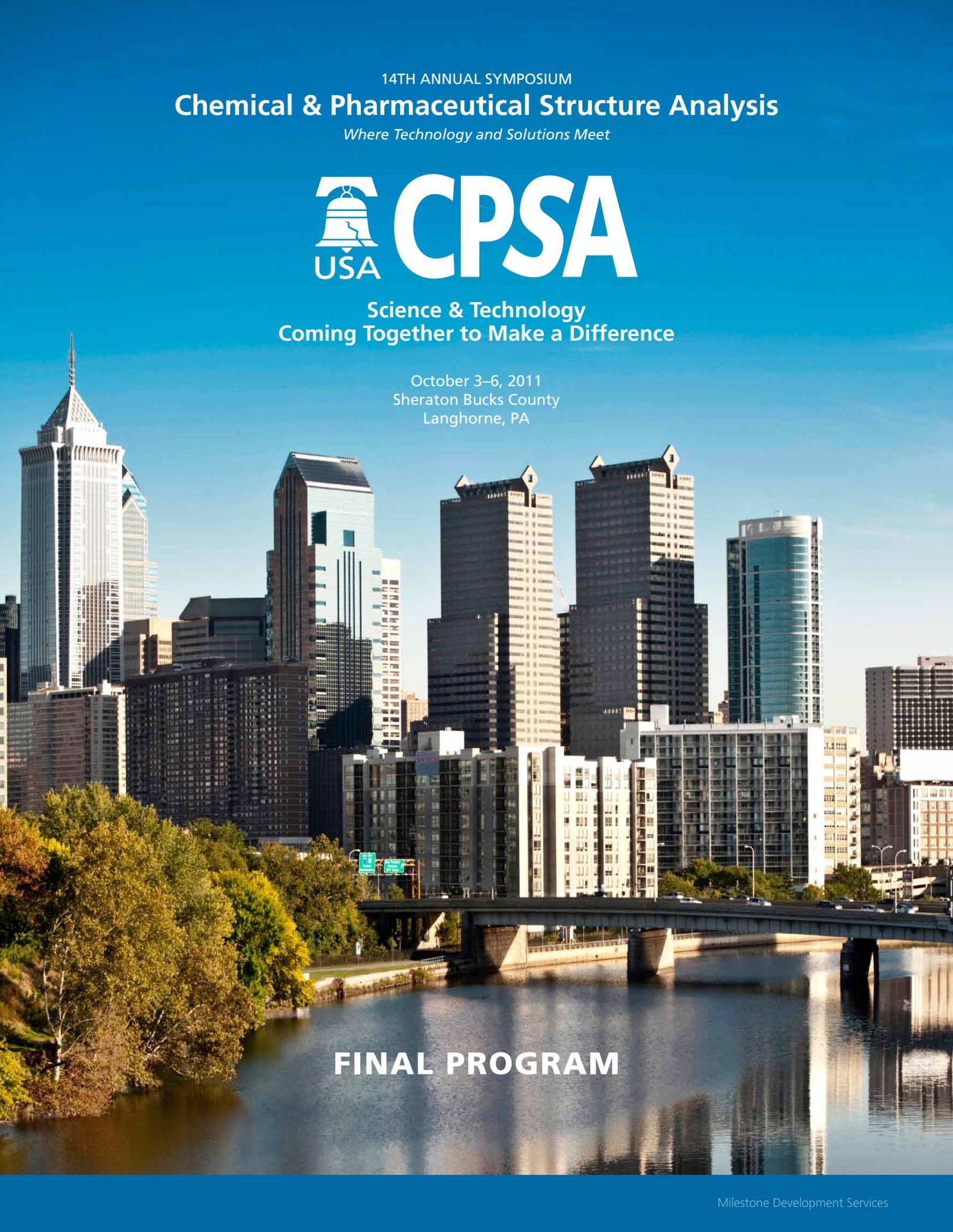


14TH ANNUAL SYMPOSIUM  
**Chemical & Pharmaceutical Structure Analysis**  
*Where Technology and Solutions Meet*



**Science & Technology  
Coming Together to Make a Difference**

October 3-6, 2011  
Sheraton Bucks County  
Langhorne, PA

A wide-angle photograph of the Philadelphia skyline, featuring several prominent skyscrapers like the Comcast Center and the Liberty City Center. In the foreground, the Schuylkill River flows under a bridge, with lush green trees on the left bank. The sky is a clear, bright blue.

**FINAL PROGRAM**

PUSHING THE LIMITS IN MASS SPECTROMETRY

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WELCOME

**Inspiration. Collaboration.**

Dear Colleague:

On behalf of our sponsors and participants, I would like to welcome you to the 14th annual Symposium on Chemical and Pharmaceutical Structure Analysis (CPSA 2011). It is a pleasure to once again host this unique event in Langhorne, PA.

A goal of the CPSA annual meetings is to provide in-depth reviews of innovative technology and industry practices through open discussion of issues and needs. The aim of this annual meeting is to promote the analytical sciences with highly interactive events where scientists openly share their experiences and visions in a collegial setting. Education and specialized training are the foundation of all CPSA events.

At last year's annual meeting, there was a sense of a new beginning when Brad Ackermann of Eli Lilly stated, "We have to move LC-MS closer to the patient before the full impact of what we can do will be realized." Such a new beginning (or challenge!) is emphasized with the CPSA 2011 theme: Science and Technology Coming Together to Make a Difference. Our CPSA 2011 program chair, Roger Hayes of Cetero Research, had a goal to feature sessions that highlight emerging technology within the CPSA environment where ideas are openly shared and observations are discussed. And in many ways, the topics reflected in each symposia session, roundtable, workshop, poster presentation, and short course attempts to move analysis "closer to the patient."

We are once again pleased to provide an expanded line-up of events at CPSA this year in conjunction with the North Jersey ACS Drug Metabolism Discussion Group (NJDMDG), Chromatography Group (NJCG), NMR Discussion Group (NJNMRDG), Mass Spectrometry Discussion Group (NJMSDG), the Greater Boston Mass Spectrometry Discussion Group (GBMSDG), the Delaware Valley Drug Metabolism Discussion Group (DVDMDG), the Chromatography Forum of the Delaware Valley (CFDV), and the Washington Chromatography Discussion Group (WCDG). We are delighted to feature symposia sessions and workshops that provide an intimate setting to expand on the knowledge of recent innovations.

As always, I encourage you to actively participate, interact, and share ideas during the event so that significant impact to the field can be made through your participation in the sciences and your leadership. Key ingredients to CPSA events are creativity and imagination. Please enthusiastically share your ideas and visions for the analytical sciences as we move closer to the patient—and perhaps consumer.

Finally, we are grateful to the sponsors of this unique event. Each sponsor shares the passion and commitment for accelerating product development. CPSA sponsors and participants are dedicated to the spirit of cooperation. Imagination needed!

Sincerely,

A handwritten signature in black ink, appearing to read "Mike S. Lee". The signature is fluid and cursive, written in a professional style.

Mike S. Lee, Ph.D.

# 2011 ORGANIZING COMMITTEE

## PROGRAM CHAIR

---

**Roger Hayes**  
Cetero Research

## SYMPOSIA & ROUNDTABLES

---

**Mark Arnold**  
Bristol-Myers Squibb

**Kevin Bateman**  
Merck

**Chad Briscoe**  
PRA International

**Guodong Chen**  
Bristol-Myers Squibb

**Lucinda Cohen**  
Merck

**Jerry Gromelski**  
QPS

**Jack Henion**  
Advion BioSciences

**Jonathan Josephs**  
Bristol-Myers Squibb

**Richard King**  
PharmaCadence

**Kenneth Lewis**  
OpAns

**Timothy Olah**  
Bristol-Myers Squibb

**Joanna Pols**  
Merck

**Ragu Ramanathan**  
Bristol-Myers Squibb

**Petia Shipkova**  
Bristol-Myers Squibb

**Ron Shoup**  
AIT Bioscience

**Gabriella Szekely-Klepser**  
Allergan

**Gary Valaskovic**  
New Objective

**Eric Woolf**  
Merck

**Nathan Yates**  
Merck

## VENDOR SESSION

---

**Mark Hayward**  
Lundbeck Research

**Ragu Ramanathan**  
Bristol-Myers Squibb

## POSTER SESSION

---

**James Stephenson**  
Thermo Scientific

**Matthew Szapacs**  
GlaxoSmithKline

**Tracie Williams**  
Centers for Disease Control &  
Prevention

**Donglu Zhang**  
Bristol-Myers Squibb

## SHORT COURSES

---

**Ayman El-Kattan**  
Pfizer

**Roger Hayes**  
Cetero Research

**Mark Hayward**  
Lundbeck Research

**Kenneth Lewis**  
OpAns

**Shane Needham**  
Alturas Analytics

**Nalini Sadagopan**  
Agilent Technologies

**Gary Valaskovic**  
New Objective

**Nathan Yates**  
Merck

## COMMUNICATION & MEDIA

---

**Carla Marshall-Waggett**  
New Objective

## CORRESPONDENCE

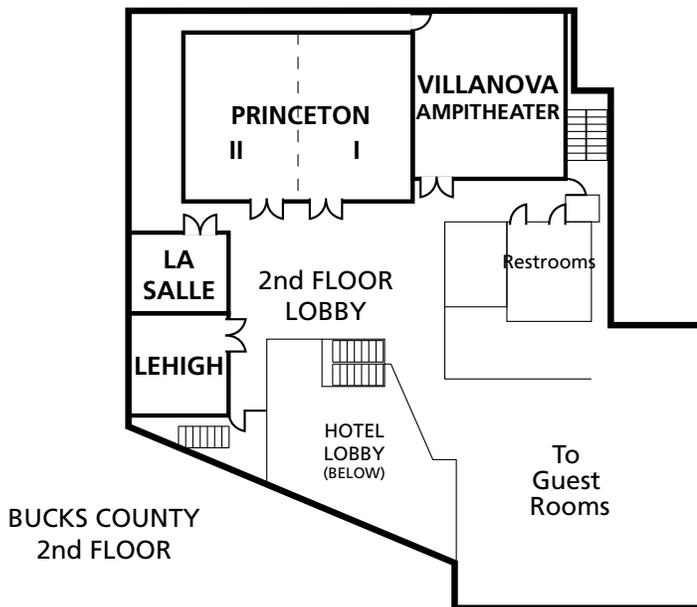
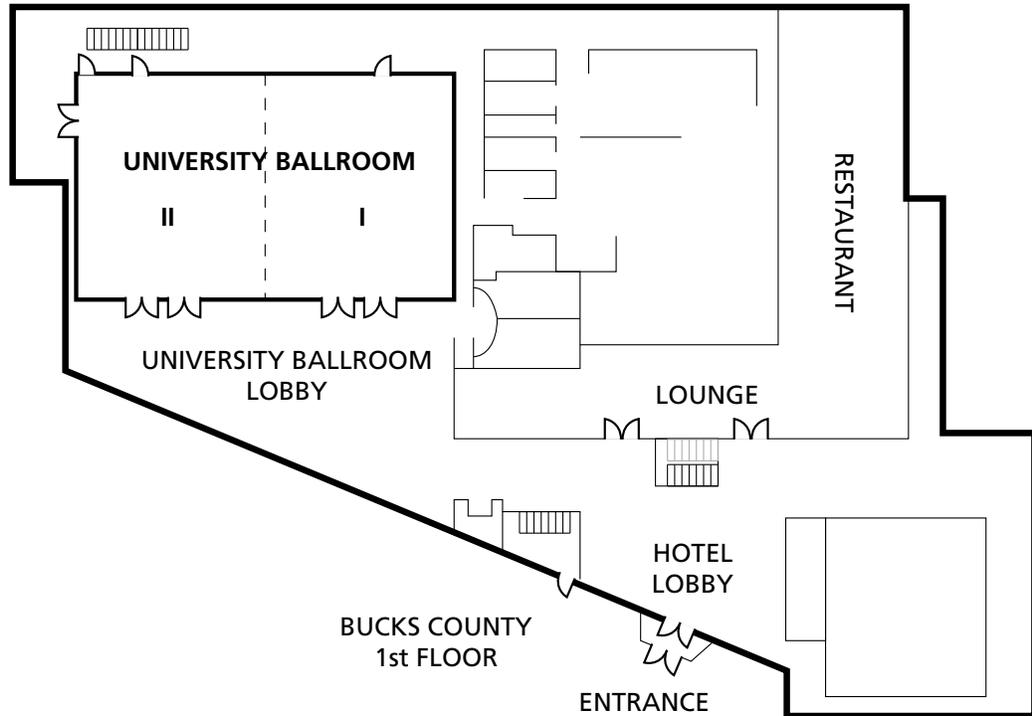
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**Mike Lee**  
Milestone Development Services

[www.cpsa-usa.com](http://www.cpsa-usa.com)

# FLOORPLAN

## Sheraton Bucks County



# EXHIBITION

## EXHIBITORS

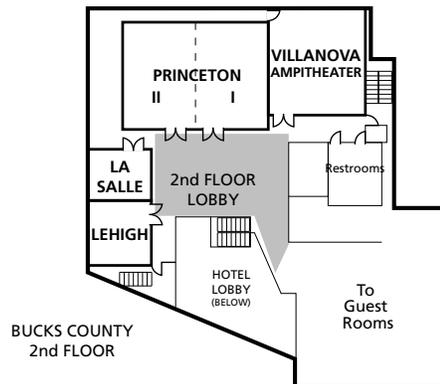
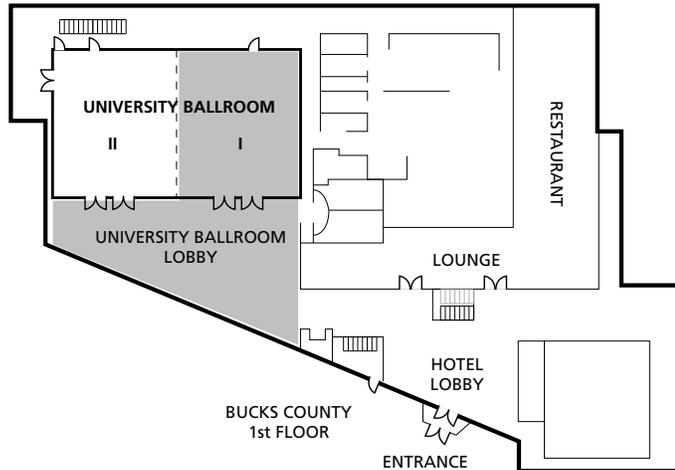
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 Alturas Analytics  
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 Biotage  
 Bonna-Agela Technologies  
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 Critical Path Services  
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 LECO Corporation  
 MAC-MOD Analytical  
 McKinley Scientific  
 Molecular Discovery  
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 Novatia  
 OpAns  
 Orochem Technologies  
 PharmaCadence  
 PRA International  
 Primera Analytical Solutions Corp.  
 QPS  
 Shimadzu  
 Tandem Labs  
 Vitalea Science  
 Waters Corporation  
 Wiley & Sons

## EXHIBIT HOURS

WEDNESDAY 12:00 PM - 2:15 PM  
 5:30 PM - 6:30 PM

## EXHIBIT LOCATIONS

Exhibit booths are located in University I Ballroom, Ballroom Lobby and in the 2nd Floor Lobby.



## FOR EXHIBITORS

Move-in: Wednesday, 9:00 am - 11:00 am  
 Move-out: Wednesday, 7:00 pm - 11:00 pm

## SPONSORS

Thank You!

The CPSA annual symposium is made possible by the broad-based support of industry sponsors. The passion for the analytical sciences and the accelerated discovery and development of pharmaceuticals is shared by each sponsor. As a result, the event is dedicated to promoting awareness and understanding of the issues and needs associated with pharmaceutical R&D in the hopes of inspiring significant advances in the field.



# SHORT COURSES & EVENTS

**Monday** October 3

**8:30 AM - 4:00 PM**

*Princeton I*

**SHORT COURSES**

**Method Development for LC/MS: Traditional Approaches and Emerging Trends**  
*Instructors: Roger Hayes, Cetero Research; Shane Needham, Alturas Analytics*

*Lehigh*

**Small Molecule Biomarkers: Strategies for Method Development, Profiling and High Throughput Workflow Solutions in Drug Discovery**  
*Instructors: Mark Hayward, Lundbeck Research; Kenneth Lewis, OpAns*

*Princeton II*

**Analysis of Peptides and Proteins: Sample Preparation to Identification to Quantitation**  
*Instructors: Nalini Sadagopan, Agilent Technologies; Gary Valaskovic, New Objective; Nathan Yates, Merck*

**9:00 AM - 3:00 PM**

**CPSA OPEN GOLF OUTING**

*Organizers: Brad Coopersmith, Waters Corporation; Ken Imatani, Agilent Technologies*  
*Makefield Highlands Golf Course, Yardley, PA*

**12:00 PM - 4:00 PM**

*Villanova*

**PHARMACEUTICAL SCIENCES WORKSHOP : IMPURITIES & DEGRADANTS**

*Discussion Leaders: Mingxiang Lin, Merck; Ron Kong, PTC Therapeutics*  
*Co-sponsored by the North Jersey Mass Spectrometry Discussion Group*

- ▶ **Characterization of Impurities and Degradants in Biologics Discovery and Development**  
*Guodong Chen, Bristol-Myers Squibb*
- ▶ **Effective Use of LC-MSn Molecular Fingerprinting for the Rapid Structure Identification of Pharmaceutical Impurities**  
*Min Li, Merck*
- ▶ **Analytical Challenges in Controlling Genotoxic Impurities**  
*David Liu, GlaxoSmithKline*
- ▶ **To Isolate or Not: The Sometimes Circuitous Characterization of a Degradant**  
*Gary Martin, Merck*

**4:30 PM - 5:30 PM**

*Princeton I & II*

**WORKSHOP & SOCIAL**

*Hosted by MAC-MOD Analytical*

**6:00 PM - 9:00 PM**

*University I & II Ballrooms*

**RECEPTION & SPONSOR'S DINNER**

*Hosted by AB SCIEX*

**New Chip to MicroLC Applications**

- ▶ **New Microfluidic cHiPLC Applications for Higher Throughput**  
*David Neyer, Eksigent part of AB SCIEX*
- ▶ **Method Development and Transfer for a Range of Linear Velocities Suitable to Scale Down to 1mm Column IDs and Beyond**  
*Rick King, PharmaCadence Analytical Services*

MONDAY, OCTOBER 3

# PROGRAM AGENDA

Tuesday October 4

<b>7:30 AM - 8:30 AM</b>	<b>REGISTRATION &amp; CONTINENTAL BREAKFAST</b> ..... <i>University Ballroom Lobby</i>
<b>7:30 AM - 8:30 AM</b>  <i>Princeton I &amp; II</i>	<b>SPONSORED BREAKFAST WORKSHOP</b> ..... Electronic Lab Notebook Special Interest Group <i>Sponsored by AIT Bioscience</i>
<b>8:30 AM – 9:00 AM</b>  <i>University I &amp; II Ballrooms</i>	<b>OPENING REMARKS</b> ..... Welcome <i>Mike Lee, Milestone Development Services</i>  Objectives, Format, and Opening Remarks <i>Roger Hayes, Cetero Research</i>
<b>9:00 AM - 9:45 AM</b>  <i>University I &amp; II Ballrooms</i>	<b>PLENARY LECTURE</b> ..... Secrets in Lipid Biochemistry Revealed by Mass Spectrometry <i>Robert Murphy, University of Colorado Denver</i>
<b>10:00 AM - 11:45 AM</b>	<b>PARALLEL SESSIONS</b>

<p><b>Biomarkers</b> <i>University I Ballroom</i></p> <p><i>Discussion Leader: Petia Shipkova, Bristol-Myers Squibb</i></p> <ul style="list-style-type: none"> <li>▶ Biomarkers for Toxicity <i>Don Robertson, Bristol-Myers Squibb</i></li> <li>▶ Lipid Analysis in Mitochondria and Serum Using High Resolution LC-MS and HCD Fragmentation <i>Susan Bird, Brigham and Women’s Hospital</i></li> <li>▶ Coupling Static and Kinetic Biomarkers in Order to Unravel Dyslipidemia <i>Stephen Previs, Merck</i></li> <li>▶ LC/MS Biomarker Assay Validation Using Surrogate Matrix and Surrogate Analyte Approaches <i>Gary Schultz, Advion BioSciences</i></li> </ul>	<p><b>Colloquium: The Science of Compliance</b> <i>University II Ballroom</i></p> <p><i>Discussion Leader: Chad Briscoe, PRA International</i></p> <ul style="list-style-type: none"> <li>▶ Holy #\$\$@! What Have We Gotten Ourselves Into? <i>Ray Farmen, Celerion</i></li> <li>▶ Carryover and Chromatographic Background Contributions: Are We Assessing Potential Bias Effects on Individual Sample Result and/or Batch Acceptance in Realistic (and Meaningful) Ways? <i>Rand Jenkins, PPD</i></li> <li>▶ Pitfalls of Whole Blood Stability and Hemolytic Plasma Assessment in Bioanalysis <i>Corey Ohnmacht, PRA International</i></li> <li>▶ The Role of Compliance in “Non-Regulated” Studies Conducted by the Pharmaceutical Industry <i>Rick Edom, Johnson &amp; Johnson</i></li> <li>▶ Pre-Compliance in Early in vitro Drug Development <i>Joanna Barbera, XenoTech</i></li> </ul>
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TUESDAY, OCTOBER 4

# PROGRAM AGENDA

**Tuesday** October 4

**12:00 PM – 1:00 PM**

*University I & II Ballrooms*

**SPONSORED LUNCH & ROUNDTABLES**

*Sponsored by Agilent Technologies*

**1:15 PM – 3:00 PM**

*University Ballroom Lobby  
2nd Floor Lobby*

**POSTER SESSION & ROUNDTABLES**

*Discussion Leaders: James Stephenson, Thermo Scientific; Matthew Szapacs, GlaxoSmithKline; Tracie Williams, Centers for Disease Control and Prevention; Donglu Zhang, Bristol-Myers Squibb*

**2:00 – 3:00 PM**

*Princeton I*

**SPONSORED WORKSHOPS**

LDTD with SelexION™ Technology and the QTRAP® 5500 System with Advanced Selectivity and High Throughput

*Sponsored by AB SCIEX*

*Yves Leblanc, AB SCIEX*

*Lehigh*

Towards Implementation of MALDI IMS into the Drug Development Workflow: Bridging Histology and Drug Tissue Distributions

*Sponsored by Bruker Daltonics*

*M. Reid Groseclose, GlaxoSmithKline*

*Villanova*

Metabolism Optimization: Future Needs and Emerging Workflows

*Sponsored by Molecular Discovery*

▶ Workflows for Efficient Data Acquisition and Processing

*Kevin Bateman, Merck*

▶ Application of Metabolite Identification Information for Drug Design

*Roy Vaz, Sanofi-Aventis*

▶ Interactive Demonstration of Software Tools for Acquisition, Processing and Design

*Ismael Zamora, Molecular Discovery*

*Princeton II*

A QbD-based Approach to LC Method Development

*Sponsored by Waters Corporation*

*Dominic Moore, Waters Corporation*

**3:00 PM – 4:30 PM**

*University I Ballroom*

**SYMPOSIA SESSION & ROUNDTABLES**

**Metabolite Identification**

*Discussion Leaders: Joanna Pols, Merck and Ragu Ramanathan, Bristol-Myers Squibb*

▶ Use of High Resolution Mass Spectrometry for Correct Structure Elucidation of Metabolites

*Natasha Penner, Biogen Idec*

▶ Advances in Metabolite Profiling Software - an Evaluation of Mass-Metasite

*Diane Grotz, Merck*

▶ Streamlining the Drug Discovery Biotransformation Workflow:

*HRMS, On-the-Fly-MDF and Metabolite Pilot Software*

*Xiaomei Gu, Bristol-Myers Squibb*

# PROGRAM AGENDA

Tuesday October 4

- ▶ A Comparison of Metabolic Profiles Following Targeted and Non-Targeted Analysis Using Q-Trap Technologies  
*Veronica Zelesky, Pfizer*

**4:45 PM – 6:15 PM**

*University II Ballroom*

## SYMPOSIA & ROUNDTABLES

### Innovation in Regulated Bioanalysis: Fact or Fantasy?

*Discussion Leaders: Kevin Bateman, Merck*

- ▶ What is Innovation?  
*Kevin Bateman, Merck*
- ▶ The Case for Innovation in Drug Discovery Bioanalysis  
*Lucinda Cohen, Merck*
- ▶ The Case for Innovation in Regulated Bioanalysis  
*Chris Evans, GlaxoSmithKline*
- ▶ Group Argument on Innovation in Bioanalysis  
*All attendees*

**6:30 PM – 9:00 PM**

*University II Ballroom*

## SPONSOR HOSPITALITY & EVENING WORKSHOPS

*Held in conjunction with the North Jersey ACS Mass Spectrometry and Delaware Valley Drug Metabolism Discussion Groups*

### Beyond Sensitivity: New Solutions for Pharmaceutical Analysis

*Sponsored by Waters Corporation*

*Ignatius Kass, Waters Corporation*

*University I Ballroom*

### Dried Blood Spot Summit

*Sponsored by Alliance Pharma and McKinley Scientific*

*Discussion Leader: Wenkui Li, Novartis*

- ▶ History, Properties, Issues and Scope of Applications for Filter Paper as a Matrix for Specimen Collection and Analysis  
*W. Harry Hannon (Retired), Centers for Disease Control and Prevention*
- ▶ New Technologies for the Direct Analysis of Analytes and Enzyme Activities in Dried Blood Spots  
*David Millington, Duke University*
- ▶ The Dried "X" Spot - Beyond Newborn Screening  
*Donald Chace, Pediatrix Analytical*
- ▶ DBS Implementation Strategies  
*Olga Kavetskaia, Abbott Labs*
- ▶ Towards Full Yet Flexible Automation of Dried Blood and Matrix Spot Analysis  
*Shane Needham, Alturas Analytics*

# PROGRAM AGENDA

**Wednesday** October 5

**7:30 AM – 8:30 AM**

**REGISTRATION & CONTINENTAL BREAKFAST**

*University Ballroom Lobby*

**7:30 AM – 8:30 PM**

**SPONSORED BREAKFAST WORKSHOP**

*Princeton I & II*

Isotope Solutions to Address Unmet Analytical Needs  
*Sponsored by Vitalea Science*

**8:30 AM – 10:30 AM**

**SYMPOSIUMS & ROUNDTABLES**

*University II Ballroom*

**Fast-to-Fail Paradigm**

*Discussion Leaders: Lucinda Cohen, Merck; Tim Olah, Bristol-Myers Squibb*

- ▶ **Optimizing the Disposition Characteristics of New Chemical Entities Using HTS ADME Screens**  
*Amit Kalgutkar, Pfizer*
- ▶ **Biochemical and Assay Screening Using High Throughput Mass Spectrometry Detection**  
*Jon Williams, GlaxoSmithKline*

**10:45 AM – 12:15 PM**

**PARALLEL TRACKS**

<p><b>Microfluidics</b> <i>Princeton I &amp; II</i></p>	<p><b>Colloquium: Globalization of Bioanalytical</b> <i>University II Ballroom</i></p>
<p><i>Discussion Leaders: Jack Henion, Advion BioSciences; Gary Valaskovic, New Objective; Nathan Yates, Merck</i></p> <ul style="list-style-type: none"> <li>▶ <b>Don't Forget the "LC" in LC-MS/MS</b> <i>Jarrold Marto, Dana-Farber Cancer Institute</i></li> <li>▶ <b>Moving Quantitative SRM-MS Toward a Faster Time-Frame: Evaluating Dual Columns and Microfluidic Chips for Peptide Quantification in Plasma</b> <i>Susan Abbatiello, Broad Institute</i></li> <li>▶ <b>Single Molecule Detection and Analysis with Nanostructures</b> <i>Benjamin Cirpriany, Cornell University</i></li> </ul>	<p><i>Discussion Leaders: Mark Arnold, Bristol-Myers Squibb; Jerry Gromelski, QPS</i></p> <ul style="list-style-type: none"> <li>▶ <b>Pharma Perspective on Globalizing Bioanalysis</b> <i>Ajai Chaudhary, Merck</i></li> <li>▶ <b>Globalizing Bioanalysis from a CRO Perspective: A Strategic Overview - Advantages and Challenges</b> <i>Jaap Wieling, QPS</i></li> <li>▶ <b>Global Bioanalysis Consortium: An update of Harmonization Activities</b> <i>Mark Arnold, Bristol-Myers Squibb</i></li> <li>▶ <b>Immunogenicity Global Guidance Harmonization</b> <i>Speaker TBA</i></li> </ul>

**12:00 PM - 2:15 PM**

**CPSA EXHIBITION OPENS**

*University I Ballroom  
University Ballroom Lobby  
2nd Floor Lobby*

*Where Technology and Solutions Meet!*

# PROGRAM AGENDA

Wednesday October 5

**12:15 PM – 2:15 PM**

**LUNCH & LEARN SESSIONS / POSTER SESSION**

*Princeton I*

**Business Management and Science in the 21st Century**

*Sponsored by McKinley Scientific*

*Ajai Chaudhary, Merck  
Paul Corcoran, McKinley Scientific  
Robyn Rourick, Genentech  
Shane Needham, Alturas Analytical*

*Princeton II*

**Lunch & Learn Session**

*Sponsored by Bruker Daltonics*

- ▶ **Transitioning Qual/Quan Platforms from Small Molecules to Biologics**  
*Matt Willetts, Bruker Daltonics*
- ▶ **New Horizons for MALDI-TOF MS: The MALDI Biotyper for Microbial Identification in Pharmaceutical Microbiology**  
*Gary Kruppa, Bruker Daltonics*

*Villanova*

**High-Performance Nanospray: Techniques & Technologies**

*Sponsored by New Objective*

- ▶ **Efficient Fractionation Strategies for LC-MS/MS in Proteomics**  
*Jarrod Marto, Dana-Farber Cancer Institute*
- ▶ **Challenges of Dual-Column Nanospray in Quantitative SRM-MS: Double the Speed or Double the Trouble?**  
*Susan Abbatiello, The Broad Institute*
- ▶ **Enabling Nanospray in Triple-Quad Mass Spectrometry**  
*Kenneth Lewis, OpAns*

*Lehigh*

**Biologics Discovery & Characterization**

*Sponsored by Shimadzu*

- ▶ **Can LC/MS/MS Play a Role in Biologics Development Without Solving the Sample Preparation Issue?**  
*Kevin Meyer, Perfinity Biosciences*

**2:15 PM – 3:30 PM**

**SYMPOSIA & ROUNDTABLE**

*Held in conjunction with the North Jersey ACS Mass Spectrometry and Delaware Valley Drug Metabolism Discussion Groups*

*University II Ballroom*

**Does LC/MS/MS Assay Have a Place in Biologics Development?**

*Discussion Leaders: Guodong Chen, Bristol-Myers Squibb;  
Gabriella Szekely-Klepser, Allergan*

- ▶ **The Rapid Integration of LC-MS-based Bioanalytical Methods to Quantify Protein Therapeutics in Drug Discovery**  
*Timothy Olah, Bristol-Myers Squibb*

# PROGRAM AGENDA

Wednesday October 5

► **Challenges and Solutions in the Quantitative Analysis of Large Therapeutic Peptides**

*Fabio Garofolo, Algorithme Pharma*

► **Large Therapeutic Proteins Quantification: The Best of Both Worlds**

*Jaap Wieling, QPS*

**3:45 PM – 5:30 PM**

*Princeton I & II*

**VENDOR SESSION - "5 MINUTES OF FAME"**

*Held in conjunction with the North Jersey ACS Mass Spectrometry and Delaware Valley Drug Metabolism Discussion Groups*

*Session Leaders: Mark Hayward, Lundbeck Research; Ragu Ramanathan, Bristol-Myers Squibb*

**5:30 PM – 6:30 PM**

*University Ballroom Lobby  
2nd Floor Lobby*

**EXHIBITION & SOCIAL HOUR**

*Held in conjunction with the North Jersey ACS Mass Spectrometry and Delaware Valley Drug Metabolism Discussion Groups*

WEDNESDAY, OCTOBER 5



**Your personal asset management team.**

The McKinley Scientific team of specialists has over 30 years of experience in biotech equipment leasing and financing. With demonstrated expertise in lifesciences and the biotechnology industry, McKinley's understanding of capital asset-based investing is unparalleled. We can help you manage your equipment assets throughout their entire lifecycle—from acquisition to disposal—by assisting you in selling your surplus equipment, locate needed equipment around the world, and help manage equipment appraisals.

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# PROGRAM AGENDA

Wednesday October 5

6:30 PM – 7:30 PM

University I & II Ballrooms

## DINNER

Held in conjunction with the North Jersey ACS Mass Spectrometry and Delaware Valley Drug Metabolism Discussion Groups

## ANNOUNCEMENTS

- ▶ Food Quality & Safety Summit  
*István Pelczar, Princeton University*
- ▶ CPSA SHANGHAI 2012  
*Eric Young, GlaxoSmithKline and Naidong Weng, Johnson & Johnson*

7:30 PM – 9:00 PM

University II Ballroom

## KEYNOTE LECTURES & AWARDS

Liquid Chromatography-Mass Spectrometry in Pharmacology Research and its Transition to Clinical Applications  
*Ian Blair, University of Pennsylvania*

Distinguished Analytical Scientist Award  
*Presented by Tom Covey, AB SCIEX and Rick King, PharmaCadence*

A Scientific Adventure - LC/MS: From Academia to Entrepreneurship  
*Jack Henion, Advion BioSciences & Cornell University*

WEDNESDAY, OCTOBER 5



Program Chair  
Jenny Zheng  
Pfizer

[www.cpsa-shanghai.com](http://www.cpsa-shanghai.com)

### From Bench to Decision Making From Basics to Application

3rd Annual Shanghai Symposium on  
**Chemical & Pharmaceutical Structure Analysis**

Make plans now to attend CPSA Shanghai 2012! This annual meeting is evolving into the premier industry-led event dedicated to promoting awareness of issues and needs associated with global research and development.

Short Courses • Symposia • Roundtables  
Expo • Workshops • Student Awards

---

April 25-27, 2012  
Renaissance Shanghai Pudong Hotel

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*Where Technology and Solutions Meet. Where East Meets West*

# PROGRAM AGENDA

Thursday October 6

7:30 AM – 8:30 AM

**REGISTRATION & CONTINENTAL BREAKFAST**

*2nd Floor Lobby*

8:30 AM - 4:00 PM

**SHORT COURSE:**

*Villanova*

**Is Poor Bioavailability in Early Drug Discovery a Problem and If So, How Can We Solve It?**

*Instructor: Ayman El-Kattan, Pfizer*

8:30 AM – 10:00 AM

**SYMPOSIA & ROUNDTABLE DISCUSSION**

*Princeton I & II*

**CRO-Innovator Interface**

*Discussion Leaders: Chad Briscoe, PRA International; Ron Shoup, AIT Bioscience; Eric Woolf, Merck*

- ▶ **Discovery and Development Bioanalysis Outsourcing: Similarities, Contrast, and Challenges**  
*Ajai Chaudhary, Merck*
- ▶ **Method Transfer Between Labs: The Challenges and Pitfall**  
*Yongdong Zhu, QPS*
- ▶ **Bioanalytical Offshore Outsourcing - Strategies and Challenges**  
*Pat Kadiyala, Bristol-Myers Squibb*
- ▶ **Whose SOPs? Ours or Yours?**  
*An Open Audience Debate*

10:15 AM – 11:45 AM

**SYMPOSIA & ROUNDTABLE DISCUSSION**

*Princeton I & II*

**New Technologies**

*Discussion Leaders: Kevin Bateman, Merck and Rick King, PharmaCadence*

- ▶ **Towards Nanospray for High Throughput Mass Spectrometry**  
*Gary Valaskovic, New Objective*
- ▶ **Exploiting the Orthogonality of Differential Mobility in LC-MS Analysis**  
*Yves LeBlanc, AB SCIEX*
- ▶ **Cells Instead of Microsomes: Why the HepRG Cell Line is Going to Revolutionize DMPK Screening**  
*Tom Rushmore, Life Technologies*
- ▶ **The Emerging Role of Zebrafish Embryo Models in Toxicology**  
*Jedd Hillegass, Lampire Biological Laboratories*

# PROGRAM AGENDA

Thursday October 6

**12:00 PM – 1:15 PM**

*Princeton I & II*

## SPONSORED LUNCH & ROUNDTABLES

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*Sponsored by Waters Corporation*

Coupled Workflows Enabled by HRMS:  
Integrated Data Sets to Facilitate Program Progression  
*Discussion Leader: Jonathan Josephs, Bristol-Myers Squibb*

- ▶ How Can We Acquire Integrated Datasets? Overview of Qual/Quant: What It Is and What It Is Not. A Specific Example.  
*Kevin Bateman, Merck*
- ▶ Informatics Considerations for Enabling Global Data Management  
*David Hardy, Waters Corporation*

**1:30 PM – 3:00**

*Princeton I & II*

## SYMPOSIA & ROUNDTABLES

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Clinical Diagnostics: From Biology to Analytical Chemistry  
*Discussion Leader: Kenneth Lewis, OpAns*

- ▶ Early Detection of Biomarkers for Pancreatic Cyst Management  
*Anthony Yeung, Fox Chase Cancer Center*
- ▶ Strategy, Specimens, Sensitivity, Selectivity and Success in the Development of Clinical Diagnostic Assays  
*Melissa Johnson, Duke University Medical Center*
- ▶ Life Lessons in a Clinical Diagnostic Lab  
*Bingfang Yue, NMS Labs*

**3:00 PM – 4:00 PM**

## CLOSING EVENT

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*Sponsored by PharmaCadence*

### The Flavorful Chemistry of Chocolate

*John P. Munafo, Ph.D.*  
*Mars Global Chocolate Science and Technology, Hackettstown, NJ USA*

The alluring aroma and complex taste of cocoa is a result of a collection of molecules that we perceive as they interact with our nasal olfactory epithelium and taste receptors in our oral cavity. In addition to its unique flavor, cocoa contains a wealth of phytonutrients known as cocoa flavanols, which are increasingly recognized for their beneficial effect on human health. Due to the complex nature and diversity of these molecules, different arrays of analytical techniques are required for their analysis. This talk will highlight chocolate flavor, the diversity of natural products found in cocoa, and several different analytical techniques used in studying the flavorful chemistry of chocolate.

## LOCAL AREA DISCUSSION GROUPS

**CHROMATOGRAPHY FORUM OF THE DELAWARE VALLEY**  
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[www.cfdv.org](http://www.cfdv.org)

**DELAWARE VALLEY DRUG METABOLISM DISCUSSION GROUP**  
.....

[www.dvdmdg.org](http://www.dvdmdg.org)

**GREATER BOSTON MASS SPEC DISCUSSION GROUP**  
.....

[www.gbmsdg.org](http://www.gbmsdg.org)

**NORTH JERSEY CHROMATOGRAPHY GROUP**  
.....

[www.njcg.org](http://www.njcg.org)

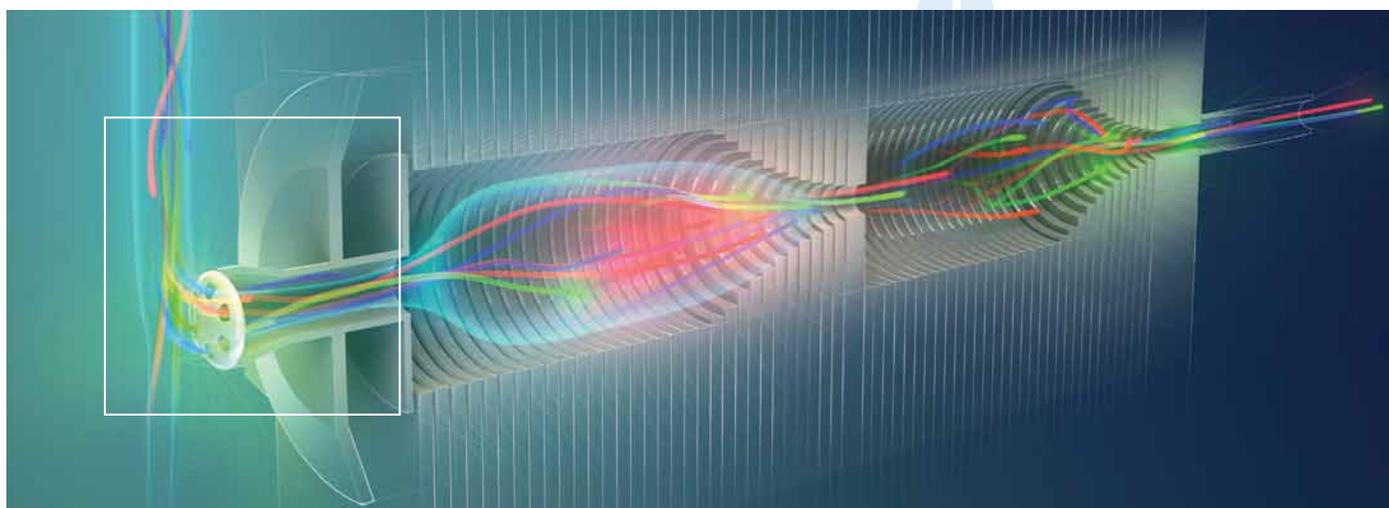
**NORTH JERSEY DRUG METABOLISM DISCUSSION GROUP**  
.....

[www.njacs.org/drugmet.html](http://www.njacs.org/drugmet.html)

**NORTH JERSEY MASS SPECTROMETRY DISCUSSION GROUP**  
.....

[www.njacs.org/msdg/index.html](http://www.njacs.org/msdg/index.html)

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# Flexibility & Performance



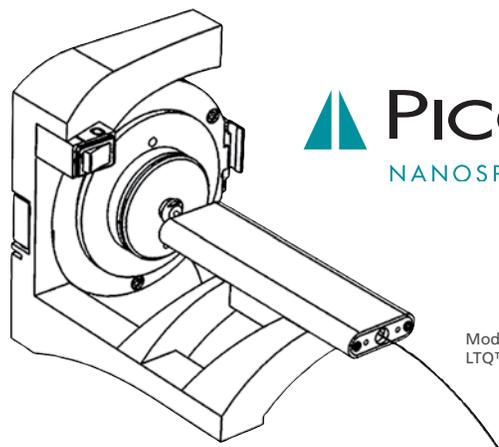
Model DPV-550 for Thermo LTQ™ and Orbitrap™.

## DIGITAL PICOVIEW® NANOSPRAY SOURCES

- Digitally-controlled tip positioning
- High-resolution digital imaging
- Stage position save and recall
- Fully-automated tip rinsing station
- Perform on- and offline analyses
- <10 nL to >10 µL/min. delivery range

### FLEXIBILITY

Digital PicoView® pushes nanospray LC-MS to a whole new level. Based on the industry-acclaimed PicoView Source, the tool-free magnetic stage, tip angle flexibility, and unique tip and spray imaging are still there, but now offer even greater control, flexibility and productivity.



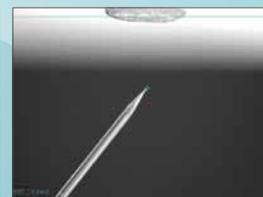
## PicoCHIP™ NANOSPRAY SYSTEM

Model PCH-550 for Thermo LTQ™ and Orbitrap™.

### PV Acquire™ Control Software



High-resolution interactive digital imaging and stage positioning controlled from your PC



Quantitative on-screen measurement cursors provide for precise tip positioning and spray optimization

### Automated Tip Rinsing



650 Injections - No rinsing



650 Injections - Rinsing

A standard-spiked plasma sample was analyzed in two separate experiments, each consisting of 650 injections. Photo A is a fritted fused-silica emitter (15µm tip) after 650 injections without tip rinsing. Photo B is also a fritted emitter after 650 injections but with tip rinsing. The rinsed emitter showed no degradation in spray stability, while the non-rinsed emitter had become virtually unusable.

### PERFORMANCE

The new PicoChip™ Nanospray System delivers what you've been asking for—simple operation, emitter/column/voltage integration—without compromising performance or sensitivity.

The industry-proven performance of the PicoFrit® column has been fused into an easy-to-use package that has the critical high-voltage connection already made inside. One quick connection to your pump or valve and you are ready to collect data.