #21,22
http://www.waters.com
Waters Corporation, the premium brand in the analytical instruments industry, creates business advantages for laboratory-dependent organizations by delivering practical and sustainable scientific innovation to enable significant advancements in healthcare delivery, environmental management, food safety, and water quality worldwide. Bringing keen understanding and deep experience to those responsible for laboratory infrastructure and performance, Waters helps customers make profound discoveries, optimize laboratory operations, deliver product performance, and ensure regulatory compliance. Pioneering a connected portfolio of separations and analytical science, laboratory informatics, mass spectrometry, as well as thermal analysis, Waters' technology breakthroughs and laboratory solutions provide an enduring platform for customer success.

Corporate Workshops

Wednesday
08:15, 14:00, 16:00

Thursday
08:15

Mozart 1-3	Ground Floor
Mozart 4-5	Ground Floor
Papageno	Ground Floor
Paracelsus	***2nd Floor***
Trakl	***3nd Floor***

As part of any MSACL registration you may attend any Corporate Workshop.
Sponsoring vendors may request that attendees register, but it is ***not*** required.
Vendors may, however, provide priority seating to pre-registered workshop attendees if there are space limitation issues.

Corporate Workshops - Wednesday
08:15 - 08:45

Thermo Scientific - Mozart 4-5

Introducing the Thermo Scientific™ Cascadion™ SM Clinical Analyzer: Accuracy. Ease-of-Use. Designed for the Clinical Lab

Sarah Robinson, PhD, Market Development Specialist, Thermo Fisher Scientific

The Cascadion SM Clinical Analyzer is the first all-in-one LC-MS/MS solution designed to meet the needs of clinical laboratories. Our fresh vision for fully automated liquid chromatography-tandem mass spectrometry (LC-MS/MS) testing was cultivated by listening to our customers. You asked for a complete solution that was accurate, easy-to-use, and designed for the clinical laboratory. The Cascadion Clinical Analyzer is designed as a turnkey solution to enable clinical labs to easily adopt the power and capabilities of LC-MS/MS as the gold standard in diagnostic testing. The Cascadion system combines assays, software, accessories, consumables and support/service in a standalone system designed to meet the regulatory requirements for routine and specialized clinical testing. This presentation will showcase the Cascadion solution.

This product is in development and not yet available for sale. *This product is not CE marked or FDA 510(k) cleared.*

SCIEX - Papageno

SWATH®-MS for Quantitation and Identification in Clinical Proteomics, Lipidomics, and Metabolomics

SWATH®-MS, a data-independent MSMS analysis (DIA) was originally developed for proteomics, to quantify thousands of tryptic peptides during one LC run without selection of a given precursor ion. Using a database containing the experimentally measured MSMS spectra, quantitative analysis of proteins has been achievable for several years. Recent software developments have permitted protein quantification to be performed in tandem with protein identification.

In lipidomics, also a complex class of compounds, the MSMS behavior of certain lipid groups is often characterized by isobaric precursors and daughter ions, but different structures. This precludes using normal SWATH®-LC applications, but by introducing ion mobility analysis with a DIA approach, isobaric lipids can be separated and quantified. By coupling direct infusion on a TripleTOF® 6600 system with high field ion mobility (using a SelexION® DMS cell), DIA is performed in 1 Da windows (MSMSALL).

The pros and cons will be shown for all the three fields of clinical proteomics, lipidomics, and metabolomics where the high numbers of samples require a robust method resulting in the use of micro-LC.

Corporate Workshops - Wednesday
14:00 - 14:30

Shimadzu - Mozart 4-5

Disruptive Technologies and Creative Solutions in Clinical Mass Spectrometry

1. **Application of the fully-automated sample preparation module, CLAM-2000, in clinical diagnostics**

Dr. Thomas Stimpfl, Medical University of Vienna - Department of Laboratory Medicine

In clinical diagnostics random access to wide range of target analytes is needed. We will present experience with a novel, fully-automated sample preparation module - directly connected to a LC-MS-system - in the routine setting of a university hospital laboratory.

2. **Rethinking library identification in quantitative clinical toxicology - transitioning towards MRM spectrum mode**

Neil Loftus - SHIMADZU Corporation (UK)

Translating information-rich mass spec data into meaningful test results is a hurdle in many labs. To help transition toward high-confidence result reporting we have been rethinking the use of MRM in compound identification. We will show how MRM can help reduce false-positive and false-negative reporting without affecting quantitative data quality.

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SCIEX - Papageno

Introducing the New SCIEX Topaz™ System, a CE-marked Integrated LC-MS-based IVD System

SCIEX is proud to launch the new TOPAZ System for Clinical Diagnostics at MSACL EU 2017. In this seminar, we will present the system and its capabilities, in particular the new ClearCore MD software designed specifically for clinical diagnostics. We will show how the system, based on strong and established mass spectrometry technology, brings enhanced ease-of-use to the diagnostic laboratory, exploiting the power of mass spectrometry to address the diagnostic challenges of today and tomorrow. Seminar delegates will have the opportunity to see and discuss real-world examples of the multitude of diagnostic applications the TOPAZ system is capable of, and meet European leaders in the diagnostics arena as well as SCIEX Diagnostics global experts in the field.

Waters - Paracelsus

Protein Quantification in the clinical laboratory. Challenges and opportunities for improved assays with LC/MS.

Although LC/MS has been successfully used and widely adopted for many small molecule clinical assays, the technique has yet to make a big impact for peptide and protein quantitation applications in the clinical laboratory. With increasingly sensitive instruments and robust micro fluidic inlet devices combined with efficient and standardised sample pre-treatment protocols LC/MS may now be ready for routine protein applications. Challenges and opportunities for LC/MS in protein and peptide biomarker assays and therapeutic drug monitoring of monoclonal antibody (mAb) drugs will be presented.

Neoteryx - Trakl

This workshop examines how two experts used Volumetric Absorptive Microsampling (VAMS™) technology to generate results comparable to those from wet blood, using a variety of analytes and eliminating the hematocrit bias associated with traditional Dried Blood Spot (DBS) cards and filter paper.

Volumetric Absorptive Microsampling (VAMS) and LC-MS/MS Analysis for Simultaneous Monitoring of 16 Antiepileptic Drugs: Workflow Development and Validation

Dr. Ugo de Grazia, Nazionale Neurologico Carlo Besta, Italy

Steroid Collection Using the Mitra Microsampling Device

Prof. Brian Keevil, University Hospital of South Manchester, United Kingdom

Corporate Workshops - Wednesday

16:00 - 16:30

Thermo Scientific - Mozart 4-5

Quantitation of endocrine markers using High Resolution Mass Spectrometry

Laura Owen – University Hospital of South Manchester

Traditionally the quantitation of endocrine biomarkers has been performed using triple quadrupole analysers whereas orbitrap technology lends itself primarily to drug monitoring and screening applications. However, in recent years, orbitrap high resolution mass spectrometry systems have proved to be a great screening and quantitation tools. Our research goal was to quantify renin activity, aldosterone and metanephrines using orbitrap HRMS, in order to bring an added level of capability and flexibility to our lab. For plasma renin analysis, data was acquired in both PRM and full scan modes while, for aldosterone analysis, extract was analysed by PRM only with negative ion mode. Renin activity was measured at concentration level typically found in Conn's syndrome with sufficient sensitivity. PRM showed slightly superior sensitivity than full scan mode. Metanephrine and normetanephrine both gave adequate sensitivity and calibration lines however 3-methoxytyramine was not sufficiently sensitive. Aldosterone demonstrated good sensitivity in sub 100pmol/L concentrations.
The QE focus demonstrated its ability to quantify difficult to measure endocrine markers offering quantitation capabilities along with full scan thus bringing screening, protein discovery and quantitative capabilities to the clinical laboratory.

Tecan - Papageno
Automation in Clinical Labs

1. **Automation and Integration of LC/MS/MS Assays into the Workflow of a Clinical Laboratory**
Emma Walker (Imperial College Healthcare NHS Trust)
Automation of sample preparation and interfacing of the LC-MS/MS system to the laboratory information system has the potential to reduce staff time and increase sample throughput. In her talk, Emma will present the approaches she has taken to streamline sample extraction utilizing Tecan Freedom Evo platforms within her laboratory. For example the endocrinology service is using the automated SPE 96-well plates format to screen patients for testosterone, androstenedione and 17-hydroxyprogesterone. The steroid panel assay runs two or three times a week, and it takes approximately 90 minutes to prepare for analysis - short overview about workflow, turnaround times, efficiency and standardization.

2. **Drug Screening in Whole Blood Using Fully Automated SPE and UHPLC-TOF-MS**
Brian Schou Rasmussen (University of Copenhagen, Forensic Chemistry)
Brian will present experiences from the automation of sample preparation in a forensic toxicology LC-MS analysis on a robotic platform. Workflow strategies, sample throughput, cost efficiencies and special considerations concerning forensic samples with be discussed.

Agilent Technologies - Paracelsus
Multiplexed Proteomic Analysis – The Need for Speed without Compromises
Dr. Cory Bystrom, VP of Research and Development Clevland Heart Laboratory

High density lipoprotein (HDL) plays a number of roles in vascular biology, including lipid and cholesterol transport, anti-oxidative and anti-thrombotic activity, endothelial regulation, and immune response regulation. Cholesterol efflux capacity (CEC), the transport of intracellular cholesterol from macrophages to an accepting HDL particle. The CEC assay is a challenging cell based assay that is labor intensive and low throughput. To enable research investigating CEC and its role in atherosclerotic plaque development we have developed a multiplex proteomic approach to estimating cholesterol efflux from a measurement of six lipoproteins.

Biocrates Life Sciences - Trakl
Targeted Metabolomics in Personalized Cancer Medicine

Although metabolites have been used in clinical diagnostics for decades, currently clinicians only use a fraction of the information contained in the metabolome. It is anticipated that the measurement of single metabolic substances will be replaced by more comprehensive metabolic signatures. Targeted metabolomics, the hypothesis driven analysis of selected metabolites, will be an important technology for the identification of such biomarker signatures. Historically, cancer has been thought to be a metabolic disorder. While the focus had turned to genetic approaches, a growing body of evidence confirms an important role for metabolic factors in the pathogenesis and outcome of many different malignancies. This has led to renewed interest into cancer metabolism. Targeted metabolomics has been instrumental for the identification of metabolic factors that modulate cancer risk, as well as blood based biomarkers for early diagnosis and prognosis. The technology has also provided predictive biomarker signatures for response to targeted and chemotherapies. This workshop will recapitulate the rationale for metabolomics in personalized cancer medicine, and provide several examples of successful biomarker research in oncology. *Products mentioned in the workshop may currently be labeled for research use only – not for use in diagnostic procedures.*

Corporate Workshops - Thursday
08:15 - 08:45

SCIEX - Papageno
New advances and technologies in Mass Spectrometry for Clinical Research

Mass Spectrometry, particularly LC-MS, has had significant impact into clinical research over a number of years now. In particular, LC-MS has revolutionised small molecule analysis, addressing analytical challenges and pushing limits in fields such as biomarker discovery and analysis of challenging compounds such as Steroids and Dihydroxyvitamin D. We present here a discussion on the novel approaches to furthering the capabilities of such applications, in particular the use of complimentary techniques such as Ion Mobility and simple sample preparation chemistries. Seminar delegates will have the opportunity to see examples of the multitude of research applications empowered by such technology advances, and discuss their impact with SCIEX experts in the field.

Podium Presentations

Tuesday, Wednesday & Thursday

Track	Room	Floor
1	Mozart 1-3	Ground
2	Mozart 4-5	Ground
3	Papageno	Ground
4	Paracelsus	***2nd***
5	Trakl	***3rd***
6	Doppler	***4th***

• Session 1 • Track 1 •

Metabolomics

Tuesday @ 15:00 in Mozart 1-3

Session Chair: Elizabeth Want - *Imperial College London*

Tuesday @ 15:00 in Mozart 1-3

Altered Brain Metabolism in Alzheimer Disease: Linking Peripheral and Central Metabolic Changes

Hector Gallart-Ayala - *Metabolomics Platform, University of Lausanne* (hector.gallartayala@unil.ch) -- *Young Investigator Grantee*

‣ Here we present a non-targeted metabolomics approach to identify a metabolic signature of Alzheimer disease (AD). This approach was applied to paired samples of peripheral plasma and CSF of cognitively impaired subjects with AD pathology confirmed by CSF biomarkers and healthy aged controls without cerebral AD pathology. Results obtained indicate common and distinctive metabolic alterations in plasma and in CSF, outlining significantly affected amino acid metabolism. Both, plasma and CSF imply the amino acid catabolism or degradation.

Tuesday @ 15:20 in Mozart 1-3

Mass Spectrometry-based Metabolic Profiling of Gut Microbiota Modulated Metabolites to Investigate Potential Health Effects on the Host

Zdenek Spacil - *Masaryk University* (spacil@recetox.muni.cz) -- *Young Investigator Grantee*

‣ Environmental factors may trigger diseases and arguably the most important of biotic factors is gut microbiota, directly affecting human health. However, molecular mechanisms underlying the interaction of microbe-derived metabolites with host signaling and metabolic pathways remain to be elucidated. Gut microbiota seems to influence physiological processes in the host, such as energy metabolism, immunomodulation or neurodevelopment. Mass spectrometry-based metabolic profiling was used to determine markers of microbial colonization, immune homeostasis, energy metabolism status and aging in various biological materials. To the best of our knowledge this is the first time metabolic profiling supported with targeted proteomics was used to simultaneously investigate several important pathways and to evaluate concentration levels of biomarkers in diverse biological materials.

Tuesday @ 15:40 in Mozart 1-3

Proton-Transfer-Reaction Time-Of-Flight Mass Spectrometry (PTR-TOF-MS) Analysis of Volatile Organic Compounds in Human Gastric Cancer Tissue

Mina Adam - *Imperial College London* (m.adam15@imperial.ac.uk) -- *Young Investigator Grantee*

‣ The detection and quantification of Volatile Organic Compounds (VOCs) has great potential in terms of disease diagnosis and measuring physiological response to treatment. In this study, Proton-Transfer-Reaction Time-Of-Flight Mass Spectrometry (PTR-TOF-MS) has been utilised for the identification of VOCs in gastric tissue samples from patients with oesphago-gastric cancer and those with healthy stomachs. A total of 41 compounds have been investigated Six VOCs including hexanoic acid, butyric acid, phenol, hexanal, nonanal and isoprene were found at higher concentrations in in cancer patients compared to non-cancer controls; these VOCs have been observed in a previous study at increased concentrations in the exhaled breath of oesophago-gastric cancer patients The preliminary results demonstrate that specific VOCs may arise directly from tissue and provide evidence for disease profiling.

• Session 1 • Track 2 •

Quality and Standardisation

Tuesday @ 15:00 in Mozart 4-5

Session Chair: Jody van den Ouweland - *Canisius-Wilhelmina Hospital, The Netherlands*

Tuesday @ 15:00 in Mozart 4-5

Application of LC-MS/MS in Routine Clinical Diagnostics: Has it Lived Up the Expectations?

Eef Lentjes - *University Medical Center Utrecht* (elentjes@umcutrecht.nl)

‣ We have investigated the performance of LC-MS/MS in comparison to immunoassays by analysis of 8 year data since the introduction of the LC-MS/MS method, from the Dutch EQAS for Endocrinology. The number of LCMSMS users is increasing each year and about 100 results are produced now per scheme by about 15 LCMSMS users. although accuracy has much improved, between laboratory CV is mostly higher for the LCMSMS group compared to immunoassay methods. We conclude that optimization and better standardization is necessary for LCMSMS methods.

Tuesday @ 15:20 in Mozart 4-5

Metrology for Clinical: From Small to Large

Christopher Hopley - *LGC* (Christopher.hopley@lgcgroup.com)

‣ Metrology research is critical to characterise higher order reference materials that are traceable to the SI. LGC is developing reference methods in the small molecule and large molecule areas to enable the production of higher order materials. This is not without its issues and challenges, some unique to the clinical area and some not. Here we present an outline of the approach taken at LGC and discuss the process of higher order material certification.

Tuesday @ 15:40 in Mozart 4-5

Quality by Design in Bioanalysis: Elvitegravir Determination

Sara Baldelli - *Clinical Pharmacology, L.Sacco University Hospital* (sara.baldelli@asst-fbf-sacco.it)

‣ The application of Quality by Design (QbD) principles in clinical laboratories can help to develop an analytical method through a systematic approach providing a significant advance over the traditional heuristic and empirical methodology. In the present work, we applied for the first time the QbD concept in the development of a method for drug quantification in human plasma using elvitegravir as the test molecule. The obtained method was validated according to EMA guidelines on bioanalytical method validation, and clinically applied with success.

• Session 1 • Track 3 •

Quantifying Proteins - Limits and Applications

Tuesday @ 15:00 in Papageno

Session Chair: Eva Hunyadi-Gulyas - *Biological Research Centre, Szeged*

Tuesday @ 15:00 in Papageno

Quantifying Proteins in Dried Blood Spots

Andy Hoofnagle - *University of Washington* (ahoof@u.washington.edu)

‣ To improve access to laboratory testing in remote sites and to facilitate more frequent measurements in longitudinal risk assessment, therapeutic monitoring, and clinical research studies, there is great interest in the use of dried blood spots in specimen collection. While there have been several studies investigating the feasibility of protein analysis in dried blood spots, comparisons with current clinically-used assays in serum and plasma are scarce. We used a precise and linear bottom-up proteomics assay to demonstrate that the measurement of apolipoproteins in dried capillary blood spots is not as accurate as needed for facile translation to clinical care.

Tuesday @ 15:20 in Papageno

How Low Can You Go? Using Flow to Measure Zero

Christopher Shuford - *Laboratory Corporation of America* (shuforc@labcorp.com)

‣ Thyroglobulin is measured in thyroid cancer patients following total-thyroidectomy as a marker for recurrent disease given circulating concentrations should be effectively zero. Although LC-MS/MS assays are resistant to autoantibody interferences (via tryptic digestion) that inhibit immunoassays, recent publications have demonstrated approximately 40% of individuals with recurrent disease go undetected by LC-MS/MS assays (Netzel et al, JCEM, 2015), suggesting autoantibodies decrease the circulating concentrations below the LLOQ of the assays used (<0.5 ng/mL). Attempting to improve the clinical sensitivity, we developed of an assay with an LLOQ of 20 pg/mL and observed a significant fraction of individuals with previously undetectable thyroglobulin did indeed have detectable/quantifiable amounts circulating.

Tuesday @ 15:40 in Papageno

Detection and Quantification of Carbohydrate Deficient Transferrin by MALDI-Compatible Protein Chips Prepared by Ambient Ion Soft Landing

Petr Pompach - *Institute of Microbiology* (petrpompach@gmail.com)

‣ The bioanalytical prospect of MALDI-compatible protein chips prepared by ambient ion soft landing is demonstrated on in-situ enrichment, detection and quantification of human transferrin and its carbohydrate deficient forms. The assay is based on the interaction between the immobilized antibody and the sampled analyte directly on the chip and subsequent analysis by MALDI mass spectrometry. The absence of any interlayer between conductive MALDI surface modified by ion landing and antibody affinity molecules reduces the non-specific interactions of other proteins in the sample and maintains the original conductivity of the MALDI plate, which provides efficient ionization.

• Session 1 • Track 4 •

Practical Training: Basic

Tuesday @ 15:00 in Paracelsus

Session Chair: Laura Owen - *University Hospital Of South Manchester*

Tuesday @ 15:00 in Paracelsus

Basics of MS/MS

Laura Owen - *University Hospital of South Manchester* (laura.owen@uhsm.nhs.uk)

‣ Tandem mass spectrometry is a technique that is often used in clinical laboratories for a wide variety of analytes. Its superior specificity is a major consideration which has led to the increase in its use over the last 10-15 years. Ionisation of the analyte of interest is essential to its measurement using this technique, with the main principle being the mass-to-charge ratio, referred to as the m/z. Understanding how a tandem mass spectrometer works and the principles behind its operation are invaluable for those interested in method development and troubleshooting.

• Session 1 • Track 5 •
Practical Training: Intermediate
Tuesday @ 15:00 in Trakl
Session Chair: Roland Geyer - *Thermo Fisher Diagnostics*

Tuesday @ 15:00 in Trakl
Quality Assurance for Clinical LC-MSMS in Production - Why, What and How
Roland Geyer *- University Institute of Clinical Chemistry, Inselspital, Bern University Hospital, University of Bern, Switzerland* (roland.geyer@gmail.com)
‣ In this practical training session we will present an overview of guidelines and recommendations for quality assurance (QA) in clinical laboratories and discuss a range of examples that are specific for the routine use of liquid-chromatography mass spectrometry (LC-MS) methods. LC-MS methods have the advantage of providing, besides the analyte concentration value, a range of additional metadata that are useful and easy to evaluate. Appropriate use of metadata can help to improve the quality of the laboratory service. As we ensure and improve the intra- and inter-lab reproducibility of results, Mass Spectrometry is moving closer to fulfilling it's potential as a gold standard for measuring the true concentration of analytes in routine clinical applications.

• Session 2 • Track 1 •

Analytical Methods in Metabolomics

Wednesday @ 10:45 in Mozart 1-3

Session Chair: Antonis Myridakis - *Imperial College London*

Wednesday @ 10:45 in Mozart 1-3

Simultaneous Quantification of Oxysterols and Bile Acids in Human Plasma by Liquid Chromatography Electrospray Ionization Tandem Mass Spectrometry

Madlen Sander - *Leipzig University* (madlen.sander@medizin.uni-leipzig.de) -- *Young Investigator Grantee*

‣ Bile acids and oxysterols are structurally related molecules derived from cholesterol. Despite evidence supporting a neuroprotective role in neurodegenerative disease, little is known about their molecular mechanisms or their physiological roles. The here described novel LC-ESI(+)MS/MS method combines the quantitation of 12 oxysterols and 17 free and conjugated bile acid without time consuming derivatization. The parameters for method validation: linear calibration range, inter-day coeffiecients of variation, lower limit of quantification, and autosampler storing stability were determined.

Wednesday @ 11:05 in Mozart 1-3

Pre-Analytic Evaluation of Volumetric Absorptive Microsampling and Integration in a Mass Spectrometry Based Metabolomics Workflow

Giuseppe Paglia - *EURAC Research* (giuseppe.paglia@eurac.edu)

‣ Integration of volumetric absorptive microsampling (VAMS) with mass spectrometry (MS) is an attractive solution for metabolomics studies. In this work, we integrated VAMS in a MS-based metabolomics workflow and investigated pre-analytical strategies such as sample extraction procedures and metabolome stability at different storage conditions. We found that the highest number and amount of metabolites were recovered upon extraction with acetonitrile:water. Prolonged storage of VAMS samples at room temperature caused significant changes in metabolome composition, but VAMS devices remained stable for up to six months at -80°C. The time used for drying the sample did also affect the metabolome. We finally employed the developed VAMS metabolomics workflow for investigating the alteration of iron homeostasis in mice fed diet rich in iron vs controls.

Wednesday @ 11:25 in Mozart 1-3

Investigating the Role of Collision Cross Section (CCS) in Metabolomics: How is CCS Used for Metabolite Identification?

Charles Nichols - *Vanderbilt University* (charles.m.nichols@vanderbilt.edu) -- *Young Investigator Grantee*

‣ Traditional global metabolomics workflows characterize molecular features by retention time (RT) and m/z. Notably, ion mobility (IM) spectrometry provides an orthogonal separation to liquid chromatography (LC) and mass spectrometry (MS). With LC-IM-MS, we gain an additional descriptor, namely collision cross section (CCS). However, CCS is not an intrensic value, and many parameters must be considered before CCS libraries can be generated and utilized for metabolite identification. This study is investigates the validity of CCS measurements alongside RT and m/z. It also investigates workflows for building CCS libraries and how to apply them to a real metabolomics dataset.

• Session 2 • Track 2 •

Androgens

Wednesday @ 10:45 in Mozart 4-5

Session Chair: Laura Owen - *University Hospital Of South Manchester*

Wednesday @ 10:45 in Mozart 4-5

Investigation of Androgen Excess in Women

Brian Keevil - *University hospital of South Manchester* (brian.keevil@uhsm.nhs.uk)

‣ Demonstration of androgen excess is important in women but there is currently no consensus on what is the best androgen to measure. LC-MS/MS is increasingly being used in the clinical laboratory for steroid measurement particularly in multiplexed panels.

Wednesday @ 11:05 in Mozart 4-5

A Broad LC-MS/MS Serum Profiling Revealed a Specific Steroid Pattern in Hirsute Women with Polycystic Ovary Syndrome

Flaminia Fanelli - *University of Bologna - S.Orsola-Malpighi Hospital* (flaminia.fanelli@gmail.com)

‣ Hirsutism and hyperandrogenemia are indistinctly used to assess hyperandrogenism in the diagnosis of polycystic ovary syndrome (PCOS), however, recent studies suggest that they have different hormonal and metabolic correlates. LC-MS/MS multianalyte potential was used to characterize steroid profile in hirsute vs not hirsute women characterized by different combination of hyperandrogenemia and ovarian dysfunction. While idiopathic hirsutism did not show relevant alteration of the steroid profile and of enzyme activity pattern, hirsute PCOS women displayed an increased P450 activity and a less severe androgen profile compared to PCOS not hirsute counterparts, combined with a less active gonad secretion and with a higher activity of the glucocorticoid pathway. Our results overall suggest an involvement of the adrenal in the hirsute PCOS phenotype.

Wednesday @ 11:25 in Mozart 4-5

Biological Variation of Testosterone, Dihydrotestosterone and their Ratio Determined in 30 Healthy Individuals with LC-MS/MS

Anna van der Veen - *University Medical Center Groningen* (a.van.der.veen03@umcg.nl) -- *Young Investigator Grantee*

‣ For correct interpretation of laboratory data, information on biological variation is essential, including within-person variation (CVi), between-person variation (CVg), analytical variation (CVa) and the reference change value (RCV). Recently, in our laboratory the biological variation was determined for plasma testosterone (T), dihydrotestosterone (DHT) and the DHT/T-ratio using online-SPE coupled to LC-MS/MS in 30 healthy individuals over a period of 4 months with 4 weeks intervals. Comparable CVi's and RCVs in men and women varied from 10-16% and 30-42%, respectively. The CVg was higher in women (35-45%) compared to men (19-31%). The data on biological variation shows a high degree of individual variation, illustrating its importance and careful interpretation of single measurements for T and DHT. The RCVs are valuable for the assessment of significant changes in patient follow-up.

• Session 2 • Track 3 •

Recent Trends in Whole-Cell MALDI-TOF

Wednesday @ 10:45 in Papageno

Session Chair: Simon Cameron - *Imperial College London*

Wednesday @ 10:45 in Papageno

Mass Spectrometry in the Micro Lab Workflow Beyond Identification

Stefan Zimmermann - *Department of Infectious Diseases* (stefan.zimmermann@med.uni-heidelberg.de)

‣ Multi-resistant Gram-negative bacteria are one of the biggest threads of global health. Mass spec-trometry opens up new possibilities for rapid and reliable detection of the underlying mechanisms. If such bugs are detected in the hospital, effective infection control is urgently necessary, which includes rapid in-house tools for outbreak analysis. New approaches show that this kind of analysis can also be done by mass spectrometry technologies.

Wednesday @ 11:05 in Papageno

Beyond "Bacterial Identification Revolution" – Detection of Resistance Markers by MALDI-TOF MS

Markus Kostrzewa - *Bruker Daltonik GmbH* (markus.kostrzewa@bruker.com)

‣ The globally increasing spread of bacterial antibiotic resistances demands for rapid detection methods. Novel applications of MALDI-TOF MS could fit this purpose; in particular, the possibility to detect specific peaks "in real time" in the bacterial identification mass spectrum, corresponding to antibiotic resistance markers, allows an innovative and extremely fast approach. Here, we investigate the use of MALDI-TOF MS (MALDI Biotyper – Bruker Daltonik, Germany) to subtype methicillin-resistant Staphylococcus aureus (testing n=1304 clinical isolates), and KPC-producing Klebsiella pneumoniae (testing n=4821 strains), and evaluate the possibility of a commercial software, to achieve an "instant resistance detection" directly during routine identification process.

Wednesday @ 11:25 in Papageno

Detection of Carbapenem-Resistance in *Bacteroides fragilis* by MALDI-TOF MS – a Quantum Leap

Miriam Cordovana - *University Hospital Sant'Orsola-Malpighi, Bologna* (miri-78@live.it)

‣ Carbapenem-resistance in Bacteroides fragilis is related to the cfiA-encoded metallo-beta-lactamase, and represents an emerging problem worldwide. Rapid detection of carbapenemase-producing strains is crucial for a proper treatment of patients, especially in bloodstream infections. While classical phenotypic and molecular methods present several key issues and limits, the latest applications of MALDI-TOF MS allow an approach that could perfectly fit this purpose.Here, n=302 Bacteroides fragilis strains were subtyped by MALDI-TOF MS (MALDI Biotyper, Bruker Daltonik) to detect cfiA-carrying strains, and the carbapenemase activity was verified and characterized by MBT STAR-CARBA hydrolysis assay. Further, 16 spiked positive blood cultures underwent the same approach, to evaluate a direct application of these methods on the primary sample.

• Session 2 • Track 4 •

Practical Training: Basic

Wednesday @ 10:45 in Paracelsus

Session Chair: Michael Vogeser - *Institute of Laboratory Medicine, Hospital of the University of Munich, Germany*

Wednesday @ 10:45 in Paracelsus

Basics of LC

Michael Vogeser - *Hospital of the University of Munich, Germany* (michael.vogeser@med.uni-muenchen.de)

‣ The aim of this session is to make users with little to no LC training familiar with the typical set-up of LC-configurations is diagnostic MS/MS assays including 2D-chromatography / on-line solid phase extraction. The session will address hardware components, basic performance descriptions and frequent problems observed in routine application.

• Session 2 • Track 5 •
Practical Training: Intermediate
Wednesday @ 10:45 in Trakl
Session Chair: Russell Grant - *Laboratory Corporation of America*

Wednesday @ 10:45 in Trakl
How to Achieve Lower Quantification Limits
Russell Grant - *Laboratory Corporation of America* (grantr@labcorp.com)
‣ This one hour session will be given as three 20 minute linked vignettes and will explore established and novel approaches to definitively improve analytical measurement performance - with the end goal of improving assay LLOQ. Part 1 "Foundations": Basis of LLOQ, signal:noise, lossless systems, and practically determining and improving measurement precision. Part 2 "Formulation": Getting the most out of your assay and system components, LC and preparative orthogonality and demystifying the black box after the LC via signal manipulation, smoothing and quadrupole resolution. Part 3 "Finesse": Tying the pieces together with assay exemplars.

• Session 2 • Track 6 •

Intraoperative Applications

Wednesday @ 10:45 in Doppler

Session Chair: Kristina Schwamborn - *Institute of Pathology, TU Munich*

Wednesday @ 10:45 in Doppler

Multimodal Molecular Profiling by Mass Spectrometry (Imaging): On its Way to Clinics?

Tiffany Porta - *Maastricht University* (t.porta@maastrichtuniversity.nl)

‣ Tissue diagnostics can be challenging due to the presence of confounding factors such as inflammation or the lack of a minimum level of differentiation of tumor cells. Recently, histological evaluation of tumor based on tissue-specific molecular signature has revealed his potential to help accurate tissue diagnosis. Here, we highlight the MS-based tissue classification techniques of tomorrow that would help clinicians with their daily practice. Namely, in the hands of surgeons, rapid evaporative ionization mass spectrometry would guide in real-time and optimize surgical resection within the anatomic boundaries reducing the incidence of incomplete tumor resection. The pathologists could greatly benefit from laser microdissection coupled to mass spectrometry to improve their diagnostics from frozen sections in a minute.

Wednesday @ 11:05 in Doppler

Nondestructive Tissue Analysis for *ex vivo* and *in Vivo* Cancer Diagnosis Using a Biocompatible Mass Spectrometry System

Marta Sans - *The University of Texas* (msans@utexas.edu) -- *Young Investigator Grantee*

‣ Conventional methods for histopathologic tissue diagnosis can delay decision-making during diagnostic procedures. We report the development of an automated and biocompatible handheld mass spectrometry device for rapid diagnosis of human cancer tissues. Statistical classifiers based on lipid and metabolites allowed prediction with high sensitivity (96.4%), selectivity (96.2%) and overall accuracy (96.3%) for breast, lung, thyroid and ovarian cancer. Lastly, we applied the device for *in vivo* cancer diagnosis during surgery performed in tumor-beating mice models. Our results suggest this technology as a potential clinical and intraoperative tool for *ex vivo* and *in vivo* cancer diagnosis.

Wednesday @ 11:25 in Doppler

Identification of Cancerous and Precancerous Cervical Abnormalities in Real-Time with the Use of Rapid Evaporative Ionization Mass Spectrometry (REIMS)

Menelaos Tzafetas - *Imperial College London* (m.tzafetas@imperial.ac.uk) -- *Young Investigator Grantee*

‣ Cervical cancer and its precancerous form cervical intraepithelial neoplasia (CIN) commonly affect women of reproductive age. Fertility-preserving procedures fail at rates of 33% due to incomplete excision. Rapid Evaporative Ionization Mass Spectrometry(REIMS) analyzes electrosurgery-generated aerosols, using time-of-flight mass spectrometry to provide real time tissue identification without the need for sample preparation, raising the potential for intraoperative use. We conducted a pilot study showing that REIMS can differentiate between cancerous and healthy cervical tissue thus presenting an innovative technique that could improve fertility-sparing operations. Currently we are investigating the application of REIMS for identification of CIN abnormalities and its direct use in the colposcopy clinic.

• Session 3 • Track 1 •

Metabolite Profiling

Wednesday @ 14:45 in Mozart 1-3

Session Chair: Hector Gallart Ayala - *University of Lausanne*

Wednesday @ 14:45 in Mozart 1-3

Optimisation and Validation of a High-Throughput Semi-Targeted Method by GC-MS with Metabolite Libraries for Large Scale Molecular Epidemiological Research

Antonis Myridakis - *Imperial College London* (a.myridakis@imperial.ac.uk) -- *Young Investigator Grantee*

‣ Metabolomics is one of the most fast growing fields in systems biology. Gas chromatography−mass spectrometry (GC-MS) approaches combine the coverage of the untargeted pipelines, with the library-facilitated, rapid metabolite identification. We developed a new holistic and high-throughput GC-MS profiling protocol samples with the use of metabolite libraries and validated for human urine and plasma samples. We optimized sample preparation, peak integration, quality control and data preprocessing steps. We compared several sample clean-up conditions and software packages for the data analysis. We present a detailed pipeline from sample aliquoting to the assigned metabolites table. The method was validated by analysing 356 human urine and plasma samples. 84 and 56 assigned metabolites passed the quality criteria, respectively for plasma and urine.

Wednesday @ 15:05 in Mozart 1-3

Quantification of Urinary Organic Acids Using Liquid Chromatography- Tandem Mass Spectrometry

Gökçe Göksu Gürsu - *JASEM Laboratory systems and solutions* (gokce.goksu@jasem.com.tr)

‣ Screening the profile of urinary organic acids can be powerful reflector for inborn errors of metabolism called organic acidurias (OAs) are characterized by defections of inherited enzymes related to amino acid, carbohydrate or lipid metabolic pathways which lead to accumulation abnormal amounts of organic acids in tissues and human urine. LC–MS/MS has arisen as a significant approach including ease of sample preparation for the quantitative analysis of metabolites from human body fluids. In our present study, we have developed OA quantification method using LC-MS/MS with excellent chromatographic separation of isomers and dilute & shoot sample preparation technique in urine.

Wednesday @ 15:25 in Mozart 1-3

Accurate and Confident Metabolic Phenotyping - Combining a Standardized and Quantitative Targeted Assay with Orbitrap™ Technology

Therese Koal - *BIOCRATES Life Sciences AG* (therese.koal@biocrates.com)

‣ Standardized, quantitative assays have increasingly been desired in metabolomics, especially in targeted studies. We developed the AbsoluteIDQ® p400 HR Kit to facilitate the quantitative analysis on Thermo Scientific™ Q ExactiveTM Orbitrap™ HRAM MS platform for the first time, bridging the gap between targeted quantitative metabolomics and profiling. The kit quantifies up to 408 metabolites of 11 classes: amino acids, biogenic amines, acylcarnitines, phosphatidylcholines, lysophosphatidylcholines, sphingomyelins, ceramides, cholesteryl esters, diglycerides, triglycerides, and hexoses. A beta-test has been carried out across 3 laboratories on different Q ExactiveTM platforms showing high inter-laboratory comparability, which is mandatory for robust, routine applications in targeted metabolomics.

• Session 3 • Track 2 •

Endocrine

Wednesday @ 14:45 in Mozart 4-5

Session Chair: Brian Keevil - *University Hospital Of South Manchester*

Wednesday @ 14:45 in Mozart 4-5

Single Assay Measurement of the Aldosterone-Renin-Ratio by Online SPE-UHPLC-MS/MS

Nicola Gray - *Shimadzu UK* (nicola.gray@shimadzu.co.uk)

‣ The measurement of the aldosterone-renin-ratio (ARR) is a recommended screening tool for primary aldosteronism. Aldosterone is classically measured in plasma/serum, while renin is often quantified by its activity, measuring angiotensin-I generation in a defined time range. Several reports describe the measurement of aldosterone or plasma renin activity (PRA) by LC-MS/MS, but no method has yet proposed a combined assay. We present an assay to measure low aldosterone levels as well as low PRA in a single sample with a simplified workflow.

Wednesday @ 15:05 in Mozart 4-5

Interference from Alpha- and Beta-Dihydrocortisone in Salivary Cortisol Assays: Ramifications for Patient Care

James Hawley - *University Hospital South Manchester* (james.hawley@uhsm.nhs.uk) -- *Young Investigator Grantee*

‣ We present a novel LC-MS/MS method for the measurement of salivary cortisol and cortisone using protein precipitation for sample preparation. Recent literature has suggested that two isobaric cortisol metabolites, alpha-dihydrocortisone and beta-dihydrocortisone, are difficult to separate chromatographically. Here, we utilise biphenyl chromatography to separate these metabolites from cortisol prior to LC-MS/MS analysis. We show that failure to separate these metabolites from cortisol may result in unnecessary over-investigation of patients. The method is well validated and with an injection-to-injection run time of only 2.5 minutes integrates well into the workflow of a busy, high-throughput clinical laboratory.

Wednesday @ 15:25 in Mozart 4-5

Derivatization as a Tool for Reaching Low pg/mL Detection Limits in Salivary Steroidomics

Cato Brede - *Stavanger University Hospital* (ca2brede@gmail.com)

‣ Measurement of multiple salivary steroid hormones requires LC-MS/MS methods with the ability to detect many of these at the low pg/mL level. Sample preparation for analyte enrichment is required. We have optimized a liquid-liquid extraction procedure for saliva, including the use of tannic acid as a novel emulsion preventing reagent, and applied robot pipetting in the 96-well plate format. We tested 5 different derivatization reagents, in order to achieve the most sensitive detection with low LC complexity. The final validated assay included cortisol, cortisone, testosterone, DHEA, progesterone, and 17-OHP.

• Session 3 • Track 3 •

Clinical Proteomics in Cancer and Immune-related Diseases

Wednesday @ 14:45 in Papageno

Session Chair: Lars Rasmussen - *Odense University Hospital*

Wednesday @ 14:45 in Papageno

Deciphering Molecular Consequences of the Prohormone Convertase 1/3 Inhibition in Macrophages for Application in Immunotherapy

Michel Salzet - *Laboratoire PRISM U1192, INSERM* (michel.salzet@univ-lille1.fr) -- *Young Investigator Grantee*

‣ The prohormone convertase 1/3 (PC1/3) is an enzyme playing an important role in the processing within the regulated secretory pathway in the nervous system. We showed by proteomic that PC1/3 is implicated un innate immunity. We demonstrated that PC1/3 inactivated macrophages express an M1-like phenotype, pro-inflammatory chemokines and cytokines secretion and TLR4 Myd88 dependent signaling activation. Under LPS/taxol challenge, PC1/3 KO cells secrete through store-operated calcium entry increase, a cocktail of pro-inflammatory factors including DAMPS. This secreted factors have been shown to favors Th1 response and inhibit viability and resistance of breast and ovarian cancer cells. This strategy can be used as a potential immune therapy for awaking intratumoral macrophages.

Wednesday @ 15:05 in Papageno

Comprehensive Proteomic Analysis of the Psoriatic Non-Lesional and Healthy Skin with Label-Free Semi-Quantitative Approach

Eva Hunyadi-Gulyas - *Laboratory of Proteomics Research, BRC, HAS* (egulyas@brc.hu)

‣ Psoriasis is a multifactorial skin disease, 2-4% of the population is affected. The subject of this investigation is its most frequent type, the psoriasis vulgaris. Our aim was to identify consistent alterations present in the non-lesional psoriatic versus healthy skin at the proteomic level. We believe, the results will provide some predetermining factor, possibly some drug target for this disease. Multi-step protein extraction followed by tryptic digestion and extensive fractionation on peptide level were applied. Spectral count based label-free semi quantitative analysis were performed. This non-hypothesis driven analysis identified several known as well as potentially novel differentially expressed psoriasis-associated proteins.

Wednesday @ 15:25 in Papageno

Quantification of PI3K p110a, PTEN and AKT I+II in Colorectal Cancer Cell Lysate and Tissue Samples Using Immuno-MALDI (iMALDI)

Björn Fröhlich - *UVic Genome BC Proteomics Centre* (bjorn@proteincentre.com) -- *Young Investigator Grantee*

‣ Colorectal cancer is one of the most common cancers in incidence and cancer-related deaths. The PI3K/AKT/mTOR pathway is commonly upregulated in colorectal cancer and is the target of many anti-cancer therapies. Immuno-MALDI (iMALDI) was used to quantify the expression levels and phosphorylation status of key proteins in this pathway, which could be useful for patient stratification. Cancer cell lysates were digested using trypsin, stable-isotope labeled standards added, enriched from the sample using anti-peptide antibodies and analysed using MALDI-TOS MS. Quantification of AKT I+II expression-and-phosphorylation levels was performed on cell lysates and tumor tissue. Endogenous PI3K p110a and PTEN was detected in cell lysate. The next steps of this project will include additional method validation and a higher degree of multiplexing.

• Session 3 • Track 4 •

Practical Training: Basic

Wednesday @ 14:45 in Paracelsus

Session Chair: Judy Stone - *Center for Advanced Laboratory Medicine (CALM) at the University of California, San Diego*

Wednesday @ 14:45 in Paracelsus

Basics of Sample Preparation - Remaining Unfazed while Your Analytes Move from Phase to Phase

Judith Stone - *Univ. of Calif. San Diego Health System* (jastone@ucsd.edu)

‣ Sample preparation for LC-MSMS is often thought of as a necessary evil. The topic is complex and there is conflicting advice about what technique to use. The default choices are dilution and protein precipitation because of their ease of use. This presentation will discuss how to proceed when a more complex and/or expensive sample preparation protocol than those defaults is under consideration. Proceeding step-by-step through an example, the goal is to demystify for the new user the processes of selecting, evaluating, comparing, optimizing and performing pre-validation studies with the common LC-MSMS sample preparation protocols used for small molecule quantitation.

• Session 3 • Track 5 •
Practical Training: Intermediate
Wednesday @ 14:45 in Trakl
Session Chair: Brian Rappold - *Essential Testing*

Wednesday @ 14:45 in Trakl
Pragmatic HILIC for the Clinic
Brian Rappold - *Essential Testing* (rappoldbr@hotmail.com)
‣ Hydrophilic-interaction-liquid chromatography (HILIC) is a separation technique orthogonal to the more commonly used reversed-phase chromatography. Reversed phase techniques are, in general, useful for non-polar compounds but poorly suited to the separation of highly polar compounds. HILIC techniques provide broad capabilities in polar separations, but the diagnostic LC-MS assays utilizing HILIC are infrequent, perhaps due to misunderstandings in the differences between HILIC and reversed-phase separations in regards to development and utility. This series will discuss development and practical fundamentals of the HILIC technique.

• Session 3 • Track 6 •
Applications in Routine Pathology
Wednesday @ 14:45 in Doppler
Session Chair: Isabelle Fournier - *Laboratoire PRISM, University Lille*

Wednesday @ 14:45 in Doppler
Imaging Mass Spectrometry - Possible Applications in Pathology
Kristina Schwamborn - *Institute of Pathology, TU Munich* (kschwamborn@tum.de)
‣ Reliable markers for diagnostic purposes or markers that correlate with prognosis and therapeutic response are needed in Pathology day to day practice. Since matrix assisted laser desorption ionization (MALDI) imaging mass spectrometry (IMS) goes far beyond microscopy it is ideal for this endeavor. MALDI IMS can generate molecular maps of tissue sections that can elucidate the underlying biochemistry or provide information on how therapeutics or toxins influence the function or misfunction of an organ. Thus, it has the potential to overcome limitations of other approaches in the identification and routine diagnostic measurement of new marker molecules/profiles.

Wednesday @ 15:05 in Doppler
Differentiating Benign and Malignant Endometrial Tissue Subtypes Using Desorption Electrospray Ionisation Mass Spectrometry Imaging (DESI-MSI)
Tanja Farrokh-Eslamlou - *Imperial College London* (ssf16@ic.ac.uk) -- *Young Investigator Grantee*
‣ Endometrial cancer (cancer of the womb lining) is the most common gynaecological cancer diagnosed in Europe. Strongly associated with obesity, the number of new cases of endometrial cancer being diagnosed is rising. DESI-MSI is an ambient ionisation technique that allows direct correlation between biochemical changes and histological features within a tissue. Detection of tissue-specific lipid ion patterns enables a novel method for tumour biology investigation by providing unique, biochemical information. This pilot study demonstrates the successful application of DESI-MSI as a tool for accurate characterisation of endometrial tissues.

Wednesday @ 15:25 in Doppler
3D Mass Spectrometry Imaging of Human FFPE Bladder Cancer Resections
Naomi Vos - *M4I division of IMS, Maastricht University* (n.vos@maastrichtuniversity.nl) -- *Young Investigator Grantee*
‣ Currently 2D MSI methods provide only a small snapshot of the chemical state of bulk tissue. Currently almost all 3D-MSI studies have been performed on lipids primarily due to their ease of detection and reproducible sample preparation requirements. However FFPE tissues, such as those stored in large biobanks worldwide, are not amenable to lipid analysis but instead require careful sample treatment to enable detection of tryptic peptides. We demonstrate among the first reports of 3D peptide MALDI-MSI of FFPE tissues. Bladder cancer resections from 11 patients were studied with MSI enabling both inter- and intra-tumour heterogeneity to be visualised in 3-dimensions.

• Session 4 • Track 1 •

Metabolite Profiling Methods

Wednesday @ 16:45 in Mozart 1-3

Session Chair: Roland Geyer - *Inselspital Bern*

Wednesday @ 16:45 in Mozart 1-3

Application of LC-MS/MS Metabolomics - Quantitative High-Throughput Method for Direct Measurements of Enterolactone Glucuronide, Sulfate and Free Enterolactone

Natalja Pustovalova Nørskov - *Aarhus University* (Natalja.Norskov@anis.au.dk) -- *Young Investigator Grantee*

‣ Enerolactone was discovered more than 30 years ago and since then it has been considered as a biomarker of healthy lifestyle in epidemiological studies. To measure enterolactone in plasma requires enzymatic hydrolyses as enterolactone is typically conjugated with glucuronic acid and sulfate. We have developed and validated a high-throughput LC-MS/MS method to quantify enterolactone without the need for hydrolysis. This has several advantages such as simple sample preparation procedure and measurement of enterolactone in its intact forms. The method has short chromatographic run time of 2.6 min with good accuracy and precision and high sensitivity, LLOQ down to 16 pM.

Wednesday @ 17:05 in Mozart 1-3

Development and Validation of an LC-MS/MS Method for Measurement of Methylmalonic Acid and Homocysteine in Human Plasma

Forough Bahadory - *SEALS, Department of Clinical Chemistry* (Forough.Bahadory@health.nsw.gov.au) -- *Young Investigator Grantee*

‣ Methylmalonic acid (MMA) is considered to be the most specific marker for vitaminB12 deficiency and methylmalonic acidaemia. VitaminB12 or folic acid deficiency can lead to hyperhomocysteinaemia. Traditionally analysis of MMA and homocysteine has been performed separately, limited by interfering substances (succinate), and required extensive sample pre-treatment. Here we present a simple, specific and time efficient LC-MS/MS assay to measure homocysteine and MMA simultaneously in plasma, free from interferences. Using protein precipitation techniques followed by a selective chromatographic separation, we have developed a fast, reliable assay readily amenable to automation into high throughput laboratories.

Wednesday @ 17:25 in Mozart 1-3

Lipidomic Evaluation of Cultured Cell Lines

Finnur Freyr Eiriksson - *University of Iceland* (finnur@arcticmass.is) -- *Young Investigator Grantee*

‣ It is now realized that lipids exhibit a wide variety of physiological functions, structural as well as regulatory. Evidence links carcinogenesis to metabolic control and indicates risk association of cancer with obesity. The aim of this project is to establish a lipidomic-based UPLC-QToF method for evaluation of lipid composition in cultured cells of normal and cancerous origin. PCA analyses revealed differences in the lipidomes of several cancer cell lines. Phosphocholins were significantly elevated in Sk-Br-3 (overexpresses fatty acid synthase) compared to other cell lines. The lipidomes of D492 and its subline D492M, which has undergone epithelial-to-mesenchymal transition, were significantly different.

• Session 4 • Track 2 •

Vitamin D

Wednesday @ 16:45 in Mozart 4-5

Session Chair: Flaminia Fanelli - *University of Bologna - S.Orsola-Malpighi General Hospital, Italy*

Wednesday @ 16:45 in Mozart 4-5

A Fast and Simple Method for Simultaneous Measurements of 25(OH)D, 24,25(OH)2D and the Vitamin D Metabolite Ratio (VMR) in Serum Samples by LC-MS/MS

Neus Fabregat-Cabello - *University of Liège, CHU de Liège* (n.fabregat@ulg.ac.be) -- *Young Investigator Grantee*

‣ We present here a rapid, easy, reliable and cost-effective method for the quantification of 25-hydryxoyvitamin D2 and D3, epi-25-hydroxyyvitamin D3 and 24,25-dihydroxyvitamin D3 by LC-MS/MS in serum samples. The proposed methodology has been strongly validated with both NIST and Labquality materials, obtaining mean intra-assay and inter-assay imprecision lower than 6 and 6.4% and mean recoveries within 95-104%. Besides we have compared satisfactorily samples from Vitamin D Standardization Program (n=80) with reference values and patient samples (n=281) with our reference LC-MS/MS method. The proposed methodology is prepared to be used in routine testing and permits the calculation of the Vitamin D Metabolite Ratio (VMR).

Wednesday @ 17:05 in Mozart 4-5

Time-Course Analysis of 3-epi-25-Hydroxyvitamin D3 Shows Markedly Elevated Levels in Early Life, Particularly from Vitamin D Supplementation in Preterm Infants

Jody van den Ouweland - *Canisius-Wilhelmina Hospital* (j.v.d.ouweland@cwz.nl)

‣ We have studied dynamics of 3-epi-25(OH)D3 formation during infancy by measuring 25(OH)D3 and 3-epi-25(OH)D3 levels by LC-MS/MS in (early)preterm and term infants up to 2 years of age. At birth, all infants showed low contribution of 3-epi-25(OH)D3, increasing the week after starting vitamin D supplementation, until three months of age. Highest levels of 3-epi-25(OH)D3 were found in early preterm infants, supporting the hypothesis that hepatic immaturity plays a role in 3-epi-25(OH)D3 formation.

Wednesday @ 17:25 in Mozart 4-5

SPME as Sample Preparation Technique Applied in Prohibited Substances Analysis from Various Matrices – Promising Tool for Doping Control Laboratories?

Krzysztof Gorynski - *Nicolaus Copernicus University Collegium Medicum* (gorynski@gmail.com) -- *Young Investigator Grantee*

‣ One of the tasks of the doping control laboratories is applying reliable techniques that are capable of multi-compound analysis at least on cut-off concentration levels. Today, the determination of substances in complex biological matrices cannot be performed without proper sample preparation, even when using highly powerful and efficient analytical instrumentation, such as LC-MS. Solid Phase Microextraction (SPME) is a sampling and sample preparation technique that has indicated its great potential for analysis of prohibited substances from complex matrices. Ongoing studies expend utilization of the technology for saliva analysis as an alternative specimen to urine and blood during doping control testing. Thus, in this talk we will describe recent developments in SPME relevant to the potential applications toward doping control of urine, plasma, blood or alternative matrices.

• Session 4 • Track 3 •

Revolutionizing Pathogen Detection by LC-MS/MS Proteotyping

Wednesday @ 16:45 in Papageno

Session Chair: Stefan Zimmerman - *University of Heidelberg*

Wednesday @ 16:45 in Papageno

Identification of Microorganisms Grown in Blood Culture Flasks Using LC-HRMS/MS

Armand Paauw - *TNO* (armand.paauw@tno.nl)

‣ Rapid and accurate identification of the causative pathogen of bloodstream infection (BSI) is key to respond adequately to the BSI. Therefore, a LC-HR-MS/MS based method was developed that was able to correctly identify 100% of the mimicked positive blood cultures (n=86). Microorganisms tested included bacteria commonly found in BSI, biological threat agents (BTAs), and species genetically closely related to BTAs. Clearly, LC-HR-MS/MS analysis of the peptidome from positive blood cultures allows for the unambiguous identification of microorganisms. This method makes it possible to identify the causative pathogen within 8 h after a positive blood culture.

Wednesday @ 17:05 in Papageno

Proteotyping: Tandem Mass Spectrometry Shotgun Proteomic Characterization and Typing of Pathogenic Microorganisms

Roger Karlsson - *Sahlgrenska Academy, University of Gothenburg* (roger.karlsson@nanoxisconsulting.com)

‣ We explore the use of proteotyping, that is, mass spectrometry and proteomic analysis for rapid and accurate detection of microorganisms, with special interest in pathogenic bacteria. Proteotyping has a higher potential in achieving strain resolution as compared to phenotyping or genotyping, and it can also be used for co-infections. Simultaneously, traits of virulence and antibiotic resistance can be detected. In doing so, the use of broad spectrum antibiotics can be reduced. The ultimate goal is to apply the methodology directly to clinical samples without the need for culturing prior analysis, thus generating a diagnostic protocol, for reliable, rapid, point-of-care diagnostics.

Wednesday @ 17:25 in Papageno

Metaproteomics for the Clinics: Quick Survey of Microbiota by MS/MS

Jean Armengaud - *CEA* (jean.armengaud@cea.fr)

‣ Characterizing human microbiota is becoming more and more important in the clinical lab. Metaproteomics aims at exploring the functional pathways present in a complex microbiota, but it may also help to establish an inventory of organisms. Evaluating parameters for tandem mass spectrometry data acquisition and bioinformatics tools for mining metaproteomics datasets is essential to establish the degree of confidence in the results obtained. We propose a microbiota reference standard, namely Mix24X, which may help in optimizing parameters for data acquisition by tandem mass spectrometry and data processing. We propose a cascaded search for interpreting tandem mass spectrometry results consisting in three query cycles that allows minimizing false-positives estimated on an experimental basis. This study paves the way to further normative approach for metaproteomics in the clinical lab.

• Session 4 • Track 4 •
Practical Training: Basic
Wednesday @ 16:45 in Paracelsus
Session Chair: Michael Wright - *LGC Group*

Wednesday @ 16:45 in Paracelsus
System Suitability Tests Part 1: Introduction to System Suitability Tests
Michael Wright *- LGC, Drug Development Services* (michael.wright@lgcgroup.com)
‣ System Suitability Tests (SST) are a valuable tool for ensuring data quality in clinical diagnostic testing. The information gleamed from running an SST prior to analysis can dictate whether a batch of samples is run and, if not, acts as an immediate troubleshooting guide. Additionally it provides data over time to determine preventative maintenance required to develop a robust platform. Focussing on LC-MS/MS this talk will cover creating an SST material, a number of different SST strategies and deciding on acceptance criteria.

Wednesday @ 17:05 in Paracelsus
System Suitability Tests Part 2: Troubleshooting Common Issues
Michael Wright *- LGC, Drug Development Services* (michael.wright@lgcgroup.com)
‣ Having set the scene on establishing System Suitability Tests (SST) the focus is now on what to do when the SST fails. Starting from the presentation of symptoms displayed by the SST chromatogram, through the process of determining the next troubleshooting experiments to be run, and finally to the diagnosis and treatment of the problem, it will soon become apparent why many call the SST "the Doctor".

Wednesday @ 17:25 in Paracelsus
System Suitability Tests 3: Case Studies
Michael Wright *- LGC, Drug Development Services* (michael.wright@lgcgroup.com)
‣ This talk will cover a series of "real world" case studies of LC-MS/MS assays where the system suitability test (SST) injection failed, or where it passed but the acceptance criteria had not been stringent enough. In each example the investigation will be walked through step by step: from the initial chromatograms, through to the troubleshooting process performed, the results from those experiments and the changes in processes that were introduced to prevent reoccurrence.

• Session 4 • Track 5 •
Practical Training: Intermediate
Wednesday @ 16:45 in Trakl
Session Chair: Chris Shuford - *Laboratory Corporation of America*

Wednesday @ 16:45 in Trakl
Getting Started with Protein Quantitation
Christopher Shuford - *Laboratory Corporation of America* (shuforc@labcorp.com)
‣ Quantification of protein biomarkers for diagnostic applications are becoming increasingly common given the analytical advantages it provides relative to conventional immunometric techniques. To that end, and overview will be given on the basics of designing a targeted protein assay, considerations in optimizing the assay work-flow, and the common pitfalls faced when standardizing a mass spectrometry-based protein assay.

• Session 4 • Track 6 •
New Technologies
Wednesday @ 16:45 in Doppler
Session Chair: Tiffany Porta - *Maastricht University*

Wednesday @ 16:45 in Doppler
The Implementation of Needle Electrospray Ionisation Mass Spectrometry for the Analysis of Aspiration Fluid Cytology in Locally Advanced Oesophageal Cancer
Pranav Patel - *Imperial College London. London, UK.* (php02@imperial.ac.uk) -- *Young Investigator Grantee*
‣ Oesophago-gastric cancer is the 5th most common cause of cancer in the world, however patients typically present late with advanced disease. Disease staging is crucial in Oesophago-gastric cancer, lymph node fluid cytology assessment is used to determine local disease spread. The accuracy of this technique can be variable. Here, we demonstrate a novel technique for the analysis of fluid cytology directly from the aspiration needle collection device using mass spectrometry. This method is based upon analysis of the cancer cell lipidome, and has proven to be rapid, easy and tissue type specific. Thereby being translational to alternative cancer cytology sub-types.

Wednesday @ 17:05 in Doppler
Can Real-Time Molecular Analyses Change the Paradigm of Dog Sarcoma Diagnosis and Classification?
Isabelle Fournier - *Laboratoire PRISM U1192, INSERM* (isabelle.fournier@univ-lille1.fr)
‣ One major difficulty of sarcoma is the fact that they have poorly defined margins. In order to improve the diagnosis and better define the margins during the surgery SpiderMass instrument will be used. Classification performance of this novel surgery instrument in pre-operative conditions on fresh biopsies has been tested. A clear differentiation between healthy and cancerous layers of different types of sarcoma have been observed. Specific markers of between tumour and heathy group have been identified by real time MS/MS. Based on such a classification, margins studies have been undertaken and compared to MALDI Mass spectrometry imaging confirming the high accuracy of SpiderMass technology.

Wednesday @ 17:25 in Doppler
Chemical Scanning of Cancer Tissues by the Combination of Mass Spectrometry with Molecular Resonance Probe Desorption
Vladimir Frankevich - *Research Center for Obstetrics and Gynecology* (vfrankevich@gmail.com)
‣ Chemical scanning of cancer tissues by the combination of mass spectrometry with molecular resonance probe desorption. Molecular composition differences in real time were shown for different cancer tissues. Multivariate analysis was used to extract useful information from mass spectrometric data. Score plots from OPLS-DA revealed good clasterization of data points with accordance to tissue source. Real-time feedback to the surgeon about margin status in patients with breast cancer was shown. High accuracy tumor boundary detection is also presented.

• Session 5 • Track 1 •
Clinical Metabolomics
Thursday @ 9:00 in Mozart 1-3
Session Chair: Oleg Mayboroda - *Leiden University Medical Center*

Thursday @ 9:00 in Mozart 1-3
Diagnosis of Multiple Myeloma by Mass Spectrometry of Peripheral Blood Plasma and Artificial Intelligence
Meritxell Deulofeu - *Masaryk University* (meritxell.deulofeu@gmail.com) -- *Young Investigator Grantee*
‣ A fast and simple method for the diagnosis of multiple myeloma by the analysis of peripheral blood plasma mass spectra has been developed. It is based on recording the Matrix Assisted Laser Desorption Ionisation Time Of Flight (MALDI TOF) mass spectra of low mass metabolites/compounds (below 2000 Daltons) and the evaluation of these data using Artificial Neural Networks (ANNs). The method, which does not require the identification of biomarkers, has been verified using clinical database of myeloma positive and negative patients.

Thursday @ 9:20 in Mozart 1-3
Vaginal Swabs Analysis Using Desorption Electrospray Ionization (DESI) MS Permits Rapid Identification of Metabolic Signatures Associated with Preterm Birth
Holly Lewis - *Imperial College London* (holly.lewis@imperial.ac.uk)
‣ Preterm birth (PTB) is the leading cause of death in children under 5 years. Approx. 30% of PTB are preceded by prelabour rupture of membranes (PPROM). We have recently described a method of medical swab analysis that permits rapid, direct assessment of the vaginal metabolome using Desorption Electrospray Ionization Mass Spectrometry (DESI-MS). In this study we show DESI-MS vaginal swab profiling can permit stratification of patients subsequently experiencing PPROM from healthy controls. Furthermore we can determine mucosal metabolic profiles for vaginal bacterial dysbiosis in women presenting with PPROM. This highlights the predictive and therapeutic potential of DESI-MS in high-risk pregnancies.

Thursday @ 9:40 in Mozart 1-3
Evidence of an Impairment of Cholesterol Metabolism Associated to Mitochondrial Dysfunction. A Metabolomic Approach Based on Mass Spectrometry
Valerio Leoni - *Lab of Clinical Chemistry, Hospital of Varese* (valerio.leoni@asst-settelaghi.it)
‣ Mitochondrial alterations are associated to tricarboxylic acid cycle and OXPHOS dysfunction which result into a reduced production of ATP, NADPH and Acetly-CoA. These dysfunctions induce changes to the lipid composition of the cellular membranes as consequence of an anabolic impairment. Isitope-dilution mass spectrometry metabolomics allo to investigate the changes in the cellular and tissue lipid profile relating functional to genetic and metabolomics evidences. It is likely that this mechanism might contribute to the process of neurodegeneration.

• Session 5 • Track 2 •
TDM/DOA
Thursday @ 9:00 in Mozart 4-5
Session Chair: Michael Vogeser - *Institute of Laboratory Medicine, Hospital of the University of Munich, Germany*

Thursday @ 9:00 in Mozart 4-5
GC-APCI-QTOFMS Coupled to Nitrogen Chemiluminescence Detector: A Tool for Identification and Quantification of New Psychoactive Substances and their Metabolites
Samuel Mesihää - *University of Helsinki* (samuel.mesihaa@helsinki.fi)
‣ Lack of authentic reference standards is a common problem in quantitative mass spectrometric analysis of new psychoactive substances (NPS) and drug metabolites. A new instrument platform was utilised for concurrent identification and quantification, by dividing the GC flow between a high resolution QTOFMS instrument and a nitrogen chemiluminescence detector. The high mass accuracy of QTOFMS combined to APCI ionisation enabled tentative substance identification relying on the accurate mass of protonated molecular ion. Quantification was based on the equimolar response of drugs to nitrogen. This concept was applied to study the concentrations of α-PVP and its metabolites in post-mortem urine samples.

Thursday @ 9:20 in Mozart 4-5
Novel LC-MS Approaches to Determination of Chemical Warfare Agents and Related Compounds in Biomedical Samples
Igor Rodin - *Moscow State University* (igorrodin@yandex.ru) -- *Young Investigator Grantee*
‣ A summary of the author's approaches for investigation of the mass spectral behavior of some chemical warfare agents (CWAs), their degradation products and metabolites, as well as the results of development of analytical methods for confirmation of nerve and blister agents application in biomedical samples are presented. Hydrolysis and oxidation metabolites of nerve agents, sulfur mustard and lewisite were used as biomarkers of the exposure. Sensitive analytical methods have been developed for their detection, based mainly on tandem mass spectrometry coupled with liquid chromatography. Several techniques for fast screening of CWAs degradation products based on capillary electrophoresis were also proposed. Some of developed approaches were successfully applied in the frame of the proficiency testing system of the Organization for the Prohibition of Chemical Weapons.

Thursday @ 9:40 in Mozart 4-5
Fake News, Alternative Facts or Just Normal Pharmacokinetics? High Urine Naloxone Concentrations in Patients Prescribed Sublingual Buprenorphine-Naloxone (BNX)
Judith Stone - *Univ. of Calif, San Diego Health System* (jastone@ucsd.edu)
‣ Sublingual buprenorphine is used for treatment of opioid abuse. Naloxone:buprenorphine coformulation is common to deter parenteral misuse. Naloxone has low sublingual bioavailability, therefore limited antagonist effect by this route, whereas intravenous naloxone is a highly effective opioid antagonist. Urine drug testing may detect diversion/misuse of BNX. Conventional wisdom is that naloxone is not detected in urine after sublingual BNX. Using LC-MSMS we quantified total urine buprenorphine, norbuprenorphine and naloxone from two patient populations prescribed BNX (A&B, nA=44,079,nB=49). We found higher than expected concentrations of naloxone. In populations A/B naloxone was detected in 91%/92% of samples with minimum-median-maximum A/B concentrations of 10/8-581/206-168,207/2,243 ng/mL. We discuss analytical, clinical and pharmacokinetic explanations for this observation.

• Session 5 • Track 3 •
Proteomic Applications
Thursday @ 9:00 in Papageno
Session Chair: Andy Hoofnagle - *University of Washington*

Thursday @ 9:00 in Papageno
Quantitative Proteome Analysis Applied to Human Arterial Tissue: Lessons in Relation to Cardiovascular Diseases
Lars Melholt Rasmussen - *Odense University Hospital* (lars.melholt.rasmussen@rsyd.dk)
‣ We have used proteome analysis on human arterial samples and find distinct protein changes in relation to diseases like diabetes, aneurysms and vascular stiffness. The observed alterations strongly support and expand our knowledge about the pathophysiology behind cardiovascular diseases.

Thursday @ 9:20 in Papageno
Quantitative Analysis of Phosphorylation Sites in the Platelet Proteome After ADP Stimulation
Christin Lorenz - *Leibniz-Institut für Analytische Wissenschaften* (christin.lorenz@isas.de)
‣ Platelets are primarily known to be key players in thrombosis and hemostasis. Targeting platelet function and signaling may represent novel therapeutic strategies in prevention of cardiovascular diseases. The absolute quantification of phosphorylation sites in actived platelets can direct the establishment of new diagnostic assays by characterization of samples with clinical relevance, including quantification of platelet receptors and signaling proteins and their regulation via posttranslational modifications in human blood. Therefore, this study aims to establish a targeted mass spectrometry based assay for quantitative analysis of the phosphorylation status in activated platelets, in particular ADP receptors and the related cAMP/PKA signalling cascade proteins.

Thursday @ 9:40 in Papageno
Clinical Applications of Universal S-Trap Sample Processing
John Wilson - *Cold Spring Harbor Laboratory* (wilsonjp@gmail.com)
‣ The widespread acceptance and application of proteomics in the clinic requires analytical reproducibility, reliability, low-cost and speed. As molecules with vastly different physiochemical properties, proteins are uniquely challenging. S-Trap sample processing unifies sample solubilization with high concentrations of SDS (5%), affords protein concentration and cleanup inexpensively with standard lab equipment and allows bottom-up proteomics sample prep in around 1 - 2 hrs. Here, we explore S-Trap clinical applications including dried blood spot protein extraction, reproducibility of sample processing and the effect of S-Trap harsh protein denaturation on antibody-antigen interactions, which may alter results in proteomics based clinical assays due to digestion differences.

• Session 5 • Track 4 •
Practical Training: Basic
Thursday @ 9:00 in Paracelsus
Session Chair: Erik Soderblom - *Duke University*

Thursday @ 9:00 in Paracelsus
Basics of LC-MS Troubleshooting
Erik Soderblom - *Duke University* (es114@duke.edu)
‣ Troubleshooting even common LC-MS related system issues can often be a daunting task, especially for inexperienced users. Here we will present a systemic and standardized approach to 1) quickly assess a wide variety of LC-MS system problems and 2) begin narrowing down and diagnosing the most likely cause of the problem – potentially saving the user valuable time (and money!). In Part 1 of this session, we will highlight and discuss this overall troubleshooting strategy, including tips and tricks to simplify the process. In Part 2 and 3 of the session, we will go through a series of “real world” problems and demonstrate the deployment of the troubleshooting workflow.

• Session 5 • Track 5 •
Practical Training: Intermediate
Thursday @ 9:00 in Trakl
Session Chair: Catarina Horro Pita - *LGC*

Thursday @ 9:00 in Trakl
Where Did My Analyte Go? – Coping with Poor Solubility and Non-Specific Binding
Catarina Horro Pita *- LGC - Drug Development Services* (catarina.horropita@lgcgroup.com)
‣ Solubility issues and non-specific binding can be insidious and often overlooked problems in method development and can subsequently cause failures during validation. Both the solubility and binding of an analyte will be affected by the pH and composition of the solution whereas non-specific binding also needs to take into account the nature of the container. These presentations will cover how to assess and differentiate between these phenomena at an early stage in development and discuss common solutions to these issues.

• Session 6 • Track 1 •

Closing Metabolomics Keynote

Thursday @ 11:00 in Mozart 1-3

Session Chair: Oleg Mayboroda - *LUMC*

Thursday @ 11:00 in Mozart 1-3

Discovery, Validation and Implementation of Biomarkers for Clinical Metabolomics

David Wishart - *University of Alberta* (dwishart@ualberta.ca)

‣ In this presentation I will provide a number of specific examples of how quantitative metabolomics has been used to discover, validate and implement a number of clinically useful biomarkers and assays. These will include examples of predictive, prognostic and diagnostic multi-metabolite markers that exhibit substantially better performance than existing single biomarker assays. I will also discuss how quantitative metabolomics is beginning to have an impact in the fields of precision/personalized medicine by providing several interesting case studies where quantitative metabolomics has been used to assist in early disease diagnosis, disease prevention and "wellness" maintenance.

• Session 6 • Track 2 •

Other Topics

Thursday @ 11:00 in Mozart 4-5

Session Chair: Christiane Auray-Blais - *Université de Sherbrooke*

Thursday @ 11:00 in Mozart 4-5

Towards Combined Determination of Paracetamol and APAP-Cys in VAMS via LC-MS/MS

Lisa Delahaye - *Ghent University* (lisa.delahaye@ugent.be) -- *Young Investigator Grantee*

‣ The risk assessment in case of a paracetamol intoxication can be improved by monitoring the NAPQI-albumin adduct, compared to the current guidelines. The potential value of this biomarker has been pointed out by several studies, using a 1 µM cut-off value for treatment. It can also be used to tailor paracetamol therapy in critically ill children and patients with liver disease, who have an increased risk for paracetamol-induced liver damage. Therefore, we aim to develop a method for the combined determination of paracetamol and the NAPQI-albumin adduct in 10 µL VAMS (volumetric absorptive microsamples) via LC-MS/MS.

Thursday @ 11:20 in Mozart 4-5

Urine Oxalate & Citrate; How Do We Get the Correct Answer?

David Marshall - *University Hospital South Manchester* (David.Marshall@UHSM.NHS.UK) -- *Young Investigator Grantee*

‣ Urine stone screens are important to identify patients at risk of nephrolithiasis. A new HPLC-MS/MS method was developed for oxalate and citrate to replace the current in house methods. Full method validation including method comparison was carried out prior to routine use. After introduction we noticed a positive bias for our EQA returns compared to WEQAS users using the oxalate oxidase enzymatic method. Recovery was good and any matrix effect was compensated for by the internal standard used therefore the differences seen may be due to variation in the sample prep, calibration and/or the enzymatic method itself.

Thursday @ 11:40 in Mozart 4-5

Isoform-Specific Quantitation of Human Growth Hormone via a Bead-based MSIA Assay

Julia Dittrich - *University Hospital Leipzig* (julia.dittrich@medizin.uni-leipzig.de) -- *Young Investigator Grantee*

‣ Human growth hormone (hGH), which is expressed in various isoforms, is essential for growth stimulation. However, commercial immunoassays are insufficiently selective and sensitive to interferences. We developed a Mass Spectrometry ImmunoAssay (MSIA) for the simultaneous quantitation of total hGH and its isoforms from 200 µL serum applying a polyclonal antibody coupled to magnetic beads. An elaborated sample preparation including protein internal standards was combined with a 5 min LC MS/MS analysis. The assay's quantitation limits facilitated a reliable analysis in the lower diagnostic decision range of <1 ng/mL.

• Session 6 • Track 3 •

Innovation for the Clinical Microbiology Lab

Thursday @ 11:00 in Papageno

Session Chair: Jean Armengaud - *CEA-Marcoule*

Thursday @ 11:00 in Papageno

Laser Assisted Rapid Evaporative Ionisation Mass Spectrometry (LA-REIMS): An Automated High-Throughput Platform for Clinical Microbiology and Beyond

Simon Cameron - *Imperial College London* (s.cameron@imperial.ac.uk)

‣ Mass spectrometry (MS) has revolutionised the workflow of clinical microbiology laboratories; allowing a substantial reduction in diagnosis times. Unlike commercially available MS platforms, rapid evaporative ionisation MS (REIMS) requires no sample preparation, such as the addition of a matrix, before sample analysis. We have recently transitioned to using a CO2 laser to complete REIMS analysis; improving the sample throughput of our automated high-throughput REIMS platform by over 30%. This platform correctly classifies clinical isolates with an accuracy of >99% for Gram stain, >97% for genus, and >95% for species. This presentation will detail the optimisation of the LA-REIMS platform, the creation of a reference spectral database for over 50 microbial species, the determination of antimicrobial susceptibilities, and direct from clinical sample pathogen detection.

Thursday @ 11:20 in Papageno

Defining Systemic Bacterial Infection Through Construction of a Murine Organ Atlas

John Lapek - *University of California, San Diego* (jlapek@ucsd.edu)

‣ Group A Streptococcus has a primary consequence of strep throat, but can also cause grossly invasive infections such as necrotizing fasciitis and bacteremia. Our understanding of the complex network of mechanisms that govern the interplay between host and pathogen during infection remains rudimentary. To better understand global host responses to systemic infection we utilize a mouse model to define niches within major organ systems in combination with multiplexed quantitative proteomics. We define organ specific markers of infection and demonstrate traceability of these markers in blood, establishing a clinically relevant link through analysis of human blood samples.

Thursday @ 11:40 in Papageno

Paper Substratum for MALDI-TOF Disposable Targets

Nadine Perrot - *R&D Microbiology Department, bioMérieux S.A.* (nadine.perrot@biomerieux.com)

‣ MALDI-TOF MS is commonly used as a tool for the rapid identification of microorganisms in clinical and industrial fields. Samples are classically loaded using either disposable plastic targets or reusable metallic slides. To reduce the environmental footprint of MALDI-TOF applications, the use of a low cost, “green target” made with paper substratum, was proposed. A proof of concept was realized with excellent results using different types of paper with a metallized side as new sample supports for microorganism identification and molecule detection (peptides and protein up to 46kDa).

Poster Presentations

Location: *Exhibit Hall (1st Floor)*

Posters by Topic: next page
Posters by Number ***with Abstract***: p. 85

Posters by Topic

Please Find Posters *with Abstracts* under
Posters by Number (starting on page 85)

Endocrinology

Endocrinology | Wednesday 9:45 Poster #A09
Heart-Cutting 2D LC-MS/MS Analysis of Estradiol in Serum
Marianne Bergmann *- Biochemistry and Immunology, Lillebaelt Hospital*

Endocrinology | Wednesday 9:45 Poster #A19
Steroids Panel by LC-MS/MS: Analytical Evaluation and Reference Ranges Establishment
Caroline Le Goff *- University Hospital of Liège, University of Liège*

Endocrinology | Thursday 10:00 Poster #B04
Reference Intervals for Plasma Concentrations of Adrenal Steroids Measured by LC-MS/MS: Impact of Gender, Age, Oral Contraceptives, BMI and Blood Pressure
Mirko Peitzsch *- Institute of Clinical Chemistry and Lab.-Medicine*

Endocrinology | Thursday 10:00 Poster #B24
Quantification of Catecholamines and Metanephrines in Urine Using the Thermo Scientific™ TSQ Endura™ Mass Spectrometer for Research Use
Sergio Indelicato *- Thermo Fisher Scientific France,Villebon surYvette*

Endocrinology | Wednesday 9:45 Poster #C09
A Versatile Workflow to Measure Plasma Renin Activity and Aldosterone for Clinical Research Using Automated On-Line Extraction Coupled to LC-MS/MS
Magnus Olin *- Thermo Fisher Scientific*

Endocrinology | Wednesday 18:30 Poster #F03
Quantitation of Plasma Metanephrine and Normetanephrine by Derivatization Using LC-MS/MS Analyzer Integrated with Fully-Automated Sample Preparation Device
Atsuhiko Toyama *- Marketing Innovation Centre, Shimadzu Corporation*

Endocrinology | Wednesday 9:45 Poster #F04
Analysis of Serum Estrogens – How Low Can Your Clinical Research Method Go?
Robert Wardle *- Waters Corporation*

Endocrinology | Wednesday 9:45 Poster #H06
LC-MS/MS Analysis of Angiotensin I for Assessment of Plasma Renin Activity in Clinical Research
Ben Dugas *- Waters Corporation*

Endocrinology | Thursday 10:00 Poster #L01
Validation of a Semi-Automated Solid Phase Extraction LC-MS/MS Method for Androstenedione, 17-Hydroxyprogesterone and Testosterone Measurement
Emma Walker *- PhD, University College London, UK*

Metabolomics

Metabolomics | Wednesday 18:30 Poster #A02
Metabolomics of Human Brain Tumor. How Far We Are to Discover Potential Biomarkers?
Paulina Zofia Gorynska *- Faculty of Pharmacy, Collegium Medicum*

Metabolomics | Wednesday 18:30 Poster #A14
An Improved MALDI-TOF MS-based Beta-Lactamase Assay Platform for Clinically Relevant Cefotaxime Resistant Bacteria
Kyoung-Soon Jang *- Korea Basic Science Institute*

Metabolomics | Wednesday 18:30 Poster #A22
Importance of Analyzing Amino Acid Concentrations on Tandem Mass Spectrometer in Monitoring the Treatment of Tyrosinemia Type 1
Ana Skaricic *- University Hospital Center Zagreb*

Metabolomics | Wednesday 18:30 Poster #B06
Diagnosis of Galactosemia by MALDI-TOF Mass Spectrometry Using a Parylene-Matrix Chip
Mira Kim *- University of Yonsei*

Metabolomics | Wednesday 9:45 Poster #B15
Quantification of 24(S)-Hydroxycholesterol and 27-Hydroxycholesterol Plasma Levels of Patients with Fragile X Syndrome by Using a LC-ESI-MS/MS Assay
Artuela Çaku *- Université de Sherbrooke*

Metabolomics | Wednesday 18:30 Poster #B18
Metabolights; an Open Source Metabolomics Resource
Keeva Cochrane *- EMBL-EBI*

Metabolomics | Wednesday 9:45 Poster #B23
Simple & Robust Approach in Urinary Metabolomics Based on UPLC-MS for Preoperative Colorectal Cancer Diagnostics
Ivan Plyushchenko *- Lomonosov Moscow State University*

Metabolomics | Wednesday 9:45 Poster #C03
Breath Biopsy with TD-EESI-FAIMS-MS: A New Approach for Rapid, Non-Invasive Measurement of the Breath Metabolome
Alasdair Edge *- Owlstone Medical Ltd.*

Metabolomics | Thursday 10:00 Poster #C08
The Role of Lipids in Diseases - Challenges of Lipid Isomers and Isobars in Mass Spectrometry-based Biomarker Research
Ulf Sommer *- Biocrates Life Sciences AG*

Metabolomics | Wednesday 9:45 Poster #C11
Towards Standardized Data Analysis Workflows in Targeted Metabolomics – Challenges and Best Practices in Biomarker Discovery
Stefan Ledinger *- Biocrates Life Sciences AG*

Metabolomics | Thursday 10:00 Poster #D01
Expanded Newborn Screening by Tandem Mass Spectrometry and Implementation of Next Generation Sequencing in Slovenia
Andraz Smon *- University Medical Centre Ljubljana*

Metabolomics | Wednesday 9:45 Poster #D06
High-Throughput Identification of Hemoglobinopathies and Thalassemia by HRAM/MS
Thomas Wiesinger *- TU Wien*

Metabolomics | Thursday 10:00 Poster #F09
Rapid-Fire Direct Metabolome Analysis by Probe Electrospray Ionization/Tandem Mass Spectrometry: its Preclinical Applications to Validate the Methods
Yumi Hayashi *- In Vivo Real-Time Omics Laboratory, Institute for*

Microbiology / Virology / Parasitology

Microbiology / Virology / Parasitology | Wednesday 9:45 Poster #A03
Simple and Rapid Assay for Simultaneous Determination of Four Triazole Antifungal Agents in Human Serum by LC-MS/MS
Hyun-Jung Choi *- Department of laboratory medicine, Chonnam Nationa*

Microbiology / Virology / Parasitology | Wednesday 9:45 Poster #B09
Rapid Discrimination Between MRSA and MSSA
Kazuyuki Sogawa *- Azabu University*

Proteomics

Proteomics | Wednesday 9:45 Poster #A05
SMART Proteomics Workflow for Automation
Christian Scherling *- Tecan*

Proteomics | Thursday 10:00 Poster #A16
Development of Parallel Reaction Monitoring (PRM) Assays for the Validation of Biomarkers Associated to Alzheimer's Disease in CSF
Claudia Fredolini *- SciLifeLab, KTH – Royal Institute of Technology*

Proteomics | Thursday 10:00 Poster #A24
Improvement of Specificity for Multiplex mAbs DMPK Triage Studies Using LC-MRM3
Tanguy Fortin *- ANAQUANT*

Proteomics | Wednesday 9:45 Poster #B05
Robust and Multiplexed Immuno-MRM Workflow for Relative Quantitation of Tumor Suppressors and Phosphopeptide Biomarkers of DNA Damage Response (DDR) Pathway
Kerstin Pohl *- SCIEX*

Proteomics | Thursday 10:00 Poster #B20
Standardizing and Harmonizing Multiple TripleTOF® Systems for DDA and DIA Using a Dedicated Performance Kit
Dietmar Waidelich *- Sciex Germany*

Proteomics | Wednesday 9:45 Poster #E04
Krabbe Disease: Quantitative Microproteomics on Specific Histological Brain Regions of the Twitcher Mouse
Davide Pellegrini *- NEST, Scuola Normale Superiore*

Proteomics | Wednesday 9:45 Poster #E08
Plasma Proteome Profiling Disentangles Caloric Restriction and Bariatric Surgery Induced Weight Loss
Philipp Geyer *- Max Planck Institute of Biochemistry*

Proteomics | Wednesday 18:30 Poster #E09
Comprehensive Proteogenomics Analysis of MCF-7 Cell Lines
Avinash Yadav *- Scuola Normale Superiore, Pisa, Italy*

Proteomics | Wednesday 9:45 Poster #F08
Quantitation of Infliximab and Adalimumab in Human Serum by Multiplex LC-MRM Using Full-Length Stable Isotope Labeled Internal Standards
Kevin Ray *- Merck KGaA*

Small Molecules

Small Molecules | Wednesday 9:45 Poster #A01
Validation of Plasma Busulfan Assay Using LC-MS/MS for Haematopoietic Stem-Cell Transplant Patients in a Cancer Hospital in India
Subhosmito Chakraborty *- Tata Medical Center*

Small Molecules | Thursday 10:00 Poster #A04
Fully Automatized LC-MS/MS Analysis of Neuroleptics Using a Novel Sample Preparation System
Sigrid Baumgarten *- Shimadzu Europa*

Small Molecules | Thursday 10:00 Poster #A08
Direct Quantitation of 25-Hydroxyvitamin D3 and D2 in Dried Blood Spots by 2D LC-MS/MS
Berit Packert Jensen *- Toxicology, Canterbury Health Laboratories*

Small Molecules | Wednesday 9:45 Poster #A11
A New Tool for the Automated Sample Preparation of Whole Blood Samples by LC-MS Using a Commercial Autosampler
Thomi Preiswerk *- CTC Analytics AG, Switzerland*

Small Molecules | Wednesday 9:45 Poster #A13
Rapid, Sensitive and High-Throughput Detection of Salivary 25-Hydroxy Vitamin D Using Ultra-High Resolution FT-ICR Mass Spectrometry
Jiyeon Hong *- Korea Basic Science Institute*

Small Molecules | Wednesday 9:45 Poster #A15
Automated Magsimus Sample Preparation for LC-MS/MS Analysis of Vitamin D on the PAL-RTC Programmable Auto Loader
Sonja Augustin *- Axel Semrau GmbH & Co. KG*

Small Molecules | Wednesday 9:45 Poster #A17
Evaluation of a New Magnetic Bead-based Biological Sample Preparation Kits for Vitamin D Analysis
Stéphanie Peeters *- University Hospital of Liege, University of Liege*

Small Molecules | Wednesday 18:30 Poster #A18
Fast and Fully Automated LC-MS/MS Approach to the Therapeutic Drug Monitoring of Immunosuppressant Drugs
Matteo Conti *- Metropolitan Laboratory of Bologna*

Small Molecules | Wednesday 9:45 Poster #B01
The CLAM-2000 Challenge: Checking the Accuracy and Reproducibility of Automatic Sample Preparation of Steroid and Glucocorticoids for Plasma and Urine Samples
Jana Rykl *- Shimadzu Schweiz AG*

Small Molecules | Wednesday 18:30 Poster #B02
Improvement in Limit of Quantitation of a Multiplex LC-MS/MS Method Using a Method Segmentation Approach
Dario Mandic *- University Hospital Osijek*

Small Molecules | Wednesday 9:45 Poster #B07
Investigation of the Metabolic Pathways of Synthetic Flavonoids Following Oral Administration by Gas Chromatography Coupled to High Acccuracy Mass Spectrometry
Michele Iannone *- Department DCT, "Sapienza" University of Rome*

Small Molecules | Thursday 10:00 Poster #B08
LC-MS/MS Quantitative Analysis of 12 Retinoids, Derivatives and Metabolites in Serum for Clinical Research
Zuzana Skrabakova *- Thermo Fisher Scientific*

Small Molecules | Thursday 10:00 Poster #B12
Quantification of Drugs of Abuse in Oral Fluid Using Online Turboflow™ Sample Extraction
Claudio De Nardi *- Thermo Fisher Scientific*

Small Molecules | Wednesday 18:30 Poster #B14
Development and Validation of a Liquid Chromatography Tandem Mass Spectrometric Assay for Plasma Bradykinin
Mikael Lindström *- HUSLAB*

Small Molecules | Thursday 10:00 Poster #B16
Rethinking Library Identification in Quantitative Clinical Toxicology – Transitioning Towards MRM Spectrum Mode
Neil Loftus *- Shimadzu Corporation*

Small Molecules | Wednesday 9:45 Poster #B17
Development of LC-MS/MS-based Method for the Analysis of mRNA 5' Cap Metabolism
Dominika Strzelecka *- University of Warsaw*

Small Molecules | Wednesday 18:30 Poster #B22
A Novel Fast and Simple Quantification Method for Bile Acids in Human Serum by LC-MS/MS
Aurore Jaffuel *- Shimadzu France*

Small Molecules | Wednesday 18:30 Poster #B26
Quantitative Toxicology Screening for Over 1000 Compounds in Whole Blood Samples; is there a Better Way of Reporting Results?
Stephane Moreau *- Shimadzu Europe*

Small Molecules | Wednesday 9:45 Poster #B27
Determination of Organophosphorus Nerve Agents Biomarkers in Urine by Ion Chromatography Tandem Mass Spectrometry
Timur Baygildiev *- Lomonosov Moscow State University*

Small Molecules | Thursday 10:00 Poster #B28
A Novel Solution for EtG/EtS Analysis in Human Urine by LC-MS/MS
Frances Carroll *- Restek Corporation*

Small Molecules | Wednesday 18:30 Poster #C02
Quebec Urinary Screening Program: From Thin Layer Chromatography to Tandem Mass Spectrometry
Christiane Auray-Blais *- Université de Sherbrooke/CIUSSS de l'Estrie-CHUS*

Small Molecules | Thursday 10:00 Poster #C04
Rapid Separation of Steroid and Secosteroid Metabolites by ultraFAIMS-MS for High-Throughput Clinical Analysis
Lauren Brown *- Owlstone Medical Ltd., 162 Cambridge Science Park,*

Small Molecules | Wednesday 9:45 Poster #C05
Universal LC-MS/MS System Configuration (Instrument, Analytical Column and Mobile Phases) for Determination of Multiple Drugs in Serum Samples
Magdalena Rajska *- Spadia Lab*

Small Molecules | Wednesday 18:30 Poster #C06
Feasibility to Screen Creatine Synthesis and Transport Disorders, Triple H Syndrome and OTC Deficiency in Newborn Urine Specimens
Pamela Lavoie *- Université de Sherbrooke*

Small Molecules | Wednesday 9:45 Poster #C07
Quantitative Analysis of 7 Antiepileptic Drugs in Human Serum for Research Using a Two-Channel LC-MS/MS System
Edward Goucher *- Thermo Fisher Scientific*

Small Molecules | Wednesday 18:30 Poster #C10
Quantitative Analysis of Heparan Sulfate and Dermatan Sulfate in MPS II Mice Tissues by UPLC-MS/MS
Iskren Menkovic *- Université de Sherbrooke*

Small Molecules | Wednesday 9:45 Poster #D02
Measurement of *in Vivo* Glycolytic Flux by Liquid Chromatography Tandem Mass Spectrometry
Bei-Tzu Wang *- University Children*

Small Molecules | Wednesday 9:45 Poster #D04
Evaluation of Blood Lysis Procedures Prior to Automated Sample Preparation for Immunosuppressant Assay by LC-MS/MS
Ryu Konoshita *- Shimadzu Europa GmbH*

Small Molecules | Wednesday 18:30 Poster #E01
Applying LCMS Methods to Instruments of Different Manufacturers – Juggling with a Variety of ESI Source Parameter Settings
Katharina Kern *- RECIPE Chemicals + Instruments GmbH*

Small Molecules | Thursday 10:00 Poster #E03
Extraction of Catecholamine Acid Metabolites from Plasma Prior to Analysis Using LC-MS/MS
Alan Edgington *- Biotage (GB) Ltd.*

Small Molecules | Wednesday 9:45 Poster #E06
Combined Screening and Quantitative Confirmation of 129 Drugs in Urine by LDTD-MS/MS Using a Generic SPE Procedure
Richard Lam *- TECAN SP*

Small Molecules | Wednesday 9:45 Poster #E10
Analysis of Plasma Free Metanephrine, Normetanephrine, and 3-Methoxytyramine by HydropHILIC Interaction Liquid Chromatography
Ute Beyer *- Restek Corporation*

Small Molecules | Wednesday 9:45 Poster #F06
Simultaneous Quantitation of 13 Psychotherapeutic Drugs in Human Plasma by UPLC-MS/MS and its Application in Therapeutic Drug Monitoring
Doudka Natalia *- Timone Hospital, Clinical Pharmacology*

Small Molecules | Wednesday 18:30 Poster #F07
Quantitative Determination of Free Hormone Fraction via Biocompatible Solid Phase Microextraction (BioSPME)
Craig Aurand *- MilliporeSigma*

Small Molecules | Wednesday 18:30 Poster #H05
Comparison of VAMS and Card Based Microsampling with LC-HRMS Analysis to Assess Cardiovascular Drug Levels
Dennis Bernieh *- De Montfort University - UK*

Small Molecules | Wednesday 9:45 Poster #L02
MagSiMUS-SteroidPREP: Automated Sample Preparation for LC-MS/MS Analysis of Steroids in Serum, Urine and Saliva on the MagSiMUSDX
Erik Ruijters *- MagnaMedics Diagnostics B.V.*

Small Molecules | Wednesday 18:30 Poster #L03
Volumetric Absorptive Microsampling (VAMS) and LC-MS/MS Analysis for Simultaneous Monitoring of 16 Antiepileptic Drugs: Workflow Development and Validation
Annachiara D'Urso *- Fondazione IRCCS Istituto Neurologico Carlo Besta*

Small Molecules | Wednesday 9:45 Poster #L04
Development of a LC-MS Method for Quantification of Six Common Pharmaceuticals in OFM Samples
Anton Mautner *- Joanneum Research, HEALTH*

Tissue Imaging

Tissue Imaging | Wednesday 18:30 Poster #A10
Contaminants Removal from Tissue Samples Using DESI Ion Mobility Imaging
Vincen Wu *- Imperial College London*

Tissue Imaging | Wednesday 9:45 Poster #B21
Metabolic Phenotyping of Cirrhotic Liver Samples by Desorption Electrospray Ionization Mass Spectrometry Imaging (DESI-MSI)
Anna Mroz *- Imperial College London*

Tissue Imaging | Wednesday 9:45 Poster #F02
Visualising Trans-Epithelial Small Molecule Transport by High Spatial Resolution Mass Spectrometry Imaging
Lennart Huizing *- M4I division of IMS, Maastricht Unviversity*

Tissue Imaging | Thursday 10:00 Poster #L05
Spatial Metabolic Profiling of Idiopathic Pulmonary Fibrosis by Mass Spectral Imaging
Shabarinath Nambiar *- Murdoch University, Western Australia*

Troubleshooting

Troubleshooting | Thursday 13:00 Poster #M01
How Do You Hit the Target for Phosphatidylethanol PEth(16:0/18:1) in External Quality Controls ?
Anne Schmedes *- Department of Clinical Biochemistry*

Troubleshooting | Thursday 13:00 Poster #M02
Column and Auto Sampler and Flow Lines Blockage After 300-400 Injections
Reena Desai *- Anzac research institute*

Troubleshooting | Thursday 13:00 Poster #M04
Troubleshooting LC-MS/MS Peak Shape and Recovery Problems for Polar Opiates
Joe Di Bussolo *- Thermo Fisher Scientific*

Troubleshooting | Tuesday 19:00 Poster #M05
Troubleshooting: Measurement of Vitamin K1, MK-4 and MK-7 in Serum – with Special Focus on Purification
Ida Bøgh Andersen *- Vejle Hospital*

Troubleshooting | Tuesday 19:00 Poster #M06
Carryover & Contamination Causes and Cures
Joe Di Bussolo *- Thermo Fisher Scientific*

Troubleshooting | Tuesday 19:00 Poster #M07
Troubleshooting in the Clinical Measurement of Iron Biomarkers Using LC-MS: Supression of Sample Losses in Autosampler Vials
Ioana-Monica Abbas *- Federal Institute for Materials Reseach and Testing (BAM) / School of Analytical Sciences Adlershof*

Various OTHER

Various OTHER | Wednesday 18:30 Poster #A06
Utilizing High Resolution Accurate Mass for the Quantitation of Therapeutic Peptides in Human Plasma for Research
Madalina Oppermann *- Thermo Fisher Scientific*

Various OTHER | Wednesday 9:45 Poster #A07
Simultaneous LC-MS/MS Quantitation of 20 Antiepileptic Drugs in Human Serum
Carrie Adler *- Agilent Technologies*

Various OTHER | Thursday 10:00 Poster #A12
Development and Validation of a Novel Mass Spectrometry Based Solution for Clinical Diagnostics
Daniel Blake *- SCIEX*

Various OTHER | Wednesday 9:45 Poster #A21
Development and Validation of a Fast UHPLC-MS/MS Dilution Method for the Quantification of Ten Antihypertensive Drugs in Urine: Application to Clinical Routine
Valeria Avataneo *- University of Turin*

Various OTHER | Wednesday 9:45 Poster #A23
Development and Full Validation of a HPLC-MS Method for Quantification of Novel Isavuconazole and Four Other Antifungal Drugs in Human Plasma Samples
Giovanna Fatiguso *- University of Turin*

Various OTHER | Wednesday 18:30 Poster #B10
Improved Sample Preparation for Whole Blood Sirolimus LC-MS/MS Assay
Anna Becker *- HUSLAB*

Various OTHER | Wednesday 9:45 Poster #B11
Hyperspectral Imaging Delineates Aβ Chemistry in Structurally Heterogenic Amyloid Plaques
Wojciech Michno *- Sahlgrenska Academy, University of Gothenburg*

Various OTHER | Wednesday 9:45 Poster #B13
Therapeutic Monitoring of Immunosuppressants: Comparison of Immunoassays with LC-MS/MS Method
Andrijana Ščavničar *- University Hospital Centre Zagreb*

Various OTHER | Wednesday 9:45 Poster #B19
Targeted Forensic Screening and Semi-Quantitation of Drugs in Plasma Using High-Resolution Accurate-Mass Detection and On-Line Sample Preparation
Valérie Thibert *- Thermo Fisher Scientific, France*

Various OTHER | Wednesday 9:45 Poster #B25
Misfortunes of a Mass Spec Start-Up
Sophie Hepburn *- The Ipswich Hospital NHS Trust*

Various OTHER | Wednesday 18:30 Poster #D03
Medicinal Compounds of Mexican Oregano Analysis by CG-MS and LC-MS
Amanda Moreno *- FESI,Universidad Nacional Autonoma de Mexico, UNAM*

Various OTHER | Wednesday 9:45 Poster #E02
Evaluation of Critical Parameters for the Establishment of a Clinical MALDI Applications Platform for Liquid Biopsy Diagnostics
Gerald Stübiger *- Medical University Vienna*

Various OTHER | Wednesday 9:45 Poster #F10
Evaluation of Hemolysate as Sample in Automated Sample Preparation for the Determination of Immunosuppressive Concentrations by LC-MS/MS - Tacrolimus Example
Matea Zorić *- Merkur University Hospital, Zagreb, Croatia*

Various OTHER | Wednesday 9:45 Poster #H02
Quantification of 31 Antidepressants in Human Serum by Using a High Resolution Orbitrap Mass Spectrometer
Johanna Lindner *- Institute of Laboratory Medicine, LMU, Munich*

Posters by Number

Poster #A01 in Exhibit Hall - *attended for 1hr on Wednesday starting at 9:45*
Topic: *Small Molecules*
Validation of Plasma Busulfan Assay Using LC-MS/MS for Haematopoietic Stem-Cell Transplant Patients in a Cancer Hospital in India
Subhosmito Chakraborty - *Tata Medical Center* (subhosmito@gmail.com)
‣ Development of a rapid liquid chromatography tandem mass spectrometry technique to measure busulfan from human plasma in bone marrow transplant patients. The method has been developed in-house and measures busulfan and the internal standard (deutarated busulfan) as ammonium adducts. The separation of the analyte is achieved using gradient mobile phases (A) containing acetonitrile with 0.1% formic acid and (B) 10 mmol/L ammonium acetate. After successful analytical validation this method has been made available for clinical use for pharmacokinetic profiling in our tertiary cancer care hospital in India.

Poster #A02 in Exhibit Hall - *attended for 1hr on Wednesday starting at 18:30*
Topic: *Metabolomics*
Metabolomics of Human Brain Tumor. How Far We Are to Discover Potential Biomarkers?
Paulina Zofia Gorynska - *Faculty of Pharmacy, Collegium Medicum* (gorynska.paulina.zofia@gmail.com)
‣ Gliomas are one of the few types of cancer, which doesn't cause any early symptoms. Current methods for brain tumor studies consist mainly of neuroimaging techniques, which cannot provide timely in vivo information regarding the biochemistry of the brain, nor quantitative information regarding concentrations of given analytes. Untargeted metabolite analysis is relatively new approach which provide comprehensive characteristic of endogenous metabolites and could improve identification of tumor types. Sample collection can be considered as the most important step in metabolomics studies. For that reason solid phase microextraction (SPME) was applied to current study as a method which has been successfully applied to metabolite analysis in the last few years.

Poster #A03 in Exhibit Hall - *attended for 1hr on Wednesday starting at 9:45*
Topic: *Microbiology / Virology / Parasitology*
Simple and Rapid Assay for Simultaneous Determination of Four Triazole Antifungal Agents in Human Serum by LC-MS/MS
Hyun-Jung Choi - *Department of laboratory medicine, Chonnam Nationa* (ideatophj@gmail.com)
‣ Therapeutic drug monitoring (TDM) is essential for optimal antifungal therapy in patients with invasive infections, because of broad inter- and intra-individual pharmacokinetic variability of these agents. We developed a simple and sensitive assay suitable for the simultaneous measurement of fluconazole, posaconazole, voriconazole, itraconazole and its metabolite (hydroxy-itraconazole) in human serum using LC-MS/MS in clinical routine laboratory practice to evaluate analytical performance. This method using LC-MS/MS can rapidly and simultaneously quantify the four triazole antifungal agents and one of their active metabolites with good analytical performance including wide analytical range and low LOQ.

Poster #A04 in Exhibit Hall - *attended for 1hr on Thursday starting at 10:00*
Topic: *Small Molecules*
Fully Automatized LC-MS/MS Analysis of Neuroleptics Using a Novel Sample Preparation System
Sigrid Baumgarten - *Shimadzu Europa* (sba@shimadzu.eu)
‣ The precise quantitation of Neuroleptics for therapeutic purpose is necessary. To avoid the sample preparation which is often tedious, involves risk of errors and increases the risk of contamination of people dealing with sample preparation The CLAM-2000 (Clinical Laboratory Automated sample preparation Module) automates the pretreatment of blood or other biological samples before LCMS analysis. By simply placing blood collection tubes in the system, the CLAM-2000 performs all processes through to LCMS analysis automatically. A complete neuroleptics analysis of Neuroleptic kit from Chromsystems was demonstrated.

Poster #A05 in Exhibit Hall - *attended for 1hr on Wednesday starting at 9:45*
Topic: *Proteomics*

SMART Proteomics Workflow for Automation

Christian Scherling - *Tecan* (christian.scherling@tecan.com)

‣ Described here is a novel workflow to streamline the pellet digestion protocol using Control Flow Plate (CFP)1, Narrow Bore Extraction Plate (NBE)1, and SMART Digest Kit. We developed a specially designed Flow Control Tube format which eliminates the centrifugation step and allows the protein denaturation and digestion steps to be performed seamlessly in a single tube. If sample matrix requires additional cleanup after protein digestion, NBE (withsorbent)can be used to further purify the samples before LC-MS/MSanalysis. Combined with SMART Digest kit, the overall sample preparation protocol is simplified, the sample digestion time is reduced from 18 hr to 1.25hr, and resulting in enhancement of assay success rate. Initiating with protein precipitation and phase seperation for other compounds, the protocol is easy transferable to an automation platform for omics sample prep.

Poster #A06 in Exhibit Hall - *attended for 1hr on Wednesday starting at 18:30*
Topic: *Various OTHER*

Utilizing High Resolution Accurate Mass for the Quantitation of Therapeutic Peptides in Human Plasma for Research

Madalina Oppermann - *Thermo Fisher Scientific* (madalina.oppermann@thermofisher.com)

‣ We investigate the advantages of a high resolution accurate mass LCMS assay for quantitation of Leuprolide. A selected ion monitoring scan experiment was performed to determine the lower limit of quantitation. Ultra high resolution settings of 70,000 and greater were also investigated to assess and evaluate the increase of method selectivity on overall assay performance. Selected ion monitoring mode was used for the quantitative evaluation, and demonstrated replicate reproducibility of <15% RSD for each group of replicate concentration points and linear signal response across the working range. The preliminary lower limit of quantitation was determined to be 5 pg/mL.

Poster #A07 in Exhibit Hall - *attended for 1hr on Wednesday starting at 9:45*
Topic: *Various OTHER*

Simultaneous LC-MS/MS Quantitation of 20 Antiepileptic Drugs in Human Serum

Carrie Adler - *Agilent Technologies* (carrie.adler@agilent.com)

‣ LC/MS/MS is particularly suited to the simultaneous analysis of multiple compounds. Further, it's detection range spans several orders of magnitude, which can enable concurrent quantification even when compounds occupy disparate concentration ranges. Here, an LC/MS/MS method was used to measure a large panel of antiepileptic drugs in human serum, rather than the small number often assayed historically due to wide concentration discrepancies. Samples were protein precipitated and diluted into water. Injection, separation of analytes, column cleaning, and column reequilibration were accomplished in <10 minutes. The analytical method was accurate (accuracies within 20% at the lowest concentration and 15% at higher concentrations), sensitive (LODs of low ng/mL), reproducible (CVs <15%, with most <10%), and robust. For Research Use Only. Not for use in diagnostic procedures.

Poster #A08 in Exhibit Hall - *attended for 1hr on Thursday starting at 10:00*
Topic: *Small Molecules*

Direct Quantitation of 25-Hydroxyvitamin D3 and D2 in Dried Blood Spots by 2D LC-MS/MS

Berit Packert Jensen - *Toxicology, Canterbury Health Laboratories* (berit.jensen@cdhb.health.nz)

‣ Measurement of vitamin D status through monitoring of circulating 25-hydroxyvitamin D is increasingly popular. Dried blood spot sampling is attractive, particularly for research studies, but a typical punch only contain about 1 microliter of serum which represents an analytical challenge. By applying heart-cutting 2D chromatography the required sensitivity was reached on a routine clinical mass spectrometer without the need to derivatise. The assay was validated and applied to a clinical study comparing results from DBS with matched serum samples (n=40). Hematocrit-corrected 25OHD3 DBS concentrations correlated strongly with serum concentrations ($p<0.001$, $R2=0.94$).This assay for direct measurement of 25OHD in dried blood spots without derivatisation was found to be a suitable alternative to measuring 25OHD in serum and applicable to clinical research studies.

Poster #A09 in Exhibit Hall - *attended for 1hr on Wednesday starting at 9:45*
Topic: *Endocrinology*
Heart-Cutting 2D LC-MS/MS Analysis of Estradiol in Serum
Marianne Bergmann - *Biochemistry and Immunology, Lillebaelt Hospital* (marianne.bergmann@rsyd.dk) -- *Young Investigator Grantee*
‣ Accurate measurement of estradiol is important in both clinical diagnostics and monitoring of various disorders. Also in clinical research, there is an increased interest for measuring estradiol in the lower concentration range. This work presents the development and validation of an LC-MS/MS method for determining estradiol in serum using heart-cutting 2D chromatography. The method was validated and displays very good analytical performance.

Poster #A10 in Exhibit Hall - *attended for 1hr on Wednesday starting at 18:30*
Topic: *Tissue Imaging*
Contaminants Removal from Tissue Samples Using DESI Ion Mobility Imaging
Vincen Wu - *Imperial College London* (v.wu15@imperial.ac.uk) -- *Young Investigator Grantee*
‣ Fresh frozen samples embedded in OCT are not suitable for DESI imaging, due to the overlap in mass peaks between the metabolites from samples and polymers from OCT. This can be overcome by combining mass spectrometry with ion mobility. Ion mobility allows for the separation of isobaric ions with similar structure based on their collisional cross-section (CCS). As a proof of concept, both pork liver embedded in OCT and pork liver embedded in water were imaged with DESI, using a high resolution mass spectrometer equipped with ion mobility.

Poster #A11 in Exhibit Hall - *attended for 1hr on Wednesday starting at 9:45*
Topic: *Small Molecules*
A New Tool for the Automated Sample Preparation of Whole Blood Samples by LC-MS Using a Commercial Autosampler
Thomi Preiswerk - *CTC Analytics AG, Switzerland* (tpreiswerk@ctc.ch)
‣ Investigation of a sensor equipped tool to perform and monitor the sample preparation of whole blood using a commercial autosampler: Here we present a new tool for liquid handling of whole blood samples and direct sample injection. The tool features an optical sensor that monitors all liquid handling steps. It detects presence or absence of sample, standards and reagents. The sensor is essential to ensure process safety for automated liquid handling steps.

Poster #A12 in Exhibit Hall - *attended for 1hr on Thursday starting at 10:00*
Topic: *Various OTHER*
Development and Validation of a Novel Mass Spectrometry Based Solution for Clinical Diagnostics
Daniel Blake - *SCIEX* (daniel.blake@sciex.com)
‣ We detail here the development of a method for automated analysis of Vitamin D utilizing the new SCIEX Topaz™ System – a CE-marked, integrated, LC-MS-based IVD system specifically designed to enable simple and rapid implementation of LC-MS technology in a clinical diagnostic environment. This approach utilizes a turnkey solution – the Vitamin D 200M Assay kit – combined with a novel, intuitive software platform - ClearCore ™ MD – which empowers new users to build proficiency quickly. Full validation has been undertaken, and the proposed assay is shows sensitivity for both 25-OH-Vitamin D2 and D3 across appropriate ranges. The assay reports a high degree of correlation with the CDC standard reference method while exhibiting minimal compound interference. The proposed application is perfectly suited to the high throughput analysis of Vitamin D in the busy clinical diagnostics laboratory.

Poster #A13 in Exhibit Hall - *attended for 1hr on Wednesday starting at 9:45*
Topic: *Small Molecules*
Rapid, Sensitive and High-Throughput Detection of Salivary 25-Hydroxy Vitamin D Using Ultra-High Resolution FT-ICR Mass Spectrometry
Jiyeon Hong - *Korea Basic Science Institute* (hjy0610@kbsi.re.kr)
‣ Measurement of endogenous levels of vitamin D is of importance for diagnosing health conditions of individuals, ranging from cardiovascular disease to cancer. In this study, rapid, sensitive and high-throughput analytical method for salivary 25-hydroxy vitamin D [25(OH)D] using an ultra-high resolution 15 Tesla Fourier transform ion cyclotron resonance mass spectrometry (15T FT-ICR MS) was developed and validated. Quantitative detection of 25(OH)D2 and 25(OH)D3 was successfully achieved by 15T FT-ICR MS using their deuterated counterparts spiked in the saliva samples. In combination with a fully automated chip-based nanoelectrospray device, high-throughput measurement of salivary 25(OH)D levels were successfully conducted. This salivary vitamin D detection platform would be utilized to rapidly and accurately monitor and determine vitamin D deficiency of subjects.

Poster #A14 in Exhibit Hall - *attended for 1hr on Wednesday starting at 18:30*
Topic: *Metabolomics*

An Improved MALDI-TOF MS-based Beta-Lactamase Assay Platform for Clinically Relevant Cefotaxime Resistant Bacteria

Kyoung-Soon Jang - *Korea Basic Science Institute* (ksjang@kbsi.re.kr) -- *Young Investigator Grantee*

‣ We demonstrate an improved MALDI-TOF MS based beta-lactamase assay platform for cefotaxime, a representative third-generation cephalosporins, resistant bacteria. Cefotaxime that was incubated with the lysates of E. coli exhibiting ESBL activity was modified by Girard"s reagent T to introduce permanent positive charge at the carboxyl functional groups of cefotaxime, resulting in dramatic advances on the ionization efficiency and quantitativeness during MS analysis. The method was validated with clinical isolates of a variety of ESBL-producing E. coli. In comparison with conventional UPLC system, it showed reliable data for distinguishing cefotaxime-resistant bacteria. This improved MS-based beta-lactamase activity assay platform would be utilized to more rapidly and accurately detect clinically relevant antibiotic resistant bacteria in clinical settings.

Poster #A15 in Exhibit Hall - *attended for 1hr on Wednesday starting at 9:45*
Topic: *Small Molecules*

Automated Magsimus Sample Preparation for LC-MS/MS Analysis of Vitamin D on the PAL-RTC Programmable Auto Loader

Sonja Augustin - *Axel Semrau GmbH & Co. KG* (augustin@axel-semrau.de)

‣ The PAL-RTC (Programmable Auto Loader) controlled by Chronos software (Axel Semrau) was configured to optimize the productivity of the MagnaMedics MagSiMUS-DPREP (25-OH-Vitamin D2/D3 for LC-MS) sample preparation product. Using a MagSiMUS-DPREP particle mix of spherical, paramagnetic beads with a unique, proprietary surface, nearly all proteins and other matrix components were efficiently removed by magnetic separation. The diagnostic levels of 25-OH-Vitamin D2 and D3 could be accurately determined in clinical serum samples, using this Programmable Auto Loader. The PAL-RTC was equipped with FlipTube® opening, transfer and vortex tools in order to optimize this automated clean-up process. This setup significantly reduces the total hands-on-time and improves the overall accuracy.

Poster #A16 in Exhibit Hall - *attended for 1hr on Thursday starting at 10:00*
Topic: *Proteomics*

Development of Parallel Reaction Monitoring (PRM) Assays for the Validation of Biomarkers Associated to Alzheimer's Disease in CSF

Claudia Fredolini - *SciLifeLab, KTH – Royal Institute of Technology* (claudia.fredolini@scilifelab.se) -- *Young Investigator Grantee*

‣ In the long path from the discovery to clinical laboratory, biomarker verification is a highly determining phase, where only the most reliable candidates are taken for validation. In this study we describe our cross-platform approach to verify candidates biomarkers for Alzheimer's disease (AD) previously discovered by suspension beads arrays. We applied parallel reaction monitoring (PRM) assays developed using heavy labeled protein fragments (QprESTs). Biomarkers were quantified in the discovery cohort of 92 cerebrospinal fluid (CSF) samples in order to verify by mass spectrometry (MS) the differential profiles observed by affinity proteomics.

Poster #A17 in Exhibit Hall - *attended for 1hr on Wednesday starting at 9:45*
Topic: *Small Molecules*

Evaluation of a New Magnetic Bead-based Biological Sample Preparation Kits for Vitamin D Analysis

Stéphanie Peeters - *University Hospital of Liege, University of Liege* (s.peeters@chu.ulg.ac.be) -- *Young Investigator Grantee*

‣ The performance of a new magnetic bead-based biological sample preparation kits for vitamin D analysis (MagSiMUS-DPREP) was compared against our reference LC-MS/MS method. Correlation was studied using Passing-Bablok analysis. The MagSiMUS-DPREP kit shows similar results compared to our Reference LC-MS/MS method and is therefore considered suitable for assessment of vitamin D status in clinical routine.

Poster #A18 in Exhibit Hall - *attended for 1hr on Wednesday starting at 18:30*
Topic: *Small Molecules*

Fast and Fully Automated LC-MS/MS Approach to the Therapeutic Drug Monitoring of Immunosuppressant Drugs

Matteo Conti - *Metropolitan Laboratory of Bologna* (m.conti@ausl.bologna.it) -- *Young Investigator Grantee*

‣ The therapeutic drug monitoring (TDM) of immunosuppressive drugs (IDs) by LC-MS/MS has become a recognized procedure in the clinical practice and various automated analytical methods are therefore emerging on the market for this analytical task. In clinical situations that require fast results turn-around time (TAT), such as in the immediacy of organ transplantation, methods relying on batch sample preparation are not suitable for fast TAT and serial sample processing would be a preferred option. We evaluated a novel automated system with serial sample processing capability based on the Zivak Multitasker™ coupled to MS/MS spectrometer (API 5500™). This system enabled us with productivity and fast TAT in the TDM of IDs.

Poster #A19 in Exhibit Hall - *attended for 1hr on Wednesday starting at 9:45*
Topic: *Endocrinology*

Steroids Panel by LC-MS/MS: Analytical Evaluation and Reference Ranges Establishment

Caroline Le Goff - *University Hospital of Liège, University of Liège* (c.legoff@chu.ulg.ac.be) -- *Young Investigator Grantee*

‣ We validated a quantification method of 13 steroid hormones to switch from the immunoassays or radiommunoassays to Liquid Chromatography triple quadrupole mass spectrometry. Finally we have established new references range values for these steroids. The method showed good precision, accuracy, detection limits, and robustness. However the sensitivity of DHT and oestradiol is still too low.

Poster #A21 in Exhibit Hall - *attended for 1hr on Wednesday starting at 9:45*
Topic: *Various OTHER*

Development and Validation of a Fast UHPLC-MS/MS Dilution Method for the Quantification of Ten Antihypertensive Drugs in Urine: Application to Clinical Routine

Valeria Avataneo - *University of Turin* (valeria.avataneo@gmail.com) -- *Young Investigator Grantee*

‣ One of the main problems in the management of resistant hypertension (RH) is the discrimination of real cases of RH from poor therapeutic adherence. We developed and validated (according to FDA and EMA guidelines) a UHPLC/MS-MS method for the Therapeutic Drug Monitoring (TDM) of antihypertensive drugs in urine samples, in order to check therapeutic adherence. By this analysis, 22% of patients resulted totally non-adherent and 39% only partially adherent. Concluding, TDM of antihypertensive drugs revealed useful in order to uncover a large fraction of cases of poor therapeutic adherence. Urine analysis is less invasive but also less precise than the plasmatic one: for this reason, we recommend urine testing for a rapid screening while plasmatic one for quantification.

Poster #A22 in Exhibit Hall - *attended for 1hr on Wednesday starting at 18:30*
Topic: *Metabolomics*

Importance of Analyzing Amino Acid Concentrations on Tandem Mass Spectrometer in Monitoring the Treatment of Tyrosinemia Type 1

Ana Skaricic - *University Hospital Center Zagreb* (askaricic@yahoo.com)

‣ A male newborn with positive family history of tyrosinemia type 1 was subjected to a metabolic work-up immediately after birth. Amino acids were quantified by tandem mass spectrometry coupled with high performance liquid chromatography. At first day of life, patient's plasma tyrosine was elevated (169 µmol/L; N: 42-135 µmol/L) while urine organic acid analysis detected succinylacetone, a tyrosine metabolite specific for tyrosinemia type 1. Patient's DNA sequencing revealed a homozygosity for the c.554-1G>T mutation in the FAH gene, which confirmed the diagnosis. Routine monitoring for amino acid concentrations continued while a patient has been examined. Regular measurement of plasma amino acid concentrations enables therapy adjustment and treatment efficiency monitoring in patients with tyrosinemia type 1.

Poster #A23 in Exhibit Hall - *attended for 1hr on Wednesday starting at 9:45*
Topic: *Various OTHER*

Development and Full Validation of a HPLC-MS Method for Quantification of Novel Isavuconazole and Four Other Antifungal Drugs in Human Plasma Samples

Giovanna Fatiguso - *University of Turin* (giofatiguso@gmail.com) -- *Young Investigator Grantee*

‣ Azole compounds are available for treatment of fungal infection diseases. The aim of this work was to develop and validate a HPLC-MS method for simulataneous quantification of novel isavuconazole and other triazoles (fluconazole, voriconazole, posaconazole and itraconazole) following FDA and EMA guidelines. After protein-precipitation, supernatant was diluted and 10 µL were injected in the system. The method resulted fully validated: accuracy and precision, recoveries, matrix effects and all requested parameters resulted within the acceptance criteria. This fast, cheap, selective and robust method is expected to be widely used in the near future for TDM routine of triazoles.

Poster #A24 in Exhibit Hall - *attended for 1hr on Thursday starting at 10:00*
Topic: *Proteomics*

Improvement of Specificity for Multiplex mAbs DMPK Triage Studies Using LC-MRM3

Tanguy Fortin - *ANAQUANT* (tanguy.fortin@anaquant.com)

‣ Monoclonal antibodies (mAbs) have emerged as a major class of therapeutics used to treat life-threatening diseases such as cancer, inflammation or autoimmune diseases. Currently over 470 therapeutic mAbs are tested in clinical trials. For clinical studies, mAbs are mainly quantified in very complex matrices such as plasma or serum and the selectivity of LC-MS-SRM technology could not be enough. In this study, we investigate the use of MRM3 for the multiplexed quantitation of comemrcial mAbs.

Poster #B01 in Exhibit Hall - *attended for 1hr on Wednesday starting at 9:45*
Topic: *Small Molecules*

The CLAM-2000 Challenge: Checking the Accuracy and Reproducibility of Automatic Sample Preparation of Steroid and Glucocorticoids for Plasma and Urine Samples

Jana Rykl - *Shimadzu Schweiz AG* (jr@shimadzu.ch)

‣ The accuracy and reproducibility of automatic sample preparation of steroid hormones and glucocorticoids for plasma and urine samples was compared with the results of manual sample preparation. Manual samples preparation of clinical samples normally include a protein precipitation step followed by centrifugation and/or extraction on SPE cartridges. Here we present an automatic sample preparation procedure using the CLAM-2000 robot coupled to an LCMS-8045 triple quadrupole mass spectrometer.

Poster #B02 in Exhibit Hall - *attended for 1hr on Wednesday starting at 18:30*
Topic: *Small Molecules*

Improvement in Limit of Quantitation of a Multiplex LC-MS/MS Method Using a Method Segmentation Approach

Dario Mandic - *University Hospital Osijek* (dario.mandic@gmail.com)

‣ Finding a right balance in multiplex LC-MS/MS methods between high signal-to-noise (S/N) ratio e.g. low limit of quantitation (LOQ) obtained by prolonged dwell times and sufficient number of peak data points may be a challenging task. A possible solution for this problem is the method segmentation which relies on sequential recording of signals corresponding to analytes eluting within a specified time-frame. S/N ratios and LOQ between segmented and non-segmented method for quantification of 13 steroid molecules were compared. Method segmentation yielded up to nine times lower LOQ without the loss of data points needed for proper integration of any peak.

Poster #B03 in Exhibit Hall - *attended for 1hr on Wednesday starting at 9:45*
Topic: *Various OTHER*

A Novel UHPLC-MS/MS Method for the Simultaneous Quantification of Buprenorphine and Methadone in Human Plasma

Fabio Favata - *University of Turin* (fabio.favata89@gmail.com) -- *Young Investigator Grantee*

‣ Today about 207,400 deaths a year are drug-related, methadone (MTD) and buprenorphine (BUP) are commonly used to prevent opioid withdrawal. These drugs have a wide inter patient variability in metabolism probably due to pharmacogenetic differences, concomitant therapy, drugs, alcohol, hepatic diseases, health state, grade of withdrawal and psychological situation. In this contest therapeutic drug monitoring could be really a useful tool for clinicians. Our UHPLC-MS/MS method for quantification of MTD and BUP in human plasma has been fully validated according to FDA and EMA guidelines; it results fast, robust, cheap, reliable and absolutely clinically applicable. We have already used this method for quantification of real sample with good and repeatable results.

Poster #B04 in Exhibit Hall - *attended for 1hr on Thursday starting at 10:00*
Topic: *Endocrinology*

Reference Intervals for Plasma Concentrations of Adrenal Steroids Measured by LC-MS/MS: Impact of Gender, Age, Oral Contraceptives, BMI and Blood Pressure

Mirko Peitzsch - *Institute of Clinical Chemistry and Lab.-Medicine* (mirko.peitzsch@uniklinikum-dresden.de)

‣ Mass spectrometry based reference intervals for 16 steroids (pregnenolone, progesterone, 11-deoxycorticosterone, corticosterone, aldosterone, 18-oxocortisol, 18-hydroxycortisol, 17-hydroxyprogesterone, 21-deoxycortisol, 11-deoxycortisol, cortisol, cortisone, dehydroepiandrosterone, dehydroepiandrosterone-sulfate, androstenedione, testosterone), established in plasma samples derived from 227 normotensive and 298 hypertensive volunteers, are presented. Besides age and gender, the most important variables for preparation of reference intervals for steroids, further parameters, such as BMI, blood pressure and the use of oral contraceptives is considered in the estimation of contineous reference interval. Those normal ranges will be useful for diagnosis and subtyping of patients with endocrine hypertension.

Poster #B05 in Exhibit Hall - *attended for 1hr on Wednesday starting at 9:45*
Topic: *Proteomics*

Robust and Multiplexed Immuno-MRM Workflow for Relative Quantitation of Tumor Suppressors and Phosphopeptide Biomarkers of DNA Damage Response (DDR) Pathway

Kerstin Pohl - *SCIEX* (kerstin.pohl@sciex.com)

‣ Direct measurement of proteins within human DNA damage response pathways and their post-translational modifications can give vital insight into key biological processes such as ageing and the manifestation of cancer. Here we present the development of a validated immuno-MRM assay utilising peptide-specific antibodies for enrichment prior to mass spectrometry detection. The assay kit contains standards for the multiplexed quantitation of 19 proteins and 42 peptide/ phosphopeptide targets implicated in DNA damage repair. Robustness of the assay was verified by analyzing multiple biological samples across multiple laboratories.

Poster #B06 in Exhibit Hall - *attended for 1hr on Wednesday starting at 18:30*
Topic: *Metabolomics*

Diagnosis of Galactosemia by MALDI-TOF Mass Spectrometry Using a Parylene-Matrix Chip

Mira Kim - *University of Yonsei* (mirakim@yonsei.ac.kr) -- *Young Investigator Grantee*

‣ The analysis of galactosemia, an inborn metabolic disease, is generally performed with various detection methods. In this work, a parylene-matrix chip was developed for the qualitative and quantitative analysis of galactose in PBS buffer and methanol using MALDI-ToF MS by reducing interference of conventional organic matrix. Parylene-N thin film was deposited on dried organic matrix (CHCA) spots with the thickness of 50 ~ 80 nm. Galactosemia can be analyzed using galactose by MALDI-ToF MS. In this work, we have quantitatively reduce o-phenylenediamine (OPD) to 2,3-diaminophenazin (DAP) using reduction power of galactose. Furthermore, it can be analyzed without noise peak using a parylene-matrix chip by MALDI-ToF MS quantitatively.

Poster #B07 in Exhibit Hall - *attended for 1hr on Wednesday starting at 9:45*
Topic: *Small Molecules*

Investigation of the Metabolic Pathways of Synthetic Flavonoids Following Oral Administration by Gas Chromatography Coupled to High Acccuracy Mass Spectrometry

Michele Iannone - *Department DCT, "Sapienza" University of Rome* (michele.iannone@uniroma1.it)

‣ Isoflavones are a group of flavonoids that may be of interest in sport doping because they can be used by athletes in recovering periods after the administration of anabolic steroids to increase the natural production of luteinizing hormone (LH) and consequently the synthesis of natural androgen. In this work we have evaluated the in vivo metabolism of two synthetic isoflavones, methoxyisoflavone (5-methyl-7-methoxy-isoflavone) and ipriflvone (7-isopropoxy-isoflavone) respectively present in a dietary supplement and in a pharmaceutical preparation. Eight metabolites of methoxyisoflavone and six metabolites of ipriflavone were identified. The accurate mass spectra revealed also a 1-3 retro Diels-Alder fragmentation. When excreted in large amounts, the metabolites of methoxyisoflavone and ipriflvone founded could interfere with the correct evaluation of the urinary steroid profile.

Poster #B08 in Exhibit Hall - *attended for 1hr on Thursday starting at 10:00*
Topic: *Small Molecules*
LC-MS/MS Quantitative Analysis of 12 Retinoids, Derivatives and Metabolites in Serum for Clinical Research
Zuzana Skrabakova - *Thermo Fisher Scientific* (zuzana.skrabakova@thermofisher.com)
‣ An analytically sensitive liquid chromatography tandem mass spectrometry (LC-MS/MS) research method for the quantification of retinoids and metabolites in serum is presented. Protein precipitation and liquid-liquid-extraction using 200 µL of serum were compared as simple sample preparation approaches. A Thermo Scientific™ Vanquish™ LC system coupled to a Thermo Scientific™ TSQ Endura™ triple quadrupole mass spectrometer were used. Acquisition was performed by selective reaction monitoring (SRM) for each analyte and internal standard in positive and negative acquisition mode. Limits of detection and quantification, linearity and reproducibility were evaluated using standard reference material and donor samples.

Poster #B09 in Exhibit Hall - *attended for 1hr on Wednesday starting at 9:45*
Topic: *Microbiology / Virology / Parasitology*
Rapid Discrimination Between MRSA and MSSA
Kazuyuki Sogawa - *Azabu University* (sogawa@azabu-u.ac.jp)
‣ The presence of MRSA in a hospital is detrimental to patients and to hospital management. Thus, rapid identification of MRSA is needed. Here, we report a prospective study of rapid discrimination of MSSA from MRSA using MALDI-TOF MS and support vector machine analysis in 160 clinical isolates of S. aureus. In blind test sets, 60 S. aureus isolates were correctly classified, with identification rates of 93.3% for MSSA and 86.7% for MRSA. The method proposed in this study using a predictive model enables detection in one colony in 5 minutes, and thus is useful at clinical sites at which rapid discrimination of MRSA from MSSA is required.

Poster #B10 in Exhibit Hall - *attended for 1hr on Wednesday starting at 18:30*
Topic: *Various OTHER*
Improved Sample Preparation for Whole Blood Sirolimus LC-MS/MS Assay
Anna Becker - *HUSLAB* (anna.becker@hus.fi)
‣ Life-long monitoring of immunosuppressive drugs in blood is essential after organ transplantation. We found poor recovery of sirolimus (86–100 %) and accuracy (77-64%) during validation of a widely employed approach [1] of protein precipitation by zinc sulphate prior to liquid chromatography tandem mass spectrometry (LC-MS/MS) to quantify cyclosporine A, tacrolimus and sirolimus in whole blood. Closer investigation revealed that sirolimus is a hydrophobic drug and has low stability in aqueous solutions [2]. Therefore, we developed a simple and fast assay for whole blood sirolimus without pretreatment with aqueous zinc sulphate. Instead, acetonitrile-methanol (50:50, vol:vol) was used for protein precipitaiton. With the newly developed assay the recovery of whole blood sirolimus was 95-106 % and accuracy 96%.

Poster #B11 in Exhibit Hall - *attended for 1hr on Wednesday starting at 9:45*
Topic: *Various OTHER*
Hyperspectral Imaging Delineates Aβ Chemistry in Structurally Heterogenic Amyloid Plaques
Wojciech Michno - *Sahlgrenska Academy, University of Gothenburg* (wojciech.michno@neuro.gu.se) -- *Young Investigator Grantee*
‣ Alzheimer's disease (AD) is a chronic, neurodegenerative disease, of which the underlying pathological mechanism is still not understood. The disease is characterized by accumulation of amyloid-B (AB) peptides into different extracellular plaques. Plaques have also been found in non-demented pathological ageing (PA) patients. Therefore, discrimination between structural and molecular plaque architecture are of essential interest to resolve Ab plaque pathology in AD. Here, hyperspectral imaging paradigm employing the AB aggregate binding luminescent conjugated oligothiophenes (LCO) in combination with an in-house software was used to differentiate between different types of AB plaques in AD mice. The approach was furher shown to be applicable for laser microdissection and offline mass spectrometric analysis, which validated the presence of various C-terminal and N-terminal Aβ.

Poster #B12 in Exhibit Hall - *attended for 1hr on Thursday starting at 10:00*
Topic: *Small Molecules*
Quantification of Drugs of Abuse in Oral Fluid Using Online Turboflow™ Sample Extraction
Claudio De Nardi - *Thermo Fisher Scientific* (claudio.denardi@thermofisher.com)
‣ An analytical method for the quantification of drugs of abuse in oral fluid using online Thermo Scientific™ TurboFlow™ sample extraction is reported. Two approaches were developed, one for tetrahydrocannabinol and its metabolites and one for basic drugs. Both methods involve a protein precipitation step followed by online sample extraction using a Thermo Scientific™ Prelude™ SPLC system; a Thermo Scientific™ TSQ Quantiva™ triple quadrupole mass spectrometer with heated electrospray ionization is used for detection by single reaction monitoring (SRM). Method performance was evaluated using oral fluid sampled using Thermo Scientific™ OralEze™ Oral Fluid collection devices and spiked with the compounds of interest.

Poster #B13 in Exhibit Hall - *attended for 1hr on Wednesday starting at 9:45*
Topic: *Various OTHER*
Therapeutic Monitoring of Immunosuppressants: Comparison of Immunoassays with LC-MS/MS Method
Andrijana Ščavničar - *University Hospital Centre Zagreb* (ascavnic@kbc-zagreb.hr) -- *Young Investigator Grantee*
‣ Immunosuppressants require therapeutic drug monitoring because of narrow therapeutic range. There are two main analytical methods to assess their concentration, i. e. immunoassays and liquid chromatography methods with various detectors (UV, mass spectrometers…). In this study, comparison of four immunoassays (ACMIA, CMIA, EMIT, ECLIA) with LC-MS/MS was done for cyclosporine and tacrolimus. Correlation coefficients for immunoassays and LC-MS/MS were relatively high for all investigated method comparisons. Passing and Bablok regression showed constant and proportional differences only for some method comparisons. The Bland-Altman plot revealed mean biases from -17.5% to 13.1%.

Poster #B14 in Exhibit Hall - *attended for 1hr on Wednesday starting at 18:30*
Topic: *Small Molecules*
Development and Validation of a Liquid Chromatography Tandem Mass Spectrometric Assay for Plasma Bradykinin
Mikael Lindström - *HUSLAB* (mikael.lindstrom@hus.fi) -- *Young Investigator Grantee*
‣ Bradykinin is a nine amino acid peptide with an important role in inflammatory response as a blood vessel dilator. It is also a major mediator for edema and shock during sepsis. We have developed a liquid chromatography tandem mass spectrometric (LC/MS-MS) assay for plasma bradykinin. Our instrumentation consisted of AB Sciex TQ5500 MS equipped with an electrospray ion source operated in positive ion mode. Chromatographic separation was achieved with biphenyl column (2.1x50mm) over 15 mins. The assay was validated for linearity, LOQ, reproducibility and sample stability. Our newly developed assay is intended for clinical and research purposes.

Poster #B15 in Exhibit Hall - *attended for 1hr on Wednesday starting at 9:45*
Topic: *Metabolomics*
Quantification of 24(S)-Hydroxycholesterol and 27-Hydroxycholesterol Plasma Levels of Patients with Fragile X Syndrome by Using a LC-ESI-MS/MS Assay
Artuela Çaku - *Université de Sherbrooke* (artuela.s.caku@usherbrooke.ca) -- *Young Investigator Grantee*
‣ Fragile X Syndrome (SXF) is a genetic condition associated with cognitive dysfunction and low cholesterol plasma levels. However, the cholesterol brain metabolism has never been studied before. 24(S)-hydroxycholesterol and 27-hydroxycholesterol are oxidized derivatives of cholesterol and their levels reflect cholesterol metabolism of the brain. Herein, we analyzed the level of 24OH-C and 27OH-C in plasma from FXS patients and matched controls. Briefly, lipids were extracted with methanol: dichloromethane, hydrolyzed with KOH, dried down, and solubilized in methanol 90%. Liquid chromatography was performed using isocratic gradient and oxysterols were measured using triple quadrupole MS. This method enabled us to determine 24OH-C and 27OH-C plasma levels of FXS subjects and would allow their quantification for other conditions as well, a measure performed only in few clinical laboratories.

Poster #B16 in Exhibit Hall - *attended for 1hr on Thursday starting at 10:00*
Topic: *Small Molecules*

Rethinking Library Identification in Quantitative Clinical Toxicology – Transitioning Towards MRM Spectrum Mode

Neil Loftus - *Shimadzu Corporation* (neil.loftus@shimadzu-mso.com)

‣ There are considerable opportunities in clinical mass spectrometry to bring about better innovations and better concepts to clinical laboratories. To help transition towards a more effective data review and higher confidence in reporting results we have been rethinking the capability of MRM in compound identification. In this poster we will show a different approach in identifying compounds by MRM Spectrum mode, an approach which can be set up in routine clinical labs helping to reduce false positive and false negative reporting without affecting quantitative data quality.

Poster #B17 in Exhibit Hall - *attended for 1hr on Wednesday starting at 9:45*
Topic: *Small Molecules*

Development of LC-MS/MS-based Method for the Analysis of mRNA 5' Cap Metabolism

Dominika Strzelecka - *University of Warsaw* (dominika.strzelecka@student.uw.edu.pl)

‣ Cap is an unusual nucleotide structure located at the 5'end of eukaryotic mRNA and it plays a major role in a variety of cellular processes such as initiation of translation, maturation, splicing, intracellular transport and turnover of mRNA. Therefore, cap analogs are useful research tools and potential therapeutics, which can influence on regulation of cellular processes. Studying degradation pathways of both natural and chemically modified cap structures can also provide new insights into mRNA turnover. We developed an LC-MS/MS method which enables qualitative and quantitative analysis of cap and cap analogs metabolism in complex matrixes, such as cell extracts.

Poster #B18 in Exhibit Hall - *attended for 1hr on Wednesday starting at 18:30*
Topic: *Metabolomics*

Metabolights; an Open Source Metabolomics Resource

Keeva Cochrane - *EMBL-EBI* (keeva@ebi.ac.uk)

‣ EMBL-EBI has established the MetaboLights database as one of the most successful international metabolomics repositories. The open access service comprises a repository database for primary metabolomic research data and metadata recommended by several leading journals, as well as a knowledge base reference layer enriched with individual metabolite information. With future developments including an integrated workspace for data management and analysis, and a secure infrastructure for clinical data through the Phenomenal project, MetaboLights aims to provide a valuable resource for the community.

Poster #B19 in Exhibit Hall - *attended for 1hr on Wednesday starting at 9:45*
Topic: *Various OTHER*

Targeted Forensic Screening and Semi-Quantitation of Drugs in Plasma Using High-Resolution Accurate-Mass Detection and On-Line Sample Preparation

Valérie Thibert - *Thermo Fisher Scientific, France* (valerie.thibert@thermofisher.com)

‣ This work presents the development and evaluation of a large forensic screening method based on liquid chromatography (HPLC) coupled to High-resolution Accurate-mass (HRAM) detection based on Orbitrap™ technology. Two different analytical methods were used, one based on HPLC, and the other based on online extraction using Thermo Scientific™ TurboFlow™ technology prior to HPLC separation. A database with retention times, compound formulas, and accurate masses for the parent ions and main fragments was obtained as well as a spectral library for forensic screening purposes. Sensitivity was also tested for 41 compounds with the on-line extraction method.

Poster #B20 in Exhibit Hall - *attended for 1hr on Thursday starting at 10:00*
Topic: *Proteomics*

Standardizing and Harmonizing Multiple TripleTOF® Systems for DDA and DIA Using a Dedicated Performance Kit

Dietmar Waidelich - *Sciex Germany* (Dietmar.Waidelich@sciex.com)

‣ To get reproducible quantitative proteomics data, proper controls are required, especially in the field of very large studies. A validated kit containing 20 peptides has been assembled to assess the performance of the TripleTOF® MS systems for IDA and SWATH® proteomics. The Stoller Biomarker Centre in Manchester has eight TripleTOF 6600 systems for IDA and SWATH analysis to help discover novel biomarkers for many different diseases. The eight systems were benchmarked using the kit in microflow during 6 months of operation. The SWATH analyses showed good instrument harmonization, with only a 5% variation in the number of proteins and 12% variation in the number of peptides quantified across all eight machines. With a 60 min gradient, over 20 samples can be run per day per instrument. At full capacity the lab could analyze over 1000 samples by microflow SWATH in one week.

Poster #B21 in Exhibit Hall - *attended for 1hr on Wednesday starting at 9:45*
Topic: *Tissue Imaging*

Metabolic Phenotyping of Cirrhotic Liver Samples by Desorption Electrospray Ionization Mass Spectrometry Imaging (DESI-MSI)

Anna Mroz - *Imperial College London* (anna.mroz@imperial.ac.uk) -- *Young Investigator Grantee*

‣ Mass spectrometry imaging, including desorption electrospray ionisation mass spectrometry imaging, is a powerful technique which can give information on the spatial distribution of metabolites, drug molecules or structural lipids in tissue sections. The spectral patterns can be directly correlated with the clinical phenotype of the disease, enabling the straightforward utilization of the information for clinical diagnostics. It has been shown that implementing DESI-MSI alongside histopathological analysis helps to understand the pathobiochemistry and thus the aetiology of diseases. This project aims to use DESI-MSI to understand the metabolic hallmarks of cirrhotic liver diseases and use this information to augment diagnostics.

Poster #B22 in Exhibit Hall - *attended for 1hr on Wednesday starting at 18:30*
Topic: *Small Molecules*

A Novel Fast and Simple Quantification Method for Bile Acids in Human Serum by LC-MS/MS

Aurore Jaffuel - *Shimadzu France* (aj@shimadzu.fr)

‣ For Research Use Only. Not for use in clinical diagnostics. Bile Acids (BAs) are steroid acids of the bile. They are fat substances solubilizers of the enterohepatic cycle and are key players of lipid and energy metabolism. Abnormal BAs profiles may be used as biomarkers of several liver diseases. Despite the clinical need of measuring BAs concentration in plasma/serum, reference separations were proved to be unsuitable for simple and rapid analysis. Here is proposed a new LC-MS/MS method for the simultaneous high sensitive quantification of 27 BAs. A quick sample preparation technique based on proteins precipitation was applied. Good repeatability was obtained (RSD<5%). Linearity was tested for 16 BAs and confirmed for all in the range 1 to 100 ng/ml. The r2 coefficients were above 0.99, with S/N>10 for LLOQ levels.

Poster #B23 in Exhibit Hall - *attended for 1hr on Wednesday starting at 9:45*
Topic: *Metabolomics*

Simple & Robust Approach in Urinary Metabolomics Based on UPLC-MS for Preoperative Colorectal Cancer Diagnostics

Ivan Plyushchenko - *Lomonosov Moscow State University* (plyush1993@bk.ru) -- *Young Investigator Grantee*

‣ We report here the results of a relatively short study in which ultra-high performance liquid chromatography mass spectrometry and multivariate statistical analysis (sPLS-DA and oPLS-DA) were applied for urinary metabolite profiling and data interpretation. The results of the statistical analysis indicated that the metabolic pattern as a whole was significantly different between the groups of preoperative colorectal cancer (CRC) patients, postoperative CRC patients, and healthy volunteers, respectively. It is especially worth noting that the complete partitioning of data into groups without overlapping was achieved without any urine concentration normalization technique and MS signal drift correction.

Poster #B24 in Exhibit Hall - *attended for 1hr on Thursday starting at 10:00*
Topic: *Endocrinology*

Quantification of Catecholamines and Metanephrines in Urine Using the Thermo Scientific™ TSQ Endura™ Mass Spectrometer for Research Use

Sergio Indelicato - *Thermo Fisher Scientific France,Villebon surYvette* (sergio.indelicato@thermofisher.com)

‣ An analytical method for the quantification of catecholamines and metanephrines in urine is reported. The method involves a liquid liquid extraction (LLE) of metanephrine, normetanephrine, epinephrine, norepinephrine and dopamine from urine followed by injection onto a Thermo Scientific™ UltiMate™ 3000 system; mass spectrometric detection is performed by Single Reaction Monitoring (SRM) on a Thermo Scientific™ TSQ Endura™ triple quadrupole mass spectrometer using heated electrospray ionization in positive mode. The method was analytically validated using charcoal stripped urine spiked with the compounds of interest for lower limit of quantification, linearity range, accuracy, intra- and inter-assay precision and matrix effect evaluation.

Poster #B25 in Exhibit Hall - *attended for 1hr on Wednesday starting at 9:45*
Topic: *Various OTHER*

Misfortunes of a Mass Spec Start-Up

Sophie Hepburn - *The Ipswich Hospital NHS Trust* (sophie.hepburn1@nhs.net) -- *Young Investigator Grantee*

‣ As the acceptance of mass spectrometry within clinical laboratories grows there is a continued push to adopt this technology, however, this acquisition should be conducted with caution. In 2014, Ipswich Hospital acquired three mass spectrometry instruments as part of a tender process. The departure of key staff, a lack of provision for the requirements of these instruments, along with a lack of in-house expertise, resulted in the instruments remaining in their delivery crates to the present day. The greatest opposition came from a restructuring of the pathology management framework in response to the Carter Report, putting a hold on development and the required structural building work. This report covers the myriad of issues that can occur with and after a tender process and offers a cautionary tale to laboratories embarking on this venture.

Poster #B26 in Exhibit Hall - *attended for 1hr on Wednesday starting at 18:30*
Topic: *Small Molecules*

Quantitative Toxicology Screening for Over 1000 Compounds in Whole Blood Samples; is there a Better Way of Reporting Results?

Stephane Moreau - *Shimadzu Europe* (sm@shimadzu.eu)

‣ Clinical pathology laboratories use highly specific, sensitive methods and technologies working across a multi-disciplinary teams delivering actionable data. However, if a false positive result is reported the downstream impact to unnecessary testing and treatment can be considerable. In this paper we present a library of product ion spectra for 1222 compounds that has been developed for clinical and forensic toxicology screening to help reduce false positive and false negative reporting. The library enables multi-targeted methods to be developed for routine screening, library identification and quantitation.

Poster #B27 in Exhibit Hall - *attended for 1hr on Wednesday starting at 9:45*
Topic: *Small Molecules*

Determination of Organophosphorus Nerve Agents Biomarkers in Urine by Ion Chromatography Tandem Mass Spectrometry

Timur Baygildiev - *Lomonosov Moscow State University* (timurbaychem@gmail.com) -- *Young Investigator Grantee*

‣ Organophosphorus nerve agents are very dangerous class of chemical weapons and methylphosphonic acid and ethylphosphonic acid are the most stable hydrolysis product of them. Methylphosphonic acid determination in urine is a direct proof of chemical weapons application. Ethylphosphonic acid is related to the chemical weapons convection and it is a possible biomarker of new nerve agents. Here we describe analytical approach that allows simultaneous determination of methylphosphonic and ethylphosphonic acid in urine with use of anion-exchange liquid chromatography with tandem mass spectrometric detection. The approach is characterized by good metrological characteristics and very low limits of detection.

Poster #B28 in Exhibit Hall - *attended for 1hr on Thursday starting at 10:00*
Topic: *Small Molecules*

A Novel Solution for EtG/EtS Analysis in Human Urine by LC-MS/MS

Frances Carroll - *Restek Corporation* (frances.carroll@restek.com)

‣ Ethyl Glucuronide (EtG) and Ethyl Sulfate (EtS) are unique biomarkers of alcohol use. EtG and EtS analysis offers many advantages for abstinence monitoring including the detection window, stability in stored specimens, and specificity. EtG and EtS are both polar, making them difficult to retain via reversed-phase chromatography. Both compounds are also very sensitive to matrix interferences which can result in being unable to achieve low limits of detection and can also make quantitation impossible. In this study, a simple dilute and shoot method was developed and validated for the analysis of EtG and EtS in human urine by LC-MS/MS.

Poster #C01 in Exhibit Hall - *attended for 1hr on Wednesday starting at 9:45*
Topic: *Tissue Imaging*

Profiling of Phospholipids Reveals Potential Biomarkers for Breast Tumor by MALDI Imaging and UPLC-MS

Geul Bang - *Korea Basic Science Institute* (bangree@kbsi.re.kr)

‣ Breast cancer is the most common cancer and the development of new technologies for enhanced understanding of the molecular alterations involved in cancer progression is important. We utilized MALDI imaging and UPLC-ESI-MS/MS method to conduct comprehensive lipid profiling in breast tumor mice in which were injected with human breast cancer cell line (MDA-MB-231). Our data showed significant alterations in the phosphatidylcholine (PC-16:0/18:1) and phosphatidylinositol (PI-18:0/20:4) in both MALDI Imaging and UPLC/MS profiling data. Our results suggest that phospholipids may have diagnostic potential as well as that changes of their metabolism may provide therapeutic opportunities in breast cancer treatment.

Poster #C02 in Exhibit Hall - *attended for 1hr on Wednesday starting at 18:30*
Topic: *Small Molecules*

Quebec Urinary Screening Program: From Thin Layer Chromatography to Tandem Mass Spectrometry

Christiane Auray-Blais - *Université de Sherbrooke/CIUSSS de l'Estrie-CHUS* (christiane.auray-blais@usherbrooke.ca)

‣ The Provincial Neonatal Urine Screening Program in the Province of Quebec and the Nunavut region began in 1971 in Sherbrooke (1) (more than 3,200,000 newborns screened). Newborn urine samples are collected on filter paper by parents at 21 days of age. The main goal is the early detection and prevention of morbidity and mortality due to inherited metabolic diseases such as urea cycle disorders, organic acidurias, disorders of amino acid metabolism and transport. Samples are analyzed using a multiplex thin layer chromatography (TLC) technique with a sequential-four reagent staining methodology. The TLC methodology transfer to tandem mass spectrometry revealed positive results for all affected patients tested. Twenty different urine metabolites are analyzed in a short 2-min UPLC-MS/MS method which might be applicable to mass and high-risk screening, and monitoring treated patients.

Poster #C03 in Exhibit Hall - *attended for 1hr on Wednesday starting at 9:45*
Topic: *Metabolomics*

Breath Biopsy with TD-EESI-FAIMS-MS: A New Approach for Rapid, Non-Invasive Measurement of the Breath Metabolome

Alasdair Edge - *Owlstone Medical Ltd.* (alasdair.edge@owlstone.co.uk)

‣ Exhaled breath contains volatile organic compounds (VOCs) that are directly linked to the body's metabolism, and constitute potential disease biomarkers. VOC metabolites in breath originate from the pulmonary tissue and circulatory system, making them relevant to both the pulmonary system and wider body. Lengthy chromatographic run times associated with GC-MS analyses of the breath metabolome limit sample throughput. A faster analytical method makes breath analysis a more viable screening technique. Here we describe a thermal desorption-extractive electrospray ionisation-field asymmetric ion mobility spectrometry-mass spectrometry (TD-EESI-FAIMS-MS) method for the analysis of VOC metabolites in exhaled breath with a 10 minute analysis time, suitable for the high throughput clinical environment.

Poster #C04 in Exhibit Hall - *attended for 1hr on Thursday starting at 10:00*
Topic: *Small Molecules*

Rapid Separation of Steroid and Secosteroid Metabolites by ultraFAIMS-MS for High-Throughput Clinical Analysis

Lauren Brown - *Owlstone Medical Ltd., 162 Cambridge Science Park,* (lauren.brown@owlstone.co.uk)

‣ The simultaneous, accurate measurement of isomeric steroid and secosteroid metabolites using mass spectrometry (MS) can be time consuming and expensive. The formation of the same mass to charge (m/z) parent and product ions presents a significant challenge for spectral interpretation and requires lengthy chromatographic runs to prevent co-elution. An alternative approach is the use of field asymmetric ion mobility spectrometry (FAIMS). FAIMS separates ions on the basis of differences in their gas-phase ion mobility under alternating low and high electric fields and is highly orthogonal to m/z separation in a mass analyser. Here we describe the application of FAIMS-MS to the analysis of hydroxyvitamin D3 epimers and isomeric testosterone metabolites, eliminating the lengthy liquid chromatography (LC) step for the high-throughput clinical laboratory.

Poster #C05 in Exhibit Hall - *attended for 1hr on Wednesday starting at 9:45*
Topic: *Small Molecules*

Universal LC-MS/MS System Configuration (Instrument, Analytical Column and Mobile Phases) for Determination of Multiple Drugs in Serum Samples

Magdalena Rajska - *Spadia Lab* (magdalena.rajska@spadia.cz)

‣ Introducing of mass spectrometry into routine clinical laboratory can benefit with optimization of workflows, especially through the introduction of versatile home-made methods in a multianalytes configuration. The aim of this work is to present universal LC-MS/MS system configuration suitable for determination of 18 drugs from different groups as antiepileptics, antibiotics, immunosupresants and benzodiazepines. All methods are designed in the way to use one analytical column with same mobile phases, methods differs in used chromatographic gradients. This approach provide optimized workflow and allows to run few methods one after another without the need for operator intervention to change system configuration.

Poster #C06 in Exhibit Hall - *attended for 1hr on Wednesday starting at 18:30*
Topic: *Small Molecules*

Feasibility to Screen Creatine Synthesis and Transport Disorders, Triple H Syndrome and OTC Deficiency in Newborn Urine Specimens

Pamela Lavoie - *Université de Sherbrooke* (pamela.lavoie@usherbrooke.ca)

‣ In the province of Quebec, newborns benefit from an additional neonatal screening performed at 21 days of age in urine specimens collected on filter paper at home by parents. Urea cycle disorders, organic acidurias, amino acid metabolism and transport disorders are targeted using a multiplex thin layer chromatography (TLC) technique. This study aimed to investigate the feasibility to increase the number of treatable disorders screened in urine, by performing tandem mass spectrometry analyses on the extracts remaining from the TLC technique. Creatine synthesis and transport disorders, Triple H syndrome and ornithine transcarbamylase deficiency were targeted using this reliable MS/MS methodology.

Poster #C07 in Exhibit Hall - *attended for 1hr on Wednesday starting at 9:45*
Topic: *Small Molecules*

Quantitative Analysis of 7 Antiepileptic Drugs in Human Serum for Research Using a Two-Channel LC-MS/MS System

Edward Goucher - *Thermo Fisher Scientific* (ed.goucher@thermofisher.com)

‣ We describe an efficient, fast and accurate LC-MS/MS method with a wide analytical range to quantitate 7 antiepileptic drugs (AEDs) - Gabapentin, Lamotrigine, Levetiracetam, 10-OH-Oxacarbazepine, Pregabalin, Topiramate and Zonisamide - in human serum for research purposes. This method employs protein precipitation followed by dilution before injection into a two-channel LC-MS/MS system, enabling analysis of 7 AEDs in each injection every 2.2 minutes. The method produced significant savings in analysis time and solvent consumption compared to traditional HPLC methods.

Poster #C08 in Exhibit Hall - *attended for 1hr on Thursday starting at 10:00*
Topic: *Metabolomics*
The Role of Lipids in Diseases - Challenges of Lipid Isomers and Isobars in Mass Spectrometry-based Biomarker Research
Ulf Sommer - *Biocrates Life Sciences AG* (ulf.sommer@biocrates.com)
‣ The distinction of different isobars and isomers is a consistent challenge in lipidomics and the attribution of the role of lipids in disease. We are discussing here the abilities and restrictions of quantitative high-resolution accurate-mass (HRAM) spectrometry versus multiple-reaction monitoring (MRM) on a triple quadrupole instrument in light of the short run times required in medical research.

Poster #C09 in Exhibit Hall - *attended for 1hr on Wednesday starting at 9:45*
Topic: *Endocrinology*
A Versatile Workflow to Measure Plasma Renin Activity and Aldosterone for Clinical Research Using Automated On-Line Extraction Coupled to LC-MS/MS
Magnus Olin - *Thermo Fisher Scientific* (magnus.olin@thermofisher.com)
‣ Researchers studying the renin-angiotensin-aldosterone system require accurate measurements of renin activity (production of angiotensin I) and of aldosterone concentration in plasma sample preparations. We report a workflow to accomplish this utilizing automated on-line extraction coupled to LC-MS/MS, which simplifies sample preparation. Only 250 µL of sample were required to achieve reliable quantitative analytical ranges for angiotensin I (1 to 500 ng/mL plasma) and aldosterone (25 to 1000 pg/mL plasma). Excluding overnight incubation time for renin activity, throughputs for quantitating angiotensin I and aldosterone were 10 and 12 samples per hour, respectively.

Poster #C10 in Exhibit Hall - *attended for 1hr on Wednesday starting at 18:30*
Topic: *Small Molecules*
Quantitative Analysis of Heparan Sulfate and Dermatan Sulfate in MPS II Mice Tissues by UPLC-MS/MS
Iskren Menkovic - *Université de Sherbrooke* (iskren.menkovic@usherbrooke.ca)
‣ Mucopolysaccharidosis type II (MPS II, Hunter syndrome) is an X-linked lysosomal storage disorder leading to an accumulation of two glycosaminoglycans, heparan sulfate (HS) and dermatan sulfate (DS) in several tissues and biological fluids. The main objective of this research project is to study the distribution of HS and DS in several MPS II tissues (brain, liver, kidney, heart and intestine), as well as biological fluids (plasma and urine) in MPS II untreated mice (n=8), MPS treated mice (n=8) and control mice (n=8) using an ultra-performance liquid chromatography tandem mass spectrometry (UPLC-MS/MS) approach.

Poster #C11 in Exhibit Hall - *attended for 1hr on Wednesday starting at 9:45*
Topic: *Metabolomics*
Towards Standardized Data Analysis Workflows in Targeted Metabolomics – Challenges and Best Practices in Biomarker Discovery
Stefan Ledinger - *Biocrates Life Sciences AG* (stefan.ledinger@biocrates.com)
‣ Despite its rapid growth and large amount of data produced, there is still a lack of awareness on the importance of targeted metabolomics data pre-processing and pre-treatment, i.e. the very first steps of data analysis. Correct data handling at this early stage may significantly enhance later statistical data analysis, biological interpretation and biomarker identification to path the way to clinical applications. This presentation addresses the cornerstones of standardized data analysis in targeted metabolomics ranging from common pitfalls in study design, to rules for harmonization of data pre-processing, as well as their impact on statistical analysis and biomarker discovery.

Poster #D01 in Exhibit Hall - *attended for 1hr on Thursday starting at 10:00*
Topic: *Metabolomics*
Expanded Newborn Screening by Tandem Mass Spectrometry and Implementation of Next Generation Sequencing in Slovenia
Andraz Smon - *University Medical Centre Ljubljana* (andraz.smon@gmail.com) -- *Young Investigator Grantee*
‣ Expansion of current screening programmes is one the major goals of health-care programmes in south-eastern Europe and Slovenia only screens for phenylketonuria and congenital hypothyroidism, we conducted a pilot study of expanded NBS for 13 inborn errors of metabolism in Slovenia. In 10048 participants we measured acylcarnitines and amino acids in dried blood spots using tandem mass spectrometry. In 5 participants an inborn error of metabolism was found, genetic confirmation was done with next generation sequencing.

Poster #D02 in Exhibit Hall - *attended for 1hr on Wednesday starting at 9:45*
Topic: *Small Molecules*

Measurement of *in Vivo* Glycolytic Flux by Liquid Chromatography Tandem Mass Spectrometry

Bei-Tzu Wang - *University Children* (bei-tzu.wang@med.uni-heidelberg.de)

‣ Glucose metabolism is essential in living organisms. The disturbance of glycolytic flux relates to several diseases, and indicated as a hallmark of cells under energetic stress. We aimed to establish a LC-MS/MS method for measuring and studying in vivo glycolytic flux . The recovery rates of the measured glucose intermediates were between 80 to 119% with the imprecision less than 10%. For the in vivo study, the increased ribulose-5-phosphate in ADP-dependent glucokinase (adpgk) deficient zebrafish embryos could be rescued when re-supplying adpgk, indicating the good specificity of the measurement. Overall, the LC-MS/MS method is reliable for detecting glucose metabolism in vivo.

Poster #D03 in Exhibit Hall - *attended for 1hr on Wednesday starting at 18:30*
Topic: *Various OTHER*

Medicinal Compounds of Mexican Oregano Analysis by CG-MS and LC-MS

Amanda Moreno - *FESI,Universidad Nacional Autonoma de Mexico, UNAM* (amanda.moreno.fesi@gmail.com) --
Young Investigator Grantee

‣ Mexican oregano is valued for its flavour and medicinal properties, which are due to the high levels of essential oils and antioxidant flavonoids. This specie is used for the treatment of gastrointestinal and respiratory ailments. Different types of abiotic stress were evaluated in greenhouse-grown and wild plants in order to compare phytochemical profile of flavonoids and terpenoids using LC-MS and GC-MS, respectively. 24 flavonoids and 48 terpenoids were identified. Water stress and foliar damage induced accumulation of some monoterpenoids, and light stress raised flavonoids concentration. The results are useful in studies of pharmacological production more predictable and sustainable.

Poster #D04 in Exhibit Hall - *attended for 1hr on Wednesday starting at 9:45*
Topic: *Small Molecules*

Evaluation of Blood Lysis Procedures Prior to Automated Sample Preparation for Immunosuppressant Assay by LC-MS/MS

Ryu Konoshita - *Shimadzu Europa GmbH* (konoshita@shimadzu.eu)

‣ CLAM-2000 (Shimadzu Corp., Japan) fully automates blood or other samples pre-treatment prior to LC-MS analysis. For measurement of immunosuppressant (ISP) in whole blood samples, most target is bound to cytoplasmic proteins in erythrocytes and it is mandatory to lyse them prior to the pre-treatment. In this study, several protocols of hemolysis were evaluated based on lysis efficiency and ISP recovery. Freeze/thaw with -80 ‹C was efficient for both 0.2mL and 1mL. -20 ‹C was also effective but the reproducibility was very low. The efficiency and recovery rate by ammonium chloride was also good but sample dilution must be taken into account.

Poster #D06 in Exhibit Hall - *attended for 1hr on Wednesday starting at 9:45*
Topic: *Metabolomics*

High-Throughput Identification of Hemoglobinopathies and Thalassemia by HRAM/MS

Thomas Wiesinger - *TU Wien* (thomas.e163.wiesinger@tuwien.ac.at)

‣ Due to their high incidence and clinical relevance, a growing interest in the development of fast and reliable methods for automated identification of pathologically relevant hemoglobin variants and disorders of impaired hemoglobin expression, which can be applied for newborn screening and selective diagnostics.[1] Even when well established methods for the characterization of hemoglobin exist for decades, their use for high throughput screening is limited. A high throughput method for the identification of selected Hb-variants and thalassemias in dried blood spots by applying a fast dual-channel size exclusion liquid chromatography analysis, with a high resolution mass spectrometer (SEC-LC-HRAM/MS), has been developed.

Poster #E01 in Exhibit Hall - *attended for 1hr on Wednesday starting at 18:30*
Topic: *Small Molecules*
Applying LCMS Methods to Instruments of Different Manufacturers – Juggling with a Variety of ESI Source Parameter Settings
Katharina Kern - *RECIPE Chemicals + Instruments GmbH* (k.kern@recipe.de)
‣ When applying our CE-IVD methods to LCMS instruments of different manufacturers, we face sensitivity differences between several instrument classes and individual instruments themselves, but we also experience the significance of appropriate set source parameters. Even though the different source gases, temperatures and voltages sound similar, they do not always have the same influence on the very same analyte. Using the example of Phenytoin, we want to demonstrate how amazingly different similar named source parameters can influence sensitivity of certain substances.

Poster #E02 in Exhibit Hall - *attended for 1hr on Wednesday starting at 9:45*
Topic: *Various OTHER*
Evaluation of Critical Parameters for the Establishment of a Clinical MALDI Applications Platform for Liquid Biopsy Diagnostics
Gerald Stübiger - *Medical University Vienna* (gerald.stubiger@meduniwien.ac.at)
‣ MALDI-MS represents a robust and easy-to-use tool for the analysis of different types of biomolecules. This makes it a very powerful and promising tool for routine clinical applications. The success of the technique mainly depends on the optimisation of individual parts of the analysis workflow including sample isolation, processing, measurement and data analysis. Here we present the evaluation of critical parameters of sample isolation and processing for the successful MALDI-based detection of biomarkers in the field of liquid biopsy.

Poster #E03 in Exhibit Hall - *attended for 1hr on Thursday starting at 10:00*
Topic: *Small Molecules*
Extraction of Catecholamine Acid Metabolites from Plasma Prior to Analysis Using LC-MS/MS
Alan Edgington - *Biotage (GB) Ltd.* (Alan.Edgington@biotage.com)
‣ Catecholamine metabolites are biomarkers for neuroblastoma and catecholamine-secreting tumors. Here we present optimization of the method development process to maximise analyte sensitivity in the extraction and quantitation of plasma catecholamine acid metabolites. Method parameters optimized for increased sensitivity: MRM transitions, chromatography and sample preparation protocols. LC-MS/MS analysis was performed using a Shimadzu Nexera UHPLC system coupled to an AB SCIEX 5500 triple quadrupole MS. Extraction methods demonstrated recoveries greater than 80% with RSDs below 10%. Calibration curves from 20 to 1000 ng mL-1 demonstrated good linearity with r2 values greater than 0.990 for all analytes.

Poster #E04 in Exhibit Hall - *attended for 1hr on Wednesday starting at 9:45*
Topic: *Proteomics*
Krabbe Disease: Quantitative Microproteomics on Specific Histological Brain Regions of the Twitcher Mouse
Davide Pellegrini - *NEST, Scuola Normale Superiore* (davide.pellegrini@sns.it)
‣ Krabbe disease is an autosomal-recessive sphingolipidosis caused by a deficiency of the enzyme galactosylceramide beta-galactosidase, and is characterized by an accumulation of psychosine in the nervous system. Here we applied ultrasensitive proteomics to investigate changes in the proteome, in specific brain regions, associated with Krabbe disease. TMT-10plex experiments were performed to compare the proteomes extracted from the corpus callosum, motor cortex and sciatic nerve. The levels of more than 3500 protein groups were compared from the specific anatomical locations. Statistical analysis revealed proteins showing a different expression profile between the Twitcher mouse model of Krabbe disease and wild type mice.

Poster #E06 in Exhibit Hall - *attended for 1hr on Wednesday starting at 9:45*
Topic: *Small Molecules*
Combined Screening and Quantitative Confirmation of 129 Drugs in Urine by LDTD-MS/MS Using a Generic SPE Procedure
Richard Lam - *TECAN SP* (richard.lam@tecan.com)
‣ Toxicology laboratories are looking for new ways to improve their analysis by lowering operating costs and increasing overall throughput while maintaining quality data reporting. The use of a generic sample preparation for presumptive analysis of all drug classes in urine and subsequent use of the same extract for definitive testing can provide a significant cost and time savings approach. To increase the sample throughput, Laser Diode Thermal Desorption Mass Spectrometry (LDTD-MS/MS) was used to screen at less than 10 seconds per sample employing a generic sample extraction. Presumptive positive samples were transferred to LC-MS/MS for confirmation using the same sample extract to separate isobaric compounds.

Poster #E08 in Exhibit Hall - *attended for 1hr on Wednesday starting at 9:45*
Topic: *Proteomics*

Plasma Proteome Profiling Disentangles Caloric Restriction and Bariatric Surgery Induced Weight Loss

Philipp Geyer - *Max Planck Institute of Biochemistry* (geyer@biochem.mpg.de)

‣ We have developed an automated and robust shotgun proteomics pipeline – called `Plasma Proteome Profiling` – to yield a global phenotype of individuals (Geyer et al. Cell Systems 2016). So far, we have applied this workflow to studies with a focus on weight loss. One study is based on weight loss induced by caloric restriction and another one by bariatric surgery. In these studies we analyzed more than 1,800 plasma proteomes using undepleted plasma and we achieved a quantitative depth of more than 500 proteins. This covered pivotal biological aspects such as the lipid homeostasis system, low level inflammation, iron metabolism, hormone differences and insulin resistance.

Poster #E09 in Exhibit Hall - *attended for 1hr on Wednesday starting at 18:30*
Topic: *Proteomics*

Comprehensive Proteogenomics Analysis of MCF-7 Cell Lines

Avinash Yadav - *Scuola Normale Superiore, Pisa, Italy* (ayavinash@gmail.com)

‣ We report a comprehensive proteogenomics analysis of MCF-7 cell lines. We demonstrate the presence of protein product from SNPs, insertions, deletions, upstream open reading frames, long non-coding RNAs, transcripts with retained introns, antisense transcripts, exon-intron boundaries, novel splice isoforms, expressed pseudogenes, and novel protein coding sequences in MCF-7 cell lines.

Poster #E10 in Exhibit Hall - *attended for 1hr on Wednesday starting at 9:45*
Topic: *Small Molecules*

Analysis of Plasma Free Metanephrine, Normetanephrine, and 3-Methoxytyramine by HydropHILIC Interaction Liquid Chromatography

Ute Beyer - *Restek Corporation* (ute.beyer@restekgmbh.de)

‣ Metanephrine, normetanephrine, and 3-methoxytyramine are methylated metabolites of epinephrine, norepinephrine, and dopamine, respectively. Measurement of these metabolites in plasma is highly sensitive for the diagnosis of pheochromocytoma and paraganglioma. Analysis of these polar compounds using typical reversed-phase liquid chromatography is difficult due to limited chromatographic retention and lack of sensitivity. As a solution, an LC-MS/MS method was developed based on hydrophilic interaction chromatography using a Raptor HILIC-Si column. Combined with a simple and fast solid-phase extraction procedure, an accurate and precise analysis of plasma free metanephrine, normetanephrine and 3-methoxytyramine can be achieved and applied to high-throughput clinical assays.

Poster #F02 in Exhibit Hall - *attended for 1hr on Wednesday starting at 9:45*
Topic: *Tissue Imaging*

Visualising Trans-Epithelial Small Molecule Transport by High Spatial Resolution Mass Spectrometry Imaging

Lennart Huizing - *M4I division of IMS, Maastricht Unviversity* (l.huizing@maastrichtuniversity.nl) -- *Young Investigator Grantee*

‣ Tofacitinib (Tofa), a Janus kinase inhibitor, used in the treatment of rheumatoid arthritis is currently being investigated in other indications like inflammatory bowel disease (IBD) and psoriasis by various drug companies. Tofa, having high epithelial membrane permeability, is a good in-vivo model compound to study intestinal membrane passage of novel drugs. Rat ileum and colon are analyzed with high spatial and high mass resolution MALDI-MSI and SIMS. MSI data reveals the exact location of Tofa, colon providing insight in uptake in and passage over the intestinal epithelium. This will greatly enhance (potential) drug discovery in e.g. IBD.

Poster #F03 in Exhibit Hall - *attended for 1hr on Wednesday starting at 18:30*
Topic: *Endocrinology*

Quantitation of Plasma Metanephrine and Normetanephrine by Derivatization Using LC-MS/MS Analyzer Integrated with Fully-Automated Sample Preparation Device

Atsuhiko Toyama - *Marketing Innovation Centre, Shimadzu Corporation* (toyama@shimadzu.com.sg)

‣ Although LC-MS/MS analysis manifests high repeatability in measurement, overall reproducibility of an assay is compromised by errors associated with manual sample pretreatment. This also hinders standardization of assay across multiple laboratories. In this investigation, we evaluated whether automated sample preparation device can be employed to carry out complex sample pretreatment procedures, such as required for chemical derivatization. As model experiment, plasma metanephrine and normetanephrine was derivatized by reductive amination to improve reversed phase column retention.

Poster #F04 in Exhibit Hall - *attended for 1hr on Wednesday starting at 9:45*
Topic: *Endocrinology*
Analysis of Serum Estrogens – How Low Can Your Clinical Research Method Go?
Robert Wardle - *Waters Corporation* (robert_wardle@waters.com)
‣ Here we address the challenges faced trying to routinely measure Estradiol (E2) and Estrone (E1) at levels of 3.7pmol/L (1pg/mL) by LC-MS/MS for clinical research applications. The quest to reach these low levels led us to investigate a range of sample preparation and liquid chromatography methods. Samples were analysed using an ACQUITY® UPLC® I-Class-FTN and Xevo® TQ-XS mass spectrometer for optimum analytical sensitivity. Limits of quantification will be presented to show how low you could go with this routine LC-MS/MS workflow without the need for derivatization. For Research Use Only, Not for use in diagnostic procedures.

Poster #F06 in Exhibit Hall - *attended for 1hr on Wednesday starting at 9:45*
Topic: *Small Molecules*
Simultaneous Quantitation of 13 Psychotherapeutic Drugs in Human Plasma by UPLC-MS/MS and its Application in Therapeutic Drug Monitoring
Doudka Natalia - *Timone Hospital, Clinical Pharmacology* (liachenko23@gmail.com)
‣ Psychiatric drugs are commonly prescribed for the treatment of mental illness. A UPLC-MS/MS method was developed and validated for the monitoring of 13 psychotherapeutic drugs and 2 main pharmacologically active metabolites. Plasmatic samples were eluted on a Luna Omega Polar C18 column (1.6µm; 100 x 2.1 mm). Intra- and inter-day precision and accuracy values ranging from 2.99% to 12.85% and from 86.45% to 109.21%, respectively. No significant matrix effect was observed for all analytes. This method was applied with success for routine patient serum analysis.

Poster #F07 in Exhibit Hall - *attended for 1hr on Wednesday starting at 18:30*
Topic: *Small Molecules*
Quantitative Determination of Free Hormone Fraction via Biocompatible Solid Phase Microextraction (BioSPME)
Craig Aurand - *MilliporeSigma* (craig.aurand@sial.com)
‣ In this study, the use of biocompatible solid phase micro extraction devices are utilized for the determination of free circulating testosterone levels in human plasma. This technique allow of rapid determination with better precision as to membrane dialysis based techniques.

Poster #F08 in Exhibit Hall - *attended for 1hr on Wednesday starting at 9:45*
Topic: *Proteomics*
Quantitation of Infliximab and Adalimumab in Human Serum by Multiplex LC-MRM Using Full-Length Stable Isotope Labeled Internal Standards
Kevin Ray - *Merck KGaA* (kevin.ray@sial.com)
‣ There is a growing demand for reliable LC-MS/MS assays to support quantitation of serum levels of Infliximab and Adalimumab monoclonal antibodies, as clinical responses differ between patients due to varying pharmacokinetics and the formation of autoantibodies. We have employed full-length stable isotope labeled Infliximab and Adalimumab monoclonal antibody internal standards to achieve significant improvements in accuracy and reproducibility in the quantitation of serum Infliximab and Adalimumab by LC-MRM assay. We will demonstrate a lower limit of quantitation, without immunoenrichment, of 500 ng/mL for Infliximab and 1 ug/mL for Adalimumab with less than 15% CV and ± 15% accuracy.

Poster #F09 in Exhibit Hall - *attended for 1hr on Thursday starting at 10:00*
Topic: *Metabolomics*
Rapid-Fire Direct Metabolome Analysis by Probe Electrospray Ionization/Tandem Mass Spectrometry: its Preclinical Applications to Validate the Methods
Yumi Hayashi - *In Vivo Real-Time Omics Laboratory, Institute for* (yhayashi@met.nagoya-u.ac.jp)
‣ Rapid-fire direct metabolome analysis was achieved by PESI/MS/MS. The present method was able to directly detect 56, 48 and 27 metabolites in the mouse brain, liver and serum, respectively, without tedious sample preparation. High-throughput analysis was demonstrated with each runtime being within 2.5 min. Application of this technique to a preclinical study using mild liver-injury model mice induced by co-administration of acetaminophen and DMSO demonstrated its ability to capture slight metabolic disruption of the model. It is highly expected that the present method will be used for clinical studies in the near future.

Poster #F10 in Exhibit Hall - *attended for 1hr on Wednesday starting at 9:45*
Topic: *Various OTHER*

Evaluation of Hemolysate as Sample in Automated Sample Preparation for the Determination of Immunosuppressive Concentrations by LC-MS/MS - Tacrolimus Example

Matea Zorić - *Merkur University Hospital, Zagreb, Croatia* (mat.zoric@gmail.com)

‣ The manual whole blood sample preparation for LC-MS/MS for quantification of immunosuppressants is currently the method of choice. In order to evaluate the suitability of hemolysate as an alternative sample, analytical results obtained with manual whole blood sample preparation versus its hemolysates were compared. Tacrolimus concentrations (N=34) were measured by LC-MS/MS method. For hemolysate preparation, aliquots of 500 µL of whole blood samples from the same patients were used by the freeze-thaw method at -80 °C for 30 minutes. Passing and Bablok regression analysis revealed satisfactory comparison (y = -0,117+ (-0,389 - 0,185) + 0,978 (0,927 - 1,024)x). Since there's no statistically or clinically significant difference, the obtained results are suggesting that hemolysate could be a good alternative for whole blood samples.

Poster #H02 in Exhibit Hall - *attended for 1hr on Wednesday starting at 9:45*
Topic: *Various OTHER*

Quantification of 31 Antidepressants in Human Serum by Using a High Resolution Orbitrap Mass Spectrometer

Johanna Lindner - *Institute of Laboratory Medicine, LMU, Munich* (johanna.lindner@med.uni-muenchen.de)

‣ Methods for quantification of antidepressants are important in the clinical routine for therapeutic drug monitoring. While most of the currently used mass spectrometry methods use triple quadrupoles as mass analyser, we developed a method for 31 antidepressants in human serum using a high resolution Q Exactive Focus Orbitrap mass spectrometer operating in full-scan mode. A Turbo Flow column upfront to the analytical LC column improved sample clean-up and stable isotope-labelled counterparts of the target analytes were used as internal standards. The method validation showed good results for precision, accuracy, recovery, matrix effect, linearity and selectivity.

Poster #H05 in Exhibit Hall - *attended for 1hr on Wednesday starting at 18:30*
Topic: *Small Molecules*

Comparison of VAMS and Card Based Microsampling with LC-HRMS Analysis to Assess Cardiovascular Drug Levels

Dennis Bernieh - *De Montfort University - UK* (P13064053@my365.dmu.ac.uk) -- *Young Investigator Grantee*

‣ An objective means of assessing medication adherence is needed to enable patients get the maximum therapeutic benefits from their medication. A bioanalytical assay using dried blood spot (DBS) and volumetric absorptive microsampling (VAMs) followed by liquid chromatography-high resolution mass spectrometry (LC-HRMS) analyses was developed and validated for quantification of 11 commonly UK prescribed cardiovascular drugs. Results from the two sampling devices showed that VAMs overcomes the limitations associated with using DBS cards for quantitative analyses.

Poster #H06 in Exhibit Hall - *attended for 1hr on Wednesday starting at 9:45*
Topic: *Endocrinology*

LC-MS/MS Analysis of Angiotensin I for Assessment of Plasma Renin Activity in Clinical Research

Ben Dugas - *Waters Corporation* (Ben_Dugas@waters.com)

‣ We have evaluated an LC-MS/MS method for the measurement of angiotensin I (Ang1) enabling investigation of Plasma Renin Activity (PRA) for clinical research activities testing biomarkers of hypertension. Renin converts angiotensinogen to Ang1, which is subsequently converted to Angiotensin II (Ang2). Ang2 is a potent vasopressor and plays a central role in regulation of blood pressure. Measurement of Ang2 is challenging due to its low circulating levels and short half life. Ang1 is more stable, and therefore, a more suitable candidate to evaluate PRA. An analytical method was developed using offline automated µElution Solid Phase Extraction (SPE), reducing sample preparation time and optimizing analytical sensitivity. For Research Use Only, Not for use in diagnostic procedures.

Poster #L01 in Exhibit Hall - *attended for 1hr on Thursday starting at 10:00*
Topic: *Endocrinology*

Validation of a Semi-Automated Solid Phase Extraction LC-MS/MS Method for Androstenedione, 17-Hydroxyprogesterone and Testosterone Measurement

Emma Walker - *PhD, University College London, UK* (emmwalker@me.com)

‣ The abstract describes the validation of a combined LC-MS/MS method for the simultaneous measurement of androstenedione, 17-OHP and testosterone using Oasis PRiME HLB solid phase extraction (SPE).

Poster #L02 in Exhibit Hall - *attended for 1hr on Wednesday starting at 9:45*
Topic: *Small Molecules*

MagSiMUS-SteroidPREP: Automated Sample Preparation for LC-MS/MS Analysis of Steroids in Serum, Urine and Saliva on the MagSiMUSDX

Erik Ruijters - *MagnaMedics Diagnostics B.V.* (eru@magnamedics.com)

‣ MagnaMedics developed two new MagSiMUS-SteroidPREP (Cortisol/Cortisone - and Universal) sample preparation products, for the simultaneous LC-MS/MS analysis of more than 13 common steroid hormones in urine, saliva and serum clinical samples. Nearly all proteins and other matrix components were efficiently removed by magnetic separation, using a novel MagSiMUS particle mix of spherical, paramagnetic beads with a unique, proprietary surface. Diagnostic levels of all of these steroids could be accurately determined, with excellent signal- to-noise ratios. For medium to high-throughput workflows, fully traceable automation is easily achieved by the MagSiMUSDX system. In the absence of a centrifugation step the MagSiMUSDX system significantly improves the total sample throughput and accuracy, and reduces total preparation time.

Poster #L03 in Exhibit Hall - *attended for 1hr on Wednesday starting at 18:30*
Topic: *Small Molecules*

Volumetric Absorptive Microsampling (VAMS) and LC-MS/MS Analysis for Simultaneous Monitoring of 16 Antiepileptic Drugs: Workflow Development and Validation

Annachiara D'Urso - *Fondazione IRCCS Istituto Neurologico Carlo Besta* (annachiara.durso@istituto-besta.it) -- *Young Investigator Grantee*

‣ Volumetric absorptive microsampling (VAMS) is a novel sampling technique for collection of capillary blood. VAMS (MitraTM) absorbs a fixed volume of blood (10 or 20 µl) from a drop or pool of blood by dipping an absorbent polymeric tip into it. The resulting blood microsample is dried and analyzed as a whole. VAMS may overcome bias issues associated with dried blood spot (DBS). In this study VAMS were applied to therapeutic drug monitoring (TDM) of 16 different antiepileptic drugs (AEDs). A liquid chromatography–tandem mass spectrometry (LC–MS/MS) workflow for analysis of VAMS sample was developed and validated. Concentration of 16 AEDs on VAMS sampler were then compared to those in venous blood.

Poster #L04 in Exhibit Hall - *attended for 1hr on Wednesday starting at 9:45*
Topic: *Small Molecules*

Development of a LC-MS Method for Quantification of Six Common Pharmaceuticals in OFM Samples

Anton Mautner - *Joanneum Research, HEALTH* (anton.mautner@joanneum.at)

‣ A fast, robust and sensitive LC-MS method was developed to quantify six common pharmaceuticals (amitriptyline, clobetasol-17-propionate, diclofenac, hydrocortisone, lidocaine and metronidazole) in samples collected by open flow microperfusion (OFM). OFM is a sampling technique for preclinical and clinical studies where it provides a few µL of specimen with very low analyte concentrations. Therefore, it is important to use a sample preparation method that offers not only efficient clean up but also high analyte recovery. We tested different SPE µ-Elution plates (solid phase extraction) materials and successfully optimised an SPE protocol for all six analytes.

Poster #L05 in Exhibit Hall - *attended for 1hr on Thursday starting at 10:00*
Topic: *Tissue Imaging*

Spatial Metabolic Profiling of Idiopathic Pulmonary Fibrosis by Mass Spectral Imaging

Shabarinath Nambiar - *Murdoch University, Western Australia* (S.Nambiar@murdoch.edu.au) -- *Young Investigator Grantee*

‣ Mass spectrometry imaging (MSI) provides a platform for the localization of a diverse range of biochemicals in a sample at high spatial resolution. This approach promises novel insights into the biochemical characteristics of lung diseases like idiopathic pulmonary fibrosis (IPF). Specifically, we will employ MSI to (1) characterize novel chemical signatures across different morphological regions of fibrotic tissue; (2) elucidate biochemical differences between IPF and healthy lung tissue; and (3) identify potential diagnostic biomarkers associated with IPF. The generation of an MSI lung database will complement existing IPF histopathological assessments and provides clinicians with an enhanced method of clinical diagnosis.

Poster #M01 in Exhibit Hall - *attended for 1hr on Thursday starting at 13:00*
Topic: *Troubleshooting*
How Do You Hit the Target for Phosphatidylethanol PEth(16:0/18:1) in External Quality Controls ?
Anne Schmedes - *Department of Clinical Biochemistry* (anne.vibeke.schmedes@rsyd.dk)
‣ During development of an LC-MS/MS method for PEth(16:0/18:1) we used an external quality control program from Equalis (Sweden). Our results were 26–53% above mean value for all participating laboratories. Whole blood calibrators were prepared several times with PEth from different sources, with the same results. Consequently, our calibrators were measured in a Swedish laboratory and the measured values used as assigned values. However the Swedish laboratory also used recalibration. The Equalis mean may therefore not be correct but more a consensus mean. We investigated the effect of different ways of adding PEth to whole blood on the concentration obtained.

Poster #M02 in Exhibit Hall - *attended for 1hr on Thursday starting at 13:00*
Topic: *Troubleshooting*
Column and Auto Sampler and Flow Lines Blockage After 300-400 Injections
Reena Desai - *Anzac research institute* (reenad2729@gmail.com)
‣ To increase the sensitivity for estradiol analysis, derivatization with a sulphonyl chloride reagent (1,2-dimethylimidazole-5-sulfonyl cholride) was performed. The reaction is similar to that for dansyl chloride, and the reaction mixture was analysed without purification. But after running few hundreds of samples we ran into problems with auto sampler and flow lines being blocked almost every time and also the deterioration in column life and so bad peak shapes. We introduced guard cartridge along with the column so as to protect the column life and have more output. This did help us to run more number of samples than previously. But the issue with auto sampler clean-ups still remained consistent.

Poster #M04 in Exhibit Hall - *attended for 1hr on Thursday starting at 13:00*
Topic: *Troubleshooting*
Troubleshooting LC-MS/MS Peak Shape and Recovery Problems for Polar Opiates
Joe Di Bussolo - *Thermo Fisher Scientific* (joe.dibussolo@thermofisher.com)
‣ Polar opiates such as morphine, normorphine, morphine glucuronides and hydromorphone from diluted urine samples experienced peak fronting, splitting and poor recoveries as some analyte molecules were poorly retained in some reversed-phase LC-MS systems. Troubleshooting investigations showed that these problems were caused by small amounts of organic solvent that mingled with samples during injections. Changes to chromatographic conditions and autosampler parameters excluded organic solvent from sample injections and resulted in symmetrical peaks with good recoveries.

Poster #M05 in Exhibit Hall - *attended for 1hr on Tuesday starting at 19:00*
Topic: *Troubleshooting*
Troubleshooting: Measurement of Vitamin K1, MK-4 and MK-7 in Serum – with Special Focus on Purification
Ida Bøgh Andersen - *Vejle Hospital* (ida.bogh.andersen@rsyd.dk) -- *Young Investigator Grantee*
‣ Vitamin K is a group of very fat-soluble vitamins, which gives rise to several challenges during purification. Vitamin K can be lost in different steps of the process, e.g. vitamin K is sticking to glass, metals and other materials used during the purification and evaporation etc., leading to low recovery. Omitting the evaporation step has markedly increased the recovery, but we are still struggling with getting consistent, high recovery. The LC-MS method works satisfactory, it is the purification we wish to improve.

Poster #M06 in Exhibit Hall - *attended for 1hr on Tuesday starting at 19:00*
Topic: *Troubleshooting*
Carryover & Contamination Causes and Cures
Joe Di Bussolo - *Thermo Fisher Scientific* (joe.dibussolo@thermofisher.com)
‣ In order to assure the quantitative accuracy of LC-MS/MS systems and methods, validation studies must demonstrate freedom from any extraneous signals that augment analyte peak areas by more than 20% of the peak areas representing the lower limit of quantitation for each analyte (1). Such signals may result from samples (carryover and/or contamination) or from non-sample sources (contamination) by the analytes themselves or by other interferences having similar chromatographic and MS/MS attributes. Ways to reveal the sources of carryover and contamination and minimize their effects will be presented.

Poster #M07 in Exhibit Hall - *attended for 1hr on Tuesday starting at 19:00*
Topic: *Troubleshooting*

Troubleshooting in the Clinical Measurement of Iron Biomarkers Using LC-MS: Supression of Sample Losses in Autosampler Vials

Ioana-Monica Abbas *- Federal Institute for Materials Reseach and Testing (BAM) / School of Analytical Sciences Adlershof* (ioana.abbas@bam.de) -- *Young Investigator Grantee*

‣ We developed a rapid and robust HPLC-MS/MS (QqQ) method for the quantification of hepcidin-25, a promising new biomarker in iron metabolism, in human samples. The novelty of the method is the use of special HPLC vials to avoid adsorptive losses due to the basic character of the peptide that causes interaction with the silanol groups of the vial's glass surface. Up to 90% decrease in the MS/MS signal was observed, when commercial HPLC vials were used, while vials treated with 3-(2-aminoethylamino)propylmethyldimethoxysilane or 1H,1H,2H,2H-perfluorooctyltriethoxysilane, leading to no losses in the range of physiological hepcidin-25 mean serum levels (10-20 µg/L).

MEET THE EXPERTS *

* THE TERM ‘EXPERT’ IS AMBIGUOUS, BUT WE’RE GOOD AT SOME THINGS RELATED TO CHROMATOGRAPHY AND MASS SPECTROMETRY IN LABORATORY MEDICINE

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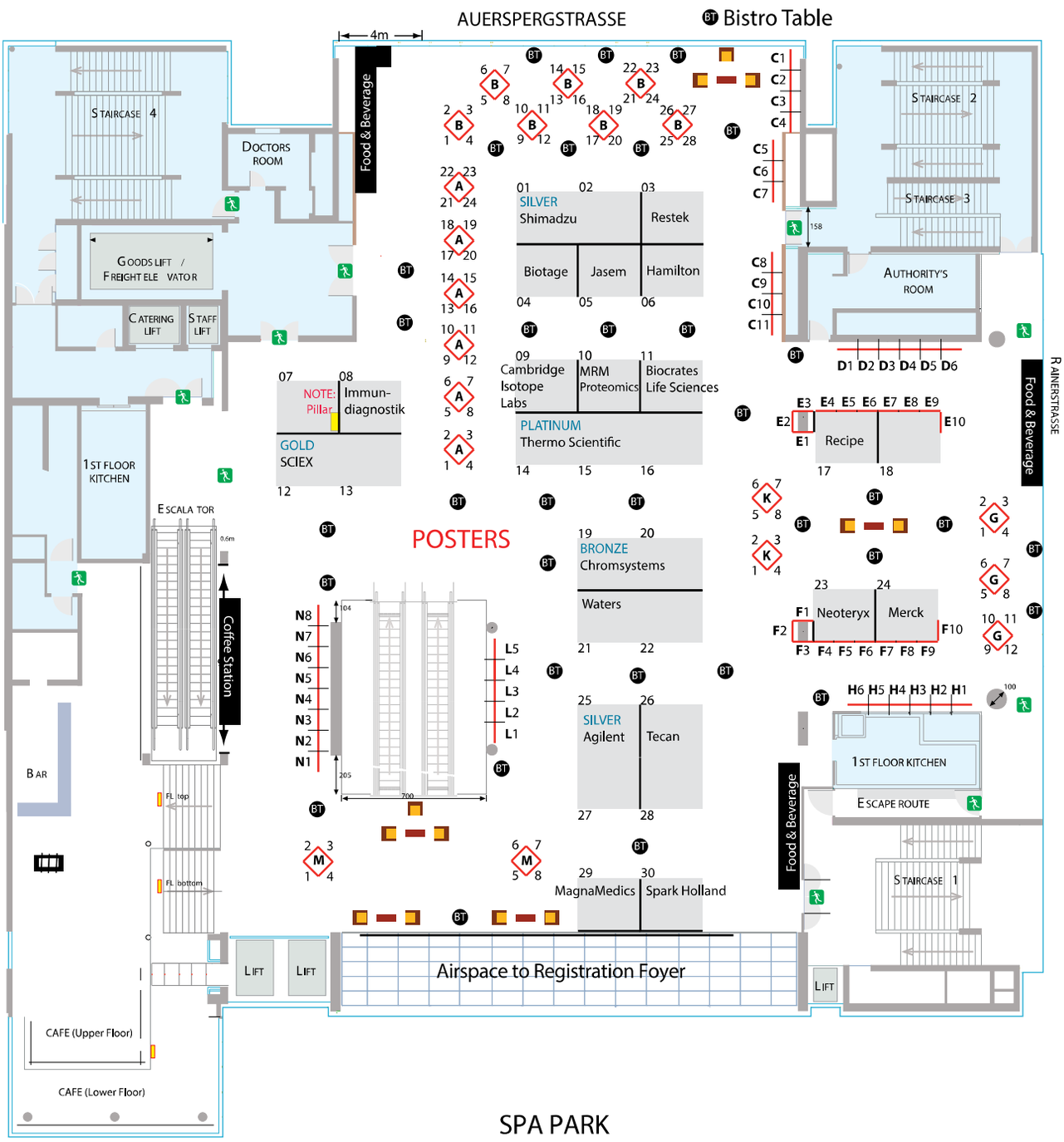
MAP: 1st Floor - *Exhibit Hall*

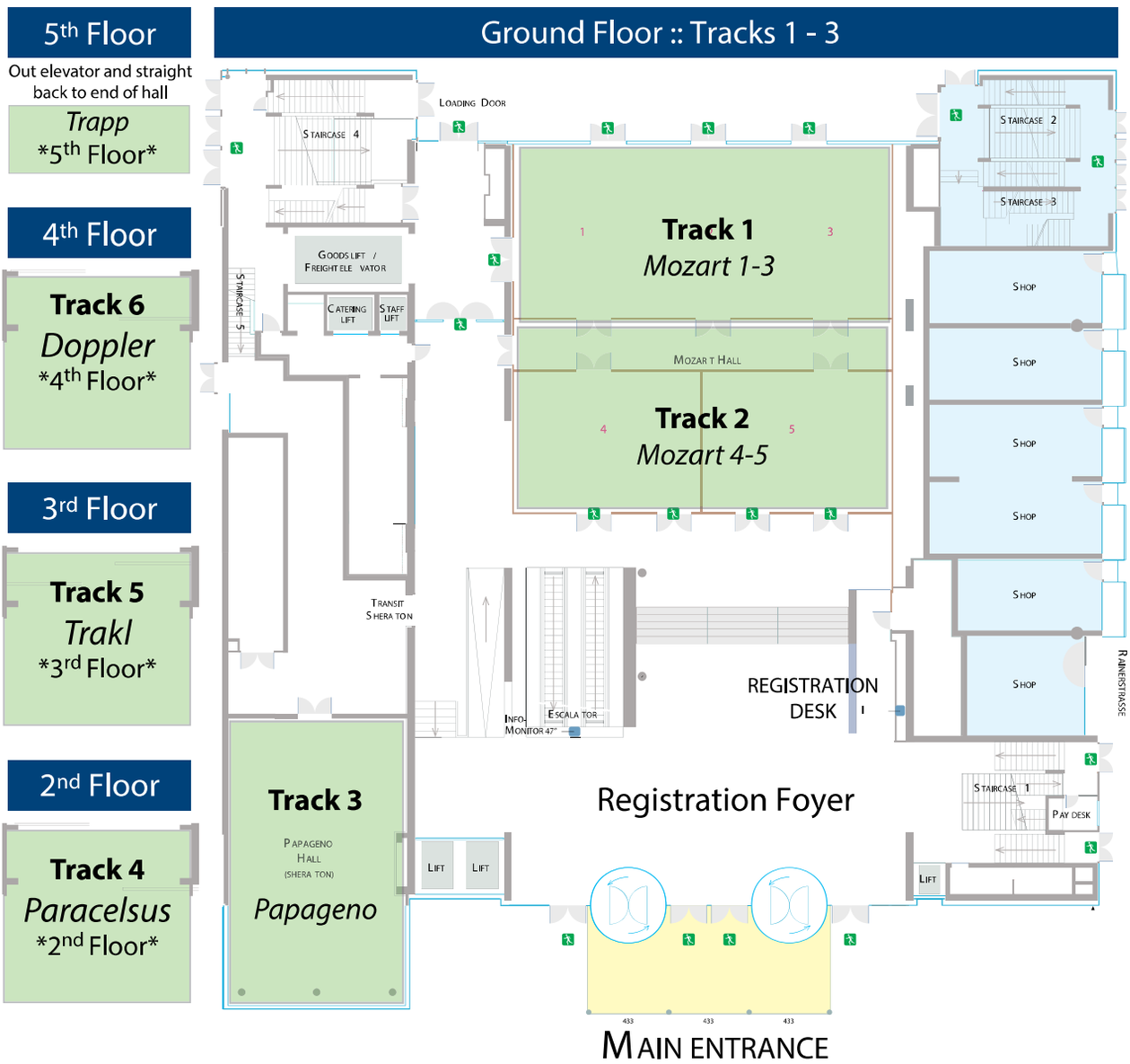
Exhibits & Posters as well as Coffee Breaks, Lunches and Receptions will be held on the 1st Floor.

Exhibit Hall / 1st Floor



MAP: Tracks and Floors

Plenary Lectures will be held in Europa (not shown, 2nd Floor) and Mozart Hall. Scientific Sessions and Corporate Workshops will be held on the Ground Floor, Paracelsus (2nd), Trakl (3rd) and Doppler (4th).



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Workshops

Wednesday, September 13, 2017 8:15 – 8:45 Location: Mozart 4-5

Introducing the Thermo Scientific™ Cascadion™ SM Clinical Analyzer: Accuracy. Ease-of-Use. Designed for the Clinical Lab.

Speaker: Sarah Robinson, Ph.D., Market Development Specialist, Thermo Fisher Scientific

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Wednesday, September 13, 2017 16:00 – 16:30 Location: Mozart 4-5

Quantitation of Endocrine Markers using High Resolution Mass Spectrometry

Speaker: Laura Owen, University Hospital of South Manchester, UK

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