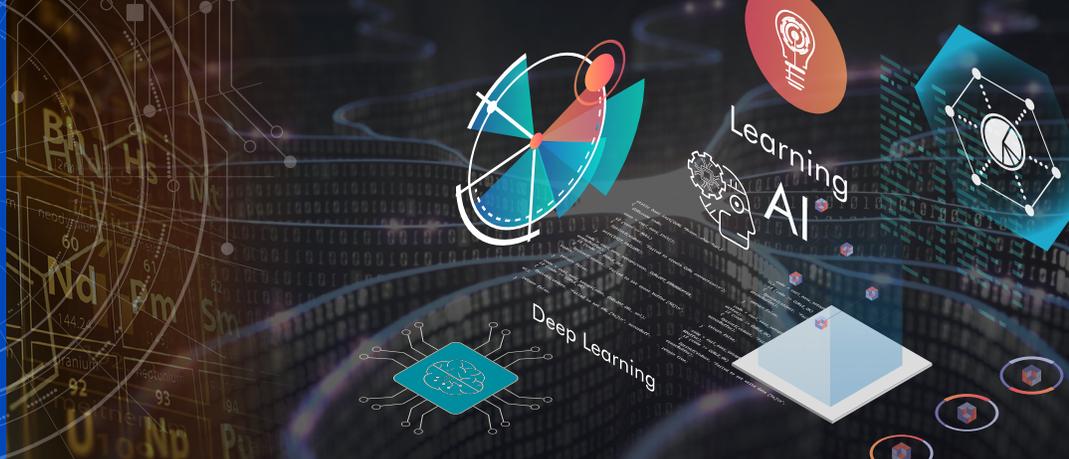




SOUTHWEST RESEARCH INSTITUTE



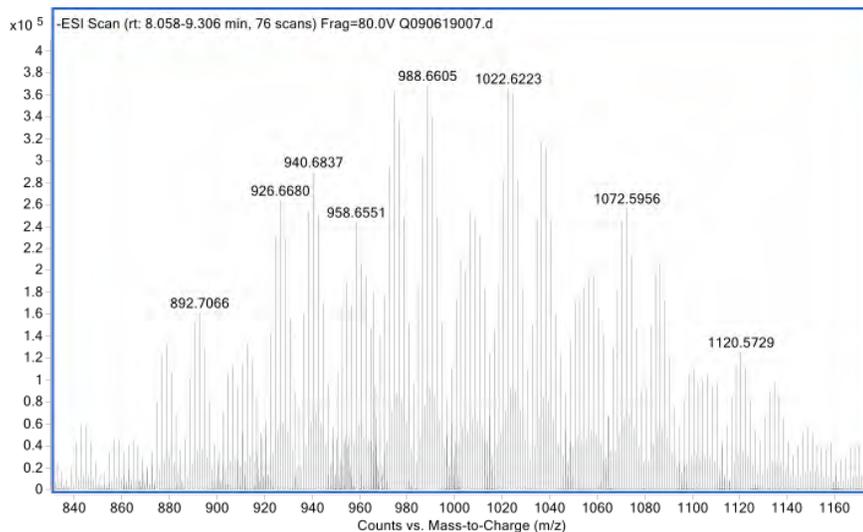
Non-Targeted Analysis Using Mass Spectrometry

Integration of Machine Learning with Mass Spectrometry to Maximize Throughput and Quality

Non-targeted analysis (NTA) is the assay of all chemicals detected by an instrument without a pre-defined list of targeted chemicals. The use of complex instrumentation such as two-dimensional gas chromatography (GCxGC) and liquid chromatography (LC) paired with high-resolution mass spectrometry (MS) often produces thousands of chemical signals for a single sample, some of which are not present in any MS library and require characterization.

NTA data review involves examining every peak, with many being poor-quality signals. Removing these poor-quality artifact peaks can be time-consuming and often causes a major bottleneck. Without automated high-throughput screening methods, tradeoffs must be made as to which samples can be investigated using a non-targeted-based workflow, resulting in unavoidable uncertainty.

Southwest Research Institute® (SwRI®) offers artificial intelligence-based solutions to complex chromatography and MS-based projects. Our expertise in analytical chemistry, machine learning and data science has uniquely positioned us to develop Floodlight™, a novel tool to automate the signal quality review in a high-throughput manner. Floodlight™ works in synergy with existing instrumental acquisition software and the extensive analytical chemistry experience of the chemists performing NTA.

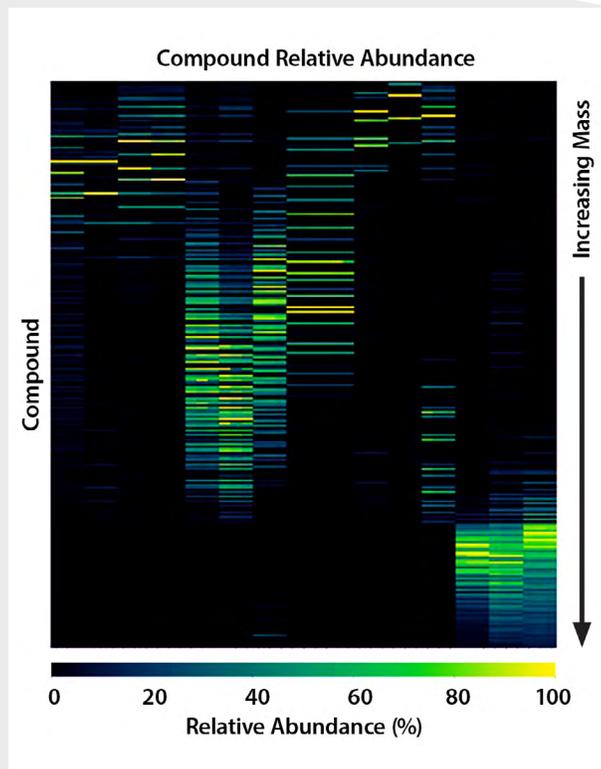
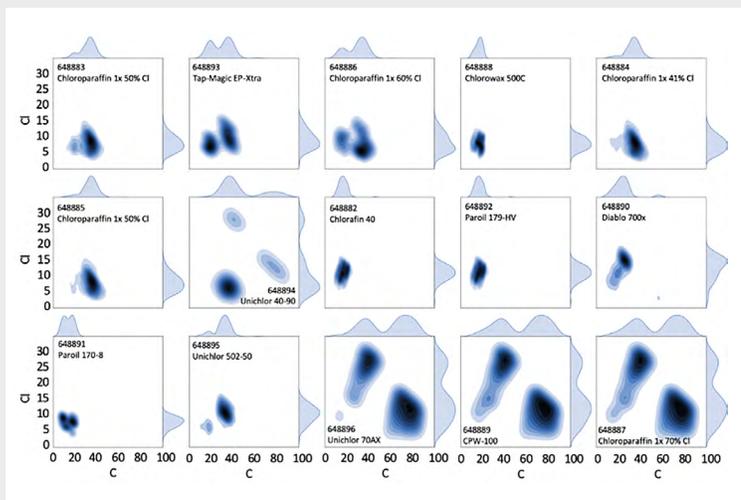


Example of overlapping signals in peaks with similar chemical composition



Floodlight™ is a novel software tool developed by the Artificial Intelligence Mass Spectrometry (AIMS) team at SwRI for rapid discovery of known and unknown chemical compounds by automating the signal quality review process. This cheminformatics machine learning tool can integrate with existing analytical chemistry workflows to support deep analysis of large data sets. The high-throughput software package can drastically reduce the amount of time, effort, and cost for signal quality interpretation, providing the highest, most comprehensive NTA results.

SwRI scientists interpret complex, overlapping signals to produce contour plots and heatmaps, revealing meaningful patterns in the samples.

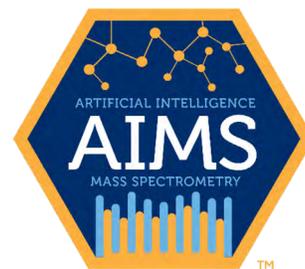


SwRI offers state-of-the-art high-resolution NTA and interpretation. We also apply our artificial intelligence tools to client-provided data sets to maximize chemical information. Our services and solutions can be customized to your unique project needs.

We welcome your inquiries.
For more information, please contact:

Kristin Favela, PhD
Analytical and Environmental Chemistry
210.522.3910
kfavela@swri.org

Michael Hartnett
Intelligent Systems
210.522.5433
mhartnett@swri.org



aims.swri.org

SOUTHWEST RESEARCH INSTITUTE

Southwest Research Institute is a premier independent, nonprofit research and development organization using multidisciplinary services to provide solutions to some of the world's most challenging scientific and engineering problems. Headquartered in San Antonio, Texas, our client-focused, client-funded organization occupies 1,500 acres, providing more than 2.3 million square feet of laboratories, test facilities, workshops, and offices for more than 2,700 employees who perform contract work for government and industry clients.

An Equal Employment Opportunity/Affirmative Action Employer
Race/Color/Religion/Sex/Sexual Orientation/Gender Identity/National Origin/Disabled/Veteran
Committed to Diversity in the Workplace

Like. Share. Follow. Listen.



swri.org

©2022 Southwest Research Institute.
All rights reserved.

Designed & printed by SwRI MPS 15-0422 JCN 267190 tp