MarkerView™ Software 1.3
New Features
MarkerView™ Software Overview

- A data visualization tool designed for scientists who wish to visualize their data in terms of sample groupings and apply statistics in order to gain valuable insight into any trends within their mass spectral data.

- MarkerView is unique in that SCIEX users can explore statistical correlations with direct connections back to the raw data. This allows them to find meaningful relationships much more quickly.

- Target Applications:
  - Metabolomics
  - Lipidomics
  - Proteomics
  - Food Authenticity
  - Water Testing
New Features

• Support for *.wiff2 format
  – X500R QTOF System
• Import wizard improves ease of learning
• Changes to t-test view
• Box and whiskers plots
• Infusion MS/MSALL Support
• SWATH® Acquisition support
• Most likely ratio (MLR) normalisation
• Custom sample columns
• ‘Set Names’ script
• Speed and other small improvements
Support for *.wiff2 Format

- Supports *.wiff2 format enabling Metabolomics and Food/Environmental workflows on the X500R QTOF System
Import Wizard

• A wizard enables several steps to be combined:
  - Selecting input files
  - Peak finding and alignment parameters
  - Sample group definition (previously set in Samples Table)
  - Point symbols for groups (previously set in Options)
  - Automatic processing such as PCA or t-test (previously done explicitly)
Updated T-tests

Unequal variance test - when the two groups have different variances and/or group sizes.

- Sorts automatically by p-value.

Profile Plot appears automatically and links to table.

New Box & Whiskers plot appears automatically.
Box and Whiskers Plots

- Standard way of visualizing statistical data across groups
- Spacing between the different parts of the box indicate the degree of spread and skewness in the data
- Highlights outliers
- Automatically generated after t-test
Infusion MS/MS\textsuperscript{ALL} acquisition is an technique in which a sample is infused and MS/MS is acquired for each precursor (at unit resolution) over a wide mass range.

- Typically used for lipidomics.
SWATH® Acquisition Support

- Import raw SWATH acquisition datafiles
- MS/MS spectra can be viewed for selected features (similar to IDA functionality).
- Targeted Spectrum Finder removes fragments with mismatching LC peak profiles
Most Likely Ratio (MLR) Normalisation

- Often need to normalize responses for a sample to allow for the fact that the *absolute* sample amount might not be constant (due to different starting amounts, sample prep differences, etc.)

- Typically used for protein/peptide normalization using large numbers of endogenous peptides (features)

For more information on the normalization strategy:

- Lambert et al. (2013) Nature Methods, 10, 1239-1245
- SCIEX Community discussion
Custom Sample Columns

- Ability to create arbitrary columns to allow metadata entry
- Allows switching between different ways of grouping data for visualisation or supervised algorithms (t-test, PCA-DA).
- Populated manually in MarkerView™ Software or by adding custom fields to Analyst® Software batch.
‘Set Names’ Feature

- Utility which allows variables to be named based on their mass and retention time.
- Assuming you have a list of such masses and retention times for known compounds
  - More useful than a list of m/z-RT ion pairs
- Unknown compounds can be excluded, otherwise they remain with the default names.
Other New Features

• Peak-finding has been made ‘multi-threaded’
  – On a multiple-core computer, processing will be faster (when there are multiple samples)

• ‘Impact’ column in PCA Loadings Table
  – Measure of the importance of each variable to separation
AB Sciex is doing business as SCIEX.

For Research Use Only. Not for use in diagnostic procedures.

© 2016 AB Sciex. The trademarks mentioned herein are the property of AB Sciex Pte. Ltd. or their respective owners. AB SCIEX™ is being used under license.
Answers for Science.
Knowledge for Life.™