



Automated Signal Review and Pattern Analysis for High-Throughput Mass Spectrometry Workflows

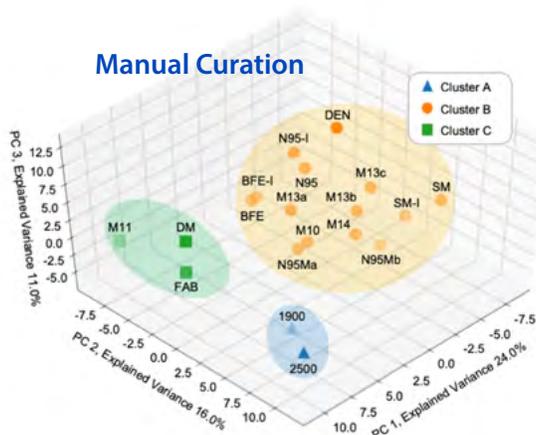
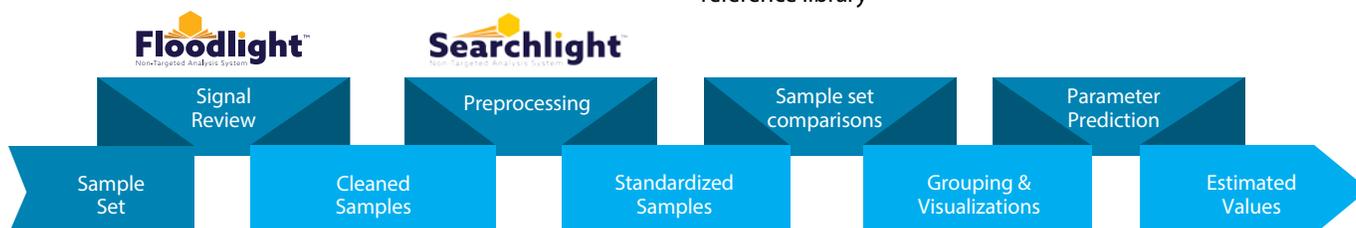
Southwest Research Institute[®] (SwRI[®]) has extensive experience in non-targeted analysis (NTA), offering a wide range of analytical chemistry services including expert evaluations of fuels and lubricants. To facilitate new state-of-the-art high-throughput workflows, SwRI developed Floodlight[™] and Searchlight[™] to rapidly screen signals, compare samples, and identify key chemical features. The machine learning (ML)-based tools can be utilized for end-to-end processing of sample sets. These tools provide user oversight and control of the analysis through a web-based interface.

Challenges of High Throughput

- Large amount of data
- Variability of multiple fields, projects, and experimental conditions
- Meaningful comparisons of multiple samples
- Identifying signals of interest
- Leveraging known samples for future analysis

Floodlight & Searchlight Features

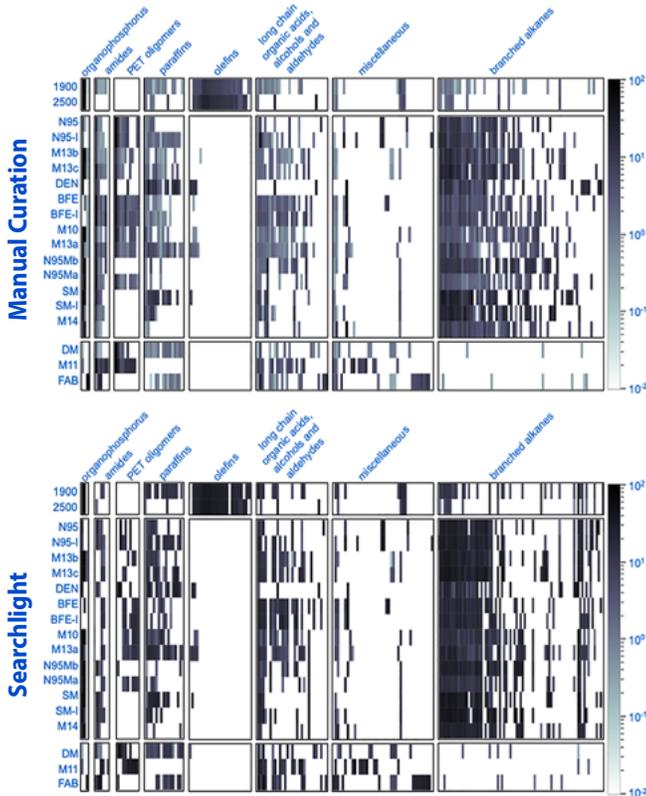
- End-to-end signal screening and processing of sample sets streamlining 75% of NTA workload
- Interactive interface for tailoring analysis to a specific sample set and automated preprocessing techniques to clean and standardize data
- Robust machine learning algorithms to cluster samples and search nearest neighbors using both peak and raw data
- Interactive visualization tools for anomaly detection, chemical fingerprinting, and display of compound groups across the sample set
- Methods for interpolating defined parameters of interest given a reference library



PCA and clustering results done manually and by Searchlight

Searchlight was compared to expert's manual technique for chemical curation during analysis of chemical exposure from facemasks.

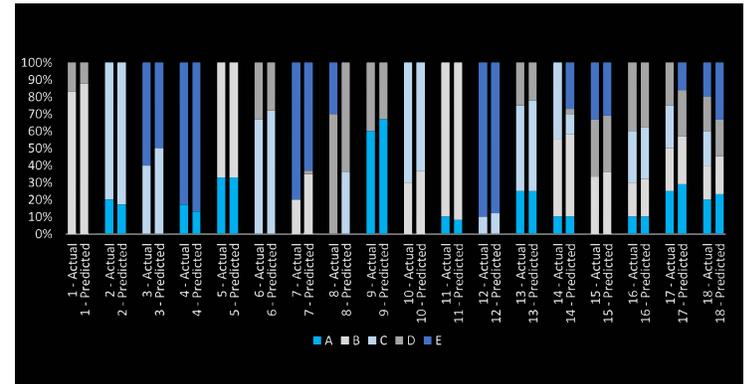
Compound selection from manual curation and Searchlight had 90% agreement with an 89% detection rate. Subsequent analysis resulted in identical clustering between the two methods.



Comparison of chemicals curated manually and with Searchlight

SwRI scientists predicted complex fuel patterns using Floodlight and Searchlight by blending five fuels in binary combinations (training set), then using ML-driven interpolation to predict blinded blends containing up to five components (validation set). Analysis was performed with minimal user effort.

The average blend ratio error was 4.4% for validation and training sets. All blends were correctly predicted except fuels C and E, which were almost identical material.



Fuel blending interpolation results on blind validation set

120x Throughput

Manual Curation: 40 hours
 Floodlight & Searchlight: 20 minutes

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

John Gomez
 Research Scientist
 210.522.5996
jgomez@swri.org

Kristin Favela, PhD
 Staff Scientist
 210.522.4209
kfavela@swri.org



aims.swri.org

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210.522.2122

ask@swri.org



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