

Release Notes

PeakView[®] Software

Qualitative Processing, Review, and Comparison Software
Version 2.1

The PeakView[®] software is a standalone, general purpose application for exploring and interpreting qualitative LC/MS data from Analyst[®] software and Analyst TF software .wiff files. The software includes tools for analyzing both nominal and accurate mass spectrometry data from single and multiple samples, as well as tools for elucidating chemical structures. The software features are described in the *Tutorial* and *Reference Guide*, available through the Help menu.

New Features and Changes

- Integration of the Bio Tool Kit MicroApp feature.
- Support for data acquired using ultraviolet (UV) detectors, diode array detectors (DAD or PDA), and analog-to-digital converters (ADC).
- Support for data acquired using QTRAP[®] and Triple Quad[™] LC/MS/MS systems.
- Support for data acquired using the 4700 MALDI TOF/TOF[™] Analyzer, the 4800 Plus MALDI TOF/TOF[™] Analyzer, and the TOF/TOF[™] 5800 Systems (.t2d format).
- Some functionality that was distributed as scripts in version 2.0 of the software has been implemented in the software as features accessible through the user interface.
- When a charge state of +1 was selected from the Charge list on the MS Details tab in the Formula Finder pane and a non-singly charged ion type was selected, the resulting found formulas were incorrect. This issue has been resolved. (PV-522)

Where to Get Help

Other Documentation

- *Reference Guide*
- *Tutorial*

Support

- support@absciex.com
- www.absciex.com
- Customer Documentation: techpubs@absciex.com

Requirements

- English (US) version of the Microsoft Windows XP operating system with SP3 or the Microsoft Windows 7 (32-bit or 64-bit) operating system with SP1.
- The user must be logged on to the computer as a user with Administrator privileges to install the software.

Supported Equipment

- Dell OptiPlex 9010, or a later model provided by AB SCIEX, is the recommended computer model.

Install the Software

1. Log on to the computer as a user with Administrator privileges.
2. If version 2.0 of the PeakView® software is already installed on the computer, then make sure that the software is closed.

To install from the Web site download:	To install from the DVD:
Select the PeakView® 2.1 software from the Other Software Downloads table at http://www.absciex.com/Downloads/Software-Downloads .	Insert the PeakView software installation DVD into the DVD drive.
Save the PeakView_2.1.zip file to the desktop of your computer.	If the PeakView® 2.1 Setup dialog does not open, navigate to the DVD drive and then double-click Setup.exe .
After the zip file is downloaded, double-click PeakView 2.1.zip and then extract all of the files to your computer.	On the Welcome to the PeakView® 2.1 Setup Wizard screen, click Next .
After the extraction is complete, browse to and then double-click PeakView 2.1.exe .	Follow the on-screen instructions.
On the WinZip Self-Extractor dialog, click Unzip . The files in the executable are extracted to C:\PeakView 2.1 .	-----
After the extraction completes, browse to and then double-click the setup.exe file.	-----
Follow the on-screen instructions.	-----

3. Install the MasterView™ software, if required.

Activate the PeakView Software

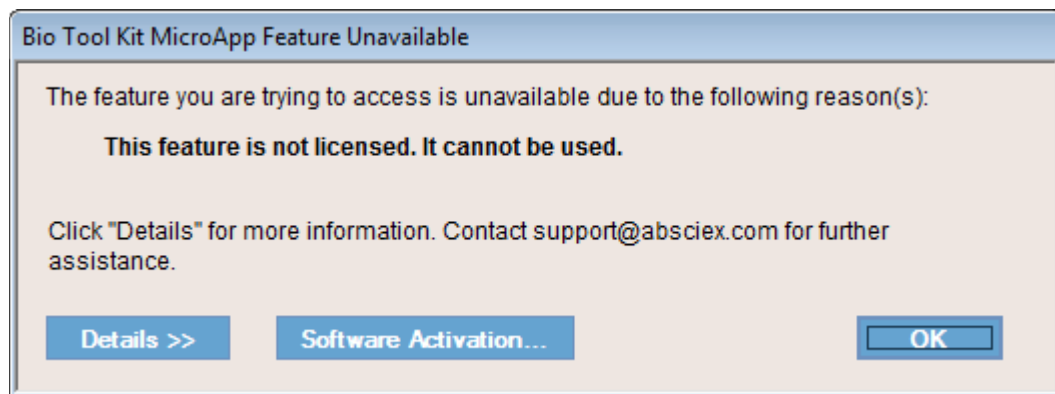
Note: When upgrading from a licensed version of the PeakView® 2.0 software, version 2.1 of the software activates automatically using the existing license.

Tip: Internet access is required to obtain a license for the software. If the computer where the PeakView software is being installed does not have Internet access, make a copy of the generated computer ID. On a computer with Internet access, go to <http://licensing.absciex.com/activation/PeakView> and follow the instructions to obtain a license.

1. Double-click the PeakView 2.1 software desktop icon to open the PeakView software.
The **PeakView Activation** dialog opens.
2. Type the license key from the license certificate in the appropriate field.
3. Click **Generate Computer ID**.
This creates a unique identifier for the workstation.
4. Click **Copy ID to Clipboard**.
5. Click the <http://licensing.absciex.com/activation/PeakView> link.
6. Follow the instructions to obtain a license.
7. After the required information is submitted, a license file is sent to all e-mail addresses provided.
8. Close the browser window.
9. When the e-mail containing the license file is received, copy the license to the workstation desktop.
10. On the **PeakView Activation** dialog, click **Install License File**.
11. On the **Select the new license file to be installed** dialog, browse to and then select the license file.
12. Click **Open**.

Both the **Select the new license file to be installed** and the **PeakView Activation** dialogs close. The PeakView software opens. The following dialog opens:

Figure 1: Bio Tool Kit MicroApp Feature Unavailable Dialog



Note: The Bio Tool Kit MicroApp feature must be licensed before the functionality can be accessed. Continue with [Activate the Bio Tool Kit MicroApp Feature](#) to activate the feature.

Tip: Click **OK** to close the dialog without activating the feature. To activate the feature at a later time, make sure that the PeakView software is open and then click **Help > Bio Tool Kit Activation**. When the **Bio Tool Kit**

MicroApp Activation dialog opens, continue with step 2 of [Activate the Bio Tool Kit MicroApp Feature](#).

Activate the Bio Tool Kit MicroApp Feature

Tip: Internet access is required to obtain a license for this feature. If the computer where the Bio Tool Kit MicroApp feature is being activated does not have Internet access, make a copy of the generated computer ID. On a computer with Internet access, go to <http://licensing.absciex.com/activation/BioToolKit> and follow the instructions to obtain a license.

1. Click **Software Activation** on the **Bio Tool Kit MicroApp Feature Unavailable** dialog. Refer to [Figure 1](#).

The **Bio Tool Kit MicroApp Activation** dialog opens.

2. Type the license key from the license certificate in the appropriate field.
3. Click **Generate Computer ID**.
This creates a unique identifier for the workstation.
4. Click **Copy ID to Clipboard**.
5. Click the <http://licensing.absciex.com/activation/BioToolKit> link.
6. Follow the instructions to obtain a license.
7. After the required information is submitted, a license file is sent to all e-mail addresses provided.
8. Close the browser window.
9. When the e-mail containing the license file is received, copy the license to the workstation desktop.
10. On the **Bio Tool Kit MicroApp Activation** dialog, click **Install License File**.
11. On the **Select the new license file to be installed** dialog, browse to and then select the license file.
12. Click **Open**.

Both the **Select the new license file to be installed** and the **Bio Tool Kit MicroApp Activation** dialogs close.

Activate the ChemSpider Web Services Feature

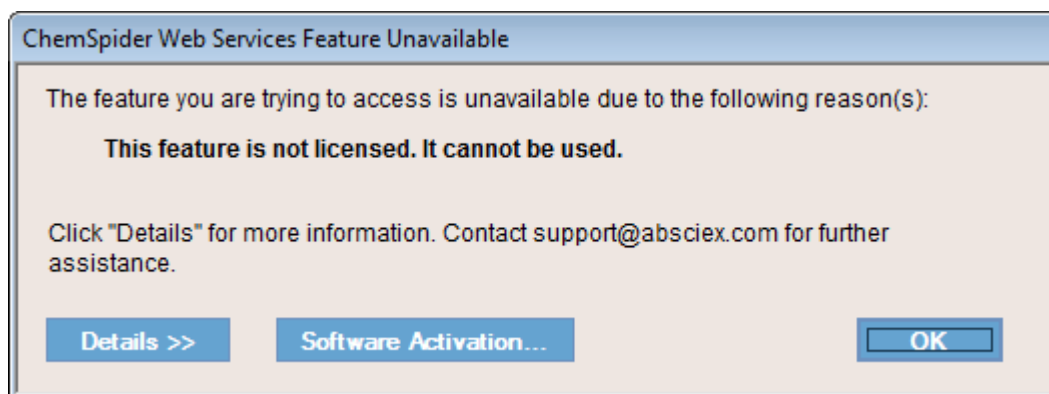
Note: The ChemSpider Web Services feature must be licensed before the ChemSpider database can be accessed. If you are upgrading from a version of the PeakView[®] 2.0 software that uses a licensed version of the ChemSpider database, then the ChemSpider Web Services feature is automatically activated during the PeakView software upgrade.

The computer where the ChemSpider Web Services feature is being used must have Internet access.

1. Open a sample and generate a spectrum from a Total Ion Chromatogram (TIC) pane. Refer to Chromatograms and Spectra on page 22 of the *PeakView® 2.1 Software Tutorial*.
2. With the Spectrum pane active, click **Show > Formula Finder**.
3. In the Formula Finder pane, click the **Show Options** icon.
4. On the **Formula Finder Settings** dialog, click the **Dictionaries** tab.
5. Select the **ChemSpider Service** check box and then click **OK**.

The following dialog opens:

Figure 2: ChemSpider Web Services Feature Unavailable Dialog



6. Click **Software Activation** on the **ChemSpider Web Services Feature Unavailable** dialog. Refer to [Figure 2](#).
- The **ChemSpider Web Services Activation** dialog opens.
7. Type the license key from the license certificate in the appropriate field.
 8. Click **Generate Computer ID**.
- This creates a unique identifier for the workstation.
9. Click **Copy ID to Clipboard**.
 10. Click the <http://licensing.absciex.com/activation/ChemSpider> link.
 11. Follow the instructions to obtain a license.
 12. After the required information is submitted, a license file is sent to all e-mail addresses provided.
 13. Close the browser window.
 14. When the e-mail containing the license file is received, copy the license to the workstation desktop.
 15. On the **ChemSpider Web Services Activation** dialog, click **Install License File**.
 16. On the **Select the new license file to be installed** dialog, browse to and then select the license file.
 17. Click **Open**.

Both the **Select the new license file to be installed** and the **ChemSpider Web Services Activation** dialogs close.

Remove the Software

1. Make sure that you are logged on to the computer as a Windows user with Administrator privileges.
2. Make sure that the PeakView® software is closed.
3. Click **Start > Control Panel**.
4. Proceed as follows, depending on the operating system:

Windows XP	Windows 7
Double-click Add or Remove Programs .	Click Programs and Features .
Click PeakView 2.1 .	Click PeakView 2.1 .
Click Remove .	Click Uninstall .

The license remains on the computer and is automatically used if the software is installed again.

Notes on Use

- If the local .mdb database cannot be accessed from the Formula Finder Option dialog, then the correct driver for the Microsoft Windows 7 operating system might need to be installed.
 - For computers configured with the Windows 7 64-bit operating system, run the AccessDatabaseEngine_x64.exe.
 - For computers configured with the Windows 7 32-bit operating system, run the AccessDatabaseEngine.exe.

These executables are located in the Setup\AccessDatabaseEngine2010 folder in the PeakView® software installer.

Note: On a computer with the Windows 7 64-bit operating system, it is possible that the 32-bit access driver is already installed. If this is the case, an error message indicating that the 64-bit version of the Access Data Provider cannot be installed because there is an existing 32-bit version is shown. To resolve this issue, remove the 32-bit version of the Access Database Provider and then install the 64-bit version.

One of the access drivers must be installed on the computer where the PeakView 2.1 software is installed. If a driver is not installed, then the Formula Finder cannot access the database and shows an error message when the **Show > Formula Finder** option is selected.

Known Issues and Limitations

Everyone should read this section of the Release Notes. This section applies specifically to issues that are known in the PeakView[®] software, version 2.1.

Note: The numbers in brackets are reference numbers to each issue in our internal tracking system.

- When exporting data to the Analyst[®] software using the **File > Export > Active Data to Analyst** and the **File > Export > All Data to Analyst** options, the labels on the x- and y-axes shown in the Analyst software graphs might be different from the labels on the x- and y-axes shown in the PeakView software. (PV-742)

Data Type	Axes Labels in Analyst Software	Axes Labels in PeakView Software
Total Ion Chromatogram (TIC)	x-axis: Time, sec	x-axis: Time, min
Analog-to-Digital Converter (ADC) Channel	x-axis: Time, sec y-axis: Intensity, cps	x-axis: Time, min y-axis: Channel 1, %
Diode Array Detector (DAD) Total Wavelength Chromatogram (TWC)	x-axis: Time, sec	x-axis: Time, min

In addition, when ultraviolet (UV), DAD, or ADC data is exported, the Analyst software and the Analyst TF software do not show any data points below 0.0 intensity.

Note: When exporting TIC data to the Analyst TF software, the labels on the x- and y-axes shown in the Analyst TF software graphs are the same as the labels on the x- and y-axes shown in the PeakView software.

- Because the algorithm being used by the protein reconstruct functionality is memory-intensive, a reasonable range should be considered for the parameters used to process the data. Computers configured with the Microsoft Windows XP operating system might experience slower performance if the algorithm is processing data with broad-range output parameters. (PV-624)

Document Revision History

Revision	Description of Change	Date
A	First release	2013/09/06
B	Added installation instructions. Updated issue PV-421 to provide information about the AccessDatabaseEngine.exe for computers configured with the Windows 7 32-bit operating system. Added procedures for removing the 32-bit Access Data Provider, if required.	2013/09/12
C	Added New Features and Changes section. Added procedure for the activation of the Bio Tool Kit MicroApp feature. Added procedure for the activation of ChemSpider Web Services feature. Added PV-742 to list of Known Issues and Limitations. Removed issue PV-522, which has been resolved. Moved issue PV-421 to Notes on Use section. Added information identifying the correct order of installation of the MasterView software and the PeakView software in the Notes on Use section.	2014/02/14
D	Removed the information identifying the correct order of installation of the MasterView software and the PeakView software from the Notes on Use section. Added step after the installation procedures for PeakView.	2014/03/07

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AB Sciex Pte. Ltd.
Blk 33, #04-06
Marsiling Ind Estate Road 3
Woodlands Central Indus. Estate
SINGAPORE 739256

