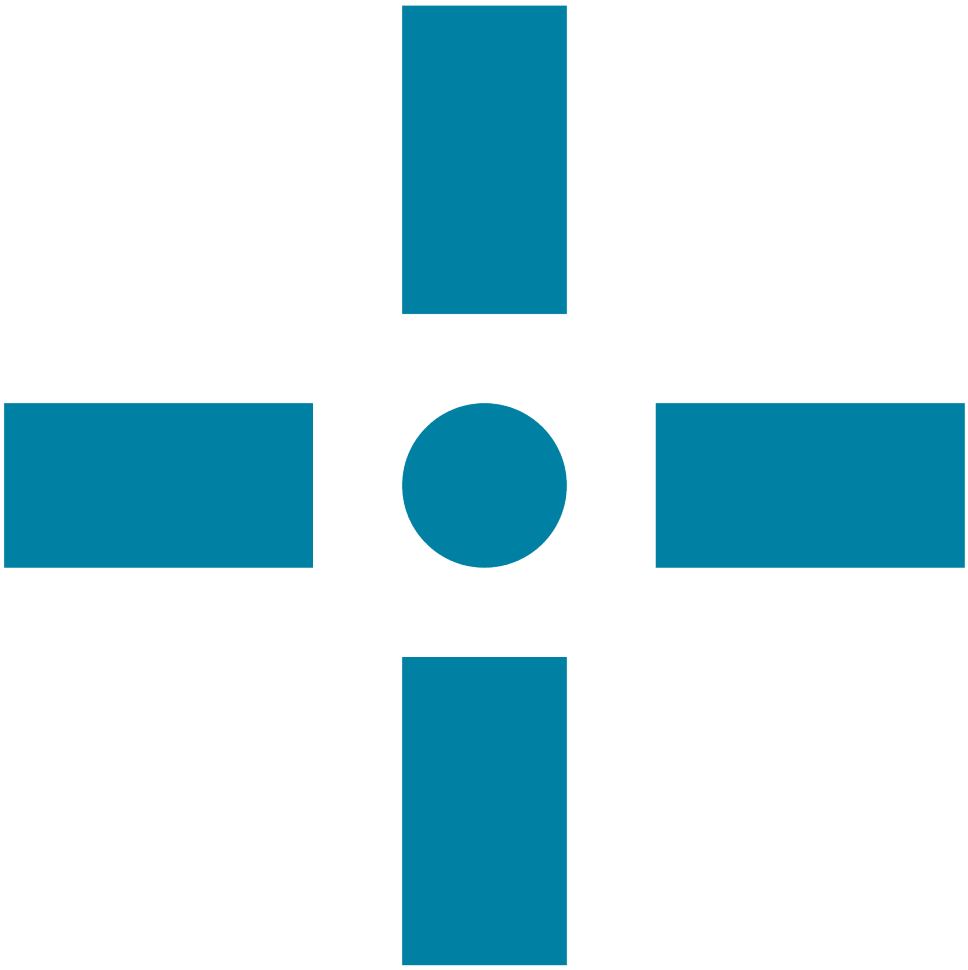
MarkerView™ Software

Release Notes



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March 2017

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Introduction 1

This document describes version 1.3.1 of the MarkerView™ software, a stand-alone application for creating aligned peak lists from LC-MS data files that were generated using SCIEX acquisition software, and for performing subsequent data processing using Principal Components Analysis (PCA), Principal Components Analysis-Discriminant Analysis (PCA-DA), or t-tests. Typical applications include: metabolomics, biomarker discovery, metabolite identification, and impurity profiling.

Where to Get Help

Click **Help** in the main menu to open the *User Guide* or the *Reference Guide*.

The *User Guide* provides a tutorial introduction to all of the main features of the software. If you have not previously used the MarkerView™ software, it is suggested that you start with this document.

The *Reference Guide* describes all of the features of the software, in detail. Unlike the *User Guide*, this document does not provide examples, but it does describe the functionality of the various menu items and options.

Changes from Version 1.3 to Version 1.3.1

- This version of the MarkerView™ software provides support for wiff2 data files generated by version 1.2 of SCIEX OS.
- This version of the MarkerView™ software enables the user to export t-test results to a text file, allowing users to integrate with the Advaita iPathwayGuide software.
- In previous releases of the MarkerView™ software, information that was exported in MGF format was not compatible with the ProteinPilot™ software search engine. This issue has been fixed.
- In previous releases of the MarkerView™ software, if peak files with identical names existed in different directories or folders, then the software incorrectly combined these files into one file. This issue has been fixed.

Contact Us

SCIEX Support

- sciex.com/contact-us
- sciex.com/request-support

Customer Training

- In North America: NA.CustomerTraining@sciex.com
- In Europe: Europe.CustomerTraining@sciex.com
- Outside the EU and North America, visit sciex.com/education for contact information.

Online Learning Center

- SCIEXUniversity

Technical Support

SCIEX and its representatives maintain a staff of fully-trained service and technical specialists located throughout the world. They can answer questions about the system or any technical issues that might arise. For more information, visit the website at sciex.com.

Workstation Requirements

CAUTION: Potential Data Loss. This software should not be installed on the acquisition computer. Software errors and data integrity issues can result if this software and acquisition software are used concurrently.

The workstation must be configured with the following applications:

- English version of the Microsoft Windows 7 (32-bit or 64-bit) operating system with SP1 or an English version of the Microsoft Windows 10 (64-bit) operating system. Other versions of Microsoft Windows have not been formally tested.
- Microsoft Office 2013 or later is required to view and print Microsoft Word reports.

  Note: If a trial version of Microsoft Office is installed on the computer as a temporary measure, then the full version of the Microsoft Office software must be activated before the trial period expires. The license can be purchased from your regional division of Microsoft or from an authorized distributor in your region.

Installation Instructions 2

Notes on Installation

CAUTION: Potential Data Loss. This software should not be installed on the acquisition computer. Software errors and data integrity issues can result if this software and acquisition software are used concurrently.

- The user must be logged on to the computer as a user with Administrator privileges.
- If version 1.3 of the MarkerView™ software is installed and licensed on the computer, then the existing version is upgraded to version 1.3.1. Version 1.3.1 automatically activates using the existing license file.
- If any other version of the MarkerView™ software is installed on the computer, for example version 1.2, then version 1.3.1 is installed as a new application and the previous version of the software remains unchanged on the computer. A new license file for version 1.3.1 is required.

Install the MarkerView™ Software

1. Log on to the computer as a Microsoft Windows user with administrator privileges.
2. If a previous version of the MarkerView™ software is installed, then make sure that the software is closed.
3. Install the MarkerView™ software as described in Table 2-1.

Table 2-1 Installation Instructions

To install from a file downloaded from the SCIEX Web site ...	To install from the MarkerView™ software installation DVD ...
Download the .zip file from http://sciex.com/products/software/markerview-software. **Tip!** To prevent potential installation issues, we recommend that the file is saved to a location other than the computer desktop.	Load the MarkerView™ software installation DVD in the DVD drive.
After the download is complete, right-click the **MarkerView_1.3.1.zip** file and then click **Extract All**. **Note:** By default, the files are extracted to the MarkerView_1.3.1 folder in the same location where the .zip was saved.	Navigate to the DVD and then double-click **setup.exe**. The MarkerView™ 1.3.1 Software – Installation Wizard dialog opens.
After the extraction is complete, browse to the extraction folder and then double-click **setup.exe**. **Note:** The Open File - Security Warning dialog might open, indicating that the publisher cannot be identified. If this dialog opens, then click **Run**.	Click **Next**.
Click **Next**.	—

4. On the License Agreement dialog, click the **I accept the terms in the license agreement** check box and then click **Next**.
5. On the Customer Information dialog, type the **User Name** and the **Organization Name**, and then click **Next**.
6. On the Destination Folder dialog, click **Next**.

   Tip! The software installation location can be changed before clicking **Next**.

7. Click **Install**.

8. After the installation is complete, click **Finish**.

Tip! When upgrading from a licensed version of the MarkerView™ 1.3 software, version 1.3.1 of the software activates automatically, using the existing license. When upgrading from any other version of the MarkerView™ software, or for a new installation, a new license file is required. Continue with License the MarkerView Software on page 8.

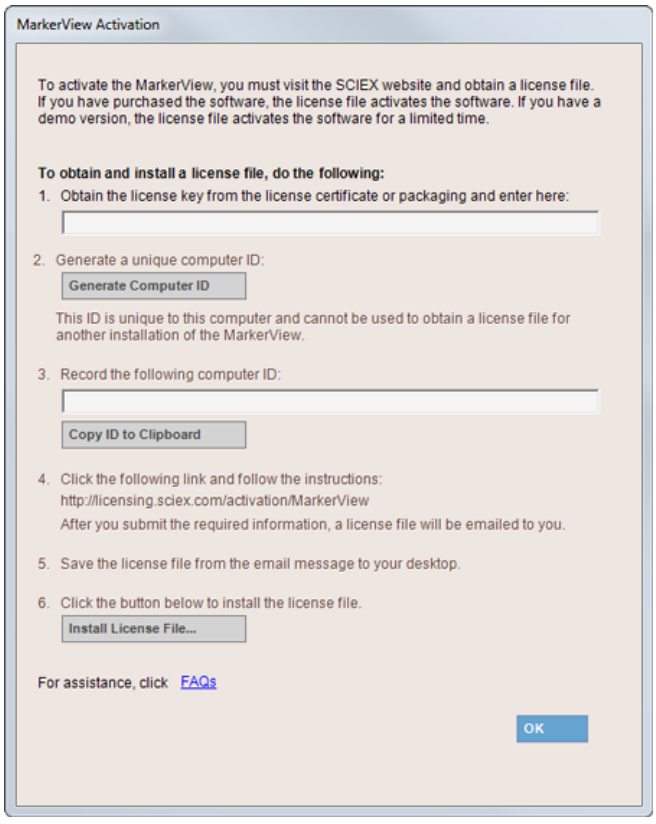
License the MarkerView™ Software

Note: Internet access is required to obtain a license for the software. If the computer where the MarkerView™ software is being installed does not have Internet access, then make a copy of the generated computer ID. On a computer with Internet access, go to http://licensing.sciex.com/activation/MarkerView and then follow the instructions to obtain a license.

1. Double-click the MarkerView™ software desktop icon.

   The MarkerView Activation dialog opens.

Figure 2-1 MarkerView Activation Dialog



2. Type the license key in the appropriate field.

   If a license key is not available, then contact sciex.com/request-support.

3. Click **Generate Computer ID**.

   This creates a unique identifier for the workstation.

4. Click **Copy ID to Clipboard**.

5. Click the http://licensing.sciex.com/activation/MarkerView link.

6. Follow the instructions to obtain the license.

   After the required information is submitted, a license file is sent to all of the e-mail addresses provided.

7. Close the browser window.

8. When the e-mail containing the license file is received, copy the license file to the workstation desktop.

9. Click **Install License File** on the MarkerView Activation dialog.

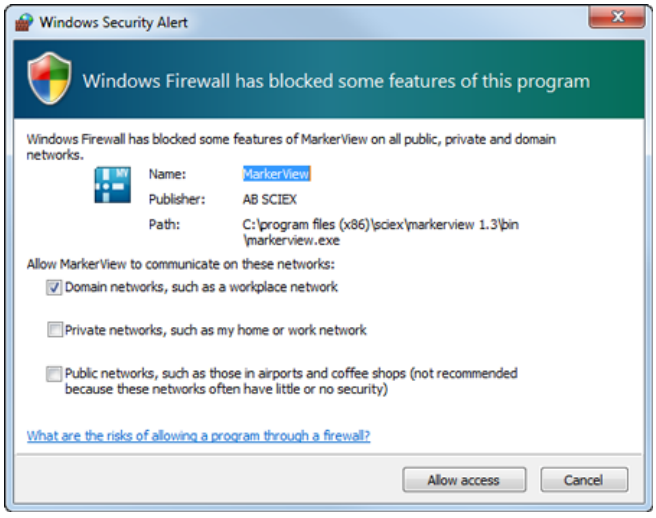
   The Select the new license file to be installed dialog opens.

10. Browse to and select the license file and then click **Open**.

    Both the Select the new license file to be installed and the MarkerView Activation dialogs close and the MarkerView™ software opens.

Tip! The first time the MarkerView™ software is opened, the dialog shown in Figure 2-2 might open. If the Windows Security Alert dialog opens, select the **Domain networks, such as a workplace network** check box and then click **Allow access**. This enables all of the external utilities included with the MarkerView™ software to communicate with the software.

Figure 2-2 Windows Security Alert Dialog



Remove the MarkerView™ Software 3

1. Log on to the computer as a Microsoft Windows user with Administrator privileges.
2. Click **Start > Control Panel > Programs and Features.**

   Tip! If the control panel components are shown by **Category**, then click **Start > Control Panel > Programs > Programs and Features > Uninstall a program.**

3. Select MarkerView™ 1.3.1 Software and then click **Uninstall**.

   The software is removed, with no user intervention required.

   During the removal, the software name is removed from the Installed Programs list, the shortcut to the MarkerView™ software is removed from the desktop, and the shortcuts to the software and the user documentation are removed from the Start menu.

   Note: If the product is licensed, then the license file is not removed and can be used if the MarkerView™ software is installed again.

Known Issues and Limitations 4

- When processing a large number of LC-MS files (or a smaller number of very large files) on a 32-bit computer, the program might run out of memory. We recommend that all peaks files for the samples are generated in smaller batches and then the Peaks Table can be generated using these peaks files. This process is described in both the *User Guide* and the *Reference Guide*.
- If the Windows Security Alert dialog shown in step 10 of License the MarkerView Software on page 8 was cancelled, then the add-on utilities cannot connect to the MarkerView™ software. This can be corrected using the Windows Firewall control panel. Contact support (sciex.com/request-support) for more information.
- The MarkerView™ software cannot process LC-MS data that was acquired in centroid mode on a QTRAP® system or other triple-quadrupole system. Profile mode data acquisition must be used.

Changes from Version 1.2.1 to Version 1.3 A

- A wizard has been added that combines many of the previously separate steps into a single workflow.
- Data created in the new wiff2 format by the SCIEX X500 QTOF system is fully supported.
- Infused MS/MS of Everything data is now supported.
- Box-and-whiskers plots are now available.
- A new normalization technique known as most-likely-ratio (MLR) normalization has been added.
- When MS/MS^{ALL} with SWATH® acquisition data are processed, it is now possible to view MS/MS spectra for the selected peaks (similar to what was previously possible for IDA data).
- An option to use the *Welch* variant has been added to the t-test.
- The Samples Table and Scores Table now have the ability to add custom columns which can be populated with arbitrary data.
- A new add-in, Set Names, is available. This add-in allows names to be assigned to peak rows for targeted workflows.
- Previously assignment of PCVG groups was available using an add-in script. This functionality is now integrated and the parameter setting has been automated.
- When creating a t-test, a Profile Plot and a Box-and-Whiskers plot are automatically generated.
- A new option to limit the time range for XIC calculation to speed processing has been added.
- The peak-finding process has been made faster when multiple samples are being processed on computers that contain more than one CPU or core.
- A licensing approach that does not require manual copying-and-pasting and e-mailing of computer IDs is being used.

Revision History

Revision	Reason for Change	Date
A	First release at software version 1.3	April 2016
B	Applied new template. Updated version information to 1.3.1. Added Changes from Version 1.3 to Version 1.3.1 section. Updated Contact Us information. Added Technical Support topic. Added Notes on Installation section. Updated Install the MarkerView™ Software and the Remove the MarkerView™ Software sections. Removed New Features in Version 1.2.1 and New Features in Version 1.1 sections.	March 2017