

Ambient Ionization & Sampling Interest Group Workshop Report 2023

“Ambient Ionization in Application Fields: *What is Required & Desired vs. What can be provided?*”

71st ASMS Conference at Houston, Texas
June 7th 2023, 5:45-7:00 PM
Wednesday Workshop 14

Coordinators and Presidents:

Anyin Li (University of New Hampshire)
Chris Gill (Vancouver Island University)
Jacob Jordan (University of California Berkeley)
Roshan Javanshad (University of Illinois Chicago)

This year’s workshop is composed of 1) a survey; 2) lightening talk; and 3) panel discussions. We observed a broad diversity of research fields involved with ambient sampling and ionization. Lightening talks and panelists were selected that represent the diversity of research topics and people. Together with the panel discussion, this workshop covers recent progress and challenges.

Conference attendees were asked to indicate which fields they are working in with Ambient Ionization. Overall, 52 entries (50% response rate) were collected, and Figure 1 displays the spread of fields in a pie chart. The majority of the responded participants were working on Fundamental Research (27%), followed by Forensic and Security (19%). Clinical and Diagnostics was tied with Environmental at 15.4%. Imaging, Manufacturing and Quality Control, and other fields represented 9.6%, 5.8% and 7.7%, respectively. A more detailed analysis of the survey will be shared online in the LinkedIn Group for Ambient Sampling and Ionization..

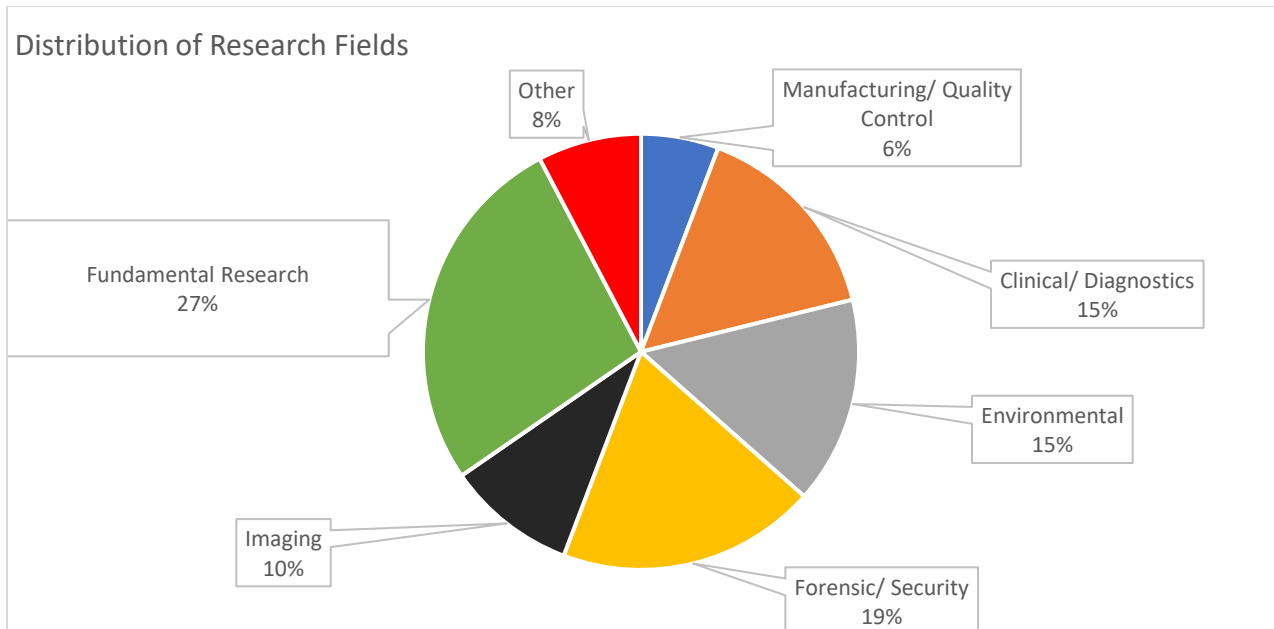


Figure 1. Pie Chart of the different fields of the participants in the survey.

3-minute lightning talks selected from poster presentations

Nicolas Morato (Purdue University)	accelerating drug discovery using an automated high-throughput desorption electrospray ionization mass spectrometry platform
Jiaxin Feng (Texas A&M University)	Accurate quantitative mass spectrometry imaging via Aziridine-based isobaric tags reveals temporal and spatial changes of isomeric lipids in medulloblastoma mice
Zoe Millbern (NC State University)	Temperature profiling and quantitative analysis of disperse dyes in polyester via DART mass spectrometry
Hannah Lawther (Smithsonian Museum Institute)	Automating minimally-invasive liquid microjunction sampling to profile large, intact objects
Lucas R. Abruzzi (University of Victoria)	High throughput quantitative algal toxin analysis by paper spray ionization tandem mass spectrometry (PS-MS/MS)
Sarah Dowling (Indiana University)	Blow flies as remote sampling devices: Detection of insensitive munitions and their degradation products in the environment using LC-MS/MS
Enoch Amoah (The Ohio State University)	Sensitive analysis and differentiation of oligosaccharides isomers by direct infusion mass spectrometry
Menin Laure (EPFL)	Interfacing LC-ESI/APCI and GC-DBDI to the same instrument: the ideal HR-MS Swiss Knife for a Mass Spectrometry Core Facility

Panelists:

Laure Menin	EPFL
Nickolas Manicke	IUPUI
Brian Musselman	Bruker
Abraham Badu-Tawiah	The Ohio State University
Andre Venter	Western Michigan University
Emma Sisley	University of Birmingham
Daojing Wang	Newomics, Inc.

Following the list of interest group's top concerns as voted in the previous ASMS conference, the workshop aimed to highlight the applications of ambient ionization while continuing our discussion of figure of merit (FoM) topics. The versatility of ambient ionization methods makes mass spectrometry approaches more accessible in a wide range of areas including forensics, security, environmental analysis, manufacturing, imaging, and clinical/point-of-care diagnostics. Each application has a set of different desired and required FoMs for analytical methods. Besides exhibiting the state of the art in ambient ionization and sampling via lightning talks selected from poster presentations, the workshop surveyed these FoMs in relevant applications by providing A) A prepared poster for attendees to vote for the desired FoMs (sensitivity, accuracy, molecular, etc.) in their application/areas and choose what they need vs. what they have and B) Expert panelists to lead a Q&A-style discussion that covers challenging aspects, recent breakthroughs, and potential research directions in our research community. The workshop aims to encourage audience participation and presentations from new investigators, postdocs, and graduate students with a balanced perspective from inside and outside academia.

Major panel Q&A discussion points:

The first point of discussion for the panel was “*So which one (method) is better?*”? Each panelist discussed their answer and their favorite method, concluding that there are multiple dimensions to this question and ultimately, there is no “best method”, it all depends on what you want to analyze. A panelist further added that while ambient ionization reduces the barrier to use/try mass spectrometry for research, drawing conclusion from data still require and understanding of capability and limitation.

The discussion led to the next question “*What is (really) ambient ionization?*” as the definition has seemed to change from the first time it was introduced to the scientific community. The panelists each described what they think of as “ambient”, admitting that the definition has indeed changed and evolved since the early 2000s, and the line between direct and ambient techniques has become blurry. In the end, it seems like as a community, we have accepted that as long as there is no chromatography and the sample is analyzed **directly ‘under ambient conditions’**, we are in the realm of ambient.

The panel discussed the question “*At what resolution is a method considered imaging?*” The highest resolution is not always necessary, and you need to find a method that is fit for purpose. The panel encouraged the community to think of the question “Do you need spatial *resolution* or spatial *information*?” The panel also discussed different ways they can control resolution in their respective techniques.

The panel next received some questions/concerns from the attendees. A concern brought forward by a physicist was ***how to get good coverage and where the community sees molecular coverage expanding to*** in the near future. The suggestions that the panel had for choosing the right method were to know the limitations of the technology, do the research before trying a technique and seek the instrument you can trust to avoid disappointment.

Another concern discussed was ***reaching the gold standard in clinical application in ambient methods.*** The panel agreed that in most cases sensitivity is no longer the issue, as several methods such as LESA or paper spray have shown to be reliable in quantification, sensitivity and diagnostic accuracy. Some problems remain to be better addressed, such as automation, specificity, coupling ambient ionization sources to MS, ion transfer efficiency, and robustness.

The workshop concluded with the takeaway message “let’s solve problems together.”

Other notes:

Noted third year as an official ASMS interest group.

Headcount of workshop attendees at 92, shows a steady increase compared to previous years.