

# Near-Real-Time Visualization and Analysis of High-Resolution Mass Spectrometric Data

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## Purpose

- Image analysis characterizes signals of interest, distinguishes them from imaging artifacts
- Identifying features is a key aspect of interpreting image signals by associating particular signals with their function regions
- Seek to establish at PNNL a set of signature capabilities for rapid image analysis and feature recognition by developing a portable, expandable, parallelized software toolkit for interpreting multi-dimensional images.

## Key Successes

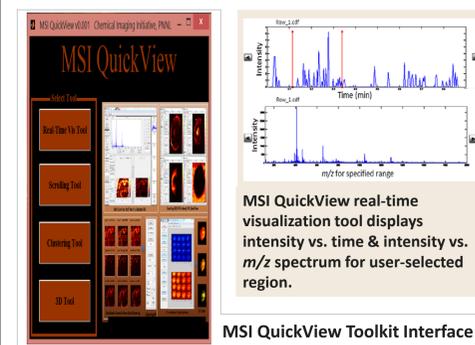
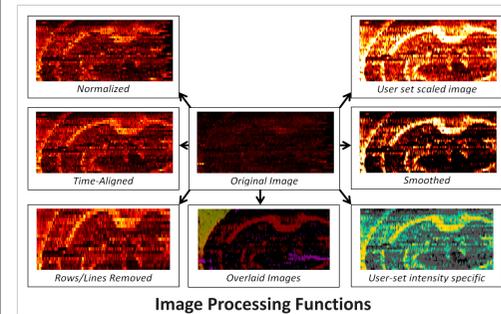
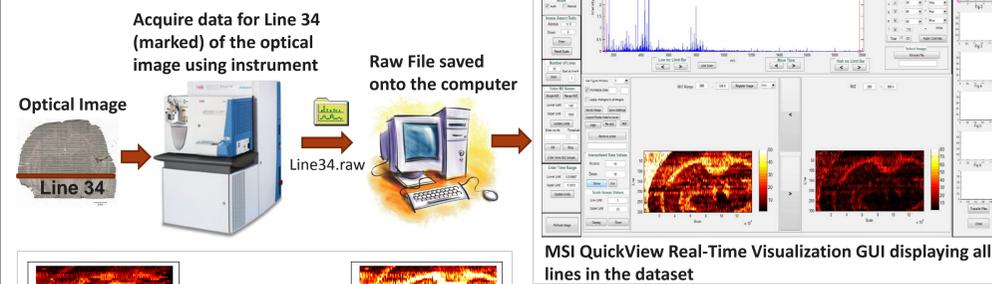
- Developed toolkit providing image analysis and feature recognition capabilities based on identified needs of data collection instruments and applications
- Established, tested toolkit links into the chemical imaging data analysis framework
- Feature recognition feeds back to other steps in the pipeline, enhancing capabilities
- Developed algorithms to generate quick views that can influence decision making during image acquisition

## Research Accomplishments

### Visual Analytics of Mass Spec Images

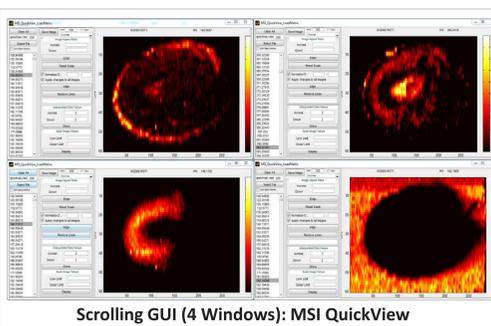
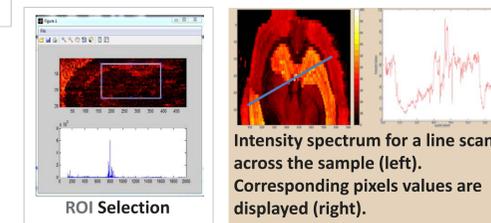
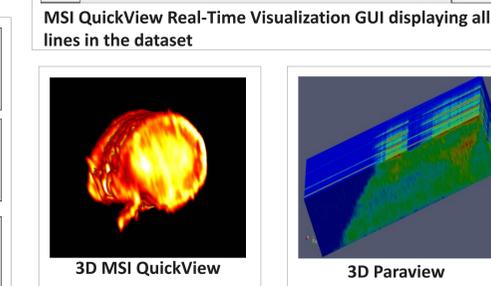
In support of **Laskin Project (CII 2.2)**,

- MSI Quickview: Process, visualize, query, analyze spatial mass spectrometry data
- On-the-fly visualization



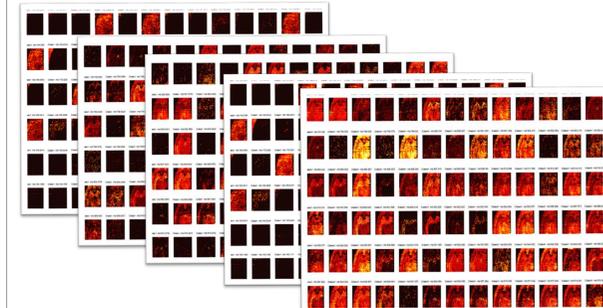
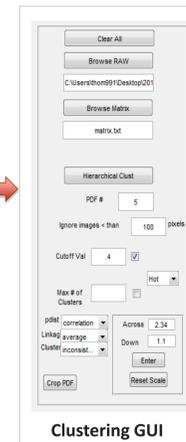
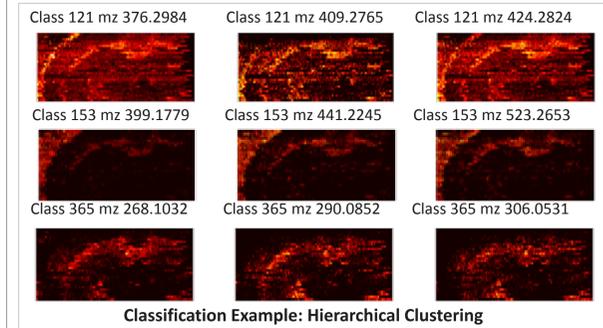
### Scrolling GUI

- Scroll through dataset images
- Generate images into PDF file
- Visualize multiple datasets



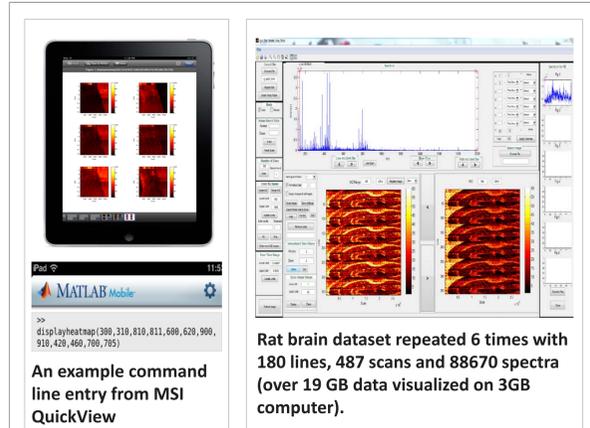
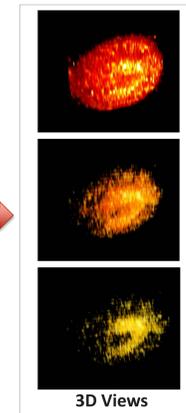
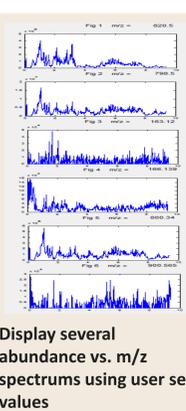
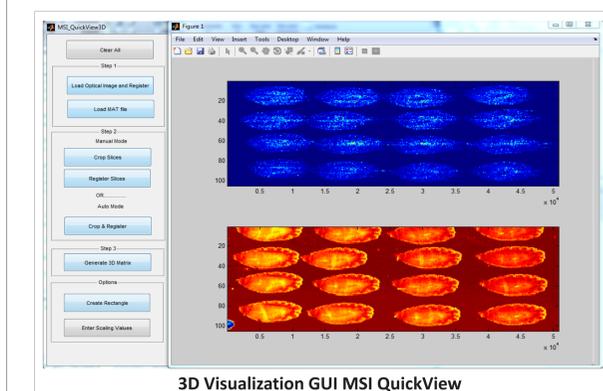
### Ion Image Classification

- Hierarchical clustering of ion images
- Visualize different classes in single PDF

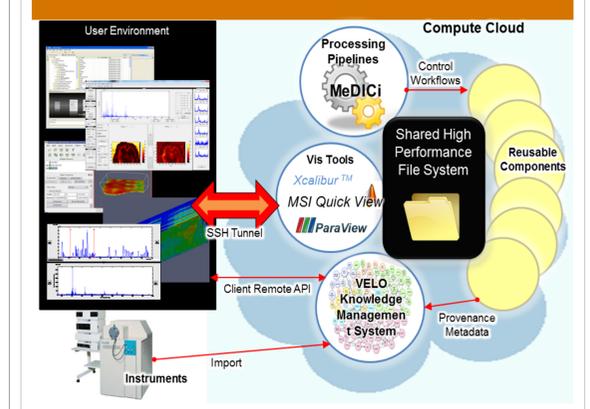


### 3D Visualization

- Create 3D stacks from 2D ion images
- Register ion images with optical image



### Behind the Scene of MSI Quickview



Data automatically transferred onto Velo, where user can organize their dataset for quick access and launch new jobs on HPC that can be accessed remotely

### Next Steps

This work is extensible to additional applications within chemical imaging and beyond. The toolkit can now be licensed and is part of funding applications from clients, including DOE, the National Institutes of Health, and Department of Homeland Security.