“Bridging the External and Internal Exposome through Advanced Mass Spectrometry”

ASMS Workshop Organized by the Exposomics Interest Group
Co-presiders: Ruth Marfil-Vega, Nina Zhao, and Adrià Sunyer Caldú
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Summary: Approximately 50 participants attended the 2026 ASMS Exposomics Interest Group workshop. The goal for this workshop is to explore how advanced mass spectrometry can connect external exposures with internal exposures and eventually with health outcomes. We designed the workshop around a case study for simulated wildfire at the wildland-urban interface, moving from urgent sampling choices to interpretation of untargeted data and public-health decisions. Panelists Adrià Sunyer Caldú, Kirsten Overdahl, and Kristin Favela led the discussions on three “Acts”.

Act 1, “The 48-hour decision window,” is led by Panelist Adrià Sunyer Caldú who brought expertise in exposomics study design. Act 1 focused on designing an exposure assessment under time and resource constraints. Adrià outlined complementary environmental and biological sampling, including air, water, dust and ash, personal samplers, and repeated collection of blood and urine alongside hair sampling. The presentation emphasized the different chemical and temporal information captured by each matrix, the value of an unexposed comparison population, and the trade-off between sampling more matrices and enrolling more participants.

Act 2, “The data complicates the story,” is led by Panelist Kirsten Overdahl who brought expertise in untargeted chemical identification. Act 2 examined recurring unknown mass-spectral features and discrepancies between environmental and biospecimen profiles. Topics included quality assurance and quality control, molecular networking, searches of public mass-spectrometry data, and possible environmental or biological transformations. These approaches offered ways to prioritize unknowns and guide additional sampling or analytical adjustments when library matches were limited.

Act 3, “The phone rings,” turned to public-health recommendations while chemical identities and health implications remained uncertain. The Act is led by Panelist Kristin Favela who brought expertise in consumer product chemistry and worked at the intersection of research and government. Topics included attributing signals to the fire, determining what evidence could support action, and communicating uncertainty to residents. Sample handling, documentation, archiving, established regulatory methods, and independent laboratory confirmation were considered alongside untargeted analysis.

Discussion followed each act, with the strongest audience engagement in Acts 1 and 3. Act 2 generated two to three questions, and participants also contributed through the online Q&A board. The format provided opportunities to examine the practical challenges of linking the external and internal exposome and using incomplete mass-spectrometry evidence to inform decisions.

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