Release Notes

PeakView® Software

Qualitative Processing, Review, and Comparison Software
Version 2.2

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

- The PeakView® 2.1 Patch for Bio Tool Kit, which was released to resolve the following issues, has been incorporated in this release of the software:

  - The Reconstruct Protein option does not function as expected when using limited mass range in the Bio Tool Kit feature. (PV-788)

  - The Bio Tool Kit MicroApp Feature Unavailable dialog is shown each time the user opens the PeakView software until the feature is activated. (PV-789)

- The pressure read-back value for the Agilent pump is 10× higher in the PeakView software than the same value in the Analyst software Explore mode. This issue has been resolved. (PV-787)

- On a computer configured with the Windows 7 (64-bit) operating system, the options for the fragment pane in the ChemSpider database view are missing when using the MasterView™ software plugin. This issue has been resolved. (PV-790)

- The PeakView 2.2 software installs the PeakViewLink.exe application in the C:\Program Files\AB SCIEX\PeakView 2\bin folder. This application enables the user to transfer data from the LipidView™ software to the PeakView software for additional processing and data review. (PV-792)

- Performance improvements have been made to the Formula Finder functionality. (PV-793)

- A new tab, AA List, has been added to the Mass Calculators pane. This tab enables users who are using non-standard amino acids (AA) to easily and efficiently create a list of custom amino acids and AA modifications for further processing. (PV-794)

- The first time that a custom element is created, the PeakView 2.2 software creates the CustomElements.xml file in the C:\ProgramData\Sciex\

ElementalCalculator folder. The first time that a custom amino acid is modified, the CustomAAData.xml file is created in the C:\ProgramData\Sciex\ ElementalCalculator folder. Users have both read and write access to the files in this folder. (PV-795) Refer to Notes on Use on page 7.

Where to Get Help

Other Documentation

- *Reference Guide*
- *Tutorial*

Support

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

Requirements

- An 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.
- A license file is required to activate the PeakView® software. Refer to Activate the PeakView® Software on page 3.
- The Bio Tool Kit MicroApp feature must be licensed before the functionality can be accessed. Refer to Activate the Bio Tool Kit MicroApp Feature on page 4.
- The ChemSpider Web Services feature must be licensed before the ChemSpider database can be accessed. The computer where the ChemSpider Web Services feature is being used must have Internet access. Refer to Activate the ChemSpider Web Services Feature on page 5.

Supported Equipment

- A 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 a previous version 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:
Download the **PeakView® 2.2 software** from the Other Software Downloads table at http://www.absciex.com/Downloads/Software-Downloads. **Note**: To prevent potential installation issues, it is recommended that you save the file to a location other than the computer desktop.	Insert the PeakView software installation DVD into the DVD drive.
After the download is complete, right-click the **PeakView_2.2.zip** file.	If the **PeakView® 2.2 Setup** dialog does not open, navigate to the DVD drive and then double-click **Setup.exe**.
Click **Extract All**. **Note**: By default, the files are extracted to the **PeakView_2.2** folder in the same location as the **PeakView_2.2.zip** file was saved.	On the **Welcome to the PeakView® 2.2 Setup Wizard** screen, click **Next**.
After the extraction is complete, browse to the extraction folder and then double-click **PeakView 2.2.exe**.	Follow the on-screen instructions.
On the **WinZip Self-Extractor** dialog, click **Unzip**. The files in the executable are extracted to **C:\PeakView 2.2**.	---
After the extraction completes, browse to and then double-click the **setup.exe** file.	---
Follow the on-screen instructions.	---

3. Activate the PeakView software, if required. Refer to Activate the PeakView® Software.

   Note: When upgrading from a licensed version of the PeakView® 2.0 or 2.1 software, version 2.2 of the software activates automatically using the existing license.

Activate the PeakView® Software

Note: Before activating the software, change the User Account Control (UAC) Settings to prevent issues with installing the license file. Refer to Change the User Account Control (UAC) Settings on page 6.

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, then make a copy of the generated computer ID. On a computer with Internet

access, go to http://licensing.absciex.com/activation/PeakView and then follow the instructions to obtain a license.

1. Double-click the PeakView 2.2 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.

Activate the Bio Tool Kit MicroApp Feature

Note: The Bio Tool Kit MicroApp feature must be licensed before the functionality can be accessed.

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, then make a copy of the generated computer ID. On a computer with Internet access, go to http://licensing.absciex.com/activation/BioToolKit and then follow the instructions to obtain a license.

1. In the PeakView® software, click **Help > Bio Tool Kit Activation**.

   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® 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® 2.2 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 Setting**s dialog, click the **Dictionaries** tab.

5. Select the **ChemSpider Service** check box and then click **OK**.

The following dialog opens:

Figure 1: ChemSpider Web Services Feature Unavailable Dialog
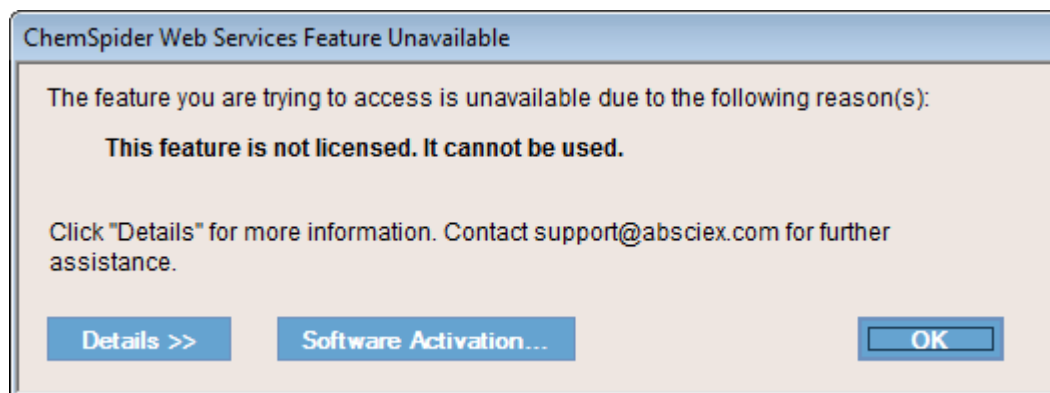
6. Click **Software Activation** on the **ChemSpider Web Services Feature Unavailable** dialog. Refer to Figure 1.

   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.

Change the User Account Control (UAC) Settings

1. Click **Start > Control Panel**.

2. Click **User Accounts > Change User Account Control settings**.

3. On the User Account Control Settings dialog, move the slider bar to **Never notify me when** and then click **OK**.

4. Continue with

Remove the Software

5. Log on to the computer as a Windows user with Administrator privileges.

6. Make sure that the PeakView® software is closed.

7. Click **Start > Control Panel**.

8. Proceed as follows, depending on the operating system:

Windows XP	Windows 7
Double-click **Add or Remove Programs**.	Click **Programs and Features**.
Click **PeakView 2.2**.	Click **PeakView 2.2**.
Click **Remove**.	Click **Uninstall**.

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

Notes on Use

- If you are upgrading the PeakView® software from an earlier version and have previously created custom elements or modified existing custom elements, a new folder must be created (refer to the New Folder column in the following table). The existing CustomElements.xml file must be copied from the original location to the new location because the previous storage location is no longer valid for this version of the software. (PV-795)

Operating System	Previous Folder	New Folder
Microsoft Windows XP	C:\Documents and Settings\All Users\Application Data\ AB SCIEX\PeakView 2\ ElementalCalculator **-OR-** C:\Documents and Settings\Administrator\Application Data\AB SCIEX\PeakView 2\ ElementalCalculator	C:\Documents and Settings\All Users\Application Data\Sciex\ ElementalCalculator **-OR-** C:\Documents and Settings\ Administrator\Application Data\ Sciex\ElementalCalculator
Microsoft Windows 7	C:\Users\[user name]\ AppData\Roaming\AB SCIEX\ PeakView 2	C:\ProgramData\Sciex\ ElementalCalculator

- 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 2.2 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 2.2.

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)

Revision History

Revision	Description of Change	Date
A	First release	2014/10/31

AB SCIEX