



Version 1.2

30-Day Trial Version and Upgrade Version

Release Notes

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Introduction

This document describes version 1.2 of the MarkerView™ Software, a stand-alone application for generating aligned peak lists from Analyst® LC/MS and other data and for performing subsequent data processing using PCA (principal components analysis), PCA-DA (PCA using discriminant analysis) or t-tests.

Please be aware that this is a demonstration version which will expire after 30 days *unless* you have previously installed and activated MarkerView 1.1.

System Requirements

MarkerView™ has been tested with both Windows® 2000 and Windows® XP; Windows NT® is not supported. A minimum of 256 MB of RAM is recommended.

Installation

If you have installed a previous version of the program, you can either remove it or leave it in place as you prefer before installing the latest version. If desired, it can be un-installed using the 'Add/Remove Programs' wizard in the Windows® 'Control Panel'. Click on the old version of MarkerView™ in the list and click the 'Remove' button.

To install the program double-click the appropriate 'Setup.exe' installer on the CD and follow the instructions presented on-screen. It is important to run the version of the installer which corresponds to the version of Analyst® which you have installed. There are separate installers provided for using with:

Analyst QS version 1.1

Analyst QS version 2.0

Analyst 1.4 (or 1.4.1 or 1.4.2) or Analyst 1.5

Other versions of Analyst are not supported. If you have no version of Analyst installed and intend to process 4700 or 4800 data in *.t2d format or text data, you can use either of the installers.

Activation

Once the program is installed, you will be prompted for an activation key the first time you run the program (assuming that you have not already registered a previous version). Follow the directions in the activation dialog; namely copy and paste the generated computer 'ID' into an e-mail message to metabolomics@sciex.com.

Documentation

There are two main help documents installed with this version of the program, both of which are available from links in the 'All Programs' section of the Windows® 'Start' menu and also from the program's 'Help' menu.

The 'User Manual.doc' document is the main user's manual. This manual should provide a good introduction to all of the main features of the program. If you have not previously

used MarkerView™ it is suggested that you start with this document. Note that the example data referred to in the manual is installed to the ‘Sample Data’ subfolder of the ‘AB-Sciex\MarkerView’ folder in the ‘Program Files’ folder.

The ‘Reference Manual.doc’ document describes all of the features of the program in detail. Unlike the user manual, this document does not provide worked examples but merely describes the various menu items, *etc.* in relative isolation.

New Features

A complete listing of features added to the 1.2 version is available in the appendix of the ‘Reference Manual.doc’ document.

A research grade script called ‘MV Metabolite Namer’ is provided on the CD in the ‘Extras’ folder. This utility is useful for metabolite ID work – it assigns specific names to MarkerView peaks based on the mass of a parent drug and expected metabolic transformations.

A second research grade script called ‘PC Variable Grouping’ is also provided on the CD in the ‘Extras’ folder. This utility is used for discovering relationships among MarkerView peaks: peaks which are correlated with one another can be automatically assigned to groups and the resulting groups can be inspected.

Known Problems and Limitations

The following known problems currently exist:

- When browsing for a folder (not a file) whose full name, including all its parent directories, is very long the program will crash. You can either move your files further up the directory structure or download a patch from Microsoft at: <http://www.microsoft.com/downloads/details.aspx?familyid=a8f5654f-088e-40b2-bbdb-a83353618b38&displaylang=en>
- When processing a large number of LC/MS files (or a smaller number of very large files) the program may run out of memory. It is recommended that you generate *.peaks files for your samples in smaller batches and generate the Peaks Table using these peaks files. This process is described in both the User Manual and the Reference Manual.
- When processing QSTAR® data, spectra are corrected for potential saturation depending on the ‘Saturation correction’ option as specified in the Analyst® QS Software. Use the checkbox on the ‘Miscellaneous’ tab of the Analyst® ‘Processing Options’ dialog to specify whether or not to enable such correction. This is not a problem *per se*, however the option is set from within Analyst®, not from within MarkerView™.
- MarkerView™ cannot process LC/MS data from QTRAP® or other triple-quadrupole instruments which was acquired in centroid mode: profile mode data acquisition must be used.