Software for Integrated and Interactive Visualization of LC-MS Data and Peptide Identification Results

Zefeng Zhang
Bioinformatics Solutions Inc, Waterloo, ON

Introduction

We present an integrated interface to visualize and navigate through your LC/MS data conveniently. The main goals of the interface combine supporting large LC/MS spectra data volume and provide easy data navigation. The spectra data can be displayed in either a 2D heatmap view or a 3D Intensity view. The free scale zooming in the 2D heatmap view makes it possible for as high as the overall LC run inspection and as low as the detailed local spectrum examination. This is further enhanced by showing intensity as spectrum peaks in the 3D view. Our optimized rendering engine and filtering mechanism make it easier to locate informative regions within massive amounts of spectra data.
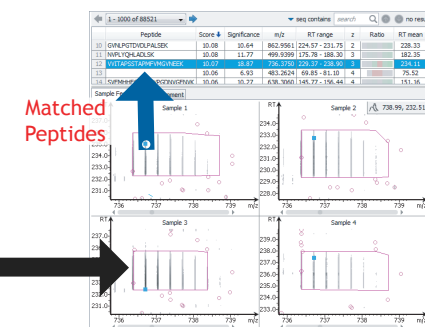
Methods

With the advancement of LC/MS technology, instruments are generating higher and higher volumes of spectra data. Dynamic loading and caching mechanisms are specially optimized in this software design to cope with this problem. The MS scans are grouped into fractions, heatmap thumbnail and TIC (total ion count) figures give an overall view of each fraction. Users can easily navigate into a region of interest and the back/forward functions make it more convenient to jump between historical view positions. For best rendering performances, only the necessary data in the current view range is loaded and processed. Data annotations such as MS/MS scans, quantified features and identified peptides can also be integrated onto the heatmap. Further detailed information can be displayed accordingly.

Experiment

To demonstrate the software interface, we loaded five fractions of Thermo raw spectrum data, with sizes ranging from 11 megabytes to 837 megabytes, with 31435 spectra in total. The data is first parsed within five minutes and stored locally as binary format on an i7 computer with 8G memory. After loading and indexing, the spectra data is ready for navigation. As indicated in the figure, the main panel contains three components: fraction selection panel, TIC figure against the retention time, and spectra view for current selected region in either 2D heatmap or 3D intensity view mode. Panels provide navigation supports for the user to easily examine the LC/MS spectra data in detail. With the optimized rendering engine, the graphical user interface responds to the user operations smoothly, even with large fractions, and operation lag time is significantly reduced. For spectra data annotation, we marked the MS/MS scans, detected features and de novo indentified peptides, processed separately. When the user hovers the cursor over a marked position for any annotation, a tooltips message will explain such annotation and the user can further examine it in detail by selecting it. The 3D view provides the user another intuitive way of understanding the spectra data. This is especially useful when the user wants to examine ion intensity shapes among adjacent scans or isotopes. With the ability to set thresholds for filtering out noise, the spectra peak regions produced from informative ion fragments are highlighted easily.
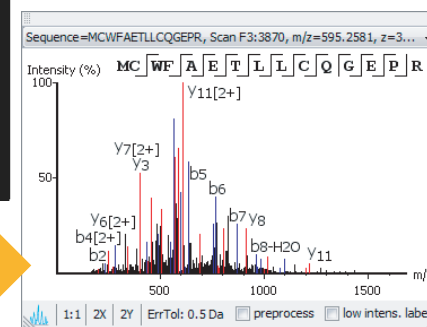
Highlights

- High volume data support
- Smooth user operation
- Convenient data navigation
- Integrated visualization
    - MS/MS scans
    - Feature detection
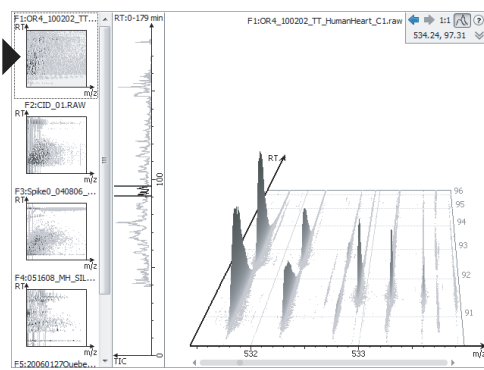   - *de novo* peptides
    - DB search result

Matched Peptides

Examine Features Across Multiple Samples

Our new feature detection engine marks features directly, and optionally matches peptide identification results.
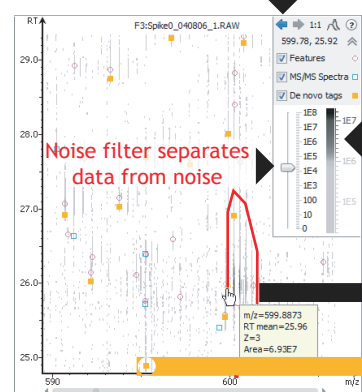

Fraction thumbnails let users easily check multiple fraction data.

LC/MS 3D Intensity View

Switch between 2D/3D views in one simple click

Navigate through historical view positions

Noise filter separates data from noise

Contrast tuner highlights signals

m/z=599.8873
RT mean=25.96
Z=3
Area=6.93E7

LC/MS 2D Heatmap View

Sequence=MCWFAETLLCQGEPR, Scan F3:3870, m/z=595.2581, z=3...

Tandem Scan with Identified Peptide