

CAID: Center for Analytical Instrumentation Development, Bindley Bioscience Center, Discovery Park, Purdue University

Workshop 2014 Report

AIM

The aims of the CAID workshop were 1) to facilitate a hands-on educational experience for undergraduate students locally and regionally 2) to demonstrate novel forensic science techniques of on-site detection of illicit drugs and explosives and 3) to expose students to novel instrumentation and the process of instrumentation development.

WHO

CAID 2014 was open to a wide audience ranging from local Purdue University undergraduates to undergraduates from nearly 40 schools in Indiana and Illinois. Graduates students from Purdue University, University of Notre Dame, Indiana University Purdue University Indianapolis and Indiana University Bloomington attended. As in past years, CAID reached beyond the college campuses with attendees from the pharmaceutical and instrumentation industries.

WHAT

CAID 2014 was a 2-day short course which combined hands-on laboratory experiments, round table discussions, and invited lectures from experts. Lecture topics focused on the CAID 2014 theme: forensic science analysis and novel instrumentation for biomedical sciences.

Speakers with titles of their talks were:

- Nick Manicke (IUPUI) – Instruments for Forensics
- Lane Baker (IU) – Unconventional Pipetting for Chem/Bioanalysis
- Marya Lieberman (ND) – Lab on Paper
- Zheng Ouyang (PU) – Miniature Mass Spectrometers

Seven experiments were performed during CAID 2014:

1. Bacterial Analysis by Touch Spray Mass spectrometry

Classify unknown bacteria by touch spray ionization using statistical multivariate methods of data analysis

2. Organic Synthesis and Reaction Monitoring by Mass Spectrometry

Synthesize 1,4-dihydropyridines by the accelerated Hantzsch reaction in electrosprayed droplets and explore the reaction mechanism

3. Nanoparticle Synthesis and Surface Enhanced Raman Spectroscopy

Ionize noble metals and use ion deposition for nanomaterials fabrication

4. Paper Spray Fundamentals

Explore the experimental effects on Taylor cone formation as observed in real time with microscopy

5. Fundamentals and Applications of Miniature Mass Spectrometry

Demonstrate a variety of applications of the Mini 12 and the Mini 10.5 mass spectrometers

6. Detection of Drugs of Abuse by Paper Spray Mass Spectrometry

Quantify drugs of abuse in blood using paper spray ionization coupled with MS/MS. Convey strategies to reach analytical figures of merit using paper spray. Demonstrate the benefits of the technique in forensic science

7. Analysis of Bomb Fragments by Desorption Electrospray Ionization Mass Spectrometry

See bomb fragments and learn to analyze using desorption electrospray ionization mass spectrometry.

Workshop Attendance

Colleges and universities participating in CAID 2014:

Aurora University, Aurora, IL
Benedictine University, Lisle, IL
Bethel College, Mishawaka, IN
Earlham College, Richmond, IN
Hanover College, Hanover, IN
Illinois Institute of Technology, Chicago, IL
Illinois State University, Normal, IL
Indiana State University, Terre Haute, IN
Indiana University, Bloomington, IN
Indiana University, Kokomo, IN
Indiana Wesleyan, Indianapolis, IN
IUPUI, Fort Wayne, IN
IUPUI, Indianapolis, IN
Kent State University, Kent, OH
Lewis University, Romeoville, IL
Loyola University, Chicago, IL

North Park University, Chicago, IL
Notre Dame University, South Bend, IN
Ohio University, Athens, OH
Olivet Nazarene University, Bourbonnais, IL
Purdue University, West Lafayette, IN
Roosevelt University, Chicago, IL
Rose-Hulman, Terre Haute, IN
Saint Joseph College, Rensselaer, IN
Saint Xavier, Chicago, IL
University of Evansville, Evansville, IN
University of Illinois-Champaign Urbana
University of Indianapolis, Indianapolis, IN
University of Southern Indiana, Evansville, IN
Valparaiso University, Valparaiso, IN
Western Michigan University, Kalamazoo, MI

Industrial attendees:

AbbVie
BASI
ThermoFisher
Evonik
FLIR

Other institutions:

Chicago Art Institute, Chicago, IL

Attendance summary:

115 Total participants:
65 undergrads attended from invited schools
50 undergrad/graduate students from Purdue attended
15 Industrial Participants

General Comments:

CAID 2014 workshop was a highly interactive conference exposing students and industrial partners to novel instrumentation through state-of-the-art experiments. There were two round table discussions and many other forums over the two days for open discussion pertaining to the experiments that were carried out as well as the future of instrumentation in the fields of forensic science and biomedical science. Participants were able to see the importance of developing novel technology to solve both new and old problems.

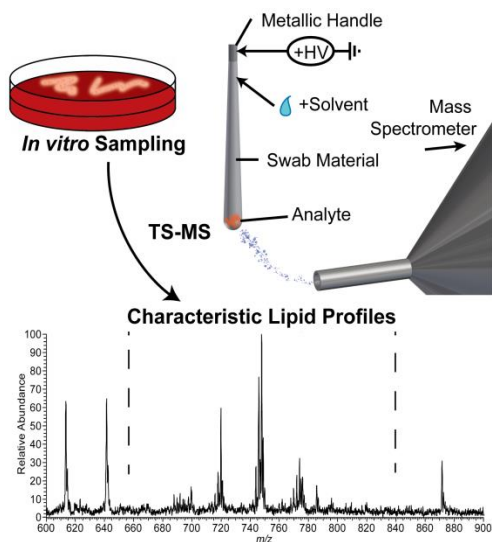
Support:

This effort was supported by the National Science Foundation and the Center for Analytical Instrumentation Development.

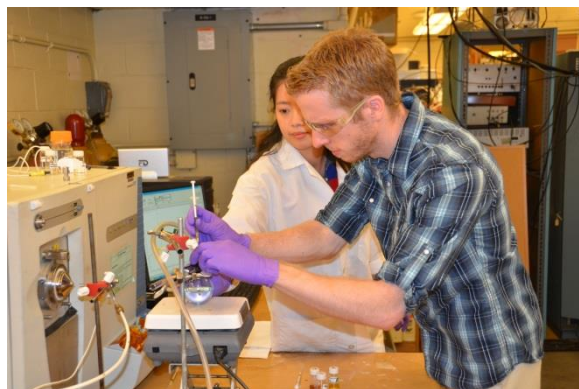
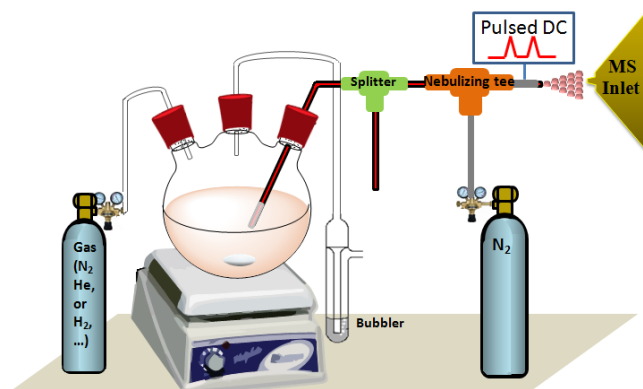


Photo/Figures

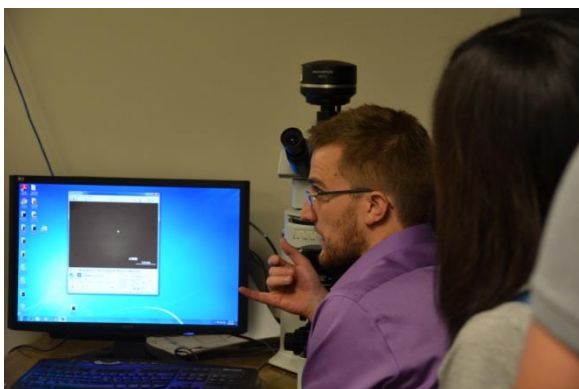
Experiment 1: Bacterial Analysis by Touch Spray Mass spectrometry



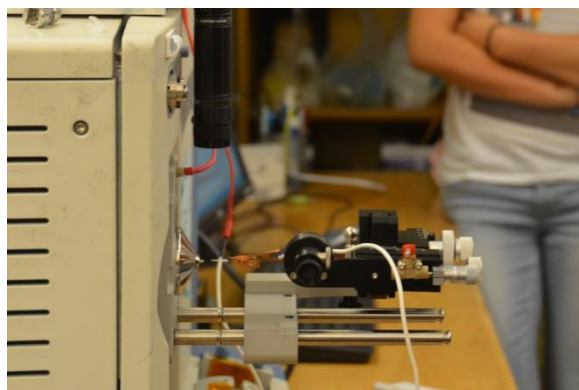
Experiment 2: Reaction Monitoring by Mass Spectrometry



Experiment 3: Nanoparticle Synthesis and Surface Enhanced Raman Spectroscopy



Experiment 4: Paper Spray Fundamentals



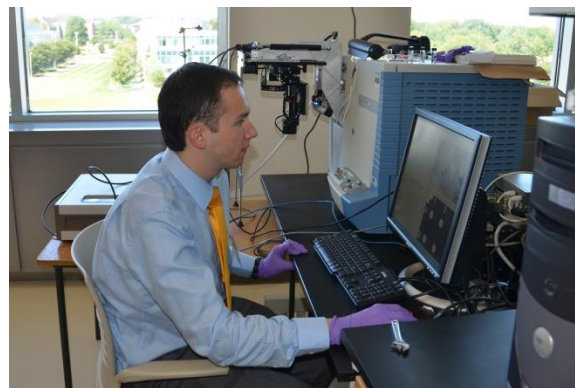
Experiment 5: Fundamentals and Applications of Miniature Mass Spectrometry



Experiment 6: Detection of Drugs of Abuse by Paper Spray Mass Spectrometry



Experiment 7: Analysis of Bomb Fragments by Desorption Electrospray Ionization Mass Spectrometry



Presentations and Discussions



Education:

A major CAID mission is education. The experiments and talks presented at CAID educated students and professionals about the development of novel instrumentation for a variety of applications. Our primary emphasis this year was **forensic science on-site measurement**. This capability was demonstrated specifically in Experiments 5,6 and 7 but carried through all the experiments. Experiments 5, 6 and 7 showed explosives analysis using ambient desorption electrospray ionization mass spectrometry, fundamentals of miniature mass spectrometry, and detection of drugs of abuse by paper spray mass spectrometry. These experiments showed the diverse approaches to analyzing potential evidence both *in situ* with the miniature mass spectrometer combined with the rapid methods of paper spray and desorption ionization analysis. All experiments were designed to engage undergraduates and graduate students. The lectures by Dr. Nick Manicke and Dr. Zheng Ouyang particularly addressed these goals.

Novel technology for biomedical applications was another major area of workshop emphasis. Attendees were able to see how bacteria can be directly sampled from a culturing plate and rapidly identified using touch spray ionization follow by multivariate statistical analysis. This methodology has the possibility to rapid improve the diagnostic capability in the medical fields for routine tests such as the rapid strep examinations. Paper spray technology demonstrated by Nick Manicke and Karen Cesafsky can be used to monitor drugs in whole blood so providing a way to determine drug concentrations in real time. The lectures of Dr. Marya Lieberman and Dr. Lane Bakers on Lab on Paper and Unconventional pipetting, respectively, aligned with this aim.

Nanoparticle synthesis, reaction monitoring, and mass spectrometric synthesis widened the scope of the workshop by demonstrating entirely new methodologies for organic chemistry and materials synthesis. Participants in these experiments were able to see traditional goals of synthesis achieved in a new manner. Dr. Anyin Li and Ryan Bain demonstrated the use of microdroplets in inorganic and organic synthesis on timescales order of magnitude faster than in bulk synthesis. Xin Yan's experiment uniquely demonstrated that with a mass spectrometer short-lived reaction intermediates can be observed and characterized very easily. Students were able to see that the unconventional techniques of today are possible gold standard methods of tomorrow.

Impact The impact of the CAID experiments go beyond the two day workshop. After the 2013 CAID one of the experiments was incorporated into the Purdue undergraduate honors organic teaching lab. The purpose of the experiment was to observe enhanced reaction rates in charged microdroplets for the Claisen-Schmidt base-catalyzed reaction (C-C bond formation) and to study substituent effects. [Bain, R. M.; Pulliam, C. J.; Yan, X.; Moore, K. F.; Müller, T.; Cooks, R. G. *Journal of Chemical Education* **2014**.] Two experiments from CAID 2014 are being integrated into Purdue's undergraduate lab courses: the bacterial analysis using touch spray and the mass spectrometric synthesis Hantzsch reaction. Exposing undergraduate students to novel technology will better suit them for the technology they will likely see after college.