

“Molecular Coverage in Ambient Ionization” – Ambient Sampling and Ionization Interest Group

Presiders:

Asher Newsome (Smithsonian Institution)

Anyin Li (University of New Hampshire)

3-minute lightning talks selected from posters:

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| Dong Zhang, | Texas Tech |
| Ayesha Seth, | Ohio State |
| Jephthe Akakpo, | Univ. Kansas Medical Center |
| Ashton Taylor, | U. South Florida |
| Jess Deng, | Queens University |
| Emma Sisley, | U. Birmingham |
| Karen Reyes, | U. North Texas |
| Kelcey Hines, | Louisiana State |

To maximize available time, audience questions were deferred to post-workshop discussion with lightning talk speakers.

Panel on Molecular Coverage:

Bindesh Shrestha, Waters

Brian Musselman, IonSense

Theresa Evans-Nguyen, U. South Florida

Chris Gill, Vancouver Island U.

Julia Balog, Waters

A wide variety of ion sources using different physical and chemical processes fall under the umbrella term of “ambient sampling and ionization” – but not every source can analyze every compound. Following the list of top concerns as voted in 2019, we will convene a panel to discuss molecular coverage in a world of unknown samples, limited budgets, and finite time to optimize methods for a given analyte. Discussion is expected to range from advantages and pitfalls of certain techniques to the mythical (but no less desirable) ion source that Does It All. The panel Q&A will be preceded by several 3-minute lightning talks selected from 2022 posters to share hot topics in ambient sampling and ionization. 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:

What technique can produce analyte ions other than protonated molecules?

Atmospheric pressure photoionization can do so, and APPI lamps can still be bought from Thermo. Hydride abstraction has been noted with SICRIT from Plasmion and DART from IonSense.

Can ambient ionization produce electron impact-type spectra?

Liquid EI and LIFTI have been performed.

Could surface acoustic wave nebulization (SAWN) methods be used for native proteins?

Perhaps, as it can be used to ionize cholesterol.

The mechanistic explanation for rapid evaporative ionization mass spectrometry (REIMS) has continued to evolve. REIMS is very good for ionizing fatty acids and phospholipids.

What are the classes of molecules that can be observed with various ionization techniques?

The panel cannot give a comprehensive list, as so many compounds have been ionized one way or another at this point. DESI is comparable to ESI; PSI applications are still growing; SAW APCI has been used for polar analytes and polyaromatic hydrocarbons (PAHs); DART has been used with derivatization

What is the best way to ionize non-polar compounds?

Dopants like CCl_4 and many others, combined techniques, and other methods have been used. Sometimes “old-fashioned” GCMS with electron ionization is the easiest way.

What about background ions?

Sometimes they are actually helpful. Pulsed DART methods had reduce background.

Off-topic points of discussion:

What ambient methods can be used without modifying the analytical system?

Paperspray (PSI) is probably the most entry-friendly.

Glyco-proteins have been studied with PSI and DESI.

Have ambient ionization methods been used with ion mobility?

PSI has, and flowing atmospheric pressure afterglow (FAPA) has been used with FAIMS.

Other business:

Noted second year as official ASMS interest group.

Applause and a good laugh for avoiding chromatography.

Call for co-organizer to join Anyin at ASMS 2023 and organize with new person in 2024.

Headcount of workshop attendees at 86, vs. 5000 attendees to full meeting; shows steady ratio compared to previous meetings (50 attendees vs. 2500-person conference in 2021, 125 attendees in 2019)