Confidence in Results

Achieve greater productivity and confidence when providing laboratory-developed test results to the healthcare professionals you serve. New Thermo Scientific™ high-performance medical devices for in vitro diagnostic use — Thermo Scientific™ Prelude MD™ HPLC, Thermo Scientific™ Endura MD™ mass spectrometer, and Thermo Scientific™ ClinQuan MD™ software — help you deliver LC-MS results easily, quickly, and with more confidence.

LC-MS for in vitro diagnostic use

Visit us in booth #12 • theoscientific.com/LCMS-IVD

MSACL 2014 EU
Salzburg, Austria
September 2-5

The 1st Annual European Congress

Supported in part by generous contributions from:
The variety of your clinical research demands a variety of technologies

No one analytical technology can adequately reveal everything you need to know about your sample. Bruker offers the broadest range of high performance, easy-to-use, and expertly supported analytical systems to overcome any clinical research challenge. Our proven, extremely robust GC-Triple Quads, LC-Triple Quads, Ion Traps and QqTOFs ensure confidence in your results for microbiology, biomarker discovery, tissue imaging, and drugs of abuse or drug monitoring research.

Get the right answer faster, more cost effectively, using the appropriate analytical technology for the job – Bruker’s complementary solutions for clinical research.

Visit us at MSACL, Booth 15 and on the Web at www.bruker.com

GC/LC/MS Systems

Innovation with Integrity

You’re not the only one who needs to trust the test results

ACCURACY THE FIRST TIME

Clinicians and patients count on the most reliable diagnostic answers. We want you to be confident that results are as timely and accurate as possible. SCIEX Diagnostics offers an in vitro diagnostics solution with exceptional assay performance that helps overcome the limitations of current testing methods. Our newly introduced assays for Vitamin D, Newborn Screening and Immunosuppressants accurately measure multiple analytes in a single run, and virtually eliminate the need for re-runs and send-outs. And not only are SCIEX Diagnostics solutions backed by over 25 years of leadership in mass spectrometry, they are surprisingly affordable, too.

Find out how SCIEX Diagnostics can help improve your accuracy, turnaround and confidence at www.sciexdiagnostics.com.

Come and visit us at MSACL, Booth 10 and 11.
The Association is a non-membership, non-profit 501(c)(3) tax-exempt California Corporation with the mission of furthering education in the field of mass spectrometry.

*Go Mobile!* Mobile Program @ https://www.msacl.org/mobile

Get Connected with BadgeScan™. The Official Contact & Lead Capture App of MSACL 2014 EU.
MSACL 2015 US
San Diego
March 28 - April 1

The 7th Annual
US Conference on
Clinical Mass Spectrometry

Travel Award & Podium Submission Deadline:
December 4, 2014

Presented by:

Supported by:
# Table of Contents

<table>
<thead>
<tr>
<th>Section</th>
<th>Page</th>
</tr>
</thead>
<tbody>
<tr>
<td>CORPORATE SPONSORS</td>
<td>4</td>
</tr>
<tr>
<td>SCIENTIFIC COMMITTEE</td>
<td>5</td>
</tr>
<tr>
<td>GENERAL INFORMATION</td>
<td>17</td>
</tr>
<tr>
<td>PRESENTER INFO AND GUIDELINES</td>
<td>18</td>
</tr>
<tr>
<td>SCHEDULE OVERVIEW</td>
<td>19</td>
</tr>
<tr>
<td><strong>Tuesday</strong></td>
<td>19</td>
</tr>
<tr>
<td><strong>Wednesday</strong></td>
<td>19</td>
</tr>
<tr>
<td><strong>Thursday</strong></td>
<td>20</td>
</tr>
<tr>
<td><strong>Friday</strong></td>
<td>21</td>
</tr>
<tr>
<td>PLENARY SPEAKER SERIES</td>
<td>23</td>
</tr>
<tr>
<td>YOUNG INVESTIGATOR AWARDS</td>
<td>25</td>
</tr>
<tr>
<td>TRAINEE AWARDS</td>
<td>26</td>
</tr>
<tr>
<td>SHORT COURSE OVERVIEW</td>
<td>27</td>
</tr>
<tr>
<td>EXHIBITS SUMMARY</td>
<td>30</td>
</tr>
<tr>
<td>EXHIBITORS</td>
<td>31</td>
</tr>
<tr>
<td>CORPORATE WORKSHOPS</td>
<td>35</td>
</tr>
<tr>
<td>PODIUM PRESENTATIONS</td>
<td>39</td>
</tr>
<tr>
<td>POSTER PRESENTATIONS</td>
<td>53</td>
</tr>
<tr>
<td><strong>Posters by Topic</strong></td>
<td>54</td>
</tr>
<tr>
<td><strong>Posters: Wednesday</strong></td>
<td>67</td>
</tr>
<tr>
<td><strong>Posters: Thursday</strong></td>
<td>77</td>
</tr>
<tr>
<td><strong>Posters: Friday</strong></td>
<td>91</td>
</tr>
<tr>
<td>PRESENTER INDEX</td>
<td>99</td>
</tr>
<tr>
<td>MAP: 2ND FLOOR</td>
<td>100</td>
</tr>
<tr>
<td>MAP: 1ST FLOOR - EXHIBIT HALL</td>
<td>101</td>
</tr>
<tr>
<td>MAP: GROUND FLOOR</td>
<td>102</td>
</tr>
</tbody>
</table>
Scientific Committee

Please take a moment to acknowledge the members of the Scientific Committee of this inaugural congress who were pivotal in the development of the Scientific Program.

Theodore Alexandrov, PhD
*University of Bremen, Germany / SCiLS, Germany / UCSD, USA*

Jean Armengaud, PhD
*CEA-Marcoule, France*

Olof Beck, PhD
*Karolinska Institutet, Sweden*

Karl-Siegfried Boos, PhD
*Professor of Clinical Chemistry
Institute of Laboratory Medicine, Medical Center of the University, Munich, Germany*

Uta Ceglarek, PhD, EurClinChem
*Leipzig University*

Olivier Gaillot, PhD
*Centre de Biologie Pathologie, CHU de Lille, France*

Roland Geyer
*Tecan Switzerland AG*

Brian Keevil, PhD
*Department of Clinical Biochemistry, University Hospital of South Manchester, Manchester, UK*

Pierre Marquet, MD, PhD
*University of Limoges, France*
Oleg Mayboroda, PhD
Leiden University Medical Center, The Netherlands

Prof. Dr. med. Soren Schubert
Ludwig-Maximilians-Universitat (LMU) Munchen

Christoph Seger, PhD
University Hospital Innsbruck

Zoltan Takats, PhD
Imperial College, London, UK

Prof. Dr. med. Michael Vogeser
Institute of Laboratory Medicine, Hospital of the University of Munich, Germany
for the working group LC-MS/MS of the DGKL

Stefan Zimmermann, MD
University Hospital Heidelberg, Germany
Changing Microbiology

- Fast and Reliable Identification of Microorganisms
- Selective Testing of Antibiotic Resistance
- The Market Leading Microbiology Mass Spectrometry System with more than 1,200 Sold Units

Visit us at Booth 15 and at www.bruker.com
SWATH™ Acquisition 2.0 with variable windows is here.

The new AB SCIEX TripleTOF® 6600 System with SWATH™ 2.0 captures virtually every detectable peptide and protein in every run, with MRM-quality quantitation and sample-to-sample reproducibility that accelerate discovery.

Maximize sample information for a more complete view of the proteome. Quantify thousands of proteins across hundreds of samples with almost no method development. Archive a digital record of every proteome you can re-interrogate at any time. Only the TripleTOF® 6600 combines increased dynamic range with the high speed, sensitivity and resolution to enable SWATH™ 2.0, unlocking the full power of data independent acquisition.

The next-generation proteomics platform has arrived.

To learn more, visit absciex.com/swath+6600

Come and visit us at MSACL, Booth 4
Confidence means a proven path to adopting mass spectrometry in the clinical research lab. The move to mass spec is inevitable, but it comes with many implementation challenges. With Agilent you will have a proven partner at your side. Our leading mass spectrometry platforms combined with our comprehensive portfolio of sample preparation and chromatography technologies deliver peak performance to help you identify and quantify both endogenous and exogenous substances in complex biological matrices with the utmost sensitivity, accuracy, productivity and reliability. And our global support network can help you get your answer with minimal ramp-up and maximum productivity. Take your clinical research lab to a new level of performance with mass spectrometry from Agilent.

Visit www.agilent.com/lifesciences/clinresMS

The Measure of Confidence
Detect more. Discover more.

Introducing the new Shimadzu LCMS-8050
Extraordinary sensitivity in the world’s fastest triple quadrupole mass spectrometer

The new Shimadzu LCMS-8050 triple quadrupole mass spectrometer delivers stunning sensitivity and exceptionally high data acquisition speed to give you accurate quantitation for the most demanding applications required by clinical research, environmental, food safety, DMPK and ADMET studies and quantitative proteomics.

Engineered with advanced ultra-fast technologies, the LCMS-8050 creates new opportunities in achieving lower limits of quantitation and, with the world’s fastest triple quadrupole delivering 30,000 u/sec scan speeds and a 5 ms/sec polarity switching time, help to enhance data quality and accelerate sample throughput – all with industry-leading reliability.

The new Shimadzu LCMS-8050 Speed and Sensitivity beyond Comparison

www.shimadzu.eu
So Smart it almost runs itself!

GCMS-TQ8040 – Smart enough for everyday use in your laboratory

Smart Productivity
- 400+ compounds in one run
- Automatic method creation

Smart Operation
- MRM Optimization tool
- Smart Database series

Smart Performance
- Scan/MRM acquisition mode
- … and much more!

www.shimadzu.eu
ACHIEVE PEAK PERFORMANCE

Confidence means a proven path to adopting mass spectrometry in the clinical research lab. The move to mass spec is inevitable, but it comes with many implementation challenges. With Agilent you will have a proven partner at your side. Our leading mass spectrometry platforms combined with our comprehensive portfolio of sample preparation and chromatography technologies deliver peak performance to help you identify and quantify both endogenous and exogenous substances in complex biological matrices with the utmost sensitivity, accuracy, productivity and reliability. And our global support network can help you get your answer with minimal ramp-up and maximum productivity. Take your clinical research lab to a new level of performance with mass spectrometry from Agilent.

Visit [www.agilent.com/lifesciences/clinresMS](http://www.agilent.com/lifesciences/clinresMS)

The Measure of Confidence

---

**Agilent Corporate Workshop - Join us....**
Friday 5th September at 13:00-14:00 in Mozart 1-3
Also visit us at booth #18-19 throughout MSACL
What’s better than a nice cup of tea and a chat?

Whilst at Riva 2014 (the 38th ISCC and 11th GCxGC Symposium), Rich Whitworth, editor of The Analytical Scientist, invited three key participants of the conference to take part in an exciting new video project: “Tea With...”, an ongoing series of informal interviews with key analytical scientists in glorious settings around the globe.

So head over to our YouTube page now to see interviews with Luigi Mondello, Chiara Cordero and James Harynuk now!

www.theanalyticalscientist.com/teawith

The Analytical Scientist
Manufacturer of innovative mobile benches for LC/GC/MS systems

- Reduce vacuum pump noise by 75%
- Overheating alarm protection
- Vibration reduced by 99%
- Safe access to solvents
- Adj. height from 22.4 to 34.3 in.
- Chemical resistant worksurface

Contact us | www.ionbench.com | contact@ionbench.com

And also... Dedicated noise reduction enclosures from MS NOISE

A wide range of noise reduction enclosures for vacuum pumps, water chillers, ultrasonic baths, nitrogen generators, ...

Contact us | www.msnoise.com | contact@msnoise.com
Confidence in Results

Achieve greater productivity and confidence when providing laboratory-developed test results to the healthcare professionals you serve. New Thermo Scientific™ high-performance medical devices for in vitro diagnostic use — Thermo Scientific™ Prelude MD™ HPLC, Thermo Scientific™ Endura MD™ mass spectrometer, and Thermo Scientific™ ClinQuan MD™ software — help you deliver LC-MS results easily, quickly, and with more confidence.

LC-MS for in vitro diagnostic use

Visit us in booth #12 • thermoscientific.com/LCMS-IVD
General Information

Smoking
Smoking is prohibited within the conference facility.

Conference Badges
Your badge constitutes your admission pass to the Conference, Receptions and the Exhibit Hall. Please display your badge prominently while attending the conference and at all associated functions. If you do not have your badge you will be escorted to the registration desk to get one, or off the premises.

Parking
Sheraton Garage - entrance via Auerspergstraße with direct access to Salzburg Congress
- Rate per hour € 2,50
- Rate 24 hours € 17,50
- Opening hours: Mo - Su, 00:00 - 24:00 hrs

Mirabell-Kongress-Garage - entrance via Mirabellplatz, 2-3 minutes walk to Salzburg Congress
- Rate per 20 min € 0,90
- Rate from the 4th hour on € 3,00 / per hour
- 24 hours € 18,00
- Opening hours: Mo - So, 00:00 - 24:00 hrs

Breakfast
It is recommended that you take breakfast before arriving at the Congress Center.

Welcome Coffee
Coffee and light pastries are served every morning from 7:30 to 8:15 am.

Lunch
Short Course Registrants: Tuesday & Wednesday
Lunch will be served in the Registration Foyer on the ground floor from 12 - 1 pm

Conference Registrants: Thursday & Friday
Buffet lunch will be served in the Exhibit Hall on the 1st Floor from 12 – 1 am.

Receptions
A buffet dinner/reception will be served each day starting at 4:15 pm

Receptions will 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 conference sessions, committee meetings, in the Exhibit Hall, and during the plenary sessions.

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

Location: Mozart Hall and Papageno

- 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 with ~5 minutes for Q&A.
- PC Laptops running Windows 7 Enterprise & Office 2010 will be provided.
- Presenters should check-in 30 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 must 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

Poster sessions are held on Wednesday, Thursday and Friday

- Poster attendance is obligatory for 1 hour,
  - Wednesday is 5:00-6:00 PM.
  - Thursday & Friday is 2:00-3:00 PM.
- Wednesday Posters
  - Place poster before 3:00 PM.
  - Attend from 5:00 - 6:00 PM.
  - Remove between 7:15 – 7:30 PM.
- Thursday & Friday Posters
  - Place on poster before 8:00 AM.
  - Attend from 2:00 - 3:00 PM.
  - Remove between 7:15 - 7:30 PM.
- Maximum Poster dimensions (for each presenter) are 1 meter wide x 2.5 meters high.
- Poster Boards are plastic.
- Tape WILL BE provided.
# Schedule Overview

## Tuesday

<table>
<thead>
<tr>
<th>Time</th>
<th>Event</th>
</tr>
</thead>
<tbody>
<tr>
<td>7:30 – 8:15 am</td>
<td><strong>Welcome Coffee</strong> - Registration Foyer</td>
</tr>
<tr>
<td>8:15 – 10:00 am</td>
<td><strong>Short Course Session 1</strong></td>
</tr>
<tr>
<td>10:00 – 10:30 am</td>
<td><strong>AM Coffee Break</strong> - Registration Foyer</td>
</tr>
<tr>
<td>10:30 – 12:00 pm</td>
<td><strong>Short Course Session 2</strong></td>
</tr>
<tr>
<td>12:00 – 1:00 pm</td>
<td><strong>Lunch</strong> - Registration Foyer &amp; Outdoor Patio</td>
</tr>
<tr>
<td>1:00 – 2:15 pm</td>
<td><strong>Short Course Session 3</strong></td>
</tr>
<tr>
<td>2:15 – 2:45 pm</td>
<td><strong>PM Coffee Break</strong></td>
</tr>
<tr>
<td>2:45 – 4:15 pm</td>
<td><strong>Short Course Session 4</strong></td>
</tr>
<tr>
<td>4:15 – 6:15 pm</td>
<td><strong>Reception</strong> - Registration Foyer &amp; Outdoor Patio</td>
</tr>
<tr>
<td>6:15 pm</td>
<td><strong>Enjoy Salzburg</strong> - Salzburg City</td>
</tr>
</tbody>
</table>

## Wednesday

<table>
<thead>
<tr>
<th>Time</th>
<th>Event</th>
</tr>
</thead>
<tbody>
<tr>
<td>7:30 – 8:15 am</td>
<td><strong>Welcome Coffee</strong> - Registration Foyer</td>
</tr>
<tr>
<td>8:15 – 10:00 am</td>
<td><strong>Short Course Session 1</strong></td>
</tr>
<tr>
<td>10:00 – 10:30 am</td>
<td><strong>AM Coffee Break</strong> - Registration Foyer</td>
</tr>
<tr>
<td>10:30 – 12:00 pm</td>
<td><strong>Short Course Session 2</strong></td>
</tr>
<tr>
<td>12:00 – 1:00 pm</td>
<td><strong>Lunch</strong> Registration Foyer</td>
</tr>
<tr>
<td>1:00 – 2:15 pm</td>
<td><strong>Short Course Session 3</strong></td>
</tr>
<tr>
<td>2:15 – 2:45 pm</td>
<td><strong>PM Coffee Break</strong> - Registration Foyer</td>
</tr>
<tr>
<td>2:45 – 4:15 pm</td>
<td><strong>Short Course Session 4</strong></td>
</tr>
<tr>
<td>4:15 – 7:30 pm</td>
<td><strong>Reception</strong> -- EXHIBITS OPEN Exhibit Hall (1st Floor)</td>
</tr>
<tr>
<td>Time</td>
<td>Event</td>
</tr>
<tr>
<td>--------------</td>
<td>-------------------------------------------------------------------------------------------</td>
</tr>
<tr>
<td>7:30 – 8:15 am</td>
<td><strong>Welcome Coffee</strong> - Registration Foyer</td>
</tr>
<tr>
<td>8:00 – 8:15 am</td>
<td><strong>Welcome, Orientation &amp;Introduction</strong></td>
</tr>
<tr>
<td>8:15 – 9:00 am</td>
<td><strong>Plenary Session 1</strong>&lt;br&gt;Chair: David Herold</td>
</tr>
<tr>
<td>8:15 – 9:00 am</td>
<td>Direct Mass Spectrometric Characterization of Fluids, Cells and Tissues – the Benefits</td>
</tr>
<tr>
<td></td>
<td>and the Price of Real-Time Analysis</td>
</tr>
<tr>
<td></td>
<td>Zoltan Takats&lt;br&gt;Imperial College London</td>
</tr>
<tr>
<td>9:00 – 9:45 am</td>
<td><strong>Metabolism and Disease Pathogenesis</strong></td>
</tr>
<tr>
<td></td>
<td>Gary Siuzdak&lt;br&gt;The Scripps Research Institute</td>
</tr>
<tr>
<td>9:45 – 10:45 am</td>
<td><strong>AM Coffee Break</strong> – Exhibit Hall (1st Floor)</td>
</tr>
<tr>
<td>10:45 – 12:00 pm</td>
<td><strong>Scientific Session 1</strong>&lt;br&gt;Track 1: Sample Prep&lt;br&gt;Track 2: Metabolomics&lt;br&gt;Track 3: Novel Methodologies</td>
</tr>
<tr>
<td>12:00 pm</td>
<td><strong>Lunch</strong> – Exhibit Hall (1st Floor)</td>
</tr>
<tr>
<td>1:00 – 2:00 pm</td>
<td><strong>Corporate Workshops</strong> – Mozart, Papageno(Ground Floor) and Paracelsus (2nd Floor)</td>
</tr>
<tr>
<td>2:00 – 3:00 pm</td>
<td><strong>Posters</strong> – Exhibit Hall (1st Floor)</td>
</tr>
<tr>
<td>2:00 – 3:00 pm</td>
<td><strong>PM Coffee Break</strong> – Exhibit Hall (1st Floor)</td>
</tr>
<tr>
<td>3:00 – 4:15 pm</td>
<td><strong>Scientific Session 2</strong>&lt;br&gt;Track 1: Small Molecule&lt;br&gt;Track 2: Proteomics&lt;br&gt;Track 3: Imaging &amp; Analytics</td>
</tr>
<tr>
<td>4:15 – 6:30 pm</td>
<td><strong>Reception</strong>&lt;br&gt;Exhibit Hall (1st Floor)</td>
</tr>
<tr>
<td>6:30 – 7:30 pm</td>
<td><strong>Plenary Session 1</strong>&lt;br&gt;Chair: Theodore Alexandrov</td>
</tr>
<tr>
<td></td>
<td>The Impact and Potential Consequences of Machine Intelligence on Healthcare</td>
</tr>
<tr>
<td></td>
<td>Randy Julian&lt;br&gt;Indigo Biosystem, Inc</td>
</tr>
</tbody>
</table>
## Friday

<table>
<thead>
<tr>
<th>Time</th>
<th>Event</th>
</tr>
</thead>
<tbody>
<tr>
<td>7:30 – 8:15 am</td>
<td><strong>Welcome Coffee</strong> - Registration Foyer</td>
</tr>
</tbody>
</table>
| 8:15 – 9:00 am| Plenary Session 3  
*Chair: Zoltan Takats*  
MALDI-TOF in Medical Microbiology  
Irene Burckhardt  
*UniversitätsKlinikum Heidelberg*  
High Resolution Proteomics for Clinical Applications  
Matthias Mann  
*Max-Planck Institute of Biochemistry*  
AM Coffee Break - *Exhibit Hall (1st Floor)* |
| 10:45 – 12:00 pm| **Scientific Session 3**  
Track 1: Small Molecule / Sample Prep  
Track 2: Metabolomics  
Track 3: Novel Methodologies |
| 12:00 – 1:00 pm| Lunch - *Exhibit Hall (1st Floor)*  
Corporate Workshops – *Mozart, Papageno (Ground Floor) and Paracelsus (2nd Floor)*  
Posters - *Exhibit Hall (1st Floor)*  
PM Coffee Break - *Exhibit Hall (1st Floor)* |
| 3:00 – 4:15 pm| **Scientific Session 4**  
Track 1: BioMarkers  
Track 2: Metabolomics  
Track 3: Toxicology |
| 4:15 – 6:15 pm| Closing Reception  
*Exhibit Hall (1st Floor)* |
| 6:15 pm       | CONFERENCE & EXHIBITION CLOSED  
*6:15 pm* |
Plenary Speaker Series

<table>
<thead>
<tr>
<th>Day</th>
<th>Time</th>
<th>Speaker(s)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Thursday</td>
<td>8:15 – 9:00 AM</td>
<td>Zoltan Takats</td>
</tr>
<tr>
<td>Thursday</td>
<td>9:00 – 9:45 AM</td>
<td>Gary Siuzdak</td>
</tr>
<tr>
<td>Thursday</td>
<td>6:30 – 7:30 PM</td>
<td>Randy Julian</td>
</tr>
<tr>
<td>Friday</td>
<td>8:15 – 9:00 AM</td>
<td>Irene Burckhardt</td>
</tr>
<tr>
<td>Friday</td>
<td>9:00 – 9:45 AM</td>
<td>Matthias Mann</td>
</tr>
</tbody>
</table>

Thursday @ 8:15 AM in Mozart Hall
**Direct Mass Spectrometric Characterization of Fluids, Cells and Tissues - The Benefits and the Price of Real-Time Analysis**
*Zoltan Takats - Imperial College London* (z.takats@imperial.ac.uk)

Development of ambient mass spectrometric techniques opened a new way of looking at clinical samples regarding the simplicity (and time demand) of analysis and the nature of data produced by these techniques. Application of these approaches in cancer surgery, histopathology, clinical microbiology and clinical chemistry has been successfully demonstrated. While these techniques mean valid alternatives to currently used technologies - with clear benefit on both cost and reliability sides - their widespread application can potentially change the current landscape of medical diagnostics. Future role of these methods in stratified clinical patient journeys will be discussed with particular emphasis on the currently unresolved problems and their future solutions regarding both regulatory and technology aspects.

Thursday @ 9:00 AM in Mozart Hall
**Metabolism and Disease Pathogenesis**
*Gary Siuzdak - The Scripps Research Institute* (siuzdak@scripps.edu)

Our lab focuses on the quantitative global analysis of endogenous metabolites (metabolomics) and the role these molecules play in disease pathogenesis. While the genome and proteome represent upstream biochemical events, metabolites correlate with the most downstream biochemistry and therefore most closely represent the phenotype. The experimental aim in our studies is to obtain a comprehensive view of the metabolome to expand our understanding of what pathways are altered in disease. We have developed a novel web-based platform for metabolomics that includes XCMS Online data analysis combined with METLIN, a comprehensive MS/MS metabolite database, as well as Nanostructure Imaging Mass Spectrometry (NIMS). These technologies will be presented in the context of pain and colorectal cancer.

Thursday @ 6:30 PM in Mozart Hall
**The Impact and Potential Consequences of Machine Intelligence on Healthcare**
*Randall Julian - Indigo BioSystems, Inc.* (rkjulian@indigobio.com)

Intelligent machines teamed with experts are superior to experts working alone. This will have profound effects on the nature of healthcare delivery. Further, the advance of automation is already having a significant effect on labor markets, and there is no reason to believe healthcare will not be impacted. In this lecture examples of human-machine teams will be given. Also, the impact on society of the increased role of smart machines will be discussed. Comparisons between the first and second machine ages will be used to draw out the consequences, benefits and difficulties we will face as a scientific community.
Friday @ 8:15 AM in Mozart Hall
MALDI-TOF in Medical Microbiology
Irene Burckhardt - UniversitätsKlinikum Heidelberg, Dept for Infectious Diseases
(irene.burckhardt@med.uni-heidelberg.de)
› Bacterial identification via MALDI-TOF has become state of the art during the last years. For susceptibility testing different very promising assays have been proposed. However, to routinely generate MALDI-TOF data for a complete antibiogram as we know it from agar diffusion or MIC determination is still not possible. To miniaturize these assays and to integrate them into a total lab automation will be the key tasks for the coming years.

Friday @ 9:00 AM in Mozart Hall
High Resolution Proteomics for Clinical Applications
Matthias Mann - Max-Planck Institute of Biochemistry (mmann@biochem.mpg.de)
› Mass spectrometry based proteomics has advanced tremendously in the last few years. We describe a shotgun proteomics workflow that allows us to detect and quantify the large majority of the proteins expressed in a biological system such as cancer cell lines. This included streamlined and highly efficient sample preparation, analysis with very high sequencing speed using modern mass spectrometers and bioinformatic analysis using the MaxQuant and Perseus platforms. Efforts in our group have focused on ‘single shot’ analysis and we demonstrate very high coverage in this mode (Mann et al., 2013).

In this talk, I will focus on applications of proteomics to questions of clinical relevance.

One of the clinically important challenges in oncology is the classification of patients into subgroups with different risk profiles and treatment modalities. Using SILAC-based or label-free proteomics, we have successfully distinguished the ABC and GBC subtypes of Germinal center B-cell like diffuse large B-cell lymphoma (DLBCLs) in cell lines derived from patients (Deeb et al., 2014; Deeb et al., 2012). We are now studying cohorts of intermediate sizes in breast, ovarian and prostate cancer. We have also revisited the analysis of body fluids, such as lung lavage and plasma, using the latest technological advances and I will discuss where these efforts stand at the moment.
Young Investigator Awards

This year twenty-eight (28) Young Investigator Travel Awards were granted. These awards support trainees (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.

Julia Balog Imperial College London
Barbara Bojko Collegium Medicum University of Nicolaus Copernicus in Torun, Poland and University of Waterloo, Canada
Hannah Bowrey The Medical University of South Carolina
Sara Capiau Ghent University
Elena Chekmeneva Imperial College London
Jennifer Colby University of California, San Francisco
Irene Costa University of Padua
Lewis Couchman King's College Hospital; University of Leicester
Pieter De Kesel Ghent University,
Julia Dittrich University Hospital Leipzig
Andrew Dowsey University of Manchester
Adrian Fontan Hospital San Pedro, Logrono, La Rioja Spain
Deborah French University of California, San Francisco
Alexander Gaudl Leipzig University
Sadakatali S. Gori University of Louisville
Kevin Kerian Purdue University
Soumen Manna National Cancer Institute
Eduardo Martinez Morillo Hospital Universitario Central de Asturias
Jessica Miller University of Arizona Cancer Center
Andrew Palmer University of Bremen
Vanessa Phelan University of California, San Diego
Madlen Sander University Hospital Leipzig, Germany
Zdenek Spacil University of Washington
Nicole Strittmatter Imperial College London
Anna Catharina Suhr Hospital of the University of Munich (LMU)
Irene van den Broek Leiden Univeristy Medical Center (LUMC)
Martijn van Faassen University Medical Center Groningen
Jane Yang University of California, San Diego
Trainee Awards

This year, ten (10) Trainee Awards were granted to 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.

Ena Melisa Canales University College London
Matteo Conti University Hospital Bologna
Morgan James Medical University of South Carolina
Manar Mashhadani Northampton General Hospital
Elizabeth Palmer Cwm Taf Health Board and Nottingham University
Sebastian Perez University of Buenos Aires
Sarah Pitkin NHS Foundation Trust
Omolara Popoola University College Hospital, Ibadan, Nigeria
Antonus van Herwaarden Radboud University Medical Center
Marija Zekušić University Hospital Centre Zagre, Croatia

Trainee Travel Awards supporting in part by:

Thermo Scientific
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 their respective course topics.

Preparing Manuscripts for Publication: Improving Your Chances for Success
Length: 1 Day (Sunday)
Location: Mozart 2
Level: 0 (General Interest)
Instructor(s): Thomas Annesley, PhD

Scientific publication is an important and necessary activity for researchers. Being a good researcher, however, does not automatically make you a good writer. Good science is the foundation of a scientific paper, but how the science is presented also strongly influences whether a paper gets accepted for publication. This session focuses on key elements of writing a scientific paper, starting with the first word put onto a page to the final printed product:

- Choosing the most effective words
- Writing clear sentences
- Developing the proper title
- Creating an informative abstract
- Organizing the Introduction
- Emphasizing results versus data
- How to start and end the Discussion
- Creating clear tables and figures
- How to correctly use citations and references
- How to choose the right journal
- How to respond to reviewer comments
- Acceptance does not mean the finish line

After this session, participants will be able to:
1. bring greater clarity and consistency to a scientific paper;
2. describe the features that distinguish papers accepted for publication;
3. organize the major sections of a scientific paper; and
4. create more effective tables and figures.

Introduction to Clinical Mass Spectrometry
Length: 2 Days (Tuesday - Wednesday)
Location: Mozart 4
Level: 1 (Beginner)
Instructor(s): Judy Stone, PhD & Daniel Holmes, MD

Course Outline

Day 1:
1. Basics of MS p1 - Principles of instruments, ionization, etc.
2. Selecting and Installing LC-MSMS - due diligence, site prep, daily maintenance & instrument startup, checklists, System Suitability testing, cutting tubing, making LC connections
3. Basics of LC - Instrument components and LC theory, gradients
4. Preparing for your first batch - selecting solvents, water, reagents, internal standards, glassware, making mobile phases (pH meter), doing infusions, calculations (salt vs free base), making calibrators
5. Basics of MS p2 - isotopes, fragmentation, isotopic overlap, cross talk, Best Practices for calibration, selecting internal standards
6. Sample Preparation Theory p1, - describe purpose of sample prep, dilute, protein crash, LLE advantages and disadvantages
7. Sample Preparation - Hands on tips, troubleshooting, case histories, Best practices
8. Sample Preparation Theory p2 - SPE, SLE & variants, PL removal, automation
Day 2:
1. Validating Assays p1 - plan, differences between validation for automated chemistry vs LC-MSMS, ion suppression, matrix effect interferences, containers (anticoagulants & tubes)
2. Troubleshooting, Maintenance & Repair1 - MSMS and IT issues, case histories, Best Practices
3. Validating Assays p2 - pre-validation stress testing, precision, accuracy, linearity, stability of samples, reagents, mobile phases, stock solutions, etc.
4. Troubleshooting, Maintenance & Repair2 - LC problems - human error, insufficiently robust methods, wear & tear
5. Validating Assays p3 - Patient sample comparisons & remaining topics
6. Troubleshooting p3 - Sample Prep, common mistakes, case histories
7. Data Analysis - calibration curve construction, evaluation, frequency, troubleshooting, QC practices, data review recommendations (MRM ratios, RRts, peak width & symmetry, internal standard recovery, etc), checklists

Detection of Pathogens and Toxins using Mass Spectrometry
Length: 2 Days (Tuesday - Wednesday)
Location: Mozart 3
Level: 2 (Intermediate)
Instructor(s): Jean Armengaud, PhD

This course will present current mass spectrometry-based technologies for the detection of pathogens and toxins. We will present established sample preparation methods, mass spectrometry tools with a brief overview of the principles of mass analysis, and analytical protocols. We will also unveil novel methodologies that are currently emerging for the analysis of difficult samples, such as mixtures of pathogens, spores, and toxin traces. We will discuss both the strengths and potential pitfalls of these methodologies.

Solid Phase Microextraction (SPME) and Other Solventless Sampling and Sample Preparation Technologies for Laboratory and On-Site
Length: 1 Day (Tuesday)
Location: Mozart 1
Level: 2 (Intermediate)
Instructor(s): Dr. Janusz Pawliszyn & Dr. Barbara Bojko

- Introduction to solventless technologies
- Theoretical principles of SPME, TFME and NT
- Sample introduction and related devices
- Calibration approaches
- Method development
- Automation
- Therapeutic drug monitoring
- Ligand-receptor binding studies
- Metabolomics and biomarkers discovery
- In vivo sampling

During the course solventless sampling and sample preparation methods such as Solid Phase Microextraction (SPME), Thin Film Microextraction (TFME) and Needle Trap (NT) will be discussed. This course will cover the main principles of the techniques, calibration methods, coupling strategies of SPME and related technologies to GC, MS and MS, method development strategy, as well as advantages and disadvantages of each technique. Applications of the technologies in the fields such as forensic, pharmaceutical and clinical analysis will be discussed. Advances in the methods will be highlighted including: ligand-receptor binding and plasma protein binding studies, breath and skin analysis, in vivo
sampling of freely moving animals for pharmacokinetic and metabolomic studies, automation in high-throughput format, direct tissue analysis with particular focus on intraoperative monitoring of drugs and biomarkers.

**How to Process Body Fluids for LC-MS/MS Analysis of Small Molecules**

*Length: 1 Day (Wednesday)*  
*Location: Mozart I*  
*Level: 2 (Intermediate)*  
*Instructor(s): Karl-Siegfried Boos, PhD*

The course covers:

1. Integration and automation of selective clean-up of complex body fluids (e.g. whole blood, plasma, urine) using SPE and column switching (SPE-LC).
2. Instrumentation, operational procedures and practical guidelines for hyphenation of SPE - LC with UV, ECD and/or MS/MS
3. Properties and performance of tailor-made SPE packing materials (e.g., restricted access materials, RAM; mixed-mode polymers, MMP; molecularly imprinted polymers, MIP)
4. POPLC: An attractive way and valuable tool to find the optimal LC-column in combination with on-line SPE
5. MS adequate processing of body fluids by means of on-line (turbulent flow) SP-LC
6. General introduction to understanding, monitoring and elimination of ion suppression / matrix effects in bioanalytical LC-MS/MS
7. Multidimensional SPE for utmost sample clean-up
8. Depletion of phospholipids for undisturbed MS/MS analysis
9. Preanalytics and processing of body fluids (Cell-Disintegrated Blood, CDB; Dried Matrix/Blood Spots, DXS; Dried Matrix/Blood Extracts, DXE)

**Development and Validation of Quantitative LC-MS/MS Assays for Use in Clinical Diagnostics**

*Length: 2 Days (Tuesday - Wednesday)*  
*Location: Papageno*  
*Level: 3 (Advanced)*  
*Instructor(s): Russell Grant, PhD & Brian Rappold*

This 2-day 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.
# Exhibits Summary

<table>
<thead>
<tr>
<th>Day</th>
<th>Time</th>
<th>Event Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Wednesday</td>
<td>8:00 am – 4:00 pm</td>
<td>Exhibitor Set-Up (EXHIBITS CLOSED) – Poster Placement for Presenters Allowed.</td>
</tr>
<tr>
<td></td>
<td>4:15 – 7:15 pm</td>
<td>Opening Reception in Exhibit Hall</td>
</tr>
<tr>
<td>Thursday</td>
<td>9:45 – 10:45 am</td>
<td>AM Coffee Break in Exhibit Hall</td>
</tr>
<tr>
<td></td>
<td>12:00 – 1:00 pm</td>
<td>Lunch provided in Exhibit Hall.</td>
</tr>
<tr>
<td></td>
<td>2:00 – 3:00 pm</td>
<td>PM Coffee Break in Exhibit Hall</td>
</tr>
<tr>
<td></td>
<td>4:15 – 6:30 pm</td>
<td>Reception in Exhibit Hall</td>
</tr>
<tr>
<td>Friday</td>
<td>9:45 – 10:45 am</td>
<td>AM Coffee Break in Exhibit Hall</td>
</tr>
<tr>
<td></td>
<td>12:00 – 1:00 pm</td>
<td>Lunch provided in the Exhibit Hall.</td>
</tr>
<tr>
<td></td>
<td>2:00 – 3:00 pm</td>
<td>PM Coffee Break in Exhibit Hall</td>
</tr>
<tr>
<td></td>
<td>4:15 – 6:15 pm</td>
<td>Reception in Exhibit Hall</td>
</tr>
<tr>
<td></td>
<td>6:15 pm</td>
<td>END OF EXHIBITS</td>
</tr>
<tr>
<td></td>
<td>11:00 pm</td>
<td>Deadline for removal of Exhibits from Exhibit Hall</td>
</tr>
</tbody>
</table>

![Exhibit Hall Map](image)
Exhibitors

**AB SCIEX** Booth #4,10-11
http://www.absciex.com
AB SCIEX helps to improve the world we live in by enabling scientists and laboratory analysts to find answers to the complex analytical challenges they face in basic research, drug discovery and development, food and environmental testing, forensics, and clinical research and diagnostics. 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.

**Agilent Technologies** Booth #19-20
http://www.agilent.com/chem
Agilent Technologies is the world-wide leader in mass spectrometry, with powerful, reliable MS systems and intuitive software suites for diverse application areas such as pharmaceutical, food safety, environmental, forensic, metabolicomic, proteomic analysis and clinical research. Key products and solutions include 1200 Infinity Series LC, Triple Quadrupole, Q-TOF and Ion Mobility LC/MS Systems and HPLC-Chip/MS; automated SISCAPA workflow; tools for protein purification and bio-separation.

**Biotage AB, Sweden** Booth #29
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. At MSACL 2014 Biotage will be presenting their EVOLUTE® and ISOLUTE® Sample Preparation Products. Biotage manufactures a range of sample preparation tools for Bioanalytical, Clinical, Environmental, Food and Forensic applications. Our focus is on developing technology to speed experimental procedures. Automation is key to controlling the reaction parameters, improving reliability and guaranteeing reproducible results.

**Bonna-Agela** Booth #03
http://www.bonnaagela.com
Bonna-Agela Technologies Inc. is a company focuses on sample separation and purification that serves chemists and biochemists in the field of drug discovery, food safety, environmental protection, forensic and clinical analysis as well as chemical research. We offer a full line in sample preparation, purification and analysis, which include. We offer a full line in sample preparation, purification and analysis, which include bulk separation media, columns and equipments. With uncompromised quality policy, our products are guaranteed for satisfaction of customers throughout North America, Asia and Europe.

**Bruker Daltonics** Booth #15-16
http://www.bdal.com/
Bruker Daltonics provides a broad range of high performance, easy to use Mass Spectrometry (MS) and analytical separation systems. Bruker delivers a series of innovative, fully integrated systems for use in the Pharmaceutical, Life Science, Applied Analytical, and Clinical Research areas, including: - Protein Characterization und Quantification - Drug Research and Development - Environmental - Forensics and Doping Analysis - Biomarker Discovery & Tissue Imaging - Metabolomics - Chemical Analysis Utilizing a product and technology portfolio which includes MALDI-TOF MS, ESI-TOF and qTOF MS, Ion Trap MS, FTMS, ICP-MS, and GC/MS as well as LC and GC systems, Bruker provides the best solutions for the very latest analytical questions. Bruker Daltonik GmbH Fahrenheitstrasse 4 28359 Bremen Germany Phone: +49 (0)421-2205-0 Fax: +49 (0)421-2205-104 sales@bdal.de http://www.bruker.com

**Cambridge Isotope Labs** Booth #17
http://www.isotope.com
Cambridge Isotope Laboratories, Inc. is the world leader in the manufacture and separation of stable isotopes and stable isotope labeled compounds. CIL offers an array of highly pure compounds that are uniformly or selectively enriched in 13C, 15N, D, 18O or 17O. Our labeled reagents are used across scientific fields including proteomics, metabolomics, metabolism and environmental applications for quantitative mass spectrometry. CIL’s products include SILAC protein quantitation kits, media and reagents, 99% enriched amino acids, MouseExpress® Lys 13C6 mouse feed and mouse tissue, MouseExpress® 15N mouse feed and mouse tissue, Spirulina 15N, intact labeled proteins, growth media for protein expression, cell-free protein synthesis products, environmental contaminants...
standards for ultratrace analysis, steroids, acylcarnitines, drug metabolites, nucleic acids, lipids and carbohydrates. CIL has GMP capabilities; a majority of substrates can be manufactured to be Q7A compliant.

**Chromsystems** Booth #25-26  
http://www.chromsystems.com  
Chromsystems is a leading global company providing ready-to-use reagent kits and supplies for routine clinical diagnostics by HPLC and LC-MS/MS, the latter representing the gold standard for a high number of parameters. Our product portfolio includes complete kits, quality controls and multilevel calibrators, all ensuring highly accurate as well as a cost-effective analysis in the laboratory. They enable any laboratory to introduce HPLC and LC-MS/MS methods into their diagnostic routine without prior technical expertise. Analyses can be started immediately and sample preparations require the minimum of laboratory time. Our products are comprehensively validated, in particular LC-MS/MS methods with all widely used tandem mass spectrometers. They are CE-IVD compliant, satisfying regulatory requirements for the laboratory. We combine these high quality products with an excellent support programme and service for our customers.

**CSols** Booth #22  
http://www.csols.com/wordpress/clinical-biochemistry/  
CSols provides powerful, transcription free software integration solutions for LC MS-MS, GC-MS, ICP-MS, LC or GC instruments and Clinical LIMS systems. CSols intelligent laboratory software solutions have been designed to reduce your laboratory costs, improve efficiency, reduce turnaround times and transcription errors. Our software solutions improve traceability, analytical performance and ensure quality lab results. We can help guide you ‘Beyond the Technology’ that you are using in your laboratory today to provide you with solutions that will streamline your lab procedures, reduce your analyst’s administration burden and help you meet your improvement goals.

**Gerstel** Booth #27  
http://www.gerstel.de  
Family-owned in the second generation since its founding in 1967, GERSTEL is focused on developing and producing systems and solutions for chemical analysis. The main focus is on automated sample preparation for Gas Chromatography / Mass Spectrometry (GC/MS) and Liquid Chromatography / Mass Spectrometry (LC/MS) as well as solvent-free thermal desorption, thermal extraction, and pyrolysis. GERSTEL delivers automated solutions, based on the GERSTEL MultiPurpose Sampler (MPS), that are focused on the needs of the customer and include integrated software control. Analytical laboratories in all branches of science and industry throughout the world use GERSTEL products for analyses in the areas of consumables, food safety, migration from packaging, flavors, fragrances, odors and off-odors, material emissions of polymers, pyrolysis, forensic toxicology, pharmaceuticals, extractable and leachable studies, biotechnology, metabolomics, and the environment.

**Indigo Biosystems** Booth #18  
http://www.indigobio.com  
Indigo Biosystems provides automated, vendor-neutral chromatogram analysis software that assists scientists’ review of LC/MS data.

**IsoSciences** Booth #28  
http://www.isosciences.com  
IsoSciences (www.isosciences.com) is a world leader in the synthesis of stable isotope labeled mass spec standards including vitamins, steroids, drug substances, metabolites and other compounds of interest. IsoSciences has an extensive catalog of stable isotope labeled standards available for immediate delivery both as solids and as CertiMass™ Reference Standards with exact concentrations for each lot. IsoSciences also specializes in the custom synthesis of any compound or metabolite, labeled or unlabeled, that you require.

**LGC Standards** Booth #09  
http://www.lgcstandards.com  
LGC is an international life sciences measurement and testing company. LGC provides reference materials, proficiency testing, genomics and analytical products and services which underpin the safety, health and security of the public to customers in the Pharmaceutical, Agricultural Bioscience, Food and Environment, Government and Academia, Security and Sports markets. With headquarters in Teddington, South West London, LGC employs over 2,000 staff, operating out of 22 countries worldwide. Its operations are extensively accredited to international quality standards such as ISO/IEC 17025 and ISO Guide 34. With a history dating back to 1842, LGC has been home to the UK Government Chemist for more than 100 years. It is the designated UK National Measurement Institute for Chemical and Bioanalytical measurement, providing metrology research, calibration and testing. LGC was privatised in 1996.
**PAS Technology** Booth #21
[http://www.pas-tec.com](http://www.pas-tec.com)
Discover advantage of NeedleTrap method! In cooperation with Prof. Pawliszyn we have realized the automation of the desorption of the NeedleTrap, a sorbent-packed needle developed by Prof. Pawliszyn. This standard needle (usually gauge 22 or 23 at 50 - 80 mm length) can be filled with up to 3 cm with a wide range of different packaging materials. Typical applications are in the field of VOC analysis. Different sampling techniques allow air sampling in the field, respiratory gas sampling, sampling from a process or reactor, from sample vials or as dynamic HS, or as purge and trap samples. The thermal desorption is carried out without further hardware directly in the S/SL injector of the GC. Detection limits are typically in the ppb to sub-ppb range and the processing of the needles can be automated for any commercial GC.

**Phenomenex** Booth #06
[http://www.phenomenex.com](http://www.phenomenex.com)
Phenomenex is a global technology leader committed to developing novel analytical chemistry solutions that solve the separation and purification challenges of researchers in industrial, clinical research, government and academic laboratories. From drug discovery and pharmaceutical development to food safety and environmental analysis, Phenomenex chromatography solutions accelerate science and help researchers improve global health and well-being. For more information, visit [http://www.phenomenex.com](http://www.phenomenex.com) or follow the company on Twitter @Phenomenex.

**Providion** Booth #23
[http://www.providion.co.uk/](http://www.providion.co.uk/)
Providion offer LCMS packages for clinical research, therapeutic drug monitoring and forensic toxicology needs. High quality ISO certified LCMS method development, instruments & customized support services are central components of efficient drug screening analysis. We know this better than anyone and have a proven record, successfully supporting the mass spectrometry industry for over 18 years! We offer entry level pre-owned certified instrumentation and support packages including installation, method development, application support, preventive maintenance & repairs. Come and visit us at our stand for more information.

**RECIPE Chemicals + Instruments** Booth #30
RECIPE was founded in Munich, Germany, in 1982 and 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 ISO 9001 and 13485.

**Shimadzu** Booth #07
[http://www.shimadzu.eu](http://www.shimadzu.eu)
Shimadzu is one of the worldwide leading manufacturers of analytical instrumentation. Its equipment and systems are used as essential tools for quality control of consumer goods and articles of daily use, in health care as well as in all areas of environmental and consumer protection. Since more than 135 years, Shimadzu is at the service of science ensuring precise, reliable diagnoses and analyses in medicine, chemistry and pharmacy. Among the leaders in Gas Chromatography coupled to Mass Spectrometry, Shimadzu has recently introduced a full range of innovative LCMS trippe quadrupole mass spectrometers that are opening new doors in the world screening and quantification of traces in complex matrices. It is creating new trends in food safety, metabolomics and lipidomics. Take the opportunity to visit our booth.

**Sigma-Aldrich** Booth #05
[http://www.sigmaaldrich.com/industries/clinical-testing.html](http://www.sigmaaldrich.com/industries/clinical-testing.html)
Sigma-Aldrich brings its high-quality MS- and LC-MS reagents, certified reference materials, kits, libraries and bioanalytical reagents to clinical diagnostics applications. Whether we are providing novel tools to explore the universe of metabolites relevant for human health, medical emergencies, acute or chronic diseases or whether we are providing targeted solutions to well-identified biomedical needs or routine diagnostic requirements, you can benefit not only from the most comprehensive metabolite program, but also from our offering of reagents, HPLC and UHPLC columns, and auxiliary products along the complete analytical workflow. Additionally, clinical, forensic and toxicology testing laboratories can take advantage of the wide range of labelled and non-labelled drugs of abuse, pharmaceutical and metabolites available in the Cerilliant CRM product portfolio.
Spark Holland Booth #02  
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 #01  
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, and 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 2013, Tecan generated sales of CHF 388 million (USD 419 million; EUR 316 million). Registered shares of Tecan Group are traded on the SIX Swiss Exchange (TECN; ISIN CH0012100191).

Thermo Scientific Booth #12-14  
http://www.thermoscientific.com  
Thermo Fisher Scientific is the world leader in serving science, enabling you to make the world healthier, cleaner and safer. With annual sales of more than $17 billion and 50,000 staff, we serve our customers worldwide within pharmaceutical and biotech companies, hospitals and clinical diagnostic labs, universities, research institutions and government agencies, as well as environmental and industrial process control settings. With four premier brands we help solve analytical challenges from routine testing to complex research and discovery. Thermo Scientific is the leading brand for technology innovation and offers customers a complete range of high-end analytical instruments as well as laboratory equipment, software, services, consumables and reagents to enable integrated laboratory workflow solutions for the clinical laboratory.

Waters Booth #31-32  
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

Thursday & Friday

1:00 – 2:00 PM

Track 1: Mozart 1-3 (Ground Floor)
Track 2: Mozart 4-5 (Ground Floor)
Track 3: Papageno (Ground Floor)
Paracelsus (2nd Floor)

As part of your registration you may attend, at no charge, 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 - Thursday
1:00 - 2:00 PM

Bruker - Mozart 1-3
Innovative Applications of Mass Spectrometry in Forensics and Clinical Research

1) An Introduction to Bruker's Chromatography and Mass Spectrometry Portfolio
   Joe Anacleto, Bruker Daltonics, Canada

2) MALDI Biotyper - Changing Microbiology: Detection of Resistance Mechanism
   Guido Mix, Bruker Daltonik GmbH, Germany

3) Toxtyper - A New Type of Forensic Evidence
   Prof. Dr. Thomas Krämer, University of Zürich, Institute of Forensic Medicine, Switzerland

4) Mass Spectrometry Meets Histology: MALDI Imaging in Clinical Research
   Dr. Sören Deininger, Bruker Daltonik GmbH, Germany

Thermo Scientific - Mozart 4-5
Novel Techniques for Toxicology Screening and Sample Extraction

› Hear our customers present their ground-breaking work using the latest innovative approach to forensic toxicology. Reserve your seat today! Novel techniques for Forensic Toxicology Screening and Sample Extraction and Analysis Without Traditional LC for Rapid Throughput of Complex Matrices Including Blood and Urine using QQQ and HR/AM Q Exactive MS Speaker: Marta Kozak, Thermo Fisher Scientific Tox library and workflow Speaker: Bénédicte Duretz, Thermo Fisher Scientific Sample Extraction and Analysis Without Traditional LC for Rapid Throughput of oncology drug measurement with HR/AM Q Exactive MS Speaker: William Clarke, John Hopkins University.

AB SCIEX - Papageno
Mass Spectrometry Applications for Clinical Research
Russell Watts & Dan Blake

› Over the last 10 years many LC/MS/MS applications have been developed by clinical research laboratories and successfully implemented as the technology has become more robust, reliable and affordable. LC/MS/MS offers many technical and financial advantages for the clinical research laboratory and is now seen as a complementary and in some cases a viable alternative to immunoassays. In this workshop we bring together scientists, clinicians and biochemists that hold an interest in the use of Mass Spectrometry in the areas of Clinical Research as we discuss what can achieved with today’s technology and what we can expect in the future.

Phenomenex - Paracelsus
Chromatographic Method Development for the LC/MS Users
Dr. James Rudge

› The advent and rapid popularity of the MS detectors has led to shorter and narrower columns and subsequently faster chromatographic run times. This presentation covers a brief discussion of chromatographic media, bonded phases and method development in connection with LC/MS and LC/MS/MS technology and requirements.
Corporate Workshops - Friday  
1:00 - 2:00 PM

**Agilent - Mozart 1-3**  
**Optimizing Mass Spec Analysis and Quantitation**

1) *Achieve Peak Performance with Agilent Technologies*  
*Kevin McCann, Agilent Technologies*

2) *Inflammatory Cytokine and Chemokine Profiles of Primary Human Cells Determined with Chip-HPLC-Triple Quadrupole Spectrometry*  
*Christopher Gerner University of Vienna, Institute of Analytical Chemistry, Austria*

3) *Quality Requirements for Quantitative Clinical Chemistry Proteomics - A Proof-of-Principle Study*  
*Christa Cobbaert, Department of Clinical Chemistry and Laboratory Medicine, Leiden University Medical Center, Leiden, The Netherlands*

**Shimadzu - Mozart 4-5**  
**Smart Solutions for Clinical Analysis**  
*Giancarlo LA MARCA / Neil LOFTUS / Emmanuel WEY*

• 1) *Newborn Screening for ADA SCID by MS/MS*  
*Giancarlo LA MARCA - Meyer Children's Hospital - Florence - Italy*

2) *Next Generation Plasma Collection Technology And Its Impact On Clinical Lc/Ms/Ms Analysis*  
*Neil LOFTUS - Shimadzu MSBU overseas - Manchester - UK*

3) *The Future Role Of Maldi Mass Spectrometry In The Evolving Challenge Of Antibiotic Resistance*  
*Emmanuel Wey MD - Royal Free Hospital, NHS Foundation Trust, London, UK*

**Waters - Papageno**  
**UPLC/MS, A Versatile Tool For The Clinical Laboratory**  
*Chair: Benjamin Dugas, Clinical Business Development Manager, Europe & India, Waters Corporation.*

1) *Using Liquid Chromatography Mass Spectrometry for the Measurement of Metabolites, Protein and Enzyme Activities*  
*Dr Robert Barouki, Professor of Biochemistry, University Paris Descartes, Head of Metabolic Biochemistry Laboratory, Necker Enfants Maladies Hospital, Paris, France*

2) *Development of a LC-MS/MS Method for Analysis of Steroids in Blood*  
*Dr Maura Brambilla, Analytical Laboratory Director, Desio Hospital, Desio, Italy*

**IsoSciences - Paracelsus**  
**Deficiencies of Deuterium as an Isotopic Label in MS Standards**  
*Scott W. Landvatter, Ph.D.*

• Stable isotope labeled standards are a critical component in quantification of analytes by LC/MS. Deuterium (2H) is most commonly used. However, deuterium suffers from inherent drawbacks that can limit the accuracy of quantification by LC/MS. These limitations include loss of deuterium in solution and loss of deuterium under mass spec conditions. Without validation of 2H stability, results can be called into question. Second generation LC/MS standards now avoid all the drawbacks of deuterium by incorporating 13C, 15N and, if necessary, 2H in chemically stable non-exchangeable positions. This talk will focus on the limitations of deuterium in LC/MS internal standards, will give examples of inappropriate 2H internal standards and will discuss the 13C/15N labeled improved standards that are now available.
Podium Presentations

**Track 1:** Mozart 1-3

**Track 2:** Mozart 4-5

**Track 3:** Papageno
Sample Prep

• Session 1 • Track 1 •

Thursday @ 10:45 AM in Mozart 1-3

Session Chair: Karl-Siegfried Boos - Medical Center of the University of Munich

Thursday @ 10:45 AM in Mozart 1-3

Immuno-MALDI for Accurate and Precise Clinical Protein Quantitation

Christoph Borchers - UVic Genome BC Proteomics Centre (christoph@proteincentre.com)

• Immuno-MALDI (iMALDI) technology combines the sensitivity of immunoaffinity capture with the specificity of mass spectrometry detection. We have now taken a multifaceted approach for translating iMALDI technology into clinical laboratories for routine protein quantification. First, we have automated the sample preparation using the Agilent Bravo liquid handling robot for improved sample throughput. Secondly, we have optimized iMALDI assays for the Bruker Microflex MALDI-TOF, a bench-top instrument that is widely used in regulated healthcare environments. We demonstrate that iMALDI technology is suitable for clinical use through the precise and accurate measurement of the plasma renin activity in >200 clinical samples.

Thursday @ 11:10 AM in Mozart 1-3

Method Development with Easy to Automate Absorptive Chemistry Extraction for LC-MS

Roland Geyer - Tecan Switzerland AG (roland.geyer@tecan.com)

• When using the innovative AC Extraction Plate(TM) for the extraction of small molecules, the method development process can be simplified due to the plate’s unique ‘pipette and shake’ workflow. Initial optimization simultaneously deals with three steps (extraction, wash and elution) in a matrix approach, the Direct Extraction-Elution Method (DEEM). This process evaluates the optimum conditions for the analyte(s) interaction with the absorptive chemistry (AC) of the extraction plate. Further optimization of conditions for the extraction step tackle the interaction of analyte with the sample matrix (e.g., protein binding). For analytes such as steroids (e.g., Testosterone, Androstendione, Estradiol) the extraction conditions must be modified and adapted to overcome protein binding. Experience with the optimization of this critical step will be outlined and interesting examples discussed.

Thursday @ 11:35 AM in Mozart 1-3

Rapid Bedside Diagnosis Tools by Coupling of Bio-compatible Solid Phase Microextraction (SPME) Devices to Mass Spectrometry

Janusz Pawliszyn - University of Waterloo (janusz@uwatuloo.ca)

• SPME is a green sample preparation technique that combines extraction and pre-concentration of analytes in one step thus simplifying the analytical process. Succinctly, SPME does not require any sample collection because extraction takes place in situ by inserting a biocompatible microfiber directly into tissue, blood or other biological matrix for a short period of time. Alternatively, the same device can be used for ex vivo analysis using a small amount of the studied sample. This work presents multiple strategies recently developed for the direct coupling of SPME to MS. In order to have a broader range of applications, different SPME geometries such coated fibers and meshes, as well as ionization approaches such DART and ESI, were studied.
Thursday @ 10:45 AM in Mozart 4-5

**Metabolic Profiling as a Tool for Investigating Diseases of Pregnancy**

*Elizabeth Want - Imperial College London (e.want@imperial.ac.uk)*

- Metabolic profiling can offer insights into disease diagnosis, progression, and responses to therapeutic intervention. Ultra-performance liquid chromatography – mass spectrometry (UPLC-MS) is a powerful tool for metabolic profiling, with excellent separation and detection capabilities. We developed a robust, reproducible UPLC-MS method for placental extract profiling and applied this to a cohort of women with intrahepatic cholestasis of pregnancy (ICP). We demonstrated clear metabolic differences between treated and untreated ICP patients, which may be reflected in plasma/serum, offering the potential for a minimally invasive diagnostic tool. This approach could be extended to study other pregnancy complications, such as pre-eclampsia and pre-term delivery.

Thursday @ 11:10 AM in Mozart 4-5

**Quantitative Multiplex Assays for Inborn Metabolic Disorders in Dried Blood Spots**

*Zdenek Spacil - University of Washington (spacil@u.washington.edu) -- *Young Investigator Awardee***

- In recent years, more efficient therapies are becoming available for inherited lysosomal storage disorders (LSDs) and timely initiation of treatment often leads to a better outcome. Consequently, tandem mass spectrometry based screening assays in newborns are being increasingly implemented in clinical laboratories. We have been developing a fully quantitative assay of nine lysosomal enzymes in dried blood spots (DBS), which screens for Niemann-Pick-A/B, Pompe, Fabry, Gaucher, Krabbe and mucopolysacharidoses I; II; IVA and VI diseases. We will present our latest progress and future directions of LSDs assay development. Further, we will demonstrate the clinical value of data from LSDs pilot studies conducted by our collaborators and worldwide.

Thursday @ 11:35 AM in Mozart 4-5

**Study of Pregnancy Outcomes: Quantification of Selected Metabolites by High-throughput Nano-electrospray HRMS-TOF Method**

*Elena Chekmeneva - Imperial College London (e.chekmeneva@imperial.ac.uk) -- *Young Investigator Awardee***

- The precise, accurate and rapid validated high-throughput direct injection nano-ESI-HRMS was applied for quantification of several selected metabolites in the urine samples of the female patients with different pregnancy outcomes (Pregnant, Non-Pregnant and Early Pregnancy Loss (EPL)). The absolute quantification of eight selected metabolites was achieved by standard addition using stable isotope labelled internal standards, using a composite urine sample to account for any matrix effect. Some other metabolites were quantified relative to these internal standards. The concentration of some metabolites showed differences for different pregnancy outcomes. The full-scan data was used for untargeted fingerprinting.
Thursday @ 10:45 AM in Papageno

A New Method to Assess Sequencing & Annotation Quality in Databases Used for Clinical Proteomics and Metaproteomics

Olivier Pible - CEA/DSV/IBEB/SBTN/LBSP (olivier.pible@cea.fr)

- Advances in next-generation genome sequencing have made proteomic experiments more successful than ever. However, genome sequences are contaminated more frequently than is admitted, with large impact on most proteomics fields. Here, we propose a new concept to highlight abnormal organism sequencing data and quickly identify the source of contamination. A specific software program was developed for a quick spotting of cross-contamination of organisms, using specific experimental MS/MS data. We highlighted two likely contaminated WGS data detected in the NCBInr database and confirmed this discovery by large scale blast analysis. Other examples related to pathogens, and associated problems will be commented. Such new concept should rapidly improve the quality of sequence databases of upmost importance for clinical proteomics analysis.

Thursday @ 11:10 AM in Papageno

Quality Assurance in Clinical Mass Spectrometry

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

- Among the analytical techniques used in clinical pathology today, mass spectrometry based methods potentially enable analyses on a unique level or reliability: signal generation is based on molecular weight and disintegration patterns of analytes, and application of stable isotope dilution internal standardisation suggests complete compensation of individual matrix effects. However, high complexity of the technology, the dynamic nature of analyte ionisation, highly variable instrument configurations, and incomplete solutions for automation challenge the quality of mass spectrometric methods. In this presentation specific requirements for quality assurance of mass spectrometry methods applied in clinical diagnostics regarding patients’ safety are discussed.

Thursday @ 11:35 AM in Papageno

Influence of Glycosylation for Providing Relevant “clinical” Protein Calibrants

Virginie Trégoat - JRC-IRMM (virginie.tregoat@ec.europa.eu)

- Sound medical decisions rely on accurate clinical measurements. To be trustable and comparable, these measurement results have to be metrologically traceable which can be established by using protein-based certified reference materials (CRMs). Many clinical diagnostic methods for proteins are based on immunoassays. Since proteins undergo post-translational modifications such as glycosylation, possible changes in glycosylation might affect protein recognition and its quantitation by immunoassays. However, this effect has hardly been studied in available CRMs. This work aims to evaluate the impact of glycosylation on the commutability and value assignment of several protein-calibrants by liquid chromatography-mass spectrometry, capillary electrophoresis and circular dichroism.
Small Molecule
• Session 2 • Track 1 •
Thursday @ 3:00 PM in Mozart 1-3
Session Chair: Michael Vogeser - Klinikum der Universität München

Thursday @ 3:00 PM in Mozart 1-3
TDM in Psychopharmacology Using LC-MS/MS – from the Complex Method to the Interpreted Result
Markus Schwarz - Klinikum der Universität München (markus.schwarz@med.uni-muenchen.de)

• Therapeutic Drug Monitoring (TDM) is an important tool for individualized psychopharmacotherapy, allowing to get a kind of ‘pharmacologic phenotyping’ of the patient. From the methodological aspect, TDM in psychopharmacotherapy is facing one major problem: Polypharmacy, leading to the necessity to use a highly specific and at the same time robust and sensitive method. LC-MS/MS for TDM of psychotropic drugs is therefore more and more becoming the gold standard. This presentation will address the major analytical, pharmacokinetic, pharmacogenetic and practical aspects of TDM in psychiatry to demonstrate how TDM can be used for individualized risk reduction.

Thursday @ 3:25 PM in Mozart 1-3
CYP1A2 Phenotyping by Measuring Paraxanthine/caffeine Concentration Ratios in Hair and Comparison with the Plasma-based Phenotype
Pieter De Kesel - Laboratory of Toxicology, Ghent University (pieter.dekesel@ugent.be) -- *Young Investigator Awardee*

• Measuring metabolite-to-parent drug concentration ratios in hair may provide a convenient tool to study drug metabolism in a non-invasive way. We evaluated whether paraxanthine/caffeine ratios measured in hair samples reflect the plasma-based CYP1A2 phenotype. Using a validated LC-MS/MS method, caffeine and paraxanthine concentrations were measured in proximal 3 cm segments of hair samples from 60 healthy volunteers and resulting paraxanthine/caffeine ratios were correlated with CYP1A2 phenotyping indices measured in plasma. Although paraxanthine/caffeine concentration ratios in hair and plasma showed overall a statistically significant correlation, large deviations between hair and plasma ratios in individual cases impede interpretation.

Thursday @ 3:50 PM in Mozart 1-3
Ultra-low Level Clinical Analysis Using LC-MS/MS Technologies
Russell Grant - Laboratory Corporation of America (grantr@labcorp.com)

• Following the explosion of steroid hormone assays in the mid 2000’s, advancements in techniques and analytical capabilities has enabled LC-MS/MS tools to supersede the performance characteristics of ELISA and RIA assays. We have leveraged these advancements to enable ultra-low level clinical biomarker analysis (<1pg/mL). This presentation will highlight the analytical challenges and solutions to realize these criterion. Specific assays for determination of estradiol/estrone (200fg/mL), free (equilibrium dialysis) and salivary Testosterone (500fg/mL), Thyroglobulin (1pg/mL peptide level) and free T3/T4 (1pg/mL) will be described. Further, multiplexing of these assays to <1500 samples/system/day will be shown.
MSIA Workflow for Comprehensive Identification and Analysis of Isobaric Insulins: An Approach to Targeted Insulin Quantitation Using HR/AM-MS and Multiplexed LC

Lewis Couchman - King’s College Hospital (lewis.couchman@nhs.net) -- *Young Investigator Awardee*

• There is a trend towards the analysis of insulins using LC-MS. We report a mass spectrometric immunoassay (MSIA) method, with high-resolution, accurate mass detection (HR/AM), and chromatographic resolution of a known isobaric insulin analogue, insulin lispro. Total analysis time was 15 minutes (without multiplexing). Analytes were detected using a Q Exactive MS (Thermo Scientific). Insulin, insulin lispro, and the internal reference standard are enriched simultaneously from samples using the insulin MSIA method. Combined with HR/AM, it is possible to acquire full-scan and MS2 data for both analytes independently, allowing (i) robust peak identification, and (ii) quantitative analysis of both compounds.

High Selectivity and Sensitivity in LC-MS Clinical Assays

Bruno Domon - Luxembourg Clinical Proteomics Center (bdomon@crp-sante.lu)

• New hybrid mass spectrometers with high resolution and accurate mass capabilities have opened new avenues in quantitative proteomics. Targeted clinical analyses, routinely performed on triple quadrupole instruments, were replicated on a high-resolution quadrupole-orbitrap instrument operated in parallel reaction monitoring (PRM) mode. The trapping capability was used to analyze peptides in tiny amounts, thus increasing the dynamic range while providing selective measurements. The PRM technique was applied to analyze makers in lung cancer markers. The gain in selectivity and an increase in the confidence of measurements in a clear discrimination of the disease stages and subtypes.

Identification of Novel Biomarkers of Brain Injury by Integrating Bioinformatics and Mass Spectrometry-based Proteomics

Eduardo Martínez Morillo - Hospital Universitario Central de Asturias (edumartinezmorillo@gmail.com) -- *Young Investigator Awardee*

• Hemorrhagic stroke (HS) is a significant cause of mortality worldwide. A blood-based diagnostic test to identify this condition would be useful. The aim was to develop selected reaction monitoring (SRM) assays to quantify “brain specific” proteins in CSF from patients with HS, ischemic stroke and controls. SRM assays for 68 proteins were developed. Six peptides from proteins GFAP, MBP, NFM, NSE, α-Inx and β-Syn were significantly elevated in the HS group. NFM was further evaluated using an ELISA. Serum NFM concentration in controls (n=46) was from 0.26 to 8.57 ng/mL, while in 78 serial samples from 7 patients with HS was from 0.97 to 42.4 ng/mL.
MALDI Molecular Imaging of Proteins, Metabolites and Drugs for Preclinical and Clinical Research

Axel Walch - Helmholtz Zentrum München
(axel.walch@helmholtz-muenchen.de)

This presentation will give an update on the application of MALDI imaging in preclinical and clinical research. We discuss the use of MALDI imaging in clinical proteomics and put it in context with classical proteomics techniques for tissue analysis. In the research area of gastrointestinal disorders MALDI imaging has already been used to address several questions of upper- and lower gastrointestinal diseases, which will be briefly presented. We also highlight a number of upcoming challenges for personalized medicine, development of targeted therapies and diagnostic molecular pathology where MALDI imaging could help.

Spatial Metabolomics: Database-Driven Metabolic Annotation for High-resolution Imaging Mass Spectrometry

Theodore Alexandrov - University of Bremen / SCiLS / UCSD (theodore@uni-bremen.de)

High-resolution Imaging Mass Spectrometry (imaging MS) is a promising technique for untargeted spatial metabolomics. We present a novel database-driven and high-throughput approach to generate hypotheses on metabolites represented in high-resolution imaging MS data. Rather than identifying molecular species for millions of individual peaks, we restricted each imaging dataset to signals potentially corresponding to molecules from metabolic databases. Sum formulas of all metabolites were considered and corresponding ion images were generated. For each sum formula, an annotation score was calculated which integrates various spatial and spectral characteristics. Hundreds of sum formulas were detected as corresponding to metabolites present in the tissue sections. The evaluation confirmed the potential of our approach to provide relevant hypotheses on metabolites present in a tissue section.

A New Approach to Biomarker Discovery in Clinical Mass Spectrometry Through Statistical Modelling of the Raw Data

Andrew Dowsey - University of Manchester (andrew.dowsey@manchester.ac.uk) -- *Young Investigator Awardee*

We present a new type of workflow for differential analysis of LC-MS data in clinical discovery. The fundamental principle is to retain and model the raw data from start to finish, thus enabling detection below the limit of current software tools, and the assessment of differential expression in overlapping peptide signals. The data is analysed entirely in raw form, so that the full profile-mode MS1 signal is retained and utilised for differential quantification. Each LC-MS dataset is denoised and converted to an image, warped by a novel LC alignment stage and then statistical analysis performed directly on the set of aligned images through a Bayesian mixed-effects model. No error-prone peak detection or deconvolution is necessary. This enables our workflow to handle complex experimental designs with multiple experimental conditions, sources of variation and batch effects.
Immunoaffinity Extraction Coupled Online with LC-MS/MS for the Quantification of Total Plasma Testosterone: A Feasibility Study

Martijn van Faassen - University Medical Center Groningen (h.j.r.van.faassen@umcg.nl) -- *Young Investigator Awardee*

- Immunoaffinity extraction was coupled online with LC-MS/MS to explore the possibility of quantifying total plasma testosterone. 25 µL plasma was analyzed using immunoaffinity- or C8-sorbents. Extraction and elution parameters were optimized. Ion suppression experiment results were comparable between immunoaffinity extraction and C8-extraction. We showed that it is feasible to combine online immunoaffinity extraction with LC-MS/MS for the determination of total plasma testosterone. Currently we are combining antibodies that capture different compounds to enable the multiplex analysis of disease specific biomarker panels.

Towards a LC-MS/MS Based Clinical-chemical Analyzer for Small Molecules in Body Fluids

Karl-Siegfried Boos - Medical Center of the University of Munich (boos@med.uni-muenchen.de)

- For a broad implementation and routine application of LC-MS/MS in clinical laboratories, sample pretreatment has to be integrated and fully automated. Towards this, we developed a novel instrumental platform which – for the first time – enables a fully automated in-line processing not only of native blood plasma, blood serum, cerebrospinal fluid, saliva and urine but also of anticoagulated whole blood samples prior to on-line SPE-LC-MS/MS analysis. Perfusion through a heated stainless-steel capillary converts whole blood into so-called cell-disintegrated blood (CDB). CDB represents a homogenous liquid composed of subcellular particles which do not sediment on standing and do not clog LC-capillaries, sieves or column packings. Target analytes present in CDB and other biofluids are extracted by on-line SPE under high flow velocity conditions.

Potassium-based Algorithm Allows Correction for the Hematocrit Bias in Quantitative Analysis of Caffeine and Its Major Metabolite in Dried Blood Spots

Sara Capiau - Laboratory of Toxicology, Ghent University (sara.capiau@ugent.be) -- *Young Investigator Awardee*

- Deviating Hct values may cause significant bias in quantitative dried blood spot (DBS) analysis. We evaluated whether a potassium-based algorithm allowed correction of the Hct bias, using caffeine as a model compound. An algorithm was constructed using data from a reference set of DBS and whole blood samples and applied to a separate test set. While at Hct levels below 0.36, caffeine concentrations in DBS were significantly underestimated compared with blood, this was no longer the case after application of the algorithm. The usefulness of this approach was further demonstrated by applying the same algorithm to paraxanthine, yielding similar results.
Friday @ 10:45 AM in Mozart 4-5

**Investigating Beneficial Changes in Human Metabolism and Immunological and Inflammatory Markers Following High Intensity Interval Or Regular Endurance Training**

*Warwick Dunn - University of Birmingham (w.dunn@bham.ac.uk)*

- Age-related declining health has a significant impact upon quality of life and healthcare costs. Exercise is a non-invasive intervention to maintain healthy status by reducing deleterious changes in immune and inflammatory status. Understanding the interactions between exercise, age and metabolism will provide insights in to how exercise interventions can maximise their effect in maintaining health as we age. The presentation will discuss a mass spectrometry metabolomics study of changes in the plasma metabolome related to two different exercise regimes, age and inflammatory/immunological status. The presentation will also discuss the importance of quality assurance and metabolite annotation in these discovery studies.

Friday @ 11:10 AM in Mozart 4-5

**Spatial Metabolomics of Three-dimensional Cell Culture Systems**

*Andrew Palmer - University of Bremen (palmer@uni-bremen.de) – Young Investigator Awardee*  

- 3D cell cultures of colon adenocarcinoma provide an advanced in vitro model for studying metabolic processes within tumours, and their response to drug treatment. However, system-wide analysis requires untargeted detection of metabolites inside these spheroid cultures and localization to a particular spheroid layer. We addressed this analytical challenge using our newly developed spatial metabolomics approach, which combines high mass-resolution imaging mass spectrometry with high-throughput database-driven molecular annotation of imaging mass spectrometry data. Our approach allowed us to detect hundreds of signals and transform the large high mass resolution data into an easily interpretable form for experts in cancer metabolomics.

Friday @ 11:35 AM in Mozart 4-5

**Application of Oxylipin Profiling to a Sulindac Intervention of Pain.**

*Jessica Miller - University of Arizona Cancer Center (jam1@email.arizona.edu) – Young Investigator Awardee*  

- Despite successful use of selective estrogen receptor modulators (SERMs) and aromatase inhibitors (AIs) for the treatment of estrogen receptor positive (ER+) breast tumors, 25-30% of ER+ patients still die from their disease. High rates of early discontinuation of AIs (estimated at 30% by year 3) due to intolerance to side effects, notably musculoskeletal pain or AI-induced musculoskeletal syndrome, are now linked to reduced benefit. Here, within the context of an ongoing clinical trial using UPLC-QTRAP, we have profiled the biologically active oxylipin metabolites of ω-6 and ω-3 fatty acids in plasma and urine in order to understand their relationship to AI-induced pain as well as response to the pain-reducing drug, sulindac. Profiles were highly interconnected with ~1/3rd of the first set of 10 patients harboring a theoretical systemic pro-inflammatory metabolome.
Novel Methodologies
• Session 3 • Track 3 •
Friday @ 10:45 AM in Papageno
Session Chair: Matthias Mann - Max Planck Institute of Biochemistry

Friday @ 10:45 AM in Papageno
Quantitation of Soluble Transferrin Receptor (sTfR) in Human Serum Using SISCAPA Immunocapture Enrichment and MALDI-TOF Mass Spectrometry
Selena Larkin - SISCAPA Assay Technologies (selenalarkin@siscapa.com)
‣ A sensitive, accurate, high-throughput and automated assay was developed for LC-free SISCAPA-MALDI quantification of sTfR. The traditional ELISA assay for quantitation of sTfR in human serum is suspected to be subject to protein interferences that can lead to inaccurate results. Here we present an alternative approach to the ELISA assay. This approach consists of automated digestion of the sample, including any present protein interferences, followed by automated, parallel analyte enrichment in 96-well format and quantitation using MALDI-TOF mass spectrometry. The approach was assessed for sensitivity and precision and was determined to be suitable for clinical analysis of patient samples.

Friday @ 11:10 AM in Papageno
Real-time Identification of Gastrointestinal Polyps and Other Alterations During Endoscopic Procedures: The iEndoscope
Julia Balog - Imperial College London (j.balog@imperial.ac.uk) -- *Young Investigator Awardee*
‣ Endoscopic screening is routinely used for the early stage detection of gastrointestinal tumours. Our aim is to create a fast, in-situ endoscopic tissue identification tool based on rapid evaporative ionization mass spectrometry (REIMS). The iEndoscope method has been shown to be capable of differentiating between healthy mucosa, cancer, adenomatous polyps and other tissue degenerations based on the REIMS fingerprint of each tissue type. The novel iEndoscope is a feasible technique for rapid identification of human tissue in-vivo during endoscopic interventions, and it can also be used as a safety tool giving a warning signal if the submucosal region becomes damaged.

Friday @ 11:35 AM in Papageno
Rapid Characterization and Identification of Clinically Relevant Microorganisms Using Rapid Evaporative Ionization Mass Spectrometry
Nicole Strittmatter - Imperial College London (n.strittmatter12@imperial.ac.uk) -- *Young Investigator Awardee*
‣ The capabilities of rapid evaporative ionization mass spectrometry (REIMS) as a general identification system for microorganisms are presented. Strains of 28 clinically relevant bacterial species were analyzed in negative ion mode and corresponding data subjected to unsupervised and supervised multivariate statistical analyses. The created supervised model yielded correct cross-validation results of 95.9%, 97.8% and 100% on species-, genus- and Gram-stain-level, respectively. Additionally, the technique proved suitable to distinguish five pathogenic Candida species with 98.8% accuracy without any further modification to the experimental workflow. Subspecies specificity is shown in case of seven Escherichia coli strains and three different Clostridium difficile ribotypes.
A Proteogenomic Strategy for Defining Biomarkers for Quick Identification of Francisella Subspecies by MALDI-TOF MS

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

- The Francisella tularensis pathogen is the causative agent of tularemia and a potential bioweapon of category A due to its high virulence. By means of an original proteogenomics strategy relying on a large panel of genomic data on Francisella bacteria and the combination of shotgun proteomics and whole-cell MALDI-TOF mass spectrometry, we established that a unique set of three protein biomarkers could enable the identification of Francisella species and subspecies, thus predicting its virulence level. Their detection as intense peaks in the most virulent subspecies of Francisella confirmed the validity of this approach that could be extended to any pathogens.

Identification of Noninvasive Biomarkers of Coordinate Metabolic Reprogramming Associated with Colorectal Cancer

Soumen Manna - National Cancer Institute, USA (soumenmanna@gmail.com) -- *Young Investigator Awardee*

- Tandem tissue and urinary metabolomic profiling revealed early noninvasive biomarkers of colorectal tumorigenesis in ApcMin/+ mice. Transcriptomic analysis in ApcMin/+ and mice with colon-specific disruption of Apc gene showed that these biomarkers were reflection of coordinate reprogramming metabolic pathways including methylation during colorectal carcino genesis. AOM-induced colorectal carcinogenesis mouse model showed that such metabolic reprogramming-associated biomarkers were a conserved feature of colorectal carcinogenesis in mice irrespective of etiology and genetic background. Analysis of paired non-tumor and tumor tissues from colorectal cancer patients showed that such metabolic derangements are also associated with human colorectal carcinogenesis in stage-dependent manner.

Touch Spray Mass Spectrometry (TS-MS) Used for Rapid Diagnosis of Kidney and Prostate Cancer Using Tissue Specimen Obtained from Surgery

Kevin Kerian - Purdue University (kkieran@purdue.edu) -- *Young Investigator Awardee*

- Touch spray uses a small probe to pick up sample and an application of voltage and solvent to cause field-induced droplet emission for MS analysis. TS was used in a study of 18 prostatectomy cases to differentiate prostate cancer and healthy tissue with 95% accuracy based on initial cross validation results of the first 12. A blind validation was performed on the latter six patients to confirm TS as a possible in vivo surgical tool. For a professional assessment of TS-MS, Dr. Timothy Masterson performed the technique in vitro on a radical nephrectomy specimen targeting diseased and normal tissue.
Friday @ 3:00 PM in Mozart 4-5
**Rapid Quantification of Cortisol, Cortisone, Dexamethasone and Prednisolone in Human Saliva and Hair by Liquid Chromatography – Tandem Mass Spectrometry**

*Alexander Gaudl* - Leipzig University (alexander.gaudl@medizin.uni-leipzig.de) -- *Young Investigator Awardee*

- Reliable determination of cortisol and cortisone concentration in saliva and hair is of interest in the assessment of stress-associated adrenocortical function. To this purpose we developed a robust method for the reliable, simultaneous quantification of glucocorticoids via LC-MS/MS, overbearing the shortcomings of immunological analysis. With excellent precision (2-7%), very good recovery rates (95-115%) and a total runtime of 4.5 min we proved the benefits of LC-MS/MS over immunoassays. Moreover, we analysed 2500 samples of the LIFE Child Depression study and demonstrated the massive impact of preanalytical factors on hair analysis, enabling proper evaluation in clinical routine diagnostics and epidemiological studies.

Friday @ 3:25 PM in Mozart 4-5
**Profiling Thiol Metabolites and Quantification of Cellular Glutathione Using FT-ICR-MS**

*Sadakatali S. Gori* - University of Louisville (sadakatali.gori@louisville.edu) -- *Young Investigator Awardee*

- We describe preparation and use of the quaternary ammonium-based α-iodoacetamide QDE and its isotopologue *QDE as reagents for chemoselective derivatization and analysis of cellular thiols using FT-ICR-MS. Examination of A549 human lung adenocarcinoma cells using this approach revealed cysteine, cysteinylglycine, glutathione and homocysteine as principal thiol metabolites as well as the sulfinic acid hypotaurine. The method was readily applied to quantify the thiol metabolites glutathione and glutathione disulfide in A549 cells and the concentrations were found to be 34.4 ± 11.5 nmol/mg protein and 10.1 ± 4.0 nmol/mg protein, respectively.

Friday @ 3:50 PM in Mozart 4-5
**A Protective Lipidomic Biosignature Associated with a Balanced Omega-6/omega-3 Ratio in Fat-1 Transgenic Mice**

*Giuseppe Astarita* - Georgetown University (Giuseppe_Astarita@waters.com)

- A balanced omega-6/omega-3 polyunsaturated fatty acid (PUFA) ratio has been linked to health benefits and the prevention of many chronic diseases. Current dietary intervention studies with different sources of omega-3 fatty acids (omega-3) lack appropriate control diets and carry many other confounding factors derived from genetic and environmental variability. In this study, we used a multi-platform lipidomic approach to phenotype the molecular phenotype of plasma samples from an animal model of long term omega-3 supplementation. Integration of the results of untargeted and targeted analyses has identified a lipidomic biosignature that may underlie the healthful phenotype associated with a balanced omega-6/omega-3 ratio, and can potentially be used as a circulating biomarker for monitoring the health status and the efficacy of omega-3 intervention in humans.
Friday @ 3:00 PM in Papageno

Five Years of Urinary Screening for Drugs of Abuse by Tandem Mass Spectrometry and the Evolution to Pain Management Testing for Compliance and Diversion

Jeff Eichhorst - Saskatchewan Disease Control Laboratory (jeichhorst@health.gov.sk.ca)

‣ We have been providing high volume drugs of abuse screening by tandem mass spectrometry for over 40 different drugs/metabolites to clinicians for more than five years. For the last few years, physicians have been asking for changes to our program, which would provide them improved information about low dose opioid/synthetic pain medication usage, compliance and possible diversion detection. This is logical given that the greatest increase in drug misuse is of prescription drugs; specifically pain medications. The major obstacles to this request were establishing lower, yet reliable cut-off values and providing quantitative data over a very broad dynamic range.

Friday @ 3:25 PM in Papageno

Detection of Allenic Norleucine, a Nephrotoxic Amino Acid from Amanita Smithiana and Related Mushrooms

Daniel Holmes - St. Paul's Hospital, Vancouver (dtholmes@mail.ubc.ca)

‣ Amanita smithiana is a poisonous mushroom, causing acute renal failure, that grows along the Pacific coast of North America. Several European Amanita species are thought to share this same toxin, a non-protein amino acid called allenic norleucine. Previously, thin layer chromatography was the method used to confirm presence of the toxin, however, this was labour-intensive and subjective in its interpretation. We have now developed an LC-MS/MS method for allenic norleucine. Apart from its potential clinical utility in poisoning cases, we have used the assay to screen a large number of mushroom species for the toxin.

Friday @ 3:50 PM in Papageno

On the Possibility of Using Exhaled Breath for Toxicological Investigations

Olof Beck - Karolinska University Hospital (olof.beck@karolinska.se)

‣ Exhaled breath has recently been proposed as a matrix for drug testing. A serie of investigations have demonstrated that most common drugs of abuse are detectable in breath following intake. The normal breathing process creates aerosol micro-particles that are exhaled in breath. These particles are formed from the airway lining fluid during the normal breathing process. The airway lining fluid can become contaminated with drugs present in the body. These aerosol particles constitutes a way for non-volatile compounds to exit lung. This presentation will give an update on the present status in the field of drug testing in exhaled breath.
Poster Presentations

Location: *Exhibit Hall (1st Floor)*
## Posters by Topic

Please Find *Extended Poster Abstracts* under Posters by Day/Time (starting on page 67)

<table>
<thead>
<tr>
<th>Topic</th>
<th>Poster</th>
<th>Date</th>
<th>Time</th>
<th>Title</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Data Analytics</strong></td>
<td>Poster #4</td>
<td>Wednesday</td>
<td>5:00 PM</td>
<td><strong>Analysis of Amphetamines in Urine Sample Using the Atmospheric-pressure Solids Analysis Probe for Ionization</strong>&lt;br&gt;<strong>Fernanda Salami</strong> - Universidade de São Paulo</td>
</tr>
<tr>
<td><strong>Disease Markers</strong></td>
<td>Poster #36</td>
<td>Wednesday</td>
<td>5:00 PM</td>
<td><strong>A Rapid Clinical Research Method for the Simultaneous Analysis of Urinary Catecholamines and Metanephrines by Mixed-Mode SPE and HILIC LC/MS/MS</strong>&lt;br&gt;<strong>Donald Mason</strong> - Waters Corporation</td>
</tr>
<tr>
<td><strong>Disease Markers</strong></td>
<td>Poster #14</td>
<td>Thursday</td>
<td>2:00 PM</td>
<td><strong>Plasma Metanephrines by LC-MS/MS: Method Development, Validation and Application in a Tertiary Referral Centre</strong>&lt;br&gt;<strong>Sarah Pitkin</strong> - UCL Hospitals NHS Foundation Trust</td>
</tr>
<tr>
<td><strong>Disease Markers</strong></td>
<td>Poster #16</td>
<td>Thursday</td>
<td>2:00 PM</td>
<td><strong>Quantitative Target Metabolomics Using LCMS/MS Improves the Diagnosis of Vitamin B12 Deficiency and Saves Huge Cost and Time</strong>&lt;br&gt;<strong>Rima Obeid</strong> - University Hospital of the Saarland</td>
</tr>
<tr>
<td><strong>Disease Markers</strong></td>
<td>Poster #31</td>
<td>Thursday</td>
<td>2:00 PM</td>
<td><strong>A Rapid Clinical Research Method for the Simultaneous Analysis of Plasma Catecholamines and Metanephrines by Mixed-Mode SPE and HILIC LC/MS/MS</strong>&lt;br&gt;<strong>Donald Mason</strong> - Waters Corporation</td>
</tr>
<tr>
<td><strong>Disease Markers</strong></td>
<td>Poster #40</td>
<td>Thursday</td>
<td>2:00 PM</td>
<td><strong>Sensitive 2D-UHPLC-MS/MS-Method for Simultaneous Quantification of Seven Corticosteroids to Investigate Adreno-cortical Dysfunction in Critically Ill Patients</strong>&lt;br&gt;<strong>Anna Catharina Suhr</strong> - Institute of Laboratory Medicine</td>
</tr>
<tr>
<td><strong>Disease Markers</strong></td>
<td>Poster #47</td>
<td>Thursday</td>
<td>2:00 PM</td>
<td><strong>Biological Variability of Plasma 5-HIAA</strong>&lt;br&gt;<strong>Joanne Adaway</strong> - University Hospital South Manchester</td>
</tr>
<tr>
<td><strong>Disease Markers</strong></td>
<td>Poster #52</td>
<td>Thursday</td>
<td>2:00 PM</td>
<td><strong>Measuring Protein Analyte Panels in Dried Blood Spots (DBS) Using an Automated SISCAPA Workflow</strong>&lt;br&gt;<strong>Selena Larkin</strong> - SISCAPA Assay Technologies</td>
</tr>
<tr>
<td><strong>Disease Markers</strong></td>
<td>Poster #8</td>
<td>Friday</td>
<td>2:00 PM</td>
<td><strong>Proteomics and Biomarkers in Osteoarthritis</strong>&lt;br&gt;<strong>Bryan Krastins</strong> - Thermo Fisher Scientific</td>
</tr>
</tbody>
</table>
Disease Markers | Friday 2:00 PM Poster #32
New LC-MS/MS Method for the Determination of Total Homocysteine in Whole Blood (Dried Blood Spots) and Serum/Plasma
Silvia Bächer - Recipe GmbH

Disease Markers | Friday 2:00 PM Poster #48
Serum 5-HIAA – a Better Marker of Neuroendocrine Tumour Than Urine 5-HIAA
Joanne Adaway - University Hospital South Manchester

Disease Markers | Friday 2:00 PM Poster #54
Determination of Insulin-Like Growth Factor-1 in Plasma by HRAM LC/MS for Clinical Research
Christopher Benton - Agilent Technologies

ICP-MS

ICP-MS | Wednesday 5:00 PM Poster #56
Improving Turnaround Times for Trace Element Screening of Hip Replacement Patients Using the CSols Links for LIMS System and Thermo X Series ICP-MS Spectrometer
Kevin Jones - CSols

Imaging

Imaging | Wednesday 5:00 PM Poster #54
Identification of Bruch’s Membrane Composition by Imaging Mass Spectrometry
Hannah Bowrey - The Medical University of South Carolina

Imaging | Thursday 2:00 PM Poster #33
Glycopathology of Aggressive Prostate Cancers Using N-Glycan MALDI Mass Spectrometry Imaging of FFPE Tissues and Biopsy Samples
Richard Drake - Medical University of South Carolina

Imaging | Thursday 2:00 PM Poster #51
A Spatially-aware Peak Picking Method for MALDI-imaging Data from TOF and FTICR Mass Analyzers
Jan Hendrik Kobarg - Steinbeis Innovation Center SCiLS Research

Inborn Errors of Metabolism

Inborn Errors of Metabolism | Wednesday 5:00 PM Poster #10
Selective Screening for Inborn Errors of Metabolism by Tandem Mass Spectrometry in Egyptian Children
Dina Mehaney - Faculty of Medicine Cairo University

Inborn Errors of Metabolism | Thursday 2:00 PM Poster #39
UPLC-MS/MS Based Activity Assay for Determination of Mevalonate Kinase
Barbara Maier - Institute of Laboratory Medicine

Inborn Errors of Metabolism | Friday 2:00 PM Poster #15
Evaluation of a New Commercial Complete Solution for New Born Screening and Comparisons with Established Methods
Daniel Blake - ABSCIEX

55
Inborn Errors of Metabolism | Friday 2:00 PM Poster #22
**Evaluation of Derivatised and Non-derivatised Methods for Analysis of Amino Acids and Acylcarnitines in Dried Blood Spots Using a Novel Triple Quadrupole Mass**
*Benedicte Duretz - ThermoFisher*

Inborn Errors of Metabolism | Friday 2:00 PM Poster #36
**The Use of a New Meta-calculation Software for Automated Data Processing of Tandem MS for Inborn Error Metabolism Research**
*Jason Lai - Thermo Fisher Scientific*

---

**Metabolomics**

Metabolomics | Wednesday 5:00 PM Poster #18
**Shortened Validation Procedure for a Method of Quantitative Analysis of 45 Amino Acids in Plasma on Tandem Mass Spectrometer**
*Marija Zekušić - University Hospital Centre Zagreb*

Metabolomics | Wednesday 5:00 PM Poster #25
**Back to the Future of Human Metabolites for Central Biochemical Pathways**
*Roland Wohlgemuth - Sigma-Aldrich*

Metabolomics | Wednesday 5:00 PM Poster #53
**LC-MS of Chiral Hydroxycarboxylic Acids**
*Roland Wohlgemuth - Sigma-Aldrich*

Metabolomics | Thursday 2:00 PM Poster #2
**Metabolomics Approach to the Study of Allergic Disease in Paediatric Research**
*Irene Costa - Department of Woman and Children’s Health*

Metabolomics | Thursday 2:00 PM Poster #3
**High-Throughput Metabolomics in the Epidemiological Study of Metabolic Disease**
*Luke Marney - Medical Research Council Human Nutrition Research*

Metabolomics | Thursday 2:00 PM Poster #13
**Preeclampsia Risk Stratification Early in Pregnancy: Conversion of a Promising Metabolomics Discovery into a LC-MS Based Clinical Assay**
*Liz Bond - Metabolomic Diagnostics*

Metabolomics | Thursday 2:00 PM Poster #29
**Identification of Marinobufagenin in Plasma as a Promising LC-MS Assay for Preeclampsia Risk Assessment**
*Charline Lenaerts - UMONS*

Metabolomics | Thursday 2:00 PM Poster #36
**Rapid Quantification of Cortisol, Cortisone, Dexamethasone and Prednisolone in Human Saliva and Hair by Liquid Chromatography – Tandem Mass Spectrometry**
*Aлексander Gaudl - Leipzig University*

Metabolomics | Thursday 2:00 PM Poster #53
**Metabolic Phenotyping of Bile Acids - Standardized Quantitative Bile Acids Analysis in Human Plasma/serum and Mouse Plasma on Different (U)HPLC-MS/MS Platforms**
*Therese Koal - BIOCRATES Life Sciences AG*
**Metabolomics**

**Thursday 2:00 PM Poster #54**

**Metabolic Phenotyping: A New Tool Enabling Drug Response Prediction and Personalized Medicine**

_Therese Koal - Biocrates Life Science_

**Thursday 2:00 PM Poster #55**

**Impact of Pre-analytical Variations in Metabolic Phenotyping**

_Therese Koal - BIOCRATES Life Sciences AG_

**Friday 2:00 PM Poster #7**

**Characterizing the Chemotypic Landscape of Cystic Fibrosis Sputum**

_Vanessa Phelan - University of California, San Diego_

**Friday 2:00 PM Poster #10**

**Analysis of Isoprenoid Pathway Metabolites by LC-MS**

_Rudolf Köhling - Sigma-Aldrich_

**Microbiology/Virology**

**Wednesday 5:00 PM Poster #30**

**Mass Spectral Advances in Diagnostic Microbiology: from Electrophoretic Typing to LC-MS/MS-based Approaches**

_Min Fang - PRU, Culture Collection, Public Health England_

**Thursday 2:00 PM Poster #24**

**Validation and Implementation of MALDI-TOF: A Quick and Easy Method for Bacterial Identification from Clinical Samples**

_Manar Mashhadani - Northampton General Hospital_

**Thursday 2:00 PM Poster #42**

**Drug Monitoring of Antibiotics in Critically Ill Patients**

_Johannes Zander - Institute of Laboratory Medicine_

**Friday 2:00 PM Poster #30**

**Quantitative MALDI-TOF MS for Rapid Susceptibility Testing in Septic Patients**

_Christina Hamacher - Max von Pettenkofer-Institut_

**Friday 2:00 PM Poster #34**

**A MALDI-TOF MS and Stable Isotopes-based Approach Towards Rapid and Reliable Detection of Resistance Against Bacteriostatic Antibiotics**

_Lukas Schmidt - University of Salzburg_

**Friday 2:00 PM Poster #42**

**Evaluation of the Bruker Biotyper and VITEK MS MALDI-TOF MS systems for the identification of difficult-to-identify bacteria isolated from clinical specimens**

_Erin McElvania - Children’s Medical Center_

**Molecular Diagnostics**

**Thursday 2:00 PM Poster #49**

**An Evaluation of Biphenyl Chemistry to Aid in High-Throughput Bioanalytical LC-MS/MS Analyses**

_Hansjoerg Majer - Restek Corporation_
New Advances

New Advances | Wednesday 5:00 PM Poster #16
Enhanced Quantitation of Structurally Similar Proteins Using a Novel Acquisition Protocol and Mass Spectrometric Analysis
Sibylle Heidelberger - ABSCIEX

New Advances | Wednesday 5:00 PM Poster #50
High-Throughput Validated Method for the Quantification of Rufinamide in Serum Using Ultra Fast SPE-MS/MS
Loralie Langman - Mayo Clinic

New Advances | Thursday 2:00 PM Poster #5
Rapid, Fully-automated Plasma Clozapine and Norclozapine Analysis Using AC Extraction Plate Technology and Isotopic Internal Calibration MS/MS
Lewis Couchman - King's College Hospital

New Advances | Thursday 2:00 PM Poster #9
An Innovative Variable-energy Electron Ionisation Technology Applied to GC-TOF MS Metabolomics Applications
Warwick Dunn - University of Birmingham

New Advances | Thursday 2:00 PM Poster #20
Next Generation Plasma Collection Technology for the Clinical Analysis of Temozolomide by HILIC/MS/MS
Neil Loftus - Shimadzu

New Advances | Thursday 2:00 PM Poster #34
Simultaneous Identification and Quantification of Triacylglycerol Species in Human Plasma by Flow Injection Electrospray Ionization Tandem Mass Spectrometry
Madlen Sander - Institute of Laboratory Medicine, Clinical Chemist

New Advances | Friday 2:00 PM Poster #16
Single Step Separation of Plasma from Whole Blood without the Need for Centrifugation Applied to the Quantitative Analysis of Warfarin
Alan Barnes - Shimadzu

New Advances | Friday 2:00 PM Poster #56
LC-MS Analysis of Non-labeled Amino Acids on a Novel Mixed-mode HPLC Column
Itaru Yazawa - Imtakt Corporation

Pain Management

Pain Management | Wednesday 5:00 PM Poster #15
Analysis of Pain Panel Medications in Urine on Raptor™ Biphenyl by LC-MS/MS
Hansjoerg Majer - Restek Corporation

Pain Management | Wednesday 5:00 PM Poster #23
Confirmatory Determination of Buprenorphine and Norbuprenorphine in Urine Using a High-Throughput LC-HRAM-MS/MS Methodology
Marta Kozak - ThermoFisher
Proteomics | Wednesday 5:00 PM Poster #32
Performance Evaluation of the Thermo Fisher Q Exactive HF Hybrid Quadrupole-Orbitrap Mass Spectrometer for High-throughput Top-down Microbial Proteomics
Ping Yip - ThermoFisher Scientific

Proteomics | Thursday 2:00 PM Poster #12
Studying the Effect of Natural Genetic Variation on Protein Abundance in C. elegans
Kapil Dev Singh - University of Zurich

Proteomics | Thursday 2:00 PM Poster #15
Application of Multiple Protease Digestion with Shotgun Protein Sequencing De novo Approach to the Characterization of Hemoglobin Variants
Jane Yang - University of California, San Diego

Proteomics | Thursday 2:00 PM Poster #18
Quantitative phosphoproteomics Analysis of Malignant Ovarian Tumors in Mice by LC-MS and Labelling with Tandem Mass Tags
Changde Zhang - Xavier University

Proteomics | Thursday 2:00 PM Poster #25
Developments Towards High-throughput Plasma Proteomics Platform for the Clinic
Garwin Pichler - Max Planck Institute of Biochemistry

Proteomics | Thursday 2:00 PM Poster #35
Standardized Targeted Proteomics Approach for the Simultaneous Determination of Eight Apolipoproteins in the Leipzig Heart Study
Julia Dittrich - University Hospital Leipzig

Proteomics | Thursday 2:00 PM Poster #45
Towards Clinically Actionable Quantification of Proteins by Mass Spectrometry: A Critical Appraisal of Bias and Imprecision for Serum Apolipoproteins A-I and B
Irene van den Broek - Leiden University Medical Center (LUMC)

Proteomics | Thursday 2:00 PM Poster #46
Quantitation of Multiplexed Serum Apolipoproteins by Stable Isotope Dilution-Multiple Reaction Monitoring-LC-MS/MS
Nico Smit - Leiden Universitary Medical Center (LUMC)

Proteomics | Friday 2:00 PM Poster #14
Kappa and Lambda Light Chain Molecular Mass Distribution Using Mass Spectrometry
Adrian Fontan - Hospital San Pedro
Absolute and Multiplex Quantification of Therapeutic Monoclonal Antibodies in Serum Samples by LC-SRM Using PSAQ Standards
Dorothee Lebert - PROMISE Advanced Proteomics

Regulations, Standards & Proficiency
Regulations, Standards & Proficiency | Wednesday 5:00 PM Poster #34
LC-MS Candidate Reference Methods for the Harmonisation of Parathyroid Hormone (PTH) Measurement: A Review of Recent Developments and Future Considerations
Lewis Couchman - King's College Hospital

Sample Prep & Automation
Sample Prep & Automation | Wednesday 5:00 PM Poster #8
A Rapid Clean-up Procedure for Monitoring the Biomarker of Dimethylformamide in Hemoglobin by LC-MS/MS
Xiaohua Chen - Bonna-Agela Technologies

Sample Prep & Automation | Wednesday 5:00 PM Poster #9
Automating an Assay for 25-OH Vitamin D in a Clinical Research Laboratory to Reduce Training Requirements for Mass Spectrometry
Daniel Blake - ABSCIEX

Sample Prep & Automation | Wednesday 5:00 PM Poster #12
A Novel Online Cleanup Valve Solution for Quantitative Analysis of Testosterone in Serum Utilizing LC-MS/MS
Peter Christensen - Agilent Technologies

Sample Prep & Automation | Wednesday 5:00 PM Poster #28
Evaluation of Supported Liquid Extraction for Vitamin D: 25-hydroxy and 1,25-dihydroxyvitamin D2/D3, PTAD Derivatization and Analysis Using UPLC-MS/MS
Lee Williams - Biotage GB Limited

Sample Prep & Automation | Wednesday 5:00 PM Poster #29
Improved Sample Preparation and HPLC-MS Analysis of Vitamin D Metabolites from Human Plasma
Rudolf Köhling - Sigma-Aldrich

Sample Prep & Automation | Wednesday 5:00 PM Poster #38
High-throughput LC-MS/MS Analysis of 25-OH-Vitamine D2/D3 in Serum Using Online SPE and Automated Sample Preparation
Silvia Bücher - Recipe GmbH

Sample Prep & Automation | Wednesday 5:00 PM Poster #43
A Study of Stability, Robustness and Time Efficiency of a New HPLC and a New Tandem MS
Jason Lai - Thermo Fisher Scientific
Estradiol - Investigation of Two Sample Preparation Procedures for Quantitative Analysis by LC-MS/MS Michal Svoboda and Ursula Turpeinen

Michal Svoboda - Tecan Schweiz AG

Analysis of Serum Testosterone and Androstenedione for Clinical Research Using Either Manual Or Automated Extraction

Dominic Foley - Waters

iST: Sample Preparation for High Throughput Clinical Proteomics

Nils A. Kulak - Max Planck Institute of Biochemistry

TICE – an Innovative, Easy-to-automate Extraction Technique for Small Molecule Analytes from Biological Fluids for LC-MS/MS Analysis

Roland Geyer - Tecan Switzerland AG

High-throughput LC-MS/MS Analysis of Immunosuppressants in Whole Blood Using On-line SPE and Automated Sample Preparation

Silvia Bürcher - Recipe GmbH

A Simple High-throughput SPE Method to Support the Biomonitoring of Phthalate Metabolites in Human Urine Prior to LC-MS/MS

Lee Williams - Biotage GB Limited

Targeted Quantitation of Insulin and Its Therapeutic Analogs

Ravindra Chaudhari - Thermo Fisher Scientific

Development of SPME-LC-MS/MS Method for Concomitant Extraction of Rocuronium Bromide and Tranexamic Acid from Plasma

Barbara Bojko - University of Waterloo

Comparison Between Different Process Methods of Arachidonic Acid in Plasma

Xiaohua Chen - Bonna-Agela Technologies

Comparison of SPE Approaches for the Extraction of Thyroid Hormones: T3, RT3 and T4 Prior to LC-MS/MS Analysis

Lee Williams - Biotage GB Limited

The Utilization of In Vivo and In Situ Solid Phase Microextraction in Clinical Analysis

Barbara Bojko - University of Waterloo
Highly Automated, High Precision Tryptic Digestion and SISCAPA-MS Quantification of Human Plasma Proteins Using the Agilent Bravo Platform

Selena Larkin - SISCAPA Assay Technologies

Small Molecule Analytes

Determinition of 25-hydroxyvitamin D3 and D2 in Plasma Using Online SPE in Combination with UPLC-MS/MS

Martijn van Faassen - University Medical Center Groningen

Benefits of the Orbitrap Technology in LCMS for Therapeutic Monitoring of Baclofen and Its Metabolites in Plasma and Urine Samples.

Benedicte Duretz - ThermoFisher

Serum Aldosterone Measurement by Liquid Chromatography-tandem Mass Spectrometry

Jody van den Ouweland - Canisius-Wilhelmina Hospital

Enhanced Resolution of Vitamin D Metabolites Utilizing Chromatographic Selectivity and Novel Sample Preparation Techniques

Craig Aurand - Sigma Aldrich

Development and Validation of a Liquid Chromatography-tandem Mass Spectrometry (LC-MS/MS) Assay for Voriconazole

Deborah French - University of California San Francisco

Determination of Urinary Ethyl Glucuronide and Ethyl Sulfate by LC/MS/MS for Clinical Research

Kevin McCann - Agilent Technologies

UPLC-MS/MS Measurement of Triazole Antifungals and Metabolites in Serum

Sankha Basu - Brigham and Women's Hospital

Analysis of Tramadol and Its Three Desmethyl Metabolites in LCMS Using High Resolution and Accurate Mass Mass Spectrometry. Monitoring in Clinical Toxicology

Claudio De Nardi - Thermo Fisher Scientific

Performance Evaluation of Serum 25-hydroxyvitamin D2 and 25-hydroxyvitamin D3 Using PerkinElmer MSMS Vitamin D Kit

Hee-Jung Chung - Cheil General Hospital & Women's Healthcare Center
Small Molecule Analytes | Wednesday 5:00 PM Poster #46
25-Hydroxy-Vitamin D- Which Sample Preparation Technique Offers the Best and Most Effective Results
Rory Doyle - Agilent Technologies, Inc

Small Molecule Analytes | Wednesday 5:00 PM Poster #49
Simultaneous Determination of 5 Steroids in Serum Using LC-MS/MS for the Diagnosis of Congenital Adrenal Hyperplasia
Hyeon Ju Oh - Samsung Medical Center

Small Molecule Analytes | Thursday 2:00 PM Poster #1
Development of a LC-MS/MS-Method for the Determination of Colistin and Colistin Methanesulfonate and Application to Plasma-Samples of Critically Ill Patients
Matthias Weber - MVZ LaborDiagnostik Karlsruhe

Small Molecule Analytes | Thursday 2:00 PM Poster #4
Quantitative Androgen Profile in Plasma Using Online SPE in Combination with UPLC Tandem Mass Spectrometry
Martijn van Faassen - University Medical Center Groningen

Small Molecule Analytes | Thursday 2:00 PM Poster #6
Development of an LC-MS/MS Method for Separate Quantification of 25-hydroxyvitamin D3, 3-epi-25-hydroxyvitamin D3 and 25-hydroxyvitamin D2 in Human Serum
Jody van den Ouweland - Canisius-Wilhelmina Hospital

Small Molecule Analytes | Thursday 2:00 PM Poster #7
Therapeutic Drug Monitoring (TDM) of Various Types of Antibiotics by a Single Multi-purpose LC-MS Method
Matteo Conti - S.orsola-Malpighi Hospital Central Laboratory

Small Molecule Analytes | Thursday 2:00 PM Poster #8
Fast and Robust LC-MS/MS Method for Determination of the Alcohol Biomarker Phosphatidylethanol (PEth) in Whole Blood Using Automated Extraction
Anders Blomgren - University Hospital of Lund

Small Molecule Analytes | Thursday 2:00 PM Poster #17
Development of a Turboflow™-LC-MS/MS Method for Determination of 17-Hydroxyprogesterone in Human Serum
Jacopo Gervasoni - Policlinico Gemelli

Small Molecule Analytes | Thursday 2:00 PM Poster #19
A Fast and Effective Approach for the Analysis of Urinary Cortisol, Cortisone, Prednisolone and Prednisone Using SPE and LC-MS/MS
Sean Orlowicz - Phenomenex

Small Molecule Analytes | Thursday 2:00 PM Poster #21
Maximizing Triple Quadrupole Mass Spectrometry Productivity Through the Automated Use of an Expanded Dual-Channel HPLC System with Online Sample Cleanup
Kevin McCann - Agilent Technologies
The Separation and Analysis of Opiates and their Glucuronide Metabolites in Urine Matrix Negating the Need for Hydrolysis During Sample Preparation

*Peter Christensen* - *Agilent Technologies*

Online Analysis of 25-OH-vitamin D2/D3 in Plasma and Serum with the Evoq Triple Quad

*Rafaela Martin* - *Bruker Daltonik GmbH*

Development of an LC-MS/MS Method to Determine Insulin and Synthetic Analogs in Human Plasma

*Yasin Bekkach* - *Laboratory of Endocrinology*

A Dutch Study into the Analysis of Vitamin B6 in Whole Blood

*Bertrand van Zelst* - *Department of Clinical Chemistry NA-420*

Development of a UPLC-MS/MS Method to Measure Next Generation Antiepileptic Medications in Serum

*Sankha Basu* - *Brigham and Women's Hospital*

Evaluation of New PreludeTM SPLC System Coupled with EnduraTM Triple Quadrupole MS Using Analysis of Testosterone and Cortisol in Biological Matrixes

*Claudio De Nardi* - *ThermoFisher*

Increased Throughput for the Analysis of Delta-9-THC in Oral Fluids Using Triple Quadrupole Mass Spectrometry Coupled with an Automated Dual-Channel HPLC System

*Kevin McCann* - *Agilent Technologies*

Overestimation of 25-hydroxyvitamin D3 by Increased Ionisation Efficiency of 3-epi-25-hydroxyvitamin D3 in LC-MS/MS Methods Not Separating Both Metabolites

*Jody van den Ouweland* - *Canisius-Wilhelmina Hospital*

Ultra High Throughput Analysis of Immunosuppressants in Whole Blood by Microflow LC-MS/MS

*Daniel Blake* - *ABSCIEX*

25-Hydroxy-Vitamin D- Which Ionization Mode and Column Type Gives the Best Analytical Results

*Rory Doyle* - *Agilent Technologies, Inc*

Multiplexing Multiple Methods to Maximize Workflow Efficiency in LC-MS Laboratories

*Marta Kozak* - *ThermoFisher*
Small Molecule Analytes | Friday 2:00 PM Poster #44
Analysis of Aldosterone in Plasma for Clinical Research Using Automated Extraction

Dominic Foley - Waters

Small Molecule Analytes | Friday 2:00 PM Poster #46
Measurement of C3-epimer Form of 25-hydroxyvitamin D3 in Korean Children

Hee-Jung Chung - Cheil General Hospital & Women's Healthcare Center

Small Molecule Analytes | Friday 2:00 PM Poster #52
Ultra-high Throughput Quantitation of Immunosuppressants in Human Whole Blood

Peter Christensen - Agilent Technologies

Toxicology

Toxicology | Wednesday 5:00 PM Poster #17
Method for Drug Screening in Exhaled Breath Using Liquid Chromatography – Tandem Mass Spectrometry

Niclas Stephanson - Clinical Pharmacology

Toxicology | Wednesday 5:00 PM Poster #20
Urine Drug Screening by GC-MS/MS and LC-MS/MS

Jennifer Colby - University of California San Francisco

Toxicology | Thursday 2:00 PM Poster #10
Screening for Psychotropic Medical Drugs in Serum using Ion Trap MS – Customizing a Screening Approach to Specific Needs in the Lab

Jürgen Kempf - Institute of Forensich Medicine

Toxicology | Thursday 2:00 PM Poster #11
An Automated LC-Ion Trap MS Screening for Synthetic Cannabinoids

Laura Huppertz - Institute of Forensic Medicine

Toxicology | Thursday 2:00 PM Poster #23
Rapid and Simple Confirmation and Quantification of 11-Nor-Δ9-Tetrahydrocannabinol-9-Carboxylic Acid (THC-COOH) in Human Urine by 2D-LC-MS/MS

Berit Jensen - Toxicology, Canterbury Health Laboratories

Toxicology | Thursday 2:00 PM Poster #38
Comprehensive Drugs of Abuse Identification in Urine by LC-MSn Combined with MS Spectral Library Matching

Ulrike Burmester - Bruker Daltonics

Toxicology | Thursday 2:00 PM Poster #50
A Method for the Determination of Desomorphine, Heroin, Methadone, Buprenorphine and Metabolites in Urine Using LC/MS QQQ

Christopher Benton - Agilent Technologies

Toxicology | Friday 2:00 PM Poster #4
Analysis of Cannabinoids in Whole Blood: Above and Beyond State of Art

Alexandre Paccou - ABSCIEX
Toxicology | Friday 2:00 PM Poster #26  
**Evaluating ToxFinder™ New Data Processing Software in Targeted Screening Applications Implemented on LC/MS Mass Spectrometers**  
*Marta Kozak* - *ThermoFisher*

---

Various OTHER | Wednesday 5:00 PM Poster #22  
**Comparison of 25-hydroxyvitamin D Assays in Korean with Detectable Ergocalciferol**  
*Misuk Ji* - *Konkuk University School of Medicine*

---

Various OTHER | Thursday 2:00 PM Poster #48  
**Development and Validation of a Candidate Reference Method for the Measurement of Serum Cortisol Using Supported Liquid Extraction and UPLC-MS/MS**  
*James Hawley* - *University Hospital South Manchester*
**Posters: WEDNESDAY**

**Wednesday 5:00 PM**
**Poster #2 in Exhibit Hall**
**Determination of 25-hydroxyvitamin D3 and D2 in Plasma Using Online SPE in Combination with UPLC-MS/MS**

**Martijn van Faassen - University Medical Center Groningen (h.j.r.van.faassen@umcg.nl) -- *Young Investigator Awardee* **

- 25-hydroxyvitamin D3 in plasma is the established marker to detect vitamin D deficiency. Several methods have been published to analyze 25-hydroxyvitamin D3 by LC-MS/MS. Most of these methods use protein precipitation or/and offline SPE methods. Here we present a fully automatable method by combing online SPE with UPLC-MS/MS. Total run-time was 6.5 min, resulting in baseline separation between 25-hydroxyvitamin D3 and D2. Intra- and inter-assay analytical variation were <5% for both vitamins. Linearity in the calibration range for D3 and D2 was excellent (r² >0.99). In summary, we have developed a selective and reproducible mass spectrometric analysis for the measurement of 25-hydroxyvitamin D3 and D2 in plasma which can be completely automated.

**Wednesday 5:00 PM**
**Poster #3 in Exhibit Hall**
**Benefits of the Orbitrap Technology in LC-MS for Therapeutic Monitoring of Baclofen and Its Metabolites in Plasma and Urine Samples.**

**Benedicte Duretz - ThermoFisher (benedicte.duretz@thermo.com)**

- Baclofen is a centrally acting muscle relaxant, prescribed in France for the treatment of cerebral spasticity. It has recently attracted considerable attention as a potential medication for alcoholism. Variability in efficient dose has been observed in patients. Therefore it is of interest to monitor baclofen and its major metabolites in plasma. We describe a method to semi-quantify baclofen’s metabolites in a single run by liquid chromatography coupled to high resolution mass spectrometry (LC-HRMS). Tests were initially carried out on samples collected from patients treated in context of alcohol withdrawal and/or in cases of overdose for forensic toxicology purposes.

**Wednesday 5:00 PM**
**Poster #4 in Exhibit Hall**
**Analysis of Amphetamines in Urine Sample Using the Atmospheric-pressure Solids Analysis Probe for Ionization**

**Fernanda Salami - Universidade de São Paulo (fernandasalami@yahoo.com.br)**

- Analysis of amphetamines in urine sample using the atmospheric-pressure solids analysis probe for ionization. Fernanda Helena Salami, Eduardo José Crevelin and Luiz Alberto Beraldo de Moraes Stimulants are substances capable of reducing tiredness and increasing alertness, competitiveness and aggression because of these effects. They are used by drivers and also as appetite suppressant for weight reduction or in sports competition and training to increase athlete performance. Here, atmospheric-pressure solids analysis probe for ionization coupled to MS/MS (ASAP-MS/MS) was utilized in the analysis of amphetamines and cocaine in urine samples. Limits of detection for stimulants were determined 1ng mL-1. ASAP-MS/MS was rapid and sensitive technique with potential for determination of amphetamines and cocaine in urine simple.

**Wednesday 5:00 PM**
**Poster #6 in Exhibit Hall**
**Serum Aldosterone Measurement by Liquid Chromatography-tandem Mass Spectrometry**

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

- We have developed an UPLC–MS/MS method for the quantitation of aldosterone using LLE and SPE prior to RP chromatography. Transitions for aldosterone m/z 359.0 > 189.1 and d7-aldosterone 366.0 > 338.3 were used for monitoring using –ESI mode. Accuracy was verified by analysis of GC-MS certified aldosterone materials (n=3; RFB, Bonn, Germany)(UPLC-MS/MS= 0.96 RFB + 34.1; r²=0.999). A preliminary method comparison with a second LC-MS/MS method (Vancouver, Canada) showed a good correlation (UPLC-MS/MS= 0.98 LC-MS/MS + 15.4 (r²=0.990; n=5). LLOQ was 30 pmol/L and intra- and inter-assay imprecision were <10%. The assay was linear up to 3140 pmol/L.
**Wednesday 5:00 PM**
**Poster #8 in Exhibit Hall**

**A Rapid Clean-up Procedure for Monitoring the Biomarker of Dimethylformamide in Hemoglobin by LC-MS/MS**

**Xiaohua Chen - Bonna-Agela Technologies** (xiaohua.chen@agela.com.cn)

• This paper described a method for monitoring 3-Methyl-5-Isopropylhydantoin (MVH), a biomarker of the degradation of dimethylformamide (DMF) in hemoglobin. Cleanert MAS-B Plate with 96-well format was used for rapid clean-up of the samples. 3-Methy-5-isobutylhydantion (MIH) was applied as internal standard to quantify MVH in hemoglobin. A clean fraction was obtained for high throughput monitoring of MVH by LC-MS/MS without further concentration. Recoveries for MVH were range from 100.4% to 102.5% with RSDs were £¼4.6%. LOD of MVH and MIH were 1.0ng/mL. The study provided a solution for assessing cumulative exposure to DMF.

---

**Wednesday 5:00 PM**
**Poster #9 in Exhibit Hall**

**Automating an Assay for 25-OH Vitamin D in a Clinical Research Laboratory to Reduce Training Requirements for Mass Spectrometry**

**Daniel Blake - ABSCIEX** (daniel.blake@absciex.com)

• The analysis of 25-OH Vitamin D within the clinical research laboratory is a high throughput assay. As a consequence of the high number of samples, automation and simplification of assay is an attractive proposal to minimise sources of error and staff training requirements, reducing the need to train staff in additional Mass Spectrometry and sample preparation theories. In addition, automated handling of sample and result data significantly reduces errors associated with manual transcription. We propose here an elegant and cost effective solution for this application.

---

**Wednesday 5:00 PM**
**Poster #10 in Exhibit Hall**

**Selective Screening for Inborn Errors of Metabolism by Tandem Mass Spectrometry in Egyptian Children**

**Dina Mehaney - Faculty of Medicine Cairo University** (drдинa.mеhanеу@kаsrаlаinе.еdu.еg)

• In order to enhance awareness and promote registry for inborn errors of metabolism (IEMs) in Egypt, we aimed to evaluate the prevalence and main clinical findings of IEMs detectable by tandem mass spectrometry (MS/MS) among high risk pediatric patients presenting to our tertiary care facility at Cairo University Children's Hospital over a period of 5years. During this period 3380 Egyptian children suspected of having IEMs were analyzed by MS/MS. A relatively high number of patients (203/3380 (6%)) were confirmed with 17 different types of IEMs. The development of a nationwide screening program for IEMs is mandatory.

---

**Wednesday 5:00 PM**
**Poster #12 in Exhibit Hall**

**A Novel Online Cleanup Valve Solution for Quantitative Analysis of Testosterone in Serum Utilizing LC-MS/MS**

**Peter Christensen - Agilent Technologies** (peter.christensen@agilent.com)

• Determination of testosterone levels in serum is an important measurement in clinical research. Liquid chromatography triple quadrupole mass spectrometry (LC/MS/MS) is an essential tool in the analytical laboratories due to its high sensitivity and specificity, excellent reproducibility, and it can be used in simultaneous analysis of multiple analytes. This work describes a novel integrated valve and liquid metering system used for on-line sample cleanup coupled with a MS/MS.

---

**Wednesday 5:00 PM**
**Poster #14 in Exhibit Hall**

**Enhanced Resolution of Vitamin D Metabolites Utilizing Chromatographic Selectivity and Novel Sample Preparation Techniques**

**Craig Aurand - Sigma Aldrich** (craig.aurand@sial.com)

• Analysis of Vitamin D metabolites has continued to be a topic of interest in recent publications, primarily as biomarkers for possible disease states and vitamin sufficiency. While Vitamin D is present in two forms, current ELISA methods cannot distinguish D2 and D3 forms of the vitamin metabolites resulting in a reporting of total 25-hydroxyvitamin D. In this study, an LC/MS method for the analysis of Vitamin D metabolites is expanded to include dihydroxy metabolites along with the epi-homologs. Chromatographic resolution is utilized for the quantitation of hydroxy and dihydroxy Vitamin D2 and D3 metabolites including the isobaric epimers. In addition, sample preparation techniques are evaluated for the impact of biological matrix ionization effects.
Wednesday 5:00 PM
Poster #15 in Exhibit Hall
Analysis of Pain Panel Medications in Urine on Raptor™ Biphenyl by LC-MS/MS
Hansjoerg Majer - Restek Corporation (Hansjoerg.Majer@restek.com)
- Restek Corporation, 110 Benner Circle, Bellefonte, PA 16823 For nearly a decade, the Restek™ Biphenyl has been the column of choice for clinical diagnostic and Pain Management drug screening testing because of its ability to provide highly retentive, selective, and rugged reversed-phase separations of drugs and metabolites. By bringing the speed of Superficially Porous Particles to the Biphenyl family, Restek’s Raptor™ Biphenyl provides clinical labs with an even faster option for a wide variety of clinical assays. Drug Screening applications can be difficult to optimize and reproduce due to the limited selectivity of C18 and phenyl-hexyl phases. Using Raptor™ Biphenyl columns pain management analysis can be performed with a 5-minute cycle time and complete isobaric resolution. Popular competitor methods have tailing peaks, longer run times, and co-elutions.

Wednesday 5:00 PM
Poster #16 in Exhibit Hall
Enhanced Quantitation of Structurally Similar Proteins Using a Novel Acquisition Protocol and Mass Spectrometric Analysis
Sibylle Heidelberger - ABSCIEX (Sibylle.Heidelberger@absciex.com)
- Metabolism of drugs by the Cytochrome P450 superfamily is pivotal in determining their disposition, safety and efficacy. Since drugs may induce expression of several isoforms of Cytochrome P450, they may enhance their own turnover, increasing the risk of toxic metabolite formation or adverse interactions with co-ingested compounds. Thus P450 profiling is a fundamental aspect of drug safety evaluation. The Cytochromes P450 share extensive structural similarity, so that antibodies are incapable of discriminating every isoform, plus mRNA levels do not correlate well with protein. SWATH™ is a data-independent MS method for label-free quantification which enables closely-related proteins to be quantified retrospectively through post-acquisition extraction of specific peptide ions, and is thus perfectly suited to P450 profiling.

Wednesday 5:00 PM
Poster #17 in Exhibit Hall
Method for Drug Screening in Exhaled Breath Using Liquid Chromatography – Tandem Mass Spectrometry
Niclas Stephanson - Clinical Pharmacology (Niclas.stephanson@karolinska.se)
- A mass spectrometric multicomponent method for analysis of drugs of abuse in aerosol particles collected from exhaled breath employing a new sampling device was developed and applied in routine. Analytes comprised morphine, 6-acetylmorphine, amphetamine, methamphetamine, benzoylecgonine, cocaine, diazepam, oxazepam and tetrahydrocannabinol. The methods involved a simple sample preparation procedure for eluting drugs with methanol from the collection filter, quantification using deuterated analogues (internal standards), reversed phase chromatography with gradient elution, positive electrospray ionization and monitoring of two product ions per analyte in selected reaction monitoring mode (Thermo Fisher Scientific TSQ Vantage instrument). The measuring range was 6.0–1000.0 pg/sample and the reporting level in routine analysis was set to 18 pg/sample for all analytes.

Wednesday 5:00 PM
Poster #18 in Exhibit Hall
Shortened Validation Procedure for a Method of Quantitative Analysis of 45 Amino Acids in Plasma on Tandem Mass Spectrometer
Marija Zekušić - University Hospital Centre Zagreb (zekusicm@yahoo.com) -- *Young Investigator Awardee*
- The validation was carried out using aTRAQ™ reagent manufactured by AB Sciex. Amino acids were quantified on API 3200 mass spectrometer. Shortened validation procedure for the method included testing of between-run and within-run imprecision, inaccuracy, limit of detection, limit of quantitation and linearity. Calculated values of the coefficient of variation (CV) for within-run and between-run imprecision and inaccuracy for most amino acids were lower than 20%, with the exception of glutamine (CV=24%). Limit of detection (LoD) and limit of quantitation (LoQ) were lower than 2 µmol/L for most amino acids except for serine, glycine and β-alanine which had somewhat higher LoQ. The method was linear up to 1000 µmol/L for most amino acids. Based on results of shortened validation procedure, it was concluded that the method is acceptable for routine laboratory practice.
Wednesday 5:00 PM
Poster #20 in Exhibit Hall
Urine Drug Screening by GC-MS/MS and LC-MS/MS

Jennifer Colby - University of California San Francisco (jennifer.colby@ucsf.edu) -- *Young Investigator Awardee*

- Clinical toxicology services are routinely offered by laboratories and can play an important role in patient management. Our laboratory offers a liquid chromatography tandem mass spectrometry (LC-MS/MS) method to screen urine samples for a diverse group of compounds. Immunoassays are not available for many of the analytes, making it challenging to verify results. Here we report the development and validation of a gas chromatography tandem mass spectrometry method for comprehensive urine drug screening of underivitized samples, which we use to corroborate our LC-MS/MS results.

Wednesday 5:00 PM
Poster #22 in Exhibit Hall
Comparison of 25-hydroxyvitamin D Assays in Korean with Detectable Ergocalciferol

Misuk Ji - Konkuk University School of Medicine (msji0402@gmail.com)

- Among two forms of 25-hydroxyvitamin D, ergocalciferol (D2) is usually not detected in the majority of Korean. This study was to evaluate the performance of two vitamin D immunoassays with samples of detectable D2. Fifty serum samples were analyzed with LC-MS/MS, ADVIA Centaur and Elecsys Vitamin D Total Assay. The mean difference of Centaur and Elecsys were -7.2 ng/mL and +1.1 ng/mL, respectively. The correlation of Elecsys with LC-MS/MS was better (R=0.8635) than that of Centaur (R=0.6234). The correlation of Centaur was inferior compared to previous studies. There might be underestimation of D2 levels in some vitamin D immunoassays.

Wednesday 5:00 PM
Poster #23 in Exhibit Hall
Confirmatory Determination of Buprenorphine and Norbuprenorphine in Urine Using a High-Throughput LC-HRAM-MS/MS Methodology

Marta Kozak - ThermoFisher (marta.kozak@thermofisher.com)

- Forensic toxicology labs monitor levels of buprenorphine and its major active metabolite, norbuprenorphine, in urine in order to determine compliance with treatment for chronic pain or opioid addiction. LC-MS/MS is currently the most popular method used for confirmation. Here we demonstrate that the use of a two-channel UHPLC system with a high resolution accurate mass MS equipped with segmented quadrupole allowed for highest specificity, sensitivity, and sample throughput as compared to conventional LCMS/ MS. This methodology resulted in achieving a sample cycle time of 1.07 minutes and dynamic linearity range of 5 – 2000ng/mL with correlation coefficients > 0.996 for both analytes.

Wednesday 5:00 PM
Poster #24 in Exhibit Hall
Development and Validation of a Liquid Chromatography-tandem Mass Spectrometry (LC-MS/MS) Assay for Voriconazole

Deborah French - University of California San Francisco (deborah.french@ucsf.edu) -- *Young Investigator Awardee*

- Background: Our institution currently sends serum samples for voriconazole testing to a reference laboratory. Objective: Develop a LC-MS/MS assay for voriconazole. Results: Six calibrators were used (0-10 µg/mL) and the reportable range was 0.1-40 µg/mL. The LOQ=0.1 µg/mL. Extraction recovery was ~69% and ion suppression was ~13%. Run time was 4 minutes. Precision studies yielded CVs <5% at LOQ and <4% through the linear range. Conclusions: An accurate, sensitive and rapid LC-MS/MS assay for voriconazole was developed. Method comparison, cost-analysis and electronic data upload to the laboratory information system studies are ongoing.

Wednesday 5:00 PM
Poster #25 in Exhibit Hall
Back to the Future of Human Metabolites for Central Biochemical Pathways

Roland Wohlgemuth - Sigma-Aldrich (roland.wohlgemuth@sial.com)

- The understanding of central biochemical pathways and their regulation is key for molecular descriptions of human health and disease. Although central pathways are well-established milestone discoveries of classical biochemistry, many metabolites of such central pathways have not been available. As mass spectrometry analyses require pure metabolite standards, an initiative to fill these gaps has been started. New tools for the analysis of highly polar carboxylated and phosphorylated metabolites have not only proven useful for the development of new metabolite standards, but also in such widely different applications like analysing inborn errors of metabolism, cancer- and other disease-related metabolites.
**Determination of Urinary Ethyl Glucuronide and Ethyl Sulfate by LC/MS/MS for Clinical Research**

*Kevin McCann - Agilent Technologies (kevin_mccann@agilent.com)*

- Liquid chromatography triple quadrupole mass spectrometry (LC/MS/MS) is ideally suited for the rapid analysis of multiple analytes. A highly sensitive and specific LC/MS/MS method has been developed for the quantitation of ethyl glucuronide and ethyl sulfate. A dilution procedure and a solid phase extraction (SPE) procedure are evaluated and compared based on ease of use, analyte recovery and post-extraction cleanliness. The described method achieves the required sensitivity and is capable of quantitating analytes over a wide dynamic range. Excellent reproducibility was observed for all compounds (CV < 5%). All calibration curves displayed linearity with an R2 > 0.995.

**Evaluation of Supported Liquid Extraction for Vitamin D: 25-hydroxy and 1,25-dihydroxyvitamin D2/D3, PTAD Derivatization and Analysis Using UPLC-MS/MS**

*Lee Williams - Biotage GB Limited (lee.williams@biotage.com)*

- Vitamin D analysis has important clinical relevance with levels needing to be measured for a wide variety of reasons. This poster demonstrates a simple supported liquid extraction protocol, derivatization with PTAD and subsequent detection of both the traditional hydroxy metabolites and the biologically active dihydroxy metabolites in serum. Extracts were analysed using a Waters ACQUITY UPLC system coupled to a Quattro PREMIER XE triple quadrupole mass spectrometer. Positive ions were acquired using ESI operated in the positive MRM mode. Method performance demonstrated high analyte recoveries and low ion suppression, allowing a quantifiable range matching levels therapeutically expected for each metabolite.

**Improved Sample Preparation and HPLC-MS Analysis of Vitamin D Metabolites from Human Plasma**

*Rudolf Köhling - Sigma-Aldrich (rudolf.koehling@sial.com)*

- The analysis of Vitamin D metabolites has continued to be a topic of interest in current research, because those serve as biomarkers for possible disease states and for vitamin sufficiency. Vitamin D is present in two forms, vitamin D2 and D3. In this work, a LC-MS method for the analysis of Vitamin D metabolites was developed to include dihydroxy metabolites along with the epi-homologs. Special focus of this development was the chromatographic resolution of the isobaric compounds. In addition, sample preparation techniques are evaluated to reduce the impact of biological matrix ionization effects.

**Mass Spectral Advances in Diagnostic Microbiology: from Electrophoretic Typing to LC-MS/MS-based Approaches**

*Min Fang - PRU, Culture Collection, Public Health England (min.fang@phe.gov.uk)*

- SDS-PAGE combined with electrospray tandem MS (GelC-MS/MS) is frequently used for proteomic analysis. However, its use as a platform for microbial proteotyping has not been systematically investigated. Here, we subjected members of the family Enterobacteriaceae including taxonomically indistinguishable species such as E. coli and Shigella spp. to such analyses to explore the potential of this approach. By using the optimised database and proteome profiling, we could confidently identify E. coli and characterise strain-specific virulence factors, differentiate shiga-toxin negative from positive strains, and demonstrate that GelC-MS/MS has the potential to simultaneously combine strain identification with key pathogenic properties of an isolate.

**Performance Evaluation of the Thermo Fisher Q Exactive HF Hybrid Quadrupole-Orbitrap Mass Spectrometer for High-throughput Top-down Microbial Proteomics**

*Ping Yip - ThermoFisher Scientific (ping.yip@thermofisher.com)*

- By using the Q Exactive HF mass spectrometer in conjunction with a new charge assignment and protein deconvolution algorithm, we demonstrate improved performance in protein identification in a series of high-throughput top-down proteomics experiments with complex E. coli extract.
The analysis of intact PTH (PTH1-84) is important in the diagnosis of hyperparathyroidism, and in the clinical management of bone mineral disorders. Recently, LC-MS methods have been developed for quantitation of PTH1-84 using tryptic peptides, but these methods are subject to interferences due to the presence of modified (oxidised/phosphorylated) PTH species, which accumulate in patient samples. The tryptic digestion process produces non-specific tryptic peptides which cannot be used as surrogates for PTH1-84. Further work, including the use of high-resolution MS, to allow the analysis of PTH without protease digestion is required before these approaches can be considered as reference methods.

Laser diode thermal desorption coupled with high-resolution accurate-mass spectrometry was evaluated to support forensic toxicology screening of benzodiazepines in urine and was compared to traditional LC-MS approach. Samples were processed by hydrolysis and liquid-liquid extraction. All compounds were linear from 1000 ng/mL to 1 to 10 ng/mL using LDTDMS. Results from LDTD compared to LC-MS were good with correlations >0.9. QCs had accuracies and precisions within 30%. Internal standards in donor samples show limited and acceptable matrix effects. LDTD coupled to HRAM mass spectrometer offers semi-quantitative screening solution making it an attractive choice for forensic toxicology laboratories seeking high throughput.

A single extraction and analysis method has been developed for urinary catecholamines and metanephrines. Analytes were extracted using weak cation exchange SPE and analyzed using HILIC LC/MS/MS. Extraction efficiencies and matrix effects were characterized. Replicate analyses of QC material displayed excellent accuracy and precision across the measurement range. This method enables rapid, simultaneous and accurate LC/MS/MS analysis of these challenging compounds without the need for reversed-phase separations employing ion-pairing reagents. For Research Use Only. Not for Use in Diagnostic Procedures.

The determination of 25-OH-Vitamin D is widely used for the assessment of the vitamin D status, which is important for many chronic conditions and latency diseases. For high throughput analysis RECIPE has developed an automated ClinMass® LC-MS/MS Complete Kit MS7000 - 25-OH-Vitamin D2/D3 in Plasma and Serum working with liquid handling systems and two-dimensional LC-MS/MS. The fully CE IVD certified kit shows outstanding validation results. A comparison between automation and manual sample preparation shows close agreement of the concentrations of the analytes for both variants. Full automation increases significantly sample traceability and process security suiting very well into clinical routine analysis.
Wednesday 5:00 PM
Poster #39 in Exhibit Hall

**Metabolic Phenotyping of Bile Acids - Standardized Quantitative Bile Acids Analysis in Human Plasma/serum and Mouse Plasma on Different (U)HPLC-MS/MS Platforms**

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

- Bile acids are considered not only as endogenous markers for liver cell functions, but also as signaling molecules regulating triglycerides, cholesterol and glucose metabolism as well as inflammatory processes and apoptosis. Accurate determination of individual bile acids and their conjugates is very important in accessing liver damages as well as hepatic and biliary tract diseases, colon cancer, atherosclerosis and type 2 diabetes. We have developed and validated a standardized (U)HPLC-ESI-MSMS assay for the analysis of ca. 20 bile acids from only 10 µL human plasma/serum or mouse plasma samples. The panel consists of cholic acid, deoxycholic acid, chenodeoxycholic acid, ursodeoxycholic acid, hyodeoxycholic acid, muricholic acids and their glycine as well as taurine conjugates.

---

Wednesday 5:00 PM
Poster #40 in Exhibit Hall

**UPLC-MS/MS Measurement of Triazole Antifungals and Metabolites in Serum**

*Sankha Basu - Brigham and Women's Hospital (sbasu2@partners.org)*

- There is growing clinical demand for therapeutic drug monitoring of triazole antifungals and their metabolites, particularly in immunosuppressed populations. Here, we present a simple and rapid stable isotope dilution liquid chromatography tandem mass spectrometry method to measure fluconazole, voriconazole, voriconazole-N-oxide, posaconazole, itraconazole, and hydroxyitraconazole in serum. Simple protein precipitation was followed by reversed phase UPLC coupled to ESI-MS/MS providing a short run time (3 min), with each analyte showing linearity \((r^2 > 0.99)\) from 0.01 µg/mL to 10 µg/mL (0.1 to 100 µg/mL for fluconazole), precision (CV < 15% at 7 concentrations) and a high degree of accuracy when cross-compared to reference clinical samples \((r^2 > 0.98)\).

---

Wednesday 5:00 PM
Poster #42 in Exhibit Hall

**Analysis of Tramadol and Its Three Desmethyl Metabolites in LCMS Using High Resolution and Accurate Mass Spectrometry. Monitoring in Clinical Toxicology**

*Claudio De Nardi - Thermo Fisher Scientific (claudio.denardi@thermofisher.com)*

- A new LC-MS method for quantitation of tramadol and the three metabolites O-desmethyltramadol, N-desmethyltramadol and O,N-didesmethyltramadol in human plasma is described. Sample preparation was based on liquid-liquid extraction. Mass spectrometric analysis was performed on an Exactive Plus (Thermo ScientificTM) using electrospray ionization. Data were acquired in full scan MS in positive mode at a resolution of 70,000 at m/z 200. The method was successfully validated in the concentration range 10-2000 ng/mL; accuracy, precision and total extraction recovery were also evaluated. This method was applied to quantify the analgesic in plasma and also evaluate metabolites ratios in some clinical intoxication cases.

---

Wednesday 5:00 PM
Poster #43 in Exhibit Hall

**A Study of Stability, Robustness and Time Efficiency of a New HPLC and a New Tandem MS**

*Jason Lai - Thermo Fisher Scientific (jason.lai@thermofisher.com)*

- Stability, robustness and time efficiency of HPLC-tandem MS are three major challenges in laboratories where a large number of samples are analyzed routinely. Here we report a study of a new design of two channels HPLC and a new design of tandem mass spectrometer to address these three challenges. A total of 1241 crashed synthetic serum samples spiked with alprazolam and isotopic internal standard were analyzed continuously in 60 hours, with additional 25 QC samples inserted. On-line turboflow column help removing sample matrix. RSD% of retention time and concentration was observed at 0.94%, 2.02%, respectively.
Estradiol - Investigation of Two Sample Preparation Procedures for Quantitative Analysis by LC-MS/MS
Michal Svoboda and Ursula Turpeinen
Michal Svoboda - Tecan Schweiz AG (michal.svoboda@tecan.com)

Sample preparation of Estradiol (E2) for LC-MS/MS analysis was investigated using the AC Extraction Plate™ featuring TICE™ (Tecan Immobilized Coating Extraction) technology in comparison to a Liquid-Liquid-(LL)-extraction procedure. Using the AC Extraction Plate workflow quantifiable signals for E2 were obtained down to levels around 500pmol/l of E2 on an ABSciex 4000 LC-MS/MS system while less serum was required compared to LL-extraction. For these concentrations the workflow offers the possibility of complete automation with walk-away capability. For levels below 500pmol/l of E2 an additional evaporation/reconstitution step was added to enhance signal intensity.

Performance Evaluation of Serum 25-hydroxyvitamin D2 and 25-hydroxyvitamin D3 Using PerkinElmer MSMS Vitamin D Kit
Hee-Jung Chung - Cheil General Hospital & Women's Healthcare Center (vivid.hee@gmail.com)

We evaluated the performance of the recently introduced PerkinElmer vitamin D kit. Accuracy, precision, linearity, LLOQ, recovery and carry-over of MSMS Vitamin D kit were evaluated. The MSMS Vitamin D kit was found to produce intra-assay and inter-assay CV of less than 6% for precision and showed a bias of less than 5%. The vitamin D kit displayed linearity in the range of 25OHD levels of 4.5-150 ng/mL, and the LLOQ for 25OHD was 0.38 ng/mL. The RIA measurements of 25OHD showed a correlation of y=0.9931x+0.2216 (r²=0.74) with LC-MS/MS values. This LC-MS/MS assay of 25OHD3 and 25OHD2 showed an excellent performance from the application of the MSMS Vitamin D kit. Assays using the MSMS Vitamin D kit are considered as more standardized methods that enable quicker and more accurate analysis than other existing methods and help reduce inter-laboratory variation.

25-Hydroxy-Vitamin D- Which Sample Preparation Technique Offers the Best and Most Effective Results
Rory Doyle - Agilent Technologies, Inc (rory_doyle@agilent.com)

25-Hydroxyvitamin D can be analyzed by liquid chromatography triple quadrupole mass spectrometry. Using a LC/MS/MS analytical method for the quantitation of 25-Hydroxyvitamin D2 and D3 by QQQ, sample preparation techniques such as protein crash, liquid-liquid extraction, supported liquid extraction and solid phase extraction were evaluated and compared based on their ease of use, analyte recovery, post-extraction cleanliness and overall effectiveness. The sample preparation methods achieved the required sensitivity, specificity and capability of quantitating the analytes over a relevant dynamic range. Excellent reproducibility was observed for all compounds (CV < 5%) with calibration curves displaying linearity with an R² > 0.995. LLE offered the best overall effectiveness as well as cost but the other techniques presented equivalent results and effectiveness.

Analysis of Serum Testosterone and Androstenedione for Clinical Research Using Either Manual Or Automated Extraction
Dominic Foley - Waters (dominic_foley@waters.com)

Here we evaluate a UPLC/MS/MS method for the measurement of serum testosterone and androstenedione enabling investigation of metabolic dysfunction for clinical research. An analytically selective method was developed using a mixed-mode Solid Phase Extraction (SPE) sorbent in 96-well plate format. Either manual or automated extraction was employed, providing flexibility in sample preparation options. Analysis was performed using an ACQUITY UPLC® I-Class system, samples were injected onto a 2.1 x 50 mm Waters ACQUITY UPLC HSS C18 SB column using a water/methanol/ammonium acetate gradient and quantified with a Waters Xevo® TQD mass spectrometer. For Research Use Only, Not for Use in Diagnostic Procedures.
Simultaneous Determination of 5 Steroids in Serum Using LC-MS/MS for the Diagnosis of Congenital Adrenal Hyperplasia

Hyeon Ju Oh - Samsung Medical Center (hyeonju.oh@samsung.com)

We developed and validated more specific and selective method for measurement of serum cortisol, 21-deoxycortisol, 11-deoxycortisol, 4-androstenedione and 17-hydroxyprogesterone using LC-MS/MS. The steroids were extracted with methyl-tert-butyl ether and separated by using Kinetex XB C18 column and Water-methanol gradient as mobile phase. The five steroids were measured in MRM mode with positive electrospray mode. The method showed good precision, specificity, sensitivity and linearity. It is expected that more specific method presented might be a useful tool for the diagnosis and follow up of CAH patients.

High-Throughput Validated Method for the Quantification of Rufinamide in Serum Using Ultra Fast SPE-MS/MS

Loralie Langman - Mayo Clinic (langman.loralie@mayo.edu)

A fast, sensitive and specific method has been developed and validated for the quantitation of rufinamide in serum. This method utilizes an online SPE extraction using a Rapidfire 300 system and detection with an Agilent 6490 MS/MS using electrospray ionization in positive ion mode. The assay is linear from 0.5 – 60.0 µg/mL with an r²= 0.9997. The intra-day and inter-day assays (n=20) showed CVs of <8% and sample comparison samples showed good correlation demonstrated by a slope= 0.9916 and r²= 0.9739. This robust method for the quantitation of rufinamide offers cycle times of <20 seconds per sample.

iST: Sample Preparation for High Throughput Clinical Proteomics

Nils A. Kulak - Max Planck Institute of Biochemistry (kulak@biochem.mpg.de)

Rapid and robust workflows are crucial for day-to-day clinical applications. Especially sample preparation procedures are time consuming and limit the overall technical reproducibility of MS-based proteomics. Here we present the in-StageTip (iST) method for streamlined sample processing of complete proteomes. This simplified 3-step procedure is performed in a single, enclosed volume and allows peptide pre-fractionation in a high-throughput fashion. Applying the procedure to the cancer cell line HeLa allowed us to estimate copy-numbers of 9,667 proteins with excellent reproducibility (R² = 0.97) in quadruplicates measurements. The in-StageTip method allows high-throughput applications with near complete proteomic coverage of highly complex samples.

LC-MS of Chiral Hydroxycarboxylic Acids

Roland Wohlgemuth - Sigma-Aldrich (roland.wohlgemuth@sial.com)

Optically active hydroxycarboxylic acids which have been related to inherited and acquired diseases are of great interest for biomedical research and applications in clinical metabolomics. LC-MS methods for the direct separation of the D- and L-enantiomers of a series of chiral 2-hydroxycarboxylic acids and 2-hydroxyglutaric acids, without the need for derivatization, have been developed. The chiral differentiation and quantification of (S)-2-hydroxyglutaric acids and (R)-2-hydroxyglutaric acids is not only important for the analysis of inborn errors of metabolism like the D-2-hydroxyglutaric aciduria type I and type II as well as L-2-hydroxyglutaric aciduria, but also for oncometabolite analysis in gliomas and glioblastomas.

Identification of Bruch’s Membrane Composition by Imaging Mass Spectrometry

Hannah Bowrey - The Medical University of South Carolina (bowrey@musc.edu) -- *Young Investigator Awardee*

Identification of the molecular constituents involved in Bruch’s membrane changes is necessary for understanding age-related macular degeneration (AMD). By utilizing MALDI-IMS, we determined the spatial localization of molecules present in Bruch’s membrane of an AMD patient and a control patient. We characterized regions abundant in the autofluorescent extracellular material, drusen, as well as features corresponding to lesions in the posterior pole. AMD had a specific molecular signature distinct from normal aging. These data show that imaging of Bruch’s membrane by MALDI-IMS will be a useful tool for the identification of the molecules responsible for diagnostically relevant clinical features of AMD.
Improving Turnaround Times for Trace Element Screening of Hip Replacement Patients Using the CSols Links for LIMS System and Thermo X Series ICP-MS Spectrometer

Kevin Jones - CSols (kevin.jones@csols.com)

Metal-on-Metal (MoM) hip replacement devices are used extensively to help patients with hip damage caused by arthritis or fracture. In 2012 the UK’s MHRA issued an alert advising that chromium and cobalt whole blood screening should be undertaken on all patients with MoM hip replacements. Faced with a large increase in Co/Cr testing to meet the demand for screening the Supra-Regional Trace Element Assay Service laboratories in Guildford deployed CSols’ Links for LIMS software to electronically report results analysed on their X Series ICP-MS spectrometers to the Clinisys’ WinPath LIMS system, reducing transcription and saving analysis times.
Posters: THURSDAY

Thursday 2:00 PM
Poster #1 in Exhibit Hall
Development of a LC-MS/MS-Method for the Determination of Colistin and Colistin Methanesulfonate and Application to Plasma-Samples of Critically Ill Patients
Matthias Weber - MVZ LaborDiagnostik Karlsruhe (matthias.weber@labor-karlsruhe.de)

- A LC-MS/MS method was developed for the determination of colistin and colistin methanesulfonate (CMS) in plasma samples of critically ill patients. More than 800 patient-samples have been analyzed. The sample preparation includes the extraction and protein precipitation with TFA/isopropanol using polymyxin B as internal standard. CMS was determined by hydrolysis prior to the determination of total colistin. The analysis was performed using ESI in positive mode. Special problems concerning standardization, stability and extraction yield will be addressed. PK-Data are derived from the measurement of patient samples under renal replacement therapy and will be compared with already published results.

Thursday 2:00 PM
Poster #2 in Exhibit Hall
Metabolomics Approach to the Study of Allergic Disease in Paediatric Research
Irene Costa - Department of Woman and Children’s Health (irene.costa.1@studenti.unipd.it) -- *Young Investigator Awardee*

- Metabolomics characterized all metabolites in a biological sample. Since allergy has a high incidence in children, we apply metabolomics and mass spectrometry to the study of metabolites present in urine to highlight the possible markers. We recruited 25 children: positive (15) and negative (10) to allergy. The analysis was performed by mass spectrometry coupled to Ultra Performance Liquid Chromatography with two chromatographic columns, the samples were analysed by ESI positive and negative and the data were processed by multivariate statistical analysis; that revealed 4 variables are particularly significant of witch two were able us to predict the response to the test.

Thursday 2:00 PM
Poster #3 in Exhibit Hall
High-Throughput Metabolomics in the Epidemiological Study of Metabolic Disease
Luke Marney - Medical Research Council Human Nutrition Research (luke.marney@mrc-hnr.cam.ac.uk)

- At the MRC HNR Lipid Profiling and Signalling group, we are performing high-throughput liquid chromatography and mass spectrometry analysis in large-scale epidemiological studies (>5000 samples ~ 600 per week). We aim to elucidate the involvement of metabolic pathways in the progression and diagnosis of metabolic disease through the detailed profiling of lipids and other metabolites. Currently, two epidemiological cohorts are being investigated with different chromatography and mass spectrometry approaches. While having similar aims for the elucidation of important metabolic pathways for metabolic disease, the scaling of different instrumental and data processing methods requires careful consideration of a few critical details.

Thursday 2:00 PM
Poster #4 in Exhibit Hall
Quantitative Androgen Profile in Plasma Using Online SPE in Combination with UPLC Tandem Mass Spectrometry
Martijn van Faassen - University Medical Center Groningen (h.j.r.van.faassen@umcg.nl) -- *Young Investigator Awardee*

- The use of mass spectrometric based assays for the determination of steroids is finding its way into the clinical laboratory as the bar for steroid testing is continually being raised. Improved accuracy and sensitivity enhance the clinical use of these biomarkers and routinely applicable methods using generic chromatographic procedures are needed. In this light we developed an LC-MS/MS method for the combined quantification of the androgens: progesterone (P), dehydroepiandrosterone (DHEA), 17-á-hydroyprogesterone (17OHP), testosterone (T), androstenedione (A) and dihydrotestosterone (DHT) in plasma with limited hands-on sample preparation. Total run-time was 7 min. Intra- and inter-assay analytical variation were <10% for all steroids. Linearity in the calibration range for each respective steroid was excellent (r2 >0.99).
Thursday 2:00 PM
Poster #5 in Exhibit Hall
**Rapid, Fully-automated Plasma Clozapine and Norclozapine Analysis Using AC Extraction Plate Technology and Isotopic Internal Calibration MS/MS**

*Lewis Couchman - King's College Hospital* (lewis.couchman@nhs.net) -- *Young Investigator Awardee*

- The analysis of plasma clozapine and N-desmethylclozapine (norclozapine) for therapeutic drug monitoring (TDM) purposes is well-established. Liquid-liquid extraction combined with isotopic internal calibration provides flexible and robust analytical methodology. To further develop sample processing fully-automated sample preparation using novel AC Extraction PlatesTM and a robotic liquid-handling platform (both Tecan Schweiz AG) has been adopted. Clozapine, norclozapine, and deuterated internal calibrators were simultaneously extracted from plasma samples (approximately 20 minutes/96 samples) and extracts were analysed directly using strong cation-exchange LC-MS/MS. The total LC analysis time was 4 minutes.

---

Thursday 2:00 PM
Poster #6 in Exhibit Hall
**Development of an LC-MS/MS Method for Separate Quantification of 25-hydroxyvitamin D3, 3-epi-25-hydroxyvitamin D3 and 25-hydroxyvitamin D2 in Human Serum**

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

- An LC-MS/MS method was developed for simultaneous quantification of (3-epi-)25-(OH)D3 and 25(OH)D2 in human serum using PFP column chromatography followed by SRM registration using +ESI-MS/MS. Accurate measurement was achieved by use of separate calibration curves and SIL-IS for each compound and was checked from measurement of samples with NIST RMP assigned values. Sample preparation consisted of PP followed by SPE. Inter-assay precision was less than 7.5% for all metabolites; LLOQ were 1, 1 and 2 nmol/L and linearity were 1-500, 1-200 and 2-500 nmol/L for 25(OH)D3, 3-epi-25(OH)D3 and 25(OH)D2, respectively. The PFP method showed minimal bias to the NIST RMP.

---

Thursday 2:00 PM
Poster #7 in Exhibit Hall
**Therapeutic Drug Monitoring (TDM) of Various Types of Antibiotics by a Single Multi-purpose LC-MS Method**

*Matteo Conti - S.orsola-Malpighi Hospital Central Laboratory* (matteo.conti@aosp.bo.it) -- *Young Investigator Awardee*

- LC-MS is the method of choice for therapeutic drug monitoring of a variety of drugs, including antibiotics. Despite methods for the search of a number of antibiotics in food matrices are present in the literature, no LC-MS method is published for multi-drug quantitation of high impact antibiotics in the blood of patients treated with these drugs. We developed, validated and applied to clinical research cases an original, high throughput LC-MS method for the simultaneous analysis of cephalosporins, carbapenems, aminoglycosides and other classes of antibiotics in blood plasma of patients. The method has currently been put in clinical use for the TDM of these drugs in various clinical settings in hospitals of our region. It is apparently providing clinicians with a helpful tool for the management of severely ill patients suffering infections by various types of drug-resistant life-threatening germs.

---

Thursday 2:00 PM
Poster #8 in Exhibit Hall
**Fast and Robust LC-MS/MS Method for Determination of the Alcohol Biomarker Phosphatidylethanol (PEth) in Whole Blood Using Automated Extraction**

*Anders Blomgren - University Hospital of Lund* (Anders.Blomgren@skane.se)

- Phosphatidylethanol (PEth) is a direct alcohol biomarker with higher sensitivity and specificity than other indirect alcohol biomarkers used, e.g. GGT, CDT. There is also a correlation between reported alcohol intake and PEth-concentration in the blood. PEth is formed in the cell membrane of the erythrocytes only when ethanol is present in the blood. LC-MS/MS is a necessity because of the many forms of PEth, with similar retention time and mass, present. The most abundant form, PEth 16:0/18:1, was used for quantitation. This poster presents the whole method, from sample preparation to LC-MS/MS detection together with the validation results.
An Innovative Variable-energy Electron Ionisation Technology Applied to GC-TOF MS Metabolomics Applications

Warwick Dunn - University of Birmingham (w.dunn@bham.ac.uk)

Traditionally, GC-MS instrumentation is operated at a single electron energy of 70 eV to maximise ionisation efficiency. However, this often results in significant fragmentation and loss of the molecular ion signal. The presence of the molecular ion can substantially increase the confidence in metabolite identification. Recently, a new and innovative variable-energy electron ionisation source, Select-eV, has been marketed by Markes International to allow data acquisition at both high (70eV) and low (<15eV) energies with no loss in sensitivity. The presentation will compare GC-MS data acquired at energies of 14eV and 70eV and assess the applicability of applying this novel methodology for the study of mammalian biofluid metabolomes.

Screening for Psychotropic Medical Drugs in Serum using Ion Trap MS – Customizing a Screening Approach to Specific Needs in the Lab

Jürgen Kempf - Institute of Forensich Medicine (juergen.kempf@uniklinik-freiburg.de)

Prescription volumes of psychotropic medical drugs increased over the last years and so did their occurrence in cases of intoxication or driving under the influence of drugs. The aim of this project was to develop a screening method for these compounds in serum by customizing the ToxtyperTM screening approach. Serum samples fortified with low therapeutic concentrations of 105 compounds and several samples of authentic cases were analyzed using data dependent acquisition of spectra to evaluate the method. For the majority of compounds automatic identification of low therapeutic levels could be shown, making the screening suitable for clinical and forensic applications.

An Automated LC-Ion Trap MS Screening for Synthetic Cannabinoids

Laura Huppertz - Institute of Forensic Medicine (laura.huppertz@uniklinik-freiburg.de)

Due to the high potency of synthetic cannabinoids, hyphenated and sensitive mass spectrometry is required for the detection of these drugs in biological specimens. This project aims at developing and implementing an automated screening procedure for the detection of synthetic cannabinoids in serum using a liquid chromatography-ion trap-MS system and a spectra library-based approach. In the process of method development a new ion-source type and its effect on the ionization efficiency of the investigated synthetic cannabinoids was evaluated and compared to a conventional ESI-source. All compounds could automatically be identified in human serum at concentrations of 0.5 ng/mL or less.

Studying the Effect of Natural Genetic Variation on Protein Abundance in C. elegans

Kapil Dev Singh - University of Zurich (kapil.singh@uzh.ch)

Complex diseases (eg cancer) are caused by a combination of genetic and environmental factors, including lifestyle. Many of the signaling pathways involved in these diseases are conserved among species and also present in Caenorhabditis elegans a microscopic nematode. To study the influence of natural genetic variation on the abundance of proteins involved in signaling pathways, we used selected reaction monitoring and quantitative trait loci mapping. We analyzed recombinant inbred lines generated from the two genetically divergent C. elegans wild-type strains Bristol N2 and Hawaii CB4856. Our data suggest that protein levels are under strong evolutionary control than transcript levels.
Thursday 2:00 PM  
Poster #13 in Exhibit Hall  
Preeclampsia Risk Stratification Early in Pregnancy: Conversion of a Promising Metabolomics Discovery into a LC-MS Based Clinical Assay  
Liz Bond - Metabolomic Diagnostics (liz.bond@metabolomicdiagnostics.com)  
‣ Basic metabolomics research has uncovered that combinations of blood borne metabolites can risk-stratify women early in pregnancy according to their risk of developing pre-eclampsia later in their pregnancy. Since then, a company has been established which is dedicated to translating this finding into a tool for health care providers and pregnant women. A targeted approach is being developed whereby ca. 40 metabolites are (semi-) quantified using liquid chromatography-tandem mass spectrometry. An update on the method development progress as well as an overview of the clinical studies lined-up to verify and validate the pre-eclampsia risk stratification test will be discussed.

Thursday 2:00 PM  
Poster #14 in Exhibit Hall  
Plasma Metanephrines by LC-MS/MS: Method Development, Validation and Application in a Tertiary Referral Centre  
Sarah Pitkin - UCL Hospitals NHS Foundation Trust (sarah.pitkin@nhs.net) -- *Young Investigator Awardee*  
‣ A novel LC-MS/MS method for the simultaneous quantification of normetanephrine, metanephrine and 3-methoxytyramine was developed and validated. The assay displayed acceptable precision and sensitivity. Comparative sample analysis (n=215) with the LC-MS/MS method at Newcastle Upon Tyne Hospitals NHS Foundation Trust, showed a bias of +141pmol/L for normetanephrine (r²=0.97) and +26pmol/L for metanephrine (r²=0.98). The assay was consistently within the acceptable performance limits of the RCPAQAP plasma metanephrines EQA scheme for all three analytes. The assay was implemented for the diagnosis and monitoring of catecholamine-secreting tumours and retrospective review of the results revealed that the diagnostic cut-offs implemented were appropriate.

Thursday 2:00 PM  
Poster #15 in Exhibit Hall  
Application of Multiple Protease Digestion with Shotgun Protein Sequencing De novo Approach to the Characterization of Hemoglobin Variants  
Jane Yang - University of California, San Diego (jyy011@ucsd.edu) -- *Young Investigator Awardee*  
‣ Hemoglobin variants may be related to pathologies. To characterize hemoglobin variants, we digested hemoglobin with trypsin, lysC, and wild type and mutant alpha lytic proteases, acquired data-dependent LC-MS/MS spectra on an AB SCIEX TripleTOF 5600, and subjected the data to shotgun protein sequencing (SPS) with meta-contig assembly. As proof of concept, the analysis of human hemoglobin samples consistent with HbAE and HbAS/HbSS included contigs that contained the E26K and the E6V mutations, corroborating the HPLC results for samples consistent with hemoglobin E and S trait, respectively. Overall coverage was 90.8% for hemoglobin alpha chain and 94.6% for beta.

Thursday 2:00 PM  
Poster #16 in Exhibit Hall  
Quantitative Target Metabolomics Using LCMS/MS Improves the Diagnosis of Vitamin B12 Deficiency and Saves Huge Cost and Time  
Rima Obeid - University Hospital of the Saarland (rima.obeid@uks.eu)  
‣ Early diagnosis of vitamin B12 deficiency can prevent irreversible complications. Plasma metabolite, methylmalonic acid (MMA) and active-B12 have made their way into modern routine laboratories to replace the traditional assay of total B12 determination. MMA was measured in a 2-step-algorithm after total or active-B12 in 1034 samples. MMA analysis reduced false negative results that were produced using total or active-B12 alone. Plasma MMA levels were explained by diet, renal function and supplementation. A new LC-MS/MS assay for MMA is comparable to the reference GC-MS assay. It is considerable cheaper and takes up less time from sample preparation to reporting results.
Thursday 2:00 PM
Poster #17 in Exhibit Hall
**Development of a Turboflow™-LC-MS/MS Method for Determination of 17-Hydroxyprogesterone in Human Serum**

*Jacopo Gervasoni - Policlinico Gemelli (jacopo.gervasoni@unicatt.it)*

Despite characterized by high rate of positive results the more widespread methods for 17-OHP quantification are the immunometric ones. We have developed a TurboFlow™-LC-MS/MS method using a Vantage triple quadrupole spectrometer (Thermo Scientific) equipped with an atmospheric pressure chemical ionization source. Method was fully validated and results compared with radioimmunoassay (RIA) currently used in our laboratory. The method was linear from 0.02 ng/mL to 50 ng/mL. Total imprecision was lower than 5%. The Bland-Altman plot indicates an overestimation of RIA method with respect to TurboFlow™-LC-MS/MS method. The method, is rapid, sensitive and then suitable for routine purpose.

Thursday 2:00 PM
Poster #18 in Exhibit Hall
**Quantitative Phosphoproteomics Analysis of Malignant Ovarian Tumors in Mice by LC-MS and Labelling with Tandem Mass Tags**

*Changde Zhang - Xavier University (czhang1@xula.edu)*

Ovarian cancer ranks the fifth in cancer deaths among women. Mass spectrometer based phosphoproteomics analysis can provide important insight in understanding the molecular mechanism in this disease development process. In our study, C57BL/6 mice were challenged with MOSE IG-10 cell line for producing later stage ovarian cancer. The malignant tumors were then lysed, reduced, alkylated, digested, and labeled with 6-plex tandem mass tag reagents. The labelled phosphopeptides were enriched with TiO2 column and were analyzed on a LTQ-Orbitrap mass spectrometer coupled with a nano flow HPLC. We identified several proteins with enhanced phosphorylation activity in malign ovarian cancer.

Thursday 2:00 PM
Poster #19 in Exhibit Hall
**A Fast and Effective Approach for the Analysis of Urinary Cortisol, Cortisone, Prednisolone and Prednisone Using SPE and LC-MS/MS**

*Sean Orlowicz - Phenomenex (seano@phenomenex.com)*

The existing methods for the quantification of cortisol, cortisone, prednisolone and prednisone are very diverse. While liquid-liquid extraction, protein precipitation and “dilute and shoot” procedures offer quick and dirty methodologies, these same methodologies risk increases in instrument down time and analytical column costs. We evaluated a variety of silica-based and polymer-based SPE sorbents, each of which provides a different retention mechanism, including; hydrophobic, anion-exchange, pi-pi interactions, and any combination thereof. The evaluation showed that a modified polymeric sorbent, with a unique elution solvent has been found to be a robust, reproducible and cost effective solution for the laboratory, while providing a LLOQ of 10 ng/mL in human urine, for all four corticosteroids.

Thursday 2:00 PM
Poster #20 in Exhibit Hall
**Next Generation Plasma Collection Technology for the Clinical Analysis of Temozolomide by HILIC/MS/MS**

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

A novel approach has been developed for the quantitative determination of circulating drug concentrations using a plasma extraction technology. Plasma extraction was achieved by applying a blood sample to a laminated membrane stack which allowed plasma (or non-red cell matrix) to flow through the asymmetric filter whilst retaining the cellular components of the blood sample. This technology has the potential for a simplified clinical sample collection including the finger prick approach. Plasma separation card technology was applied to the quantitative analysis of temozolomide (an oral imidazotetrazine alkylating agent used for the treatment of Grade IV astrocytoma, an aggressive form of brain tumour) in blood samples by HILIC/MS/MS.
Maximizing Triple Quadrupole Mass Spectrometry Productivity Through the Automated Use of an Expanded Dual-Channel HPLC System with Online Sample Cleanup

Kevin McCann - Agilent Technologies (kevin_mccann@agilent.com)

This work explores increasing mass spectrometer productivity through the automated use of an expanded dual channel high performance liquid chromatography system. The complete, integrated LC/MS/MS system is comprised of a triple quadrupole mass spectrometer coupled to a configurable HPLC system, all controlled by a single software application. A previously developed method for the analysis of 25-OH vitamin D has been used for testing the capabilities of this new instrument. By staggering injections on parallel streams and switching between the two streams at the appropriate time, throughput of the integrated expanded system can double the throughput of the standard method.

TICE – an Innovative, Easy-to-automate Extraction Technique for Small Molecule Analytes from Biological Fluids for LC-MS/MS Analysis

Roland Geyer - Tecan Switzerland AG (roland.geyer@tecan.com)

Tecan Immobilized Coating Extraction™ (TICE™) – a sample preparation technique for LC-MS/MS analysis – uses a simple to automate plate format for analyte extraction from biological fluids. This extraction device was applied for extraction of various 25-hydroxyvitamin D (25OHD) metabolites from serum at a robotic liquid handling system. A LC-MS/MS method was developed for quantitation. The AC Extraction Plate™ was found to be suitable for extraction of 25OHD3/2, their epimeric forms and the metabolite 24R,25-(OH)2D3. Within a set of 47 human serum samples significant amounts of 3-epi-25OHD3 were detected in infants. TICE™ enables automated extraction of various 25OHD metabolites with different polarity.

Rapid and Simple Confirmation and Quantification of 11-Nor-Δ9-Tetrahydrocannabinol-9-Carboxylic Acid (THC-COOH) in Human Urine by 2D-LC-MS/MS

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

Cannabinoids commonly detected compounds in toxicology screening programs and workplace drug testing. Urine is tested for 11-nor-Δ9-tetrahydrocannabinol-9-carboxylic acid (THC-COOH) including its ester-glucuronides. Traditionally this has involved hydrolysis, SPE, derivatisation and GC-MS detection. We sought to replace this with a rapid 2D-LC-MS/MS method. Samples were hydrolysed by NaOH directly in the injection vial, neutralised and injected into the 2D-LC-MS/MS with a total runtime of 2.2 min. The assay was validated over 5-1000 ng/ml with minimal matrix effects. It performed well on external quality control samples and is to be used for >60 samples/day for medical screening and workplace confirmations meeting AS/NZS 4308:2008 standards.

Validation and Implementation of MALDI-TOF: A Quick and Easy Method for Bacterial Identification from Clinical Samples

Manar Mashhadani - Northampton General Hospital (manar.mashhadani@nhs.net) -- *Young Investigator Awardee*

The Department of Microbiology at Northampton General Hospital used clinical samples to evaluate the performance of the Bruker Biotyper MALDI-TOF-MS system for the routine identification of bacterial and yeast isolates from cultures compared to conventional identification methods. The results validated microbial identification using MALDI-TOF and support the replacement of existing identification methods. Because of its simplicity, speed, and accuracy, the MALDI-TOF whole cell approach promises to become a standard method of bacterial identification in clinical laboratories. Related to this, the project developed the workflow in the laboratory and looked at the turnaround time and cost associated with the implementation.
Thursday 2:00 PM
Poster #25 in Exhibit Hall

**Developments Towards High-throughput Plasma Proteomics Platform for the Clinic**  
*Garwin Pichler - Max Planck Institute of Biochemistry (pichler@biochem.mpg.de)*

- Fast and in-depth proteomics of blood samples has been a long-standing but unachieved goal. Here we apply a novel sample-preparation pipeline in combination with high-throughput LC-MS measurement technologies to identify and accurately quantify important clinical in short mass spectrometric measurements. Preliminary results demonstrate a depth of more than 600 proteins in less than 2 h of LC-MS time. Very short gradients (10 min) still enabled measurements of more than 200 proteins, including 42 FDA-approved biomarkers. These developments contribute to opening plasma proteomics up for routine, quantitative analysis of patient samples in clinical settings.

Thursday 2:00 PM
Poster #26 in Exhibit Hall

**High-throughput LC-MS/MS Analysis of Immunosuppressants in Whole Blood Using On-line SPE and Automated Sample Preparation**  
*Silvia Bächer - Recipe GmbH (baecher@recipe.de)*

- For accurate, sensitive and fast therapeutic drug monitoring (TDM) of immunosuppressants in clinical routine analysis, RECIPE has developed its ClinMass® LC-MS/MS Complete Kit, advanced - Immunosuppressants in Whole Blood (MS1100). High-throughput LC-MS/MS analysis can be realized using liquid handling systems and two-dimensional LC-MS/MS. The method shows outstanding validation results for all analytes. Close agreement of results was found for clinical samples which were processed applying automated and manual sample preparation. High throughput TDM enables preparation of 96 samples <45 minutes. Full automation is realized which significantly increases sample traceability and process security very well suited for clinical routine analysis.

Thursday 2:00 PM
Poster #27 in Exhibit Hall

**A Simple High-throughput SPE Method to Support the Biomonitoring of Phthalate Metabolites in Human Urine Prior to LC-MS/MS**  
*Lee Williams - Biotage GB Limited (lee.williams@biotage.com)*

- An SPE-LC-MS/MS method to quantify nine phthalate metabolites in human urine was developed. To facilitate the sample preparation of glucuronidase-treated urine samples prior to LC-MS/MS analysis, three sorbent chemistries (ISOLUTE ENV+, ISOLUTE Myco, EVOLUTE ABN) were evaluated. We found ISOLUTE ENV+ to be most suitable for the efficient and reproducible recovery of phthalate metabolites in human urine. The run time for 40 samples and 8 calibrators was 30 minutes. The optimized method allowed for LODs in the range of 0.05-0.2 ng/mL with at least four orders of magnitude in linear dynamic range for all analytes.

Thursday 2:00 PM
Poster #28 in Exhibit Hall

**Targeted Quantitation of Insulin and Its Therapeutic Analogs**  
*Ravindra Chaudhari - Thermo Fisher Scientific (rav.chaudhari@thermofisher.com)*

- Detection and quantification of insulin and its analogs has become paramount for medical and athletic doping. Traditional assays lack the ability to differentiate insulin and insulin analogs due to the lack of selectivity. Therefore, a Mass Spectrometric Immunoassay was developed. Capitalizing on conserved sequences, a single antibody is used to simultaneously enrich for insulin and insulin therapeutics, while LC/MS enables differentiation of the sequence variances. A robust clinical research assay able to concurrently measure multiple insulin analogs, providing a 15 pM lower limit-of-quantification and a dynamic range of 15-960 pM, is demonstrated.

Thursday 2:00 PM
Poster #29 in Exhibit Hall

**Identification of Marinobufagenin in Plasma as a Promising LC-MS Assay for Preeclampsia Risk Assessment**  
*Charline Lenaerts - UMONS (charline.lenaerts@umons.ac.be)*

- Marinobufagenin (MBG) is a bufadienolide cardiac inotrope which has a growing interest in the early diagnosis of volume expansion-mediated hypertensive states such as preeclampsia. This endogenous compound inhibits the α1 isoform of Na+,K+-ATPase, resulting in hypertension and natriuresis. The enhanced production of MBG in preeclamptic patients has been described, and demonstrated the need for a sensitive analytical method to detect MBG in plasma at low levels. Currently, only marinobufagenin-like material has been found in humans. The identification of marinobufagenin in non-pregnant human plasma utilising a LC-MS assay will be presented, leading to a promising perspective concerning the preeclampsia risk assessment.
Thursday 2:00 PM  
Poster #30 in Exhibit Hall  
**Development of SPME-LC-MS/MS Method for Concomitant Extraction of Rocuronium Bromide and Tranexamic Acid from Plasma**  
*Barbara Bojko - University of Waterloo (bbojko@uwaterloo.ca) --- *Young Investigator Awardee*  
† The presented work shows new method for determination of rocuronium bromide and tranexamic acid. The major challenges related to the analytical procedure are different properties of the drugs, their expected concentrations and instability of rocuronium in plasma samples. The proposed protocol is based on thin film solid phase microextraction followed by LC-MS/MS analysis. The developed approach offers high throughput of sample preparation and very good sample clean up thus improving time and quality of the data. Simplicity of the method and potential of coupling SPME device directly with mass spectrometer make the method applicable for onsite use in clinical facilities.

---

Thursday 2:00 PM  
Poster #31 in Exhibit Hall  
**A Rapid Clinical Research Method for the Simultaneous Analysis of Plasma Catecholamines and Metanephrines by Mixed-Mode SPE and HILIC LC/MS/MS**  
*Donald Mason - Waters Corporation (donald_mason@waters.com)*  
† An analytical method was developed for plasma catecholamines and metanephrines for clinical research purposes. Analytes extracted using weak cation exchange SPE were analyzed using HILIC LC/MS/MS. Extraction efficiencies and matrix effects were characterized. Replicate analyses of QC material showed imprecision (CV) and bias < 10% across the measurement range. This method enables rapid, simultaneous and accurate LC/MS/MS analysis of these analytically challenging compounds, obviating the use of reversed-phase separations employing ion-pairing reagents. For Research Use Only. Not for Use in Diagnostic Procedures.

---

Thursday 2:00 PM  
Poster #32 in Exhibit Hall  
**The Separation and Analysis of Opiates and their Glucuronide Metabolites in Urine Matrix Negating the Need for Hydrolysis During Sample Preparation**  
*Peter Christensen - Agilent Technologies (Peter.christensen@agilent.com)*  
† Opiates and their metabolites can be challenging to analyze using LC/MS due to a relatively large number of their analytes having the identical empirical mass and subsequent similar fragmentation patterns in MS/MS. The need for good chromatographic separation is therefore paramount as is the need to reduce complicated sample preparation techniques. Opiate glucuronides pose the greater separation challenge in reverse phase chromatography due to their highly polar nature and are, therefore, routinely hydrolyzed during sample preparation, a process that removes any sugar group returning the metabolite to its original parent form. This work describes a 4 minute LC/MS/MS method that eliminates the need for sample hydrolysis.

---

Thursday 2:00 PM  
Poster #33 in Exhibit Hall  
**Glycopathology of Aggressive Prostate Cancers Using N-Glycan MALDI Mass Spectrometry Imaging of FFPE Tissues and Biopsy Samples**  
*Richard Drake - Medical University of South Carolina (draker@musc.edu)*  
† A new MALDI imaging mass spectrometry workflow for simultaneous analysis of multiple N-linked glycans in standard FFPE tissue slides, tissue microarrays and biopsy cores for prostate cancers will be presented. Following antigen retrieval processing and on-tissue digestion with peptide N-glycanase, over 50 glycan species can be simultaneously detected. The approach is being applied to identify glycans that distinguish indolent from aggressive forms of prostate cancers. Methods to confirm on-tissue confirmation of glycan compositions, and efficient computational analysis workflows will also be described. The advantage of the approach, especially for heterogeneous prostate tumors, is the spatial correlation of the glycan distributions with standard pathology scoring.
Simultaneous Identification and Quantification of Triacylglycerol Species in Human Plasma by Flow Injection Electrospray Ionization Tandem Mass Spectrometry

Madlen Sander - Institute of Laboratory Medicine, Clinical Chemist (madlen.sander@medizin.uni-leipzig.de) -- *Young Investigator Awardee*

- Civilization diseases like atherosclerosis and type II diabetes are associated with elevated levels of triacylglycerol (TAG). Using conventional enzymatic methods, the fatty acid distribution in TAGs cannot be differentiated. With increasing knowledge of the effects of fatty acid distribution in TAGs, it is necessary to study the TAG molecular species. Tandem mass spectrometric detection was performed by neutral loss scans on an AB Sciex API 4000 triple quadrupole mass spectrometer with positive electrospray ionization. By coupling flow injection analysis with electrospray ionization tandem mass spectrometry, we had been able to establish a novel, reproducible and semi-quantitative method for the identification and quantification of 19 TAG molecular species in human blood plasma. Sample preparation was simple protein precipitation with toluene/methanol (1:1 v/v).

Standardized Targeted Proteomics Approach for the Simultaneous Determination of Eight Apolipoproteins in the Leipzig Heart Study

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

- Sample preparation strategies for absolute quantification of eight apolipoproteins including Apo E and J in human plasma by microLC-MS/MS using proteotypic tryptic peptides and corresponding isotope labeled peptides as internal standards were investigated to establish a standardized sample pretreatment protocol for high-throughput analysis using only 3 µL of sample material. Method validation revealed adequate lower limits of quantification as well as coefficients of variation < 13%. Method comparison with commercial immunoassays for Apo A-I and Apo B-100 in 1000 samples of the Leipzig Heart study showed good agreement. Consequently, the distribution of eight apolipoproteins in cardiovascular disease was reliably determined.

Rapid Quantification of Cortisol, Cortisone, Dexamethasone and Prednisolone in Human Saliva and Hair by Liquid Chromatography – Tandem Mass Spectrometry

Alexander Gaudl - Leipzig University (alexander.gaudl@medizin.uni-leipzig.de) -- *Young Investigator Awardee*

- Reliable determination of cortisol and cortisone concentration in saliva and hair is of interest in the assessment of stress-associated adrenocortical function. To this purpose we developed a robust method for the reliable, simultaneous quantification of glucocorticoids via LC-MS/MS, overbearing the shortcomings of immunological analysis. With excellent precision (2-7%), very good recovery rates (95-115%) and a total runtime of 4.5 min we proved the benefits of LC-MS/MS over immunoassays. Moreover, we analysed 2500 samples of the LIFE Child Depression study and demonstrated the massive impact of preanalytical factors on hair analysis, enabling proper evaluation in clinical routine diagnostics and epidemiological studies.

Online Analysis of 25-OH-vitamin D2/D3 in Plasma and Serum with the Evoq Triple Quad

Rafaela Martin - Bruker Daltonik GmbH (rafaela.martin@bdal.de)

- A robust and reliable research method to quantitate 25-OH-vitamin D2 and D3 in plasma and serum samples using the Bruker Advance UHPLC with OLE coupled to the EVOQ Elite triple quad is demonstrated. The integrated online extraction option of the UHPLC together with the ClinMass® LC-MS/MS complete kit (MS7000) provides fast and easy sample cleanup. Interlacing the online extraction and chromatographic separation reduces the overall run time to 3 minutes per sample. The calibrations showed excellent linearity with $r^2 \geq 0.999$. The assay had a very good interday and intraday precision with RSD <6.5% as well as high accuracy with bias < ±6%.
Thursday 2:00 PM
Poster #38 in Exhibit Hall
Comprehensive Drugs of Abuse Identification in Urine by LC-MSn Combined with MS Spectral Library Matching
Ulrike Burmester - Bruker Daltonics (ulrike.burmester@bdal.de)
‣ Due to the ease of noninvasive sampling, urine has become a sample of choice for drugs-of-abuse identification. Detection is traditionally achieved by immunoassays. Their simplicity and speed enable high-throughput analysis. However, immunoassays cover only a limited number of drugs. Many assays identify only drug classes producing a significant rate of false-positives due to antibody cross-reactivities. Thus, often a secondary, more specific analysis such as LC-MS/MS is required. Here we present an ion trap LC-MSn-method using full scan MS, MS2 and MS3 spectra from +ESI and -ESI polarities with retention time matching for a broad automated screening based on spectral libraries.

Thursday 2:00 PM
Poster #39 in Exhibit Hall
UPLC-MS/MS Based Activity Assay for Determination of Mevalonate Kinase
Barbara Maier - Institute of Laboratory Medicine (barbara.maier@med.uni-muenchen.de)
‣ Mevalonate kinase (MK) catalyzes the transformation of mevalonic acid to mevalonate-5-phosphate (MVAP). Mevalonate kinase deficiency is an autosomal recessive disorder, which can lead to various clinical manifestations reaching from the milder hyperimmunoglobulinemia D with periodic fever syndrome to the more severe mevalonic aciduria. The disease severity correlates closely with the residual activity of the enzyme. To characterize the in vitro activity of recombinant human MK protein variants we developed an assay, which was based on the quantification of MVAP by isotope dilution UPLC-MS/MS. MVAP was detected with high accuracy (± 2.7%). The total precision of the whole assay was 8.3%.

Thursday 2:00 PM
Poster #40 in Exhibit Hall
Sensitive 2D-UHPLC-MS/MS-Method for Simultaneous Quantification of Seven Corticosteroids to Investigate Adreno-cortical Dysfunction in Critically Ill Patients
Anna Catharina Suhr - Institute of Laboratory Medicine (anna.suhr@med.uni-muenchen.de) -- *Young Investigator Awardee*
‣ The role of adreno-cortical dysfunction in septicaemia is a widely discussed topic in clinical research worldwide. In order to improve the biochemical description of this condition a highly sensitive and very selective 2D-UHPLC-MS/MS-method was developed addressing cortisol, cortison and aldosterone as well as their four precursors (corticosterone, 11-desoxycortisol, 17-hydroxyprogesterone, 11-desoxycorticosterone). Since large clinical studies require a high-througput method we decided to apply two-dimensional chromatography with protein precipitation as the only manual step of sample preparation.

Thursday 2:00 PM
Poster #41 in Exhibit Hall
Development of an LC-MS/MS Method to Determine Insulin and Synthetic Analogs in Human Plasma
Yasin Bekkach - Laboratory of Endocrinology (y.bekkach@amc.uva.nl)
‣ Several synthetic insulin analogs are available for the treatment of diabetes. These analogs differ in some amino acids from endogenous insulin. Routine diagnostic assays for insulin, usually immunoassays on automated platforms, show highly variable results for recombinant insulin analogs. Therefore an LC-MS/MS method for the quantitative determination of endogenous and synthetic insulin forms was developed and validated. This method can be of clinical importance i.e. for patients with unexplained hypoglycemia and can provide extra information for research questions where both endogenous and exogenous insulin(s) are present.
Thursday 2:00 PM
Poster #42 in Exhibit Hall

**Drug Monitoring of Antibiotics in Critically Ill Patients**

*Johannes Zander - Institute of Laboratory Medicine (Johannes.Zander@med.uni-muenchen.de)*

- Therapeutic drug monitoring (TDM) is well established for aminoglycosides and glycopeptides. However, there is currently no TDM for various other classes of frequently used antibiotics. Substantial variability of serum concentrations of several antibiotics with often inappropriate levels have been described in previous studies on critically ill patients. Here we present our results of a prospective observational study measuring antibiotic blood concentrations in critically ill patients with infections. The variability of blood concentrations of antibiotics was evaluated by LC-MS/MS and related to preliminary therapeutic ranges. This study should help to implement a routine TDM for different antibiotics in future.

---

Thursday 2:00 PM
Poster #43 in Exhibit Hall

**A Dutch Study into the Analysis of Vitamin B6 in Whole Blood**

*Bertrand van Zelst - Department of Clinical Chemistry NA-420 (b.vanzelst@erasmusmc.nl)*

- In this study, different commercial and homemade HPLC-methods for measuring vitamin B6 in whole blood were compared with a homemade LC-MS/MS method using different sample types. The comparison of whole blood showed a proportional bias of 40% for the Chromsystems method when compared with the LC-MS/MS method whereas the INstruchemie and the homemade HPLC methods showed no bias towards the LC-MS/MS method. Surprisingly, the comparison of lyophilized blood showed no bias between methods. This lack in standardization or harmonization between methods is hampered by the absence of a reference technique or reference material for measuring vitamin B6 in whole blood.

---

Thursday 2:00 PM
Poster #44 in Exhibit Hall

**Development of a UPLC-MS/MS Method to Measure Next Generation Antiepileptic Medications in Serum**

*Sankha Basu - Brigham and Women's Hospital (sbasu2@partners.org)*

- Next generation antiepileptic medications have revolutionized the treatment of epilepsy as well as other neurological disorders. As with traditional anticonvulsant therapy, however, inter-individual variability in pharmacokinetics has increased the need for therapeutic drug monitoring for effective dosing and decreased toxicity. In this study, we developed a fast and simple stable isotope dilution UPLC-MS/MS method to measure levetiracetam, lamotrigine, gabapentin, zonisamide and topiramate in serum. A total method run time of three minutes allowed adequate separation of all analytes with sensitivity and linearity covering the relevant serum concentration range found in humans.

---

Thursday 2:00 PM
Poster #45 in Exhibit Hall

**Towards Clinically Actionable Quantification of Proteins by Mass Spectrometry: A Critical Appraisal of Bias and Imprecision for Serum Apolipoproteins A-I and B**

*Irene van den Broek - Leiden University Medical Center (LUMC) (i.van_den_broek@lumc.nl) -- *Young Investigator Awardee*"

- Test results in medical laboratories should be traceable to standards of higher order, and within predefined criteria for analytical quality. In this study, we describe a thorough evaluation of bias and imprecision, according to CLSI-guidelines EP15 and EP9, for mass spectrometry-based quantification of serum apolipoprotein A-I (Apo A-I) and apolipoprotein B (Apo B). The results provide (1) a systematic overview of the impact of trypsin digestion, calibration, internal standardization, peptide selection, LC-MS/MS performance, and matrix-effects on analytical performance, and (2) a proof-of-concept to achieve metrologically traceable results within the minimal total allowable error based on biological variation.
Quantitation of Multiplexed Serum Apolipoproteins by Stable Isotope Dilution- Multiple Reaction Monitoring-LC-MS/MS

Nico Smit - Leiden University Medical Center (LUMC) (n.p.m.smit@lumc.nl)

An LC-MS/MS method was developed for simultaneous measurement of six serum apolipoproteins: apo A-I, B100, C-I, C-II, C-III, and E. The analytical performance was evaluated using CLSI EP15 and EP9 protocols, demonstrating a total CVa below 15 % for all twelve peptides. In addition, LC-MS/MS results correlated well with CE-marked immunoassays for quantitation of serum apo A-I and apo B100 (R > 0.975) in 100 normo- and hypertriglyceridemic sera. No interference was found in hypertriglyceridemic sera as compared to normotriglyceridemic sera. The laboratory-developed test has potential to improve cardiovascular disease risk stratification and treatment monitoring.

Biological Variability of Plasma 5-HIAA

Joanne Adaway - University Hospital South Manchester (jo.adaway@uhsm.nhs.uk)

Plasma 5-hydroxyindole acetic acid (5-HIAA) measurement is used in the diagnosis and management of serotonin-secreting neuroendocrine tumours (NET). In order to calculate the reference change value of an assay it is important to know the biological variability of the analyte, so we carried out a study to determine this. Plasma was collected from 37 post-menopausal women beyond the age of 50. Eight samples were collected over 4-8 weeks with a day interval of 6 days. The analytical CV of the assay was 4.9%. The mean inter-individual CV was 29.47%, the mean intra-individual CV was 13.46%, with an overall variance of 32.77%. The reference change interval for plasma 5-HIAA is 23.8 nmol/L. This will be of use when monitoring the treatment of patients with serotonin-secreting NET.

Development and Validation of a Candidate Reference Method for the Measurement of Serum Cortisol Using Supported Liquid Extraction and UPLC-MS/MS

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

We present a novel candidate reference method for the measurement of serum cortisol using SLE and UPLC-MS/MS. National quality assurance (QA) schemes have demonstrated that cortisol measurements are inaccurate and display high variability. This method utilises certified reference material to ensure results are traceable to the International System of Units (SI). The analytical quality specifications have been validated against a panel of 34 certified European Reference Materials (ERM-DA451). The excellent accuracy and precision of this method qualify it as a candidate reference method that can be utilised to underpin QA schemes by assigning traceable target values.

An Evaluation of Biphenyl Chemistry to Aid in High-Throughput Bioanalytical LC-MS/MS Analyses

Hansjoerg Majer - Restek Corporation (Hansjoerg.Majer@restek.com)

LC-MS/MS has become commonplace in the bioanalytical laboratory, as it can produce high throughput, high data quality analyses. The use of fully porous UHPLC and superficially porous HPLC columns are often used to increase the efficiency and peak capacity, and to decrease the analysis times. While these column advancements do impact efficiency, they do not directly impact selectivity or retention, which are the prominent parameters to analyte resolution. We investigated a biphenyl based column chemistry to determine the effect on sample throughput and data quality in bioanalytical separations. From these applications we hope to demonstrate the advantages of the biphenyl-based stationary phase on throughput, data quality, sensitivity, and compound resolution.
Thursday 2:00 PM  
Poster #50 in Exhibit Hall  
A Method for the Determination of Desomorphine, Heroin, Methadone, Buprenorphine and Metabolites in Urine Using LC/MS QQQ  
Christopher Benton - Agilent Technologies (christopher_benton@agilent.com)  
Analytical measurement of opioid panels commonly include a number of compounds such as heroin, methadone and buprenorphine. Research methods with sufficient flexibility are of value to respond to the need to measure new compounds resulting from clandestine production. Desomorphine, also known as Krokodil, is an emerging synthetic opioid, sometimes used as a heroin substitute. This poster describes the development of an LC/MS QQQ research method that rapidly quantifies desomorphine together with heroin, buprenorphine, methadone and their metabolites 6-acetylmorphine, norbuprenorphine and EDDP over a concentration range of 1-5000 ng/ml. Precision data, LLOQ and calibration linearity will be reported for each analyte.

Thursday 2:00 PM  
Poster #51 in Exhibit Hall  
A Spatially-aware Peak Picking Method for MALDI-imaging Data from TOF and FTICR Mass Analyzers  
Jan Hendrik Kobarg - Steinbeis Innovation Center SCiLS Research (kobarg@scils.de)  
MALDI-imaging is a spatially-resolved mass spectrometric technique which can obtain the spatial distribution of hundreds of molecules in a thin tissue section. Manual analysis is tedious since it requires visual examination of all m/z-images. We introduce a novel method that automatically detects structured m/z-values without specifying a region of interest and without manual visual examination. Our parameter-free and unsupervised method provides fully-automatic selection of spatially informative m/z-images. The method also complements spectrum-wise peak picking increasing its sensitivity, as it does not depend on peak intensity, but is based on the novel measure of spatial chaos of the corresponding m/z-image.

Thursday 2:00 PM  
Poster #52 in Exhibit Hall  
Measuring Protein Analyte Panels in Dried Blood Spots (DBS) Using an Automated SISCAPA Workflow  
Selena Larkin - SISCAPA Assay Technologies (selenalarkin@siscapa.com)  
An automated SISCAPA method was devised using a Bravo liquid handling robot to extract proteins from dried blood spots, digest with trypsin and enrich specific proteotypic peptide analytes in 96-well plate format. This was followed by LCMS quantitation versus stable isotope labeled internal standards. A set of high-abundance proteins of plasma and red cells was measured to yield surrogate hematocrit and total plasma load and establish a normalization algorithm. Two 11-plex panels of clinically-proven cardiovascular and inflammation markers were measured from a single DBS punch across longitudinally-collected patient samples. The panel proteins span 8 orders of magnitude in abundance, with lowest present at 1-10 ng/mL range. Up to 400 patient samples were processed and analyzed in a working day.

Thursday 2:00 PM  
Poster #55 in Exhibit Hall  
Impact of Pre-analytical Variations in Metabolic Phenotyping  
Therese Koal - BIOCRATES Life Sciences AG (therese.koal@biocrates.com)  
MS-based metabolic phenotyping is a powerful tool with a variety of application areas in life sciences. Blood samples are a key resource for the biomedical research, but there is no consensus on the sample type, especially the choice of anticoagulant. This study compared the concentrations of 186 endogenous metabolites in different plasma types and serum, collected from the same person at the same time, by the application of the AbsoluteIDQ p180 Kit, a MS-based quantification assay. Our study showed that the different methodologies used for blood sampling did not affect the analytical performance. However, significant differences in the metabolomic profiles were found between the sample types. In conclusion, the sample type should be clearly defined and maintained throughout a study. And, thus, it is not recommended to compare data obtained from different samples types.

Thursday 2:00 PM  
Poster #56 in Exhibit Hall  
Multiplexing Multiple Methods to Maximize Workflow Efficiency in LC-MS Laboratories  
Marta Kozak - ThermoFisher (marta.kozak@thermofisher.com)  
Many research laboratories run several different LC-MS methods in series on a single channel LC-MS system. If the methods involve different columns and mobile phases, the changeover is time consuming, labor intensive and increases the risk of mistakes and contamination. A four-channel UHPLC system multiplexed into one mass spectrometer permits parallel batches of up to four different methods utilizing unique columns and mobile phases to be completed in a fraction of the time and effort.
Posters: FRIDAY

Friday 2:00 PM
Poster #2 in Exhibit Hall
**Increased Throughput for the Analysis of Delta-9-THC in Oral Fluids Using Triple Quadrupole Mass Spectrometry Coupled with an Automated Dual-Channel HPLC System**
Kevin McCann - Agilent Technologies (kevin_mccann@agilent.com)

- In this work we demonstrate increased mass spectrometer productivity through the automated use of a dual channel high performance liquid chromatography system. The integrated LC-MS/MS system is comprised of a triple quadrupole mass spectrometer coupled to a configurable dual HPLC system, all controlled by a single software. The analysis of delta-9-THC from oral fluids was used to demonstrate capabilities of this system. The new HPLC system mirrors certain components of this single stream system to provide a second stream, operating in parallel to the first stream. By staggering injections on parallel streams, throughput can double as compared to standard method.

Friday 2:00 PM
Poster #4 in Exhibit Hall
**Analysis of Cannabinoids in Whole Blood: Above and Beyond State of Art**
Alexandre Paccou - ABSCIEX (alexandre.paccou@absciex.com)

- Since the Decree-law of 22 February 1990, the Cannabis, in any form is classified as a narcotic in France. After consumption, 9-tetrahydrocannabinol (THC), the major active form, is metabolized primarily as 11OH-A9-tetrahydrocannabinol (THC-OH) and acid 11nor-A9-tetrahydrocannabinol (THC-COOH). THC is detectable within seconds after first inhalation and maximum concentration in blood is obtained in less than 10 minutes. The maximum concentration of THC-OH is generally reached in less than 30 minutes, and THC-COOH in less than 2 hours. The recommended limits of quantification are 0.5 ng/mL for THC and THC-11OH and 2 ng/mL for THC-COOH. In this workflow, we describe a new approach allowing the quantification of the three analytes respecting the new guidelines of French Analytical Toxicology Society (SFTA) on Cannabis quantitation in whole blood.

Friday 2:00 PM
Poster #6 in Exhibit Hall
**Overestimation of 25-hydroxyvitamin D3 by Increased Ionisation Efficiency of 3-epi-25-hydroxyvitamin D3 in LC-MS/MS Methods Not Separating Both Metabolites**
Jody van den Ouweland - Canisius-Wilhelmina Hospital (j.v.d.ouweland@cwz.nl)

- Using an LC-MS/MS method for separate quantification of (3-epi-)25-(OH)D3 and 25(OH)D2 we could show that in LC-MS/MS methods, not resolving 25(OH)D3 from 3-epi-25(OH)D3, the 3-epi-25(OH)D3 contribution not only is overestimated from its co-elution with 25(OH)D3, but that an additional 37% overestimation is caused by differences in ionisation efficiency between both isomers. Due to its increased ionization efficiency, the contribution of the 3-epi-25(OH)D3 metabolite to the total 25(OH)D3 concentration is significantly overestimated in MS methods that do not resolve 3-epi-25(OH)D3 from 25(OH)D3 which may compromise its use in infant samples, known to have significant amounts of 3-epi-25(OH)D3.

Friday 2:00 PM
Poster #7 in Exhibit Hall
**Characterizing the Chemotypic Landscape of Cystic Fibrosis Sputum**
Vanessa Phelan - University of California, San Diego (vphelan@ucsd.edu) -- *Young Investigator Awardee*

- In cystic fibrosis (CF) patients, mutations within the CF transmembrane conductance regulator (CFTR) lead to decreased mucociliary clearance and accumulation of thick and sticky bronchial mucus providing a nutrient rich environment for opportunistic pathogens to flourish. It is well established that microbes produce a number of organism specific molecules to interact with their environment. These specialized metabolites function as toxins, antibiotics, redox active molecules and nutrient scavenging entities. With the advent of modern mass spectrometry techniques, we can begin to unravel the hidden chemical communication in complex microbial communities. Herein, we describe the application of MS/MS based molecular networking to identify key Pseudomonas aeruginosa metabolites in clinical CF sputum samples.
The application of proteomic techniques to disease states affords the opportunity to identify deregulated pathways that contribute to pathogenesis. These discoveries in turn may lead to new therapeutic targets, as well as biomarkers that aid in diagnosis, prognosis and the prediction of treatment responses. Osteoarthritis (OA) is a disease of all joint structures and synovial fluid (SF) may represent a synthesis of inputs from these structures. We compared the proteomic profile of knee joint SF from patients with early and late stage OA to unaffected controls by mass spectrometry. In our recent publication, 66 proteins were reported as differentially represented in healthy vs. OA. Pathway analysis identified three biologic processes among these proteins: the complement and coagulation systems and the acute phase response. Early and late OA manifested a very similar proteomic profile.

Isoprenoid pathway metabolites such as the isoprenoidphosphates and isoprenoid-pyrophosphates are central metabolites leading to sterols, dolichols, ubiquinones, prenylated natural products and proteins. It is therefore of much interest to develop new high-performance separation methods which are able to determine the whole range of isoprenoid- (pyro)phosphates. New HPLC-MS methods for the simultaneous analysis of the stereoisomeric dimethylallyl- and isopentenyl-(pyro)phosphates respectively have been established using the cyclo-dextrine-based stationary phase. Whereas the separation of these polar single unit isoprenoid-(pyro)-phosphates is based on selective ionic interactions on a cyclodextrin-based stationary phase, the separation of the larger isoprenoid-(pyro)phosphates has been achieved with IPC-UHPLC-MS.

Rapid turnaround of immunosuppressant samples, as with all therapeutic drug monitoring, is necessary in a clinical research laboratory. Additionally, as financial and environmental concerns become more prevalent, heavy use of solvents for high flow LC-MS/MS methods, particularly those involving online extraction, can be an issue. Microflow LC offers a solution to these concerns, whilst greatly enhancing on column sensitivity and chromatography performance, reducing sample consumption and improving system robustness and uptime. As the sample injection volume is minimized, robustness and reproducibility of the entire method is dramatically increased as matrix effects are significantly reduced.

Mass spectrometry (MS) can be used to characterize intact immunoglobulin light chains (ILC). In this study we qualitatively and quantitatively evaluated serum kappa and lambda total light chains in normo-, hypo- and hyper-gamma patients using immunonephelometry and MS on an ABSciex-TripleTOF 5600 (microLC-ESI-Q-TOF-MS). A pre-analytical purification step for IgG using Melon Gel (Thermo Scientific) was used for the MS method, and IgG recovery estimated. Nephelometric quantitation and microLC-ESI-Q-TOF-MS calculation of the kappa/lambda ratio were compared yielded an equation y=1.4x+1.37 and R2 of 0.64. The results encourage us to pursue MS approaches to detect and quantitate ILC abnormalities in the study of monoclonal gammopathies, polyclonal light chains elevation in autoimmune diseases, immunodeficiencies, and post-vaccination.
**Friday 2:00 PM**
**Poster #15 in Exhibit Hall**

**Evaluation of a New Commercial Complete Solution for New Born Screening and Comparisons with Established Methods**

*Daniel Blake - ABSCIEX* (daniel.blake@absciex.com)

- LC-MS/MS is a powerful tool for the study of metabolic disorders. The simultaneous analysis of amino acid and acylcarnitine panels can provide information on over 40 metabolic disorders such as Phenylketonuria (PKU) and Medium Chain Acyl-CoA Dehydrogenase Deficiency (MCAD). We present here a discussion of the results obtained using a new commercially available kit for the LC-MS/MS analysis of these compounds, with performance comparison and evaluation with existing commercial kits on the market today.

---

**Friday 2:00 PM**
**Poster #16 in Exhibit Hall**

**Single Step Separation of Plasma from Whole Blood without the Need for Centrifugation Applied to the Quantitative Analysis of Warfarin**

*Alan Barnes - Shimadzu* (alan.barnes@shimadzu-mso.com)

- Achieving a dried plasma sample from whole blood without the need for centrifugation creates new opportunities in blood sampling strategies for quantitative LC/MS/MS bioanalysis. Dried plasma samples were generated by gravity filtration of a whole blood sample through a laminated membrane stack allowing plasma (or what may be referred to as a non-red cell matrix) to be collected, dried, transported and analysed by LC/MS/MS. The process of gravity filtration takes 3 minutes to complete and a further 15 minutes to air-dry the 2.5uL plasma sample. The dried plasma sample disc can then be removed from the base card and stored, transported or analysed. This novel plasma separation technology was applied to the quantitative LC/MS/MS analysis of the coumarin anticoagulant, warfarin, in blood samples.

---

**Friday 2:00 PM**
**Poster #18 in Exhibit Hall**

**Comparison Between Different Process Methods of Arachidonic Acid in Plasma**

*Xiaohua Chen - Bonna-Agela Technologies* (xiaohua_chen@agela.com.cn)

- This poster was a comparative study of different sample pretreatment processes to extract Arachidonic Acid (AA) from plasma, which involved 96-well protein precipitation plate, Brand W 96-well plate and Cleanert MAS-M 96-well plate. Protein precipitation method enjoyed a convenience due to its minimum procedures, but its recoveries of AA were 129.32%~149.02%, implying the worst purification effect which caused the matrix enhancement on mass spectrum. The recoveries of AA on Brand W 96-well plate were 5.45%~70.15%, while the recoveries of Cleanert MAS-M 96-well plate were 99.19%~106.38 which ensured an extraction procedure without reconstitution to support a rapid, high throughput assay of AA in plasma.

---

**Friday 2:00 PM**
**Poster #20 in Exhibit Hall**

**25-Hydroxy-Vitamin D- Which Ionization Mode and Column Type Gives the Best Analytical Results**

*Rory Doyle - Agilent Technologies, Inc* (rory_doyle@agilent.com)

- 25-Hydroxyvitamin D can be analyzed by liquid chromatography triple quadrupole mass spectrometry with Electrospray or Atmospheric Pressure Chemical Ionization using various column types. LC/MS/MS analytical methods were developed for the quantitation of 25-Hydroxyvitamin D2/D3 by QQQ in ESI and APCI modes to evaluate which was more sensitive and specific. Using protein crash sample preparation, various column types were evaluated and compared based on their chromatographic resolution, separation, matrix effect, robustness and response. The methods achieved the required sensitivity, specificity and capability of quantitating the analytes over a relevant dynamic range. Excellent reproducibility was observed for all compounds (CV < 5%) with calibration curves displaying linearity with an R2 > 0.995. ESI mode with a Poroshell Bonus RP achieved the best overall analytical results.
Friday 2:00 PM
Poster #22 in Exhibit Hall
**Evaluation of Derivatised and Non-derivatised Methods for Analysis of Amino Acids and Acylcarnitines in Dried Blood Spots Using a Novel Triple Quadrupole Mass**

*Benedicte Duretz* - *ThermoFisher* (benedicte.duretz@thermo.com)

- Flow injection tandem mass spectrometry (FIA-MS/MS) has been routinely used for analysis of amino acids and acylcarnitines in dried blood spots from newborns in order to detect inborn errors of metabolism. We evaluated a commercially available kit and an in-house developed assay, on both derivatised and non-derivatised methods, using a novel Thermo Scientific™ TSQ Endura™ Triple Quadrupole MS. The exceptional sensitivity and specificity of TSQ Endura™ MS SRM mode enabled us to reach or exceed the LOQ of amino acids and acylcarnitines well accepted in the industry, prove robust and precise method, on either derivatised or non-derivatised method.

Friday 2:00 PM
Poster #26 in Exhibit Hall
**Evaluating ToxFinder™ New Data Processing Software in Targeted Screening Applications Implemented on LC/MS Mass Spectrometers**

*Marta Kozak* - *ThermoFisher* (marta.kozak@thermofisher.com)

- Targeted screening applications are commonly used in forensic toxicology laboratories. Screening applications utilize all kind of mass spectrometers, each with advantages and limitations. User friendly software that fully utilizes screening data and simplifies data interpretation is a critical component. Here we evaluate new data processing software which supports two screening methods or orbitrap mass spectrometers and one with SRM transitions on triple quadrupole mass spectrometers. The software provides intuitive data processing workflow, rapid data review and custom reporting. It supports requirements for relative retention time and semi-quantitative assessment, as well as output for easy data transfer to laboratory LIMS system.

Friday 2:00 PM
Poster #28 in Exhibit Hall
**Comparison of SPE Approaches for the Extraction of Thyroid Hormones: T3, RT3 and T4 Prior to LC-MS/MS Analysis**

*Lee Williams* - *Biotage GB Limited* (lee.williams@biotage.com)

- Thyroid hormones are extremely important physiologically and involved in many biological processes such as growth and development. Reverse T3 is only produced at low levels compared to T3 and most notably T4 so it is important to have a robust assay capable of detecting these low levels. This poster evaluates the performance of various resin-based ion exchange SPE chemistries for the extraction of thyroid hormones prior to LC-MS/MS analysis. Method performance will be investigated from an analyte recovery perspective with particular emphasis on extract cleanliness.

Friday 2:00 PM
Poster #29 in Exhibit Hall
**Evaluation of New Prelude™ SPLC System Coupled with Endura™ Triple Quadrupole MS Using Analysis of Testosterone and Cortisol in Biological Matrixes**

*Claudio De Nardi* - *ThermoFisher* (claudio.denardi@thermofisher.com)

- Growing demand for cost-efficient and easy to use LC-MS solutions has resulted in development of new instrumentation now available to laboratories. We evaluated the Prelude SRLC system coupled to an Endura triple quadrupole mass spectrometer for the analysis of testosterone and cortisol in plasma and urine, respectively. The Prelude system offers cost efficient methods by providing on-line sample clean up, low solvent consumption, and increased sample throughput with dual channel multiplexing. Additionally, syringe pumps give reproducible gradients which improve data quality. Data obtained met analytical laboratory requirements for LOQ, linear range, precision and accuracy. No matrix effects were observed.
New methods for rapid detection of antibiotic resistance are a timely topic in clinical microbiology. We evaluated the use of a novel quantitative MALDI-TOF MS approach for rapid detection of antibiotic resistances directly from patient derived blood cultures. A total of 30 consecutive blood cultures microscopically diagnosed with Gram-negative rods were tested for resistance against Cefotaxime and Ciprofloxacin. Our classification into susceptible and resistant strains was in complete accordance with the conventional method (E-test). In combination with direct identification of the pathogen the novel method could be a promising option for early therapeutic guidance in septic patients.

A LC-MS/MS method was developed allowing now the determination of total homocysteine (tHcy) in Dried Blood Spots (DBS) and in plasma/serum as well. While the LC-MS/MS method is the same, there are just slight changes in sample preparation for both matrices. It includes reduction of protein-bound or dimerized homocysteine, followed by extraction for DBS samples and protein precipitation for plasma/serum samples, respectively. With an injection interval of only 1 minute, the fast, easy and reliable determination of tHcy in DBS and Plasma/ Serum is now possible.

Since the first approval of a therapeutic monoclonal antibody drug in the late nineties, over 400 therapeutic monoclonal antibodies (mAbs) were undergoing in preclinical development or clinical evaluation. Due to high specificity and efficacy, therapeutic mAbs have become a major class of therapeutic compounds for the treatment of cancers, infectious diseases, allergies, inflammation, and auto-immune diseases. To date, immunoassays, such as ELISA, remain the most sensitive, specific and selective technologies used for quantifying mAbs in biological fluids. However, it requires specific developments for each mAb, suffers from matrix-effect and is species-dependant, what is time-consuming, costly and not really suited for early phases of developments. Thus, the development of innovative and fit-for-purpose MS-based quantification methods represents a challenge for pharmacokinetics studies.

Recently a method based on stable isotope labelling by amino acids in cell culture was introduced for rapid detection of antibiotic resistance. Instead of visible growth the novel method measures bacterial protein biosynthesis in the presence of antibiotics. So far the method has been described to be successful for several bactericidal substances. This proof of principle study demonstrates that the method works equally well for bacteriostatic antibiotics (Linezolid, Erythromycin, Clindamycin). 49 Staphylococcus spp. isolates were analysed, where clear distinction between resistant and susceptible isolates was achieved within an incubation time of 1.5 h.
The Use of a New Meta-calculation Software for Automated Data Processing of Tandem MS for Inborn Error Metabolism Research

Jason Lai - Thermo Fisher Scientific (jason.lai@thermofisher.com)

- The use of Tandem MS for inborn error metabolism research started in 1990. With advancement of Tandem MS technology, more compounds can be detected and quantified using a simple sample introduction method such as flow injection with isotopic internal standards. A major challenge is to process a large quantity of generated data efficiently without transcription errors. We compared the result from a new meta-calculation software with a manual process on 100 donor samples for a total 3200 calculations. The new software significantly reduced processing time from hours to minutes and showed agreement with the manual calculations.

Metabolic Phenotyping: A New Tool Enabling Drug Response Prediction and Personalized Medicine

Therese Koal - Biocrates Life Science (fabio.polato@biocrates.com)

- Metabolic phenotyping provides a surrogate marker of individual genetic disposition, somatic changes, acquired adaptations and exposition to pathogens, environment and alimentation. Allowing disease diagnosis and subclassification, treatment prediction, drug response and identification of pathophysiological processes of different diseases. Therefore enabling an early diagnosis and prognosis of diseases yet lacking of precise diagnostic parameters. Biocrates’ AbsoluteIDQ® Kit solutions and the in-house lab service enable the standardized, quantitative, and quality controlled analysis of over 630 relevant metabolites. These data allow metabolic pathway analyses and identification of potential drug targets as well as their mode of action. Combined with other “omics”-techniques, metabolic phenotyping provides a system biological diagnosis for an improved personalized medicine approach.

The Utilization of In Vivo and In Situ Solid Phase Microextraction in Clinical Analysis

Barbara Bojko - University of Waterloo (bbojko@uwaterloo.ca) -- *Young Investigator Awardee*

- Solid phase microextraction (SPME) was used as a novel approach for in vivo and in situ extraction of drugs and endogenous metabolites from lung during in vivo and ex vivo lung perfusion (IVLP and EVLP, respectively). The concentration profile of the chemotherapeutic and its distribution in the organ as well as changes of global metabolome were analyzed with the used of LC-MS(ESI) platforms. Due to the minimum invasiveness and easy direct coupling of SPME probe with mass spectrometer the method shows great potential to be used on-site as rapid diagnostic tool.

Evaluation of the Bruker Biotyper and VITEK MS MALDI-TOF MS systems for the identification of difficult-to-identify bacteria isolated from clinical specimens

Erin McElvania - Children’s Medical Center (erin.mcelvania@childrens.com)

- The purpose of this investigation was to evaluate the analytical performance characteristics of matrix-assisted laser desorption/ionization time-of-flight mass spectrometry (MALDI-TOF MS) for the identification of unusual organisms. We evaluated the accuracy of two MALDI-TOF MS systems, bioMérieux VITEK MS (database v2.0) and Bruker Biotyper (software version 3.0), for the identification of the most difficult and/or unusual microorganisms isolated from clinical specimens. Our study included 174 bacterial isolates recovered from clinical cultures at Barnes-Jewish Hospital, St. Louis, MO, USA from 2009 to 2013, representing 50 genera and 52 species. We found there was no significant difference in the number of organisms identified to the genus level, species level, unidentified, or misidentified by the two MALDI-TOF MS systems.
Friday 2:00 PM
Poster #44 in Exhibit Hall

**Analysis of Aldosterone in Plasma for Clinical Research Using Automated Extraction**

*Dominic Foley - Waters* (dominic_foley@waters.com)

- Here we evaluate a UPLC/MS/MS method for the measurement of plasma aldosterone for clinical research purposes. An analytically sensitive method was developed using a mixed-mode Solid Phase Extraction (SPE) sorbent in 96-well plate format. Automated extraction was employed, enabling high throughput of samples. Analysis was performed using an ACQUITY UPLC® I-Class system, samples were injected onto a 2.1 x 50 mm Waters ACQUITY UPLC BEH Phenyl column using a water/methanol gradient and quantified with a Waters Xevo® TQ-S mass spectrometer to obtain the optimal sensitivity. For Research Use Only, Not for Use in Diagnostic Procedures.

Friday 2:00 PM
Poster #46 in Exhibit Hall

**Measurement of C3-epimer Form of 25-hydroxyvitamin D3 in Korean Children**

*Hee-Jung Chung - Cheil General Hospital & Women's Healthcare Center* (vivid.hee@gmail.com)

- Using PerkinElmer MSMS Vitamin D Kit using LC-MS/MS, we established and validated measurement method of C3-epimer-25OHD3(3-EpiD3). We measured 3-EpiD3 in 91 Korean children by this method. This assay showed high accuracy, precision and sensitivity. Measurements of 3-EpiD3 ranged from less than LoQ level(1.30 ng/mL) to 3.35 ng/mL. Proportion of 3-EpiD3 among 25OHD3 ranged from 3% to 38%(median 6%). Before 12 mo of age, high 3-EpiD3 level more than 2.0 ng/mL was often(27%) observed(median 1.6 ng/mL). While after 12mo, 3-EpiD3 decreased overall showing median level of 1.3 ng/mL and high 3-EpiD3 level more than 2.0 ng/mL was rare(5%). We can successfully measure 3-EpiD3 with PerkinElmer MSMS Vitamin D Kit using LC-MS/MS. And 3-EpiD3 level of Korean children was relatively high in infants and it showed decreasing change with time.

Friday 2:00 PM
Poster #48 in Exhibit Hall

**Serum 5-HIAA – a Better Marker of Neuroendocrine Tumour Than Urine 5-HIAA**

*Joanne Adaway - University Hospital South Manchester* (jo.adaway@uhsm.nhs.uk)

- We compared urine and serum 5-HIAA to assess whether serum 5-HIAA could replace urine 5-HIAA in the diagnosis and monitoring of neuroendocrine tumours (NET). We measured 5-HIAA in 233 paired serum and urine samples from 26 healthy volunteers and 151 patients with known NET Linear regression showed a correlation coefficient of 0.64. The sensitivity of urine 5-HIAA was 75.8%, with a specificity of 96.2%. The sensitivity of serum 5-HIAA was superior to this at 80.3%, and the test had a specificity of 100%. We have demonstrated a strong correlation between serum and urine 5-HIAA results. The clinical sensitivity of serum 5-HIAA is superior to that of urine 5-HIAA, as is the specificity. This supports the assertion that serum 5-HIAA is a better test than urine 5-HIAA for the diagnosis and monitoring of NET.

Friday 2:00 PM
Poster #49 in Exhibit Hall

**Highly Automated, High Precision Tryptic Digestion and SISCAPA-MS Quantification of Human Plasma Proteins Using the Agilent Bravo Platform**

*Selena Larkin - SISCAPA Assay Technologies* (selenalarkin@siscapa.com)

- We report here the development of a highly reproducible, automated “addition only” method for tryptic digestion of plasma, followed by bead-based SISCAPA enrichment of target proteotypic peptides, driven through a simple software user interface. The combined protocols, taking as little as four hours total, were coupled with high throughput LC-MRM for multiplexed quantitation of plasma proteins over a wide range of abundance. The complete workflow was demonstrated for suitability for routine quantitation of target plasma proteins based upon sensitivity, multiplexing capability, scalability, reproducibility, and throughput. These characteristics make the workflow an appropriate platform for routine measurement of clinically relevant proteins.

Friday 2:00 PM
Poster #50 in Exhibit Hall

**Ultra-high Throughput Quantitation of Immunosuppressants in Human Whole Blood**

*Peter Christensen - Agilent Technologies* (Peter.christensen@agilent.com)

- The purpose of this study was to evaluate the usability of the Agilent RapidFire-MS/MS system using solid phase extraction (SPE) cartridges instead of chromatography columns for the quantitative analysis of cyclosporine A, everolimus, sirolimus and tacrolimus in a clinical research laboratory. Results of more than 1100 samples were compared between LC-MS/MS system and the RapidFire 366 system coupled to an Agilent 6460 QQQ mass spectrometer. Sample preparation and measurement were performed using a commercial kit, imprecision and accuracy were investigated analyzing three concentration levels of commercial QC samples.
Determination of Insulin-Like Growth Factor-1 in Plasma by HRAM LC/MS for Clinical Research

Christopher Benton - Agilent Technologies (christopher_benton@agilent.com)

- High Resolution Accurate Mass (HRAM) Liquid Chromatography Mass Spectrometry (LC/MS) is ideally suited for the rapid analysis of biomolecules. A highly sensitive and specific HRAM LC/MS method has been developed for the quantitation of Insulin-Like Growth Factor-1 (IGF-1). This method uses a simple sample preparation combined with an online sample cleanup procedure coupled to a high resolution accurate mass quadrupole time-of-flight mass spectrometer. The described method achieves the required functional sensitivity and is capable of quantitating IGF-1 over a sufficiently wide dynamic range at R² > 0.999. Intra- and inter-day CVs are below 5 and 10% respectively.

LC-MS Analysis of Non-labeled Amino Acids on a Novel Mixed-mode HPLC Column

Itaru Yazawa - Imtakt Corporation (yazawa@imtakt.com)

- There are several established methods for analyzing amino acids, but each of these methods has disadvantages. The pre-labeled method has problems with derivitization efficiency and cost, while the post-labeled method is usually not compatible with LC-MS due to non-volatile mobile phases. We have developed a novel amino acid separation column for LC-MS/(MS) which can analyze the complete array of 55 amino acids: 1) high throughput separation with Leu/Ile separation in 5min, and 2) simple gradient separation in 1 min or 10min. In addition, no prederivitization is required, and a standard LC-MS/(MS) system is sufficient for the analysis. In this presentation, we will show the sensitivity and application for amino acids in serum.
## Presenter Index

### A
- Adaway, Joanne 88, 97
- Alexandrov, Theodore 45
- Armengaud, Jean 49
- Asturina, Giuseppe 50
- Aurand, Craig 68

### B
- Bächler, Silvia 72, 83, 95
- Balog, Julia 48
- Barney, Alan 93
- Basu, Sankha 73, 87
- Beck, Olof 51
- Bejjack, Yasin 86
- Benton, Christopher 89, 94
- Blake, Daniel 68, 92, 93
- Blomgren, Anders 46
- Bojko, Barbara 84, 96
- Bond, Liz 80
- Boos, Karl-Siegfried 46
- Borchers, Christoph 40
- Bowrey, Hannah 75
- Burckhardt, Irene 24
- Burmester, Ulrike 86

### C
- Capiau, Sara 46
- Chaudhari, Ravindra 83
- Chekmeneva, Elena 41
- Chen, Xiaohua 68, 93
- Christensen, Peter 68, 84, 97
- Chung, Hee-Jung 74, 97
- Colby, Jennifer 70
- Conti, Matteo 78
- Costa, Irene 77
- Couchman, Lewis 44, 72, 78

### D
- De Kesel, Pieter 43
- De Nardi, Claudio 73, 94

### E
- Eichhorst, Jeff 51

### F
- Fang, Min 71
- Foley, Dominic 74, 97
- Fontan, Adrian 92
- French, Deborah 70

### G
- Gaudl, Alexander 50, 85
- Gervasoni, Jacopo 81
- Geyer, Roland 40, 82
- Gori, Sadakat Ali 50
- Grant, Russell 43

### H
- Hamacher, Christina 95
- Hawley, James 88
- Heidelberger, Sibylle 69
- Holmes, Daniel 51
- Hornshaw, Martin 72
- Huppertz, Laura 79

### J
- Jensen, Berit 82
- Ji, Misuk 70
- Jones, Kevin 76
- Julian, Randall 23

### K
- Kempf, Jürgen 79
- Kerian, Kevin 49
- Koal, Therese 73, 89, 96
- Kobarg, Jan Hendrik 89
- Köhling, Rudolf 71, 92
- Kozak, Marta 70, 89, 94
- Krastins, Bryan 92

### L
- Lai, Jason 73, 96
- Langman, Loranal 75
- Larkin, Selena 48, 89, 97
- Leber, Dorothée 95
- Lenaerts, Charline 83
- Loftus, Neil 81

### M
- Maier, Barbara 86
- Majer, Hansjoerg 69, 88
- Mann, Matthias 21, 23, 24, 48
- Manna, Soumen 49
- Marney, Luke 77
- Martin, Rafaela 85
- Mashhadani, Manar 82
- Mason, Donald 72, 84
- McCann, Kevin 71, 82, 91
- McElvania, Erin 96
- Mehany, Dina 68
- Miller, Jessica 47
- Morillo, Eduardo Martinez 44

### O
- Obeid, Rima 80
- Oh, Hyeon Ju 75
- Orlovic, Sean 81
- Ouwehand, Jody van den 67, 78, 91

### P
- Paccou, Alexandre 91
- Palmer, Andrew 47
- Pawliszyn, Janusz 40
- Phelan, Vanessa 91
- Plbhi, Olivier 42
- Pichler, Garvin 83
- Pitkin, Sarah 80

### S
- Salmi, Fernanda 67
- Sander, Madlen 85
- Schmidt, Lukas 95
- Schwarz, Markus 43
- Singh, Kapil Dev 79
- Sluzak, Gary 23
- Smid, Nico 88
- Spacił, Zdenek 41
- Stephanson, Nicolas 69
- Strittmatter, Nicole 48
- Suhr, Anna Catharina 86
- Svoboda, Michal 74

### T
- Takats, Zoltan 23
- Trégoat, Virginie 42

### V
- van den Broek, Irene 87
- van Faassen, Martijn 46, 67, 77
- van Zelst, Bertrand 87
- Vogeser, Michael 42

### W
- Walch, Axel 45
- Want, Elizabeth 41
- Weber, Matthias 77
- Williams, Lee 71, 83, 94
- Wolhgemuth, Roland 70, 75

### Y
- Yang, Jane 80
- Yazawa, Itaru 98
- Yip, Ping 71

### Z
- Zander, Johannes 87
- Zekúšič, Marija 69
- Zhang, Changde 81
Select Corporate Workshops will be held in Paracelsus on the 2nd Floor on Thursday and Friday from 1-2 PM.

Thursday: Phenomenex
Friday: IsoSciences
MAP: 1st Floor - Exhibit Hall

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

Plenary Lectures, Scientific Session Presentations and Corporate Workshops will be held on the Ground Floor. Corporate Workshops will also be held on the 2\textsuperscript{nd} Floor in Paracelsus.
The variety of your clinical research demands a variety of technologies

No one analytical technology can adequately reveal everything you need to know about your sample. Bruker offers the broadest range of high performance, easy-to-use, and expertly supported analytical systems to overcome any clinical research challenge. Our proven, extremely robust GC-Triple Quads, LC-Triple Quads, Ion Traps and QqTOFs ensure confidence in your results for microbiology, biomarker discovery, tissue imaging, and drugs of abuse or drug monitoring research.

Get the right answer faster, more cost effectively, using the appropriate analytical technology for the job – Bruker’s complementary solutions for clinical research.

Visit us at MSACL, Booth 15 and on the Web at www.bruker.com

You’re not the only one who needs to trust the test results

ACCURACY THE FIRST TIME

Clinicians and patients count on the most reliable diagnostic answers. We want you to be confident that results are as timely and accurate as possible. SCIEX Diagnostics offers an in vitro diagnostics solution with exceptional assay performance that helps overcome the limitations of current testing methods. Our newly introduced assays for Vitamin D, Newborn Screening and Immunosuppressants accurately measure multiple analytes in a single run, and virtually eliminate the need for re-runs and send-outs. And not only are SCIEX Diagnostics solutions backed by over 25 years of leadership in mass spectrometry, they are surprisingly affordable, too.

Find out how SCIEX Diagnostics can help improve your accuracy, turnaround and confidence at www.sciexdiagnostics.com.

Come and visit us at MSACL, Booth 10 and 11.
Confidence in Results

Achieve greater productivity and confidence when providing laboratory-developed test results to the healthcare professionals you serve. New Thermo Scientific™ high-performance medical devices for in vitro diagnostic use—Thermo Scientific™ Prelude MD™ HPLC, Thermo Scientific™ Endura MD™ mass spectrometer, and Thermo Scientific™ ClinQuan MD™ software—help you deliver LC-MS results easily, quickly, and with more confidence.

LC-MS for in vitro diagnostic use

Visit us in booth #12 • thermo scientific.com/LCMS-IVD