The Association for
Mass Spectrometry:
Applications to the Clinical Lab

MSACL 2018 US

10th Annual Conference & Exhibits

January 21-25

Palm Springs, CA

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MSACL
Clinical Mass Spectrometry

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For over 140 years, Shimadzu has been developing instrumentation for a broad range of applications in a variety of markets. This history is rivaled only by the passion we have for the future. We encourage you to **visit us at MSACL 2018** to discover our extensive portfolio of innovative, proven products designed to address your specific laboratory workflows.

BE SURE TO ATTEND OUR WORKSHOPS:

Implementation of a Fully Integrated Automated Sample Preparation System for Routine Clinical LC-MS/MS Analysis

Wednesday, January 24th, 12:30 – 1:15 pm in the Madera Room

Presentation by Lorin Bachmann, PhD, DABCC, Associate Professor of Pathology, Co-Director of Clinical Chemistry, Virginia Commonwealth University

Simultaneous Analysis of Multiple Steroid Hormones by LC-MS/MS

Thursday, January 25th, 1:30 – 2:00 pm in the Madera Room

Presentation by David Erikson, Ph.D., Director of the Endocrine Technologies Support Core at OHSU

Find out more at Booth #15

www.ssi.shimadzu.com

The Association for
Mass Spectrometry:
Applications to the Clinical Lab

MSACL 2018 US

The 10th Annual North American Congress
of
The Association for

Mass Spectrometry:
Applications to the Clinical Lab

Palm Springs, California

January 21 - 25, 2018

Renaissance Hotel & Palm Springs Convention Center

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.

clinical mass spectrometry
cms
an international journal

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Be someone's hero.

Who knows what lies ahead? What we know is the work you do can make an impact on whatever comes next. And we share that quest with you, providing the tools and confidence to improve lives every day. Leveraging our years of experience to help advance clinical research to routine testing with the most comprehensive, most innovative mass spectrometry-based workflows on the planet. We both know, the faster the results, the faster decisions can be made. So samples to data, knowledge to answers, cancer to Alzheimer's, we never forget those samples aren't just samples. Each is a person. A person for whom your work can make all the difference in their world. **ThermoFisher.com/ClinicalResearchSolutions**

Thermo Scientific™ Q Exactive™ hybrid quadrupole-Orbitrap MS and Vanquish™ UHPLC System

Thermo Scientific™ TSQ Altis™ triple quadrupole MS and Vanquish™ UHPLC System

Thermo Scientific™ iCAP™ TQ ICP-MS

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Platirum	$17,900	thermo scientific; SHIMADZU Excellence in Science
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Bronze	$2,900	PerkinElmer For the Better
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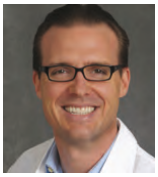

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:: Metabolomics

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:: Tissue Imaging

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Aegis Sciences Corporation
:: Cannabinoids

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Achieve greater productivity and confidence when providing laboratory-developed test results to the healthcare professionals you serve. Thermo Scientific™ high-performance LC-MS Class I medical devices for in vitro diagnostic use — Thermo Scientific™ Prelude LX-4 MD™ HPLC, 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.

Prelude LX-4 MD HPLC

Prelude MD HPLC

Endura MD Mass Spectrometer

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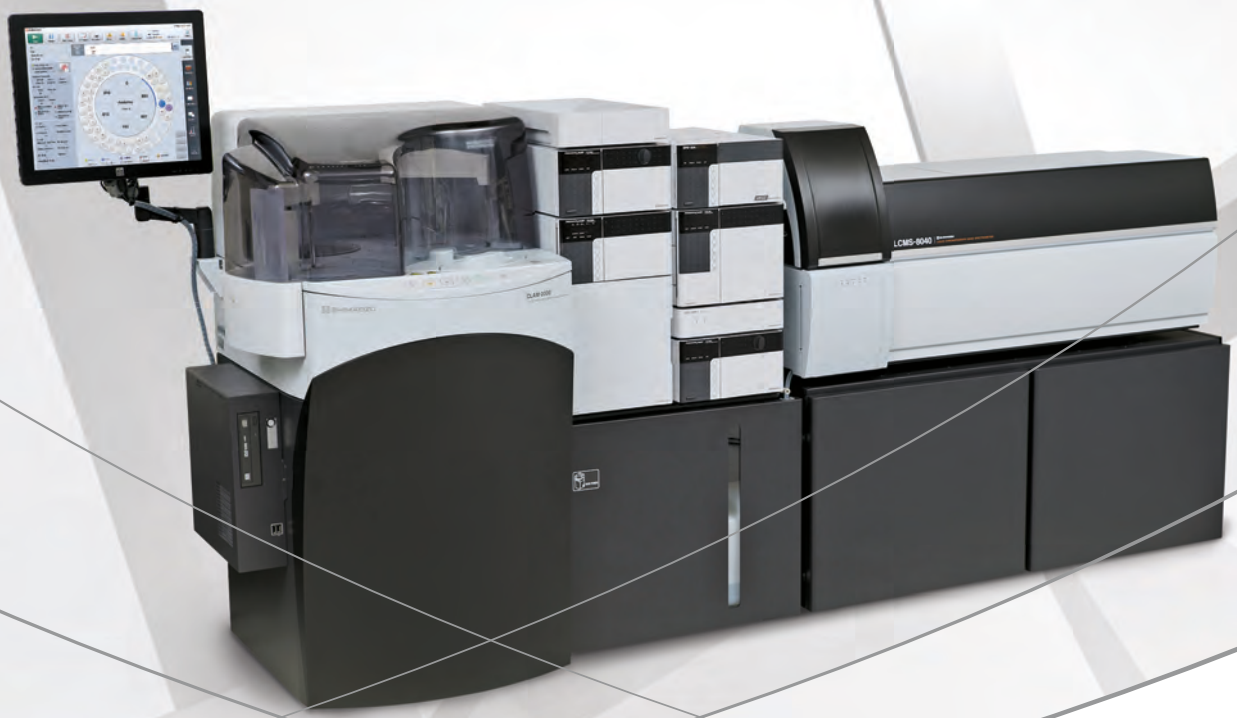

Seamless Integration of Sample Preparation to LC-MS/MS Analysis

Simplify workflows and improve lab efficiency with Shimadzu's industry-first automated sample prep module

Shimadzu's **CLAM-2000** Clinical Laboratory Automation Module is a fully automated sample prep module for LC-MS/MS that integrates common clinical sample prep workflows, such as protein precipitation and chemical derivatization, to the mass spec. By requiring no intervention from sample loading to results, it improves data reproducibility and accuracy, provides uniform pretreatment times between samples, and minimizes operator error.

Learn more about Shimadzu's CLAM-2000. Call (800) 477-1227 or visit us online at **www.ssi.shimadzu.com/CLAM**

Order consumables and accessories on-line at http://store.shimadzu.com
Shimadzu Scientific Instruments Inc., 7102 Riverwood Dr., Columbia, MD 21046, USA
For Research Use Only. Not for use in diagnostic procedures.

Key features/benefits include:

- **Offers exceptional data accuracy and reproducibility by performing all processes from pretreatment of samples to analysis automatically.**
- **Increases laboratory efficiency by processing each sample successively in parallel.**
- **Allows any level of user to prepare samples and operate the LCMS like an expert using a simplified user interface.**
- **Provides a flexible platform to suit the specific application's needs.**

It's Time to Embrace the Future of Diagnostic Accuracy

Learn more at Booth 12-13 and join our Corporate Workshops on Wednesday and Thursday at 8 AM in Madera Room 3

Introducing the new SCIEX Topaz™ System, an FDA Class I and CE-marked integrated LC-MS-based IVD system

Designed with new mass spec users in mind, the Topaz System now makes LC-MS/MS accessible to the entire hospital lab. ClearCore™ MD software is specifically designed for the clinical lab to simplify and streamline workflows and method development, enabling your lab to adopt the power of SCIEX LC-MS/MS technology to:

- Expand in-house test menus
- Reduce turn-around times
- Embrace gold standard accuracy
- Avoid costly send-out testing.

Delivering accuracy without complexity seen with traditional MS, the SCIEX Topaz System provides the confidence in test results critical to your hospital lab.

For more information visit
sciex.com/MassSpecMadeSimple

SCIEX
Diagnostics

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What couldn't be done. Until now.

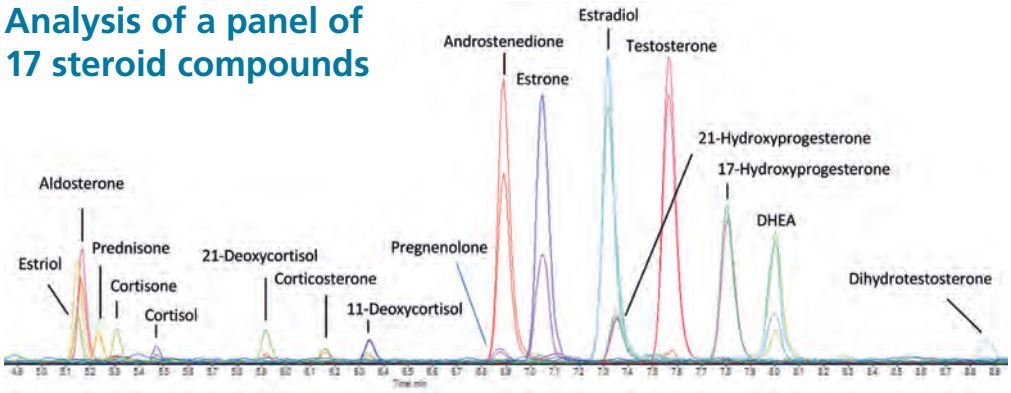
Our Fastest, Most Sensitive Mass Spec, Available as a Medical Device*

The SCIEX Citrine™ System – an *in vitro* diagnostic MS/MS system provides you with the highest performance and reliability to tackle today's difficult assays, and the versatility to address tomorrow's challenges.

- Monitor 100's of MRM transitions per analysis with uncompromised accuracy, precision, and sensitivity
- Experience faster data acquisition with 5 msec polarity switching
- Detect reliably down to picomole levels for clinically relevant biomarkers and metabolites
- Perform qualitative and quantitative analysis in a single injection with QTRAP® technology
- Enjoy the confidence of a medical device that meets the high quality and safety standards required by FDA regulations

Do everything. See everything. Citrine MS/MS – one solution for every challenge.

Analysis of a panel of 17 steroid compounds



Quantify trace levels of steroids, using rapid polarity switching to detect both positive and negative ions in a single injection.

SCIEX Diagnostics

sciex.com/diagnostics

*Product not currently available for sale pending registration and listing in the U.S. and CE marking for EU.

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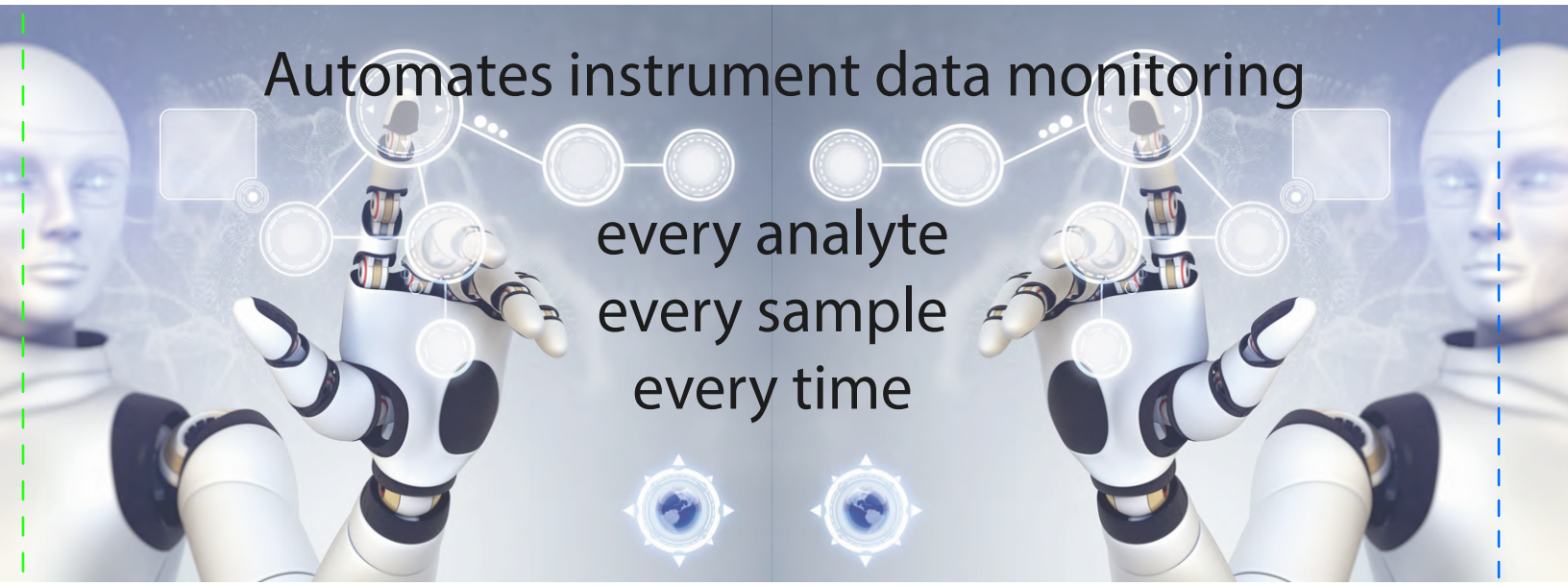
consistent and correct results



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IT'S TIME TO SET A PINT-SIZED POWERHOUSE LOOSE IN YOUR LAB.

Meet Agilent's new, revolutionary Ultivo Triple Quadrupole LC/MS. It's packed full of the same power and accuracy you'll find in the big guys but at a fraction of the size. It's on a transformative mission to reshape expectations, reinvent capabilities, and redefine what's possible when small meets powerful.

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Analytical sensitivity **and** robustness—for proteomics studies that are not sample limited!

Based on Agilent's revolutionary Jet Stream source, the Agilent Jet Stream proteomics solution achieves near-nanoflow analytical sensitivity with the robustness, reproducibility, and ease-of-use of standard-flow chromatography.

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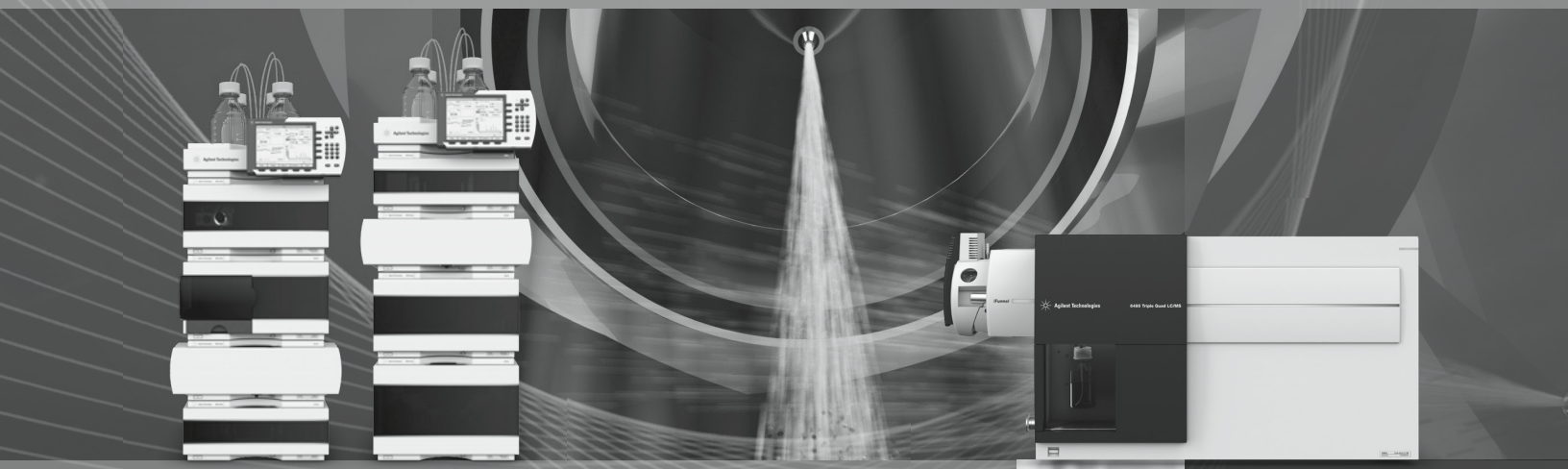

Don't miss Steve Pennington's presentation on Wednesday at 12:30pm in the Renaissance Ballroom Foyer, Room 4

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Agilent Technologies

The Triple Quad That Knows The Value Of Time

The QSight® LC/MS/MS includes unique patented technologies such as:

- **Dual Source technology** providing true multiplexing
- **StayClean™ Source** that virtually eliminates maintenance
- **Laminar Flow Ion Guide™** highly efficient field-free transmission, providing virtually no maintenance requirements

Please visit our posters on Wednesday, Jan. 24 at 1:30pm

Poster #14C – *Robustness Evaluation of the QSight® 210 MD Triple-Quadrupole Mass Spectrometer Against "Dirty" Samples*

Poster #4C – *Non-Derivatized LC-ESI-MS/MS Method for Determination of Vitamin D and 10 Steroid Hormones Using New PerkinElmer QSight® Triple Quadrupole Mass Spectrometer*

Visit PerkinElmer at Booth #8 to Learn More.

Products may not be available in all countries.
Please contact your local PerkinElmer Representative.

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For better & smarter working conditions

-15 db(A) up to -20 db(A). About 75% reduction in noise perception.

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LC-MS Solutions

From discovery to clinical utility.

Please join us at MSACL 2018!

Visit us at Booth 39/40/44 to speak with a specialist and to register for our workshops.

Workshops

Wednesday, 12:30 – 1:15 p.m. Location: Catalina, Room #2

Mass Spectrometry Approaches to the Opioid Epidemic

Speaker: Dr. Marilyn Huestis, Retired Chief, Chemistry and Drug Metabolism, NIDA
Huestis & Smith Toxicology, LLC, U.S.A.

Thursday, 8:00 – 8:45 a.m. Location: Catalina, Room #2

Comparison of Sample Purification Methods for Therapeutic Monoclonal Antibody Quantitation in Human Serum

Speaker: Dr. Mohsin el Amrani
University Medical Center, University of Utrecht, The Netherlands

Thursday, 1:30 – 2:15 p.m. Location: Catalina, Room #2

Introducing the Thermo Scientific™ Cascadion™ SM Clinical Analyzer

Speaker: Peter Cooke, Maket Development Specialist
Thermo Fisher Scientific

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thermofisher.com/ClinicalResearchSolutions

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Liquid Chromatograph Mass Spectrometer

LCMS-8060

CHANGES EVERYTHING

Shimadzu's New Triple Quad LCMS-8060 Expands the Limits of LC-MS/MS Quantitation for Applications Requiring the Highest Sensitivity

The newest model in the Ultra-Fast Mass Spectrometry (UFMS) series, the **LCMS-8060** offers an incomparable fusion of LC-MS/MS speed and sensitivity to achieve new levels of data quality.

Ultrafast Technologies

The LCMS-8060 incorporates Shimadzu's proprietary ultrafast technologies (UF Technologies) to enable:

- polarity switching time of 5 msec
- data acquisition scan speed of 30,000 u/sec
- ultra-fast MRM measurements up to 555 ch/sec

Highest Sensitivity

A redesigned UF-Qarray ion optical system increases ion transmission and signal intensity while reducing background noise for the utmost in quantitative detection.

Outstanding Durability

A robust design and easy maintenance allow highly reliable data even for high-throughput analysis of samples in challenging matrices.

Time for a change? Discover the **LCMS-8060**, the ideal solution for better data quality and higher throughput for a wide array of challenging and routine applications.

Learn more about Shimadzu's Triple Quad LCMS-8060.
Call (800) 477-1227 or visit us online at
www.ssi.shimadzu.com/8060

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General Information

Continuing Education Credits
MSACL strives to provide Continuing Education credits for the short courses and the Scientific Sessions through ACCENT by AACC. ***However***, there was a personell change at AACC in the CE department at the end of November, and there has been a bit of a delay in processing our CE request for 2018 US. It does appear they will be processed, but it might a little later than usual. We will keep you posted.

Conference Badges
Your badge constitutes your admission pass to the Conference, receptions and the Exhibit Hall. **YOU ARE REQUIRED TO 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.

If you have an **EXHIBITS ONLY** badge **YOU ARE NOT PERMITTED IN THE SCIENTIFIC SESSIONS**, except the Plenary. Violation may result in registration revokation without refund.

Yoga
Yoga will be held daily starting ***Monday*** from at 6:00 – 7:00 AM in San Jacinto in the Renaissance Hotel. MSACL will be providing a limited number of yoga mats and other related accoutrements.

Smoking
*Smoking is **prohibited** within the conference facility and outside within 50 ft of the building*.

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, in the Exhibit Hall, and during the plenary sessions

NOTE: Throughout the conference 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.

Short Course Meals on Monday and Tuesday
If you are registered for a short course, you will receive meal vouchers when you pick up your registration materials; 4 for 3-day courses and 2 for 2-day courses. These voucher(s) are for use Monday (breakfast , lunch) and Tuesday (breakfast, lunch) in the Date Restaurant located in the Renaissance Hotel. You MUST sign present the bottom part of your voucher to receive a comped meal.

The Date Restaurant is openly accessible even without a meal voucher.

Presenter Info and Guidelines

Podium Presentations

Locations: Rooms 1-6 (*i.e., Mojave, Catalina, Madera, Pasadena, Sierra, SmokeTree*), Pueblo, Chino and Andreas.

- If an individual is unable to present or does not show, the presentation time slot will be left open. ***IT WILL NOT BE FILLED BY THE NEXT SPEAKER***. The next speaker will begin presenting at his/her scheduled time.
    - **Back-Up Presenters**: If a presenter does not show, a back-up presenter may be called to fill-in the open spot. *Session Chairs, please contact registration immediately on determining that a speaker may not show so that efforts may be put in place to locate a back-up speaker*
- Speakers: Please make an effort to repeat any questions from the audience before answering.
- Podium presentations are ***20 minutes*** including Q&A.
- PC Laptops running Windows OS and Powerpoint.
- Presenters should check-in at least 15 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 may 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: *Exhibit Hall*

Posters will be placed for the entire conference starting on Tuesday at 16:00 and ending on Thursday at 17:45. Posters are only required to be attended for one hour on a selected day (specific to each poster), but are up for the duration of the congress. Please see poster abstract information for attendance details.

- Poster dimensions: 42x42 inches.
- Poster Boards are fabric.
- Push pins will be provided.

SUNDAY

08:00 18:00	Badge Pickup @ *Renaissance Foyer*
08:00 12:00	Agilent Breakfast Workshop @ *Rm 3 (Madera)*
11:00 14:00	Lunch On Your Own @ *Your Decision*
14:00 18:00	Short Courses @ *Various Rooms*
EVERY :50 MINS FOR 10 MINS	Coffee Break @ *Renaissance Foyer*
18:00 20:00	Dinner On Your Own @ *Your Decision*
18:00 22:00	Hospitality @ *Santa Rosa and/or Rocks Terrace*
18:30 20:00	Private: Scientific Committee Discussion Group @ *Pueblo*

MONDAY

06:00 07:00	Yoga @ *San Jacinto*
06:00 09:00	Breakfast @ *Date Restaurant*
07:00 20:00	Badge Pickup @ *Renaissance Foyer*
08:00 12:00	Short Courses: Group A @ *Various*
08:30 12:30	Short Courses: Group B @ *Various*
09:00 13:00	Short Courses: Group C @ *Various*
:20 or :50 FOR 10 MINS	Coffee Break @ *Renaissance Foyer*
12:00 14:00	Lunch @ *Date Restaruant & Patio*
13:00 17:00	Short Courses: Group A @ *Various*
13:30 17:30	Short Courses: Group B @ *Various*
14:00 18:00	Short Courses: Group C @ *Various*
:20 or :50 FOR 10 MINS	Coffee Break @ *Renaissance Foyer*
17:00 20:00	Dinner On Your Own @ *Your Decision*
17:00 22:00	Hospitality @ *Santa Rosa and /or Rocks Terrace*

TUESDAY

06:00 07:00	Yoga @ *San Jacinto*
06:00 09:00	Breakfast @ *Date Restaurant*
07:00 20:00	Badge Pickup @ *Renaissance Foyer*
08:00 12:00	Short Courses: Group A @ *Various*
08:30 12:30	Short Courses: Group B @ *Various*
09:00 13:00	Short Courses: Group C @ *Various*
:20 or :50 FOR 10 MINS	Coffee Break @ *Renaissance Foyer*
11:00 16:00	Place Posters @ *Exhibit Hall*
12:00 14:00	Lunch @ *Date Restaruant & Terrace*
14:00	End Of Short Courses
14:00 14:15	Welcome Orientation @ *Rms 2 - 4*
14:15 15:00	Opening Plenary Lecture @ *Rms 2 - 4*
15:00 15:30	Coffee Break @ *Renaissance Foyer*
15:30 16:15	Plenary Panel: The Future of Clinical MS @ *Rms 2 - 4*
16:15 16:30	Intermission @ *Renaissance Foyer*
16:30 17:00	Poster Lightning Talks @ *Rms 2 - 4*
17:00 17:30	Exhibitor Lightning Talks @ *Rms 2 - 4*
17:30 20:00	Exhibits Dinner Reception @ *Exhibit Hall*
18:00 19:00	Meet-The-Experts: Booth Tours @ *Exhibit Hall*
19:00 20:00	Troubleshooting Forum: Poster Rounds @ *Exhibit Hall - Poster Board 40*
20:00 22:00	Discussion Groups: 1) CDC Standardization Programs Forum @ *Rm 2* 2) FDA Overview of the Process for Clearance & Approval of MS-based In vitro Diagnostic Devices @ *Rm 3*
20:00 22:00	Hospitality @ *Santa Rosa and Rocks Terrace*

WEDNESDAY

06:00 07:00	Yoga @ *San Jacinto*
06:30 08:15	Workshop Breakfast @ *Renaissance Foyer*
07:00 07:45	Corporate Workshops Am β @ *Rm2, Rm4, Rm5*
07:45 08:00	Intermission @ *Renaissance Foyer*
08:00 08:45	Corporate Workshops Am γ @ *Rm1 - Rm5*
08:45 09:00	Intermission @ *Renaissance Foyer*
09:00 10:00	Scientific Session 1 @ *Various Track Rooms*
10:00 11:00	Exhbiits and Poster Session @ *Exhibit Hall*
10:00 11:00	Meet-The-Experts: Poster Tours 1 @ *Exhibit Hall: Meet-the-Experts Rally Point*
11:00 12:00	Scientific Session 2 @ *Various Track Rooms*
12:00 13:30	Lunch @ *Renaissance Foyer*
12:30 13:15	Corporate Workshops PM @ *Rm1 - Rm5*
13:30 14:30	Exhibits & Poster Session @ *Exhibit Hall*
13:30 14:30	Meet-The-Experts: Poster Tours 2 @ *Exhibit Hall: Meet-the-Experts Rally Point*
14:30 15:30	Scientific Session 3 @ *Various Track Rooms*
15:30 17:00	Exhibits & Appetizers @ *Exhibit Hall*
15:45 16:45	Meet-The-Experts: Office Hours @ *Exhibit Hall: Meet-the-Experts Rally Point*
17:00 18:00	Distinguished Contribution Award Plenary Lecture @ *Rms 2 - 4*
18:00 22:00	Free Evening / Off-Site Meetings / Dinner on own
18:00 22:00	Hospitality @ *Santa Rosa and/or Rocks Terrace*

THURSDAY

06:00 07:00	Yoga @ *San Jacinto*
06:30 08:15	Workshop Breakfast @ *Renaissance Foyer*
07:00 07:45	Corporate workshops Am β @ *Rm2 (Catalina)*
07:45 08:00	Intermission @ *Renaissance Foyer*

THURSDAY (cont)

08:00 09:00	Private: Scientific Committee Discussion Group @ *Mesquite H*
08:00 08:45	Corporate Workshops Am γ @ *Rm1 - Rm4*
08:45 09:00	Intermission @ *Renaissance Foyer*
09:00 10:00	Scientific Session 4 @ *Various Track Rooms*
09:00 10:00	Exhibitor Feedback Meeting @ *Mesquite H*
10:00 11:00	Exhibits & Poster Session @ *Exhibit Hall*
10:00 11:00	Meet-The-Experts: Poster Tours 3 @ *Exhibit Hall: Meet-the-Experts Rally Point*
11:00 12:00	Scientific Session 5 @ *Various Track Rooms*
12:00 13:30	Lunch & Exhibits @ *Exhibit Hall*
12:30 13:30	Exhibits & Poster Session @ *Exhibit Hall*
12:30 13:30	Meet-The-Experts: Poster Tours 4 @ *Exhibit Hall: Meet-the-Experts Rally Point*
13:30 14:00	Corporate Workshops PM @ *Rm2 - Rm3*
14:00 14:15	Intermission @ *Renaissance Foyer*
14:15 15:15	Scientific Session 6 @ *Various Track Rooms*
15:15 15:30	Intermission @ *Renaissance Foyer*
15:30 16:30	Scientific Session 7 @ *Various Track Rooms*
16:30 18:00	Closing Exhibits Reception @ *Exhibit Hall*
16:30 17:30	Poster Finalists to Attend Posters @ *Exhibit Hall*
16:45 17:45	Troubleshooting Forum: Poster Rounds @ *Exhibit Hall - Poster Board 41*
17:45 18:00	Remove Posters From Exhibit Hall @ *Exhibit Hall (Storage Available @ Reg Desk)*
18:00	Exhibits Closed
17:45 18:15	Plenary Reception @ *Renaissance Foyer*
18:15 18:30	Poster Awards @ *Rms 2 - 4*
18:30 19:15	Closing Plenary Lecture @ *Rms 2 - 4*
19:15 21:00	Closing Dinner: Mexican Fiesta @ *Rms 2 - 4, Renaissance Foyer & Patio*
21:00 22:00	Hospitality @ *Rocks Terrace / Santa Rosa*
22:00	Conference Closed

Plenary Speaker Series

Community-Scale Translation of Mass Spectrometry Big Data into Crowdsourced Proteomics and Metabolomics Resources
Nuno Bandeira
University of California, San Diego

Tuesday @ 14:15 in California Ballroom (Rms 2-4)

Translating the growing volumes of proteomics mass spectrometry data into reusable evidence of the occurrence and provenance of proteomics and metabolomics events requires the development of novel community-scale computational workflows. We show how advanced distributed computing algorithms can be used to process tens of terabytes of public data to reveal hundreds of millions of new identifications, including the discovery of novel proteins and hypermodified peptides with over 100 modification variants. We further show how large scale reanalyses can be reliably aggregated into community-scale crowdsourced spectral libraries enabling high-throughput detection and discovery in newly acquired data.

MSACL 2017 US - Distinguished Contribution Awardee
The Triple Quadrupole: Innovation, Serendipity and Persistence
Richard Yost
University of Florida

Wednesday @ 17:00 in California Ballroom (Rms 2-4), *includes Award Presentation*

In this presentation I will provide a personal perspective on the conceptualization, development and demonstration of the analytical capabilities of the triple quadrupole mass spectrometer. And in that perspective, I will try to illustrate the roles of innovation, serendipity and persistence that are fundamental to scientific research. The triple quadrupole mass spectrometer has become the most common mass spectrometer in the world today, with sales of over $1 billion per year. It is today the gold standard for quantitative analysis in metabolomics, clinical analysis, drug discovery and development, environmental analysis, and a wide variety of other application areas. That invention and related research have helped propel mass spectrometry into the most commonly used analytical method in the world.

A New Approach to Genome Editing
Alexis Komor
University of California, San Diego

Thursday @ 18:30 in California Ballroom (Rms 2-4)

The CRISPR-Cas9 RNA-guided DNA endonuclease has contributed to an explosion of advances in the life sciences that have grown from the ability to edit genomes within living cells. Here I describe the development of base editing, a new approach to genome editing that enables the direct, irreversible conversion of one target DNA base into another in a programmable manner, without requiring double-stranded DNA backbone cleavage or a donor template. Base editing is one of many recent developments in the genome editing field that advances both the scope and effectiveness of genome editing.

Young Investigator Grants

Young Investigator Travel Grants (n=80) are provided to support trainees (MD/residents/fellows and PhD - students / post-docs) and young faculty members (fewer than 4 years since appointment) who submitted abstracts that have been accepted for presentation at the conference.

Mina Adam *Imperial College London UK*
Yehia Baghdady *The University of Texas at Arlington*
Brenda Bakker *University of Twente*
Emmanuelle Bardin *Imperial College London*
Sankha (Bobby) Basu *Brigham and Women's Hospital*
Marianne Bergmann *Lillebaelt Hospital*
Zsolt Bodai *Imperial College London, London, United Kingdom*
Anne-Claire Boschat *Institut Imagine*
Theresa Boyle *Moffitt Cancer Center*
Adam Burke *Imperial College London*
Simon Cameron *Imperial College London*
Sean Campbell *University of Virginia*
Anaamika Campeau *University of California, San Diego*
Casey Chamberlain *University of Florida*
Andreas Dannhorn *Imperial College London*
Noortje de Haan *Leiden University Medical Center*
Diogo de Oliveira *University of Campinas*
Rahul Deshpande *Greenwood Genetic Center, Greenwood, SC*
Andrei Drabovich *University of Toronto*
Stephenie Droll *National Institutes of Health*
Mans Ekelof *North Carolina State University*
Jia Fan *Arizona State University*
Clara Feider *University of Texas at Austin*
Kyana Garza *University of Texas at Austin*
Noah Giese *University of Texas at Austin*
Begona Gimenez-Cassina Lopez *Brigham and Women´s Hospital, Harvard University*
German Gomez-Rios *University of Waterloo*
Jörg Hanrieder *University of Gothenburg*
Lidong He *Florida State University*
Max Hecht *University of Tartu*
Kelly Hines *University of Washington*
Melissa Hoffman *Moffitt Cancer Center/University of South Florida*
Xinying Hong *University of Washington*
Melissa Hughs *ARUP Institute for Clinical and Experimental Pathology*
Carl Jenkinson *University of Birmingham*
Kirk Jensen *Osaka University*
Marissa Jones *Vanderbilt University*
Rutchanna Jongejan *Erasmus Medical Centre*
Raghavi Kakarla *Cleveland State University*
Martin Kaufmann *Queen's University/Kingston General Hospital*
Robin Kemperman *University of Florida*
Antony Lehtikoski *Orise Fellow at CDC*
Jieli Li *MD Anderson Cancer Center*
Estela Lima *University of Campinas*

Danting Liu *Cleveland State University*
Yiqi Ruben Luo *University of California, San Francisco*
Carlo Martins *Memorial Sloan Kettering Cancer Center*
Vandana Megaraj *Cincinnati Children's Hospital*
Robert Mills *University of California, San Diego*
Anna Mroz *Imperial College London*
Nicholas Oranzi *University of Florida*
Abed-Hamlet Pablo *Johns Hopkins University*
William Perry *Vanderbilt University*
William Phipps *UT Southwestern*
Deema Qasrawi *University of Calgary*
Elizabeth Randall *Brigham and Women's Hospital, Harvard Medical School*
Carlos Fernando Odir Rodrigues Melo *University of Campinas*
Lucia Renee Ruhaak *Leiden University Medical Center*
Triniti Scroggin *ARUP Laboratories*
Rohan Shah *Cleveland State University*
Junyan Shi *University of British Columbia*
Elisβngela Silva *A.C.Camargo Cancer center*
Sandra Spencer *University of Washington*
Madeleine Swortwood *Sam Houston State University*
Raf Van de Plas *Delft University of Technology*
Xander van Wijk *The University of Chicago*
Ruta Veigure *University of Tartu*
Stephanie Vuong *University of Saskatchewan*
Dawei Wang *University of Pittsburgh*
Joesph Wiencek *University of Virginia School of Medicine*
Jacob Wozniak *University of California, San Diego*
Jikang Wu *The Ohio State University*
Vincen Wu *Imperial College London*
Yi Xiao *Children's Hospital Los Angeles*
Karen Yannell *Purdue University*
Fan Yi *University of Washington*
Marina Zajec *Erasmus University Medical Center*
Shenyan Zhang *Cedars Sinai Medical Center*
Yuzi (Emma) Zheng *Cleveland Clinic*
Xueyun Zheng *Pacific Northwest National Laboratory*

Lab Director Grants

Lab Director Travel Grants (n=17) are provided to individuals leading clinical labs. These individuals have had minimal exposure to mass spectrometry and are interested in gaining more understanding of its clinical applications.

Jing Cao *Texas Children's Hospital*
Subhosmito Chakraborty *Tata Medical Center*
Taraka Donti *Greenwood Genetic Center*
Xiaowei Fu *University of Southern California*
Qin Fu *Cedars Sinai Medical Center*
Angela Fung *St. Paul's Hospital*
Ronald Henriquez *Walter Reed National Military Medical Center*
Nichole Korpi-Steiner *University of North Carolina*
Vathany Kulasingam *University Health Network and University of Toronto*
David Lin *Ann & Robert H. Lurie Children's Hospital / Northwestern University*
Anna Merrill *University of Iowa*
Arthur Moseley *Duke University School of Medicine*
Khushbu Patel *UT Southwestern Medical Center*
Jennifer Powers *Washington University in St. Louis*
Margrét Thorsteinsdóttir *University of Iceland*
Sjoerd van den Berg *Erasmus MC*
Zhen Zhao *The National Institutes of Health*

Trainee Grants

Trainee Grants (n=35) were provided 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.

Dennis Adams *UC San Diego*
Aaron Barnes *University of Minnesota - Lab Medicine & Patholgy*
Anne Bendt *National University Of Singapore*
Daniel Biocini *Santa Clara Valley Medical Center*
Miranda Brun *University of Alberta, Alberta Health Services*
Dustin Bunch *Yale New Haven Hospital*
Catherine Cheng *University of British Columbia*
Sarah Delaney *Hospital for Sick Children*
Carmen Gherasim *University of Utah School of Medicine, Department of Pathology*
Keisha Hardeman *Vanderbilt University*
Alexey Hodkoff *University of California San Diego*
Rongrong Huang *Houston Methodist Hospital*
Jacqueline Hubbard *University of California, San Diego*
Leroy Hubert *Baylor College of Medicine*
Lisa Johnson *University of Minnesota*
Claire Knezevic *Johns Hopkins Medical Institutes*
Ning Liu *Baylor College of Medicine*
Katelyn Ludwig *University of Notre Dame*
Maximo Marin *University of Chicago*
Lauren Moore *Memorial Sloan Kettering Cancer Center*
penn Muluhngwi *University of Louisville*
Jaime Noguez *University Hospitals Cleveland Medical Center*
Nicola Rutherford *Vanderbilt University Medical Center*
Maryam Salehi *Emory University School of Medicine & Emory University Hospital*
Kwabena Sarpong *University of Virginia School of Medicine*
Serena Singh *St. Paul's Hospital (Pathology & Laboratory Medicine)*
Philip Sobolesky *University of California San Diego*
Heather Stieglitz *University of North Carolina*
Stefani Thomas *Johns Hopkins University*
Katherine Turner *Mayo Clinic*
Cameron Wales *UCSD pathology*
Jeffrey Whitman *University of California, San Francisco*
Grace Williams *Dartmouth-Hitchcock medical Center*
Gabrielle Winston-McPherson *University of Washington*
Emily Wysocki *University of Chicago*

clinical mass spectrometry

cms

an international journal

Subject areas include:

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

Types of papers:

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

MSACL
Clinical Mass Spectrometry
m/z

Official Journal of MSACL

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

Short Course Overview

Clinical MS 301 : **A Comprehensive Review of Clinical Mass Spectrometry Technology & Techniques, including Miniaturization**
Duration: *Sunday 14:00 → Tuesday 12:00 (Group A)*
Location: *Mesquite D*
Level: *2-3 (Intermediate - Advanced)*
Instructor(s): **Jack Henion, PhD**

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

Data Science 201 : **Going Further With R: Tackling Clinical Laboratory Data Manipulation and Modeling**
Duration: *Sunday 14:00 → Tuesday 12:30 (Group B)*
Location: *Room 1 (Mojave Learning Center)*
Level: *2 (Intermediate)*
Instructor(s): **Patrick Mathias, MD, PhD & Randall Julian, PhD**

Forensic Toxicology 101 : **Basic Forensic Toxicology**
Duration: *Monday 14:00 → Tuesday 12:30 (Group B)*
Location: *Pueblo A*
Level: *1 (Beginner)*
Instructor(s): **Jarrad Wagner, Ph.D., F-ABFT, Allison Veitenheimer, Ph.D., Russell Lewis, Ph.D., F-ABFT**

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

LC-MSMS 101 : **Getting Started with Quantitative LC-MS/MS in the Diagnostic Laboratory**
Duration: *Sunday 14:00 → Tuesday 12:00 (Group A)*
Location: *Room 3 (Madera)*
Level: *1-2 (Beginner - Intermediate)*
Instructor(s): **Judy Stone, PhD, Lorin Bachmann, PhD & Grace van der Gugten**

LC-MSMS 201 : **Understanding and Optimization of LC-MS/MS to Develop Successful Methods for Identification and Quantitation in Complex Matrices**
Duration: *Sunday 14:00 → Tuesday 13:00 (Group C)*
Location: *Andreas*
Level: *2 (Intermediate)*
Instructor(s): **Robert D. Voyksner, PhD**

LC-MSMS 202 : **Practical LC-MS Maintenance and Troubleshooting**
Duration: *Sunday 14:00 → Tuesday 13:00 (Group C)*
Location: *Mesquite H*
Level: *2 (Intermediate)*
Instructor(s): **J. Will Thompson, PhD, Erik J. Soderblom, PhD & Chris Shuford, PhD**

LC-MSMS 301 : **Development and Validation of Quantitative LC-MS/MS Assays for Use in Clinical Diagnostics**
Duration: *Sunday 14:00 → Tuesday 12:00 (Group A)*
Location: *Room 4 (Pasadena)*
Level: *3 (Advanced)*
Instructor(s): **Russell Grant, PhD & Matthew Crawford**

MALDI 102 : **Practical Considerations for MALDI Imaging Mass Spectrometry**
Duration: *Sunday 14:00 → Tuesday 13:00 (Group C)*
Location: *Snowcreek*
Level: *1-2 (Beginner - Intermediate)*
Instructor(s): **Michelle Reyzer, PhD**

MALDI 103 : **MALDI-MS Fundamentals and its Emerging Role in Pathology and Laboratory Medicine**
Duration: *Sunday 14:00 → Tuesday 12:30 (Group B)*
Location: *Mesquite G*
Level: *1-2 (Beginner - Intermediate)*
Instructor(s): **Mark W. Duncan, PhD & Mari L. DeMarco, PhD**

Metabolomics 201 : **Application of High Resolution Mass Spectrometry and Metabolomics in Clinical Analysis**
Duration: *Sunday 14:00 → Tuesday 12:30 (Group B)*
Location: *Mesquite F*
Level: *2 (Intermediate)*
Instructor(s): **Timothy Garrett, PhD & Erin Baker, PhD**

Microbiology 201 : **Mass Spectrometric Methods of Microbial identification**
Duration: *Monday 14:00 → Tuesday 12:30 (Group B)*
Location: *Pueblo B*
Level: *2 (Intermediate)*
Instructor(s): **John Lapek, PhD & Chris Cox, PhD**

Presentations 101 : **How to Maximize Your Influence Through Creating Compelling Presentations**
Duration: *Sunday 14:00 → Tuesday 12:30 (Group B)*
Location: *Chino A*
Level: *1-2 (Beginner - Intermediate)*
Instructor(s): **Karen Mahooti, MBA**

Proteomics 201 : **Clinical Proteomics**
Duration: *Sunday 14:00 → Tuesday 12:30 (Group B)*
Location: *Room 5 (Sierra/Ventura)*
Level: *2-3 (Intermediate - Advanced)*
Instructor(s): **Andy Hoofnagle, MD, PhD, Cory Bystrom, PhD & Chris Shuford, PhD**

Proteomics 202 : **Practical Proteomics Using the Skyline Software Ecosystem**
Duration: *Sunday 14:00 → Tuesday 12:00 (Group A)*
Location: *Chino B*
Level: *1-3 (Beginner -Advanced)*
Instructor(s): **Mike MacCoss, PhD, Brendan MacLean, Lindsay Pino, and Sandi Spencer**

Sample Prep 201 : **Sample Preparation and Alternative Matrices for LC-MS Assays**
Duration: *Sunday 14:00 → Tuesday 13:00 (Group C)*
Location: *Mesquite E*
Level: *Beginner / Intermediate*
Instructor(s): **William Clarke, PhD & Mark Marzinke, PhD**

Discussion Groups

***PRIVATE*: Scientific Committee Discussion Group**

Sunday 18:30 - 20:00
Pueblo
Lead: David Herold

CDC Standardization Programs Forum

Tuesday 20:00 - 21:00+
Rm 2: Catalina
Leads: Julianne Botelho & Hubert Vesper
Participants will discuss how CDC Standardization Programs support laboratories with improving measurements for key hormones such as 25-hydroxyvitamin D, estradiol, and testosterone. Included will be additional discussions about new projects and tools available in CDC Standardization Programs.

FDA Overview of the Process for Clearance and Approval of MS-based In vitro Diagnostic Devices

Tuesday 20:00 - 22:00+
Rm 3: Madera
Leads: Doug Jeffery & Matthew Humbard

***PRIVATE* : Scientific Committee Discussion Group**

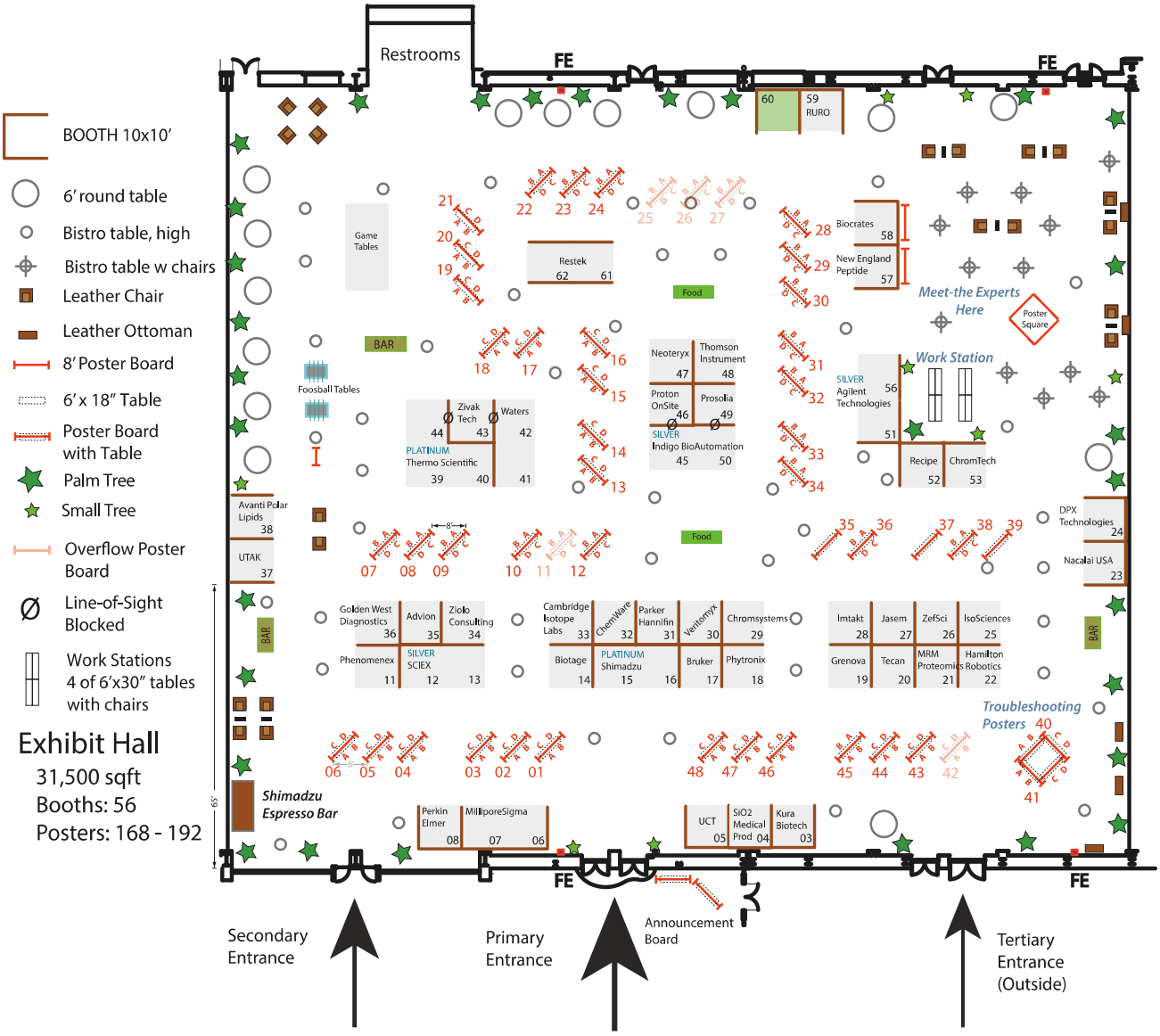
Thursday 8:00-9:00
Mesquite H
Lead: David Herold

Exhibitor Feedback Meeting

Thursday 9:00-10:00
Mesquite H
Lead: Chris Herold

Exhibits Summary

Tuesday	
8:00 – 16:00	Exhibitor Set-Up (EXHIBITS CLOSED) – Poster Placement for Presenters Permitted.
17:30 – 20:00	**Opening Reception** in Exhibit Hall
Wednesday	
10:00 – 11:00	**Exhibit & Poster Session** in Exhibit Hall
9:45 - 10:45	**Posters** in Exhibit Hall
13:30 – 14:30	**Exhibit & Poster Session** in Exhibit Hall
15:30 – 17:00	**Exhibits & Appetizers** in Exhibit Hall
Thursday	
10:00 – 11:00	**Poster Session** in Exhibit Hall
12:00 – 13:30	**Lunch & Poster Session** in Exhibit Hall
16:30 – 18:00	**Lunch** provided in the Exhibit Hall.
18:00	**EXHIBITS CLOSE**
18:00 – 23:00	***Exhibitor Breakdown and Packing***



Exhibitors

Advion Booth #35
http://www.advion.com
With over 20 years of mass spectrometry and chemistry expertise, Advion offers the expression family of compact mass spectrometers designed for the chemist. The affordability, small size and ease-of-use make them ideal for use directly at the chemist's bench, giving immediate answers and informed decisions instead of waiting in line at a central analytical service laboratory. Quickly and effortlessly analyze samples from Flash chromatography, Prep-LC, SFC, TLC, (U)HPLC, or manual syringe injection. Now every synthetic chemist can have a mass spec that works the same hours that they do. Learn more at www.expressioncms.com

Agilent Technologies Booth #51,56
http://www.agilent.com/en-us/solutions/clinical-diagnostics
Agilent Technologies delivers premiere analytical technologies for clinical research ensuring your success from sample prep to final answer. These include a comprehensive portfolio of innovative automation, chemistries, GC, GC/MS, ICP/MS, LC, and LC/MS solutions which enables the identification and quantification of both endogenous and exogenous substances in complex biological matrices with the utmost accuracy and reliability. Coupled with our dedicated global support network, we will get you to your final answer with minimal ramp-up and maximum productivity.

Avanti Polar Lipids Booth #38
http://www.avantilipids.com
No summary as of press time.

Biocrates Life Sciences Booth #58
http://www.biocrates.com
Biocrates provides the fast track to metabolic biomarker signatures, with standardized and highly reproducible solutions for the quantitative analysis of hundreds of endogenous metabolites. Biocrates' metabolic phenotyping technology is among the most widely used approaches in metabolomics. It has contributed to more than 800 scientific publications in a large variety of applications. Targeted Metabolomics kits build the cornerstone of Biocrates' portfolio. These allow for metabolomics analyses in your own laboratory, eliminating the need to invest resources into method development. A new kit for broad lipid and metabolic profiling with HRAM mass spectrometers has recently been introduced. Biocrates' targeted metabolomics kits have proven excellent analytical performance in international ring trials, as well as in proficiency tests organized by national clinical chemistry societies. Biocrates also operates an analytical services laboratory, which can provide quantitative analysis of more than 700 metabolites.

Biotage Booth #14
http://www.biotage.com/
Biotage is a leading provider of sample preparation instrumentation and consumables for a wide range of applications, including pharmaceutical, clinical, forensic, environmental, and agrochemical/food. ISOLUTE® and EVOLUTE® brand solid-phase extraction (SPE) and Supported Liquid Extraction (SLE) products can be run in either a manual or automated environment. The new RapidTrace+ SPE workstation and TurboVap® Solvent evaporators are ideal for increasing throughput and achieving accurate results. Stop by our booth for the latest innovations and applications for Evaporation and Sample preparation.

Bruker Booth #17
http://www.bruker.com
For more than 55 years, Bruker has enabled scientists to make breakthrough discoveries and develop new applications that improve the quality of human life. Bruker's high-performance scientific instruments and high-value analytical and diagnostic solutions enable scientists to explore life and materials at molecular, cellular and microscopic levels. In close cooperation with our customers, Bruker is enabling innovation, productivity and customer success in life science molecular research, in applied and pharma applications, and in microscopy, nano-analysis and industrial applications. In recent years, Bruker has also become a provider of high-performance systems for cell biology, preclinical imaging, clinical phenomics and proteomics research, clinical microbiology, and for molecular pathology research.

Cambridge Isotope Labs Booth #33
http://www.isotope.com
Cambridge Isotope Laboratories, Inc. is the world leader in the manufacture and separation of stable isotopes and isotope-labeled compounds. CIL and Euriso-Top (a European subsidiary of CIL) offer highly pure compounds that are uniformly or selectively enriched in ^{13}C, ^{15}N, D, ^{18}O or ^{17}O. CIL's labeled reagents are used in proteomics, metabolomics, metabolism, and environmental applications for quantitative mass spectrometry. Our products include MRM PeptiQuantTM assay kits, SILAC protein quantitation kits, media and reagents, 99% enriched amino acids, Mouse Express® Lys $^{13}C_6$ and ^{15}N mouse feed and tissue, ^{15}N spirulina, intact labeled proteins, growth media for protein expression, cell-free protein synthesis products, environmental contaminants standards for ultra-trace analysis, steroids, acylcarnitines, drug metabolites, nucleic acids, lipids and carbohydrates. CIL has cGMP capabilities; a majority of substrates can be manufactured to Q7A compliance.

ChemWare Booth #32
http://www.horizonlims.com
HORIZON is today's approach to lab information management, based on more than 30 years of industry leadership. Originally developed by ChemWare, HORIZON is a part of Red Arrow Labs, a member of the Dohmen family of companies. Some of the most mission-critical marketplaces apply our product – each one important to millions every day. From large government public health labs to small, private clinical ones, HORIZON is designed to be the LIMS of choice for any lab. If you collect, process and test samples, HORIZON is your lab's solution.

Chrom Tech Booth #53
http://www.chromtech.com
Distributor of Chromatography consumables, instrumentation and supplies. Featuring: Sample Preparation Products, 96 Well Plates for MS, 96-well Multi-Tier™ Micro Plate System with Glass Inserts, Columns, Instrument consumables and replacement parts, Pumps, Gas Generators. Featured Suppliers include: Agilent Technologies, Thermo Scientific, Sigma Aldrich, Idex (Upchurch and Rheodyne), Parker Balston, Hamilton, Restek.

Chromsystems Booth #29
http://www.chromsystems.com/en-gb
Chromsystems is a leading global company providing ready-to-use kits, multilevel calibrators and quality controls for routine clinical diagnostics by LC-MS/MS and HPLC. Our parameter menu covers a range of areas such as newborn screening, therapeutic drug monitoring, steroid analysis, vitamin profiling and more. We continuously expand our portfolio with additional tests all ensuring a highly accurate and cost-effective analysis. We enable laboratories to add new parameters into their diagnostic routine and expand their testing menu without prior technical expertise. They can immediately start the analysis with a minimum of time for the sample preparation. The products are comprehensively validated, and in particular LC-MS/MS methods with all widely used tandem mass spectrometers. They are CE-IVD compliant, satisfying regulatory requirements in the laboratory. We combine these high quality products with an excellent support programme and service for our customers.

DPX Technologies Booth #24
http://www.dpxlabs.com/
At DPX Labs we believe that your sample preparation should be fast and easy. That is why we have incorporated the benefits of solid-phase extraction into a simple to use pipette tip. The patented Dispersive Pipette Extraction (DPX) tip functions by dispersive SPE, requiring only seconds of mixing within the DPX tip to complete the sample preparation process. Now anyone can rapidly extract samples with high recoveries prior to LC/MS analysis. Whether your laboratory uses a single channel pipettor or a fully robotic liquid handler, there is a DPX tip compatible with your analysis method and throughput. Contact DPX Labs so we can help you eliminate matrix interferences and make ion suppression a thing of the past.

Golden West Diagnostics Booth #36
http://www.goldenwestdiagnostics.com
Golden West Diagnostics, Inc. addresses the need for quality, cost effective biological raw materials for the development of immunoassays and LC-MS applications. GWD provides manufacturers and laboratories with over 80 products including Vitamin D free human serum, serum for ultra-sensitive testing, HSA, HGG, and RGG. Please visit us at www.goldenwestdiagnostics.com.

GRENOVA Booth #19
http://www.grenovasolutions.com
Grenova's proven technology offers labs the option to safely reuse plastic pipette tips several times, cutting associated costs by up to 90%. Grenova TipNovus is a benchtop, high-throughput, automated device that will enable labs to wash and sterilize contaminated pipette tips in large quantities for re-use with no carryover. TipNovus' unique, patented method of washing and sterilization is safe for both laboratory personnel and the environment, and has been implemented in CAP and CLIA certified labs for over 3 years now.

Hamilton Robotics Booth #22
http://www.hamiltonrobotics.com
Hamilton Robotics is dedicated to the design and manufacture of automated liquid handling workstations. We offer a several types workstations for direct sale and OEM. Key to our products is our air displacement pipetting and monitoring technology as well as the software controlling our systems. We believe every laboratory automation project is unique. Our workstations and software serve as a common high precision and flexible base upon which to provide automated solutions. To this end we employ teams of highly skilled and experienced application and hardware customization specialists around the world to provide our customers with unique solutions to automate their assays successfully and within budget. Please come explore our products and contact us to discuss your automated liquid handling needs further.

Imtakt USA Booth #28
http://www.imtaktusa.com
We are advancing HPLC science by creating unique columns with novel chemistries that provide enhanced selectivity and resolution. We offer a wide range of innovative stationary phases compatible with HPLC, UPLC and LC-MS. Our columns have 25-50% lower pressure and excellent batch-to-batch reproducibility. For more information, please visit our website to view our Product Guide and Application Library.

Indigo BioAutomation Booth #45,50
http://www.indigobio.com/
Indigo BioAutomation, founded in 2004, is an established leader in software automation for the applied and health sciences. Indigo's flagship system, ASCENT, is a hosted system for automating the processing, reviewing, and reporting of LC-MS/MS data. ASCENT has helped automate the review of tens of millions of samples, in a variety of clinical/toxicology laboratories. In addition to daily workflows, Indigo's systems also provide laboratory analytics dashboards. Looking ahead, Indigo will continue to create world-class computational decision-making tools and laboratory automation systems.

IsoSciences Booth #25
http://isosciences.com/
IsoSciences, LLC is a world leader in the synthesis of stable isotope labeled vitamins, steroids, drug substances, metabolites and other compounds of interest. IsoSciences is ISO9001 certified and has an extensive catalog of stable isotope labeled standards available for immediate delivery both as solids and as CertiMass™ exact concentrations solutions. IsoSciences has added over 200 new products over the past year including an extensive range of $^{13}C_3$ labeled steroids, Vitamin D metabolites, $^{13}C_7$-Vitamin B_{12}, $^{13}C_6$-Vitamin K2 MK4,MK7 and MK9. Contact info@isosciences.com for any internal standard needs you may have!

Jasem Booth #27
http://www.jasem.com.tr
Adapting diagnostics in chromatography coupled mass spectrometry Jasem serves customers ready-to-use diagnostic kits for clinical analysis based on HPLC and mass spectrometry. Providing innovative trustworthy and accurate results constitutes the core viewpoint of us. Hence, our straightforward and economic solutions are being used extensively in clinical and food laboratories. Foundation purpose is clinical and food analysis kit development; Simple and practical sample preparation Short analysis time Reliable and sensitive analysis Low analysis cost (without derivatization, SPE or concentration) Longer column life-time

Kura Biotec Booth #03
http://www.kurabiotec.com/
Growing clinical tox-lab? Thinking of adding more centrifuges, more technicians and more HPLC / LCMS to keep up with growing demand and turnaround time? ... Before that ... have you actually streamlined and scaled-up sample-prep? ... Discover how BGTurbo™ FLASH HYDROLYSIS and FLASH SAMPLE PREP cuts your hydrolysis bottle-neck while securing 90% upstream hydrolysis recovery, codeine included. ... HYDROLYZE.ANALYZE. Your DOWNstream quality and accuracy relies on your UPstream hydrolysis recovery. ... The top toxicology labs in the US, Australia and Europe trust Kura Biotec®´s enzymes for consistent, fast, accurate screening and quantification of conjugated drugs and xenobiotics. What are you waiting for? Step on the BGTurbo™ fast-train and ride away!

MilliporeSigma Booth #6,7
http://www.Sigma-Aldrich.com/clinical
MilliporeSigma provides the innovative solutions you need to advance your research, and more importantly, the support and expertise to utilize them successfully in your lab. You'll identify more than analytes, target molecules and contaminants. Our full range of water purification products provides accurate lab results, high reliability, low maintenance, predictable and economical running costs and total support. In cellular analysis, protein detection, separation science and membrane filtration, we continue to set the standard for analytical research by providing the highest quality bioanalysis platforms, sample preparation solutions, essential biochemicals, and analytical separation tools.

MRM Proteomics Booth #21
http://www.mrmproteomics.com
MRM Proteomics Inc. is at the leading edge of proteomics technology. We offer a wide range of proteomics services and easy-to-use kits for do-it-yourself protein quantitation. We are also currently involved in developing clinical diagnostics. Our technologies include: MRM-MS with paired heavy/light peptide standards for high-precision highly-multiplexed quantitation of hundreds of proteins from low-volume samples; Patented iMALDI-MS technology for robust high-throughput clinical proteomics; HDX structural characterization of proteins and biosimilars, approaching single-residue resolution; and Tissue imaging of peptides and >500 lipids using innovative matrices and techniques (patent pending). Our mission is to offer the highest quality of proteomics technologies on the market today. Although our services fit with many diverse applications, we recognize that research projects are not "one-size-fits-all." Our expertise allows us to offer custom-tailored solutions for your specific research needs.

Nacalai USA Booth #23
http://www.nacalaiusa.com
Nacalai provides HPLC and SFC columns with alternate selectivity for difficult-to-separate compounds. The core-shell Cosmocore Cholester HPLC column can baseline separate 25-OH vitamin D_2 and D_3 metabolites and their epimers in isocratic reversed-phase condition. The same Cosmocore Cholester HPLC column can also detect Δ-8 THC and Δ-9 THC and metabolites. Additionally, we provide SunShell HPLC/SFC columns in the US. Free column screening is available in our San Diego lab.

Neoteryx Booth #47
http://www.neoteryx.com
Neoteryx delivers on the promise of microsampling technology, enabling biological specimen collection anytime, anywhere, by anyone, while reducing costs and improving the clinical experience. Benefits of Volumetric Absorbtive Microsampling (VAMS™) technology include improved comfort (particularly for children and the elderly), reduced animal usage, and a more economical specimen collection method for low-resourced regions.

New England Peptide Booth #57
http://www.newenglandpeptide.com/
New England Peptide (NEP, Gardner, Massachusetts) has designed and produced high quality custom peptides, polyclonal and monoclonal antibodies for research organizations worldwide since 1998. Our chemists and immunological experts have over 100 years of experience and deliver a full range of peptide and antibody services for biotech and pharmaceutical applications. These include custom peptide synthesis, custom peptide arrays, polyclonal antibodies, quantitative proteomics via our NEPTune™ platform, and analytical services such as mass spec and AAA. Learn more at www.newenglandpeptide.com.

Parker Hannifin Booth #31
http://www.labgasgenerators.com
Our company manufactures high efficiency gas generators to eliminate high pressure cylinders from the laboratory. Gas generators provide increased safety, free up laboratory space, save money and produce ultra high purity gasses for your laboratory instruments. With a gas generator you are in control. These state-of-the-art gas generators continuously produce ultra-high purity gases for LC/MS, GC, FT-IR, TOC, ICP, AA and other instrumentation. All products are backed by fully staffed field sales and service organizations and one-year warranty. Preventative maintenance programs and extended warranties are available for all Parker Balston products.

PerkinElmer Booth #08
https://www.perkinelmer.com
PerkinElmer, Inc. is a global leader focused on improving the health and safety of people and their environment. PerkinElmer is dedicated to the quality and sustainability of the environment. With our analytical instrumentation, illumination and detection technologies, and leading laboratory services, we focus on improving the integrity and safety of the world we live in.

Phenomenex Booth #11
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, government and academic laboratories. Phenomenex's core technologies include products for liquid chromatography, gas chromatography, sample preparation, bulk purification chromatographic media, and chromatography accessories and equipment. For more information, visit www.phenomenex.com.

Phytronix Technologies Booth #18
http://www.phytronix.com/
The leader in quantitative ultra-fast high-throughput analysis for mass spectrometry presents the new LUXON ION SOURCE with a sample to sample speed below one second . The Luxon process can be integrated with automated liquid handling and robotic transfer arm systems to provide real high-throughput and continuous automation for your laboratory workflow. This patented ionization source offers outstanding analytical performance in pharmaceutical, bioanalytical, forensic, food and environmental industries and performs exceptionally well in other analytical fields. The Luxon Ion Source is the second generation sample introduction and ionization source based on the LDTD® technology to provide the fastest and most robust process in mass spectrometry.

Prosolia Booth #49
http://www.prosolia.com
Prosolia's DESI, Flowprobe and Velox 360 products empower scientists in the pursuit of obtaining better chemical data for better decisions in science and medicine. Our portfolio of scientific analytical tools includes innovative sample introduction systems and intuitive software - all of which are part of workflows that reduce complexity and accelerate results.

Proton OnSite Booth #46
http://protononsite.com/
Proton OnSite is the world’s leading supplier of on-site generators for laboratories. Proton Onsite offers a safe, affordable and high performance solution for onsite hydrogen generators, nitrogen generators, air compressors, air generators and zero air purifiers. Proton’s units are manufactured in a wide range of space saving stackable systems and we offer a complete line of advanced equipment for the LCMS and GC lab market.

RECIPE Chemicals & Instruments Booth #52
http://www.recipe.de/en/index.html
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.

Restek Booth #61,62
http://www.restek.com
A leading innovator of chromatography solutions for both LC and GC, Restek has been developing and manufacturing columns, reference standards, sample preparation materials, accessories, and more since 1985. We provide analysts around the world with products and services to monitor the quality of air, water, soil, food, pharmaceuticals, chemicals, and petroleum products. Our experts have diverse areas of specialization in chemistry, chromatography, engineering, and related fields as well as close relationships with government agencies, international regulators, academia, and instrument manufacturers. www.restek.com

RURO Booth #59
https://ruro.com/
RURO, Inc. is a cutting-edge software development company committed to building modern and comprehensive solutions for laboratories. RURO develops state of the art software for research, biotechnological, pharmaceutical, healthcare and government (homeland security) laboratories in the US and worldwide. Our recent line of biological applications is designed to increase the productivity of scientific, biotech and pharmaceutical laboratories while maintaining the highest level of security, versatility and knowledge.

SCIEX Booth #12,13
http://sciex.com/applications/clinical-research
SCIEX helps to improve the world we live in. SCIEX LC-MS/MS solutions enable clinical researchers to push the limits of analysis across a wide variety of applications, including quantitation of steroids, vitamin D, immunosuppressants or drugs of abuse, by harnessing the power of mass spectrometry through exceptionally simple-to-use tools. SCIEX offers the most comprehensive portfolio of pre-configured LC-MS/MS methods and software for clinical research and toxicology. All based on the proven reliability of SCIEX systems, including the SCIEX QTRAP® 5500 system, the most sensitive LC-MS/MS system for trace level analysis -- all backed by the most comprehensive service and support organization in the industry. For more information, go to www.sciex.com/clinicalresearch

Shimadzu Booth #15,16
http://www.shimadzu.com/
Founded in 1875, Shimadzu is a global corporation with three major divisions: Medical Diagnostics, Aerospace/Industrial, and Analytical Instruments. The Analytical Division is one of the world´s largest manufacturers of analytical instrumentation, supporting a broad range of applications including life sciences, pharmaceuticals, food safety, environmental, cannabis QC testing, chemicals/energy, and forensics. Shimadzu expanded the scope of its ISO-13485 certification to include LC and LCMS instruments, and supports the growing demand for LC and LCMS in clinical testing markets. Visit our booth to learn more about new Shimadzu platforms, including our ultra-fast LCMS-8060 triple quadrupole MS, our CLAM-2000 clinical lab MS automation platform, automated protein digestion workstations and Noviplex Plasma Prep Cards (Novilytic, LLC).

SiO2 Medical Products Booth #04
http://www.sio2med.com/
SiO2 Medical Products' Advanced Bioscience Labware division combines plastic molding and materials expertise with plasma-based coating and treatment technologies to create labware products that offer multiple benefits, including Ultra-Low Binding, Ultra-Low Extractable, and Ultra-Clean technology. - “Ultra-Low Binding” Treatment Technology: Minimizes protein/peptide binding to bioscience labware at low concentrations - “Ultra-Low Extractable” Technology: Minimizes extractables of the plastic labware into the sample - “Ultra-Clean” Coating Technology: Incorporates an SiO2 coating to replace glass insert microplates

Tecan Booth #20
http://www.tecan.com
Tecan is a leading global provider of laboratory instruments and solutions in biopharmaceuticals, forensics, and clinical diagnostics. Had enough of tedious mass spectrometry sample preparation? Tecan offers Freedom EVO®-based end-to-end process automation for even the most challenging protocols, liberating you from the bottleneck of manual sample preparation. Keep up with ever-increasing demands with Tecan Freedom EVO • Solid phase extraction • Liquid liquid extraction • Protein purification AC Extraction Plate™ The Tecan AC Extraction Plate with TICE™ (Tecan Immobilized Coating Extraction) technology revolutionizes your sample preparation routine. A simple pipette and shake sequence, with no filtration, centrifugation or solvent evaporation, is all that is required. The AC Extraction Plate is easily integrated into automated processes, making it a perfect match with Tecan's Freedom EVO® liquid handling platform.

Thermo Scientific Booth #39,40,44
http://www.thermoscientific.com
From proven clinical laboratory services and diagnostics to scalable translational research solutions, we are a partner you can trust who will help you efficiently develop and apply clinical applications today, and for many years into the future. Our portfolio of Chromatography and Mass Spectrometry solutions are designed to empower clinical laboratories around the world with flexible research to lab developed test solutions and fully automated diagnostic testing capabilities. Our product portfolio offers a full range of benefits from systems with complete assay kits, to scalable systems providing you flexibility in providing laboratory developed testing services. Visit us in booth #39, 40,44 to see how we can help you achieve greater flexibility, productivity and confidence in your test results to serve the healthcare professionals.

Thomson Instrument Co Booth #48
http://htslabs.com/
Thomson Instrument Company is a leading-edge manufacturer and supplier of consumable products for the Chemistry and Biological fields. Our SINGLE Step Filter Vials (450uL capacity), Nano Filter Vials (10uL minimum sample volume), and eXtreme Filter Vials (>30% particulates) are used in many labs for all your sample preparation needs and are compatible with most standard autosamplers for HPLC, GC, LC/MS. We provide a number of simple standard and custom products to meet our customer's needs. Please look at our website at www.htslabs.com. We are committed to competitive pricing and quality customer service. Ph: 800-541-4792 or 760-757-8080 Fax: 760-757-9367 E-Mail: folks@htslabs.com

UCT Booth #05
http://www.unitedchem.com
UCT is a vertically integrated manufacturer of high quality Sample Prep and HPLC column products. We combine this with world class technical support. Product lines include Solid Phase Extraction (SPE) cartridges/well plates, QuEChERS tubes, Selectra® HPLC columns, manifolds, Selectrasil® reagents and enzymes, and newly launched Ultra Flash® purification columns. Also, UCT in collaboration with Obotics and Hudson Robotics are excited to present OB-1, the world's first truly intelligent robotic lab assistant. This automated platform provides a complete solution that fully accommodates the needs of the forensic toxicology community.

UTAK Laboratories Booth #37
http://www.utak.com
Since 1973, UTAK Laboratories, Inc., has been connecting Research and Commercial Laboratories with the most comprehensive menu of Stock and Custom manufactured Quality Controls available. Our Products offer complete commutability with many methods of evaluation including; Immunoassay, ELISA, HPLC, UHPLC, ICPMS, GC/MS, and LC/MS, TOF, etc. Our entire line of 100% REAL Human Matrix products along with our Specialty Matrix (SMx™) products come together to offer Laboratorians a true 3rd party Quality Control, especially for Laboratory Developed Tests or LDT's. Ask us about QC for your LDT. UTAK, createCONTROL

Veritomyx Booth #30
http://www.veritomyx.com/msacl.pdf
Veritomyx® delivers unprecedented mass spectral analysis quality and completeness, through advanced signal processing and identification algorithms applied to raw MS data. PeakInvestigator® software differentiates peak signals from noise with statistical confidence intervals, and deconvolves overlapped peaks with 5-6x higher resolution, revealing critical hidden information. PeakInvestigator operates on raw profile MS data from ion trap, TOF, Orbitrap and FTICR mass analyzers. PeptideDetective® software (alpha collaborations phase), outperforms current market leaders in de novo peptide identifications. This more accurate and complete information helps to minimize inefficient misdirected R&D by accelerating metabolomic and proteomic biomolecular identifications.

Waters Booth #41,42
http://wvmc.waters.com
At Waters Corporation, we understand the factors necessary to succeed at each stage of the health sciences continuum, from the challenges of biomarker discovery and translation to validation and commercialization of innovative clinical diagnostics. We draw on first class scientific expertise to bridge the translation gap and help further the understanding and management of disease. Driven by purposeful innovation, we have created a comprehensive line of scientific products and services designed to support the entire continuum of biomedical research. These include state of the art analytical tools such as chromatography and mass spectrometry, associated informatics, and supportive sample preparation and diverse column chemistries. www.waters.com/msacl

Zef Scientific Booth #26
http://www.zefsci.com
•Is your Mass Spectrometer showing the uptime that you expect? •Do the different vendors tend to blame each other—or your method—for an issue? •Are you looking for a more harmonized and seamless experience in maintaining your LC-MS/MS? ZefSci is the country's premier independent LC-MS/MS engineering firm. A network of experienced field service and qualification engineers are strategically positioned nationwide supplying our customers with the highest level of services on AB/Sciex, Thermo, Waters, Agilent, and Shimadzu. 1- Service Contracts 2- Preventative Maintenance 3- Repair 4- GxP Compliance IQ/OQ/PQ

Ziolo Consulting Booth #34
http://www.zioloconsulting.com
Ziolo Consulting provides a wide variety of laboratory services including: Laboratory management, technical consulting, lab setup, instrument validation and lab personnel for toxicology and genetics labs. Ziolo Consulting was founded on the idea that every lab is different, and they all face different obstacles. Our goal is to adapt to each of our client's specific needs. As a relatively new company, we are highly adaptable and very competitive. At this conference we will be launching our newest service, the ZC Proficiency Testing Network. Stop by Booth #34 to learn more and discover how Ziolo Consulting can improve your lab today.

Zivak Technologies Booth #43
http://www.zivak.com
Based in Istanbul, Turkey, Zivak Technologies provides ready to use LC-MS/MS and HPLC analysis kits in the clinical diagnostic field. The company also offers its own fully automated sample preparation and injection system which enables laboratories around the globe to make efficient use of their LC-MS/MS instruments as well as HPLC instruments in a fast, accurate and cost efficient way.The company focuses on automation of processes in labs, HPLC and LC-MS/MS analysis kits, and consumabled. Sales and marketing activities are carried out in more than 70 countries.

Corporate Workshops

Corporate Sponsor Workshop - Sunday
8:00 - 12:00

Agilent Technologies - Room 3 (Madera)

Join Agilent for breakfast and meet a few of our Mass Spectrometry Experts. We will be covering the following material:
- MassHunter Software Overview: Review by Exception and PDF Reporting.
- New Innovations and New Synthetic Opioids. Introducing the Agilent Ultivo Miniature Tandem LC/Mass Spectrometer with clinical research application to Toxicological analytes of interest.
- Jet Steam Proteomics with Automated Sample Prep for High-Throughput Peptide Quantitation in Clinical Research.

Corporate Workshops - Wednesday AM β
7:00 - 7:45

MilliporeSigma - Room 2 (Catalina)
Biompatible Solid Phase Microextraction Coupled to MS for Improved Analysis of Biological Fluids

Microextraction using newly developed biocompatible solid phase microextraction (BioSPME) devices can be used to directly sample from complex biological matrices without significant co-extraction of interferences. BioSPME extractions may be coupled with a mass spectrometer directly or analyzed via a standard LC/MS workflow. This sample preparation methodology has evolved into a useful tool for clinical applications. Performing direct MS analysis eliminates time-consuming and costly steps specific to LC and GC separations. This rapid detection technique facilitates fast screening methods and, due to analyte concentration as well as extraction from matrix interferences, often provides highly quantitative results. This workshop will provide an overview of the technique including method development and optimization schemes. Applications including analysis of drugs of abuse, steroids and hormones from a variety of biological matrices including plasma, urine and saliva, will be explored and contrasted to conventional approaches.

Waters - Room 4 (Pasadena)
It's all about the Base: How much Simpler, Cleaner and Faster can Mixed Mode Ion Exchange SPE Methods get?
Kim Haynes, Principal Product Marketing Manager, Chemistry Technology Center

Mixed-mode ion exchange solid phase extraction (SPE) is an extremely powerful sample cleanup tool when higher degrees of analyte specificity and sample cleanliness are required. However, these methods are often associated with extra method development time and complicated processes.
In this seminar we will explore the compromise scientists have had to make between analyte specificity, sample cleanliness and simple workflows. We will then introduce an easy-to-implement solution to this problem using a new solid phase extraction product recently developed by scientists at Waters Corporation. Finally, we will demonstrate how this new product simplifies workflows, reduces method development and processing time, while improving sample cleanliness in applications.

Veritomyx - Room 5 (Sierra/Ventura)
Discover a new era of mass spectrometry effectiveness - revealing the power hidden in your existing MS data!

Transform your existing mass spectral data sets and subsequent analyses to unexpected new levels of quality and effectiveness. Discover how to employ fully-automated PeakInvestigator® advanced post-processing software to open a new era of effective life sciences problem solving with the introduction of statistically-valid MS peak determinations, including error bars on every mass and abundance call.

Learn how PeakInvestigator can transform your existing MS results into more powerful and complete data sets by deconvolving overlapped peaks, extracting remarkably improved sensitivity with noise rejection, and providing higher

precision in peak determinations. These remarkable improvements extracted from your existing MS data outputs enable you to open a new era of effectiveness in subsequent data analysis, discoveries and confirmations.

Join the Veritomyx team and renowned guest speakers for presentations and Q&A including:
“Fully-Automated, Advanced Mass Spectral Data Analysis”
“Increased Quantity & Quality Of Proteomics Identifications"
“Transformation in Metabolic Biomarkers Blind Discovery Effectiveness”

Corporate Workshops - Wednesday AM γ

8:00 - 8:45

Restek - Room 1 (Mojave)

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

Neoteryx - Room 2 (Catalina)

The Patient & Lab Perspective: Capillary vs. Venous Monitoring of Immunosuppressants

Dr. Paul Jannetto, Mayo Clinic, Director, Clinical Mass Spectrometry Lab, Clinical and Forensic Toxicology Lab, and Metals Lab

This session will provide a brief summary of a clinical pilot study where 100 patients were enrolled to compare the analytical results and patient satisfaction from a traditional venous whole blood draw versus a capillary collected whole blood sample using the Mitra microsampling collection device. In addition, the operational and analytical validation of the new automated Mitra workflow will be discussed.

SCIEX - Room 3 (Madera)

Endocrine Applications requiring high sensitivity: performance of the new SCIEX Citrine™ Mass Spectrometry System for measuring Thyroglobulin and 1,25 dihydroxyvitamin D

Dr. Daniel T. Holmes, MD; FRCPC Division Head, Clinical Chemistry,
St. Paul's Hospital Department of Pathology and Laboratory Medicine Vancouver, BC, Canada

SCIEX is very pleased to invite you to attend the unveiling of the Citrine™ MS/MS system, our fastest, most sensitive IVD mass spectrometer. The Citrine MS/MS system provides the clinical lab with the performance and robustness to address the most challenging applications. In this session, data will be presented to highlight the performance of the Citrine MS/MS system for (i) the measurement of 1,25-dihydroxyvitamin D, and (ii) the measurement of thyroglobulin, using the SISCAPA workflow.

Waters - Room 4 (Pasadena)

Measurement of Eicosanoids and their Urinary Metabolites using Mass Spectrometry

Ginger L. Milne, PhD, Research Associate Professor, Director, Eicosanoid & Neurochemistry Core Laboratories, School of Medicine, Vanderbilt University, TN

Eicosanoids are important signaling molecules central to many critical physiological processes such as inflammation, pregnancy and childbirth, and cardiovascular function. Dysregulation of eicosanoid production has been implicated in a number of diseases such as oncology, metabolic syndrome, and cardiovascular disease. Derived by the enzymatic or non-enzymatic oxidation of arachidonic acid or other 20 carbon length polyunsaturated fatty acids (PUFAs), eicosanoids are challenging to quantitatively measure due to their inherent structural and chemical similarities. This workshop will demonstrate how targeted mass spectrometry workflows are key to accurate and precise measurement of eicosanoids for clinical research and why they are required to further biomedical research of these important class of biochemicals. For Research Use Only. Not for use in Diagnostic Procedures.

Indigo BioAutomation - Room 5 (Sierra/Ventura)
The Batch and Beyond - LCMS Result Automation Strategies and Analytics
Jim Edwards

The utilization of self-aware peak processing algorithms, a comprehensive quality architecture, and a streamlined, exception-based data/result review process have proven to be a successful strategy for improving both quality and throughput of LCMS analysis. The positive impacts of these batch-oriented optimizations can be significantly magnified by an additional layer of analytics and visualization which provide comprehensive information across instruments, assays, and batches over time. Please join us for a discussion on how these analytics are used to diagnose and prevent issues, target quality improvement efforts where they will be most effective, improve the quality and speed of automated result release, and align both the business and science aspects of the laboratory for an elevation in the efficiency and effectiveness of both.

Corporate Workshops - Wednesday PM

12:30 - 13:15

DPX Technologies - Room 1 (Mojave)
Innovative Filtration Method to Rapidly Remove Protein from Biological Matrices Prior to LC/MS/MS Analyses
Daniel B. Kassel, Ph.D., Founder & CEO, SciAnalytical Strategies, Inc., La Jolla, CA; Kaylee R. Mastrianni, Ph.D., Applications Chemist, DPX Technologies, LLC, Columbia, SC

Conventional protein precipitation methods require centrifugation and oftentimes offline sample handling prior to LC/MS/MS analyses. We introduce a rapid and readily automated patent pending method for protein precipitation with automated filtration. The method utilizes Tip-On-Tip (ToT) technology for the streamlined analysis of urine, whole blood, and serum/plasma. We will discuss numerous applications such as filtration of hydrolyzed urine samples, comprehensive drug testing in whole blood, and steroid analysis in serum. We will also present a validated method for the analysis of total testosterone in serum, and show detailed patient results obtained from a collaborative clinical laboratory. Using this ToT technology, up to 96 serum samples were processed simultaneously in less than 10 minutes using a Hamilton Nimbus96, providing clean extracts immediately ready for injection into LC/MS instrumentation.

Thermo Scientific - Room 2 (Catalina)
Mass Spectrometry Approaches to the Opioid Epidemic
Marilyn Huestis, Retired Chief, Chemistry and Drug Metabolism, NIDA, Huestis & Smith Toxicology, LLC, USA

The opioid epidemic began when pain became the 6th vital sign. More than 100 million US citizens report chronic pain that requires treatment. Physicians rapidly moved to potent opioid analgesics rather than other non-steroidal anti-inflammatory drugs, leading to opioid dependence. Prescription opioid abuse is estimated to cost $72.5 B annually in health-care costs. The Drug Enforcement Agency's increased controls on health care providers and clandestine laboratories offerings of designer opioids and synthetic fentanyls resulted in opioid-dependent users moving to these new potent opioid drugs. These developments challenge laboratories to identify and quantify a wide variety of prescription opioids, heroin, and novel psychoactive opioids. Laboratories need analytical solutions to address the opioid epidemic. Liquid chromatography tandem mass spectrometry (LC-MS/MS) offers the power of multi-opioid analysis and rapid quantification of numerous analgesics. To determine the utility of high resolution accurate mass spectrometry (HRAM) to enable broad spectrum screening for prescription, illicit and clandestine laboratory opioids in clinical research will be discussed.

Shimadzu - Room 3 (Madera)
Implementation of a fully integrated automated sample preparation system for routine clinical LC-MS/MS analysis
Lorin Bachmann, PhD, DABCC, Associate Professor of Pathology, Co-Director of Clinical Chemistry, Virginia Commonwealth University

Lack of availability of a fully automated LC-MS/MS system has been one of the largest barriers to meaningful adoption of mass spectrometry in the routine clinical laboratory. Our laboratory evaluated the workflow attributes and analytical performance characteristics of the Clinical Laboratory Automation Module 2000 (CLAM-2000) integrated with the Prominence LCMS-8050 platform for routine analysis of total 25-OH Vitamin D (25-OHD). This configuration enabled complete integration of automated sample preparation with LCMS analysis during the validation study. The

method validation included patient samples obtained from our academic medical center and was performed according to Clinical and Laboratory Standards Institute (CLSI) guidelines. The CLAM-2000 Prominence LCMS-8050 method was linear from 2ng/mL- 150 ng/mL for 25-OH D3, 3-epi 25-OH D3 and 25-OH D2. Precision was excellent with coefficients of variation < 6%. The method agreed with our validated manual LCMS method, however the CLAM-2000 Prominence LCMS-8050 system had the additional advantage of resolving the 3-epimer of 25-OH Vitamin D3. Trueness was confirmed using NIST 972a Vitamin D reference materials.

Agilent Technologies - Room 4 (Pasadena)

Despite a few decades of proteomics research and the apparent discovery of multiple protein biomarkers to support the diagnosis and treatment of patients, the number of protein biomarkers that have been developed to the stage of being used routinely is disappointingly low. So, it's clear that whilst there's huge interest in the field of research for development of new protein biomarkers and major drivers for this to happen: including the pharmaceutical industry's need to better stratify patients for effective treatment, as yet biomarker development and delivery is proving very challenging. Why is this?
By enabling rapid assay development and evaluation, SRM/MRM on triple quadrupole mass spectrometers holds huge potential as a platform for the development of specific and sensitive 'biomarker signatures' comprising multiple proteins. However, once such prototype signatures are developed can they be clinically validated and then delivered to a clinical test environment? Addressing this current bottleneck may be dependent on the implementation of robust and reliable workflows with methods that are easy, quick and inexpensive and may be automated.
For Research Use Only. Not for use in diagnostic procedures.

Biognosys - Room 5 (Sierra/Ventura)
Next-Generation Proteomics Technology to Increase Depth of Coverage and Data Reproducibility In Clinical Proteomics

Recent major advancements in label free mass spectrometry based proteomics have enabled deeper and more reproducible quantification of thousands of proteins in a single measurement. This next generation proteomics technology is based on data independent acquisition (DIA) which overcomes the technical limitation of sampling speed of mass spectrometers by isolating broad ranges of peptide ions in parallel and utilizing powerful data deconvolution algorithms. DIA technology is only limited by the sensitivity of the detector, and not the sequential speed of the instrument. Researchers can now carry out deeper analysis of proteins in clinical samples and with new chromatographic set-ups the studies can be extended to hundreds of samples without any loss in depth, coverage and reproducibility.
During the lunch symposium proteomics experts from Biognosys will present the latest improvements in data acquisition, analysis and interpretation. Attendees will learn how to identify more than 8`000 protein groups in single shot DIA with almost no missing values across technical replicates.
Further we will present an optimized capillary flow system coupled to the Thermo Fisher Orbitrap Fusion Lumos. This system was used to analyse over 1500 human plasma samples.

Corporate Workshops - Thursday AM β
7:00 - 7:45

MilliporeSigma - Room 2 (Catalina)
Sample Preparation for Meaningful LC-MS

Mass spectrometry-based analysis is playing an increasingly vital role in basic research and more significantly, clinical applications. Sample preparation is an integral, but often overlooked, component of a successful LC-MS experiment. However, given the highly manual nature of the process, dearth of efficient standardized methods, and the wide variability in sample content, sample processing is the predominant source of errors and reporting bias. Due to the nature of the workflow, sample prep errors remain undetected until the final data analysis step; such issues are particularly costly in clinical settings where samples are precious or access is limited.
This workshop will offer simple tips and tricks to expedite sample preparation while ensuring sample integrity is maintained. Aspects of sample preparation to be covered in the workshop include:

- Quick guidance to filtration membrane selection allowing efficient and contamination (extractables) free sample

cleanup
- Importance of plate selection for high throughput removal of matrix components while retaining desired analyte(s)
- Filter Aided Sample Preparation (FASP) and attempts on quantitative analysis
- Quick ZipTip based sample pre-treatment to enhance LC-MS quality.

Corporate Workshops - Thursday AM γ

8:00 - 8:45

Biotage - Room 1 (Mojave)

Achieving Low Level Detection of Clinical Samples Prior to LC-MS/MS Analysis through efficient Sample Prep

Dr. Lee Williams, Biotage GB Limited, UK

The use of LC/MS analysis in the clinical lab has increased exponentially over the last 10 years. Modern mass spectrometers are extremely sensitive allowing low level detection of many target analytes. However, this sensitivity can come at a price, in that levels of contamination not previous detected with less sensitive instruments can now have larger impact on analysis. The complexity of common matrices such as plasma/serum and urine while presenting different challenges can have a marked influence on method performance. As a result sample preparation is an extremely important part of the process in order to provide robust methods. This seminar will focus on some of the method development challenges our lab faced when looking at two clinical assays; Endogenous steroid hormone extraction from serum, and catecholamine extraction from plasma and urine. Particular emphasis will be placed on the various sample preparation options we looked at for the extraction of these analytes. Optimization of the extraction process we investigated included recovery, co-extractable matrix components, HPLC column degradation, calibration curve performance and limits of quantitation.

Thermo Scientific - Room 2 (Catalina)

Comparison of Sample Purification Methods for Therapeutic Monoclonal Antibody Quantitation in Human Serum

Mohsin el Amrani, University Medical Center, University of Utrecht, The Netherlands

In recent years, there has been growing interest in quantifying biopharmaceuticals such as monoclonal antibodies (mAbs) with liquid chromatography coupled to tandem mass spectrometry (LC-MS/MS) in biological matrices for clinical research and drug monitoring research. LC-MS/MS possesses notable advantages over several other technologies with capabilities that ensure faster method development, wider linear dynamic range, and most importantly, higher selectivity. However, it can be challenging to select an appropriate and feasible sample purification method for absolute quantification of the target mAb with LC-MS/MS. In this study, a comparison between various sample purification methods for the quantification of total mAbs, including fast, economical and easy pre-analytical sample work-up will be shown. Furthermore, optimized workflow enabling the use of a stable isotopically labelled (SIL) peptide instead of SIL proteins which are commercially unavailable for most mAbs and a successful validation of quantitation assays of mAbs following EMA guidelines using the therapeutic mAbs infliximab and dinutuximab will be discussed.

SCIEX - Room 3 (Madera)

The Vitamin D 200M Assay for the Topaz™ System as a Model for LC-MS-based Diagnostics

Jason Cournoyer, Ph.D. Senior Development Scientist, SCIEX R&D

The SCIEX Vitamin D 200M Assay for the Topaz™ System is the first FDA-cleared LC-MS/MS assay for Vitamin D. It represents an evolution towards simple, turnkey solutions that enable rapid adoption of this powerful technology in a standard clinical diagnostic lab setting. This workshop will review the development and performance characteristics and advantages of this novel assay, and it's streamlined utilization on the intuitive ClearCore™ MD software platform.

Waters - Room 4 (Pasadena)

Automation and Integration of LC/MS/MS Assays into the Workflow of a Clinical Laboratory

Dr. Emma Walker, Charing Cross Hospital, London, UK

LC-MS/MS has been utilized in the clinical laboratory for approximately two decades and offers increased specificity over more traditional immunoassay based techniques. Widespread adoption of this technique has been hindered as a

result of the high capital cost of the equipment, need for highly trained laboratory personnel and the often labor intensive sample preparation required. Automation of sample preparation and interfacing of the LC-MS/MS system to the laboratory information system has the potential to reduce staff time and increase sample throughput. The options available to improve automation and to integrate LC-MS/MS into the workflow of the clinical laboratory will be discussed, including the steps that we have taken within the laboratory at Charing Cross hospital.

Corporate Workshops - Thursday PM

13:30 - 14:00

Thermo Scientific - Room 2 (Catalina)

Introducing the Thermo Scientific Cascadion SM Clinical Analyzer

Peter Cooke, Market Development Specialist, Thermo Fisher Scientific

The Thermo Scientific Cascadion SM Clinical Analyzer will be the first all-in-one LC-MS/MS solution designed to meet the needs of clinical laboratories. Our fresh vision for fully automated liquid chromatography-tandem mass spectrometry (LC-MS/MS) testing is cultivated by listening to our customers. You asked for a complete solution that was accurate, easy-to-use, and designed for the clinical laboratory. The Cascadion Clinical Analyzer is designed as a turnkey solution to enable clinical labs to easily adopt the power and capabilities of LC-MS/MS as the gold standard in diagnostic testing. The Cascadion system will combine assays, software, accessories, consumables and support/service in a standalone system designed to meet the regulatory requirements for routine and specialized clinical testing. This presentation will showcase the Cascadion solution.
Product under development, not CE/IVD marked nor FDA cleared yet.

Shimadzu - Room 3 (Madera)

Simultaneous analysis of multiple steroid hormones by LC-MS/MS

David Erikson, PhD, Director of the Endocrine Technologies Support Core at OHSU

Measurement of steroid hormones has been traditionally performed by radioimmunoassay (RIA) or automatic immunoassay (AI). Recently, liquid chromatography-tandem mass spectrometry (LC-MS/MS) has emerged as the "gold standard" for steroid analysis in the clinical laboratory, as this method offers dramatic improvements in sensitivity, specificity, and automation of serum steroid measurements over immunoassay.

Our laboratory has focused on simultaneous, sensitive measurement of multiple steroid hormones in nonhuman primate and human samples for basic and clinical research using a Shimadzu Nexera-LCMS-8050 platform. Using this technology we are often able to quantify as low as 10 pg/ml using as little as 200 ul of serum from a single sample. The purpose of this presentation is to describe methodology for quantitation of endogenous steroid hormones in serum samples, as well as methods for quantitation of synthetic hormones used for contraception and therapeutic reasons.

We will discuss application of an analytical method for quantitating synthetic hormone levels in women for the purpose of monitoring systemic exposure to determine drug interactions, nonadherence, misreporting, and proper dosing.

Podium Presentations

Wednesday & Thursday

	Room #	Room Name
Track 1	1	Mojave
Track 2	2	Catalina
Track 3	3	Madera
Track 4	4	Pasadena
Track 5	5	Sierra
Track 6	6	Smoketree
Track 7	--	Pueblo
Track 8	--	Chino
Track 9	--	Andreas

• Session 1 • Track 1 •

Keynote - Cannabinoids

Wednesday @ 9:00 in Room 1 (Mojave Learning Center)

Session Chair: David Schwope - *Aegis Labs*

Wednesday @ 9:00 in Room 1 (Mojave Learning Center)

Mass Spectrometry Meets Medical and Legal Cannabis

Marilyn Huestis - *University of Maryland School of Medicine* (marilyn.huestis@gmail.com)

‣ Currently, 8 states legalized cannabis and 29 approved medical cannabis increasing laboratory requests for cannabinoids quantification. There are now more daily cannabis users with resultant increases in stored THC in adipose, brain and organs tissues. Stored THC produces pharmacokinetic differences between daily and occasional intake. Cannabis-impaired driving increased and rapid blood THC decreases provided the impetus for roadside oral fluid cannabinoid testing. Also, new synthetic cannabinoids challenged laboratories to identify these toxic chemicals and tie their presence to accompanying adverse effects. These public health and safety challenges were met with sensitive and specific mass spectrometric methods for an expanded range of cannabinoids and their synthetic counterparts, and with greater utilization of high resolution mass spectrometry to identify NPS urinary metabolites.

• Session 1 • Track 2 •

Keynote - Informatics

Wednesday @ 9:00 in Room 2 (Catalina)

Session Chair: Patrick Mathias - *University of Washington*

Wednesday @ 9:00 in Room 2 (Catalina)

On the Building of the Skyline Targeted Mass Spec Software

Brendan MacLean - *University of Washington* (brendanx@uw.edu)

‣ The Skyline project started in August, 2008 as a 2-year effort to bring better SRM/MRM software tools to the NCI Clinical Proteomics Technology Assessment for Cancer (CPTAC) Verification Working Group that could support the variety of mass spectrometers in use in participating laboratories. Over 9 years later, the Skyline project is a thriving proteomics community open-source collaboration supporting 6 mass spec instrument vendors, integrated with a wide variety of external software, with thousands of users worldwide and many thousands of instances started each week with expanding support for small molecules, absolute quantification and ion mobility.

• Session 1 • Track 3 •

Mobilize, Derivatize and Free: Novel Approaches to Vitamin D

Wednesday @ 9:00 in Room 3 (Madera)

Session Chair: Joe El-Khoury - *Yale*

Wednesday @ 9:00 in Room 3 (Madera)

Using Ion Mobility to Reduce Chromatography Time for Liquid Chromatography-Ion Mobility-Mass Spectrometry Quantitation of 25-Hydroxyvitamin D in Human Serum

Nicholas Oranzi - *University of Florida* (noranzi555@ufl.edu) -- *Young Investigator Grantee*

‣ The evidence of links between vitamin D deficiency and many diseases has led to a dramatic increase in the demand for vitamin D testing. Quantitation of the vitamin D metabolite 25-hydroxyvitamin D (25OHD) by liquid chromatography-mass spectrometry (LC-MS) provides high accuracy but suffers from long analysis times needed to resolve 25OHD from its epimer 3-epi-25-hydroxyvitamin D. Ion mobility is coupled with LC-MS, to rapidly separate the epimer based on differences in their gas-phase conformations, and significantly reduce liquid chromatography time to two minutes. Quantitation was demonstrated for 25-hydroxyvitamin D2 and D3 in human serum without interference from the epimer. Experimental conditions were investigated to ensure ion mobility did not bias quantitation. At high ion density, RF-heating reduces the unique conformer of 25OHD, potentially impacting quantitation.

Wednesday @ 9:20 in Room 3 (Madera)

LC-MS/MS Method for Measurement of Free 25-Hydroxy Vitamin D

Mark Kushnir - *ARUP Institute for Clinical and Experimental Patho* (kushnmm@aruplab.com)

‣ 25-hydroxy vitamin D (25OHD) is widely used as biochemical marker for assessment of status of vitamin D. It was demonstrated that the majority of cells in the human body respond to free rather than total 25OHD, therefore measurement of free 25OHD should be more relevant than total 25OHD to assess the physiological actions of vitamin D. We developed an LC-MS/MS method that allows accurate measurement of free 25OHD in biological samples and evaluated its performance. Sensitivity and specificity of the method are sufficient to quantify free 25OHD in samples of healthy and pathologic individuals.

Wednesday @ 9:40 in Room 3 (Madera)

Optimized Derivatization Techniques for Quantitation of Vitamin D in Serum by LC-MS/MS

Carl Jenkinson - *University of Birmingham* (C.Jenkinson@Bham.ac.uk) -- *Young Investigator Grantee*

‣ Clinical analysis of vitamin D continues to be focussed primarily on the highly abundant circulating 25-hydoxyvitamin D (25OHD) despite being an inactive form. However quantitation of the active hormonal form 1,25(OH)2D3 may provide further information on the physiology of vitamin D in health and disease. Circulating concentrations of 1,25(OH)2D3 range between 15-75 pg/mL and often cannot be measured by LC-MS/MS owing to LLOQ levels above these ranges. The aim of this project was to determine the optimum derivatization approach for measuring dihydroxy metabolites of vitamin D, including 1,25(OH)2D3 to ensure accurate routine measurements at endogenous concentrations.

• Session 1 • Track 4 •

Therapeutic Proteins

Wednesday @ 9:00 in Room 4 (Pasadena)

Session Chair: Andy Hoofnagle - *University of Washington*

Wednesday @ 9:00 in Room 4 (Pasadena)

Tumor Tissue Proteomics in the CAP/CLIA Laboratory: A 5-year Update

Maryann Vogelsang - *NantOmics* (Maryann.Vogelsang@nantomics.com)

‣ By 2024, an estimated 19 million cancer survivors will be living in the United States. Successful treatment is increasingly dependent on detailed molecular characterization of a patient's cancer to inform selection of personalized therapies. Targeted mass spectrometry can provide precise, multiplexed analysis of treatment-related tumor biomarkers. During the past 5 years, thousands of formalin-fixed, paraffin-embedded tumor samples have been submitted to our CAP/CLIA-certified laboratory for proteomic and genomic profiling. This talk will share data and lessons learned from quantitative mass spectrometric analysis of clinical tumor samples and from research on the relationships between tumor protein expression and response to cancer therapies.

Wednesday @ 9:20 in Room 4 (Pasadena)

Stop the Inflixi-Madness: Comparison of Immunometric and Mass Spectrometric Therapeutic Drug Monitoring Assay

Grace van der Gugten - *St Paul's Hospital* (gvandergugten@providencehealth.bc.ca)

‣ Infliximab (IFX) is an anti-TNF monoclonal antibody therapy used to treat autoimmune disorders such as Crohn's disease and ulcerative colitis. A significant portion of patients receiving IFX therapy will develop signs of loss of response, making therapeutic drug monitoring necessary for rational therapeutic decision making. Immunometric assays have been routinely used for the measurement of IFX in serum, but do not correlate with one another and share issues common to immunoassays. By contrast, mass spectrometry has the potential to enable harmonization of IFX assays including development of common therapeutic cut-points.

Wednesday @ 9:40 in Room 4 (Pasadena)

Comparison of Protein Extraction, Detection, and Quantitation Methods for Therapeutic Monoclonal Antibodies; LC-MS/MS Tryptic Peptide vs Intact LC-MS

Paula Ladwig - *Mayo Clinic* (ladwig.paula@mayo.edu)

‣ The established method of choice for protein quantitation has been tryptic peptide by liquid chromatography-tandem mass spectrometry. While some monoclonal antibody therapeutics (t-mAb) may fit this paradigm, developing assays to monitor more humanized t-mAbs has become challenging given the high homology with human immunoglobulin sequences. An alternative is to pursue t-mAb intact light chain quantitation by liquid chromatography-mass spectrometry. Here we present an assessment of extraction, detection and quantitation methodologies for t-mAbs, using eculizumab as an example. The methods discussed are readily transferrable to different mass spectrometry platforms as well as to new t-mAbs that may require therapeutic drug monitoring.

• Session 1 • Track 5 •

Targeted Metabolomics Analysis

Wednesday @ 9:00 in Room 5 (Sierra)

Session Chair: Erin Baker - *Pacific Northwest National Laboratory*

Wednesday @ 9:00 in Room 5 (Sierra)

Measurement of Underivatized Amino Acids in Dried Blood Spots by Isocratic LC-MS/MS to Diagnose and Monitor Multiple Metabolic Disorders

Cheryl Garganta - *University of Florida* (cgarganta@ufl.edu)

‣ Measurement of amino acids is important for diagnosis and management of disorders such as MSUD, PKU and tyrosinemia. Newborn screening allows early detection of these disorders but is limited by lack of separation of allo-isoleucine, a specific marker of MSUD. This method allows isocratic separation of leucine isomers within 3 minutes. It is suitable for use as a second tier test in newborn screening labs to evaluate specimens with elevated "leu" on flow-injection analysis. Preparation of calibrators in blood with hematocrit of 35-40% yields results that correlate well with results from plasma amino acid analysis. Multiple disorders can be monitored in a single assay.

Wednesday @ 9:20 in Room 5 (Sierra)

Persistently Increased Alloisoleucine in a Patient without Maple Syrup Urine Disease

Joesph Wiencek - *University of Virginia School of Medicine* (joesph.wiencek@virginia.edu) -- *Young Investigator Grantee*

‣ Quantitative analysis of plasma amino acids is a useful laboratory test in the investigation of metabolic diseases. In 1999, Schadewaldt et al. published in Clinical Chemistry the significance of alloisoleucine (allo-ile) in plasma for diagnosis of maple syrup urine disease (MSUD). Their findings indicated that the identification of allo-ile >5 µmol/L is pathognomonic for MSUD. In this study, we identified a 3-year-old patient with persistently (n=3) elevated allo-ile without clinical history or genetic confirmation of MSUD. Through the use of tandem mass spectrometry and our in-house liquid chromathography method, we were able to confirm a suspected interference.

Wednesday @ 9:40 in Room 5 (Sierra)

Multiple Reaction Monitoring (MRM) Profiling: Metabolomics Discovery Methodology Demonstrated with a Human Plasma Coronary Artery Disease Study

Karen Yannell - *Purdue University* (kcesafsk@purdue.edu) -- *Young Investigator Grantee*

‣ Multiple reaction monitoring (MRM)-profiling is demonstrated with a human plasma coronary artery disease (CAD) study. This semi-targeted first pass metabolomics methodology explores a sample for biological functional groups with precursor and neutral loss scans. Peaks from those scans are converted to transitions in a MRM method for rapid screening of samples. Univariate and multivariate statistics are used to determine which transitions are potential biomarkers. This CAD study (N>1000) found 177 transitions separating CAD from control samples with an agreement of 91% for males and 92% for females which shows the effectiveness of this methodology. Identification of these transitions is ongoing.

• Session 1 • Track 6 •

Keynote - Tissue Imaging

Wednesday @ 9:00 in Room 6 (SmokeTree)

Session Chair: Jeff Spraggins - *Vanderbilt*

Wednesday @ 9:00 in Room 6 (SmokeTree)

Application of N-Glycan MALDI MS Imaging to Identify Biomarker Signatures of Advanced Cancers in FFPE Tissues

Richard Drake - *Medical University of South Carolina* (draker@musc.edu)

‣ Alterations in cell surface glycosylation during tumorigenesis are well documented, and most current FDA approved cancer biomarkers are glycoproteins or glycan antigens. A MALDI mass spectrometry imaging method to spatially profile N-linked glycans in formalin-fixed paraffin-embedded (FFPE) tissue sections and tissue microarrays (TMAs) has been applied to nearly 1000 patient samples of breast and prostate cancer tissues. Analysis was done using MALDI-FTICR MS and a new rapid MALDI-TOF MS TissueTyper. Classes of N-glycans representing the most lethal forms of each cancer will be described. The goal will be to develop the approach as a prognostic assay for disease stratification at the time of diagnosis.

• Session 1 • Track 9 •
Microbiology Identification
Wednesday @ 9:00 in Andreas
Session Chair: Kent Voorhees - *Colorado School of Mines*

Wednesday @ 9:00 in Andreas
Metal Oxide Laser Ionization MS Bacterial Fatty Acid Composition for Rapid ID and Antibiotic Resistance Determination
Chris Cox - *Colorado School of Mines* (crcox@mines.edu)
‣ MALDI-TOF MS protein profiling has emerged as a rapid approach for clinical bacterial diagnostics. However, current methods do not address the increasing demand for antibiotic resistance profiling and often cannot accurately ID closely related phylotypes. As a result, additional culture-based tests are required to inform antibiotic therapy and confirm ID if protein-based methods fail. This adds significant time and expense, further delaying patient treatment and reducing the likelihood of positive therapeutic outcomes. We investigated metal oxide laser ionization (MOLI) MS fatty acid analysis as an alternative and achieved highly accurate simultaneous strain-level ID and resistance profiling of methicillin resistant *Staphylococcus aureus* and aminoglycoside, cephalosporin and fluoroquinolone resistant *Pseudomonas aeruginosa*.

Wednesday @ 9:20 in Andreas
Laser Assisted Rapid Evaporative Ionisation Mass Spectrometry (LA-REIMS): An Automated High-Throughput Platform for Clinical Microbiology and Beyond
Simon Cameron - *Imperial College London* (s.cameron@imperial.ac.uk) -- *Young Investigator Grantee*
‣ Rapid evaporative ionization mass spectrometry (REIMS) is a novel technique for the identification of microorganisms, and unlike commercially available MS platforms, does not require sample preparation such as the addition of a matrix. Previously, REIMS used an electrical current to heat a sample, causing it to evaporate and produce gas-phase ions which could be aspirated directly to a mass spectrometer and analysed in real-time. Here, we detail the transition to using a CO2 laser for biomass heating; removing the necessity for contact to be made with the sample and allowing sample throughput to be increased by approximately 50%. This presentation will detail optimisation of the laser assisted REIMS platform, the creation of a reference spectral database for over 60 microbial species, the determination of antimicrobial susceptibilities, and direct from clinical sample pathogen detection.

Wednesday @ 9:40 in Andreas
Metabolic Phenotyping of *Pseudomonas aeruginosa* Using Rapid Evaporative Ionization Mass Spectrometry: Strain Characterization and Clinical Applications
Emmanuelle Bardin - *Imperial College London* (e.bardin15@imperial.ac.uk) -- *Young Investigator Grantee*
‣ Rapid evaporative ionization mass spectrometry (REIMS) competes, in terms of performance, cost, and ease of use, with other technologies currently available in clinical laboratories such as matrix assisted laser desorption ionisation mass spectrometry (MALDI). Here, we used REIMS to further study bacterial variability, at the sub-species level within Pseudomonas aeruginosa. REIMS allowed the detection of a highly diversified metabolome with variable levels of virulence-related metabolites, such as quorum sensing molecules and rhamnolipids, thereby supporting its role as a monitoring tool for infection exacerbation. We also demonstrated as a proof of concept that REIMS can achieve a strain classification for MLST types of 84% accuracy.

• Session 2 • Track 1 •

Cannabinoids - Alternative Matrices

Wednesday @ 11:00 in Room 1 (Mojave Learning Center)

Session Chair: Jackie Hubbard - *UCSD*

Wednesday @ 11:00 in Room 1 (Mojave Learning Center)

Simple and Rapid LC-MS/MS Methods for Quantitation of Five Cannabinoids in Breath and Blood Samples – Correlation in the Two Sample Forms

Y. Ruben Luo - *University of California, San Francisco* (ruben.luo@ucsf.edu) -- *Young Investigator Grantee*

‣ Due to the legalization of recreational cannabis use in some states in the US, simple and rapid cannabis use monitoring under certain circumstances is in urgent demand for both public health and safety concerns. A prototype breathalyzer for real-time cannabis use monitoring was built allowing for the collection of liquid-form breath samples. Two LC-MS/MS methods with simple and rapid sample preparation procedures were developed for quantitation of 5 cannabinoids THC, THCCOOH, 11-OH-THC, CBN, CBD in both blood (serum) and breath samples. The serum samples were "crashed" to remove proteins, filtered, and directly analyzed in LC-MS/MS without sample dry-down and reconstitution. The breath samples were simply diluted and directly analyzed in LC-MS/MS. Validation of the LC-MS/MS methods was carried out in terms of precision, accuracy, linear range, limit of quantitation (LOQ), and carryover.

Wednesday @ 11:20 in Room 1 (Mojave Learning Center)

Detection of *in utero* Exposure to Cannabis, What Are We Missing?

Triniti Scroggin - *ARUP Laboratories* (triniti.scroggin@aruplab.com) -- *Young Investigator Grantee*

‣ Detection of in utero exposure to drugs is critical to the immediate and long term medical and social management of newborns. Our objective was to develop an LC-MS/MS method for the detection and quantification of 5 cannabis analytes in the traditional neonate specimen type (meconium) and a relatively new specimen type (umbilical cord tissue) considering the wide usage of cannabis amongst pregnant women. This method could support studies designed to evaluate the patterns and concentrations of cannabis analytes observed in newborns exposed to cannabis in utero, as well as correlate such data with clinical and social outcomes.

Wednesday @ 11:40 in Room 1 (Mojave Learning Center)

Cannabinoids in Oral Fluid: Roadside Screening & Markers of Recent Use

Madeleine Swortwood - *Sam Houston State University* (mjs079@shsu.edu) -- *Young Investigator Grantee*

‣ Oral fluid (OF) is an important alternative matrix for monitoring drug use. Cannabis remains the most commonly used illicit drug worldwide. Oral fluid is easily collected under direct observation, deterring adulteration, and does not require specialized personnel for collection. High concentrations of tetrahydrocannabinol (THC) result primarily from oral mucosa contamination from smoking or vaporizing cannabis and can persist. Concentrations of carboxy-THC vary considerably between frequent and occasional smokers. This presentation will examine and compare two roadside screening devices to detect recent cannabis use in oral fluid in frequent and occasional cannabis smokers following controlled smoked, vaporized, and oral cannabis administration. Additionally, presence of minor cannabinoids present in oral fluid will be discussed as potential markers of recent cannabis intake.

• Session 2 • Track 2 •

Keynote - Joint Informatics and Microbiology

Wednesday @ 11:00 in Room 2 (Catalina)

Session Chair: Brendan MacLean - University of Washington

Wednesday @ 11:00 in Room 2 (Catalina)

Can We Advance Health Monitoring the Way Google Has Advanced Text Mining for the General Population?

Pieter Dorrestein - *UCSD* (pdorrestein@ucsd.edu)

‣ While significant advances have been made in proof-of-principle approaches in mass spectrometry, they are not yet used by the general population. Yet, and although still far away, the future potential exists that one day every person with a smart toilet, smart mirror and if size of instrumentation can be solved, a smart phone, will perform molecular analysis of any object/sample they want. While it is clear that such capabilities do not yet exist for mass spectrometry, we will highlight the potential with experiments from our own laboratories with our longterm longitudional data collections, crowdsourced sample collections and our patient at home freezer collection program so that episodes of disease can be characterized.

• Session 2 • Track 3 •

Keynote - Endocrine

Wednesday @ 11:00 in Room 3 (Madera)

Session Chair: Dan Holmes - *St. Paul's Hospital*

Wednesday @ 11:00 in Room 3 (Madera)

24,25(OH)$_2$ Vitamin D and Vitamin D Metabolite Ratio: New Players in the Exploration of Non-Parathyroid Hypercalcemia

Etienne Cavalier - *University of Liege* (etienne.cavalier@chu.ulg.ac.be)

‣ While the activation pathway of vitamin D (VTD) is well known, its catabolism through CYP24A1 or 24-hydroxylase, remains unknown to the vast majority of clinicians. The metabolism product of CYP24A1, 24,25(OH)2D, is of great clinical interest because it reflects both vitamin D (VTD) intake and the first step in VTD catabolism and thus the physiologic response to sufficient VTD. It has been shown that changes in serum 24,25(OH)2D are associated with changes in calcium absorption, bone turnover and PTH. The only way to measure 24,25(OH)2D is LC-MS/MS. We have recently published a method for simultaneous measurements of 25(OH)D, 24,25(OH)2D and the Vitamin D Metabolite Ratio (VMR) in serum samples by LC-MS/MS. The assessment of 24,25(OH)2D by LC-MSMS is an under-recognized clinical tool in the evaluation of patients presenting with hypercalcemia and low PTH.

• Session 2 • Track 4 •

Proteomics and Precision Medicine

Wednesday @ 11:00 in Room 4 (Pasadena)

Session Chair: Tim Collier - *Cleveland Heart Laboratory*

Wednesday @ 11:00 in Room 4 (Pasadena)

Proteomics Identifies DNAJB9 as a Pathogenic Protein in Fibrillary Glomerulonephritis

Surendra Dasari - *Mayo Clinic* (Dasari.Surendra@mayo.edu)

‣ Fibrillary glomerulonephritis (FGN) is a rare primary glomerular disease with unknown pathogenesis. A proteomic analysis of FGN glomeruli in patient biopsies detected six-fold overexpression of DNAJB9 protein when compared to amyloid glomeruli. DNAJB9 was not detected in glomeruli of healthy subjects and 19 types of non-FGN glomerular diseases. This highlights 100% sensitivity and 100% specificity of DNAJB9 as an FGN biomarker. Additional experiments showed that DNAJB9 was deposited extracellularly, localized to fibrils, and co-localized with Ig-gamma chains in FGN glomeruli. With this evidence, we propose that DNAJB9 is a strong biomarker for rapid diagnosis of FGN in renal biopsies.

Wednesday @ 11:20 in Room 4 (Pasadena)

Differential Processing of High-Molecular-Weight Kininogen Throughout Normal Pregnancy

Stephenie Droll - *National Institutes of Health* (stephenie.droll@nih.gov) -- *Young Investigator Grantee*

‣ Preeclampsia is a serious disorder of pregnancy resulting in adverse maternal and neonatal outcomes. Aberrant processing of high-molecular-weight kininogen(HK) in early pregnancy has been indicated preceding the onset of preeclampsia. HK derived peptides are possible biomarkers for the early detection of preeclampsia. The present study characterized the cleavage pattern of HK in longitudinal serum samples during normal pregnancy. Western blotting analysis demonstrated significantly decreased inactive HK and significantly increased active heavy chain (HC) and light chain (LC). LC-MS/MS analysis revealed significantly increased concentrations of HK peptide fragments during pregnancy. A large number of the cleavage peptide fragments mapped to LC-HK Domain 5, which down-regulates angiogenesis, inhibits endothelial cell proliferation and migration, and induces apoptosis of endothelial cells.

Wednesday @ 11:40 in Room 4 (Pasadena)

MALDI-TOF MS Profiling of Biological Fluids in Precision Medicine

Mark Duncan - *Biodesix Inc.* (mark.duncan@biodesix.com)

‣ The cost-effective, sensitive and practical identification and quantification of tear peptides and proteins is critical if we are to exploit the diagnostic potential of tear fluid. In the era of precision medicine, we will require methods that can precisely quantify multiple components simultaneously and deliver sensitive detection. The approach developed for this study is a non-targeted MALDI-MS based method for the analysis of human tear fluid. Our findings demonstrate that sensitive, practical and precise quantification of multiple components is achievable (CV values of 10% or less). This method described allows detection, identification, and quantification of potential biomarkers that relate to eye injury and/or disease. The results of this study further reinforce the view that tear analysis can serve as a diagnostic tool, and illustrate the Clinical potential of MALDI-TOF MS.

• Session 2 • Track 5 •

Direct Analysis in Metabolomics

Wednesday @ 11:00 in Room 5 (Sierra)

Session Chair: Gary Patti - Washington University, St. Louis

Wednesday @ 11:00 in Room 5 (Sierra)

Metabolic Phenotyping of *ex vivo* Human Lung Perfusion

Vincen Wu - *Imperial College London* (v.wu15@imperial.ac.uk) -- *Young Investigator Grantee*

‣ Many patients with end stage lung disease die on the transplant waiting list due to shortages of suitable donor lungs. Ex vivo lung perfusion (EVLP) is a novel technology in the field of lung transplantation for evaluation and reconditioning donor lungs to facilitate transplantation, thereby decreases waiting time and increases the availability of suitable donor lungs. We have utilised perfusate samples from the DEVELOP-UK national multicentre EVLP trial to gain insights into global metabolic changes during EVLP, as well as the efficacy between two different EVLP techniques, acellular and blood perfused approaches. From the results, it was shown that the blood perfused method has induced the increase of lactate, pyruvate, phenylalanine, and xanthine, and the decrease of glucose. Whereas, the levels of these metabolites in acellular method has remained relatively stable during EVLP.

Wednesday @ 11:20 in Room 5 (Sierra)

Innovations for Direct Tissue Analysis and Imaging with Mass Spectrometry

Richard Yost - *University of Florida* (ryost@ufl.edu)

‣ Direct analysis of tissue by mass spectrometry, including extensions to mass spectrometric imaging (MSI), permits rapid and direct analysis of tissue (when an image is not of interest) as well as providing a level of chemical information unmatched by any other imaging modality (including histopathology, MRI, and PET scans). This presentation will explore innovations in direct tissue analysis and MSI, focusing on new sampling methods (including real-time in situ microextraction using the flowprobe and desorption electrospray, and MALDI) and strategies for increasing the speed, spatial resolution, information content, and quantitative performance of the methods.

Wednesday @ 11:40 in Room 5 (Sierra)

Targeted Full-Scan Data Analysis Using the ChromXtractor Tool Suite

Adam Rosebrock - *Stony Brook University* (adam.rosebrock@stonybrookmedicine.edu)

‣ Ongoing advances in sensitivity, resolution, and acquisition speed of mass spectrometers are driving adoption in a growing range of research and clinical applications. New approaches for data storage, analysis, and review are necessary to deal with the increased volume and information density of new and emerging platforms. I will discuss how our open-source ChromXtractor software suite enables targeted analysis of full-scan LC/GC/CE-MS data, including the ability to (1) quickly analyze full scan mass spec data in a feature-centric fashion, (2) perform robust feature-level local chromatographic/electropherographic alignment, (3) streamline review of individual compounds within a sample or group, (4) enable project-wide consensus-bounded integration, (5) correct data to spiked-in mass labeled standards, while (6) passing data to and from other open-source and commercial tools.

• Session 2 • Track 6 •

New Applications

Wednesday @ 11:00 in Room 6 (SmokeTree)

Session Chair: Stephanie Cologna - *University of Illinois at Chicago*

Wednesday @ 11:00 in Room 6 (SmokeTree)

Assessing the Effect of Immunization on the Global Lipidome of Mouse Spleen Using MALDI FTICR IMS

Marissa Jones - *Vanderbilt University* (marissa.a.jones@vanderbilt.edu) -- *Young Investigator Grantee*

‣ Hypoxia plays a key role in immune response and can have mechanistic downstream effects on B cell survival, proliferation, and differentiation. Germinal Center (GC), where B cell undergoes proliferation, selection and differentiation, consists of light and dark zones in which the native oxygen levels vary. Immunization increases the size and number of GCs. While the connection between hypoxia and inflammation is widely understood, the effect of these hypoxic regions on biomolecular modification and distribution within activated lymphoid tissue structures are largely uncharacterized. Herein we propose using high mass and spatial resolution MALDI FTICR IMS to examine the effect of immunization on the differential expression of biomolecules within spleen.

Wednesday @ 11:20 in Room 6 (SmokeTree)

Spatially Resolved Profiling of Polymyxin B Induced Acute Kidney Injury

Andreas Dannhorn - *Imperial College London* (a.dannhorn16@imperial.ac.uk) -- *Young Investigator Grantee*

‣ The global problem of advancing antimicrobial resistance led to a renewed interest in Polymyxin antibiotics. These antibiotics are commonly used as a last resort in cases of uncontrolled infection with gram-negative bacteria. Polymyxin efficacy is linked to known neuro- and nephrotoxicity in the clinic. We applied multimodal Mass Spectrometry Imaging (MSI) to investigate Polymyxin induced acute kidney injury in a rat model. We were able to correlate drug accumulation in the organ with dose dependent effects it caused to the tissue metabolome. MSI analysis revealed drug induced phospholipidoses after receiving a low dose of PMB, whist a high dose induced acute kidney injury.

Wednesday @ 11:40 in Room 6 (SmokeTree)

Ambient Ionization Mass Spectrometry for Molecular Characterization and Surgical Diagnosis of Endometriosis

Clara Feider - *University of Texas at Austin* (clfeider@utexas.edu) -- *Young Investigator Grantee*

‣ Here, we describe the use of ambient ionization mass spectrometry (MS) techniques towards the molecular analysis of endometrial glands and stroma found within both healthy endometrial tissue and endometriosis lesions. Using ambient ionization MS analysis of the lipid and metabolite species in endometriosis lesions, we aim to find molecular ions that are indicative of endometriosis compared to normal endometrium from the same patients. The information gathered in this studied will be used to: 1) evaluate statistically significant alterations between healthy and diseases endometrium to yield insights into endometriosis pathogenesis; and 2) investigate the usefulness of intraoperative ambient MS during conservative endometriosis surgery to improve precision in endometriosis resection, reduce disease recurrence, and ultimately improve patient outcome.

• Session 2 • Track 7 •

Practical Training Intermediate: How to Achieve Lower Quantitation Limits

Wednesday @ 11:00 in Pueblo

Session Chair: Russell Grant - *LabCorp*

Wednesday @ 11:00 in Pueblo

How to Achieve Lower Quantification Limits : Part 1 : Foundations

Russ Grant - *LabCorp* (grantr@labcorp.com)

‣ This one hour session will be given as three 20 minute linked vignettes and will explore established and novel approaches to definitively improve analytical measurement performance - with the end goal of improving assay LLOQ. Part 1 "Foundations": Basis of LLOQ, signal:noise, lossless systems, and practically determining and improving measurement precision. Part 2 "Formulation": Getting the most out of your assay and system components, LC and preparative orthogonality and demystifying the black box after the LC via signal manipulation, smoothing and quadrupole resolution. Part 3 "Finesse": Tying the pieces together with assay exemplars.

Wednesday @ 11:20 in Pueblo

How to Achieve Lower Quantification Limits : Part 2 : Formulation

Russ Grant - *LabCorp* (grantr@labcorp.com)

‣ This one hour session will be given as three 20 minute linked vignettes and will explore established and novel approaches to definitively improve analytical measurement performance - with the end goal of improving assay LLOQ. Part 1 "Foundations": Basis of LLOQ, signal:noise, lossless systems, and practically determining and improving measurement precision. Part 2 "Formulation": Getting the most out of your assay and system components, LC and preparative orthogonality and demystifying the black box after the LC via signal manipulation, smoothing and quadrupole resolution. Part 3 "Finesse": Tying the pieces together with assay exemplars.

Wednesday @ 11:40 in Pueblo

How to Achieve Lower Quantification Limits : Part 3 : Finesse

Russ Grant - *LabCorp* (grantr@labcorp.com)

‣ This one hour session will be given as three 20 minute linked vignettes and will explore established and novel approaches to definitively improve analytical measurement performance - with the end goal of improving assay LLOQ. Part 1 "Foundations": Basis of LLOQ, signal:noise, lossless systems, and practically determining and improving measurement precision. Part 2 "Formulation": Getting the most out of your assay and system components, LC and preparative orthogonality and demystifying the black box after the LC via signal manipulation, smoothing and quadrupole resolution. Part 3 "Finesse": Tying the pieces together with assay exemplars.

• Session 2 • Track 8 •

Practical Training Basic: Introduction to Quantitative LC-MSMS

Wednesday @ 11:00 in Chino

Session Chair: Alec Saitman - *Providence Regional Laboratory*

Wednesday @ 11:00 in Chino

Clinical Mass Spectrometry Case Studies: How We Can "Read Between the Lines"

Alec Saitman - *Providence Regional Laboratories* (alec.saitman@providence.org)

‣ This session talk provides case studies which highlight the superiority of mass spectrometry when compared to other methodologies. Each case study describes how an added piece of mass spectrometry data can alter the entire clinical interpretation of a patient sample.

Wednesday @ 11:20 in Chino

Clinical Mass Spectrometry: Benefits and Considerations

Jeff Young - *Providence Health And Services* (jeffrey.young@providence.org)

‣ Implementation of liquid chromatography tandem mass spectrometry (LC-MS/MS) testing in a clinical laboratory is major undertaking. This presentation will focus on the operational benefits and drawbacks of performing LC-MS/MS testing. It will compare traditional immunoassay testing to LC-MS/MS and will include discussion on validation, costs, and staffing.

Wednesday @ 11:40 in Chino

A Brief Introduction to the Basics of LC-MS in the Clinical Laboratory

Nandu Chindarkar - *Kaiser Permanente Regional Lab* (nandkishor.s.chindarkar@kp.org)

‣ Bio: Nandu Chindarkar, PhD, is a Technical Director (Clinical Chemistry) at the Kaiser Permanente Regional Laboratory, Berkeley, CA. Dr. Chindarkar has worked on various mass spectrometry platforms over the last 14 years. He has extensive experience in developing LC-MS methods for clinical/toxicology applications. Short Abstract: The goal of this presentation is to introduce the audience to liquid LC-MS platform used in clinical laboratories. It provides a brief introduction to LC, ESI, and tandem quadrupole mass analyzer. Furthermore, an overview of detection and quantitation of an analyte using LC-MS will be provided.

• Session 3 • Track 1 •

Synthetic Cannabinoids Detection

Wednesday @ 14:30 in Room 1 (Mojave Learning Center)

Session Chair: Madeline Swortwood - *Sam Houston State University*

Wednesday @ 14:30 in Room 1 (Mojave Learning Center)

The Utility of LC-QTOF/MS in Proactive Synthetic Cannabinoid Testing in the Psychoactives Surveillance Consortium and Analysis Network (P SCAN)

Roy Gerona - *University of California, San Francisco* (Roy.Gerona@ucsf.edu)

‣ The ability to identify previously unreported new psychoactive substance (NPS) is a challenging task even for well-equipped laboratories. We developed a proactive approach to NPS testing that couple metabolite prediction and proactive synthesis of "prophetic" synthetic cannabinoid reference standards with targeted and suspect screening using LC-QTOF/MS in a recently established NPS surveillance network, the Psychoactives Surveillance Consortium And Analysis Network (P SCAN). We will present initial data to illustrate how this approach is used to identify, confirm and quantify analytes in biological samples in cases involving synthetic cannabinoids in the first 100 P SCAN cases.

Wednesday @ 14:50 in Room 1 (Mojave Learning Center)

Screening for Synthetic Cannabinoids in Blood Using LC-QTRAP

Matthew McMullin - *NMS Labs* (matthew.mcmullin@nmslabs.com)

‣ Since 2009 when we first encountered synthetic cannabinoids in blood the structural diversity has created analytical challenges with variable and for some poor ionization efficiencies. The enhanced sensitivity and specificity of the 2-dimensional QTRAP has made it possible to detect 36 analytes in a single method; and we can easily update the scope of analysis without major changes to the basic analytical method. The results from testing of 1241 blood samples in 2017 shows that 5-ADB, FUB-AMB and ADB-FUBINACA are currently the three most prevalent drugs in this case.

Wednesday @ 15:10 in Room 1 (Mojave Learning Center)

A Sustainable LC-MS/MS Testing Platform for K2 Synthetic Cannabinoids

Jeffery Moran - *University of Arkansas for Medical Sciences* (jeff.moran@pinpointtesting.com)

‣ The objective of this study is to validate a high-throughput analytical method for quantifying low levels of synthetic cannabinoids (SCBs) in human blood. The fully-customizable 96-well plate ToxBox® uses supported liquid extraction (SLE) to streamline sample preparation (<30 min) of high priority SCBs and over 100 potential confounding drugs. Fast LC-MS/MS procedures (< 7 min) also meet data quality objectives established for forensic and clinical applications and provide a high level of precision that enable low levels of quantification (< 1 ng/ml). Case studies presented as part of this study demonstrate utility in identifying specific metabolic products and provide insight for understanding the clinical consequences of SCB exposure, while controlling for potential confounding drug effects.

• Session 3 • Track 2 •
Clinical Operations
Wednesday @ 14:30 in Room 2 (Catalina)
Session Chair: Shannon Haymond - *Lurie Children's Hospital*

Wednesday @ 14:30 in Room 2 (Catalina)
Current Perspectives on Clinical Mass Spectrometry Auto-Data Review: An Innovative Solution
Alec Saitman - *Providence Regional Laboratories* (alec.saitman@providence.org)
‣ Dynamic mass spectrometry auto-data review is a concept that is not entirely new, but currently requires individual laboratories to produce highly customized, in-house solutions. There needs to be an easier way for laboratories to access these solutions, preferably using technologies and strategies many labs have already acquired. This presentation provides insight into a new driver developed by the middleware company, Data Innovations. The driver has the unique advantage of providing dynamic information using calibrator averages of important data elements. By elevating and incorporating clinical mass spectrometry data into middleware, we bridge the gap between mass spectrometry and automated instrumentation platforms.

Wednesday @ 14:50 in Room 2 (Catalina)
Interfacing MS Instrumentation in a Clinical Chemistry Routine Laboratory: Squeezing Standards vs Real Life Constraints
Pierre-Alain Binz - *CHUV Lausanne University Hospital* (pierre-alain.binz@chuv.ch)
‣ Automation is a key feature in today's laboratory medicine practice. Many industrial robotic and automated analyzers are interfaced with Laboratory Informatics Systems (LIS) and electronic patient record systems (EPR) using standard protocols and formats such as HL7 and ASTM. This also implies the use of middleware, data backup and archive architecture. Reaching this level of interoperability with current mass spectrometry equipment is not straightforward. Although specific data exchange formats exist in addition to the generic industrial ones (HUPO-PSI mzML and mzTAB for instance), the task is challenging due to heterogeneity of instrumentation, of vendors constraints, of data types and of result reporting format requirements. We will discuss how we have integrated our MS instruments into our clinical routine, from sample reception to results reporting.

Wednesday @ 15:10 in Room 2 (Catalina)
A Survey of Clinical Laboratories to Determine Needs for Clinical Mass Spectrometry Data Exchange
Patrick Mathias - *University of Washington* (pcm10@uw.edu)
‣ Mass spectrometry is a valuable platform for many clinical laboratories, but setting up data exchange between these instruments and laboratory information systems can be challenging. Instrument vendors utilize proprietary file formats and there is no standardization of data for clinical purposes. The Mass Spectrometry Data Interface Standardization (MSDIS) working group is assessing these challenges and distributed a survey to clinical laboratories to understand their data exchange needs. A variety of laboratory settings were represented and most laboratories had successfully interfaced their instruments. Data mapping and the need for verification rules were cited as important requirements among the surveyed laboratories.

• Session 3 • Track 3 •

Clinical Nuances in Ion Ratios, Intensive Care TDM And Assessment Of Malabsorption

Wednesday @ 14:30 in Room 3 (Madera)

Session Chair: Michael Chen - *Royal Jubilee Hospital, Victoria*

Wednesday @ 14:30 in Room 3 (Madera)

Simvastatin as a Biomarker for Intestinal Villous Health for Celiac Disease Patients

Robert Voyksner - *ImmunogenX* (robert_voyksner@lcmslimited.com)

‣ This work is leading to a minimally-invasive diagnostic for celiac disease (CD) management as an alternative to an invasive and expensive biopsy. The method uses administration of a drug biomarker simvastatin that is strongly metabolized by the CYP3A4 enzyme on the villi of the small intestine. Therefore, its concentration in subsequently drawn blood samples, as measured by LC/MS, is directly related to villous health. Here we report new trial data conducted at the Mayo Clinic that substantiates data from an initial feasibility study and further refines the method for extracting SV Cmax from just two blood draw time points.

Wednesday @ 14:50 in Room 3 (Madera)

A Sensitive Method for the Simultaneous UHPLC-MS/MS Analysis of Milrinone and Dobutamine in Blood Plasma Using NH4F as the Eluent Additive

Ruta Veigure - *University of Tartu* (ruta.veigure@ut.ee) -- *Young Investigator Grantee*

‣ We aimed to develop an HPLC-MS/MS method suitable for quantifying milrinone and dobutamine – two important cardiovascular drugs, in the limited sample volume conditions – from neonatal and paediatric patients' blood plasma samples. Sufficiently low LLOQ levels were necessary for obtaining adequate pharmacokinetic data for the evaluation of optimal dosing in the future. The developed and validated method facilitates only 20 µl of human plasma sample needed for the analysis with the quantification limit of 0.97 ng/mL. The matrix matched calibration was linear in the range of 1 - 300 ng/mL for both analytes. In addition, between-run accuracy remained within 87.5 – 114.8 %, and precision within 4.8 – 7.4 % for both analytes at all concentration levels (including LLOQ level) over the calibration range (including LLOQ level).

Wednesday @ 15:10 in Room 3 (Madera)

Matrix and Instrument Effects on Analyte Fragmentation and Ion Ratios

Geoffrey Rule - *ARUP Laboratories* (geoffrey.s.rule@aruplab.com)

‣ Unlike pharmaceutical bioanalysis, clinical mass spec labs use two ions to identify/confirm the identity of each analyte reported. The ratio of the quantitative and qualitative ions is generally required to be within certain limits of an expected value in order to confirm identity and report a result. Oftentimes these limits are arbitrarily set to +/- 35% with values falling outside these limits possibly given as "unreportable due to an interfering substance". This presentation explores several factors, including tube type, matrix and instrument effects that may influence fragment ion ratios from a given precursor.

• Session 3 • Track 4 •

Applications of High Resolution Mass Spectrometry

Wednesday @ 14:30 in Room 4 (Pasadena)

Session Chair: Jennifer Van Eyk - *Cedars-Sinai*

Wednesday @ 14:30 in Room 4 (Pasadena)

Everything You Wanted to Know (sort of) about High Resolution Q-TOF Quantitation of Peptides But Were Afraid to Ask

Michael Lassman - *Merck & Co* (michael_lassman@merck.com)

‣ The application of high resolution mass spectrometry (HR-MS) has drawn considerable attention by researchers interested in protein and peptide quantitation. HR-MS could replace traditional QQQ, requiring reduced method development time for targeted quantitation of peptides. Perhaps the paucity of published HR-MS quantitation assays is a direct result of uncertainty regarding how and even if HR-MS can be used for reliable quantitation of peptides. In this study, using oxyntomodulin as a test molecule, we evaluate the effects of different instrument acquisition and processing methods on the sensitivity of a Q-TOF instrument, as defined by accuracy and precision.

Wednesday @ 14:50 in Room 4 (Pasadena)

Top-Down Quantitative Determination of Intact Proteins in Serum by Multi-Dimensional LC/QTOF Mass Spectrometry

Jack Henion - *Q2 Solutions* (henionj@advion.com)

‣ A top-down LC/MS/MS method has been developed for the quantitative determination of an intact model protein (SigmaMab) in mouse plasma. Both the intact denatured protein and its intact native form have been studied with the goal of quantifying this protein using its commercially available stable isotope internal standard, SILUMab. SEC, HIC and weak cation exchange chromatography was coupled in an automated multi-dimensional manner to a QTOF MS system. A linear dynamic range from 0.2 to 20 ug/mL plasma was accomplished for this protein in its denatured form. Results of another biotherapeutic protein from incurred monkey serum will also be reported.

Wednesday @ 15:10 in Room 4 (Pasadena)

Quantitation of the Therapeutic Monoclonal Antibody Eculizumab Using High Resolution Accurate Mass Spectrometry

Ann Rivard - *Mayo Clinic Clincal Mass Spec Dev Lab- DLMP* (rivard.ann@mayo.edu)

‣ Eculizumab is a humanized IgG2/4¥ê monoclonal antibody therapeutic (t-mab) targeting complement component C5 of the alternative pathway. It is prescribed for rare, chronic conditions such as atypical hemolytic uremic syndrome (aHUS) and paroxysmal nocturnal hemoglobinuria (PNH). As an expensive t-mab, therapeutic monitoring is desired in attempt to decrease the high cost of therapy. A previously published method using the molecular mass of the intact light chain of the t-mab by microLC-ESI-Q-TOF mass spectrometry was adapted into a sensitive and specific assay, validated on a multiplexed HPLC-high resolution accurate mass spectrometer.

• Session 3 • Track 5 •

Ion Mobility and High Resolution in Metabolomics

Wednesday @ 14:30 in Room 5 (Sierra)

Session Chair: Adam Rosebrock - *Stony Brook*

Wednesday @ 14:30 in Room 5 (Sierra)

Lipidomic and Metabolomic Profiles Investigating the Role of Alzheimer's Disease and Genotype

Xueyun Zheng - *Pacific Northwest National Laboratory* (xueyun.zheng@pnnl.gov) -- *Young Investigator Grantee*

‣ The metabolism of metabolites and lipids have been shown to play important roles in Alzheimer's disease. However the mechanism of how they involved in the AD pathology remain unclear. In this study, we aimed to profile the presence of lipids and how they change in patient with AD. In this study, 126 brain tissue samples that were grey matter from the frontal cortex and cerebellum (disease control tissue) and 63 plasma samples were investigated. In order to study the differences in metabolites and lipid between AD and control grey matter, both metabolomics and lipidomics studies were performed by using ion mobility spectrometry coupled with mass spectrometry (IMS-MS), in combination with an ultra-fast sub-minute Rapidfire SPE or LC separations.

Wednesday @ 14:50 in Room 5 (Sierra)

Interest of High Resolution Mass Spectrometry in Metabolomics Studies for a Better Characterization of Primary Immunodeficiency in Humans

Anne Claire Boschat - *Institut Imagine* (anne-claire.boschat@institutimagine.org) -- *Young Investigator Grantee*

‣ We recently identified a mutation in Cytosine 5'-Triphosphate Synthase 1 (CTPS1) leading to a severe immunodeficiency, characterized by an impaired capacity of activated T and B cells to proliferate. To better assess the role of CTPS in the onset of immunodeficiency, we first developed mass spectrometry targeted assays for measuring CTPS activity, nucleotides and deoxynucleotides. We are now developing large-scale metabolomics in order to provide usable data to further explore the altered metabolic pathways during the immune response and better characterize immune deficiencies. As a first attempt, we compared the metabolome of resting and stimulated lymphocytes. These first experiments validated our methodology and we are now in progress to perform studies on precious cells from PIDs patients.

Wednesday @ 15:10 in Room 5 (Sierra)

Isotopic Ratio Outlier Analysis (IROA) in Combination with Ion Mobility/Mass Spectrometry for Higher Quality Metabolomic Profiling

Robin Kemperman - *University of Florida* (rkemperman@ufl.edu) -- *Young Investigator Grantee*

‣ Isotopic ratio outlier analysis (IROA) has been used for metabolite profiling studies by LC-MS. This powerful methodology can identify biochemical compounds using its characteristic isotope pattern created by a 5% and 95% 13C-labeled media. Although significant differences between chemical noise and biological signals are obtained, complex mass spectra cause difficulties in interpretation and mass overlap. This study will show how ion mobility spectrometry (IM) can assist deconvolution of IROA patterns and add a significantly higher confidence level to compound identification using IM drift times and collision cross sections.

• Session 3 • Track 6 •
Intraoperative Diagnosis
Wednesday @ 14:30 in Room 6 (SmokeTree)
Session Chair: David Muddiman - *North Carolina State University*

Wednesday @ 14:30 in Room 6 (SmokeTree)
An International "iKnife" Network to Validate Tissue-Specific Database Across Multi-Centers
Zsolt Bodai - *Imperial College London* (z.bodai@imperial.ac.uk) -- *Young Investigator Grantee*
‣ Rapid evaporative ionization mass spectrometry (REIMS) has been recently introduced and showed great promises to improve margin assessment in situ, opening up new perspectives in surgery management. REIMS analyses in real time the chemical composition of aerosols produced by electrosurgical devices and provides enough selectivity and specificity for differentiating tissues based on specific molecular signatures. But can other hospitals immediately implement the technology and use the previously built database? What is the inter- hospital and intra- hospital repeatability and reproducibility? In order to answer these questions, an international iKnife network was created. One of the first goals of the network is to monitor and assess reproducibility across different sites, identify pitfalls, and harmonize the protocols for surgical iKnife applications.

Wednesday @ 14:50 in Room 6 (SmokeTree)
Advanced Development of the MasSpec Pen Technology for Laparoscopic and Robotic Surgical Applications
Noah Giese - *University of Texas at Austin* (ngiese@utexas.edu) -- *Young Investigator Grantee*
‣ We describe the design and development of the MasSpec Pen for use in laparoscopic and robotic surgery. We have recently reported the development of the MasSpec Pen, a handheld device that allows non-destructive molecular analysis of tissue samples. The Laparoscopic MasSpec Pen allows comparable acquisition of molecular information from tissues while operating at extended lengths and increased resolution suitable for minimally invasive surgeries. We plan to apply this technology for accurate cancer prediction from normal and tumorous human tissue. Our results provide preliminary evidence that the laparoscopic MasSpec Pen will be suitable for minimally invasive surgical procedures.

Wednesday @ 15:10 in Room 6 (SmokeTree)
Towards *in situ* Tissue Classification to Improve Prostate Cancer Diagnosis Using Mass Spectrometry Imaging
Elizabeth Randall - *Brigham and Women's Hospital, Harvard Medical Scho* (erandall@bwh.harvard.edu) -- *Young Investigator Grantee*
‣ We present a workflow for the identification of biomarkers of prostate cancer and Gleason grade. High resolution matrix assisted laser desorption ionization mass spectrometry imaging (MALDI MSI) was performed on prostate tissue from patients with Gleason grade from 6 to 9. Unsupervised data analysis revealed ions that were differentially expressed between tumor and normal tissue, and between different Gleason grades. Ions were assigned based on high mass accuracy data searched using the Human Metabolome Database (HMDB). MALDI results were then correlated with a fast, ambient MS method for validation as a clinical tool to support image-guided prostate biopsy.

• Session 3 • Track 7 •

Practical Training Intermediate: Pharmacogenetics & MALDI-TOF

Wednesday @ 14:30 in Pueblo

Session Chair: Fang Wu - *St. Paul's Hospital*

Wednesday @ 14:30 in Pueblo

Getting Started with Pharmacogenetics Testing and Mass Spectrometry - I

Fang Wu *- St. Paul's Hospital, Saskatoon Health Region* (fang.wu@saskatoonhealthregion.ca)

‣ This session will discuss current strategies and applications for pharmacogenetics (PGx) testing using matrix assisted-laser desorption/ionization time-of-flight mass spectrometry (MALDI-TOF/MS) with the focus on single nucleotide variant (SNV) and copy number variant (CNV) analysis. The MALDI-TOF/MS basics and the workflow for SNV and CNV analysis will be explained. Guidance/recommendations on method validation will be discussed. The advantages and challenges of implementing MALDI-TOF/MS PGx in clinical laboratories will be presented using the presenters' laboratory data and data from publications from several key points, e.g. turnaround time, cost, personnel and technical issues associated with CNV analysis.

Wednesday @ 14:50 in Pueblo

Getting Started with Pharmacogenetics Testing and Mass Spectrometry - II

Fang Wu *- St. Paul's Hospital, Saskatoon Health Region* (fang.wu@saskatoonhealthregion.ca)

‣ After an overview of background information in Segment I, attendees are encouraged to take part in classroom discussions on the challenges of implementing MALDI-TOF/MS PGx tests. Afterwards, the presenter will summarize the discussions and further the topic with the main focus on cost, personnel, turnaround time and technical difficulties to further describe this topic. Several practical considerations for the implementation will also be considered, e.g. space and workflow automation.

Wednesday @ 15:10 in Pueblo

Getting Started with Pharmacogenetics Testing and Mass Spectrometry - III

Fang Wu *- St. Paul's Hospital, Saskatoon Health Region* (fang.wu@saskatoonhealthregion.ca)

‣ The last 20-minute segment will cover the method validation/evaluation for MALDI-TOF/MS PGx testing. Recommendations on accuracy, method comparison, reproducibility (within run and between run), sensitivity, carryover and specimen requirements will be given.

• Session 3 • Track 8 •

Practical Training Basic: Purchasing Your First LC-MSMS

Wednesday @ 14:30 in Chino

Session Chair: Deborah French - *UCSF*

Wednesday @ 14:30 in Chino

Selecting and Planning for the Right Mass Spectrometer_i

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

‣ Starting mass spectrometry testing in your laboratory, or adding a new mass spectrometer, is a daunting task. How do you make the right decision? And how do you finance this purchase? This 60 minute session will discuss: 1st 20 minutes: The different types of mass spectrometer that are available and what type of analyses they are best suited for. 2nd 20 minutes: Questions you should ask mass spectrometry vendors and colleagues and how you should test different instruments so that you are comparing apples to apples. 3rd 20 minutes: Financial considerations of purchasing a mass spectrometry system as well as return on investment calculation and negotiation with vendors. Audience participation will be encouraged!

Wednesday @ 14:50 in Chino

Making the Most of Vendor Visits and Discussions with Colleagues during Instrument Vendor Selection_II

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

‣ Starting mass spectrometry testing in your laboratory, or adding a new mass spectrometer, is a daunting task. How do you make the right decision? And how do you finance this purchase? This session will discuss questions you should ask mass spectrometry vendors and colleagues and how you should test different instruments so that you are comparing apples to apples. Audience participation will be encouraged!

Wednesday @ 15:10 in Chino

Financial Considerations for Purchasing a Mass Spectrometer_III

Joe El-Khoury - *Yale University* (deborah.french@ucsf.edu)

‣ Starting mass spectrometry testing in your laboratory, or adding a new mass spectrometer, is a daunting task. How do you make the right decision? And how do you finance this purchase? This session will discuss the financial considerations of purchasing a mass spectrometry system as well as return on investment calculation and negotiation with vendors. Audience participation will be encouraged!

• Session 3 • Track 9 •
Keynote - Microbiology
Wednesday @ 14:30 in Andreas
Session Chair: Chris Cox - *Colorado School of Mines*

Wednesday @ 14:30 in Andreas
Microbial Applications of Mass Spectrometry
Kent Voorhees - *Colorado School of Mines* (kvtv@comcast.net)
‣ Mass spectrometry for bacterial identification has a long history. The first studies of this application were reported in the 1960s. Since then, pyrolysis, gas chromatography, liquid chromatography, and Lasers have been combined with mass spectrometry to characterize bacteria. The application of MALDI to whole cell bacteria for protein profiling is relatively new and was first reported in 1996. This foundation research lead to the commercialization of the technique and has resulted in sales of approximately 4000 units. Although popular, protein profiling has its drawbacks and does not work well with closely related bacterial species. We have extended MALDI to fatty acid analysis using metal oxide as a catalytic matrix free platform to overcome the protein profiling shortfalls. This presentation will present a historical summary of bacterial mass spectrometry applications.

• Session 4 • Track 1 •

Driving and MJ: Analytical Approaches and the Washington State Experience

Thursday @ 9:00 in Room 1 (Mojave Learning Center)

Session Chair: Jack Henion - *Advion, Inc.*

Thursday @ 9:00 in Room 1 (Mojave Learning Center)

Method Development and Validation of LC-MS/MS Assay for Quantification of Cannabinoids in Whole Blood

Breland Smith - *InSource Diagnostics* (besmith8984@gmail.com)

‣ A majority of US states have passed laws allowing either medical or recreational use of marijuana. The method development and validation of an LC-MS/MS assay to quantify Δ9-tetrahydrocannabinol (THC) and 9 other cannabinoids in whole blood will be discussed in this presentation. Cannabinoids are isolated from 200 µL of whole blood to achieve an LLOQ of 0.5 – 1.0 ng/mL for all analytes. This assay is currently being used to support studies in conjunction with the Center for Medical Marijuana Research (CMCR) aimed at understanding the pharmacokinetics of cannabinoids for the purpose of identifying biomarkers that can accurately predict impairment.

Thursday @ 9:20 in Room 1 (Mojave Learning Center)

Detection and Levels of Cannabinoids in Whole Blood and Oral Fluid After Recent Marijuana Inhalation

Jacqueline Hubbard - *University of California, San Diego* (jahubbard@ucsd.edu)

‣ Marijuana use is growing in popularity in the United States due to it being legalized in several states and U.S. territories. This has raised concerns regarding the impact of marijuana on driving performance. Therefore, it is critical to have ways to accurately measure levels of cannabinoids. Using liquid chromatography- tandem mass spectrometry (LC-MS/MS), levels of Δ9-tetrahydrocannabinol (THC), the main psychoactive compound in marijuana, and several of its metabolites were measured in whole blood (WB) and oral fluid (OF) after recent cannabis inhalation. In this presentation, preliminary data on the detection and levels of cannabinoids observed in WB and OF will be discussed. Both the utility and limitations of confirming recent marijuana use through cannabinoid monitoring with LC-MS/MS will be conveyed.

Thursday @ 9:40 in Room 1 (Mojave Learning Center)

The Prevalence of Marijuana in Suspected Impaired Driving Cases in Washington State

Brianna Peterson - *Washington State Patrol* (brianna.peterson@wsp.wa.gov)

‣ The prevalence of both active THC and its metabolite carboxy-THC (THCCOOH) detected in suspected impaired driving cases pre-legalization was compared to the prevalence post-legalization for the state of Washington.

• Session 4 • Track 2 •

Proteomic Analysis

Thursday @ 9:00 in Room 2 (Catalina)

Session Chair: Pierre-Alain Binz - *CHUV Lausanne University Hospital*

Thursday @ 9:00 in Room 2 (Catalina)

Statistical Identification and Quantitative Deconvolution of Hemoglobin Beta Chain Isotypes Unresolved by LC-MS by Isotopic Vector Angle Analysis

Luke Schneider - *Target Discovery, Inc./ Veritomyx, Inc.* (luke_schneider@targetdiscovery.com)

‣ Isotopic Vector Angle (IVA) analysis is a new approach to statistically detect and quantitatively deconvolve nearly complete overlapping isotopic patterns within one spectrum. This method is based on the computational representation of isotopic abundance patterns as vectors and comparison between patterns via calculation of vector angles. In this paper, IVA analysis statistically detects and deconvolves chromatographically unresolved hemoglobin variants with a mass difference of less than 4 mass units from normal hemoglobin beta chain.

Thursday @ 9:20 in Room 2 (Catalina)

Using Data Independent Acquisition to Develop a Targeted Assay for the Generation of Molecular Signatures of Neurodegenerative Disease in Biological Fluids

Sandra Spencer - *University of Washington* (sespence@uw.edu) -- *Young Investigator Grantee*

‣ Alzheimer's disease (AD) represents an increasing and unchecked burden on the population and the economy, projected to affect 16 million people with a healthcare cost of $1.1 trillion by 2050.1 Definitive diagnosis of AD uses outdated technology and can only be performed post-mortem; far too late to inform treatment and prognosis. We use data independent acquisition (DIA) of MS data to establish a well characterized proteomic profile of cerebrospinal fluid (CSF) from patients with AD). A molecular signatures of AD in CSF and plasma is developed and a targeted assay for each of the reliably detected peptides will be developed and validated- in essence an expanded version of an assay offered by Caprion for CSF2 but designed based on deep-dive empirical data. This work is expected to improve early detection of AD using a biofluid that can be safely collected during a routine clinical visit.

Thursday @ 9:40 in Room 2 (Catalina)

A Systematic Approach to Data-Independent Acquisition-MS for Plasma-based Proteomics Analyses

Shenyan Zhang - *Cedars Sinai Medical Center* (shenyan.zhang@cshs.org) -- *Young Investigator Grantee*

‣ Plasma is one of the most common matrices for clinical proteomics analyses. The advent of data-independent acquisition(DIA) mass spectrometry has enabled the simultaneous quantitative analysis of hundreds of proteins in plasma samples in support population and disease studies. Unlike MRM workflows that target a constrained number of peptides for accurate quantitation, DIA workflows cannot be simultaneously tailored to suit all plasma protein subsets. We sought to identify the subset of proteins that are most amenable to quantitative analysis by DIA-MS from depleted- and undepleted-plasma samples, respectively. In the process, we built a QC strategy for DIA-MS that monitors the digestion, desalting, and LC-MS steps inherent to plasma proteomics workflows. This strategy serves as a useful guide for DIA-MS analysis of large cohort studies.

• Session 4 • Track 3 •

LC Free: Is it for me?

Thursday @ 9:00 in Room 3 (Madera)

Session Chair: Jennifer Colby - *Vanderbilt*

Thursday @ 9:00 in Room 3 (Madera)

Can LC-MS be Replaced by Direct Coupling of SPME to MS in Clinical Applications?

German Gomez-Rios - *University of Waterloo* (tutogomez1@gmail.com) -- *Young Investigator Grantee*

‣ This work presents most recent developments in Coated Blade Spray (CBS)-Mass Spectrometry towards the analysis of small molecules in biofluids. For instance, we explore novel strategies for analysis of small sample volumes (blood droplets) as well as a new methodology for rapid analysis of controlled substances in urine and plasma samples (under 15s per sample).

Thursday @ 9:20 in Room 3 (Madera)

Evolution of Sponge Spray for Direct Sampling and Analysis by MS

Max Hecht - *University of Tartu* (hecht@ut.ee) -- *Young Investigator Grantee*

‣ Sample preparation for the analysis of clinical samples with the mass spectrometer (MS) can be extensive and expensive. With the novel sampling and MS analysis technique we call sponge spray, we can circumvent this and directly analyse blood, plasma and urine. A volumetric absorption microsampling (Neoteryx Mitra) device is used to take up an exact amount of sample and from that same tip an electrospray can be directed into a mass spectrometer. We demonstrated that although with significant matrix effects, quantitation of penicillin G, a common antimicrobial, is possible in plasma and urine.

Thursday @ 9:40 in Room 3 (Madera)

Multiple Point-of-Care Applications of Ambient Mass Spectrometry for the Emergency Department

Jentaie Shiea - *National Sun Yat-Sen University* (jetea@fac.nsysu.edu.tw)

‣ We have developed a multi-tasking ambient mass spectrometry platform which is capable of rapidly identifying pesticides in suicide patients, abused drugs in overdosed patients, and herbal toxic ingredients in intoxicated patients in the emergency department. The specimens collected from the patients include gastric lavage fluid, urine and real samples of herbal plants or herbal decoction. The turnaround time of the technique is less than one minute per sample analysis. Its limit-of-detection is at sub-ppm levels. Good reproducibility of the tests (RSD < 15%) reflects its high precision. This platform provides the information for emergency physicians to decide correct treatment in the shortest possible time.

• Session 4 • Track 4 •

Keynote - Proteomics

Thursday @ 9:00 in Room 4 (Pasadena)

Session Chair: Michael Lassman - *Merck & Co.*

Thursday @ 9:00 in Room 4 (Pasadena)

Protein Biomarker Immunoaffinity Mass Spectrometry: Enabling Translational Pharmacology of Biologics in Pharma

Hendrik Neubert - *Pfizer Inc* (hendrik.neubert@pfizer.com)

‣ Significant efforts are spent in the pharmaceutical industry to execute translational pharmacology strategies aiming to reduce costly compound attrition in phase 2 clinical trials. A key element is to develop a deep understanding of the properties of human drug targets early on in discovery phases as well as to predict and assess using clinical bioanalysis how targets are engaged by biologics. This leads to better target selection, improved prediction of drug exposure and clinical dosing regimen. To this end, the pharmaceutical industry has been applying quantitative protein mass spectrometry for over a decade now. This presentation will illustrate this development with case studies and share our future vision for quantitative protein biomarker mass spectrometry in biopharmaceutical research.

• Session 4 • Track 5 •
Biomarkers in Metabolomics
Thursday @ 9:00 in Room 5 (Sierra)
Session Chair: Xueyun Zheng - PNNL

Thursday @ 9:00 in Room 5 (Sierra)
***In vitro* Volatile Compound Bacterial Profiling Using GC-MS and their Potential Role for the Diagnosis of Oesophago-Gastric Cancer**
Mina Adam - *Imperial College London UK* (m.adam15@imperial.ac.uk) -- *Young Investigator Grantee*
‣ The potential role of bacteria in Oesophago-Gastric(OG) tumorigenesis and their influence on Volatile Organic Compounds (VOCs) produced within the upper gastrointestinal tract is currently unknown. The detection and quantification of VOCs has great potential in terms of disease diagnosis. In this study, Gas Chromatography Mass Spectrometry has been utilised for the identification of VOCs from bacteria that are present in OG cancer. Data demonstrated the presence of specific predominant bacteria in cancer patients producing acetic acid, phenol, acetaldehyde and 2-pentene. Similar compounds have previously been identified at increased concentrations in exhaled breath and the headspace of tissue biopsies from OG cancer patients. These findings support further culturing investigations to understand the role of microbiome with VOCs and their potential diagnostic and therapeutic significance.

Thursday @ 9:20 in Room 5 (Sierra)
Metabolomic Profiling of a Large Cohort of Glioblastoma Stem Cell Lines Identifies Metabolites Associated with Clinical Outcome
Amy Caudy - *University of Toronto* (amy.caudy@utoronto.ca)
‣ Glioblastoma multiforme tumors are driven by a rare stem cell population. In an effort to identify metabolic pathways active in these tumors as new therapeutic targets for a disease with few available drug therapies, we have profiled the metabolome of patient-derived glioblastoma stem cell lines cultured in vitro. To enable this large-scale project with samples arriving over a period of years, we have developed stable, reliable LC-MS methods and a biologically derived stable isotope reference material to enable comparison across different sample sets. We observe differences among patients in levels of 2-hydroxyglutarate and alpha-aminoadipic-acid, two metabolites whose levels have been linked to the progression of glioblastoma, and we observe many other known and unidentified metabolites whose levels vary across patients.

Thursday @ 9:40 in Room 5 (Sierra)
Metabolomic Biomarkers for Human Plasma Quality
Casey Chamberlain - *University of Florida* (chamberlainc@ufl.edu) -- *Young Investigator Grantee*
‣ This study seeks to define global trends in human plasma under various storage conditions to identify biomarkers for sample age and quality. Plasma was obtained through American Red Cross (pooled from approximately 5,000 individuals) as well as from four individual subjects. Analysis by UHPLC-HRMS was conducted using a Thermo Scientific Q Exactive coupled to a Dionex Ultimate 3000 UHPLC System. The effect of butylated hydroxytoluene (BHT) in stabilizing plasma metabolites was also investigated. Many significantly-changing metabolites were identified and evaluated as biomarkers for sample quality. Plasma showed to be largely unstable when left at ambient temperature even for short periods of time.

• Session 4 • Track 6 •

Biomarker Discovery and Validation

Thursday @ 9:00 in Room 6 (SmokeTree)

Session Chair: Clara L. Feider - *University of Texas at Austin*

Thursday @ 9:00 in Room 6 (SmokeTree)

Lipid Mapping in Niemann-Pick Disease, Type C1

Stephanie Cologna - *University of Illinois at Chicago* (cologna@uic.edu)

‣ Niemann-Pick Disease, type C1 (NPC1) is a fatal, genetic, neurodegenerative disease that is characterized by the accumulation of unesterified cholesterol and sphingolipids in the endo/lysosomal system. A hallmark of NPC1 includes progressive neurodegeneration of the cerebellum. In this study, we performed mass spectrometry imaging on cerebellar tissue from control and mutant NPC1 mice. Additionally, we developed an algorithmic platform to analyze technical and biological replicate similarity. Finally, our LC-MS studies have been used to confirm potential lipid alterations in NPC1. The results of these studies will be presented.

Thursday @ 9:20 in Room 6 (SmokeTree)

Combining MALDI MS Imaging with 2D Gel-based Proteomics to Reveal Potential Penile Carcinoma Biomarkers

Elisangela Silva - *A.C.Camargo Cancer center* (esilva@cipe.accamargo.org.br) -- *Young Investigator Grantee*

‣ Penile cancer (PeCa) is a mutilating men's malignant tumor, especially in underprivileged socioeconomic regions of developing countries. New markers are still needed for early diagnosis, prognosis and prediction of therapy. Supervised and unsupervised analysis, using MALDI Mass Spectrometry Imaging (MSI) integrated with 2D gel data, provided evidence that the protein calreticulin might be a potential biomarker of PeCa. Immunohistochemistry validation was performed in PeCa tumors and controls. Calreticulin expression was associated with poorly prognosis in PeCa patients. Our approach proved to be useful for the in situ analysis of target protein and for the development of biomarkers with clinical value.

Thursday @ 9:40 in Room 6 (SmokeTree)

Mitochondrial Changes of Articular Cartilage by Oxygen

Brenda Bakker - *University of Twente* (b.bakker-1@utwente.nl) -- *Young Investigator Grantee*

‣ In this study we employed several mass spectrometry modalities to identify molecular changes by oxygen in chondrocytes. We found changes in the lipidome, proteome and metabolome that all signify alterations in mitochondria. These mitochondrial changes may explain why chondrocytes perform poorly and lose their phenotype in supraphysiological oxygen levels and cartilage degenerative disease such as osteoarthritis. Targeting these specific molecular changes may be relevant for retaining the chondrogenic phenotype which has important implications for the treatment of bone and cartilage diseases.

• Session 4 • Track 7 •

Practical Training Intermediate: LC-MSMS Interference Testing

Thursday @ 9:00 in Pueblo

Session Chair: Zlatuse Clark - *ARUP Laboratories*

Thursday @ 9:00 in Pueblo

Taking Aim at Interference (Without Shooting Yourself in the Foot) : Part 1

Zlatuse Clark - *ARUP Laboratories* (zlatuse.d.clark@aruplab.com)

‣ The popularity of LC-MS/MS-based methods for clinical testing continues to rise. However, despite their superior analytical specificity, these methods may still suffer from interference affecting method accuracy and precision, and hence negatively impacting patient care. Examples of interference issues in various methods and how they were resolved will be shown throughout the entire session. This session segment will discuss: • Sources of guidelines for interference testing in method development/validation and routine testing (CLSI, CAP, SWGTOX) • What is analytical interference and where does it come from? • How do we define acceptable interference levels?

Thursday @ 9:20 in Pueblo

Taking Aim at Interference (Without Shooting Yourself in the Foot) : Part 2

Zlatuse Clark - *ARUP Laboratories* (zlatuse.d.clark@aruplab.com)

‣ This session segment will discuss: • How do we test for interference in LC-MS/MS? • When do we test for interference?

Thursday @ 9:40 in Pueblo

Taking Aim at Interference (Without Shooting Yourself in the Foot) : Part 3

Zlatuse Clark - *ARUP Laboratories* (zlatuse.d.clark@aruplab.com)

‣ This session segment will discuss: • The use of internal standard in mitigating interference • How do we monitor for interference?

• Session 4 • Track 8 •

Practical Training Basic: LC Theory for Troubleshooting

Thursday @ 9:00 in Chino

Session Chair: Autumn Breaud - *Johns Hopkins University*

Thursday @ 9:00 in Chino

LC Basics Part I: Demystifying Liquid Chromatography Separations and Hardware

Autumn Breaud - *Johns Hopkins University* (abreaud1@jhmi.edu)

‣ In this course, we will introduce LC basics including: principles of separation; liquid handling system hardware, including plumbing, pumps, valves, and autosamplers; and variations on traditional liquid chromatography systems including UHPLC, two-dimensional separations, and multiplexing.

Thursday @ 9:20 in Chino

LC Basics Part II: Troubleshooting and Staying Productive, or Up a Creek? Pick a Paddle

Autumn Breaud - *Johns Hopkins University* (abreaud1@jhmi.edu)

‣ In part II of this session, we will introduce diagnostic tools commonly used to troubleshoot LC systems, including pressure trace analysis and lot check-in record-keeping and review. We will then introduce the six most common LC problems observed in our production laboratory and how to determine them.

Thursday @ 9:40 in Chino

LC Basics Part III: Case Studies in Separations Sleuthing

Autumn Breaud - *Johns Hopkins University* (abreaud1@jhmi.edu)

‣ In part III of this course, we will introduce case studies in troubleshooting which incorporate the principles introduced throughout the session.

• Session 4 • Track 9 •
Analysis of Microbial Antibiotic Resistance
Thursday @ 9:00 in Andreas
Session Chair: John Lapek - *UCSD*

Thursday @ 9:00 in Andreas
A Rapid, Functional, Mass Spectrometry-based Assay for Detecting Carbapenemase Activity and Differentiating Carbapenemase Class
Joshua Hayden - *Weill Cornell Medical College* (jah9108@med.cornell.edu)
‣ Our objective was to develop a rapid, functional assay for carbapenemase activity that could potentially differentiate the various classes (A, B and D). The assay uses dilute-and-shoot liquid chromatography tandem mass spectrometry (LCMS) to monitor meropenem degradation in tryptic soy broth inoculated with bacterial isolates. The method showed excellent agreement with the modified carbapenemase inactivation method (mCIM) on 74 clinical isolates. Ethylenediaminetetraacetic acid inhibited the class B zinc-dependent carbapenemases (IMP, NMD and VIM), allowing segregation of this class. The class D (OXA-type) carbapenemases exhibited slower meropenem degradation at early time points, differentiating them from class A serine (IMI and KPC) enzymes. This method represents a rapid, functional assay that can offer valuable insight into carbapenem resistance mechanisms in clinical isolates.

Thursday @ 9:20 in Andreas
Resistome Profiling in Gram Negative Bacteria to Identify Selection-Averse Antimicrobial Drug Targets
Anaamika Campeau - *University of California, San Diego* (acampeau@ucsd.edu) -- *Young Investigator Grantee*
‣ The advent of Gram negative bacterial strains increasingly resistant to standard regimens of antibiotics represents an imminent public health crisis. Given the long-term unsustainability of traditional antimicrobial drug development, novel, systems-based strategies that combat bacterial infection from multiple angles are needed. Here, we performed adaptive laboratory evolution (ALE) on a model Gram negative, E. coli, and on a closely-related human pathogen, K. pneumoniae. Following the evolution of these strains, we performed whole genome sequencing and quantitative mass spectrometry-based proteomic profiling of evolved strains. This work will ultimately lead to the functional characterization of new, selection-averse drug targets.

Thursday @ 9:40 in Andreas
Lipid Signatures as Diagnostic Predictors of β-Lactam "Seesaw Effect" in Glycopeptide, Lipopeptide, and Lipoglycopeptide Resistance
Kelly Hines - *University of Washington* (kmhines5@uw.edu) -- *Young Investigator Grantee*
‣ Lipopeptide and lipoglycopeptide antimicrobials daptomycin and dalbavancin, respectively, were developed as last-resort therapies for the management of MRSA, but emerging cross-resistance among these therapies and the glycopeptide vancomycin is a threat to patient outcomes. β-Lactam antimicrobials are known to exhibit a "seesaw effect" with vancomycin and daptomycin, whereby β-lactam minimum inhibitory concentrations (MICs) decrease as daptomycin and vancomycin MICs increase. We have evaluated membrane lipid content, β-lactam susceptibilities and genetic mutations of in vitro derived mutants of MRSA strain N315 with resistance to vancomycin, daptomycin and dalbavancin to develop predictive signatures of cross-resistance and the β-lactam "seesaw effect".

• Session 5 • Track 1 •

Certifying Marijuana for Consumption

Thursday @ 11:00 in Room 1 (Mojave Learning Center)

Session Chair: Brianna Peterson - *Washington State Patrol*

Thursday @ 11:00 in Room 1 (Mojave Learning Center)

Analysis of Cannabis-Related Samples for Composition via LC-MS Employing a Compact Mass Spectrometer

Jack Henion - *Advion, Inc* (henionj@advion.com)

‣ The analyses of cannabis-related plant materials and products are being performed using techniques ranging from the very simple, unsophisticated 'tests' to highly selective, very expensive analytical approaches. This presentation will describe an approach which uses generally accepted analytical methods, as well as a technique that uses a compact mass spectrometer equipped for LC/MS, to assure accuracy and precision for the qualitative and quantitative determination of potency and pesticides in cannabis-related samples. A comparison of LC/UV coupled in-line with selected ion monitoring (SIM/MS) will be shown for both potency and pesticide measurements from plant materials.

Thursday @ 11:20 in Room 1 (Mojave Learning Center)

Mass Spectrometric Analysis of Medicinal Cannabis and Synthetic Cannabinoids at a State Public Health Laboratory

Kenneth Aldous - *Wadsworth Center , NY State Department of Health* (kenneth.aldous@health.ny.gov)

‣ Medicinal cannabis (MC) is available in 28 States of the US. The lack of standardized state regulations and testing has resulted in inconsistent quality and potency of products. NY State's Public Health Laboratory has been required to develop validated methods for testing and confirm the quality and potency of distributed products to meet MC program regulations and identify illegal synthetic cannabinoids. We present the laboratory assays developed, applying mass spectrometry methods, for the analysis of final MC products that are approved under the current NY state program regulations. Methods developed for determining 9 major phytocannabinoids and contaminants such as pesticides, growth regulators and trace elements are presented.

Thursday @ 11:40 in Room 1 (Mojave Learning Center)

A New Approach for Phytocannabinoids Comprehensive Metabolic Profiling: A Step Towards Understanding the Clinical Effects of Cannabis

Paula Berman - *Technion - Israel Institute of Technology* (bermansh@gmail.com)

‣ Medical Cannabis today is prescribed to patients primarily by its content of (-)-Δ9-trans-tetrahydrocannabinol (Δ9-THC) and cannabidiol (CBD), regardless of the fact that the plant contains over 100 additional phytocannabinoids whose therapeutic effects and interplay have not yet been fully elucidated. In this study we suggest a new LC/MS/MS approach to identify phytocannabinoids from 10 different subclasses, and comprehensive profiling of the identified compounds in different medical Cannabis plants. This method is important for the successful medicalization and standardization of Cannabis, and critical when performing biological, medical and pharmacological-based research using medical Cannabis.

• Session 5 • Track 2 •

Machine learning and Data mining

Thursday @ 11:00 in Room 2 (Catalina)

Session Chair: Steve Master - *Children's Hospital of Philadelphia*

Thursday @ 11:00 in Room 2 (Catalina)

Data Mining Routine Results for Reference Intervals: Common Errors and Modern Techniques

Daniel Holmes - *St. Paul's Hospital, Univ. of British Columbia* (dr.daniel.holmes@gmail.com)

‣ Commonly employed graphical techniques (Hoffman and Bhattacharya) for parameter estimation of Gaussian Mixture Models will be demonstrated and discussed in application to "mining" reference intervals from the results of routine analyses. A frequent error in the implementation of the Hoffman Method and its ramifications will be demonstrated. The modern approach to this parameter estimation problem is maximum likelihood (ML) through the expectation maximization algorithm. This approach is implemented in a number of packages in the R programming language and will also be demonstrated. The benefit of ML approach is that it is not necessarily constrained by the assumption that the underlying mixture is Gaussian. This allows for fitting of skewed distributions without the application of normalizing transformations affording better results.

Thursday @ 11:20 in Room 2 (Catalina)

Data Mining at Scale – Turning the Data Gaze into the Data Result

Adam Zabell - *Indigo BioAutomation* (azabell@indigobio.com)

‣ When data retention rates scale from thousands of observations into billions, the opportunity to discover an outlier event goes up even as the ability to identify it goes down. The common methods of outlier detection in LC-MS/MS are designed to provide answers to an established question on a limited timescale. Expanding that timescale to use all of the available data is as much about the answer as it is the discovery of what question to ask. It is in this middle ground where data gazing, focused on human-centered pattern recognition, is essential prior to question codification and answer automation. We present several recent examples showing different patterns in the clinical setting, and work backwards to show the necessarily human process of 'query and revise.' In this intermediate step, it is the capacity for data curation which causes the biggest gap in understanding the system.

Thursday @ 11:40 in Room 2 (Catalina)

High-Throughput Mass Spectrometry Coupled to Machine Learning Algorithms to Enable Accelerated Biomarker Discovery

Jacques Corbeil - *Laval University* (jacques.corbeil@fmed.ulaval.ca)

‣ We developed a very efficient methodology coupling high throughput mass spectrometry and machine learning algorithms to reliably identify the minimum set of biomarkers (metabolites) that can be used as classifiers or predictors for specific phenotypes of interest.

• Session 5 • Track 3 •

Neonatal Toxicology: from bench to bedside

Thursday @ 11:00 in Room 3 (Madera)

Session Chair: Mark Marzinke - *Johns Hopkins*

Thursday @ 11:00 in Room 3 (Madera)

Analysis of 44 Drugs and their Metabolites in Umbilical Cord by LC-MS/MS

Vandana Megaraj - *Cincinnati Childrens Hospital* (vandana.megaraj@cchmc.org) -- *Young Investigator Grantee*

‣ Detection of in utero drug exposure in pregnant women at the time of delivery is critical to implementing effective treatment of the newborn for withdrawal symptoms of neonatal abstinence syndrome. Umbilical cord tissue offers an alternative to urine and meconium for the detection of drugs of abuse during pregnancy. A validated LC-MS/MS method for the simultaneous detection of 44 drugs and metabolites in umbilical cord was developed using a novel sample preparation followed by hydrolysis of the conjugates and solid phase extraction. The method was rapid, making it suitable for routine clinical use and had high sensitivity, accuracy and precision.

Thursday @ 11:20 in Room 3 (Madera)

Performance of Umbilical Cord Tissue and Meconium Toxicology Testing in a Population of Subjects Diagnosed with Neonatal Abstinence Syndrome

Jennifer Colby - *Vanderbilt University* (jennifer.colby@vanderbilt.edu)

‣ Exposure to drugs in utero has negative health consequences for neonates, and through the involvement of social services, may carry legal ramifications for parents. Drug exposure is confirmed using mass spectrometry based tests of specimens from the neonate, typically meconium or cord tissue. In this study, paired cord tissue and meconium samples were collected from neonates who were diagnosed with a drug withdrawal syndrome. A comparison of drug detection in cord tissue and meconium showed fair concordance, and that in spite of more sensitive analytical methods, fewer drugs were detected in cord tissue than in meconium.

Thursday @ 11:40 in Room 3 (Madera)

Method Performance and Clinical Workflow Outcomes Associated with Meconium and Umbilical Cord Toxicology Testing

Steven Cotten - *Ohio State University Wexner Medical Center* (Steven.Cotten@osumc.edu)

‣ Umbilical cord tissue testing for neonatal drug exposure enables proactive intervention to mitigate withdrawal symptoms and potential adverse effects in neonatal abstinence syndrome. Switching from meconium to UCT demonstrated reductions in collect to result time and positively impacted the nursing clinical workflow. Additionally the number of QNS specimens and missed collections was minimized compared to meconium. The clinical sensitivity and specificity evaluated through ICD9 and ICD10 codes showed mixed results for both specimen types. UCT showed increased clinical sensitivity and NPV for NAS relative to meconium. However, neither specimen showed a calculated sensitivity for NAS >80%.

• Session 5 • Track 4 •

Proteome methods and insights

Thursday @ 11:00 in Room 4 (Pasadena)

Session Chair: Mari DeMarco - *The University of British Columbia*

Thursday @ 11:00 in Room 4 (Pasadena)

Potential Clinical Implications for Measuring Thyroglobulin in Human Serum on a Micro-Flow LC-MS/MS System

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

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

Thursday @ 11:20 in Room 4 (Pasadena)

Multiplexed Quantification of Proteins in Dried Blood Spots

Clark Henderson - *University of Washington* (cmhende@uw.edu)

‣ Blood samples collected during clinical and epidemiological investigations are often archived using dried blood spots for future retrospective investigations of novel biomarkers of human disease. Several recent studies have investigated protein quantification using dried bloods spots, however few studies have determined their performance compared to matched plasma or serum samples measured using validated clinical assays. We developed a precise and linear bottom-up proteomic method for quantification of proteins in dried blood spots that demonstrated poorer accuracy than anticipated with matched plasma samples analyzed using clinically validated immunoassays.

Thursday @ 11:40 in Room 4 (Pasadena)

Albumin Oxidizability: A Rigorous Yardstick of Plasma/Serum Exposure to Thawed Conditions

Chad Borges - *Arizona State University* (chad.borges@asu.edu)

‣ Every year, improprieties in the pre-analytical handling & storage of blood plasma/serum (P/S) specimens employed in clinical laboratory research produce false leads--particularly in the world of biomarker discovery. Temporary exposure to the thawed state (> -30°C) is difficult if not impossible to comprehensively track. We have developed a low sample-volume (≤10 µL), dilute-and-shoot, intact protein mass spectrometric assay of albumin proteoforms, “ΔS-Cys-Albumin”, that estimates the equivalent number of room temperatures hours to which stored P/S samples have been exposed over the course of their lifetimes. The assay is based on the known population reference ranges for albumin, cystine, free cysteine and adventitious Cu2+ in P/S used in conjunction with our newly determined multiple-reaction rate law that accurately predicts the ex vivo formation of S-Cys-Albumin over time.

• Session 5 • Track 5 •
Keynote - Joint Metabolomics and Microbiology
Thursday @ 11:00 in Room 5 (Sierra)
Session Chair: Tim Garrett - *University of Florida*

Thursday @ 11:00 in Room 5 (Sierra)
Early Detection of Cystic Fibrosis Acute Pulmonary Exacerbations by Exhaled Breath Condensate Metabolomics
Facundo Fernández - *Georgia Institute of Technology* (facundo.fernandez@chemistry.gatech.edu)
‣ Progressive lung function decline in cystic fibrosis (CF) patients often does not proceed in a linear fashion, rather is punctuated by acute pulmonary exacerbations (APEs). The frequency of APEs severe enough to require hospitalization is a crucial factor of death in CF patients and the diagnosis remains challenging. The objective of this research is to develop reliable methods to predict oncoming APEs in order to prevent associated lung function loss, mortality and morbidity. In this study, non-targeted metabolomics profiling of exhaled breath condensate (EBC) samples from 36 pre-APE (CF patients 1 to 3 months before an APE) and 97 stable CF patients (CF subjects who are clinically stable without an APE for ?3 months) was performed using ultra performance liquid chromatography coupled to ultra-high resolution accurate mass high-field Orbitrap mass spectrometry. A supervised orthogonal partial least squares discriminant analysis (OPLS-DA) model, was able to distinguish pre-APE from stable CF samples with good accuracy (88.5-89.7%), sensitivity (81.0-84.6%) and specificity (89.6-93.6%), suggesting significant alterations in epithelial lining lung fluid monitored through EBC could be useful to detect APEs early, therefore improving patient outcomes.

• Session 5 • Track 6 •

New Developments and Technologies

Thursday @ 11:00 in Room 6 (SmokeTree)

Session Chair: Raf Van de Plas - *Delf University of Technology*

Thursday @ 11:00 in Room 6 (SmokeTree)

Metabolic Phenotyping of Fresh Frozen and Formalin-Fixed, Paraffin-Embedded Colorectal Tissue Samples Using DESI-MSI

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

‣ Colorectal cancer is one of the leading causes of cancer-related deaths and it is thought to be the third most commonly diagnosed type of cancer. In routine histopathology laboratories majority of samples are fixed in formalin and embedded in wax to allow further diagnosis. In this study we have assess the feasibility of DESI-MSI to distinguish between different tissue types in both fresh and paraffin-embedded colorectal samples. When normal versus tumour fresh samples were analysed, an accuracy of 87% and 91% was achieved, respectively. In case of the FFPE samples, metabolic information remaining in the tissue sections after standard histological processing was enough to discriminate between different tissue types in multiple samples (overall accuracy over 95%). This study has proven that DESI-MSI can be successfully employed not only for analysing fresh frozen but also FFPE samples.

Thursday @ 11:20 in Room 6 (SmokeTree)

Hyperspectral Chemical Imaging to Probe Amyloid Pathology in Alzheimer's Disease

Jörg Hanrieder - *University of Gothenburg* (jh@gu.se) -- *Young Investigator Grantee*

‣ The major pathological hallmarks of Alzheimer's disease (AD) is the progressive accumulation and aggregation of beta-amyloid (A) and hyperphosphorylated-tau, into neurotoxic deposits. A aggregation has been suggested as a possibly critical, early inducer driving the disease progression. However, the exact mechanisms underlying A pathology remain unknown, which hampers the development of effective AD treatment strategies. We here, developed a multimodal chemical imaging paradigm employing hyper spectral fluorescent amyloid imaging together with MALDI imaging mass spectrometry to probe Abeta plaque pathology in transgenic AD mice. The results show distinct localisation of e.g. ceramides to compact deposits, while phospho-ceramides localise to diffuse aggregates. The results highlight the potential of IMS for discovering novel pathological mechanisms underlying neurodegeneration.

Thursday @ 11:40 in Room 6 (SmokeTree)

Optimised Desorption Electrospray Ionisationmass Spectrometry Imaging (DESI-MSI) Method for the Analysis of Proteins/Peptides Directly from Tissue Sections

Emmanuelle Claude - *Waters Corporation* (emmanuelle_claude@waters.com)

‣ The detection of large biomolecules such as peptides and proteins directly from tissue sections by DESI-MSI has proven to be extremely challenging. Here we describe a newly developed method combining a series of optimized parameters and conditions (gas pressure, solvent composition and flow rate) which allow the extraction of large biomolecules from the tissue in droplet form. These droplets are desorbed/ionized using a heated MS capillary into multiply charged ions Detection of these multiply charged ions is enhanced using Ion Mobility which enables separation from the intense endogenous ion species and chemical background.

• Session 5 • Track 7 •

Practical Training Intermediate: Quality Assurance - The Path to Peace of Mind

Thursday @ 11:00 in Pueblo

Session Chair: Kara Lynch - *UCSF*

Thursday @ 11:00 in Pueblo

A Regulatory Review of QA Monitoring for LC-MS/MS: the Real Work Begins After Validation : Part 1

Kara Lynch - *University of California San Francisco* (kara.lynch@ucsf.edu)

‣ For mass spectrometry testing in the clinical laboratory, post-implementation monitoring for quality is just as important as method development and validation but often receives less attention. Assuring that your laboratory has designed and implemented a quality management system for LC-MS/MS testing is vital to maintaining quality. This talk will review available guidelines (CLSI C62A, CLSI EP23, CLSI QMS01, QMS06, QMS12) and typical parameters that are used to monitor the entire testing process. Example tools for monitoring quality assurance will be presented.

Thursday @ 11:20 in Pueblo

Design a Customized and Effective Quality Assurance Program for Your Laboratory : Part 2

Kara Lynch - *University of California San Francisco* (kara.lynch@ucsf.edu)

‣ Current laboratory practice guidelines outline metrics that should be monitored in LC-MS/MS QA programs; however, few resources provide specific steps on how to design a value-added QA program. In this session, practical examples and step-by-step instructions will be provided to demonstrate how to effectively select QA parameters, establish QA acceptability criteria, monitor QA data and utilize QA metrics to critically assess test performance. The first half will cover how meta-data can be used to define QA goals and catch problems early. The last half will demonstrate how to establish custom QA metric acceptability criteria using a statistical data-driven approach.

Thursday @ 11:40 in Pueblo

Potential New Approaches for Quality Assurance Monitoring : Part 3

Lorin Bachmann - *Virginia Commonwealth University* (lorin.bachmann@vcuhealth.org)

‣ Current method validation protocols and quality assurance programs may be insufficient to identify sample-specific interferences that contribute to erroneous results. In this 20 min session, examples will be provided to demonstrate how new approaches to quality assurance monitoring may be used to identify potentially inaccurate results. Learning objectives include: 1)Explain why LCMS/MS methods are not immune to sample-specific influences and review sources of sample-specific errors, 2)Explain concepts around cluster ion monitoring as an indicator of ionization effectiveness, 3)Show how cluster ion monitoring can be used as a QA monitor, 4)Participate in a 5 min brain storming session on ways to improve QA monitoring strategies.

• Session 5 • Track 8 •

Practical Training Basic: MSMS Survival Training

Thursday @ 11:00 in Chino

Session Chair: Phil Sobolesky - *UCSD*

Thursday @ 11:00 in Chino

Understanding the Importance of System Suitability Testing for Monitoring Instrument Health

Philip Sobolesky - *University of California San Diego* (psobolesky@ucsd.edu)

‣ High performance liquid chromatography tandem mass spectrometry is becoming a fixture in the modern clinical laboratory. The ability to describe the health status of your instrument is essential for accurate and reproducible patient results. The purpose of this presentation will be on the significance of selecting, developing, and monitoring a system suitability test for your triple quadrapole mass spectrometer. The focus will be on addressing the use of the system suitability test for monitoring the health of your instrument demonstrated by examples of troubleshooting abnormal system suitability results.

Thursday @ 11:20 in Chino

Zen and the Art of LC-MS/MS Maintenance: Assuring Optimal Instrument Performance

Joshua Akin - *UC San Diego Health* (jakin@ucsd.edu)

‣ LC-MS/MS instruments are continually becoming faster, more accurate and easier to use. With this demand for performance comes a need to assure quality results in a dependable manner. Reliability and reproducibility can be greatly improved with a small amount of consistent, preventative maintenance. We will discuss several steps to assure reliable results by minimizing system contamination and degradation. These steps will also be contrasted with examples of poor instrument performance, and how to prevent it. In addition, we will provide a framework for daily, weekly, monthly and annual maintenance.

Thursday @ 11:40 in Chino

Choosing the Right Internal Standard for Good LC-MS/MS Method Development

Imir Metushi - *Endocrine Sciences (LabCorp)* (imirmetushi@gmail.com)

‣ Developing good methods for analyte quantification by liquid chromatography (LC) triple quadrupole mass spectrometry (MS/MS) is an important first step when developing new assays. The choice of internal standard is critical for optimal performance. This session will use examples to discuss why choosing the right internal standard is important, when it should be added and what can go wrong.

• Session 6 • Track 1 •

Endnote - Cannabinoids

Thursday @ 14:15 in Room 1 (Mojave Learning Center)

Session Chair: Marilyn Huestis - *Huestis & Smith Toxicology, LLC*

Thursday @ 14:15 in Room 1 (Mojave Learning Center)

***Cannabis sativa L.*: Cultivation, Chemistry, Analysis and Prospect Therapeutic Cannabis-based Pharmaceutical Products**

Mahmoud ElSohly - *University of Mississippi* (melsohly@olemiss.edu)

‣ Cannabis is an annual, dioceous (occasionally monoecious) and wind pollinated plant. The plant has been reported to contain >500 different compounds, of which 120 are the cannabinoids. Delta-9-tetrahydrocannabinol (Delta-9-THC), the major biologically active compound and cannabidiol (CBD), a non-psychoactive cannabinoid are the most studied cannabinoids for various indications. This presentation will address the cannabis plant, its cultivation/propagation, its chemistry and preparations derived from the plant on both licit and illicit markets. The widespread legalization of cannabis for medical and to a lesser extent recreational purposes by many states poses new challenges to both clinical and forensic laboratories. Analytical methods for the quantitation of cannabinoids will be discussed and the development of cannabis based therapeutics will be elaborated.

• Session 6 • Track 3 •

Global Reach: MS Public Health Applications

Thursday @ 14:15 in Room 3 (Madera)

Session Chair: Xander van Wijk - *University of Chicago*

Thursday @ 14:15 in Room 3 (Madera)

Detection of Synthetic Opioids Using High Resolution Mass Spectrometry

Kara Lynch - *University of California San Francisco* (kara.lynch@ucsf.edu)

‣ The emergence of illicitly manufactured synthetic opioids including fentanyl and analogues represents a significant escalation of the ongoing opioid overdose epidemic in the United States. Synthetic opioids have been identified as adulterants in heroin and counterfeit opioid pills and are often consumed unknowingly. The purpose of this project was to validate the detection of 13 fentanyl analogues/synthetic opioids using a high resolution mass spectrometry drug screen and develop a comprehensive suspect analysis approach for the detection of synthetic opioid metabolites and emerging synthetic opioids.

Thursday @ 14:35 in Room 3 (Madera)

High-Throughput Sample Preparation and LC-MS/MS Determination of Menthol, Nicotine and its Metabolites, Minor Tobacco Alkaloids, and Cessation Drugs in Urine

Sujeewa Piyankarage - *Centers for Disease Control and Prevention (CDC)* (ysq5@cdc.gov)

‣ Characterization of menthol and nicotine and its metabolites in human samples in large-scale epidemiological studies is important when determining the role of menthol in tobacco use. This method quantifies menthol-glucuronide, nicotine and its unconjugated metabolites, minor tobacco alkaloids, and smoking-cessation drugs in human urine. The automated sample preparation process includes cleaning urine with mixed-mode solid-phase extraction. Compounds separated with reversed-phase liquid chromatography are detected with polarity-switching tandem mass spectrometry. Separation of 14 different compounds is achieved in 4.3 minutes while a linear calibration range from 1-80,000 ng/mL is maintained for the analytes that showed a broad concentration range in urine.

Thursday @ 14:55 in Room 3 (Madera)

High-Throughput UPLC-MS/MS Analysis of 28 Urinary Metabolites of Toxic and Carcinogenic Volatile Organic Compounds

Victor De Jesus - *Centers for Disease Control and Prevention* (vdejesus@cdc.gov)

‣ Volatile organic compounds (VOCs) are ubiquitous in the environment. Long-term exposure to certain VOCs may increase the risk for cancer and birth defects. In the U.S. tobacco smoke is the major non-occupational source of exposure to harmful VOCs. Characterizing human exposure to carcinogenic VOCs is of significant public health interest. We developed a UPLC-ESI-MS/MS method to quantify urinary VOC metabolites to detect 28 metabolites from exposure to 20 VOCs. The method is rugged and allows high-throughput analysis of urine specimens. It improves studies related to human exposure and health effects by providing reliable estimates of population exposure to VOCs.

• Session 6 • Track 4 •

Cardiovascular Proteomics

Thursday @ 14:15 in Room 4 (Pasadena)

Session Chair: Surendra Dasari - *Mayo Clinic*

Thursday @ 14:15 in Room 4 (Pasadena)

Rapid, Accurate, and Cost-Effective Quantification of C-Reactive Protein in Plasma by High-Performance LC-MS/MS

Junyan Shi - *University of British Columbia* (jyshi.bj@gmail.com) -- *Young Investigator Grantee*

‣ We developed a simple and rapid workflow for quantitative analysis of C-reactive protein in plasma. The method uses 10 uL of plasma, and avoids the use of analyte cleanup/enrichment steps and reduction/alkylation steps prior to tryptic digestion, thus facilitating a rapid turnaround time and minimal reagent costs. The new method has a cost-per-test of a few pennies, and requires 15-times less sample volume and has an analytical range 50-times greater than that of a commercial immunometric method. HPLC-MS/MS provides an alternative and cost-effective method for CRP quantification in plasma that is benchmarked against gravimetric targets.

Thursday @ 14:35 in Room 4 (Pasadena)

Development and Characterization of a High-Throughput Method for the Enrichment of ApoA-I Associated High-Density Lipoproteins

Timothy Collier - *Cleveland Heartlab, Inc.* (tcollier@clevelandheartlab.com)

‣ The purification of high density lipoprotein (HDL) for structural and functional studies typically utilizes ultracentrifugation that is time-consuming and challenging to scale-up for large clinical studies. As interest increases in the relevance of HDL composition and function as it relates to cardiovascular health, a significant need exists for high-throughput methodologies. We present an approach which relies on association of recombinant His-tagged ApoA-I with HDL, allowing subsequent immobilized metal affinity purification of ApoA-I associated high density lipoproteins (AA-HDL). The enrichment procedure takes minutes and provides a pool AA-HDL which retains close agreement in structure, composition, and enzymatic activity to HDL isolated by ultracentrifugation. Additionally, the use of mild elution conditions yields a sample readily amenable for proteo-/metabolomic MS analysis.

Thursday @ 14:55 in Room 4 (Pasadena)

Development of a Multiplexed Mass Spectrometry-based Method for Absolute Quantitation of Serum Apolipoprotein (A), Independent of its Size Polymorphism

Lucia Renee Ruhaak - *Leiden University Medical Center* (l.r.ruhaak@lumc.nl) -- *Young Investigator Grantee*

‣ Apolipoprotein (a) (Apo(a)) is believed to be an independent risk factor for cardiovascular disease. Because of its size polymorphism, quantitation of apo(a) is inherently challenging, but the LC-MS technique has potential for accurate quantitation of apo(a) irrespective of its size polymorphisms. We here present the addition of medium abundant serum apo(a) to our previously developed test for absolute quantitation of high abundant serum apolipoproteins A1, B, C-I, C-II, C-III and E. By including an SPE step to enhance sensitivity, we were able to reach total CV's below 5% for the quantitative peptide LFLEPTQADIALLK, while maintaining desirable precision for the high abundant apolipoproteins. Value-assigned matrix based serum pools were used for Apo(a) calibration, and a method comparison to an immunoassay based method showed results were exchangeable with mean bias of 4%.

• Session 6 • Track 5 •

Discovery Metabolomics

Thursday @ 14:15 in Room 5 (Sierra)

Session Chair: Karen Yannell - *Purdue University*

Thursday @ 14:15 in Room 5 (Sierra)

Target Metabolomics Analysis Reveals Alteration in Pathways in 5p minus Patients by UPLC-MS/MS

Nilson Assuncao - *UNIFESP* (nilson.assuncao@gmail.com)

‣ We analyzed urine and plasma samples from healthy and unhealthy people of both sexes aged 1–38 years old by UPLC-MS/MS. Student's statistical test and metabolomic pathway analysis were applied. Increases in alanine, asparagine, aspartate, citrulline, glutamine, histidine, phenylalanine, leucine, methionine, serine, threonine, tyrosine, tryptophan, methionine sulfoxide, kyneurine, trans-4-hydroxyproline and sarcosine were found. In general, the catabolism of some metabolic pathways is affected in CDCS patients, primarily the TCA cycle; glycine, serine and threonine metabolism; histidine metabolism; phenylalanine metabolism and tryptophan metabolism. Furthermore, the disease has been shown to be related to the ageing process and folate deficiency.

Thursday @ 14:35 in Room 5 (Sierra)

Evaluation of the Lipid Profile in the Saliva of Children Affected by Zika Virus Infection

Diogo de Oliveira - *University of Campinas* (diogo1986@gmail.com) -- *Young Investigator Grantee*

‣ This work applies high-resolution mass spectrometry to identify lipidomic differences between the saliva of infants with microcephaly that were exposed to Zika virus during pregnancy vs. control infants (i.e. no microcephaly and no exposure to Zika virus). We intend to identify and characterize lipids and related molecules that are directly linked to compromised metabolic pathways due to Zika infection, potentially providing insight on how the infection affects fetal development during pregnancy.

Thursday @ 14:55 in Room 5 (Sierra)

High-Throughput Screening of Enzymatic Reactions Using IR-MALDESI

Mans Ekelof - *North Carolina State University* (moekeloe@ncsu.edu) -- *Young Investigator Grantee*

‣ The ability to rapidly and accurately characterize samples is of critical importance in the drug discovery process as well as in the clinical testing laboratory. For many screens and assays, the benefits of mass spectrometric analysis are outweighed by sample compatibility concerns and low throughput. We present a method for high-throughput measurement of analytes in the IDH1-catalyzed conversion of isocitric acid to 2-oxoglutaric acid, sampled directly from the reaction vessel with no sample treatment, using infrared matrix assisted laser desorption electrospray ionization (IR-MALDESI) coupled to a Q Exactive Plus mass spectrometer.

• Session 6 • Track 6 •

Joint Informatics and Tissue Imaging

Thursday @ 14:15 in Room 6 (SmokeTree)

Session Chair: Livia Eberlin - *University of Texas, Austin*

Thursday @ 14:15 in Room 6 (SmokeTree)

Linking Exploratory Tissue Analysis to Established Clinical Targets: Automated Discovery of Bio-Molecular Relationships Between Stained Microscopy and IMS

Raf Van de Plas - *Delft University of Technology* (raf.vandeplas@tudelft.nl) -- *Young Investigator Grantee*

‣ Clinical pathology employs a broad array of targeted microscopy stains to drive diagnosis. While commonly employed, their labeled nature makes stains inherently targeted, yielding only narrow insight into underlying patho-mechanisms. Imaging MS (IMS) does not require labeling and can map thousands of chemical species in a single experiment, providing an excellent imaging modality for exploratory tissue analysis and discovery of disease markers. Here, we employ machine learning techniques to automatically learn correlative relationships between microscopy and biomolecular species reported by IMS. The ability to empirically capture microscopy-IMS relationships in mathematical models, and open up those models for biological interpretation, enables a novel link between medical practice and exploratory biology and has potential as a new multi-modal pipeline for discovery of clinical markers.

Thursday @ 14:35 in Room 6 (SmokeTree)

Identifying Predictive Markers of Breast Cancer Receptor Status and Molecular Subtypes Using DESI-MS Imaging

Kyana Garza - *University of Texas at Austin* (kygarza@utexas.edu) -- *Young Investigator Grantee*

‣ Breast cancer receptor status is indicative of patient prognosis as well as determines the appropriate treatment option for the patient. Here, desorption electrospray ionization mass spectrometry, together with the Lasso, were used to characterize breast cancer receptor status. Statistical classifiers were generated for the prediction of breast cancer receptor status, and an overall accuracy of 88.7%, 89.0%, and 34.9% was achieved for estrogen receptor (ER), progesterone receptor (PR) and human epidermal growth factor receptor 2 (HER2) status, respectively. Metabolic signatures predictive of breast cancer receptor status were also identified using the Lasso method.

Thursday @ 14:55 in Room 6 (SmokeTree)

IR MALDESI: from Technological Innovations to Cancer, HIV Treatment and Exposomics

David Muddiman - *North Carolina State University* (david_muddiman@ncsu.edu)

‣ This presentation will cover new technology developments including new mid IR lasers, new optical trains for improved spatial resolution, and several interesting applications of the platform technology for MSI.

• Session 6 • Track 7 •

Practical Training Intermediate: A Method Development Case History

Thursday @ 14:15 in Pueblo

Session Chair: Stephanie Marin - *Biotage*

Thursday @ 14:15 in Pueblo

Method Development Case History Part 1: Development and Validation

Stephanie Marin - *Biotage* (stephanie.marin@biotage.com)

‣ The development and validation of an LDT for drug detection implementing a new specimen type for routine clinical use creates multiple challenges. A clinical assay to detect neonatal drug exposure using umbilical cord tissue was developed and validated. Part 1 of the case history will review assay conception, clinical utility, proof-of-concept studies, method development and validation for this complex biological matrix. Homogenization techniques, drug extraction, sample clean-up, and LC-MS detection platforms that were evaluated will be discussed. Results used to determine final method parameters and conditions, and criteria for routine clinical use will be presented.

Thursday @ 14:35 in Pueblo

Method Development Case History Part 2: Can't You Do this Faster and Better? Understanding and Addressing Needs of Clinicians, Technical Staff and Operations

Gwen McMillin - *ARUP Laboratories* (gwen.mcmillin@aruplab.com)

‣ Within the first two years of testing, volumes were taxing the laboratory resources such that the original assay was not sustainable. We were also starting to understand the strengths and weaknesses (clinical and analytical) of the assay so we wanted to make some improvements. In this section changes in homogenization and assay design, as well as a switch to LC-MS/MS will be discussed with outcomes on throughput and quality of results.

Thursday @ 14:55 in Pueblo

Method Development Case History Part 3: Re-Development and Re-Validation

Simuli Wabuyele - *ARUP Institute for Clinical and Experimental Pathology* (simuli.wabuyele@aruplab.com)

‣ The development of an effective and robust sample preparation method for analysis of complex biological matrices is critical for LC-MS/MS-based LDTs in the clinical laboratory as it may significantly impact the quality of results and ultimately increase time and cost of analysis. This section of the case history will focus on the re-development of the sample preparation method and LC-MS/MS method improvements for the analysis of a broad range of drugs in a complex biological matrix (i.e., tissue) and the validation of the assay for implementation into routine clinical use.

• Session 6 • Track 8 •

Practical Training Basic: Staff Training for Mass Spectrometry

Thursday @ 14:15 in Chino

Session Chair: Shannon Haymond - *Northwestern University*

Thursday @ 14:15 in Chino

Developing a Curriculum for MS Training_i

Faye Vicente - *Ann & Robert H Lurie Children's Hospital Chicago* (fvicente@luriechildrens.org)

‣ This is the first segment of a 60 min workshop session that will involve short lectures and small-group work on how to develop an effective training curriculum for clinical mass spectrometry assays. This session will cover the first 20 min and include two talks: Tips on Training Documents -- Faye Vicente; Using Online Content for Curricula & Competencies -- Judy Stone.

Thursday @ 14:35 in Chino

Developing a Curriculum for Training_II

Shannon Haymond - *Northwestern University* (shaymond@luriechildrens.org)

‣ This is the second segment of a 60 min workshop session that will involve short lectures and small-group work on how to develop an effective training curriculum for clinical mass spectrometry assays. In this segment, small groups will work through development of a training curriculum. This includes defining training activities, learning resources, and competency assessments for a given learning objective.

Thursday @ 14:55 in Chino

Developing a Curriculum for Training_III

Shannon Haymond - *Northwestern University* (shaymond@luriechildrens.org)

‣ This is the final segment of a 60 min workshop session that will involve short lectures and small-group work on how to develop an effective training curriculum for clinical mass spectrometry assays. In this segment, the small group work conducted in session, Developing a Curriculum for Training_II, will be aggregated and discussed by the large group. This will allow attendees an opportunity to view a completed training curriculum, reflect on the process, and to identify areas with gaps or opportunities for development of additional learning resources.

• Session 6 • Track 9 •
Microbiology Metabolomics
Thursday @ 14:15 in Andreas
Session Chair: Kelly Hines - *University of Washington*

Thursday @ 14:15 in Andreas
Untargeted Metabolomics of 2400 Fecal Samples from American Gut Participants and ICU Subjects Reveals Information about Our Health, Behavior, and Microbiota
Alan Jarmusch - *University of California, San Diego* (ajarmusch@ucsd.edu)
‣ The metabolome of our gut is complex and understudied. The American Gut, a crowd-sourced citizen scientist project, aims to explore how our health, behaviors, and environment influence our gut microbiota. Untargeted metabolomic analysis of fecal samples from >2400 subjects in the American Gut and ICU Microbiome Project revealed compounds related to health, behavior, and those created by or modified by gut microbes. Fecal samples from the United States, United Kingdom, and Australia were compared, as well as subjects with various diagnosed diseases. Molecular networking and automatic annotation of MS/MS spectra using GNPS allowed for in depth exploration of the data as well as providing the frequency of compounds detected in the cohort.

Thursday @ 14:35 in Andreas
Daily Dynamics of the Microbiome and Metabolome in Chronically Infected Lungs
Robert Quinn - *University of California at San Diego* (rquinn@ucsd.edu)
‣ This study describes the largest longitudinal sampling of microbiome and metabolome data ever collected on a chronic disease. We integrate microbial and metabolite information from patient samples collected on a daily basis, showing connections between metabolite production, microbial abundances and clinical disease state.

Thursday @ 14:55 in Andreas
Integration of Non-Targeted Metabolic and Metagenomic Profiling of Feces After Chemical- and Salmonella-Induced Inflammation of Murine Intestines
Jikang Wu - *The Ohio State University* (wu.2014@osu.edu) -- *Young Investigator Grantee*
‣ Salmonella is the leading cause of death from foodborne illness in the United States. While it is well documented that Salmonella infection triggers host inflammation, little is known about the interaction between Salmonella and the gut environment. Here we applied non-targeted metabolomics and metagenomics approaches to reveal the chemical and biological environment in the murine intestine with inflammation induced by a chemical (DSS) or Salmonella. Several metabolites were found to be significantly changed with inflammation and they were correlated with the changes in the abundance of some microorganisms. The enhanced understanding of Salmonella's interaction with the environment may reveal new therapeutic strategies for prebiotics or probiotics for maintaining or restoring the microbiota in response to Salmonella perturbation.

• Session 7 • Track 1 •

Beyond Cannabis: Detection of Natural Products & Alternative Medicines

Thursday @ 15:30 in Room 1 (Mojave Learning Center)

Session Chair: TBA

Thursday @ 15:30 in Room 1 (Mojave Learning Center)

Pharmacokinetic Interactions Between Drugs and Hop Botanical Dietary Supplements Used by Menopausal Women

Richard van Breemen - *Linus Pauling Institute* (vanbreer@oregonstate.edu)

‣ Among botanical supplement alternatives to hormone therapy, hops (Humulus lupulus L.) is an increasingly popular alternative and has a long history of use in the brewing industry. To ensure the safe use of hop dietary supplements, we investigated their potential for drug interactions. Standardized extracts of spent hops (pre-extracted to remove the bitter acid flavor components), which are rich in prenylated phenols and flavonoids with estrogenic and chemoprevention activities, were studied for possible inhibition or induction of cytochrome P450 enzymes involved in drug metabolism both in vitro and in a Phase I clinical trial.

Thursday @ 15:50 in Room 1 (Mojave Learning Center)

The Grapefruit Effect: Identifying Potential Drug-Food Interactions in Patients Through Mass-Spectrometric Urinary Furanocoumarin Detection

David Schwope - *Aegis Sciences Corporation* (david.schwope@aegislabs.com)

‣ Furanocoumarin effects on metabolism of cytochrome P450 subtype 3A4 (CYP3A4) substrates have been well documented (e.g. “grapefruit effect”) and are of significant concern for numerous xenobiotics. To our knowledge, no clinical laboratories are routinely testing for furanocoumarin consumption. As part of a drug-drug interaction urine testing profile, we examined the prevalence of furanocoumarins in chronic pain, addiction treatment and mental health patients. A total of 27218 urines were obtained over 10 weeks and analyzed by LC-MS/MS. Furanocoumarins (either dihydroxybergamottin [LOD 10 ng/mL] or bergaptol [LOD 50 ng/mL]) were identified in 1165 samples (4.3%). Although urine detection cannot provide direct evidence of enzyme inhibition, these data provide beneficial insight regarding furanocoumarin prevalence and potential consequences on CYP3A4 substrate metabolism.

Thursday @ 16:10 in Room 1 (Mojave Learning Center)

Method for Estimating Oxidative Stress by Quantifying Urinary 8-Isoprostane Using UPLC-MS/MS

Cory Holder - *Oak Ridge Institute of Science and Education/ Centers for Disease Control and Prevention* (mvo5@cdc.gov)

‣ A non-enzymatic peroxidation product of arachidonic acid, 8-isoprostane, is a known biomarker for estimating oxidative stress. We have developed a robust automated method for measuring urinary 8-isoprostane using polymeric weak anion exchange solid phase extraction isotope dilution ultra-high performance liquid chromatography atmospheric pressure ionization tandem mass spectrometry assay. Since 8-isoprostane exists in urine as glucuronide conjugates and free acids, we enzymatically hydrolyzed the samples with β-glucuronidase prior to UPLC-MS/MS quantification. Using 400 µL sample volume, this method returned a limit-of-detection below 8 pg/mL and a coefficient of variation (CV) below 10% with cycle times of less than 10 min.

• Session 7 • Track 2 •

Endnote - Statistics in Science

Thursday @ 15:30 in Room 2 (Catalina)

Session Chair: Randy Julian - *Indigo Bioautomation*

Thursday @ 15:30 in Room 2 (Catalina)

The Importance of Reproducible Research in High-Throughput Biology: Case Studies in Forensic Bioinformatics

Keith Baggerly - *UT MD Anderson Cancer Center* (kabagger@mdanderson.org)

‣ We present case studies in reverse engineering of high profile results from high throughput biology (forensic bioinformatics) illustrating how simple errors in experimental design and data analysis may have put patients at risk. We discuss these in the context of ongoing efforts by the NIH to enhance research reproducibility.

• Session 7 • Track 3 •

Benzodiazepines: basic applications and beyond

Thursday @ 15:30 in Room 3 (Madera)

Session Chair: Kara Lynch - *UCSF*

Thursday @ 15:30 in Room 3 (Madera)

A High-Resolution Mass Spectrometry Method for Designer Benzodiazepines

Xander van Wijk - *The University of Chicago* (xvanwijk@uchicago.edu) -- *Young Investigator Grantee*

‣ Benzodiazepines are widely used for treatment of anxiety and insomnia, however, this class of drugs is also commonly abused. Many different benzodiazepines and analogs have been produced that are not FDA-approved. We developed a liquid chromatography high-resolution mass spectrometry method for detection of 16 of these so-called 'designer' benzodiazepines in urine. The limit of detection for most of these compounds ranged from 5 to 50 ng/mL, and minor negative matrix effects were observed only in some instances. With the exception of ketazolam, all compounds showed significant reactivity with the ThermoFisher CEDIA® benzodiazepine immunoassay. Although we recently encountered three designer benzodiazepines in clinical toxicology cases (clonazolam, etizolam, and phenazepam), we did not detect any in 211 urine samples that were previously determined benzodiazepine-positive by immunoassay.

Thursday @ 15:50 in Room 3 (Madera)

Confirming 23-Benzodiazepines in Urine for Pain Management Using LC-MS/MS – a Challenging Assay Development

Richard Lahr - *Development Technologist, Mayo Clinic* (lahr.richard@mayo.edu)

‣ During the routine validation of a benzodiazepine LC-MS/MS method, it was noted that lorazepam, triazolam, and alpha-hydroxytriazolam showed a quadratic shift/bias in the calibration curve particularly at the high end. The ultimate cause of this bias was determined to be due to the natural presence of chlorine (Cl) in these benzodiazepines where the mass of the heavy isoforms of Cl was the same as the respective deuterium labeled internal standards for these compounds. One solution to this bias was to identify and use the Cl heavy isoforms of the respective labeled internal standards.

Thursday @ 16:10 in Room 3 (Madera)

Quantitation of Seven Benzodiazepines and Metabolites in Urine by LC-MSMS

Yuzi (Emma) Zheng - *Cleveland Clinic* (zhengy4@ccf.org) -- *Young Investigator Grantee*

‣ Benzodiazepines are central nervous system depressants that are prescribed to patients to prevent seizures, treat anxiety or simply help them to sleep. Benzodiazepines when overdosed can lead to addiction and sometimes cause death. Therapeutic drug monitoring of benzodiazepines in urine are used to help physicians identify the drugs used, especially in the pain management settings. Here we report a novel liquid chromatography-tandem mass spectrometry assay for measuring seven common benzodiazepines and active metabolites in urine, which has been validated for clinical testing.

• Session 7 • Track 4 •

Biomarkers

Thursday @ 15:30 in Room 4 (Pasadena)

Session Chair: Cory Bystrom - *Cleveland Heart Laboratory*

Thursday @ 15:30 in Room 4 (Pasadena)

Mass Spectrometry Analysis of Immune Checkpoint Proteins in Lung Cancer

Theresa Boyle - *Moffitt Cancer Center* (theresa.boyle@moffitt.org) -- *Young Investigator Grantee*

‣ Immunotherapy against the programmed death ligand 1 axis (PD-L1/PD-1) has revolutionized the care of lung cancer patients with dramatic response and increase in survival time observed in a subset of these patients. No biomarkers clearly predict which patients will respond, although PD-L1 IHC has been approved as an FDA-approved immunotherapy companion diagnostic. Mass spectrometry is an ideal platform for exploring the role of PD-L1 in relation to other immune checkpoint proteins because it allows for simultaneous quantification of multiple proteins with a small amount of tissue.

Thursday @ 15:50 in Room 4 (Pasadena)

Diagnosis of Male Infertility with Proteomic and Proteogenomic Biomarkers Measured in Seminal Plasma

Andrei Drabovich - *University of Toronto* (adrabovich@gmail.com) -- *Young Investigator Grantee*

‣ Non-invasive differential diagnosis of male infertility is a recognized unmet need in urology. In our search for biomarkers, we focused on testis-specific proteins secreted into seminal plasma, a proximal fluid suitable for non-invasive diagnostics. Using mass spectrometry, we previously discovered and validated TEX101 protein as a biomarker of azoospermia. In this work, we discovered and quantified by targeted proteomic assays a polymorphic TEX101 protein variant associated with idiopathic male infertility. We also identified and measured additional 45 testis-specific proteins expressed in male germ cells at different stages of spermatogenesis. Pending further validation, a comprehensive panel of these markers will facilitate diagnosis of idiopathic male infertility and prediction of sperm retrieval outcomes, thus increasing the reliability of assisted reproduction techniques.

Thursday @ 16:10 in Room 4 (Pasadena)

Anemia, Altitude, and Autologous Blood Transfusions – Applications of a Novel Method to Measure Membrane Proteins in Dried Blood Spots

Holly Cox - *Sports Medicine Research and Testing Laboratory* (hcox@smrtl.org)

‣ Membrane proteins include several important drug targets, transporters, receptors, and cell differentiation markers. We have developed a method to enrich for membrane proteins and reduce matrix interference in dried blood spot (DBS) samples. The method was applied to the measurement of four cluster of differentiation (CD) proteins, CD71, Band3, CD45, and CD41, which serve as blood cell-specific markers. The DBS method was validated and tested in subjects under several conditions including iron deficient anemia, after blood withdrawal, after autologous blood transfusion, and at high altitude, with and without iron supplementation.

• Session 7 • Track 6 •

Endnote - Tissue Imaging

Thursday @ 15:30 in Room 6 (SmokeTree)

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

Thursday @ 15:30 in Room 6 (SmokeTree)

Advanced Development of the MasSpec Pen for Cancer Diagnosis and Surgical Margin Evaluation

Livia S. Eberlin - *University of Texas at Austin* (liviase@utexas.edu)

‣ We have recently reported the development of the MasSpec Pen for rapid diagnosis of human cancer tissues. Here, new describe recent results on independent samples sets analyzed ex vivo, including new tissue types and improvements in cancer prediction. Suitability for in vivo analysis was further demonstrated by evaluating normal, cancer and margin tissue from mouse models during surgery. A laparoscopic version of the MasSpec Pen was designed and developed for minimally invasive procedures, and tested on fresh tissue samples. Our results demonstrate current efforts towards the translation of the MasSpec Pen into clinical workflows for rapid cancer tissue diagnosis.

• Session 7 • Track 9 •

Proteomic Approaches to Bacterial Analysis

Thursday @ 15:30 in Andreas

Session Chair: Anaamika Campeau - *University of California, San Diego*

Thursday @ 15:30 in Andreas

Exploring the Hidden World of MRSA Pathogenesis

Jacob Wozniak - *UCSD* (jakewozniak@gmail.com) -- *Young Investigator Grantee*

‣ Staphylococcus aureus remains the leading cause of skin and soft tissue infections in the US. During the course of S. aureus infection, the interplay between host and pathogen involves a complex crosstalk mediated by several protein factors. To date, many of the bacterial proteins remain beyond our limits of detection. Specifically, in the context of infection, high host protein levels can mask the signal of bacterial proteins. By using a targeted proteomics approach, we hope to overcome the limitations of identifying bacterial proteins that are typically lost or discarded when analyzing host-pathogen interactions. Implementation of this technique in a clinical setting would theoretically shorten time to positive diagnosis because bacterial proteins could be targeted directly from samples without the need for culture.

Thursday @ 15:50 in Andreas

Defining Systemic Bacterial Infection Through a Murine Organ Atlas of Response to Group A and B Strep Infections

John Lapek - *UCSD* (jlapek@ucsd.edu)

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

Thursday @ 16:10 in Andreas

Top-Down Proteomic Identification of Clinical Subtypes of Shiga Toxin from Shiga Toxin-Producing Escherichia coli Using MALDI-TOF-TOF Tandem Mass Spectrometry

Clifton Fagerquist - *Agricultural Research Service, USDA* (clifton.fagerquist@ars.usda.gov)

‣ We analyzed 45 Shiga toxin-producing Escherichia coli (STEC) strains (environmental isolates collected from Northern California agricultural regions) for expression of Shiga toxin (Stx) using MALDI-TOF-TOF-MS/MS and top-down proteomic analysis. Strains were grown overnight on agar supplemented with a sub-inhibitory level of DNA-damaging antibiotics. Nineteen STEC strains produced clinical subtype Stx2a, fifteen strains produced clinical subtype Stx2c, nine strains produced clinical subtype Stx2c or Stx2d (weak inducers), three strains induced but expressed an unknown protein biomarker close in mass to Stx but not Stx. Four control strains were also correctly identified.

Poster Presentations

Location: *Exhibit Hall (Oasis 3-4)*

Posters by Topic

Please Find Posters *with Abstracts* under
Posters by Number (starting on page 119)

Cannabinoids

Cannabinoids | Thursday 12:30 Poster #6D
Analysis of 12 Cannabinoids in Whole Blood by LC-MS/MS
Laura Snow *- Phenomenex, Inc.*

Cannabinoids | Thursday 12:30 Poster #12A
Medical Marijuana and Pain Medication Monitoring
Oneka Cummings *- Ameritox, LLC*

Cannabinoids | Thursday 12:30 Poster #24A
Development of a LC-MS/MS Assay for Bioactive Cannabinoids in Plasma of Pediatric Patients on Cannabis Oil Therapy
Stephanie Vuong *- University of Saskatchewan (*YI Grantee*)*

Cannabinoids | Wednesday 10:00 Poster #35D
The Grass Isn't Always Greener: Removal of Purple Pigmentation from Cannabis Using QuEChERS Extraction and Chlorofiltr® dSPE Cleanup
Danielle Mackowsky *- United Chemical Technologies, LLC*

Cannabinoids | Thursday 10:00 Poster #37C
Profiling Hemp Oils Using Liquid Chromatography-Time of Flight Mass Spectrometry
Vaughn Miller *- Agilent Technologies*

Cannabinoids | Thursday 12:30 Poster #38A
Complex Mixture Analysis by Bromobenzyl (PBr) Compare to Fluorophenyl (PFP) Core-Shell HPLC Columns
Ken Tseng *- Nacalai USA Inc.*

Cannabinoids | Thursday 12:30 Poster #46A
Detection of 22 Phytocannabinoids and Their Metabolites in Urine by LC-MS/MS and Their Evaluation as Potential Markers
Rory Doyle *- Thermo Fisher, Inc*

Endocrinology

Endocrinology | Wednesday 10:00 Poster #1D
Simultaneous Quantitation of Segesterone Acetate (Nestorone®), Estradiol, Estrone, and Progesterone in Human Sera by LC-MS/MS
David Erikson *- Oregon National Primate Research Center*

Endocrinology | Wednesday 10:00 Poster #3A
Obtaining FDA Clearance via the *de novo* Pathway, for the First IVD LC-MS/MS 25-Hydroxyvitamin D Assay
Michal Weinstock *- SCIEX*

Endocrinology | Wednesday 13:30 Poster #4B
Measurement of Serum Free Cortisol Using ED-LC-MS/MS; Revisiting the Use of Free Cortisol Measurement for Adrenal Insufficiency in Critically Ill Patients
Julie Ray *- ARUP Laboratories*

Endocrinology | Wednesday 10:00 Poster #5D
A Sensitive LC-MS/MS Method for the Determination of Nestorone in Human Serum
Feng Bai *- Los Angeles Biomedical Research Institute*

Endocrinology | Wednesday 13:30 Poster #6B
Matrix Based Calibrators for Quantification of Testosterone and Dihydrotestosterone
Linda Smith *- MilliporeSigma*

Endocrinology | Thursday 12:30 Poster #8A
Development of a Multi-Component Analytical Method for 18 Steroid Compounds in Serum Matrix Utilizing Rapid Polarity Switching and Simple Sample Preparation
Jenny Moshin *- SCIEX*

Endocrinology | Wednesday 10:00 Poster #9A
Simultaneous Measurement of T3, Reversed T3 and T4 by a Sciex™ QTRAP5500 LC-MS/MS and Comparison to (Radio)immunoassay
Rutchanna Jongejan *- Erasmus Medical Centre (*YI Grantee*)*

Endocrinology | Thursday 12:30 Poster #10A
Increasing Throughput for High Analytical Sensitivity Bioanalysis of Human Insulin and its Biotherapeutic Analogs Using Microflow LC-MS/MS for Clinical Research
Andrew Peck *- Waters Corporation*

Endocrinology | Thursday 12:30 Poster #10D
Tandem Mass Spectrometric Measurement of Seven Steroids in Dried Blood Spots to Diagnose Congenital Adrenal Hyperplasia
Deema Qasrawi *- University of Calgary (*YI Grantee*)*

Endocrinology | Wednesday 10:00 Poster #13D
25-Hydroxy Vitamin D C-3 Epimers: A Close-Up Comparison Between LC-MS/MS and BioPlex 2200
Jane Dickerson *- Seattle Children's Hospital*

Endocrinology | Thursday 10:00 Poster #17C
Analysis of Urinary Free Cortisol and Cortisone by LC-MS/MS
Frances Carroll *- Restek Corporation*

Endocrinology | Wednesday 13:30 Poster #18B
The Comparison of Aldosterone Level by Mass Spectrometry and Radioimmunoassay
Sunhyun Ahn *- Seoul Clinical Laboratories*

Endocrinology | Thursday 12:30 Poster #20A
Reliable Direct Quantitative Measurement of Total and Free Testosterone in Plasma/Serum by UHPLC-MS/MS
Ayuna Dagdanova *- Accu Reference Medical Laboratory*

Endocrinology | Wednesday 10:00 Poster #23A
A Fully Automated and Novel "Tip-On-Tip" Extraction Method for the Quantitation of Testosterone and Related Hormones in Human Serum
Daniel Kassel *- Scianalytical Strategies, Inc.*

Endocrinology | Wednesday 10:00 Poster #23D
Achieving Lower Limits of Quantitation for Testosterone and Estradiol by LC-MS/MS
Kristine Van Natta *- Thermo Fisher Sceintific*

Endocrinology | Thursday 12:30 Poster #28A
Effect of Blood Collection Tubes on Serum/Plasma Estrogen Quantitation by LC-MSMS
Carmen Gherasim *- Department of Pathology, University of Utah*

Endocrinology | Wednesday 13:30 Poster #28C
iExchange: Overcoming Extraction Challenges of T3 and rT3 from Human Serum
Shahana Huq *- Phenomenex*

Endocrinology | Thursday 10:00 Poster #31B
High-Throughput Method for Measurement of 25 -Hydroxy Vitamin D by LC -MS/MS
Canary Tennison *- ARUP Laboratories*

Endocrinology | Thursday 12:30 Poster #36D
Amino acids and metabolites analysis without derivatization using a novel mixed-mode column
Itaru Yazawa *- Imtakt Corporation*

Endocrinology | Thursday 10:00 Poster #37B
Enhancing LC-MS/MS Sensitivity for Catecholamines via a Reductive Alkylation Derivatization Strategy
Melissa Hughs *- ARUP Institute for Clinical and Experimental Pathology (*YI Grantee*)*

Endocrinology | Thursday 10:00 Poster #39C
Analytical Determination of Testosterone in Human Serum Using an Ultivo Tandem LC-MS
Yanan Yang *- Agilent Technologies Inc.*

Endocrinology | Wednesday 10:00 Poster #45D
Evaluating the Accuracy of Vitamin D Assays
Nicole Tolan *- SCIEX*

Endocrinology | Thursday 12:30 Poster #46D
High Sensitivity Assay of Estrogens in Human Plasma by UHPLC-MS/MS without Derivatization
Atsuhiko Toyama *- Shimadzu Corporation*

Endocrinology | Thursday 12:30 Poster #48D
Mass Spectrometric Studies of Apolipoprotein Proteoforms and their Role in Lipid Metabolism and Type 2 Diabetes
Dobrin Nedelkov *- Isoformix*

Informatics & Analytics

Informatics & Analytics | Wednesday 13:30 Poster #14B
Application of LIS Interface for Quality Control for LC-MS/MS in Therapeutic Drug Monitoring of Immunosuppressant
Yeo-Min Yun *- Konkuk University School of Medicine*

Informatics & Analytics | Thursday 12:30 Poster #22A
Determination of Busulfan in Human Plasma by LC-MSMS
Eun Jin Lee *- University of Ulsan College of Medicine*

Metabolomics

Metabolomics | Thursday 10:00 Poster #1C
Development of Combined LC-MS/MS Analysis for Citric Acid Cycle Intermediates, Acylcarnitines and Amino Acids
Rohan Shah *- Cleveland State University (*YI Grantee*)*

Metabolomics | Wednesday 10:00 Poster #3D
Screening for 3 LSD Using Triplex Tandem Mass Spectrometry Assays with 2 Confirmation Tests in Korea
Sung Eun Cho *- LabGenomics*

Metabolomics | Thursday 12:30 Poster #4D
Microflow LC-MS/MS Workflow Allows Up to 50% More Metabolite Coverage for Targeted Polar Metabolite Analysis
Khatereh Motamedchaboki *- SCIEX*

Metabolomics | Wednesday 10:00 Poster #7D
The Utility of Urine GAGs as a Follow-Up and Confirmatory Test in Newborn Screening of Mucopolysaccharidosis I
Haoyue Zhang *- Duke University*

Metabolomics | Wednesday 13:30 Poster #16B
Bile Acid Profiling and Quantification in Human Plasma Using LC-MS/MS
Ravali Alagandula *- Restek Corporation*

Metabolomics | Wednesday 13:30 Poster #16C
Simultaneous Analysis of Catecholamines and Metanephrines in Urine by LC-MS/MS
Rob Freeman *- Restek Corporation*

Metabolomics | Thursday 12:30 Poster #16D
Global Natural Product Social Molecular Networking (GNPS) – an Open Resource for MS-based Metabolomics Data Sharing and Analysis
Alexander Aksenov *- UC San Diego*

Metabolomics | Wednesday 10:00 Poster #19D
Analysis of Plasma Free Metanephrine, Normetanephrine, and 3-Methoxytyramine by Hydrophilic Interaction Liquid Chromatography
Ashlee Reese *- Restek Corporation*

Metabolomics | Wednesday 13:30 Poster #22C
Validation of High-Throughput MS/MS-based Amino Assay Screen Using an Automated Liquid Handler for Amino Acid Extraction and Stable-Isotope Labeling Semiautomation
William Phipps *- UT Southwestern Medical Center (*YI Grantee*)*

Metabolomics | Thursday 12:30 Poster #22D
Metabolomic Profile Change in Patients with Sepsis Compared with Normal Controls
Sang-Guk Lee *- Yonsei University College of Medicine*

Metabolomics | Wednesday 13:30 Poster #28B
Fasting Serum Levels of Bile Acid Are Associated with Insulin Resistance
Yonggeun Cho *- Yonsei University College of Medicine*

Metabolomics | Thursday 10:00 Poster #31C
Accurate and Confident Metabolic Phenotyping - Combining a Standardized and Quantitative Targeted Assay with Orbitrap™ Technology
Wulf Fischer-Knuppertz *- BIOCRATES Life Sciences AG*

Metabolomics | Thursday 12:30 Poster #32A
Feasibility of Dried Blood Spots (DBS) for Metabolomics and its Short and Long-Term Metabolome Stability
Maria Chiam *- BIOCRATES Life Sciences AG*

Metabolomics | Thursday 10:00 Poster #33B
Simultaneous Determination of 14 Biomarkers of Exposure to BTEX in Human Urine by Isotope Dilution LC-MS/MS
Yehia Baghdady *- The University of Texas at Arlington (*YI Grantee*)*

Metabolomics | Wednesday 13:30 Poster #34B
Proteometabolomics of Myeloma Drug Resistance
David Koomen *- Moffitt Cancer Center*

Metabolomics | Thursday 10:00 Poster #35B
Rapid and Simple Measurement of Plasma Amino Acids and Urinary Organic Acids Using LC-ESI-MS/MS Technology
Mehmet Balci *- JASEM Laboratory Systems and Solutions*

Metabolomics | Wednesday 10:00 Poster #43D
Quantitation of Glycocholic Acid and Bilirubin in Human Bile for Gall Bladder Diseases by Flow Injection MS/MS Using Standard Addition Method
Raghavi Kakarla *- Cleveland State University (*YI Grantee*)*

Metabolomics | Thursday 12:30 Poster #44D
Inherited Genetic Disorders Meets Untargeted Metabolomics
Rahul Deshpande *- Greenwood Genetic Center (*YI Grantee*)*

Microbiology/Virology

Microbiology/Virology | Thursday 10:00 Poster #3B
Endogenous Digoxin and Cancer Management – Would Zika Virus be the Trigger for Glioblastomas Death Through Digoxin Synthesis?
Estela Lima *- University of Campinas (*YI Grantee*)*

Microbiology/Virology | Thursday 10:00 Poster #3C
Serum Metabolic Alterations Upon Zika Infection
Carlos Fernando Odir Rodrigues Melo *- University of Campinas (*YI Grantee*)*

Microbiology/Virology | Wednesday 13:30 Poster #18C
Rapid Evaporative Ionisation Mass Spectrometry (REIMS) as a Novel Approach to Pathogen Detection Directly from Clinical Urine Samples
Adam Burke *- Imperial College London (*YI Grantee*)*

Microbiology/Virology | Thursday 10:00 Poster #29B
Regulated LC-MS/MS Bioanalysis of Therapeutic Antibodies Based on Nano-Surface and Molecular-Orientation Limited (nSMOL) Proteolysis Method Using a New Reagent
Christopher Gilles *- Shimadzu Scientific Instruments*

Proficiency, Regulations, Standards

Proficiency, Regulations, Standards | Thursday 10:00 Poster #43C
Designing the Perfect Mass Standard for Applied Mass Spectrometry
Joe Giesen *- Tulane University*

Proficiency, Regulations, Standards | Wednesday 10:00 Poster #47A
Developing a Vitamin D-Binding Protein Reference Material
Lisa Kilpatrick *- National Institute of Standards and Technology*

Proficiency, Regulations, Standards | Wednesday 13:30 Poster #48B
Worldwide Interlaboratory Study on Monoclonal Antibody Glycosylation
Maria Lorna De Leoz *- National Institute of Standards and Technology*

Proteomics

Proteomics | Thursday 10:00 Poster #1B
Using Activity-based Protein Profiling Proteomics to Determine Novel Pathways and Therapeutic Monitoring Targets
Sean Campbell *- University of Virginia (*YI Grantee*)*

Proteomics | Wednesday 10:00 Poster #5A
Monitoring Monoclonal Immunoglobulins Directly from Bone Marrow Plasma Cells Using LC-MS
David Barnidge *- Mayo Clinic and The Binding Site*

Proteomics | Wednesday 13:30 Poster #6C
Development of Simple and Rapid Workflows for Quantitation of Infliximab and Adalimumab in Human Serum by LC-MS/MS
Kevin Ray *- MilliporeSigma*

Proteomics | Thursday 10:00 Poster #7C
Proteogenomic Analysis of Clinical Samples Using a Unified Extraction Method
Jared Isaac *- Thermo Fisher Scientific*

Proteomics | Wednesday 13:30 Poster #8B
Quantitative LC-MS/MS Analysis of Intact IgF-1 and 2 on a Triple Quadrupole and Quadrupole Orbitrap Mass Spectrometers
Sherry Gregory *- Thermo Fisher, Inc*

Proteomics | Thursday 10:00 Poster #9C
Investigation of Immunoglobulins from Patients with IgA Nephropathy by Using Liquid Chromatography - Triple Quadrupole Tandem Mass Spectrometry
I-Lin Tsai *- Taipei Medical University*

Proteomics | Wednesday 10:00 Poster #9D
Development of a Novel LC Concept for Clinical Proteomics
Nicolai Bache *- Evosep Biosystems*

Proteomics | Wednesday 13:30 Poster #12B
Quantitative Proteomics of Ras Signaling to Support Translational Cancer Research
Melissa Hoffman *- Moffitt Cancer Center/University of South Florida (*YI Grantee*)*

Proteomics | Wednesday 10:00 Poster #13A
Proteomic Analysis of Therapeutic Biomarkers to Guide Treatment in Patients with Bone Metastasis
Yeoun Jin Kim *- Nantomics*

Proteomics | Thursday 10:00 Poster #13B
Personalized Proteomics of Inflammatory Bowel Disease
Robert Mills *- UC San Diego (*YI Grantee*)*

Proteomics | Thursday 12:30 Poster #14A
LC-MS/MS Quantification of Intact Insulin Like Growth Factor-I (IGF-I) from Serum for Clinical Research
Khalid Khan *- Waters Corporation*

Proteomics | Thursday 10:00 Poster #19B
An Optimized Rapid Trypsin Digestion Protocol for Proteomic Sample Preparation
Michael Rosenblatt *- Promega*

Proteomics | Thursday 10:00 Poster #23C
Development of a Robust, Routine, and Multiplexed Plasma Profiling Method Using UHPLC-MS/MS
Kerry Hassell *- Thermo Fisher Scientific*

Proteomics | Wednesday 13:30 Poster #24B
Optimization of Experimental Parameters in Data-Independent Mass Spectrometry Significantly Increases Depth and Reproducibility of Results
Florian Marty *- Biognosys AG*

Proteomics | Thursday 12:30 Poster #28D
Quantitative Proteomics-based Identification of Novel Serum Markers for First-Trimester Prediction of Gestational Diabetes Mellitus
Martin Overgaard *- University of Southern Denmark*

Proteomics | Thursday 10:00 Poster #29C
Feasibility of Mitra® Microsampling Devices in Remote, Longitudinal Monitoring of Apolipoprotein B/ApolipoProtein A-I in Patients at Risk for Cardiac Events
Kelly Mouapi *- Cedars Sinai Medical Center*

Proteomics | Thursday 12:30 Poster #30D
timsTOF Pro with PASEF for Shotgun Proteomics
Gary KRUPPA *- Bruker Dalotnics*

Proteomics | Wednesday 10:00 Poster #31A
Mass Spectrometric IgG Fc-Glycosylation Analysis in Pediatric Samples Reveals Glycosylation Changes Related to Age and Physiological State
Noortje de Haan *- Leiden University Medical Center (*YI Grantee**)*

Proteomics | Wednesday 13:30 Poster #32C
Nanopore-Enabled Circulating Peptides Extraction and Quantitative Detection Coupling with Mass Spectrometry
Jia Fan *- Arizona State University (*YI Grantee**)*

Proteomics | Wednesday 10:00 Poster #33D
Validation of ApolipoProtein A-I Associated Lipoprotein Panel for the Prediction of Cholesterol Efflux Capacity
Cory Bystrom *- Cleveland HeartLab Inc.*

Proteomics | Wednesday 10:00 Poster #35A
Discovery Proteomics and Biomarker Quantification in a Breast Tumor Tissue Microarray
John Koomen *- Moffitt Cancer Center*

Proteomics | Wednesday 10:00 Poster #37A
Role of RNase L on Kindey Function and its Effect on EGF Shedding and Excretion into Urine
Norah Alghamdi *- Cleveland State University*

Proteomics | Wednesday 10:00 Poster #37D
Identification of Novel Biomarkers for Ovarian Cancer
Danting Liu *- Cleveland State University (*YI Grantee**)*

Proteomics | Thursday 10:00 Poster #43B
Use of a MS-based Targeted Approach for Detection of Minimal Residual Disease (MRD) in Multiple Myeloma
Carlo Martins *- Memorial Sloan Kettering Cancer Center (*YI Grantee**)*

Proteomics | Wednesday 13:30 Poster #44B
An LC-MS/MS Method to Characterize *in vivo* Carbamylation of Human Serum Albumin
Collin Hill *- PerkinElmer*

Proteomics | Wednesday 10:00 Poster #45A
Detection of M-Protein in the Presence of Therapeutic Monoclonal Antibodies Using Targeted Mass Spectrometry
Marina Zajec *- Erasmus University Medical Center (*YI Grantee**)*

Proteomics | Thursday 10:00 Poster #47B
No Phlebotomy Needed: Evaluation of Protein Stability in Liquid Blood Collected with the HemoLinkTM Device for Use in Patient-Centered Sampling and Monitoring
Irene van den Broek *- Cedars Sinai Medical Center*

Proteomics | Wednesday 13:30 Poster #48C
The First Precision Diagnosis of Multiple Myeloma by Use of 21 Tesla FT-ICR Top/Middle-Down *de novo* Sequencing
Lidong He *- Florida State University (*YI Grantee**)*

Small Molecules / Tox

Small Molecules / Tox | Wednesday 10:00 Poster #1A
A Simple and Rapid UPLC-MS/MS Assay for the Determination of Serum Free Voriconazole in Cancer Patients
Jieli Li *- MD Anderson Cancer Center (*YI Grantee**)*

Small Molecules / Tox | Thursday 12:30 Poster #4A
Evaluation of Matrix Component Removal Using a Novel Flow-Through Scavenging Plate for Drugs of Abuse Testing in Urine
Lee Williams *- Biotage GB Limited*

Small Molecules / Tox | Thursday 10:00 Poster #5B
Comparison of Sample Preparation Options for the Extraction of a Panel of Endogenous Steroids from Serum Prior to UHPLC-MS/MS Analysis
Katie-Jo Teehan *- Biotage GB Limited*

Small Molecules / Tox | Thursday 10:00 Poster #5C
Extraction of Catecholamine Acid Metabolites from Plasma Prior to Analysis Using UHPLC-MS/MS
Elena Gairloch *- Biotage GB Limited*

Small Molecules / Tox | Thursday 12:30 Poster #6A
Rapid Quantification of 90+ Drugs in Urine Using Citrine™ QTRAP® MS/MS System
Amol Kafle *- SCIEX*

Small Molecules / Tox | Wednesday 10:00 Poster #7A
Elucidation of a Naproxen Metabolite Interference in Total Bilirubin Testing on a Routine Chemistry Analyzer System Using LC-MS/MS
Aaron Barnes *- University of Minnesota (*YI Grantee*)*

Small Molecules / Tox | Thursday 12:30 Poster #8D
Quantification of 11-nor-9-Carboxy-THC and Panel of 22 Drugs in Hair Using Citrine™ QTRAP® MS/MS System
Xiang He *- SCIEX*

Small Molecules / Tox | Thursday 10:00 Poster #13C
Better Hydrolysis and Increased Efficiency for Urine Drug Testing Using Mixed-Mode Solid Phase Extraction with In-well Hydrolysis
Stephanie Marin *- Biotage*

Small Molecules / Tox | Thursday 12:30 Poster #14D
UPLC-MS/MS Analysis of Oncology Drugs in Plasma for Clinical Research
Stephen Balloch *- Waters Corporation*

Small Molecules / Tox | Wednesday 10:00 Poster #15A
Therapeutic Drug Monitoring of lacosamide, a newer antiepileptic drug, by LC-MS/MS
Sarina Yang *- Quest Diagnostics Nichols Institute of Valencia*

Small Molecules / Tox | Thursday 10:00 Poster #15C
Development and Validation of a Dried Urine Spot Assay as a Toxicology Screening Method Using LC-MS/MS
Abed-Hamlet Pablo *- Johns Hopkins University (*YI Grantee*)*

Small Molecules / Tox | Thursday 12:30 Poster #16A
How Low Can Your Clinical Research Method Go for the Analysis of Serum Estrogens?
Robert Wardle *- Waters Corporation*

Small Molecules / Tox | Wednesday 10:00 Poster #17D
A Novel Solution for EtG/EtS Analysis in Human Urine by LC-MS/MS
Richard Cummings *- Restek Corporation*

Small Molecules / Tox | Thursday 12:30 Poster #18D
A Simple Method for the Analysis of Methylmalonic Acid in Human Plasma by LC-MS/MS
Susan Steinike *- Restek Corporation*

Small Molecules / Tox | Wednesday 10:00 Poster #19A
Development and Validation of a LC-MS/MS Method for the Determination of Tenofovir Alafenamide in Human Plasma Over a 10,000-Fold Calibration Range
Kimberly Blake *- UNC Center for AIDS Research*

Small Molecules / Tox | Wednesday 13:30 Poster #20B
Effect of Enzyme Titer and pH on Hydrolysis Efficiency Using Recombinant Limpet Beta-Glucuronidase
Jim Blasberg *- MilliporeSigma*

Small Molecules / Tox | Wednesday 13:30 Poster #20C
Practical Considerations Using Quantisal Oral Fluid Collection Devices & SPE Method Development by Polymeric Mixed-Mode Cation Exchange
Dan Menasco *- Biotage*

Small Molecules / Tox | Thursday 12:30 Poster #20D
Novel Sensitive LC-MS/MS-based 25(OH)D Assays and Vitamin D Status of 150,000 Chinese Population
Zhouyang Kang *- Hangzhou Calibra Diagnostics*

Small Molecules / Tox | Wednesday 10:00 Poster #21A
LC-MS/MS Validation Using Natural Isotopes of Stable Labeled Internal Standards to Overcome Crosstalk for Three Brominated or Chlorinated Antiretrovirals
Amanda Schauer *- University of North Carolina-Chapel Hill*

Small Molecules / Tox | Thursday 10:00 Poster #21B
A Case Study on Ion Suppression: Analysis of 17a-Hydroxyprogesterone by ESI Mass Spectrometry
Andrew Tromans *- Canterbury Health Laboratory (NZ)*

Small Molecules / Tox | Thursday 10:00 Poster #21C
Approaching a Random Access Calibration Design for LC-MS/MS – Performance in Production
Heather Hochrein *- UC San Diego Health*

Small Molecules / Tox | Wednesday 10:00 Poster #21D
Addition of Supercharging Agents to Lower Detection Limits of Phosphorylated Compounds by LC-MS/MS
Bryan Guzman Rodriguez *- University of North Carolina at Chapel Hill*

Small Molecules / Tox | Wednesday 13:30 Poster #22B
Rapid LC-MS/MS Detection of Opiates, Opioids, Benzodiazepines, Amphetamines, and Cannibinoids in Urine in Clinical Research
Carrie Adler *- Agilent Technologies*

Small Molecules / Tox | Wednesday 10:00 Poster #29A
A Comprehensive Method for Analysis of Pain Management Drugs Employing Simplified and Rapid LC-MS/MS Workflow for Clinical Research
Jonathan Danaceau *- Waters Corporation*

Small Molecules / Tox | Wednesday 10:00 Poster #29D
An Easy-to-Use Automated Solid-Phase Extraction Method for Quantification of Serum Nicotine and Metabolites Using LC-MS/MS
Rongrong Huang *- Houston Methodist Hospital (*YI Grantee*)*

Small Molecules / Tox | Thursday 12:30 Poster #30A
Lowering the Bar for Mass Spec: A Comparison Between Immunoassay and Rapid LC-TOF-MS for Presumptive Analytical Screening of Drugs in the Clinical Research Lab
Natalie Rasmussen *- Agilent Technologies*

Small Molecules / Tox | Wednesday 13:30 Poster #30B
Glyphosate and Aminomethylphosphonic Acid (AMPA) Analysis in Biological Matrices Using LC-MS/MS
Evelyn Wang *- Shimadzu Scientific Instruments*

Small Molecules / Tox | Wednesday 13:30 Poster #30C
The Detection and Analytical Confirmation of Synthetic Fentanyl Analogues in Human Urine & Serum Using an Ultivo LC/TQ
Peter Stone *- Agilent Technologies Inc*

Small Molecules / Tox | Wednesday 13:30 Poster #32B
Rapid Analysis of Fentanyl and Other Synthetic Opioids Using Paperspray-Mass Spectrometry: Comparison to Current Technologies
Joseph Kennedy *- Prosolia.com*

Small Molecules / Tox | Wednesday 10:00 Poster #33A
A UPLC-MS/MS Method for Therapeutic Drug Monitoring of Oxcarbazepine
Chia-Ni Lin *- Chang Gung Memorial Hospital*

Small Molecules / Tox | Wednesday 13:30 Poster #34C
Development of the Comprehensive Method for Steroid Analysis by GCxGC-HR TOFMS
Viatcheslav Artaev *- LECO Corp*

Small Molecules / Tox | Thursday 10:00 Poster #35C
eXtreme Filter Vial Extraction for the Detection of Fentanyl and Analogues in Oral Fluid Samples
Lisa Wanders *- Thomson Instrument Company*

Small Molecules / Tox | Thursday 12:30 Poster #36A
Applying LCMS Methods to Instruments of Different Manufacturers – the Diverging Influence of Same-Named ESI Source Parameters
Katharina Kern *- RECIPE Chemicals + Instruments GmbH*

Small Molecules / Tox | Wednesday 13:30 Poster #36B
Development and Validation of LC-MS/MS Approach for Quantification of Haloperidol and Several Atypical Antipsychotics and their Metabolites in Serum Samples
Magdalena Rajska *- Spadia Lab*

Small Molecules / Tox | Wednesday 13:30 Poster #38B
Multi-Residue Analysis of Abuse Drugs in Whole Blood Using In-well Protein Precipitation Followed with Captiva EMR-Lipid Cleanup by LC-MS/MS
Limian Zhao *- Agilent Technologies*

Small Molecules / Tox | Wednesday 13:30 Poster #38C
The Rise of Loperamide and Desmethyl Loperamide Abuse in the Wake of the Opioid Crisis: Development and Validation of Loperamide and Metabolite by LC-MS/MS
Rebecca Mastrovito *- NMS Labs*

Small Molecules / Tox | Wednesday 10:00 Poster #39A
Determination of Urine Copper and Zinc Concentrations by ICP-MS in UPEC Infections
Jisook Yim *- Green Cross Laboratories*

Small Molecules / Tox | Thursday 10:00 Poster #39B
Analysis of Antiepileptic Drugs in Human Serum Using an Ultivo LC/TQ
Jennifer Hitchcock *- Agilent Technologies*

Small Molecules / Tox | Thursday 12:30 Poster #44A
A Rapid and Simple HPLC-MS/MS Method for Personalized Busulfan Dosing in Pediatric Patients Undergoing Hematopoietic Stem Cell Transplantation (HSCT)
Yi Xiao *- Children's Hospital Los Angeles (*YI Grantee*)*

Small Molecules / Tox | Thursday 10:00 Poster #45B
Measurement of a Panel of Water Soluble Vitamins in Serum Using the Sciex Citrine™ Triple Quad™ MS/MS System
Michael Jarvis *- SCIEX*

Small Molecules / Tox | Wednesday 13:30 Poster #46B
Evaluation of Tip-Washing Technology for Forensic and Clinical Applications
Allison Veitenheimer *- Oklahoma State University*

Small Molecules / Tox | Wednesday 13:30 Poster #46C
Cross Validation of Immunosuppressant Quantification in Whole Blood by LDTD-MS/MS and LC-MS/MS Using Triple Ion Source
Pierre Picard *- Phytronix Technologies, Inc*

Small Molecules / Tox | Wednesday 10:00 Poster #47D
Fast LC-MS/MS Analytical Method with Alternate Column Regeneration for the Analysis of >100 Various Drugs and Their Metabolites in Urine in Clinical Research
Andre Szczesniewski *- Agilent Technologies*

Small Molecules / Tox | Thursday 12:30 Poster #48A
New Analytical Tool for Urine Sample Screening and Confirmation Analysis: Combined LDTD-MS/MS and LC-MS/MS Ion Source
Jean Lacoursière *- Phytronix*

Tissue Imaging & Analysis

Tissue Imaging & Analysis | Wednesday 13:30 Poster #8C
Mass Spectrometry Imaging Enables Molecular Diagnosis of Melanocytic Lesions
Erin Seeley *- Protea Biosciences*

Tissue Imaging & Analysis | Thursday 10:00 Poster #9B
Pharmaco-Metabolomics in the Clinical Lab
Begona Gimenez-Cassina Lopez *- Brigham and Women´s Hospital, Harvard University (*YI Grantee*)*

Tissue Imaging & Analysis | Wednesday 13:30 Poster #10C
Smartphone Whole Slide Imaging: the Slide Scanner Already in Your Lab
David Farnell *- McMaster University*

Tissue Imaging & Analysis | Wednesday 13:30 Poster #12C
Data Fusion of Polarity Switched DESI Mass Spectrometry Imaging Data for Enhanced Histological Classification of Clinical Tissue Samples
James McKenzie *- Imperial College London*

Tissue Imaging & Analysis | Thursday 12:30 Poster #12D
3D Volume Cartography of Diseased Human Lungs
Alexey Melnik *- UCSD*

Tissue Imaging & Analysis | Wednesday 10:00 Poster #17A
In vitro **Liquid Extraction Surface Analysis Mass Spectrometry (IV-LESA MS) for Direct Analysis of Adherent Cells in Culture**
Sankha (Bobby) Basu *- Brigham and Women's Hospital (*YI Grantee*)*

Tissue Imaging & Analysis | Thursday 10:00 Poster #17B
Multimodal Imaging of AD-Associated Lipid Species in Structurally Distinct Plaques
Wojciech Michno *- Sahlgrenska Academy, University of Gothenburg*

Tissue Imaging & Analysis | Thursday 10:00 Poster #19C
Detection of Renal Cell Carcinoma Multikinase Inhibitors in Hair by Mass Spectroscopy Imaging to Measure Patient Adherence
Nicole White *- University of North Carolina at Chapel Hill*

Tissue Imaging & Analysis | Wednesday 10:00 Poster #31D
Visualizing Differential Molecular Abundance in Staphylococcal Infectious Interfaces Using Imaging Mass Spectrometry
William Perry *- Vanderbilt University (*YI Grantee*)*

Tissue Imaging & Analysis | Thursday 12:30 Poster #34A
Potential Role of Desorption Electrospray Ionization (DESI) Mass Spectrometry Imaging for Intra-Operative Margin Assessment of Basal Cell Carcinoma Resections
Martin Kaufmann *- Queen's University (*YI Grantee*)*

Tissue Imaging & Analysis | Thursday 12:30 Poster #34D
Liquid Extraction Surface Analysis Mass Spectrometry (LESA-MS): Examples of a New Surface Probing Technique for Clinical and Pre-Clinical Applications
Daniel Eikel *- Advion Inc.*

Tissue Imaging & Analysis | Thursday 10:00 Poster #45C
Pathological Assessment of Prostate Cancer Biopsies by DESI Mass Spectrometry Imaging
Nicole Morse *- Queen's University*

Troubleshooting

Troubleshooting | Tuesday 19:00 Poster #40A
Charge Wars of Ion Suppression - Awakening the Force for the Analysis of Estrogens in Clinical Research
Robert Wardle *- Waters Corporation*

Troubleshooting | Tuesday 19:20 Poster #40B
Metformin Interference in LC-MS/MS Analysis of Plasma Methoxycatecholamines
Marianne Bergmann *- Lillebaelt Hospital (*YI Grantee*)*

Troubleshooting | Tuesday 19:40 Poster #40C
Fat Loving Vitamins – the Struggle is Real
Matthew Crawford *- LabCorp*

Troubleshooting | Thursday 17:00 Poster #41B
Low Extraction Rate of 6-Methylmercaptopurine in RBC
Soo Young Moon *- Seoul National University Hospital*

Troubleshooting | Thursday 17:15 Poster #41C
Autosampler Tray Troubleshooting Tales
Kristine Van Natta *- Thermo Fisher Scientific*

Troubleshooting | Thursday 10:00 Poster #47C
Troubleshooting the Urine Interferences Present in the LC-MS/MS Analysis of Ethyl Glucuronide and Ethyl Sulfate
Rory Doyle *- Thermo Fisher Scientific, Inc*

Various OTHER

Various OTHER | Wednesday 13:30 Poster #4C
Non-Derivatized LC-ESI-MS/MS Method for Determination of Vitamin D and 10 Steroid Hormones Using New PerkinElmer Qsight® Triple Quadrupole Mass Spectrometer
Jordan Haddock *- PerkinElmer*

Various OTHER | Thursday 10:00 Poster #7B
Multiplexed, High-Throughput LCMS Methods for Non-Polar and Polar Lipid Quantification in Size Separated Lipoproteins
Antony Lehtikoski *- Orise Fellow at CDC (*YI Grantee**)*

Various OTHER | Wednesday 13:30 Poster #14C
Robustness Evaluation of the Qsight® 210 MD Triple-Quadrupole Mass Spectrometer Against "Dirty" Samples
Sumeet Kaushal *- Perkin Elmer Inc*

Various OTHER | Thursday 10:00 Poster #15B
Regulation Mechanisms on Vascular Functions in sEH KO Mice Revealed by High-Throughput Mass Spectrometry-based Proteomics
Dawei Wang *- University of Pittsburgh (*YI Grantee**)*

Various OTHER | Wednesday 10:00 Poster #15D
Novel Plasma Card for Shipping Clinical Samples
Tim Schlabach *- Novilytic LLC*

Various OTHER | Thursday 12:30 Poster #18A
A Single High-Throughput UPLC-MS/MS Platform for Targeted Metabolomic, Lipidomic and Proteomic Studies (Targeted Multi-OMICS)
Billy Molloy *- Waters*

Various OTHER | Thursday 10:00 Poster #23B
Integrating Inborn Errors of Metabolism and Hemoglobin Variant Clinical Research into a Single High Resolution Accurate Mass Based Mass Spectrometer Workflow
Xiaolei Xie *- Thermo Fisher Scientific*

Various OTHER | Thursday 12:30 Poster #24D
Development of a Reliable Mass Spectrometric Enzymatic Assay for Mucopolysaccharidosis Type III (MPS III)
Fan Yi *- University of Washington (*YI Grantee**)*

Various OTHER | Thursday 12:30 Poster #32D
A Multiplex UPLC-MSMS Method for Newborn Screening of 13 Lysosomal Storage Diseases Plus Adrenoleukodystrophy
Xinying Hong *- University of Washington (*YI Grantee**)*

Various OTHER | Thursday 10:00 Poster #33C
Meeting the Challenges of Large Molecule Bioanalysis: Demonstration of an Automated & Standardized, Kit-based Workflow for LC-MS/MS Protein Quantification
Keil Brinster *- Waters Technologies*

Various OTHER | Wednesday 10:00 Poster #43A
Quantification of Simvastatin and its Metabolites in Plasma Samples
Jenni Viinamäki *- University of Helsinki*

Various OTHER | Wednesday 13:30 Poster #44C
Statistical Classification Analysis of Mass Spectral Data of Biological Samples: A Basic Introduction
Kirk Jensen *- Osaka University (*YI Grantee**)*

Posters by Number

Poster #1A in Exhibit Hall - *attended for 1 hr on Wednesday starting at 10:00*
Topic: *Small Molecules / Tox*
A Simple and Rapid UPLC-MS/MS Assay for the Determination of Serum Free Voriconazole in Cancer Patients
Jieli Li - *MD Anderson Cancer Center* (jli28@mdanderson.org) *YI Grantee*
‣ Therapeutic drug monitoring (TDM) may miss the window of dose adjustment for cancer patients who exhibit normal total VOR but higher unbound VOR concentrations due to hypoalbuminemia. Thus we report an accurate, simple and fast UPLC-MS/MS method to measure unbounded VOR concentrations in human serum. This assay is suitable for routine VOR monitoring in clinical laboratories for better therapeutic outcome.

Poster #1B in Exhibit Hall - *attended for 1 hr on Thursday starting at 10:00*
Topic: *Proteomics*
Using Activity-based Protein Profiling Proteomics to Determine Novel Pathways & Therapeutic Monitoring Targets
Sean Campbell - *University of Virginia* (STC2M@virginia.edu) *YI Grantee*
‣ Kinases, through their function of phosphorylating various substrates, control a wide range of cellular functions. However, as a result of this important role, most cellular kinases exist in auto-inhibited states. Activity Based Protein Profiling (ABPP), allows us to monitor only active kinases in both gel and MS systems. In the Hsu lab, we have managed to leverage a number of different technologies, including classic substrate assays, ABPP, and mass spectrometry-based proteomics, to determine previously unknown downstream targets of a potential immune-modulating therapeutic, Ritanserin. This points the way to further proteomic investigation of new and current drugs to determine new targets for susceptibility and therapeutic monitoring.

Poster #1C in Exhibit Hall - *attended for 1 hr on Thursday starting at 10:00*
Topic: *Metabolomics*
Development of Combined LC-MS/MS Analysis for Citric Acid Cycle Intermediates, Acylcarnitines and Amino Acids
Rohan Shah - *Cleveland State University* (r.r.shah22@vikes.csuohio.edu) *YI Grantee*
‣ Citric Acid Cycle (CAC) intermediates, acylcarnitines, and amino acids are key metabolites that serve vital roles in the maintenance of cellular homeostasis. Monitoring these metabolites facilitates the understanding of aberrant metabolic processes which occur due to various disease states. We have developed a new LCMS/MS based workflow to analyze these metabolites. Currently, acylcarnitines and amino acids are screened clinically via FIA-MS, whereas organic acids like citric acid cycle intermediates are analyzed using GC-MS which includes extensive sample preparation steps. Our method streamlines the analytical approach to detect and quantify these metabolites via a single sample preparation technique and increased throughput for further application in clinical settings. We applied the developed platform to analyze all target metabolites in various biological matrices.

Poster #1D in Exhibit Hall - *attended for 1 hr on Wednesday starting at 10:00*
Topic: *Endocrinology*
Simultaneous Quantitation of Segesterone Acetate (Nestorone®), Estradiol, Estrone, and Progesterone in Human Sera by LC-MS/MS
David Erikson - *Oregon National Primate Research Center* (erikson@ohsu.edu)
‣ Precise measurement of synthetic and natural steroid hormones is critical to assess pharmacokinetic and pharmacodynamic effects of novel contraceptive methods. We have developed a method to simultaneously quantitate serum levels of the 19-norprogesterone derivative, segesterone acetate (Nestorone®), and the endogenous steroid hormones estradiol, estrone, and progesterone by liquid chromatography-tandem mass spectrometry. This method is rapid, sensitive, precise, and accurate. It can be used to monitor adherence to contraceptive methods using Nestorone®, and also for development of new contraceptive protocols using Nestorone®.

Poster #3A in Exhibit Hall - *attended for 1 hr on Wednesday starting at 10:00*
Topic: *Endocrinology*

Obtaining FDA Clearance via the *de novo* Pathway, for the First IVD LC-MS/MS 25-Hydroxyvitamin D Assay

Michal Weinstock - *SCIEX* (michal.weinstock@sciex.com)

‣ We present here the data from our FDA submission to obtain clearance for the first LC-MS/MS Vitamin D Assay, granted by the FDA via the de novo pathway. The assay independently quantitates 25(OH)D3 and 25(OH)D2, while separating the isobaric 3-epimer forms and other potential interferences using Topaz™ LC-MS/MS System (SCIEX). In addition, it is certified by the CDC Vitamin D Standardization Certification Program and is traceable to the NIST and Ghent University reference measurement procedure. The verification studies were performed at three clinical trial sites following the standard clinical diagnostics guidelines for each study.

Poster #3B in Exhibit Hall - *attended for 1 hr on Thursday starting at 10:00*
Topic: *Microbiology/Virology*

Endogenous Digoxin and Cancer Management – Would Zika Virus be the Trigger for Glioblastomas Death Through Digoxin Synthesis?

Estela Lima - *University of Campinas* (eoliv.lima@gmail.com) *YI Grantee*

‣ Zika virus (ZIKV) has been associated with microcephaly cases in babies from mothers infected during pregnancy. Cell death has been reported in neural progenitor cells and glioblastoma cells infected with ZIKV, corroborating with virus tropism for brain progenitor cells. What would be the metabolic changes caused by ZIKV that allow these phenomena? The present study has evaluated the metabolomic profile of ZIKV infection over glioblastoma cells through MALDI-MSI. We found out an interesting biomarker, endogenous Digoxin, a Na+/K+-ATPase pump inhibitor, previously reported at tumors recovering. So, we suggest ZIKV would be an interesting oncolytic tool for neural tumors through induction of endogenous digoxin synthesis.

Poster #3C in Exhibit Hall - *attended for 1 hr on Thursday starting at 10:00*
Topic: *Microbiology/Virology*

Serum Metabolic Alterations Upon Zika Infection

Carlos Fernando Odir Rodrigues Melo - *University of Campinas* (carlosfernandomelo1@gmail.com) *YI Grantee*

‣ Zika virus (ZIKV) has recently emerged as a major concern worldwide due to its strong association with nervous system malformation (microcephaly) of fetuses in pregnant women who were infected by the virus. This has brought much attention from the medical community, and understanding the mechanism of viral infection has become an important research focus. Within this context, the present work analyzed blood plasma from a total of 79 subjects, including: (i) patients with positive ZIKV diagnosis, (ii) patients with negative ZIKV diagnosis, but presenting symptoms like ZIKA infections, and (iii) healthy subjects. Through sample direct infusion associated with mass spectrometry and statistical analysis, it was possible to describe seven lipid markers that are related to the pathophysiological process of ZIKV replication.

Poster #3D in Exhibit Hall - *attended for 1 hr on Wednesday starting at 10:00*
Topic: *Metabolomics*

Screening for 3 LSD Using Triplex Tandem Mass Spectrometry Assays with 2 Confirmation Tests in Korea

Sung Eun Cho - *LabGenomics* (secho0824@gmail.com)

‣ LabGenomics Clinical Laboratories used UPLC-MS/MS (Waters CSH C18 column and TQD in MRM mode) following the methods of our previous study to screen the 3 LSDs, Pompe, Fabry, and Gaucher diseases. The purpose of this study was to evaluate the prevalence of selective screening tests for these LSDs with 2 confirmation tests, which were leukocyte enzymatic activity test and genotyping tests such as NGS or Sanger sequencing method. The % of the suspected diseases of the positive screening samples was 5.72% in 9,160 dried blood spots from the patients visiting various departments of general hospitals or clinics in Korea. Of these screened positive samples, 11 samples were both positive assessed by above 2 confirmation tests.

Poster #4A in Exhibit Hall - *attended for 1 hr on Thursday starting at 12:30*
Topic: *Small Molecules / Tox*

Evaluation of Matrix Component Removal Using a Novel Flow-Through Scavenging Plate for Drugs of Abuse Testing in Urine

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

‣ Dilute and shoot is the most common form of sample preparation for the analysis of drugs of abuse in urine. High analyte cutoffs combined with sensitive mass spectrometers allow substantial sample dilution while still reaching desired limits of quantitation. However, this technique presents various issues resulting in increased MS downtime. This poster evaluates the extraction of a range of drugs of abuse from hydrolysed and non-hydrolysed urine using a novel flow-through matrix scavenging plate. Specific investigation of matrix component removal in terms of creatinine and urea, salt residue, pigmentation associated with urobillin content and protein removal will be demonstrated.

Poster #4B in Exhibit Hall - *attended for 1 hr on Wednesday starting at 13:30*
Topic: *Endocrinology*

Measurement of Serum Free Cortisol Using ED-LC-MS/MS; Revisiting the Use of Free Cortisol Measurement for Adrenal Insufficiency in Critically Ill Patients

Julie Ray - *ARUP Laboratories* (julie.ray@aruplab.com)

‣ Free cortisol (fC) provides an accurate measure of adrenal function in the critically ill. An equilibrium dialysis (ED)-LC-MS/MS method was developed with imprecision <10% and LOQ and ULOL of 0.06 and 60.00 µg/dL respectively. The method agreed poorly with an electrochemiluminescent immunoassay (slope=0.41, r=0.52) but well with another ED-LC-MS/MS method (slope=0.82, r=0.98). Time-specific transformed parametric reference intervals were: 0.21–1.04 µg/dL (8-10AM) and 0.10 –0.63 µg/dL (4-6PM). 100 samples from critically ill patients showed loss of diurnal variation of total cortisol with mean fC in samples with low albumin concentrations being 3.1 times higher than healthy samples.

Poster #4C in Exhibit Hall - *attended for 1 hr on Wednesday starting at 13:30*
Topic: *Various OTHER*

Non-Derivatized LC-ESI-MS/MS Method for Determination of Vitamin D and 10 Steroid Hormones Using New PerkinElmer Qsight® Triple Quadrupole Mass Spectrometer

Jordan Haddock - *PerkinElmer* (jordan.haddock@perkinelmer.com)

‣ The preferred use of LC-MS/MS over immunoassays is ever increasing as mass spectrometry continually demonstrates superior performance in its accuracy, precision and ability to multiplex. In this study, we determined the feasibility of measuring Vitamin D and Steroids using both ESI and APCI ionization modes without sample derivatization. Here, we demonstrate 2 separate non-derivatized LC-ESI-MS/MS assays for determining Vitamin D metabolites, 25(OH)D3 and 25(OH)D2, and 10 steroid hormones in human serum on the new PerkinElmer QSight® Triple Quadrupole Mass Spectrometer.

Poster #4D in Exhibit Hall - *attended for 1 hr on Thursday starting at 12:30*
Topic: *Metabolomics*

Microflow LC-MS/MS Workflow Allows Up to 50% More Metabolite Coverage for Targeted Polar Metabolite Analysis

Khatereh Motamedchaboki - *SCIEX* (khatereh.motamedchaboki@sciex.com)

‣ Identifying metabolites from urine and plasma are essential to understanding diseases and developing novel therapeutics. Liquid chromatography–tandem mass spectrometry (LC-MS/MS) analysis has become an essential tool for the identification and quantification of metabolites in complex matrices. Here, we describe a robust and sensitive workflow using microflow LC and targeted MS for qualitative and quantitative analysis of polar metabolites. A colon cancer study is presented to evaluate the assay performance for biological sample sets.

Poster #5A in Exhibit Hall - *attended for 1 hr on Wednesday starting at 10:00*
Topic: *Proteomics*

Monitoring Monoclonal Immunoglobulins Directly from Bone Marrow Plasma Cells Using LC-MS

David Barnidge - *Mayo Clinic and The Binding Site* (david.barnidge@thebindingsite.com)

‣ In this abstract we demonstrate the ability of mass spectrometry to identify monoclonal immunoglobulins directly from plasma cells isolated from a bone marrow biopsy. Plasma cells were isolated from the biopsy using anti-CD138 antibodies bound to magnetic beads. Monoclonal immunoglobulins were then purified from plasma cell cytoplasm by incubating with camelid nanobody beads. The molecular masses of monoclonal light chains and heavy chains were matched in cell lysates and serum from patients with multiple myeloma. The glycosylation pattern on monoclonal heavy chains isolated from cytoplasm often did not match the glycosylation pattern observed serum, suggesting plasma cell specific glycoforms.

Poster #5B in Exhibit Hall - *attended for 1 hr on Thursday starting at 10:00*
Topic: *Small Molecules / Tox*

Comparison of Sample Preparation Options for the Extraction of a Panel of Endogenous Steroids from Serum Prior to UHPLC-MS/MS Analysis

Katie-Jo Teehan - *Biotage GB Limited* (Katie-Jo.Teehan@biotage.com)

‣ This poster compares sample preparation options for the extraction of a panel of endogenous steroids from serum. Method parameters were optimized for increased sensitivity: MRM transitions, chromatography and mobile phase additives due to the necessity of positive and negative ionisation modes. LC-MS/MS analysis was performed using a Shimadzu Nexera UHPLC system coupled to an 8060 triple quadrupole MS. Solid phase extraction was compared to supported liquid extraction and methods optimized for a steroid panel including and without DHEAS. Final optimized methods were compared for extract cleanliness by investigation for phospholipid content.

Poster #5C in Exhibit Hall - *attended for 1 hr on Thursday starting at 10:00*
Topic: *Small Molecules / Tox*

Extraction of Catecholamine Acid Metabolites from Plasma Prior to Analysis Using UHPLC-MS/MS

Elena Gairloch - *Biotage GB Limited* (Elena.Gairloch@biotage.com)

‣ Catecholamine metabolites are biomarkers for neuroblastoma and catecholamine-secreting tumors. Here we present optimization of the method development process to maximise analyte sensitivity in the extraction and quantitation of plasma catecholamine acid metabolites. Method parameters optimized for increased sensitivity: MRM transitions, chromatography and sample preparation protocols. LC-MS/MS analysis was performed using a Shimadzu Nexera UHPLC system coupled to an AB SCIEX 5500 triple quadrupole MS. Extraction methods demonstrated recoveries greater than 80% with RSDs below 10%. Calibration curves from 20 to 1000 ng/mL demonstrated good linearity with r2 values greater than 0.990 for all analytes.

Poster #5D in Exhibit Hall - *attended for 1 hr on Wednesday starting at 10:00*
Topic: *Endocrinology*

A Sensitive LC-MS/MS Method for the Determination of Nestorone in Human Serum

Feng Bai - *Los Angeles Biomedical Research Institute* (fbai@labiomed.org)

‣ We have developed and validated a highly sensitive and accurate LC-MS/MS assay for the measurement of serum Nestorone for clinical research. The Nestorone (371.4.3/253.1) with 13C3-NES ISTD (374.4/253.1) were separated on a Kinetex C18 column within 5 minutes with a gradient profile from 45% to 100% methanol at 0.6 mL/min. The calibration curve was linear over a concentration range of 10 to 30,000 pg/mL. The intra-assay and inter-assay precision expressed as coefficient of variation (%CV) were less than 10. The accuracy were from 88.0% to 104.7% in spanning different Nes concentrations.

Poster #6A in Exhibit Hall - *attended for 1 hr on Thursday starting at 12:30*
Topic: *Small Molecules / Tox*

Rapid Quantification of 90+ Drugs in Urine Using Citrine™ QTRAP® MS/MS System

Amol Kafle - *SCIEX* (amol.kafle@sciex.com)

‣ We developed a 5 min method for the quantitation of 90+ drugs in urine using the new Citrine™ QTRAP® MS/MS system. This method utilizes the fast polarity switching as well as low dwell time capabilities of the new LC-MS/MS system. We monitored 2 transitions per analyte as well as 1 transition per internal standard for a total of 197 MRM transitions in positive ionization mode and 15 MRM transitions in negative ionization mode. Sample preparation consists of a 30 min enzymatic hydrolysis followed by centrifugation, dilution and injection.

Poster #6B in Exhibit Hall - *attended for 1 hr on Wednesday starting at 13:30*
Topic: *Endocrinology*

Matrix Based Calibrators for Quantification of Testosterone and Dihydrotestosterone

Linda Smith - *MilliporeSigma* (Linda.Smith@sial.com)

‣ Development of accuracy-based calibrators in biological matrices requires measurement methods with high accuracy, precision and sensitivity. We present a method for quantitation of Testosterone in serum and Dihydrotestosterone in synthetic serum by Isotope Dilution Liquid Chromatography Mass Spectrometry (ID-LC-MS/MS). Data presented will address validation of the method, validation of the product and provide long term evidence of stability through the use of control charting.

Poster #6C in Exhibit Hall - *attended for 1 hr on Wednesday starting at 13:30*
Topic: *Proteomics*

Development of Simple and Rapid Workflows for Quantitation of Infliximab and Adalimumab in Human Serum by LC-MS/MS

Kevin Ray - *MilliporeSigma* (kevin.ray@sial.com)

‣ There is a growing demand for reliable LC-MS/MS assays to support quantitation of serum levels of Infliximab and Adalimumab monoclonal antibodies, as clinical responses differ between patients due to varying pharmacokinetics and the formation of autoantibodies. We have optimized a simple “pellet digestion” sample preparation workflow that can be completed for 96 samples in under 4 hours. A lower limit of quantitation of 1 µg/mL for Adalimumab and Infliximab from 20 µL of serum was achieved with the optimized workflow. We have also evaluated the optimized “pellet digestion workflow” in a Control Flow Plate (CFP) format. We find that the CFP protocol provides greater automation potential by eliminating manual processing steps, but the CFP protocol is less sensitive, with lower limit of quantitation of 8 µg/mL for Infliximab and 16 µg/mL for Adalimumab.

Poster #6D in Exhibit Hall - *attended for 1 hr on Thursday starting at 12:30*
Topic: *Cannabinoids*

Analysis of 12 Cannabinoids in Whole Blood by LC-MS/MS

Laura Snow - *Phenomenex, Inc.* (laurasn@phenomenex.com)

‣ In addition to the psychoactive cannabinoid THC, there is growing interest in the potential medicinal benefits of the plant’s other major cannabinoids which are non-psychoactive. This work presents a LC-MS/MS method for analysis of 12 cannabinoids and 2 metabolites from whole blood. Cannabinoids are very hydrophobic compounds which elute late in reversed phase chromatography. Since phospholipids also elute in this region, matrix effects/ion suppression can be a concern. Through a simple sample preparation technique utilizing a phospholipid removal cartridge, removal of phospholipids, reduced matrix effects, and good recovery were achieved while avoiding the added inconvenience of a dry down step.

Poster #7A in Exhibit Hall - *attended for 1 hr on Wednesday starting at 10:00*
Topic: *Small Molecules / Tox*

Elucidation of a Naproxen Metabolite Interference in Total Bilirubin Testing on a Routine Chemistry Analyzer System Using LC-MS/MS

Aaron Barnes - *University of Minnesota* (barnesa@umn.edu) *YI Grantee*

‣ The CYP450-based demethylation of the anti-inflammatory drug naproxen leads to a metabolite – O-desmethylnaproxen – that rapidly reacts with the sulfanilic acid-based chemistry in the classic Jendrassik & Grof method for total bilirubin. This chemistry is currently used in a significant number of automated clinical analyzer systems. Here we found experimental mass spectrometric along with spectroscopic data that is consistent with formation of a novel substituted naphthalene ring-based azo dye related to the Orange G histochemical stain. This compound is likely responsible for the positive test interference seen in patients with markedly elevated serum naproxen levels when using chemistry platforms employing such reagents.

Poster #7B in Exhibit Hall - *attended for 1 hr on Thursday starting at 10:00*
Topic: *Various OTHER*

Multiplexed, High-Throughput LCMS Methods for Non-Polar and Polar Lipid Quantification in Size Separated Lipoproteins

Antony Lehtikoski - *Orise Fellow at CDC* (nkg2@cdc.gov) *YI Grantee*

‣ Lipid metabolism research and risk assessment studies requires separation of lipoproteins into high, low and very low density fractions (HDL, LDL and VLDL) and sub-fractions. Fractionation needs to be followed by sensitive and multiplexed quantitative analysis. Conventional liquid-liquid extraction of lipids are labor intensive limiting sample throughput. We present two simple “one-pot” lipid extraction protocols performed in high throughput 96-well format using <1 µL serum or plasma or diluted lipoprotein fractions from 50 µL serum. The extraction protocols were coupled with corresponding high-throughput UPLC-MS/MS methods for non-polar and polar lipid classes. The reproducibility and accuracy meet requirements of clinical application.

Poster #7C in Exhibit Hall - *attended for 1 hr on Thursday starting at 10:00*
Topic: *Proteomics*

Proteogenomic Analysis of Clinical Samples Using a Unified Extraction Method

Jared Isaac - *Thermo Fisher Scientific* (jared.isaac@thermofisher.com)

‣ The Thermo Scientific™ KingFisher™ Flex Purification System and MagMAX FFPE DNA/RNA kit were optimized for DNA, RNA and protein extraction for proteogenomics in a Unified Method (UM). Fresh frozen and formalin fixed paraffin embedded tissues from breast and lung cancer tissues were fixed and processed and/or sectioned followed by nucleic acid and peptide extraction, QC analyses, and “omics” techniques. NGS and LC-MS were performed on UM biomolecules using panels of cancer biomarkers producing quantitative data. This study shows that Proteogenomics in Pathology can provide Quantitative data to supplement Qualitative interpretation and speculation.

Poster #7D in Exhibit Hall - *attended for 1 hr on Wednesday starting at 10:00*
Topic: *Metabolomics*

The Utility of Urine GAGs as a Follow-Up and Confirmatory Test in Newborn Screening of Mucopolysaccharidosis I

Haoyue Zhang - *Duke University* (zhang053@mc.duke.edu)

‣ A pilot study of newborn screening for mucopolysaccharidosis (MPS) I was conducted based on alpha-iduronidase (IDUA) activity in dried blood spots (DBS) with Sanger sequencing of the IDUA gene as a second tier test. Urinary glycosaminoglycans (GAGs) analysis by UPLC-MS/MS was used as a confirmatory test in conjunction with repeat blood IDUA activity, and targeted mutation testing. Specific GAGs (heparan sulfate and dermatan sulfate) were markedly elevated in an infant with confirmed MPS I based on mutation testing, but were not elevated in infants who were heterozygous for pathogenic gene variants, or those with one or more pseudodeficiency alleles.

Poster #8A in Exhibit Hall - *attended for 1 hr on Thursday starting at 12:30*
Topic: *Endocrinology*

Development of a Multi-Component Analytical Method for 18 Steroid Compounds in Serum Matrix Utilizing Rapid Polarity Switching and Simple Sample Preparation

Jenny Moshin - *SCIEX* (jenny.moshin@sciex.com)

‣ The analysis of steroid hormones in serum is of high importance in modern research mass spectrometry laboratory portfolios. To maximize the efficiency and return on investment in research mass spectrometry, many laboratories look to exploit the power of mass spectrometry to run multi-component analyses and simplify and/or standardize their sample preparation. We present here a methodology that employs the sensitivity and rapid polarity switching of the new Sciex Citrine™ MS/MS system to achieve these goals, giving significant advantages over established methodologies for the analysis of steroids in serum.

Poster #8B in Exhibit Hall - *attended for 1 hr on Wednesday starting at 13:30*
Topic: *Proteomics*

Quantitative LC-MS/MS Analysis of Intact IgF-1 and 2 on a Triple Quadrupole and Quadrupole Orbitrap Mass Spectrometers

Sherry Gregory - *Thermo Fisher, Inc* (sherry.gregory@thermofisher.com)

‣ An LC-MS/MS analytical method was developed for the quantitation of intact IgF-1 and 2 on triple quadrupole and orbitrap platfroms. An acidic ethanol precipitation and solid phase extraction sample preparations were evaluated. Thermo Fisher tandem mass spectrometer and orbitrap platforms in positve Electrospray mode with a Vanquish Horizon HPLC system were used. 100 ul of serum with an Accucore Vanquish 100 x 2.1 mm, 1.5 mm using water:acetonitrile mixture containing formic acid achieved baseline separation within 6 minutes. The limits of detection and quantitation were determined to be 2.5 and 5 ng/ml for the orbitrap and tandem mass spectrometer respectively.

Poster #8C in Exhibit Hall - *attended for 1 hr on Wednesday starting at 13:30*
Topic: *Tissue Imaging & Analysis*

Mass Spectrometry Imaging Enables Molecular Diagnosis of Melanocytic Lesions

Erin Seeley - *Protea Biosciences* (erin.h.seeley@gmail.com)

‣ Mass spectrometry imaging (MSI) is an emergent technology for the analysis of clinical samples. Here, we present an application of MSI to the molecular diagnosis of human melanocytic skin lesions. Seven different subtypes of malignant melanoma as well as 3 subtypes of benign nevi were evaluated to determine a molecular classifier able to provide an accurate diagnosis. Overall classification accuracy of 94% for malignant melanomas and 92% for benign nevi was achieved within an independent validation sample set. Ongoing work involves increasing samples numbers of underrepresented subtypes to improve classification accuracies.

Poster #8D in Exhibit Hall - *attended for 1 hr on Thursday starting at 12:30*
Topic: *Small Molecules / Tox*

Quantification of 11-nor-9-Carboxy-THC and Panel of 22 Drugs in Hair Using Citrine™ QTRAP® MS/MS System

Xiang He - *SCIEX* (xiang.he@sciex.com)

‣ We developed a MS/MS/MS mass spectrometric method that reproducibly detects and quantifies 11-nor-9-Carboxy-THC levels in hair down to 0.1 pg/mg with Citrine™ QTRAP® MS/MS system. Using the same system a method was evaluated that allows the identification with simultaneous quantification and confirmation through MS/MS library matching and ion ratio values, for a panel of commonly analyzed forensic drugs in hair.

Poster #9A in Exhibit Hall - *attended for 1 hr on Wednesday starting at 10:00*
Topic: *Endocrinology*

Simultaneous Measurement of T3, Reversed T3 and T4 by a Sciex™ QTRAP5500 LC-MS/MS and Comparison to (Radio)immunoassay

Rutchanna Jongejan - *Erasmus Medical Centre* (r.jongejan@erasmusmc.nl) *YI Grantee*

‣ Immunoassays are often plagued by cross-reactivity. Our objective was to compare immunoassay and LC-MS/MS measurements of T3, rT3 and T4 . Passing & Bablok-fit showed a constant positive bias (+0.3nM) for T3, but not for rT3 or T4, when measured by immunoassay. This was likely explained by interference of T4 in the T3 immunoassay. In contrast, proportional bias was found for rT3 (-30%), likely due to a calibration problem in the rT3 radioimmunoassay. We developed a superior LC-MS/MS method for the simultaneous measurement of T3, rT3 and T4, which enables us to minimize sample volume.

Poster #9B in Exhibit Hall - *attended for 1 hr on Thursday starting at 10:00*
Topic: *Tissue Imaging & Analysis*

Pharmaco-Metabolomics in the Clinical Lab

Begona Gimenez-Cassina Lopez - *Brigham and Women´s Hospital, Harvard University* (bgimenez-cassinalopez@bwh.harvard.edu) *YI Grantee*

‣ A major challenge in drug development is getting the drug to arrive to the place of action inside the body. This challenge is further compounded for drugs directed towards the central nervous system (CNS), as they first need it to pass through the blood brain barrier (BBB), which presents additional chemical and biological features to be considered in drug development1. Besides the mathematical models that calculate the propensity of a drug to permeate into the CNS, mass spectrometry imaging (MSI) provides the ability to directly map and quantify the spatial distribution of a drug in the brain. To this end, a workflow was created using MALDI MS and LESA MS to assess the pharmacokinetics (mainly distribution and metabolism) and pharmacodynamics (pharmacological effect) of different targeted therapeutics in the CNS as they relate to tissue architecture.

Poster #9C in Exhibit Hall - *attended for 1 hr on Thursday starting at 10:00*
Topic: *Proteomics*

Investigation of Immunoglobulins from Patients with IgA Nephropathy by Using Liquid Chromatography - Triple Quadrupole Tandem Mass Spectrometry

I-Lin Tsai - *Taipei Medical University* (isabel10@tmu.edu.tw)

‣ Immunoglobulin A nephropathy (IgAN) is a kidney disease characterized by IgA deposition in the glomerular mesangial cells. Until now, kidney biopsy is the only way to confirm the disease. To investigate all the immunoglobulins from patient plasma, we used three platforms to detect IgG, IgA, and total Ig, respectively. Bead volume, time of incubation, and temperature of incubation were optimized to achieve the best purification efficiency. Samples were introduced to liquid chromatography-triple quadruple mass spectrometry for analysis. Multiple reaction monitoring was used to detect the tryptic peptides.

Poster #9D in Exhibit Hall - *attended for 1 hr on Wednesday starting at 10:00*
Topic: *Proteomics*

Development of a Novel LC Concept for Clinical Proteomics

Nicolai Bache - *Evosep Biosystems* (nb@evosep.com)

‣ Here we describe a conceptually novel low-flow chromatography system that delivers the robustness and throughput required for clinical applications while maintaining the sensitivity of current nano-flow LC instrumentation. Low pressure pumps elute the sample from a disposable trap while also forming a chromatographic gradient that is stored in a long holding loop. An auxiliary gradient creates an offset, ensuring that peptides are fully re-focused before being separated on the analytical column by a single high-pressure pump. We demonstrate the performance over thousands of samples and emphasises the clinical potential by re-analysing longitudinal plasma proteome weight loss study.

Poster #10A in Exhibit Hall - *attended for 1 hr on Thursday starting at 12:30*
Topic: *Endocrinology*

Increasing Throughput for High Analytical Sensitivity Bioanalysis of Human Insulin and its Biotherapeutic Analogs Using Microflow LC-MS/MS for Clinical Research

Andrew Peck - *Waters Corporation* (andrew_peck@waters.com)

‣ A higher throughput microfluidic analysis was developed for insulin and 5 analogs that delivers pg/mL analytical sensitivity with a 2x faster run time. A novel multidimensional microflow LC approach, coupled to a tandem quadruple MS, delivered highly analytically sensitive results with throughput comparable to analytical scale, a requirement by many routine bioanalytical labs. LLOQs were in the range of 25-100 pg/ml with standard curves over 3 orders with R2 values >0.99 and mean accuracy values >93% for all analytes.

Poster #10C in Exhibit Hall - *attended for 1 hr on Wednesday starting at 13:30*
Topic: *Tissue Imaging & Analysis*

Smartphone Whole Slide Imaging: the Slide Scanner Already in Your Lab

David Farnell - *McMaster University* (davefarnell@gmail.com)

‣ Mass spectrometry imaging is an exciting technique with the ability to drastically improve the practice of surgical pathology. Access to slide scanners is a potential limiting factor in the development and implementation of mass spectrometry. I have demonstrated an inexpensive and accessible way to create a slide scanner using equipment which is readily available in most research laboratories: a light microscope, a smartphone, and a computer. This method can be used by anyone and will hopefully increase the use of mass spectrometry imaging in surgical pathology.

Poster #10D in Exhibit Hall - *attended for 1 hr on Thursday starting at 12:30*
Topic: *Endocrinology*

Tandem Mass Spectrometric Measurement of Seven Steroids in Dried Blood Spots to Diagnose Congenital Adrenal Hyperplasia

Deema Qasrawi - *University of Calgary* (doqasraw@ucalgary.ca) *YI Grantee*

‣ Congenital adrenal hyperplasia (CAH) is a group of inherited disorders that lead to a reduction production of cortisol and overproduction of androgen due to mutations in those enzymes responsible for steroidogenesis. Defects in adrenal gland steroidogenesis is most commonly detected by immunoassay measurement of serum 17-hydroxyprogesterone (17-OHP). The low specificity and high costs associated with immunoassays have led to the development of multiplexed liquid chromatography tandem mass spectrometry (LC-MS/MS) methods for CAH diagnosis. Development of a LC-MS/MS for steroids measurement in dried blood spots (DBS) would be beneficial for patients because it reduces specimen volume, is less invasive and easy to collect, handle, transport and store.

Poster #12A in Exhibit Hall - *attended for 1 hr on Thursday starting at 12:30*
Topic: *Cannabinoids*

Medical Marijuana and Pain Medication Monitoring

Oneka Cummings - *Ameritox, LLC* (Oneka.Cummings@ameritox.com)

‣ As states continue to legalize both medical and recreational marijuana, pain medication monitoring laboratories are increasingly finding positive THCCOOH samples from both patients prescribed (Marinol®) or recommended marijuana (plant) as well as recreational users. This work is a retrospective look at data from patients prescribed Marinol® or recommended marijuana in the context of pain medication monitoring. Additional information includes: the identity and concentrations of other drugs prescribed, what illicit drugs proved positive, and what were the prescribed Marinol® dosing paradigms.

Poster #12B in Exhibit Hall - *attended for 1 hr on Wednesday starting at 13:30*
Topic: *Proteomics*

Quantitative Proteomics of Ras Signaling to Support Translational Cancer Research

Melissa Hoffman - *Moffitt Cancer Center/University of South Florida* (Melissa.Martinez@moffitt.org) *YI Grantee*

‣ Aggressive Ras-mutant tumors, which represent~30% of all cancers, have limited treatment options, leading to poor patient prognosis. To address challenges in translating basic research into tumor analysis for discovery of effective therapies and companion biomarker assays, a multiplexed LC-MRM assay was developed to quantify 167 tryptic peptides corresponding to 30 signaling proteins and 35 phosphorylation sites relevant to Ras signaling. Assay feasibility was demonstrated in cell lines to evaluate signaling changes caused by BRAF inhibitor treatment in sensitive and drug resistant cells. This resource will support the development of novel therapeutics and companion biomarkers for patients with Ras-driven cancers.

Poster #12C in Exhibit Hall - *attended for 1 hr on Wednesday starting at 13:30*
Topic: *Tissue Imaging & Analysis*

Data Fusion of Polarity Switched DESI Mass Spectrometry Imaging Data for Enhanced Histological Classification of Clinical Tissue Samples

James McKenzie - *Imperial College London* (j.mckenzie@imperial.ac.uk)

‣ Polarity switched desorption electrospray ionisation mass spectrometry imaging (DESI MSI) allows for acquisition of positive and negative ion modes. We present a workflow for acquiring and processing such data from clinical tissue samples. We employ linear interpolation to impute missing spectra, and as each pixel of the image is described by one positive and one negative mode spectrum, data fusion methods were employed to leverage the complementary nature of the data. Enhanced classification rates of various tissue types were observed in multiple samples when compared to either of the positive or negative mode data. DESI MSI can provide more objective classification than conventional histopathology, and polarity switched acquisition enhances its capabilities by using the complementarity of both positive and negative ion modes.

Poster #12D in Exhibit Hall - *attended for 1 hr on Thursday starting at 12:30*
Topic: *Tissue Imaging & Analysis*

3D Volume Cartography of Diseased Human Lungs

Alexey Melnik - *UCSD* (alexvmelnik@gmail.com)

‣ Our knowledge about the distributions of pathogenic microbes, antibiotics and their metabolites in Cystic Fibrosis affected lungs is limited. As a result, lungs are often treated as homogeneous entities. To gain insight into the chemical environment of the microbial habitat in human lungs, we created digitized maps of six explanted lungs from three patients with cystic fibrosis onto the 3D models generated from CT scans at both the chemical and microbial level. Except for the most dominant genera, the microbial constitution, also reflected in the chemistry, varied to a great extent in the lung. The chemical diversity between lobes of the same individual was sometimes greater than the inter-individual variation. The spatial maps revealed that the distribution of pharmaceuticals, microbial molecules, and host factors is unique to each patient and heterogeneously localized.

Poster #13A in Exhibit Hall - *attended for 1 hr on Wednesday starting at 10:00*
Topic: *Proteomics*

Proteomic Analysis of Therapeutic Biomarkers to Guide Treatment in Patients with Bone Metastasis

Yeoun Jin Kim - *Nantomics* (YeounJin.Kim@nantomics.com)

‣ Decalcification of bone can destroy protein and DNA, precluding personalized cancer therapy for some patients. We applied MS to quantify expression of treatment-related biomarkers in decalcified neoplastic bone samples. We compared protein expression in samples of primary cancer with their paired bone metastases. The 23 bone samples expressed 19 of 27 protein targets tested. 83% of samples expressed one or more markers of chemotherapy response, and 52% expressed at least one marker of response to targeted therapy. Eleven samples expressed HER2 (marker for trastuzumab). Mutated KRAS protein (marker of cetuximab resistance) was detected with MS. Acid decalcification had no discernable effect on MS-based protein quantification in archived tumor samples. Reproducible quantitation of drug targets in bone provides valuable information to inform personalized cancer treatment.

Poster #13B in Exhibit Hall - *attended for 1 hr on Thursday starting at 10:00*
Topic: *Proteomics*

Personalized Proteomics of Inflammatory Bowel Disease

Robert Mills - *UC San Diego* (rhmills@ucsd.edu) *YI Grantee*

‣ Inflammatory bowel disease is an autoimmune condition where inflammation and microbiome dysbiosis occur concurrently (1-3). Within the microbiome field, there is a distinct under-representation of proteome-level information. Proteomics holds the potential to elucidate functional mechanisms associated with IBD etiology. Here, we characterize the fecal metaproteome associated with disease states both in a time series of a patient with colonic Crohn's disease and in 40 patients with varying severity of Ulcerative Colitis. Results quantify over 29,000 proteins revealing potential pathways such as maltose metabolism and an increased IgA response associated with decreased inflammation.

Poster #13C in Exhibit Hall - *attended for 1 hr on Thursday starting at 10:00*
Topic: *Small Molecules / Tox*

Better Hydrolysis and Increased Efficiency for Urine Drug Testing Using Mixed-Mode Solid Phase Extraction with In-well Hydrolysis

Stephanie Marin - *Biotage* (stephanie.marin@biotage.com)

‣ Most drugs and metabolites are conjugated prior to excretion in the urine. Methods to detect drug analytes in urine usually include enzyme hydrolysis to convert glucuronide metabolites to their free form to maximize sensitivity. Four glucuronidase enzymes at different times and temperatures were evaluated to determine hydrolysis efficiency for seven glucuronide metabolites in a 100 compound urine drug panel. Offline hydrolysis with mixed-mode SPE (EVOLUTE EXPRESS CX, Biotage) was compared to results using a new SPE plate with in-well hydrolysis capability (EVOLUTE HYDRO CX, Biotage). Comparable hydrolysis, recovery and matrix effects were observed using both offline hydrolysis and in-well hydrolysis.

Poster #13D in Exhibit Hall - *attended for 1 hr on Wednesday starting at 10:00*
Topic: *Endocrinology*

25-Hydroxy Vitamin D C-3 Epimers: A Close-Up Comparison Between LC-MS/MS and BioPlex 2200

Jane Dickerson - *Seattle Children's Hospital* (jane.dickerson@seattlechildrens.org)

‣ C-3 epimers of 25-hydroxy vitamin D2 and D3 (3-epi-25(OH)D or epimers) are stereoisomers of 25-hydroxy vitamin D2 and D3, and require chromatographic separation in LC-MS/MS analyses. Epimers have been reported to cause positive interference in LC-MS/MS methods and commercially available immunoassays that measure total Vitamin D (3). The purpose of this study was to examine any interference of total 3-epi-25(OH)D in the BioPlex 2200 25-hydroxy vitamin D assay. Although there is a small positive bias overall, the BioPlex shows no consistent or significant positive bias in samples with significant epimer present, suggesting epimers are detected to some degree, but not at equimolar concentration to 25(OH) D.

Poster #14A in Exhibit Hall - *attended for 1 hr on Thursday starting at 12:30*
Topic: *Proteomics*

LC-MS/MS Quantification of Intact Insulin Like Growth Factor-I (IGF-I) from Serum for Clinical Research

Khalid Khan - *Waters Corporation* (khalid_khan@waters.com)

‣ Insulin-like Growth Factor I (IGF-I) is a 70 amino acid (7.6 kDa) peptide hormone which plays a significant role in mediating the effects of Growth Hormone (GH). Challenges with current immunoassay (lack of specificity, dynamic range) and LC-MS methods (digestion, immunoaffinity, nano-LC or its combination) make routine analysis difficult. Here, we highlight a simplified sample preparation workflow using SPE for quantification of intact IGF-I from human serum using analytical LC and a tandem quadrupole instrument achieving LLOQ's (5 ng/mL), linearity (5-1000 ng/mL) and CV's <10%. We further compare its performance to a targeted HRMS approach for quantification in clinical research.

Poster #14B in Exhibit Hall - *attended for 1 hr on Wednesday starting at 13:30*
Topic: *Informatics & Analytics*

Application of LIS Interface for Quality Control for LC-MS/MS in Therapeutic Drug Monitoring of Immunosuppressant

Yeo-Min Yun - *Konkuk University School of Medicine* (ymyun@kuh.ac.kr)

‣ The quality control of LC-MS/MS is important for reliable results supporting precise medical decision. We describe new laboratory information system interface (ACK Co., Ltd, Korea) for quality control for LC-MS/MS. We designed LIS interface for quality control for LC-MS/MS (Waters Xevo TQD, MA, USA). We implemented the standard of QC acceptable limits of retention time, internal standard peak area, ion ratio, and percent deviation based on CLSI guideline; ±2.5% in RT between runs, < 20% in IS peak area, ±20% in ion ratio, and ±15% in percent deviation. This LIS interface can enable efficient QC of LC-MS/MS, simplification of workflow (manual calculation and review of QC results), reduction of the time to review the QC, automatic data transmission, and early detection of instrument failure.

Poster #14C in Exhibit Hall - *attended for 1 hr on Wednesday starting at 13:30*
Topic: *Various OTHER*

Robustness Evaluation of the Qsight® 210 MD Triple-Quadrupole Mass Spectrometer Against "Dirty" Samples

Sumeet Kaushal - *Perkin Elmer Inc* (Sumeet.Kaushal@perkinelmer.com)

‣ The QSight® 210 MD triple-quadrupole mass spectrometer is uniquely equipped with a StayClean™ source and novel "heated solvent induced desolvation" (HSID™) interface for robust performance against dirty samples. Newborn screening laboratories routinely use "dirty" samples - with minimal sample clean-up and no chromatography - for quantitating amino acids and acylcarnitines from neonatal dried blood spots. Here, we evaluated the robustness of the QSight® 210 MD system to "dirty" samples by monitoring its quantitative performance through sustained injections of newborn screening controls/samples. Our results demonstrate highly reliable quantitation by the QSight® 210 MD for 30 different amino acids and acylcarnitines over 25,000 sample/control equivalent injections.

Poster #14D in Exhibit Hall - *attended for 1 hr on Thursday starting at 12:30*
Topic: *Small Molecules / Tox*

UPLC-MS/MS Analysis of Oncology Drugs in Plasma for Clinical Research

Stephen Balloch - *Waters Corporation* (stephen_balloch@waters.com)

‣ Here we describe separate UPLC-MS/MS methods for plasma busulfan and 5-fluorouracil (5-FU) for clinical research applications using an ACQUITY® UPLC® I-Class-FTN and Xevo® TQ-XS mass spectrometer. Following CLSI guidelines, carryover, linearity, matrix effects, precision and specificity were evaluated. Additionally, a comparison was performed for busulfan with an independent method. Analytically sensitive and specific methods may play a role in assessing the pharmacokinetic and pharmacodynamic effects of administration of these drugs in clinical research.

Poster #15A in Exhibit Hall - *attended for 1 hr on Wednesday starting at 10:00*
Topic: *Small Molecules / Tox*

Therapeutic Drug Monitoring of lacosamide, a newer antiepileptic drug, by LC-MS/MS

Sarina Yang - *Quest Diagnostics Nichols Institute of Valencia* (sarina.h.yang@questdiagnostics.com)

‣ Therapeutic drug monitoring (TDM) of the newer generation of anticonvulsant drugs (AEDs) is of great importance in treatment of seizure disorders and prevention of adverse effects. Automated immunoassay is only available for some of the newer AEDs, and antibodies used in these methods have cross-reactivity with drug metabolites, causing overestimation of concentration. We report the development and validation of a lacosamide LC-MS/MS assay as an example of a procedure for specific and accurate measurement of the newer AEDs in blood. Sensitivity, linearity, precision, accuracy, comparison of different specimen types, extracted specimen stability, and interference were validated for this assay.

Poster #15B in Exhibit Hall - *attended for 1 hr on Thursday starting at 10:00*
Topic: *Various OTHER*

Regulation Mechanisms on Vascular Functions in sEH KO Mice Revealed by High-Throughput Mass Spectrometry-based Proteomics

Dawei Wang - *University of Pittsburgh* (daw156@pitt.edu) *YI Grantee*

‣ Soluble epoxide hydrolase (sEH) is the key enzyme in arachidonic acid metabolic pathways, which hydrolyzes Epoxyeicosatrienoic acids to inactive dihydroxyeicosatrienoic acids. We utilized mass spectrometry-based proteomics to analyze aortic protein profile in sEH knockout mice. We found 237 significantly altered proteins, which were further shown to be enriched in TCA cycle and respiratory electron transport, oxidative phosphorylation, extracellular matrix organization, collagen formation and so on. Of note, a group of proteins which might mediate the effects of sEH in vascular functions was uncovered. We further revealed that sEH inhibited angiogenic potential of endothelial cells by down-regulating focal adhesion protein Parvb.

Poster #15C in Exhibit Hall - *attended for 1 hr on Thursday starting at 10:00*
Topic: *Small Molecules / Tox*

Development and Validation of a Dried Urine Spot Assay as a Toxicology Screening Method Using LC-MS/MS

Abed-Hamlet Pablo - *Johns Hopkins University* (apablo1@jhu.edu) *YI Grantee*

‣ Dried urine spot samples offer an alternative to storing and shipping liquid urine samples which is useful in locations where resources are limited. We describe the development and validation of an LC-MS/MS toxicology screening method using dried urine spot (DUS) samples. The method described enables the identification of 41 compounds in human urine samples. Validation of the screening method was performed and the method was shown to be precise and accurate.

Poster #15D in Exhibit Hall - *attended for 1 hr on Wednesday starting at 10:00*
Topic: *Various OTHER*

Novel Plasma Card for Shipping Clinical Samples

Tim Schlabach - *Novilytic LLC* (tschlabach@novilytic.com)

‣ Clinical trials often collect blood at a medical center and spin down the plasma. But the plasma has to be frozen for shipment to a LCMS testing lab. The cost of shipping clinical trial samples to laboratories is estimated to be more than $3 billion dollars this year. Dried plasma spots(1) on DBS paper allow a great cost savings in transport, but do not support variable and quantitative amounts of plasma. A new product allows quantitative plasma volumes from 3 to 20 µL to be shipped in a dry form.

Poster #16A in Exhibit Hall - *attended for 1 hr on Thursday starting at 12:30*
Topic: *Small Molecules / Tox*

How Low Can Your Clinical Research Method Go for the Analysis of Serum Estrogens?

Robert Wardle - *Waters Corporation* (robert_wardle@waters.com)

‣ Here we address the challenges faced trying to routinely measure 17β-Estradiol (E2) and Estrone (E1) at levels of 3.7pmol/L (1pg/mL) by LC-MS/MS for clinical research applications. The quest to reach these low levels led us to investigate a range of sample preparation and liquid chromatography methods. Samples were analyzed using an ACQUITY® UPLC® I-Class-FTN and Xevo® TQ-XS mass spectrometer for optimum analytical sensitivity. Limits of quantification will be presented to show 'how low you could go' with this routine LC-MS/MS workflow without the need for derivatization. For Research Use Only, Not for use in diagnostic procedures.

Poster #16B in Exhibit Hall - *attended for 1 hr on Wednesday starting at 13:30*
Topic: *Metabolomics*

Bile Acid Profiling and Quantification in Human Plasma Using LC-MS/MS

Ravali Alagandula - *Restek Corporation* (Ravali.Alagandula@restek.com)

‣ Bile acids are a group of major catabolic products of cholesterol. They are important biomarkers for signaling potential harmful side effects for new drug development. Quantitation of bile acids in matrices proves to be very challenging due to a number of factors, including, the similarity of structures, varying polarities and stereochemistries, limited fragmentation for unconjugated bile acids in mass spectrometer, high endogenous levels, and matrix effects caused by phospholipids or triglycerides. In this study, a rapid, robust, selective and reliable LC-MS/MS method was established and validated in human plasma using a Raptor C18 column with baseline separation of 17 bile acids in 6 minutes.

Poster #16C in Exhibit Hall - *attended for 1 hr on Wednesday starting at 13:30*
Topic: *Metabolomics*

Simultaneous Analysis of Catecholamines and Metanephrines in Urine by LC-MS/MS

Rob Freeman - *Restek Corporation* (Rob.Freeman@restek.com)

‣ Measurements of catecholamines and their methylated metabolites in urine are commonly used for the clinical diagnosis and monitoring of pheochromocytoma and paraganglioma. Although reversed-phase LC-MS/MS has been the method of choice for this type of analysis, challenges still remain for insufficient retention, urine matrix interference, and inconsistent chromatographic performance. To solve these problems, a simple and fast solid phase extraction (SPE) procedure was developed and followed by LC-MS/MS analysis using a Raptor Biphenyl column.

Poster #16D in Exhibit Hall - *attended for 1 hr on Thursday starting at 12:30*
Topic: *Metabolomics*

Global Natural Product Social Molecular Networking (GNPS) – an Open Resource for MS-based Metabolomics Data Sharing and Analysis

Alexander Aksenov - *UC San Diego* (aaaksenov@ucsd.edu)

‣ GNPS (Global Natural Products Social networking) is an open, crowd-sourced mass spectrometry based metabolomics platform. One of the defining features of GNPS is so-called “living data” - a feedback loop with scientists to convey community knowledge that has been captured since the study was done. Currently, GNPS provides capabilities to store, share and annotate tandem MS data, and also offers several additional utilities such as molecular networking.

Poster #17A in Exhibit Hall - *attended for 1 hr on Wednesday starting at 10:00*
Topic: *Tissue Imaging & Analysis*

***In vitro* Liquid Extraction Surface Analysis Mass Spectrometry (IV-LESA MS) for Direct Analysis of Adherent Cells in Culture**

Sankha (Bobby) Basu - *Brigham and Women's Hospital* (sbasu@bwh.harvard.edu) *YI Grantee*

‣ Conventional metabolomics can involve significant sample preparation and analytical time, limiting high throughput applications and potentially inducing metabolic artifacts. Here, we present in vitro liquid extraction surface analysis mass spectrometry (IV-LESA MS), an adaptation of LESA MS, performed directly on adherent cells grown in 96-well plates, with total extraction and analysis time in as little as one minute per well. Using this platform, we demonstrated distinct and reproducible lipid signatures from four different breast cancer cell lines (MCF-7, ZR-75-1, MDA-MB-231 and MDA-MB-453). IV-LESA MS represents a simple and fast technique to directly analyze adherent cells in culture, and can be applied to drug screening or other high throughput applications.

Poster #17B in Exhibit Hall - *attended for 1 hr on Thursday starting at 10:00*
Topic: *Tissue Imaging & Analysis*

Multimodal Imaging of AD-Associated Lipid Species in Structurally Distinct Plaques

Wojciech Michno - *Sahlgrenska Academy, University of Gothenburg* (wojciech.michno@neuro.gu.se)

‣ Alzheimer's disease (AD) is a neurodegenerative disease, of which the underlying pathological mechanism is still not understood. The disease is characterized by accumulation of Amyloid-β (Aβ) peptides into different extracellular plaques. Plaques have also been found in non-demented pathological aging patients. Therefore, discrimination between structural and molecular plaque architecture are of interest to resolve Aβ plaque pathology in AD. MALDI IMS was utilized to elucidated lipid environment in AD tissue. Then, a hyperspectral imaging paradigm employing Aβ aggregate binding LCOs and an in-house software was used to differentiate between different types of plaques. Clear localization of several sphingolipids in plaques, as well as lipid composition differences between the different Aβ plaques, were identified through a true multimodal imaging paradigm.

Poster #17C in Exhibit Hall - *attended for 1 hr on Thursday starting at 10:00*
Topic: *Endocrinology*

Analysis of Urinary Free Cortisol and Cortisone by LC-MS/MS

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

‣ Determination of urinary free cortisol and cortisone is used to test for various types of adrenocortical dysfunction. Liquid chromatography-tandem mass spectrometry (LC-MS/MS) is the preferred screening methodology since it can eliminate interferences which affect immunoassay-based results. Here, a fast and selective 3 minute LC-MS/MS assay is described using a Raptor Biphenyl 2.7 µm, 50x2.1mm LC column. Linearity, precision, and accuracy were assessed and complete resolution from both endogenous and potential drug interferences was achieved. Samples were extracted using Biotage Isolute SLE+ supported liquid extraction plates to maximize instrument up time while removing potential data compromising matrix interferences.

Poster #17D in Exhibit Hall - *attended for 1 hr on Wednesday starting at 10:00*
Topic: *Small Molecules / Tox*

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

Richard Cummings - *Restek Corporation* (Richard.Cummings@restek.com)

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

Poster #18A in Exhibit Hall - *attended for 1 hr on Thursday starting at 12:30*
Topic: *Various OTHER*

A Single High-Throughput UPLC-MS/MS Platform for Targeted Metabolomic, Lipidomic and Proteomic Studies (Targeted Multi-OMICS)

Billy Molloy - *Waters* (billy_molloy@waters.com)

‣ Targeted liquid chromatography - mass spectrometry (LC-MS) assays, using unit mass resolution, tandem quadrupole mass spectrometers, and standard analytical flow UPLC, are increasingly being used in the discovery omics arena. This approach offers an alternative to the un-targeted, high-resolution approach traditionally applied in these types of studies, using time of flight instruments and micro/nano flow LC. These methods offer increased simplicity and throughput, while still offering the level of sensitivity and specificity required. Here, this methodology is applied to metabolomic, lipidomic and proteomic preparations of a set of human plasma samples, using the same LC-MS platform. The ability to run these 3 different analysis types on the same LC-MS platform facilitates the consecutive analysis of multiple sample sets from different sample preparations with virtually no down time.

Poster #18B in Exhibit Hall - *attended for 1 hr on Wednesday starting at 13:30*
Topic: *Endocrinology*

The Comparison of Aldosterone Level by Mass Spectrometry and Radioimmunoassay

Sunhyun Ahn - *Seoul Clinical Laboratories* (ash1008@naver.com)

‣ To compare MS/MS with radioimmunoassay to measure aldosterone level, 64 samples were used. Aldosterone by MS/MS and RIA ranged from 0.378 to 322 (median 65.574)ng/dL and from 0.6 to 958.9 (median 167.285)ng/dL, respectively. 10 out of 64 samples(15.6%) recorded higher than the reference value by MS/MS, and 36 out of 64 samples(56%) by RIA. Linear regression analysis revealed the following equation: MS/MS = 0.978 x RIA - 12.161 (R2 = 0.9132). MS/MS showed better selectivity, and RIA showed false elevation of aldosterone level. MS/MS should be considered the first choice to measure aldosterone level reflecting its accuracy and selectivity.

Poster #18C in Exhibit Hall - *attended for 1 hr on Wednesday starting at 13:30*
Topic: *Microbiology/Virology*

Rapid Evaporative Ionisation Mass Spectrometry (REIMS) as a Novel Approach to Pathogen Detection Directly from Clinical Urine Samples

Adam Burke - *Imperial College London* (a.burke@imperial.ac.uk) *YI Grantee*

‣ Current diagnostic microbiology laboratory MS systems rely on pure microbial culture isolation, followed by subsequent sample preparation for MALDI-ToF. These approaches suffer from poor identification accuracy when more than one microbial species is present. Rapid evaporative ionisation mass spectrometry (REIMS) has shown robust identification at the species level for a range of clinically important microorganisms. Here, we present a methodology for species specific biomarker detection direct from clinical urine samples using REIMS. 240 clinical urine samples have been analysed directly with automated Laser Assisted REIMS, with >50 species specific biomarkers identified for each species present. A database of these is in population with the intention of expanding capability to other clinical samples including faeces; removing the requirement for pre-isolation and culturing.

Poster #18D in Exhibit Hall - *attended for 1 hr on Thursday starting at 12:30*
Topic: *Small Molecules / Tox*

A Simple Method for the Analysis of Methylmalonic Acid in Human Plasma by LC-MS/MS

Susan Steinike - *Restek Corporation* (Susan.Steinike@restek.com)

‣ Vitamin B12 deficiency can manifest itself in a wide variety of physical and behavioral signs and symptoms. A specific marker for diagnosing vitamin B12 deficiency is methylmalonic acid (MMA). In a part of the metabolic cycle for energy production, vitamin B12 promotes the conversion of methylmalonyl CoA to succinyl CoA. If there is not enough B12 available, blood levels of MMA begin to rise. The MMA test typically requires extensive sample pre-treatment incorporating liquid-liquid extraction, derivatization, solvent evaporation and/or SPE. Additionally, chromatographic resolution can be difficult to achieve between MMA and its naturally occurring isomer, succinic acid. Herein we present a simple sample preparation method without derivatization which allows for the direct injection of protein crash supernatant while still maintaining resolution in a 5-minute cycle time.

Poster #19A in Exhibit Hall - *attended for 1 hr on Wednesday starting at 10:00*
Topic: *Small Molecules / Tox*

Development and Validation of a LC-MS/MS Method for the Determination of Tenofovir Alafenamide in Human Plasma Over a 10,000-Fold Calibration Range

Kimberly Blake - *UNC Center for AIDS Research* (khandy@email.unc.edu)

‣ The rapid metabolism (0.5hr half-life) of tenofovir alafenamide (TAF) necessitates a large calibration range to quantify concentrations around the Cmax and subsequent collection times in pharmacokinetic studies. Here we present a fully validated LC-MS/MS assay for TAF in human plasma over the 10,000-fold range of 0.05-500ng/mL that uses a highly sensitive transition to quantify samples in the lower part of the range with a less sensitive transition utilized for the upper end of the range. This method allows quantitation of samples over the entire range without losing linearity or requiring dilutions for samples around the Cmax.

Poster #19B in Exhibit Hall - *attended for 1 hr on Thursday starting at 10:00*
Topic: *Proteomics*

An Optimized Rapid Trypsin Digestion Protocol for Proteomic Sample Preparation

Michael Rosenblatt - *Promega* (mike.rosenblatt@promega.com)

‣ We have developed a novel Rapid Trypsin/Lys-C digestion protocol that is compatible with proteolysis of complex mixture and quantitation of analytes within theses mixtures. The protocol requires a 5-60 minute digestion step and is fully compatible with reduction/alkylation and denaturation. The system is also highly flexible and compatible with multiple sample types. The protocol does not involved immobilized enzymes nor does it require off-line desalting. The protocol is also compatible with other workflow steps that require affinity enrichment steps. This procedure can be easily adapted to clinical samples derived from serum/plasma or complex samples derived from cell culture.

Poster #19C in Exhibit Hall - *attended for 1 hr on Thursday starting at 10:00*
Topic: *Tissue Imaging & Analysis*

Detection of Renal Cell Carcinoma Multikinase Inhibitors in Hair by Mass Spectroscopy Imaging to Measure Patient Adherence

Nicole White - *University of North Carolina at Chapel Hill* (nwhite@med.unc.edu)

‣ A non-invasive technique to evaluate patient adherence to oral chemotherapy has been developed. Utilizing infrared matrix assisted laser desorption electrospray ionization (IR-MALDESI) mass spectrometry imaging (MSI), five oral multikinase inhibitor chemotherapeutics used for metastatic renal cell carcinoma (mRCC) have been detected in single, incubated hair strands over a 40-fold concentration range. We anticipate that this approach will provide a longer-term (weeks to months) retrospective measure of patient adherence, when compared to routine plasma or urine testing (days), and will provide critical information that will improve patient-clinician communication.

Poster #19D in Exhibit Hall - *attended for 1 hr on Wednesday starting at 10:00*
Topic: *Metabolomics*

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

Ashlee Reese - *Restek Corporation* (Ashlee.Gerardi@restek.com)

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

Poster #20A in Exhibit Hall - *attended for 1 hr on Thursday starting at 12:30*
Topic: *Endocrinology*

Reliable Direct Quantitative Measurement of Total and Free Testosterone in Plasma/Serum by UHPLC-MS/MS

Ayuna Dagdanova - *Accu Reference Medical Laboratory* (adagdanova@accureference.com)

‣ Blood levels of total (TT) and free (FT) testosterone are used to assess endocrine functionality in males and females. We validated two methods to reliably measure TT in males and females plasma/serum with a range of 2.5 to 3000.0 ng/dL, and FT in males with a range of 25.0 to 5000.0 pg/mL, using UHPLC-MS/MS after solid supported - liquid extraction (SLE) for TT, and ultrafiltration - solid-phase extraction (SPE) for FT.

Poster #20B in Exhibit Hall - *attended for 1 hr on Wednesday starting at 13:30*
Topic: *Small Molecules / Tox*

Effect of Enzyme Titer and pH on Hydrolysis Efficiency Using Recombinant Limpet Beta-Glucuronidase

Jim Blasberg - *MilliporeSigma* (jim.blasberg@sial.com)

‣ Here we evaluate the impact of enzyme titer and pH effect on hydrolysis efficiency of a recombinant limpet beta-glucuronidase enzyme against a panel of 17 drug glucuronide substrates. A traditionally recalcitrant opioid substrate, Codeine-6-β-D-glucuronide; a quaternary amine substrate, Amitriptiyline-N-β-D-glucuronide; as well as additional opioids, benzodiazepines, and steroid drugs are represented in the panel. We found that enzyme titer and solution pH effect on hydrolysis efficiency varied widely among tested substrates. Based on this data, optimal experimental conditions of titer, pH, and hydrolysis time can be recommended for each substrate of interest.

Poster #20C in Exhibit Hall - *attended for 1 hr on Wednesday starting at 13:30*
Topic: *Small Molecules / Tox*

Practical Considerations Using Quantisal Oral Fluid Collection Devices & SPE Method Development by Polymeric Mixed-Mode Cation Exchange

Dan Menasco - *Biotage* (dan.menasco@biotage.com)

‣ With the resurgence of oral fluids (OF) as testing matrix for drugs of abuse (DOA), the need to provide larger and more comprehensive panels for drugs is required. However, to reach the lower limits of quantitation necessary for nominal analyte detection in oral fluids, both biological matrix and the storage buffers used in the collection OF present obstacles to this end. Here, we implement the use of a mixed-mode cation exchange SPE and survey the effects of altering the polarity of organic wash against 85 analytes comprised of 12 different drug classes.

Poster #20D in Exhibit Hall - *attended for 1 hr on Thursday starting at 12:30*
Topic: *Small Molecules / Tox*

Novel Sensitive LC-MS/MS-based 25(OH)D Assays and Vitamin D Status of 150,000 Chinese Population

Zhouyang Kang - *Hangzhou Calibra Diagnostics* (kangzy@dazd.cn)

‣ Vitamin D deficiency has become a worldwide problem that not only for elderly, but also found common in children and adults. Serum level of total 25-hydroxy Vitamin D (sum of 25(OH)D2 and 25(OH)D3) is a key indicator to determine a person"s vitamin D status. In recent years, mass spectrometry based assay has been recognized as ¡°Gold-standard¡± method for 25-hydroxy Vitamin D measurement in clinical labs. Here we report the development of two novel sensitive LC-MS/MS methods for measuring 25-hydroxy Vitamin D in serum and in dried blood spot. We have tested more than 150 thousand samples since the adoption of the methods and the statistical findings were also reported.

Poster #21A in Exhibit Hall - *attended for 1 hr on Wednesday starting at 10:00*
Topic: *Small Molecules / Tox*

LC-MS/MS Validation Using Natural Isotopes of Stable Labeled Internal Standards to Overcome Crosstalk for Three Brominated or Chlorinated Antiretrovirals

Amanda Schauer - *University of North Carolina-Chapel Hill* (aps5@email.unc.edu)

‣ The use of a stable-isotopically labeled (SIL) internal standard is highly recommended in quantitative bioanalytical LC-MS/MS assays. This approach requires sufficient mass differences between the analyte and SIL internal standard to overcome crosstalk at high analyte concentrations. Analytes that are brominated or chlorinated can present significant crosstalk due to their high abundance of natural isotopes. An LC-MS/MS method was fully validated for three brominated or chlorinated antiretrovirals, elvitegravir, etravirine, and efavirenz over a 400-fold range in human plasma using natural isotopes (81Br or 37Cl) of the SIL internal standards to increase mass difference and eliminate crosstalk at high analyte concentrations.

Poster #21B in Exhibit Hall - *attended for 1 hr on Thursday starting at 10:00*
Topic: *Small Molecules / Tox*

A Case Study on Ion Suppression: Analysis of 17a-Hydroxyprogesterone by ESI Mass Spectrometry

Andrew Tromans - *Canterbury Health Laboratory (NZ)* (Andrew.Tromans@cdhb.health.nz)

‣ LC-MS/MS methods are susceptible to ion suppression during electrospray ionisation and this phenomenon can have dramatic effects on the analyte sensitivity and the accuracy of results. We present a case study on the analysis of 17a-hydroxyprogesterone by LC-QQQ detailing our methods to reduce loss of sensitivity from ionisation suppression and to quantify the resulting bias in test results. Post column infusion experiments were performed to adjust chromatographic conditions to avoid co-elution with interfering species. Isotope dilution mass-spectrometry (IDMS) was used to accurately define 6 levels of IQC. A GC-QQQ method was developed to determine method bias between the LCQQQ method and reference method.

Poster #21C in Exhibit Hall - *attended for 1 hr on Thursday starting at 10:00*
Topic: *Small Molecules / Tox*

Approaching a Random Access Calibration Design for LC-MS/MS – Performance in Production

Heather Hochrein - *UC San Diego Health* (hhochrein@ucsd.edu)

‣ A retrospective analysis of historical calibration for an LC-MS/MS urine amphetamines assay was presented previously. Promising results lead to a pilot study performed in parallel with twice-weekly production batches that included a 5-level (Intensive) calibration with each run. Good performance was observed in the pilot study and subsequently in production after the historical calibration scheme was implemented for routine patient sample testing. Preparing smaller, daily-batches with a single calibrator, used in conjunction with an intensive monthly calibration curve, halved the mean turn-around-times (TAT) from 3.5 to 1.7 days with similar accuracy and precision to the in-batch intensive calibration scheme.

Poster #21D in Exhibit Hall - *attended for 1 hr on Wednesday starting at 10:00*
Topic: *Small Molecules / Tox*

Addition of Supercharging Agents to Lower Detection Limits of Phosphorylated Compounds by LC-MS/MS

Bryan Guzman Rodriguez - *University of North Carolina at Chapel Hill* (bryanbg@ad.unc.edu)

‣ The active form of several drugs used for HIV treatment and prevention are phosphorylated intracellularly and can exist in very low concentrations in cells and tissues requiring highly sensitive LC-MS/MS assays. Here, we investigated whether dimethyl sulfoxide (DMSO) or sulfolane added to the mobile phases would result in a lower limit of detection for these metabolites. DMSO was found to increase the sensitivity of tenofovir diphosphate, emtricitabine triphosphate, lamivudine triphosphate, dATP, and dCTP up to 7-fold when analyzed in negative ionization mode.

Poster #22A in Exhibit Hall - *attended for 1 hr on Thursday starting at 12:30*
Topic: *Informatics & Analytics*
Determination of Busulfan in Human Plasma by LC-MSMS
Eun Jin Lee *- University of Ulsan College of Medicine* (hjejyk@gmail.com)
‣ We suggest a rapid and simple method for measuring accurate concentration of plasma Busulfan (Bu) using Liquid chromatography-tandem mass spectrometry (LC-MS/MS). Bu is separated and detected with internal standard (Bu-2H8) in positive ion multiple reaction monitoring (MRM) mode at m/z 264.1 → 151.1 and 272.2 → 159.1, respectively. Our rapid and simple LC-MS/MS method for Bu showed great analytical performance.

Poster #22B in Exhibit Hall - *attended for 1 hr on Wednesday starting at 13:30*
Topic: *Small Molecules / Tox*
Rapid LC-MS/MS Detection of Opiates, Opioids, Benzodiazepines, Amphetamines, and Cannibinoids in Urine in Clinical Research
Carrie Adler *- Agilent Technologies* (carrie.adler@agilent.com)
‣ A rapid liquid chromatography-mass spectrometry method was developed to quickly determine the presence or absence of a panel of exogenous compounds in human urine for research purposes. Injection of sample, separation of 36 compounds, and cleaning and reequilibration of the column were accomplished in a 2.3 minute total runtime. A single point calibration was used as a reference, and negative (0.25x calibrator concentration) and positive (1.5x calibrator concentration) samples all quantified as expected. Commercially available controls also gave consistent and reproducible results when prepared and analyzed in 5 separate runs over three days.

Poster #22C in Exhibit Hall - *attended for 1 hr on Wednesday starting at 13:30*
Topic: *Metabolomics*
Validation of High-Throughput MS/MS-based Amino Assay Screen Using an Automated Liquid Handler for Amino Acid Extraction and Stable-Isotope Labeling Semiautomation
William Phipps *- UT Southwestern Medical Center* (william.phipps@phhs.org) *YI Grantee*
‣ Liquid-chromatography coupled with tandem mass spectrometry (LC/MS/MS) provides a rapid and highly specific method for identifying and quantifying amino acids. However, sample preparation involves laborious extraction and derivatization procedures, thus limiting throughput. Here we present our validation of a semi-automated method using an automated liquid handler (QIAGEN QIAgility) for amino acid extraction and labeling to speed processing and improve reproducibility. 30 Amino acids can be quantified with a dynamic range of 5 M to 1500 M within 20 min after sample injection. Sample preparation can be completed with 30-45 minutes of hands on time with the QIAgility liquid handler.

Poster #22D in Exhibit Hall - *attended for 1 hr on Thursday starting at 12:30*
Topic: *Metabolomics*
Metabolomic Profile Change in Patients with Sepsis Compared with Normal Controls
Sang-Guk Lee *- Yonsei University College of Medicine* (comforter6@yuhs.ac)
‣ We tried to find metabolomic signature of sepsis compared with healthy controls using a commercial metabolomics platform and mass spectrometry. We measured 188 metabolites in 49 patients with sepsis, 12 patients with pneumonia, and 10 healthy controls. We found 22 statistically different metabolites, nine metabolites increased and thirteen metabolites decreased in patients with pneumonia and sepsis compared with normal control. Especially, 6 of 9 increased metabolites were phosphatidylcholines (PCs); PC diacyl C34:1, PC acyl-alkyl C36:0, PC acyl-alkyl C34:0, PC diacyl C32:1, PC diacyl C32:0, PC acyl-alkyl C30:0. Further large population studies including patients with sepsis or systemic inflammation and healthy controls are needed to determine metabolic signature of sepsis. In addition, mechanisms of PCs'increase in sepsis and their metabolic role should be addressed.

Poster #23A in Exhibit Hall - *attended for 1 hr on Wednesday starting at 10:00*
Topic: *Endocrinology*
A Fully Automated and Novel "Tip-On-Tip" Extraction Method for the Quantitation of Testosterone and Related Hormones in Human Serum
Daniel Kassel *- Scianalytical Strategies, Inc.* (dkassel@scianalytical.com)
‣ A novel and automated liquid handling method for the extraction of testosterone and related hormones from human serum is presented. The method involves the use of a novel "tip-on-tip" liquid handling technique, which allows serum to be extracted in situ (within the extraction tip) and transfer of extracted sample via automated coupling of the extraction tip to a specially designed filter tip to allow for collection of supernate into a microtiter plate for analysis without any user intervention in the process. The method greatly simplifies and streamlines the sample preparation process prior to LC-MS-MS analysis.

Poster #23B in Exhibit Hall - *attended for 1 hr on Thursday starting at 10:00*
Topic: *Various OTHER*

Integrating Inborn Errors of Metabolism and Hemoglobin Variant Clinical Research into a Single High Resolution Accurate Mass Based Mass Spectrometer Workflow

Xiaolei Xie - *Thermo Fisher Scientific* (xiaolei.xie@thermofisher.com)

‣ Inborn Errors of Metabolism clinical research has been conducted conventionally by tandem mass spectrometry. Meanwhile, hemoglobin variant related research was mostly carried out using either HPLC or IEF. Thus labs must use two different platforms for two tests. Here we developed an integrated workflow incorporating two tests into one platform, high-resolution accurate-mass (HRAM) technology based mass spectrometer. Using the single platform, we were able to quantify small molecules, amino acids and acylcarnitines, as well as identify hemoglobin variants with high resolution from dried blood spot samples. The new workflow also provided high throughput benefit by integrating multi-channel HPLC.

Poster #23C in Exhibit Hall - *attended for 1 hr on Thursday starting at 10:00*
Topic: *Proteomics*

Development of a Robust, Routine, and Multiplexed Plasma Profiling Method Using UHPLC-MS/MS

Kerry Hassell - *Thermo Fisher Scientific* (kerry.hassell@thermofisher.com)

‣ TMT tags are used to increase sample throughput while maintaining normalization and quality control for large-scale plasma sample analysis. A universal standard was labeled with TMT 0 and used for quality control and normalization against plasma labeled with different TMT6 tags. Sample analysis utilized high resolution chromatography and precursor isolation on a triple quadrupole mass spectrometer to increase selectivity and maintain confident quantitation. Over 2200 time-selected SRM transitions were monitored in a 30 minute gradient and SRM transitions were monitored using dynamic dwell times (ranging from 1-15 msec). A wide set of samples with varying TMT0/6 levels were analyzed.

Poster #23D in Exhibit Hall - *attended for 1 hr on Wednesday starting at 10:00*
Topic: *Endocrinology*

Achieving Lower Limits of Quantitation for Testosterone and Estradiol by LC-MS/MS

Kristine Van Natta - *Thermo Fisher Sceintific* (kristine.vannatta@thermofisher.com)

‣ Researchers want to measure low levels of steroids without derivatization. We report a research method that achieves a lower limit of quantitation (LLOQ) of 2 pg/mL for testosterone and 20 pg/mL for estradiol in human blood-plasma using liquid chromatography coupled to tandem mass spectrometry (LC-MS/MS). Liquid-liquid extractions of donor plasma samples (400 µL) were evaporated and reconstituted with mobile phase (200 µL) followed by 10 µL injections into the LC-MS/MS. Recent experiments imply LLOQs of 0.25 pg/mL for testosterone are possible using on-line extraction/concentration.

Poster #24A in Exhibit Hall - *attended for 1 hr on Thursday starting at 12:30*
Topic: *Cannabinoids*

Development of a LC-MS/MS Assay for Bioactive Cannabinoids in Plasma of Pediatric Patients on Cannabis Oil Therapy

Stephanie Vuong - *University of Saskatchewan* (steph.vuong@usask.ca) *YI Grantee*

‣ A sensitive and efficient liquid chromatography-tandem mass spectrometry method is under development to identify and quantify cannabidiol, Δ9-tetrahydrocannabinol, and metabolite 11-hydroxy-Δ9- tetrahydrocannabinol in plasma volumes from pediatric patients undergoing Cannabis oil therapy for refractory epileptic encephalopathy. Plasma sample processing involves solvent protein precipitation, evaporation of supernatant under nitrogen, and reconstitution with mobile phase.The LC-MS/MS method demonstrates acceptable sensitivity, linearity, precision, and accuracy. We currently are in process of determining recovery, carryover, and stability. This method will be applied in clinical tolerability and efficacy studies and for oral pharmacokinetic studies that will further help us determine the dosage requirements for oral administration of cannabis oil in children.

Poster #24B in Exhibit Hall - *attended for 1 hr on Wednesday starting at 13:30*
Topic: *Proteomics*

Optimization of Experimental Parameters in Data-Independent Mass Spectrometry Significantly Increases Depth and Reproducibility of Results

Florian Marty - *Biognosys AG* (florian.marty@biognosys.com)

‣ Comprehensive, reproducible and precise analysis of large sample cohorts is one of the key objectives of quantitative proteomics. Here, we present an implementation of DIA that surpasses the limitation of serial MS2 acquisition of DDA. In deep single shot DIA, we identified and quantified over 7,100 proteins in human cell lines. In mouse tissues 8,121 proteins were identified and quantified. Missing values for proteins were within 0.3 to 2.1% and median coefficients of variation of 4.7 to 6.2% among technical triplicates. In very complex mixtures, we could quantify 12,192 proteins in total showing that DIA is not limited to low complexity samples.

Poster #24D in Exhibit Hall - *attended for 1 hr on Thursday starting at 12:30*
Topic: *Various OTHER*

Development of a Reliable Mass Spectrometric Enzymatic Assay for Mucopolysaccharidosis Type III (MPS III)

Fan Yi - *University of Washington* (yif1860@uw.edu) *YI Grantee*

‣ The development of reliable Mass Spectrometric enzymatic assays for Mucopolysaccharidosis type III (MPS III) subtype A and B are presented here. Synthetic substrates are made to mimic the natural ones for the target enzymes – Heparan N-sulfatase (MPS III A) and α-N-acetylglucosaminidase (MPS III B), respectively. Using the synthetic substrates together with internal standards, which are isotope-labeled enzymatic products, the true activity of the target enzymes can be extrapolated with the help of tandem mass spectrometer. More importantly, these assays are done on dried blood spot(DBS), which allows a simple sample transportation if no local laboratory can perform the assay.

Poster #28A in Exhibit Hall - *attended for 1 hr on Thursday starting at 12:30*
Topic: *Endocrinology*

Effect of Blood Collection Tubes on Serum/Plasma Estrogen Quantitation by LC-MSMS

Carmen Gherasim - *Department of Pathology, University of Utah* (carmen.gherasim@aruplab.com)

‣ Reliable measurement of estrogens in children, males and postmenopausal females is crucial for workup of pathophysiological conditions including precocious or delayed puberty, oligomenorrhea and amenorrhea, gynecomastia, estrogen deficiency and antiestrogen treatment efficiency. Here, we have assessed the effect of three collection tubes (Becton Dickinson (BD) Vacutainer red top (RTs), Barricor (BTs) and serum separator tubes (SSTs)) on the performance of a laboratory-developed liquid chromatography-tandem mass spectrometry (LC-MS/MS) assay for estrogens. Our results indicate that BTs have similar performance characteristics with the RTs for measurement of estrogens whereas SSTs exhibit interferences that increase with the length of time on the gel.

Poster #28B in Exhibit Hall - *attended for 1 hr on Wednesday starting at 13:30*
Topic: *Metabolomics*

Fasting Serum Levels of Bile Acid Are Associated with Insulin Resistance

Yonggeun Cho - *Yonsei University College of Medicine* (yonggeuncho@yuhs.ac)

‣ The alterations in variety of bile acid (BA)s have been linked to type 2 diabetes mellitus (T2DM) or insulin resistance (IR). We conducted an in depth profiling study of representative BAs in drug-naive patients with T2DM (n=72) or impaired fasting glucose (IFG) (n=97), and healthy controls (n=75). The levels of most BA species were significantly elevated in people who are obese or have IR, irrelevantly of the disease status. Also, most BAs were positively correlated with and were contributor of HOMA-IR. Meanwhile, HbA1c and fasting glucose level were not contributing factor of BAs.

Poster #28C in Exhibit Hall - *attended for 1 hr on Wednesday starting at 13:30*
Topic: *Endocrinology*

iExchange: Overcoming Extraction Challenges of T3 and rT3 from Human Serum

Shahana Huq - *Phenomenex* (shahanaH@phenomenex.com)

‣ Thyroid hormones are essential for the regulation of development and growth in human. T3, rT3 hormones, produced by thyroid are crucial parameters for researching optimum thyroid function.1 In this communication we will discuss a few of the method development challenges encountered when trying to quantitatively measure these hormones from human serum. We demonstrate a step by step sample preparation approach that successfully targets a neutral polymeric sorbent, Strata-X® for solid phase extraction (SPE) out of a wide variety of chemistry. A Kinetex® 2.6µm, 100x2.1mm dimension C18 HPLC column was employed for analytical measurement of these hormones.

Poster #28D in Exhibit Hall - *attended for 1 hr on Thursday starting at 12:30*
Topic: *Proteomics*

Quantitative Proteomics-based Identification of Novel Serum Markers for First-Trimester Prediction of Gestational Diabetes Mellitus

Martin Overgaard - *University of Southern Denmark* (martin.overgaard@rsyd.dk)

‣ Gestational diabetes mellitus (GDM) is associated with an increased risk of preeclampsia, caesarean section, macrosomia and future development of type 2 diabetes mellitus (T2DM) in both mother and child. The aim of this study was to identify new protein signatures that in combination with maternal risk factors, improve first trimester prediction for later development of GDM among obese women. By the use of quantitative mass spectrometry (MS) based proteomics we profiled 60 sera and identified five combinations of 4-plex protein signatures that each increased the ROC AUC of maternal risk factors from 0.730 to a range of 0.946-0.965.

Poster #29A in Exhibit Hall - *attended for 1 hr on Wednesday starting at 10:00*
Topic: *Small Molecules / Tox*

A Comprehensive Method for Analysis of Pain Management Drugs Employing Simplified and Rapid LC-MS/MS Workflow for Clinical Research

Jonathan Danaceau - *Waters Corporation* (jonathan_danaceau@waters.com)

‣ A rapid and efficient LC-MS/MS method has been developed for a variety of pain management compounds. This method employs an efficient mixed-mode SPE strategy that eliminates sample transfer and evaporation steps. The analytical method quantitates 80 unique compounds in 3 minutes with accurate and precise results. The combination of sample preparation, chromatography and tandem MS analysis results in a complete, comprehensive workflow for a wide variety of relevant compounds.

Poster #29B in Exhibit Hall - *attended for 1 hr on Thursday starting at 10:00*
Topic: *Microbiology/Virology*

Regulated LC-MS/MS Bioanalysis of Therapeutic Antibodies Based on Nano-Surface and Molecular-Orientation Limited (nSMOL) Proteolysis Method Using a New Reagent

Christopher Gilles - *Shimadzu Scientific Instruments* (CTGilles@shimadzu.com)

‣ Traditionally, antibody quantitation in serum is performed with ligand-binding assays, such as ELISA. These assays typically require a number of variables that need to be considered during the development, all of which take time to evaluate. The nano-surface and molecular-orientation limited (nSMOL) proteolysis. This new approach to therapeutic monoclonal antibodies (mAbs) quantitation allows for better sensitivity while minimizing sample complexity and preparation. IgGs are collected from serum and immobilized on a collection resin, with only the Fab region exposed. Trypsin-immobilized nanoparticles then proteolyze the exposed Fab region while the Fc region is protected by the collection resin. By excluding both tryptic fragments other than those around the Fc region and trypsin enzyme, selective quantification of target mAb peptides is performed via LC/MS/MS.

Poster #29C in Exhibit Hall - *attended for 1 hr on Thursday starting at 10:00*
Topic: *Proteomics*

Feasibility of Mitra® Microsampling Devices in Remote, Longitudinal Monitoring of Apolipoprotein B/ApolipoProtein A-I in Patients at Risk for Cardiac Events

Kelly Mouapi - *Cedars Sinai Medical Center* (kellynjine.mouapi@cshs.org)

‣ In this pilot study, we evaluate the feasibility of remote longitudinal sample collection using Mitra® microsampling devices in a subset (n=40) of stable ischemic heart disease patients included in a study for early prediction of major adverse cardiac events (MACE). Blood was collected from a fingerprick at four time-points: baseline, one-month, two-months and three months. Ratios of apolipoprotein B (apoB) to apolipoprotein A-I (apoA-I) were measured using targeted multiple reaction monitoring (MRM) mass spectrometry. Analysis of the dried blood samples showed an average intra-individual %CV in apoB/apoA-I ratio of 9.5 %, whereas the inter-individual %CV was 37.5 %.

Poster #29D in Exhibit Hall - *attended for 1 hr on Wednesday starting at 10:00*
Topic: *Small Molecules / Tox*

An Easy-to-Use Automated Solid-Phase Extraction Method for Quantification of Serum Nicotine and Metabolites Using LC-MS/MS

Rongrong Huang - *Houston Methodist Hospital* (rhuang@houstonmethodist.org) *YI Grantee*

‣ A simple, programmable automated solid-phase extraction (SPE) method has been developed and validated for simultaneous measurement of nicotine, cotinine and trans-3'-hydroxycotinine (3OH-cotinine) in patient serum using liquid chromatography-tandem mass spectrometry (LC-MS/MS). A batch of 24 samples can be prepared in approximately 30 minutes. The eluent is directly collected in a glass vial and ready for LC-MS/MS analysis. The assay is validated and will be used to evaluate patients' recent nicotine-intake for surgery qualification purpose. The described automated SPE method greatly decreases the need for manual labor and is also easily adaptable for uses with other LC-MS/MS assays that require SPE.

Poster #30A in Exhibit Hall - *attended for 1 hr on Thursday starting at 12:30*
Topic: *Small Molecules / Tox*

Lowering the Bar for Mass Spec: A Comparison Between Immunoassay and Rapid LC-TOF-MS for Presumptive Analytical Screening of Drugs in the Clinical Research Lab

Natalie Rasmussen - *Agilent Technologies* (natalie.rasmussen@agilent.com)

‣ Immunoassay-based techniques have been the choice analytical method for drug screening in a clinical research laboratory. Then, positive results are typically confirmed by GC/MS or LC-MS/MS. Incorrect presumptive results with immunoassay techniques are common problems. This research outlines a simple sample preparation analytical method, and rapid LC-TOF-MS analytical methods used for screening to reduce these. Eighty-four analytes were included and reported qualitatively, while creatinine was reported quantitatively. 420 biological specimens were compared to immunoassay results. The LC-TOF-MS analytical method is shown to be a sensitive and more specific way to screen for drugs providing creatinine quantitation. For Research Use Only. Not for use in diagnostic procedures.

Poster #30B in Exhibit Hall - *attended for 1 hr on Wednesday starting at 13:30*
Topic: *Small Molecules / Tox*

Glyphosate and Aminomethylphosphonic Acid (AMPA) Analysis in Biological Matrices Using LC-MS/MS

Evelyn Wang - *Shimadzu Scientific Instruments* (ehwang@shimadzu.com)

‣ The potential health effects of exposure to glyphosate and its degradant, AMPA, have been a growing concern. To meet this increasing demand, an LCMS-8060 triple quadrupole mass spectrometer was used to analyze glyphosate and AMPA in ESI negative mode. Separation was done on a Bio-Rad Micro-Guard Cation H+ Cartridge. Optimized MRM transitions for glyphosate and AMPA were used for quantitation. Respectable linearities were obtained from 0.1 ppb to 10 ppb. Glyphosate and AMPA were spiked into biological matrices to show feasibility of future clinical research applications.

Poster #30C in Exhibit Hall - *attended for 1 hr on Wednesday starting at 13:30*
Topic: *Small Molecules / Tox*

The Detection and Analytical Confirmation of Synthetic Fentanyl Analogues in Human Urine & Serum Using an Ultivo LC/TQ

Peter Stone - *Agilent Technologies Inc* (peter_j_stone@agilent.com)

‣ During this research study, a sensitive, robust and relatively fast targeted analytical method was developed for the quantitation of 12x synthetic fentanyl opioids, 4-ANPP the synthetic precursor molecule and a similar powerful opioid-like synthetic known as W-18. Simple sample preparation routines were employed to make samples ready for analysis using an Ultivo triple quadrupole mass spectrometer LC/MS (LC/TQ) from both human serum and urine matrices. A comparison of the analytical performance of each analyte for both urine and serum matrices will be outlined. For Research Use Only. Not for use in diagnostic procedures.

Poster #30D in Exhibit Hall - *attended for 1 hr on Thursday starting at 12:30*
Topic: *Proteomics*
timsTOF Pro with PASEF for Shotgun Proteomics
Gary Kruppa - *Bruker Dalotnics* (Gary.Kruppa@bruker.com)
‣ First results for ion mobility spectrometry with parallel accumulation – serial fragmentation (TIMS-PASEF) : pushing the limits of shotgun proteomics analysis.

Poster #31A in Exhibit Hall - *attended for 1 hr on Wednesday starting at 10:00*
Topic: *Proteomics*
Mass Spectrometric IgG Fc-Glycosylation Analysis in Pediatric Samples Reveals Glycosylation Changes Related to Age and Physiological State
Noortje de Haan - *Leiden University Medical Center* (n.de_haan@lumc.nl) *YI Grantee*
‣ Immunoglobulin G (IgG) fragment crystallizable (Fc) N-glycosylation has a large influence on immune effector functions. IgG Fc-glycosylation has been widely studied in the adult population, however, knowledge of IgG Fc-glycosylation in children lags behind. We developed fast and robust mass spectrometric methods for the subclass-specific analysis of human IgG Fc-glycosylation and applied these on various pediatric cohorts. In this way we revealed how IgG Fc-glycosylation changes with age in children and what the effects of infectious diseases, like meningitis, are on Fc-glycosylation. In addition, IgG glycosylation changes were studied before and after hematopoietic stem cell transplantation in children, showing that recipient IgG Fc-glycosylation does not directly mimic donor glycosylation, but is rather influenced by the host.

Poster #31B in Exhibit Hall - *attended for 1 hr on Thursday starting at 10:00*
Topic: *Endocrinology*
High-Throughput Method for Measurement of 25 -Hydroxy Vitamin D by LC -MS/MS
Canary Tennison - *ARUP Laboratories* (canary.tennison@aruplab.com)
‣ Measurement of concentration 25-Hydroxyvitamin D (25OHD) is considered to be the best test for evaluation of status of vitamin D in blood and tissues. We developed a simple, high throughput method for measurement of 25OHD. Sample preparation was performed using automated liquid-liquid extraction; HPLC separation was performed using an automated alternating column regeneration setup. Using this approach, the column was washed and re-equilibrated, while the next analysis was already performed on another column. Compared to the other published methods for measurement of 25OHD, this method has low consumable cost and allows high throughput measurement of 25OHD2 and 25OHD3.

Poster #31C in Exhibit Hall - *attended for 1 hr on Thursday starting at 10:00*
Topic: *Metabolomics*
Accurate and Confident Metabolic Phenotyping - Combining a Standardized and Quantitative Targeted Assay with Orbitrap™ Technology
Wulf Fischer-Knuppertz - *BIOCRATES Life Sciences AG* (wulf.fischer-knuppertz@biocrates.com)
‣ Standardized, quantitative assays have increasingly been desired in metabolomics, especially in targeted studies. We developed the AbsoluteIDQ® p400 HR Kit to facilitate the quantitative analysis on Thermo Scientific™ Q ExactiveTM Orbitrap™ HRAM MS platform for the first time, bridging the gap between targeted quantitative metabolomics and profiling. The kit quantifies up to 408 metabolites of 11 classes: amino acids, biogenic amines, acylcarnitines, phosphatidylcholines, lysophosphatidylcholines, sphingomyelins, ceramides, cholesteryl esters, diglycerides, triglycerides, and hexoses. A beta-test has been carried out across 3 laboratories on different Q ExactiveTM platforms showing high inter-laboratory comparability, which is mandatory for robust, routine applications in targeted metabolomics.

Poster #31D in Exhibit Hall - *attended for 1 hr on Wednesday starting at 10:00*
Topic: *Tissue Imaging & Analysis*
Visualizing Differential Molecular Abundance in Staphylococcal Infectious Interfaces Using Imaging Mass Spectrometry
William Perry - *Vanderbilt University* (william.j.perry@vanderbilt.edu) *YI Grantee*
‣ Imaging Mass Spectrometry (IMS) allows for molecular abundance to be measured directly from tissue while preserving spatial distribution. Fourier transform ion cyclotron resonance (FTICR) mass spectrometry (MS) has been used to provide molecular images of the pathogen-host interface of S. aureus infection. Instrumental modifications have allowed isotopic resolution of proteins up to m/z 20,000 for IMS analysis of infected tissues. Using multimodal data-driven image fusion, we have observed differential abundance of biomolecules at the pathogen-host interface in various tissues, providing new potential targets to study bacterial pathogenesis.

Poster #32A in Exhibit Hall - *attended for 1 hr on Thursday starting at 12:30*
Topic: *Metabolomics*

Feasibility of Dried Blood Spots (DBS) for Metabolomics and its Short and Long-Term Metabolome Stability

Maria Chiam - *BIOCRATES Life Sciences AG* (maria.chiam@biocrates.com)

‣ Dried blood spots (DBS) analysis undergo an increasing interest for metabolomics research today as less-invasive blood sampling device e.g. for biomarker discovery or epidemiological studies. The stability of the metabolome on DBS is therefore of utmost importance. We will present a comprehensive stability overview of the main target metabolome in DBS with the focus on short-term (4 weeks) and long-term stability up to 2 years at room temperature and -80°C.

Poster #32B in Exhibit Hall - *attended for 1 hr on Wednesday starting at 13:30*
Topic: *Small Molecules / Tox*

Rapid Analysis of Fentanyl and Other Synthetic Opioids Using Paperspray-Mass Spectrometry: Comparison to Current Technologies

Joseph Kennedy - *Prosolia.com* (kennedy@prosolia.com)

‣ Synthetic opioids, including Fentanyl and its analogs, are now the leading cause of overdose deaths nationally. Fentanyl has been detected in illicit drug supplies since 2012 and its potency is approximately 50 times that of morphine. More potent analogs such as carfentanil have increasingly been linked to overdose cases, usually in combination with other opioids. Overdoses may be underestimated because laboratories do not have access to equipment with the sensitivity to detect these high potency compounds. Rapid, cost effective and sensitive analytical methods are needed to screen as well as quantitate these new analogs in biological matrices. PaperSpray-MS is a relatively new technique for quantitation of drugs in biological fluids. Using a cellulose matrix, fluids can be sampled and analyzed directly using the technique without chromatography or additional sample preparation.

Poster #32C in Exhibit Hall - *attended for 1 hr on Wednesday starting at 13:30*
Topic: *Proteomics*

Nanopore-Enabled Circulating Peptides Extraction and Quantitative Detection Coupling with Mass Spectrometry

Jia Fan - *Arizona State University* (jfan49@asu.edu) *YI Grantee*

‣ Circulating peptides have been recognized as useful signatures that can be used for tracking tumor progression. However, detecting low-abundance peptides from blood is still a challenge. We have established “Nanotrap” to effectively fractionate blood peptides with little to no sample processing. By coupling this nanotechnique to advanced mass spectrometry, we can bypass the limitation of current proteomic technologies. We investigated the serum peptides in 228 cancer patients at before, during and after chemoradiotherapy, and the results indicated that baseline serum peptide levels exhibit predictive value for cancer outcome in patients subsequently treated with chemoradiotherapy.

Poster #32D in Exhibit Hall - *attended for 1 hr on Thursday starting at 12:30*
Topic: *Various OTHER*

A Multiplex UPLC-MSMS Method for Newborn Screening of 13 Lysosomal Storage Diseases Plus Adrenoleukodystrophy

Xinying Hong - *University of Washington* (hxy@uw.edu) *YI Grantee*

‣ Newborn screening is often considered for those genetic disorders in which an acceptable treatment has been established and in cases where early initiation of treatment leads to a better clinical outcome. Recently, there has been interested in expanded newborn screening panels to include a subset of lysosomal storage diseases (LSD). We combined some of our previously developed tandem mass spectrometry assays for LSDs with additional diseases to enable simultaneous measurement of up to 24 diseases by enzymatic activity and/or biomarker level.

Poster #33A in Exhibit Hall - *attended for 1 hr on Wednesday starting at 10:00*
Topic: *Small Molecules / Tox*

A UPLC-MS/MS Method for Therapeutic Drug Monitoring of Oxcarbazepine

Chia-Ni Lin - *Chang Gung Memorial Hospital* (chianilin@cgmh.org.tw)

‣ Oxcarbazepine is a 10-keto analogue of carbamazepine, used for the treatment of partial seizures or generalized tonic-clonic seizures. The primary metabolite of oxcarbazepine is 10-hydroxy-carbazepine (MHD). MHD is responsible for most of the anti-convulsant activity. The plasma concentration of MHD is used as a reference for clinical dose adjustment. We have developed and validated a rapid, sensitive, and robust UPLC-MS/MS method for the quantification of oxcarbazepine and its active metabolite MHD in plasma that is clinically useful for therapeutic drug monitoring.

Poster #33B in Exhibit Hall - *attended for 1 hr on Thursday starting at 10:00*
Topic: *Metabolomics*

Simultaneous Determination of 14 Biomarkers of Exposure to BTEX in Human Urine by Isotope Dilution LC-MS/MS

Yehia Baghdady - *The University of Texas at Arlington* (yehia.baghdady@mavs.uta.edu) *YI Grantee*

‣ Benzene, toluene, ethylbenzene, and xylenes (BTEX) are ubiquitous pollutants in the surrounding environment. Because of toxic and carcinogenic effects of BTEX, their urinary metabolites are usually used for the biological monitoring of occupational human exposure to BTEX. We developed and validated a novel in situ derivatization kit for the direct simultaneous determination of 14 biomarkers of exposure to BTEX in human urine by isotope dilution liquid chromatography tandem mass spectrometry.

Poster #33C in Exhibit Hall - *attended for 1 hr on Thursday starting at 10:00*
Topic: *Various OTHER*

Meeting the Challenges of Large Molecule Bioanalysis: Demonstration of an Automated & Standardized, Kit-based Workflow for LC-MS/MS Protein Quantification

Keil Brinster - *Waters Technologies* (Keil_Brinster@waters.com)

‣ Bottom-up, protein quantification workflows are time consuming and complex. High variability in protein quantification analytical data and a general lack of expertise strongly support the requirement for simpler and standardized workflows which facilitate accurate and robust protein quantification. In this work, an automated sample preparation approach, using commercially available sample preparation kits was developed to quantify monoclonal antibody-based plasma. This standardized and automated approach yielded excellent quantification performance, meeting standard method validation criteria with excellent linearity (>0.99) and standard curve and QC accuracies between 88-109% and mean % CVs < 15%.

Poster #33D in Exhibit Hall - *attended for 1 hr on Wednesday starting at 10:00*
Topic: *Proteomics*

Validation of ApolipoProtein A-I Associated Lipoprotein Panel for the Prediction of Cholesterol Efflux Capacity

Cory Bystrom - *Cleveland HeartLab Inc.* (cbystrom@clevelandheartlab.com)

‣ We developed a rapid affinity method to enrich apolipoprotein A-I associated lipoproteins and utilized mass spectrometry-based approach for multiplex quantitation. Utilizing this technique, a multiprotein panel was developed which can be used to estimate cholesterol efflux capacity. The analytical workflow was validated according to CAP/CLIA guidelines. In a 8 week longitudinal study in normal healthy volunteers, predicted cholesterol efflux was stable.

Poster #34A in Exhibit Hall - *attended for 1 hr on Thursday starting at 12:30*
Topic: *Tissue Imaging & Analysis*

Potential Role of Desorption Electrospray Ionization (DESI) Mass Spectrometry Imaging for Intra-Operative Margin Assessment of Basal Cell Carcinoma Resections

Martin Kaufmann - *Queen's University* (martin.kaufmann@queensu.ca) *YI Grantee*

‣ Basal cell carcinoma (BCC) of the skin is the most common cancer, and often occurs in cosmetically sensitive areas. Achieving negative margins during BCC resection is essential for cure and optimizes reconstructive aesthetics. We studied 7 cases of BCC and adjacent benign tissue using DESI mass spectrometry imaging and histopathologic analysis. In most cases, we observed a range of lipid metabolites including m/z 722.51, 858.52, 748.51, 883.53 and 750.54 that were selectively enriched in cancer tissues. This work highlights a potential role for DESI and other metabolomic techniques in intra-operative assessment of BCC margins.

Poster #34B in Exhibit Hall - *attended for 1 hr on Wednesday starting at 13:30*
Topic: *Metabolomics*

Proteometabolomics of Myeloma Drug Resistance

David Koomen - *Moffitt Cancer Center* (david.koomen@moffitt.org)

‣ Drug resistance is a critical clinical problem for the treatment of multiple myeloma patients. While the arsenal of therapeutic agents continues to expand and diversify, we still lack in-depth molecular understanding of both drug mechanisms of action and cellular pathways to therapeutic escape. Therefore, preclinical models of drug resistance have been developed and characterized using proteometabolomics, leading to insights into myeloma biology and elucidating mechanisms of drug resistance.

Poster #34C in Exhibit Hall - *attended for 1 hr on Wednesday starting at 13:30*
Topic: *Small Molecules / Tox*

Development of the Comprehensive Method for Steroid Analysis by GCxGC-HR TOFMS

Viatcheslav Artaev - *LECO Corp* (slava_artaev@lecotc.com)

‣ Thirty three steroids from different classes (progestogens, androgens, estrogens, glucocorticoids, mineralocorticoids) were derivatized using MSTFA, and analyzed using comprehensive two-dimensional gas chromatography coupled to high resolution time-of-flight mass spectrometer, to achieve their reliable and sensitive detection in complex mixtures. The analytes were run as individual components first and their mass spectra were used for creating custom accurate mass library to further assist in identification in the biological matrices. Then the mixture of the steroid standards was used for developing a chromatographic method for achieving most efficient separation. The developed method was validated by analyzing urine spiked with the studied steroids.

Poster #34D in Exhibit Hall - *attended for 1 hr on Thursday starting at 12:30*
Topic: *Tissue Imaging & Analysis*

Liquid Extraction Surface Analysis Mass Spectrometry (LESA-MS): Examples of a New Surface Probing Technique for Clinical and Pre-Clinical Applications

Daniel Eikel - *Advion Inc.* (DEikel@advion.com)

‣ Overview of recent development in the field of surface analysis with focus on liquid extraction surface analysis (LESA) MS and its cousin LESA with LC separation. Brief examples for current use for biomarker detection in tumor biopsies, PKPD of small molecules from doesed mouse tissue sections and advantages for bacterial analysis from agar.

Poster #35A in Exhibit Hall - *attended for 1 hr on Wednesday starting at 10:00*
Topic: *Proteomics*

Discovery Proteomics and Biomarker Quantification in a Breast Tumor Tissue Microarray

John Koomen - *Moffitt Cancer Center* (john.koomen@moffitt.org)

‣ In order to examine the novel paradigm of targeted biomarker measurements nested in discovery proteomics experiments, we have selected the test case of LC-PRM HER2 quantification within an LC-MS/MS analysis of single tissue sections for breast tumor cores in a tissue microarray. HER2 expression levels and proteome content are compared for tumors with and without metastases.

Poster #35B in Exhibit Hall - *attended for 1 hr on Thursday starting at 10:00*
Topic: *Metabolomics*

Rapid and Simple Measurement of Plasma Amino Acids and Urinary Organic Acids Using LC-ESI-MS/MS Technology

Mehmet Balci - *JASEM Laboratory Systems and Solutions* (mehmet.balci@sem.com.tr)

‣ In recent years metabolomics has facilitated gaining insight into discovering the potential disease diagnostic markers and observing fluctuations of certain metabolite levels in body fluids. Disease-related metabolites can be uncovered by following progress of the new methodologies which enable to identify a broad range of diagnostic biomarker candidates including amino acids and organic acids. LC–MS/MS has arisen as a significant approach including ease of sample preparation for the quantitative analysis of metabolites from human body fluids. In our present study, we have developed amino acids and organic acids quantification methods using LC-MS/MS with chromatographically excellent separation of isomers.

Poster #35C in Exhibit Hall - *attended for 1 hr on Thursday starting at 10:00*
Topic: *Small Molecules / Tox*

eXtreme Filter Vial Extraction for the Detection of Fentanyl and Analogues in Oral Fluid Samples

Lisa Wanders - *Thomson Instrument Company* (lisa.wanders@htslabs.com)

‣ Fentanyl analogues have gained popularity in the illicit drug market over the last few years adding to the dangers of the opioid epidemic. A total of 100 de-identified oral fluid samples were provided for the study. Patient samples were collected using the Intercept I2he collection device and underwent a filter vial extraction using the Thomson eXtreme|FV prior to analysis. In addition to investigating this sample preparation technique, this project specifically explores the methodology efficacy to extract Fentanyl and corresponding analogues; Acetyl Fentanyl, Butyryl Fentanyl, Furanyl Fentanyl, Norfentanyl and Sufentanil from oral fluid specimens for analysis on a LC-MS/MS.

Poster #35D in Exhibit Hall - *attended for 1 hr on Wednesday starting at 10:00*
Topic: *Cannabinoids*

The Grass Isn't Always Greener: Removal of Purple Pigmentation from Cannabis Using QuEChERS Extraction and Chlorofiltr® dSPE Cleanup

Danielle Mackowsky - *United Chemical Technologies, LLC* (DMACKOWSKY@UNITEDCHEM.COM)

‣ Minimal sample preparation applications are devoted to the extraction of pigmentations that cause cannabis to have a purple hue. Using first a QuEChERS extraction, 7 dSPE sorbent blends were then evaluated for the removal of uncommon pigmentations from cannabis. The resulting extracts were visually inspected in order to determine if they effectively removed pigmentation from four strains of cannabis. Recoveries of common pesticides and mycotoxins were then determined for the two most effective blends: one featuring Chlorofiltr®, and the other utilizing graphitized carbon black. The blend containing Chlorofiltr® was the best choice for all pigmentation removal without compromising analyte recoveries.

Poster #36A in Exhibit Hall - *attended for 1 hr on Thursday starting at 12:30*
Topic: *Small Molecules / Tox*

Applying LCMS Methods to Instruments of Different Manufacturers – the Diverging Influence of Same-Named ESI Source Parameters

Katharina Kern - *RECIPE Chemicals + Instruments GmbH* (k.kern@recipe.de)

‣ When applying our CE-IVD methods to LCMS instruments of different manufacturers, we face sensitivity differences between several instrument classes and individual instruments themselves, but we also experience the significance of appropriate set source parameters. Even though acronyms for the different source gases, temperatures and voltages sound similar, they do not always have the same influence on ionisation efficiency of the very same analyte. Using the example of Phenytoin, we demonstrate how surprisingly different similar named source parameters can influence the signals of certain substances.

Poster #36B in Exhibit Hall - *attended for 1 hr on Wednesday starting at 13:30*
Topic: *Small Molecules / Tox*

Development and Validation of LC-MS/MS Approach for Quantification of Haloperidol and Several Atypical Antipsychotics and their Metabolites in Serum Samples

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

‣ The group of antipsychotics has grown and expanded over the past 50 years since its inception. As at the beginning antipsychotics were primarily used to manage psychosis, principally in schizophrenia and bipolar disorder, nowadays they are increasingly being used also in the management of non-psychotic disorders. To meet needs of physicians and due to strong recommendations for TDM of some of antipsychotics the analytical method based on LC-MS/MS approach for quantification of haloperidol and three atypical antipsychotics (Clozapine/Norclozapine, Olanzapine, Risperidone/9-OH-Risperidone) in serum samples was developed, validated and implemented into clinical laboratory. This method fulfilled requirements for validation parameters for all analytes.

Poster #36D in Exhibit Hall - *attended for 1 hr on Thursday starting at 12:30*
Topic: *Endocrinology*

Amino acids and metabolites analysis without derivatization using a novel mixed-mode column

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

‣ Current LC-MS analysis strategies of intact amino acids are quite challenging due to the compound fs polarity and ionic structures, often involving the use of complex derivatization steps and/or the use of non-volatile ion-pairing reagents. We have succeeded to develop a specialized amino acid analysis column for use in LC-MS applications, which addresses these challenges. This column has both normal-phase (NP) and ion-exchange (IEX) mixed-mode technology built into the column, with the aim of providing the best possible retention and separation of amino acids without the need for derivatization or ion-pairing. Recently, we have also found that this mixed-mode column can analyze not only amino acids but also derived metabolites. In this study, we show analysis of both amino acids and their various metabolites or related synthetic pathway compounds, using an underivatized LC-MS method.

Poster #37A in Exhibit Hall - *attended for 1 hr on Wednesday starting at 10:00*
Topic: *Proteomics*

Role of RNase L on Kindey Function and its Effect on EGF Shedding and Excretion into Urine

Norah Alghamdi *- Cleveland State University* (n.alghamdi@csuohio.edu)

‣ Renal diseases continue to be prevalent problems. 1% of patients admitted to hospitasl are diagnosed with acute kidney injury, while 5% of hospitalized patients develop AKI. We showed that ribonucleaseL(RNaseL), mediated EGF/EGFR activation. Kidneys from aged RNaseL deficient mice were smaller than wild type. Histological staining revealed higher number of vacuoles in kidneys of RNaseL deficient mice although the biological significance of the observation is unknown. Proteomic analyses of urine by LC/MS discovered that lack of RNaseL blocks EGF excretion to urine. Our findings suggest RNaseL may be a novel target in the design of therapeutic strategies for renal diseases.

Poster #37B in Exhibit Hall - *attended for 1 hr on Thursday starting at 10:00*
Topic: *Endocrinology*

Enhancing LC-MS/MS Sensitivity for Catecholamines via a Reductive Alkylation Derivatization Strategy

Melissa Hughs *- ARUP Institute for Clinical and Experimental Pathology* (melissa.hughs@aruplab.com) *YI Grantee*

‣ A quantitative method for the analysis of catecholamines (epinephrine, norepinephrine, and dopamine) in human plasma by LC-MS/MS was developed. In order to provide sensitivity adequate for analysis in the clinically relevant range, a derivatization protocol employing reductive alkylation with aldehydes was developed. Of the eleven aldehydes evaluated as derivatization agents, hexanal was found to provide the greatest signal enhancement for the analytes. Upon optimization, the method provided adequate sensitivity, linearity, and reproducibility for use in the clinical laboratory. Smaller sample volume, easier sample preparation, and shorter run times compared to the existing HPLC-ECD method were achieved.

Poster #37C in Exhibit Hall - *attended for 1 hr on Thursday starting at 10:00*
Topic: *Cannabinoids*

Profiling Hemp Oils Using Liquid Chromatography-Time of Flight Mass Spectrometry

Vaughn Miller *- Agilent Technologies* (vaughn.miller@agilent.com)

‣ Hemp is a commodity that contains less than 0.30% psychoactive delta-9-tetrahydrocannabinol (Δ9-THC) by weight as compared to its cousin, marijuana. Hemp is a complex plant and may contain high concentrations of other naturally occurring cannabinoids and chemical compounds such as terpenes and flavonoids. Due to this rich chemical diversity and the fact that foodstuffs derived from hemp are not considered controlled substances, a great many commercially available products are available. In this study, we use liquid chromatography-time of flight mass spectrometry to quantitate 10 known cannabinoids and interrogate the resulting raw data for other chemical species inherent to hemp oils.

Poster #37D in Exhibit Hall - *attended for 1 hr on Wednesday starting at 10:00*
Topic: *Proteomics*

Identification of Novel Biomarkers for Ovarian Cancer

Danting Liu *- Cleveland State University* (d.liu0718@gmail.com) *YI Grantee*

‣ Ovarian cancer has the highest mortality of all cancers associated with the female reproductive system. This is mainly due to the fact that most patients with ovarian cancer are diagnosed at an advanced stage because of lack of early symptoms and predicative biomarkers for early detection. We recently developed a mouse model to identify tumor markers for ovarian cancer. LC-MS/MS was used to analyze proteins in the plasma from xenografted ovarian cancer mice and the results showed the level of several inflammatory gene products was gradually increased along with the growth of tumor. The observation was further confirmed by Western blot analysis. Thus, our study may have identified novel candidates for ovarian cancer.

Poster #38A in Exhibit Hall - *attended for 1 hr on Thursday starting at 12:30*
Topic: *Cannabinoids*

Complex Mixture Analysis by Bromobenzyl (PBr) Compare to Fluorophenyl (PFP) Core-Shell HPLC Columns

Ken Tseng *- Nacalai USA Inc.* (ken@nacalaiusa.com)

‣ The ability for BromoBenzyl (PBr) and FluoroPhenyl (PFP) HPLC columns to retain polar molecules in reversed-phase condition allows them to provide orthogonal selectivity comparing to C18. We provide a direct experimental data showing their selectivity differences. In addition, we show the PBr core-shell HPLC column's strength in analyzing a complex mixture of polar and non-polar standard molecules. Another example of PBr for mixture analysis was show with a baseline separation of 11 cannabinoids in under 14 minutes in isocratic MS-compatible condition. This includes the separation of isobaric compounds of Δ9-THC from Δ8-THC.

Poster #38B in Exhibit Hall - *attended for 1 hr on Wednesday starting at 13:30*
Topic: *Small Molecules / Tox*

Multi-Residue Analysis of Abuse Drugs in Whole Blood Using In-well Protein Precipitation Followed with Captiva EMR-Lipid Cleanup by LC-MS/MS

Limian Zhao - *Agilent Technologies* (limian_zhao8@agilent.com)

‣ The Captiva Enhanced Matrix Removal-Lipid (EMR-Lipid) is a pass-through lipid cleanup product implemented in a convenient 96-well plate or SPE cartridge format. This study demonstrates an analytical method for analysis of 24 abuse drugs in whole blood using in-well protein precipitation (PPT) followed with Captiva EMR-Lipid cleanup by LC/MS/MS. Samples were prepared using in-well PPT for protein removal, followed by Captiva EMR-Lipid cleanup for lipids removal. The entire study was conducted in the 96-well plate as a batch process with minimal sample transfer and automatable operations. The analytical method provided >99% removal of phospholipids from whole blood, and an average of 80% absolute recoveries for target analytes. The analytical method was verified for the calibration range of 0.1(0.5) – 20 ng/mL in whole blood with superior accuracy and precision.

Poster #38C in Exhibit Hall - *attended for 1 hr on Wednesday starting at 13:30*
Topic: *Small Molecules / Tox*

The Rise of Loperamide and Desmethyl Loperamide Abuse in the Wake of the Opioid Crisis: Development and Validation of Loperamide and Metabolite by LC-MS/MS

Rebecca Mastrovito - *NMS Labs* (rebecca.mastrovito@nmslabs.com)

‣ A quantitative assay was developed for the detection of loperamide and its metabolite by LC-MS/MS in response to the rise in opioid abuse. Compounds were detected and quantified using positive-ion electrospray tandem mass spectrometry. Linearity was established from 5.0 – 500 ng/mL using six points of calibration in whole human blood. Loperamide was historically used as an anti-diarrheal; however, the levels in recent casework far exceeded therapeutic ranges. The observed concentrations in biological fluids has provided insight to the clinical toxicology community in regards to the toxicity and expected levels of loperamide in casework.

Poster #39A in Exhibit Hall - *attended for 1 hr on Wednesday starting at 10:00*
Topic: *Small Molecules / Tox*

Determination of Urine Copper and Zinc Concentrations by ICP-MS in UPEC Infections

Jisook Yim - *Green Cross Laboratories* (invincibleg17@gmail.com)

‣ We measured the copper (Cu) and zinc (Zn) in urine specimens of uropathogenic Escherichia coli (UPEC) patients using ICP-MS to investigate potential biomarkers. The test set consisted of 20 identified UPEC samples and 20 control samples. Each mean of Cu concentration were 2.45 μg/dL and 2.21 μg/dL in the UPEC and control groups, and those of Zn concentrations were 58.77 μg/dL and 67.44 μg/dL, respectively. In this study, there were no significant differences in Cu and Zn concentrations between UPEC and control groups (p=0.14, 0.52, respectively). Further studies will be required to determine if trace elements will become a useful biomarker.

Poster #39B in Exhibit Hall - *attended for 1 hr on Thursday starting at 10:00*
Topic: *Small Molecules / Tox*

Analysis of Antiepileptic Drugs in Human Serum Using an Ultivo LC/TQ

Jennifer Hitchcock - *Agilent Technologies* (jennifer.hitchcock@agilent.com)

‣ Analyzing antiepileptic drugs can be challenging in clinical research due to the disparate concentrations at which these drugs may be present in human serum. Therefore, a quality assay must be able to analyze many compounds simultaneously, over several orders of magnitude. A highly sensitive and specific analytical method for the quantitation of 15 antiepileptic drugs in human serum was tested on an innovative miniature triple quadrupole mass spectrometer, the Agilent Ultivo triple quadrupole LC/MS (LC/TQ). Samples were prepared through a simple protein precipitation/dilution protocol. Analytes could be quantified over a wide dynamic range; accuracy and reproducibility metrics, as well as R2 values, were acceptable. For Research Use Only. Not for use in diagnostic procedures.

Poster #39C in Exhibit Hall - *attended for 1 hr on Thursday starting at 10:00*
Topic: *Endocrinology*

Analytical Determination of Testosterone in Human Serum Using an Ultivo Tandem LC-MS

Yanan Yang - *Agilent Technologies Inc.* (yanan_yang@agilent.com)

‣ In this research study, a robust, sensitive and relatively fast analytical method was developed for the quantitation of free testosterone in serum using a miniature Ultivo Tandem LC/MS. Ultivo has been designed to address many challenges faced by research laboratories and this research study was conducted in order to assess how this novel tandem mass spectrometer (MS) could perform with a typical endogenous analyte of research interest. This research study will outline typical confirmation performance of free testosterone in human serum using the Ultivo Tandem LC/MS. LLOQ, chromatographic precision and calibration linearity, range and accuracy will be outlined. For Research Use Only. Not for use in diagnostic procedures.

Poster #40A in Exhibit Hall - *attended for 20 min on Tuesday starting at 19:00*
Topic: *Troubleshooting*

Charge Wars of Ion Suppression - Awakening the Force for the Analysis of Estrogens in Clinical Research

Robert Wardle - *Waters Corporation* (robert_wardle@waters.com)

‣ Ion suppression in LC-MS/MS methods can be considered the dark side of the force, possibly leading to analytical sensitivity, selectivity and accuracy goals not being met. Here we discuss the routine measurement of 17β-Estradiol (E2) and Estrone (E1) for clinical research as an example. Testing was performed to investigate the source of a disturbance in the force (labware, biological matrix or solvents), chromatographically resolve it from the analytes and identify the interferent using MS scanning techniques and accurate mass analysis. For Research Use Only, Not for use in diagnostic procedures.

Poster #40B in Exhibit Hall - *attended for 20 min on Tuesday starting at 19:20*
Topic: *Troubleshooting*

Metformin Interference in LC-MS/MS Analysis of Plasma Methoxycatecholamines

Marianne Bergmann - *Lillebaelt Hospital* (marianne.bergmann@rsyd.dk) *YI Grantee*

‣ The LC-MS/MS analysis for plasma methoxycatecholamines has been in routine use at Lillebaelt Hospital since October 2015. During the last 6 months we have experienced an increasing problem with sample chromatograms showing lower peak height for metanephrine and d3-metanephrine, but not for normetanephrine and d3-normetanephrine. The problem only affects a few samples in each run, but these samples also show poor peak shape. We discovered that the problem was caused by metformin – a drug used to treat type 2 diabetes. Metformin co-elutes with metanephrine and causes major ion suppression. Because metformin is widely used and in high doses (up to 2000 mg/day), we set out to solve this problem.

Poster #40C in Exhibit Hall - *attended for 20 min on Tuesday starting at 19:40*
Topic: *Troubleshooting*

Fat Loving Vitamins – the Struggle is Real

Matthew Crawford - *LabCorp* (crawfm1@labcorp.com)

‣ Transitioning lipophilic vitamins A (retinol), E (α- and γ/β- tocopherol), and β-carotene onto a high throughput LC-MS/MS platform provided a gamut of challenges within the laboratory. Application of troubleshooting tools such as; pairwise split sample stress testing, adsorptive loss contact studies, spike order preparative loss determination, IS binding equivalency, phospholipid elution characterization and ionization mode switching, variance reduction of precursor ion population, transition ratio monitoring for interferent identification, echo summing, pre-validation critical assay component assessment and enhancements in chromatographic efficiency were used for resolution of pre-validation challenges. Spoiler alert: We were not 100% successful.

Poster #41B in Exhibit Hall - *attended for 20 min on Thursday starting at 17:00*
Topic: *Troubleshooting*

Low Extraction Rate of 6-Methylmercaptopurine in RBC

Soo Young Moon - *Seoul National University Hospital* (symoon9@gmail.com)

‣ For measuring thiopurine nucleotides, acid hydrolysis step is required. Recovery rate of 6-methylmercaptopurine was 1~3% according to comparison of peak chromatogram before and after extraction. By using isotope-substituted internal standard, final concentration was not overly affected.

Poster #41C in Exhibit Hall - *attended for 20 min on Thursday starting at 17:15*
Topic: *Troubleshooting*

Autosampler Tray Troubleshooting Tales

Kristine Van Natta - *Thermo Fisher Scientific* (kristine.vannatta@thermofisher.com)

‣ From our experiences supporting customers over the years, many instances of bad results from LC-MS batches have been caused by problems in and around the system's autosampler tray. Bad results include abnormally low sensitivity, almost no chromatographic peaks for some specimens and chromatographic results that don't match the intended specimen injections. These problems have been caused by specimen vials with gas-tight caps that have been cooled by the autosampler, specimen vials with micro-inserts that have air trapped at their bottoms and incorrect placement of microtiter plates in the tray holder. Sample preparation procedures must include detailed instructions to avoid such problems.

Poster #43A in Exhibit Hall - *attended for 1 hr on Wednesday starting at 10:00*
Topic: *Various OTHER*

Quantification of Simvastatin and its Metabolites in Plasma Samples

Jenni Viinamäki - *University of Helsinki* (jenni.viinamaki@helsinki.fi)

‣ In this study, a quantitative method for simvastatin, a cholesterol lowering agent, and five of its metabolites in plasma was developed. Sample pre-treatment was supported liquid extraction with diatomaceous earth cartridges and of tert-butyl methyl ether as extraction solvent. Separation was performed with reversed phase liquid chromatography using gradient elution and analytes were detected with mass spectrometry with electro-spray ionization in positive mode for lactone forms and negative mode for acid forms using multiple reactions monitoring. The sensitivity of the method enabled quantification of analytes after a single dose of simvastatin up to 24 h.

Poster #43B in Exhibit Hall - *attended for 1 hr on Thursday starting at 10:00*
Topic: *Proteomics*

Use of a MS-based Targeted Approach for Detection of Minimal Residual Disease (MRD) in Multiple Myeloma

Carlo Martins - *Memorial Sloan Kettering Cancer Center* (martinsc@mskcc.org) *YI Grantee*

‣ Minimal residual disease (MRD) is the most important biomarker for management of patients with multiple myeloma. Here we developed a method to detect lower levels of peptides from variable light-chain of immunoglobulins produced in multiple myeloma, to better assess MRD. We used immunoglobulin enrichment and targeted proteomics to detect the peptides specific for each patient, to help individualized therapy.

Poster #43C in Exhibit Hall - *attended for 1 hr on Thursday starting at 10:00*
Topic: *Proficiency, Regulations, Standards*

Designing the Perfect Mass Standard for Applied Mass Spectrometry

Joe Giesen - *Tulane University* (jgiesen@tulane.edu)

‣ Traditional mass standards are selected from existing commercially available materials. However, if one could design the "perfect calibrant," what features are most important and what class of compounds is most modular to incorporate the desired features? In attempting to address these questions, we have selected monodisperse dendrimers as an appealing substrate for additional investigations. Their modular synthesis and exponential mass increase with synthetic iteration makes them particularly appealing for a range of specific mass spectrometry applications.

Poster #43D in Exhibit Hall - *attended for 1 hr on Wednesday starting at 10:00*
Topic: *Metabolomics*

Quantitation of Glycocholic Acid and Bilirubin in Human Bile for Gall Bladder Diseases by Flow Injection MS/MS Using Standard Addition Method

Raghavi Kakarla - *Cleveland State University* (r.kakarla@vikes.csuohio.edu) *YI Grantee*

‣ Bile can be an ideal fluid for diagnosing Cholangiocarcinoma (CCA) and Cholelithiasis as it is in direct contact with the epithelium and as the emergence of ERCP has made sampling possible without surgical intervention. Elevated levels of Glycocholic acid (GCA) and unconjugated Bilirubin (BLB) in bile have been found to be associated with CCA and Cholelithiasis respectively. We have developed the first mass spectrometric method that can quantify both the analytes in human bile. The method involves a simple dilute and shoot flow injection approach to solve the problems of complex sample preparation and column carry over. A standard addition strategy has been used to reduce any matrix effects if at all present in the diluted bile samples. The method is linear in the range of 12.5-200ng/mL and is validated for accuracy, precision, matrix effects and specificity.

Poster #44A in Exhibit Hall - *attended for 1 hr on Thursday starting at 12:30*
Topic: *Small Molecules / Tox*

A Rapid and Simple HPLC-MS/MS Method for Personalized Busulfan Dosing in Pediatric Patients Undergoing Hematopoietic Stem Cell Transplantation (HSCT)

Yi Xiao - *Children's Hospital Los Angeles* (mulleryi@gmail.com) *YI Grantee*

‣ Busulfan is commonly used as a conditioning regimen before hematological stem cell transplantation (HSCT). To achieve therapeutic efficacy and safety concurrently, personalized busulfan dosing, guided by pharmacokinetic study with serial plasma samples, is needed a few hours after the first dose. We have developed, validated, and implemented a faster method for busulfan measurements with high pressure liquid chromatography-tandem mass spectrometry (HPLC-MS/MS). The sample preparation procedure involves only protein precipitation and dilution, and the HPLC-MS/MS method takes only 3 minutes per sample. The method is accurate and precise. It offers a robust tool for timely dose adjustment for patients undergoing HSCT.

Poster #44B in Exhibit Hall - *attended for 1 hr on Wednesday starting at 13:30*
Topic: *Proteomics*

An LC-MS/MS Method to Characterize *in vivo* Carbamylation of Human Serum Albumin

Collin Hill - *PerkinElmer* (collin.hill@perkinelmer.com)

‣ Measurement of carbamylated albumin from human serum has been a suggested indicator of time-averaged urea concentrations. Here we characterized a previously published LC-MS/MS assay method and determined acceptable inter-site reproducibility of carbamylated albumin measurements. Our data suggests that the sample preparation procedure and analytical method to characterize the extent of albumin carbamylation are robust and can be implemented in a clinical laboratory.

Poster #44C in Exhibit Hall - *attended for 1 hr on Wednesday starting at 13:30*
Topic: *Various OTHER*

Statistical Classification Analysis of Mass Spectral Data of Biological Samples: A Basic Introduction

Kirk Jensen - *Osaka University* (jensen@mass.phys.sci.osaka-u.ac.jp) *YI Grantee*

‣ Mass spectrometry (MS) has become an increasingly valuable tool for biological sample analysis in both research and clinical laboratories. However, data analysis often relies on proprietary software, which can sometimes produce erroneous results. In order to increase understanding of the methods utilized in classification analysis, a short course on statistical classification analysis of mass spectral data of biological samples will be presented including principal component analysis, k-nearest neighbor, random forest, and cross-validation. A few case studies will be presented to highlight certain methods and give a good example of how to analyze mass spectral data.

Poster #44D in Exhibit Hall - *attended for 1 hr on Thursday starting at 12:30*
Topic: *Metabolomics*

Inherited Genetic Disorders Meets Untargeted Metabolomics

Rahul Deshpande - *Greenwood Genetic Center* (rahulrd14@gmail.com) *YI Grantee*

‣ Many inherited genetic defects result in metabolic disorders. Here we describe an untargeted metabolomics approach to screen for these metabolic defects. With this single approach we can effectively screen for multiple disorders hence offering an advantage over the targeted methods presently used.

Poster #45A in Exhibit Hall - *attended for 1 hr on Wednesday starting at 10:00*
Topic: *Proteomics*

Detection of M-Protein in the Presence of Therapeutic Monoclonal Antibodies Using Targeted Mass Spectrometry

Marina Zajec - *Erasmus University Medical Center* (m.zajec@erasmusmc.nl) *YI Grantee*

‣ In multiple myeloma monoclonal plasma cells start to proliferate in an uncontrolled way. These plasma cells produce a monoclonal immunoglobulin called M-protein. Rearranged variable regions of M-protein are patient unique, therefore M-protein can be seen as a marker for personalized cancer diagnostics . Current techniques for detecting serum M-proteins have low sensitivity and are often not able to distinguish between M-proteins and therapeutic monoclonal antibodies used in multiple myeloma. We developed a targeted mass spectrometry assay to detect M-proteins in serum in presence of therapeutic monoclonal antibodies. This assay can target specific M-protein peptides and unique peptides derived from therapeutic monoclonal antibodies enabling multiplexing without interference. Sensitivity of this assay allows deep remission monitoring and early detection of disease relapse.

Poster #45B in Exhibit Hall - *attended for 1 hr on Thursday starting at 10:00*
Topic: *Small Molecules / Tox*

Measurement of a Panel of Water Soluble Vitamins in Serum Using the Sciex Citrine™ Triple Quad™ MS/MS System

Michael Jarvis - *SCIEX* (michael.jarvis@sciex.com)

‣ One of the advantages of LC-MS/MS is the ability to monitor large numbers of analytes in a single method, across multiple compound classes. In this work we have developed an LC-MS/MS method for the measurement of a panel of water soluble vitamins in serum, consisting of: Thiamine, Riboflavin, Nicotinamide, Nicotinic acid, Pantothenic acid, Biotin, Folic acid, and Cyanocobalamin. The lower limit of the measurement range for each analyte was between 0.05 and 10 ng/mL.

Poster #45C in Exhibit Hall - *attended for 1 hr on Thursday starting at 10:00*
Topic: *Tissue Imaging & Analysis*

Pathological Assessment of Prostate Cancer Biopsies by DESI Mass Spectrometry Imaging

Nicole Morse - *Queen's University* (n.morse@queensu.ca)

‣ Accurate diagnosis of aggressive prostate cancer is needed for appropriate patient stratification but is prone to subjective error. Desorption electrospray ionization mass spectrometry imaging (DESI-MSI) was used to investigate metabolite profiles of benign and malignant prostate tissue in 30 biopsy cores across 20 cases. Mass spectra were compared using qualitative approaches and multivariate statistical analysis which revealed metabolomic profiles that distinguished benign from malignant tissue. Metabolites selectively abundant in cancer included; m/z 700.52, 863.56, and 885.55, whereas m/z 480.30, 452.28, and 465.30 were more abundant in benign tissue. Thus, DESI has the potential to identify novel metabolomic biomarkers that can improve prostate cancer diagnosis.

Poster #45D in Exhibit Hall - *attended for 1 hr on Wednesday starting at 10:00*
Topic: *Endocrinology*

Evaluating the Accuracy of Vitamin D Assays

Nicole Tolan - *SCIEX* (nicole.tolan@sciex.com)

‣ We demonstrate the prevalence of inaccurate 25(OH)D determination, as a result of poor recoveries of 25(OH)D2, and present a straightforward method for estimating the percent cross-reactivity of immunoassays. Given the relatively few number of SRMs and PT materials containing sufficient concentrations of 25(OH)D2, our study highlights the need to thoroughly evaluate the performance of commercial immunoassay methods and communicate their limitations to practicing clinicians.

Poster #46A in Exhibit Hall - *attended for 1 hr on Thursday starting at 12:30*
Topic: *Cannabinoids*

Detection of 22 Phytocannabinoids and Their Metabolites in Urine by LC-MS/MS and Their Evaluation as Potential Markers

Rory Doyle - *Thermo Fisher, Inc* (rory.doyle@thermofisher.com)

‣ 22 phytocannabinoid’s and metabolites were extracted from urine by simple sample preparation techniques of dilute and shoot and liquid-liquid. Thermo Fisher Quantis and Altis tandem mass spectrometers in positive and negative Electrospray mode with a Vanquish Horizon HPLC system were used. 100 µl of urine matrix using an Accucore C18, 100 x 2.1 mm, 2.6 µm with a water:acetonitrile mixture containing acetic acid achieved baseline chromatographic separation within 6 minutes. The limits of detection and quantitation were determined on each instrument and the presence of the various compounds detected were evaluated as potential markers for recent usage or of origin.

Poster #46B in Exhibit Hall - *attended for 1 hr on Wednesday starting at 13:30*
Topic: *Small Molecules / Tox*

Evaluation of Tip-Washing Technology for Forensic and Clinical Applications

Allison Veitenheimer - *Oklahoma State University* (allison.veitenheimer@okstate.edu)

‣ Disposable pipette tips are a large expense for clinical toxicology laboratories, so implementation of a pipette tip washing device could reduce the consumption of plastic tips by allowing for reuse after washing, thus reducing costs. Urine (50 uL) fortified with high concentrations (10 ug/mL) of analytes that might be present in specimens (opiates, benzodiazepines, stimulants, and cannabinoids) were processed for analysis by LC-MS/MS. One Way ANOVA with Tukey’s Multiple Comparisons Test showed no significant differences ($p<0.05$) in washed tips versus unwashed tips (N=6). There were no data trends indicating carryover of any of the classes of analytes.

Poster #46C in Exhibit Hall - *attended for 1 hr on Wednesday starting at 13:30*
Topic: *Small Molecules / Tox*

Cross Validation of Immunosuppressant Quantification in Whole Blood by LDTD-MS/MS and LC-MS/MS Using Triple Ion Source

Pierre Picard - *Phytronix Technologies, Inc* (p.picard@phytronix.com)

‣ The use of laser diode thermal desorption (LDTD) for immunosuppressant quantification remove the long separation of chromatography and the cost of immunoassays. We show here the ultra-fast quantification of Tacrolimus, Sirolimus, Everolimus and Cyclosporine-A. The sample preparation is a combination of protein precipitation and solid phase extraction with an OFX cartridge. The recovered solution is diluted in water mixture with BSA, HEPES and EDTA for LDTD analysis on a Shimadzu LCMS-8060 mass spectrometer equipped with a triple ion source. We have a LLOQ of 25ng/mL for Cyclosporine-A and 2.25ng/mL for the 3 other molecules. We show the linearity, intra-day and inter-day reproducibility, selectivity and carry-over measurement of our method. We also quantified 48 real samples. All results and real samples are cross-validated by LC-MS/MS on the same instrument.

Poster #46D in Exhibit Hall - *attended for 1 hr on Thursday starting at 12:30*
Topic: *Endocrinology*

High Sensitivity Assay of Estrogens in Human Plasma by UHPLC-MS/MS without Derivatization

Atsuhiko Toyama - *Shimadzu Corporation* (toyama@shimadzu.com.sg)

‣ While many laboratories still use immunoassay to measure estrogen levels in plasma, these assays suffer from several drawbacks and are not able to measure very low levels in routine. Here we present an UHPLC-MS/MS method that can measure low pg/mL of estrone, estradiol and estriol with an easy and rapid sample preparation. Limits of quantification were of 0.5, 1 and 5 pg/mL for E1, E2 and E3, respectively, using a sample volume of 200ìL. The total analysis time was of 3.5 min. Validation experiments and real samples have been assayed to demonstrate the fit-for-purpose of the method.

Poster #47A in Exhibit Hall - *attended for 1 hr on Wednesday starting at 10:00*
Topic: *Proficiency, Regulations, Standards*

Developing a Vitamin D-Binding Protein Reference Material

Lisa Kilpatrick - *National Institute of Standards and Technology* (lisa.kilpatrick@nist.gov)

‣ Vitamin D-binding protein (VDBP) is the primary transporter of vitamin D metabolites in plasma. There is a recent interest in calculating the unbound or bioavailable fractions of 25-hydroxyvitamin D which requires accurate quantification of VDBP. Recent studies show that immunoassays for VDBP may not give comparable results and there are no standards currently available to assess their accuracy. In this work, a pooled plasma sample (SRM 1950) was evaluated in two different laboratories for use as a reference material. VDBP concentrations measured by LC-MRM were 3.22 micromol/kg and 3.47 to 3.52 micromol/kg. Differences in concentrations between the laboratories had < 6.4 % CV indicating good reproducibility and suitability as a reference material.

Poster #47B in Exhibit Hall - *attended for 1 hr on Thursday starting at 10:00*
Topic: *Proteomics*

No Phlebotomy Needed: Evaluation of Protein Stability in Liquid Blood Collected with the HemoLinkTM Device for Use in Patient-Centered Sampling and Monitoring

Irene van den Broek - *Cedars Sinai Medical Center* (irene.vandenbroek@cshs.org)

‣ The HemoLink blood collection device is needle-free, easy-to-use, and allows for self-collection of up to 150 µL of liquid blood or plasma. For use with patient-centered self-sampling, stability of analytes in HemoLink liquid whole blood (or plasma) that has been remotely shipped should be understood. In this study, we evaluate the stability of ten proteins (primarily apolipoproteins) in HemoLink liquid blood, a pre-requisite for the application of this device with remote patient sampling. Preliminary data shows stability of all proteins in HemoLink whole blood and plasma during 1 and 3-day shipment at room temperature.

Poster #47C in Exhibit Hall - *attended for 1 hr on Thursday starting at 10:00*
Topic: *Troubleshooting*

Troubleshooting the Urine Interferences Present in the LC-MS/MS Analysis of Ethyl Glucuronide and Ethyl Sulfate

Rory Doyle - *Thermo Fisher Scientific, Inc* (rory.doyle@thermofisher.com)

‣ LC-MS/MS analytical method for the quantitation of Ethyl Glucuronide and Ethyl sulfate on a triple quadrupole mass spectrometer can be easy to setup with a dilute and shoot sample preparation. However, urine interferences can make consistent and accurate measurements of difficult. A Thermo Fisher Quantis mass spectrometer in negative Electrospray mode with a Vanquish Horizon HPLC system was used. 100 ul of urine matrix was diluted and a Synchronis AQ 100 x 3.0 mm, 3 um column using water:methanol mixture containing acetic acid achieved baseline separation within 3.5 minutes that limited the interferences and improved limits of detection and quantitation.

Poster #47D in Exhibit Hall - *attended for 1 hr on Wednesday starting at 10:00*
Topic: *Small Molecules / Tox*

Fast LC-MS/MS Analytical Method with Alternate Column Regeneration for the Analysis of >100 Various Drugs and Their Metabolites in Urine in Clinical Research

Andre Szczesniewski - *Agilent Technologies* (andre_szczesniewski@agilent.com)

‣ This research outlines a highly sensitive, specific and fast LC/MS/MS analytical method that was developed for the quantitation of >100 drugs from a variety of drug classes over a wide dynamic range. The Alternate Column Regeneration (ACR) hardware configuration was employed to significantly increase the sample throughput. The ability to combine many analytes into a single run coupled with a fast analytical method and ACR could improve turnaround time in a clinical research laboratory. Future work will include testing multiple sources of human urine for interferences that may impact the quantitation of any of the compounds in the analytical method.

Poster #48A in Exhibit Hall - *attended for 1 hr on Thursday starting at 12:30*
Topic: *Small Molecules / Tox*

New Analytical Tool for Urine Sample Screening and Confirmation Analysis: Combined LDTD-MS/MS and LC-MS/MS Ion Source

Jean Lacoursière - *Phytronix* (j.lacoursiere@phytronix.com)

‣ A new instrument tool was developed using a hybrid ion source. The source combines the laser diode thermal desorption source (LDTD) and a liquid chromatographic electrospray ion source (LC-ESI). Urine samples are extracted with a generic method and high-throughput screening is performed using the LDTD ion source part. Without any changes to the source inlet parts, presumptive positive samples are analyzed with LC-ESI-MS/MS for confirmation. Using a generic extraction method for all drug hydrophobicities, combined LDTD and LC system was evaluated for its precision and linearity performance for presumptive and definitive testing method. More than 50 drugs are analyzed simultaneously in urine from different classes.

Poster #48B in Exhibit Hall - *attended for 1 hr on Wednesday starting at 13:30*
Topic: *Proficiency, Regulations, Standards*

Worldwide Interlaboratory Study on Monoclonal Antibody Glycosylation

Maria Lorna De Leoz - *National Institute of Standards and Technology* (lorna.deleoz@nist.gov)

‣ An interlaboratory study was conducted by NIST to determine measurement variability in identifying and quantifying N-glycans across laboratories and to assign best values for NISTmAb, a monoclonal antibody reference material. A total 103 reports were submitted by 76 participants worldwide from industry, university, research, government, and hospital laboratories. Various methods were used for glycosylation analysis, including mass spectrometry, fluorescence detection and capillary electrophoresis. Consensus values were calculated for fifty-seven glycan compositions that were reported at least six times; some labs differentiated between isomers. Determining variability of glycosylation profiles from a larger number of laboratories and range of measurement methods provides a baseline for comparison in the rapidly developing field of glycosylation analysis.

Poster #48C in Exhibit Hall - *attended for 1 hr on Wednesday starting at 13:30*
Topic: *Proteomics*

The First Precision Diagnosis of Multiple Myeloma by Use of 21 Tesla FT-ICR Top/Middle-Down *de novo* Sequencing

Lidong He - *Florida State University* (lhe@magnet.fsu.edu) *YI Grantee*

‣ Multiple myeloma is a B cell malignancy characterized by a plasma cell clonal expansion. If there is clinical suspicion of a multiple myeloma, serum is tested for the presence of elevated levels of a monoclonal immunoglobulin (mIg) secreted by clonal plasma cells. We describe the first top/middle-down de novo sequencing of mIg in serum with the advantages of ultrahigh mass accuracy and extensive residue cleavages. There may be certain predilections for disease type based on immunoglobulin gene usage, and typical cloning experiments are expensive, invasive, and laborious. Herein we report a non-invasive method for sequencing mIg proteins from the blood.

Poster #48D in Exhibit Hall - *attended for 1 hr on Thursday starting at 12:30*
Topic: *Endocrinology*

Mass Spectrometric Studies of Apolipoprotein Proteoforms and their Role in Lipid Metabolism and Type 2 Diabetes

Dobrin Nedelkov - *Isoformix* (dobrin.nedelkov@isoformix.com)

‣ Apolipoproteins function as structural components of lipoprotein particles, cofactors for enzymes, and ligands for cell-surface receptors. Most of the apoliporoteins exhibit proteoforms, arising from PTMs such as glycosylation, oxidation and sequence truncations. Presented will be recent studies correlating apolipoproteins proteoforms with specific clinical measures of lipid metabolism and cardiometabolic risk. Mass spectrometric immunoassays toward apolipoproteins A-I, A-II, C-I, C-II, and C-III were applied on large cross-sectional and longitudinal clinical cohorts. Several correlations were observed, including greater apolipoprotein A-I and A-II oxidation in patients with diabetes and cardiovascular disease, and a divergent apoC-III proteoforms association with plasma triglycerides, indicating significant differences in the metabolism of the individual apoC-III proteoforms.

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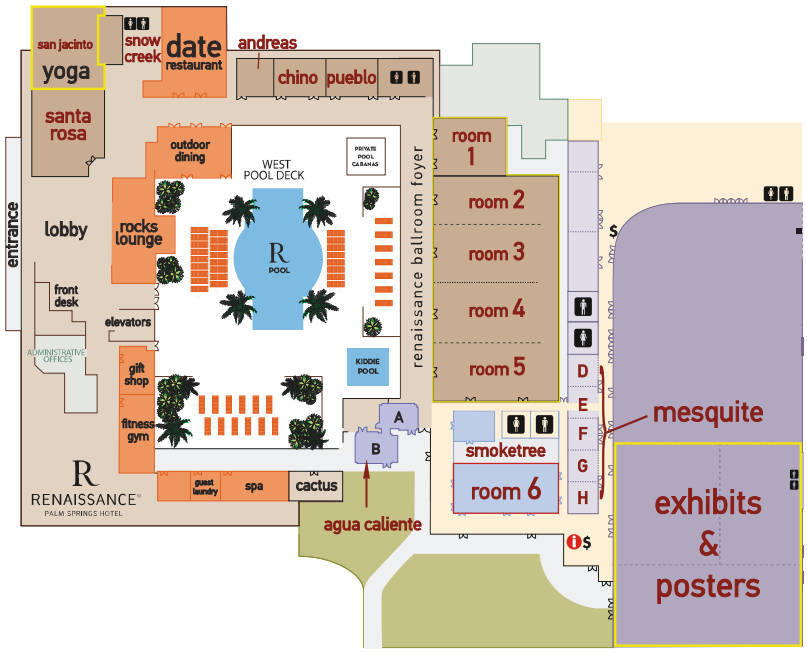

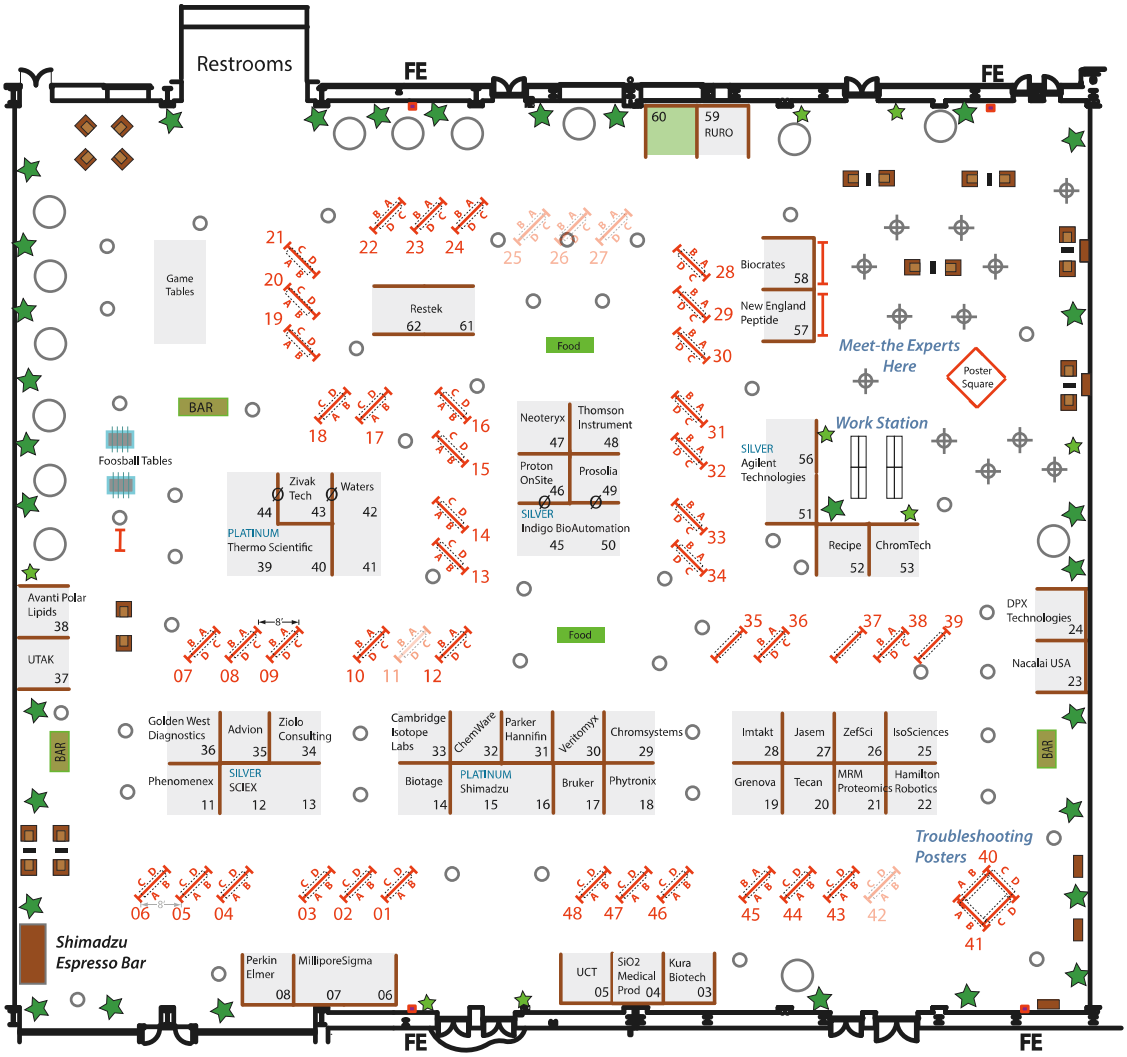

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