SCIEX

The Power of Precision

Keystone Software

User Guide

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Contents

Introduction

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The Keystone Software consists of the following applications:

- The Keystone Converter Software is: A desktop application that converts wiff, rdb, and audit trail files, generated by the Analyst® Software, to AnIML format.
- The Keystone Viewer Software is: A desktop application that is used to view the converted AnIML files.

For information on how to renew the software licenses, refer to the *Keystone Converter Software Installation* Guide.

What is AnIML?

AnIML is an open standard XML data format for storage and sharing of experiment data. The AnIML file is a human-readable format that captures analytical data generated by many different analytical techniques, such as MS, NMR, and IR, from many different analytical instrument vendors. AnIML provides a generic data container that permits the storage of analytical data, including the following:

- Sample information
- Method information
- Measurement results
- Instruments and software used
- Workflow information that ties experiments and samples together

AnIML files derived from the various analytical techniques and vendors can be opened and viewed with an AnIML file viewer. The original proprietary software that created the file is no longer required.

Configure the Analyst® Software 2

1. Make sure that the Analyst® Software is open and running in the background before converting any data.
2. Make sure that the data to be converted is in an Analyst Data Root folder and the Analyst® Software must have that data root folder set as the active data root folder.

   If wiff files are converted using the Keystone Converter Software, then two audit records are created in the Analyst® Software Project Audit Trail for every sample converted. If a large number of samples are being converted, then this behaviour might be undesirable.
3. To avoid creating two audit records, in the active Project Audit Map, clear the **Audited** checkbox for the **Closed Module** and the **Data File has been opened** fields.
4. In the Analyst® Software, update the IDA Explorer Appearance Options tab. Refer to Update Appearance Options on the IDA Explorer Tab.

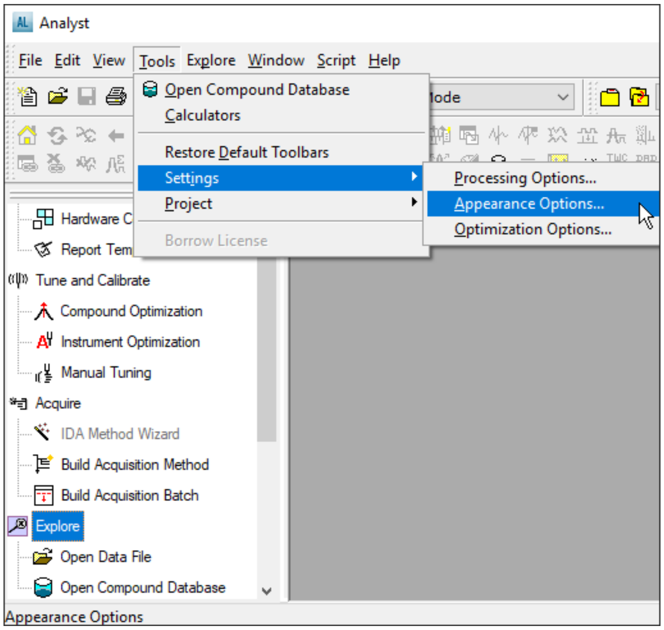
Update Appearance Options on the IDA Explorer Tab

This procedure applies to the Analyst® 1.7.2 Software.

To make sure that data is converted and shown correctly in the Keystone Viewer Software, before converting IDA data, update the IDA Explorer tab in the Appearance Options dialog.

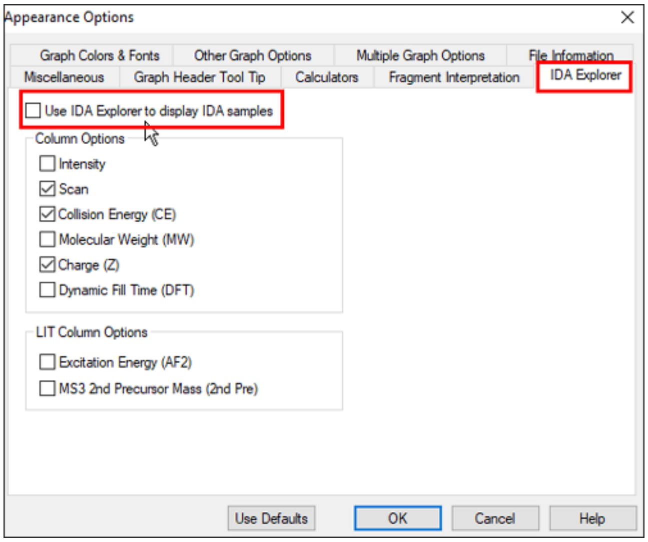
1. Open the Analyst® 1.7.2 Software.
2. On the Navigation bar, click **Explore**.
3. From the menu, select **Tools > Settings > Appearance Options**.

Figure 2-1 Menu Bar



4. Click the **IDA Explorer** tab and then clear the **Use IDA Explorer to display IDA samples** check box.

Figure 2-2 IDA Explorer Tab



☐ Use IDA Explorer to display IDA samples

Column Options
☐ Intensity
☑ Scan
☑ Collision Energy (CE)
☐ Molecular Weight (MW)
☑ Charge (Z)
☐ Dynamic Fill Time (DFT)

LIT Column Options
☐ Excitation Energy (AF2)
☐ MS3 2nd Precursor Mass (2nd Pre)

Keystone Converter Software

3

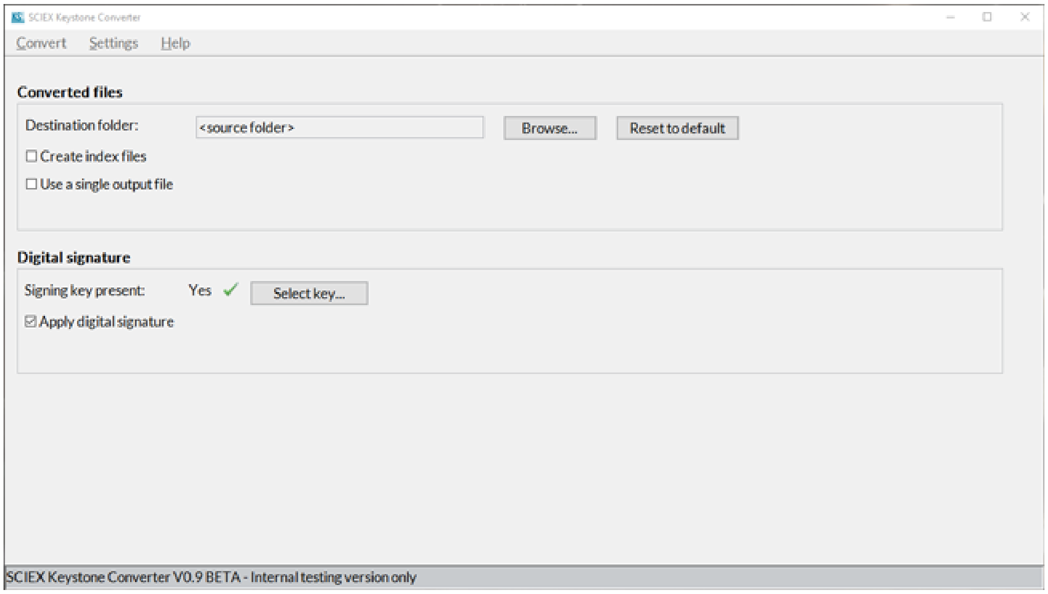
Note: Before converting data, make sure that the Analyst® Software is open and running in the background. Data to be converted must be in an Analyst Data Root folder and the Analyst® Software must have that data root folder set as the active data root folder.

Note: If the Analyst® Software version 1.7.2 is installed, then the Analyst® 1.7.2 Patch for Keystone Software must also be installed.

Configure the Keystone Converter Software

1. Click **Start > SCIEX Keystone > SCIEX Keystone Converter** to open the Keystone Converter Software.
2. Click **Settings**.

Figure 3-1 SCIEX Keystone Converter Dialog: Settings Page



Converted files

Destination folder: <source folder>

☐ Create index files

☐ Use a single output file

Digital signature

Signing key present: Yes ✓

☑ Apply digital signature

SCIEX Keystone Converter V0.9 BETA - Internal testing version only

---

Note: The following settings are automatically configured by the software:

- The **Destination folder** is **<source folder>**.
  The default destination folder is the folder that contains the source file.
- The **Create index files** check box is selected.
- The **Use a single output file** check box is cleared.
- The **Signing key present** field is set to **Yes**.
- The **Apply digital signature** check box is selected.

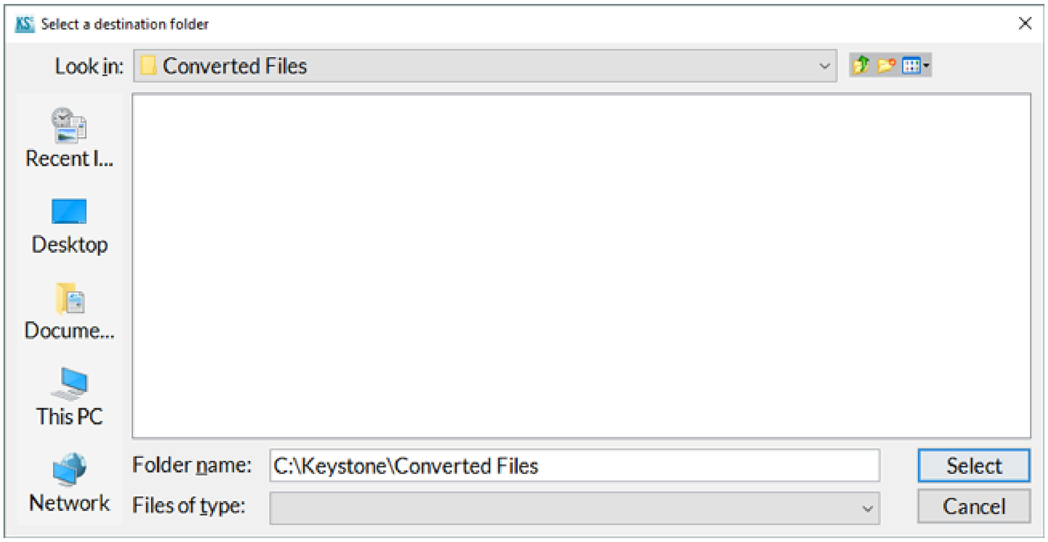
---

3. (Optional) To change the default **Destination folder**, do this:

Note: If a destination folder is not configured, then the software automatically saves the converted files in the same location as the source files.

a. Click **Browse**.

Figure 3-2 Select a destination folder Dialog



Folder name: C:\Keystone\Converted Files

b. Browse to the appropriate folder and then click **Select**.

The Settings page refreshes and the selected folder is shown in the **Destination folder** field.

4. (Optional) Clear the **Create index files** check box.

Index files are used by the Viewer to improve the loading of large files. Index files are stored in the same location as the AnIML files.

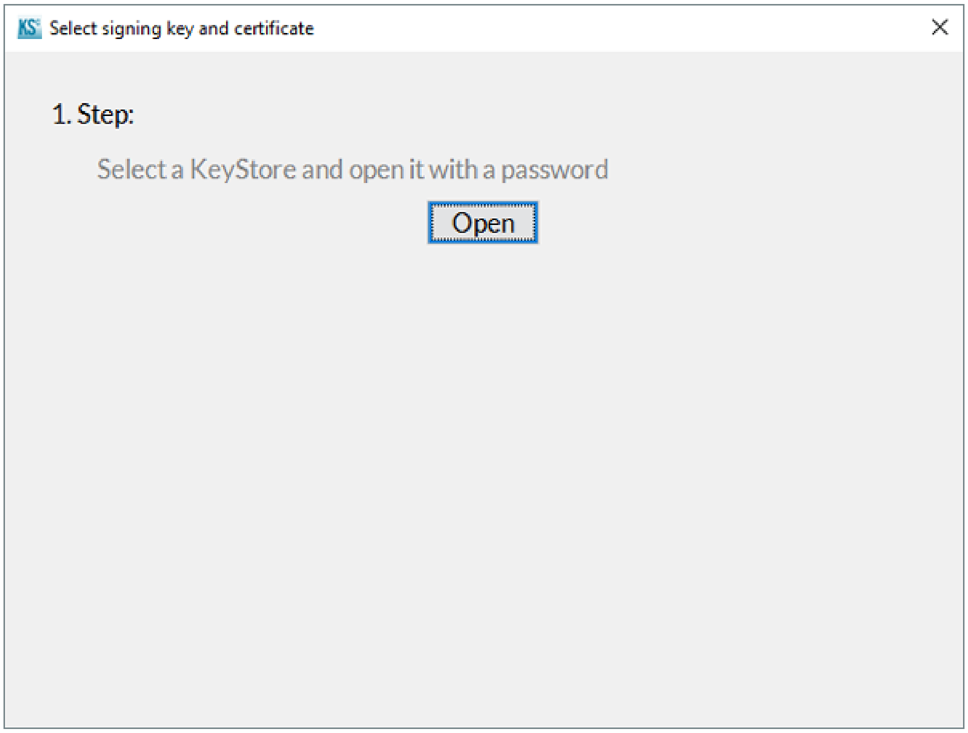
5. (Optional) Select the **Use a single output file** check box.

   If this option is selected, then all selected files are consolidated in one AnIML file.

6. (Optional) By default, the **Apply digital signature** check box is selected. To change the digital key when applying the digital signature, do this:

   a. Click **Select key**.

Figure 3-3 Select signing key and certificate Dialog



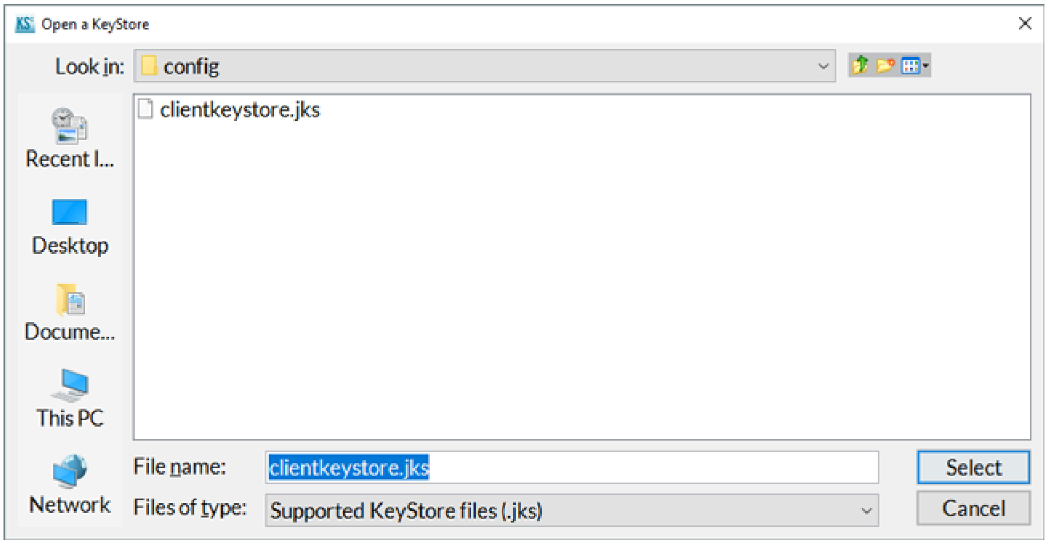
Select signing key and certificate

1. Step:

Select a KeyStore and open it with a password

b. Click **Open**.

Figure 3-4 Open a Keystore Dialog



Look in: config

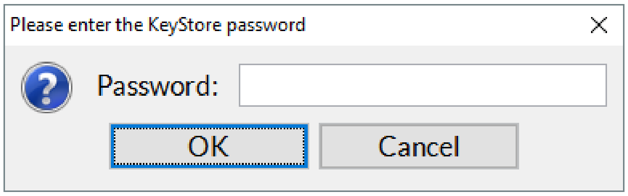
clientkeystore.jks

File name: clientkeystore.jks

Files of type: Supported KeyStore files (.jks)

c. Browse to the C:\ProgramData\KeystoneConverter\config folder, select the KeyStore file, and then click **Select**.

Figure 3-5 Please enter the KeyStore password Dialog

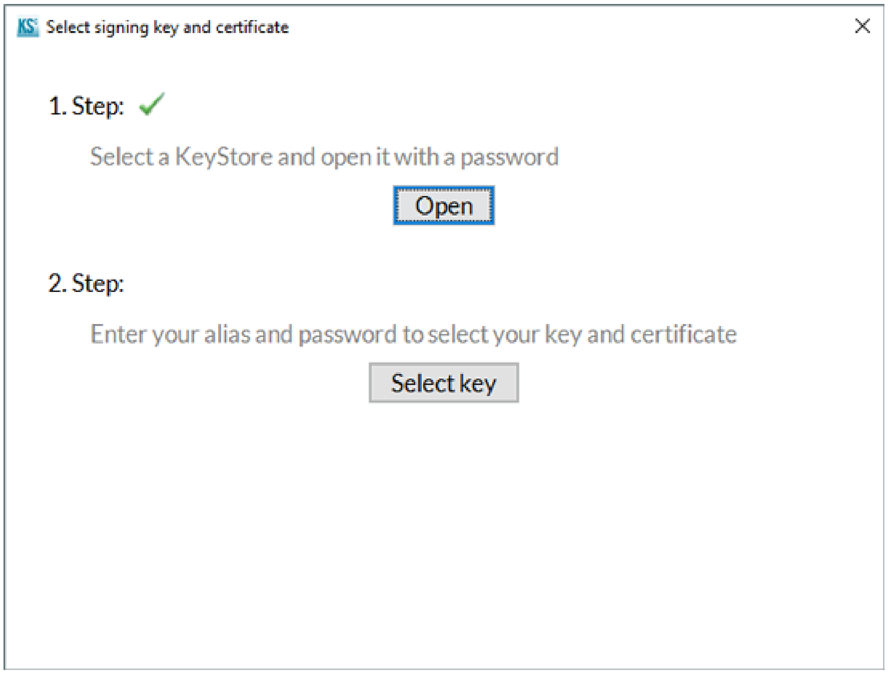


Please enter the KeyStore password

Password:

d. Type the KeyStore **Password** and then click **OK**.

Figure 3-6 Select signing key and certificate Dialog



Select signing key and certificate

1. Step: ✓

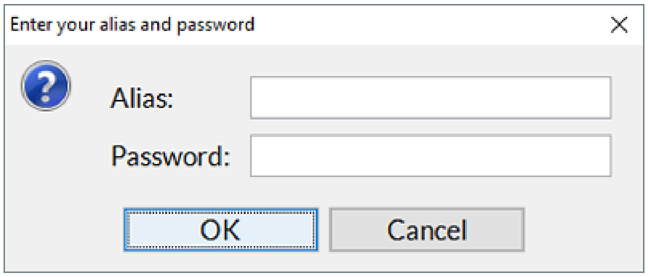
Select a KeyStore and open it with a password

2. Step:

Enter your alias and password to select your key and certificate

e. Click **Select key**.

Figure 3-7 Enter your alias and password Dialog



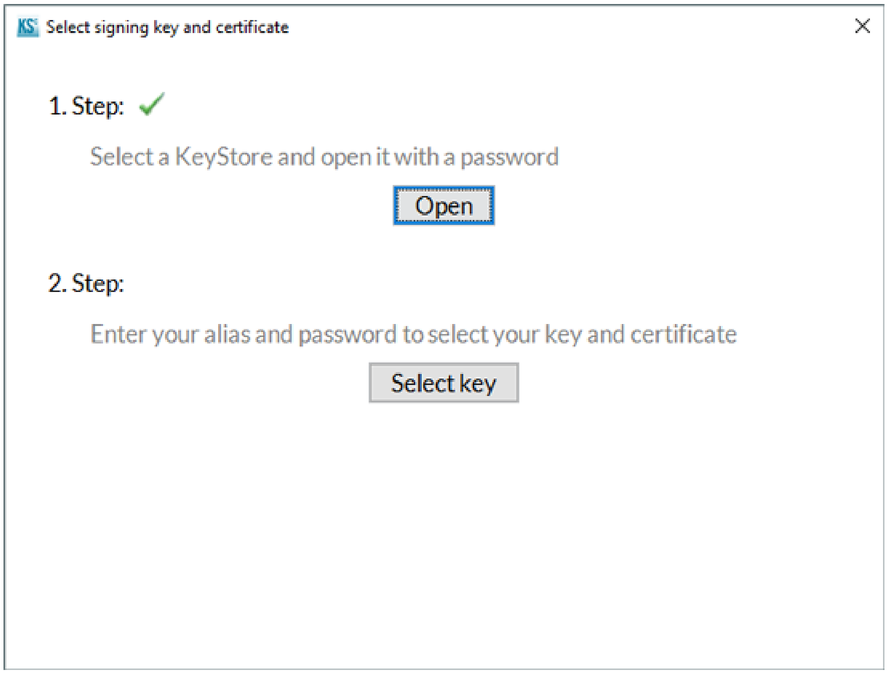
Enter your alias and password

Alias:

Password:

f. Type the **Alias** and **Password** and then click **OK**.

Figure 3-8 Select signing key and certificate Dialog



Select signing key and certificate

1. Step: ✓

Select a KeyStore and open it with a password

2. Step:

Enter your alias and password to select your key and certificate

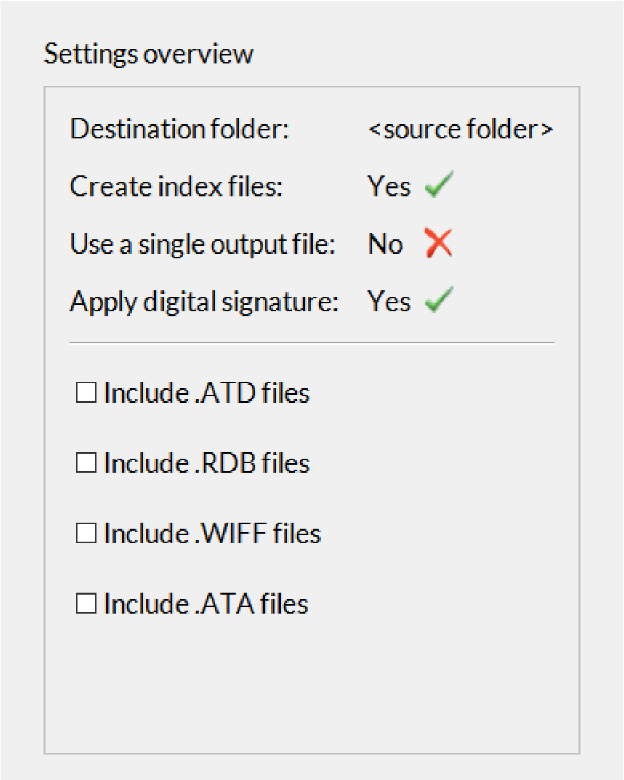
g. Click **Finish**.

A digital signature is applied to each converted file. The signature contains the name of the individual who completed the conversion and the date and time that the signature was applied.

7. Click **Convert** on the menu bar.

The Settings overview section shows a summary of the settings that were enabled.

Figure 3-9 Settings overview



Settings overview

Destination folder: <source folder>

Create index files: Yes ✓

Use a single output file: No ✗

Apply digital signature: Yes ✓

☐ Include .ATD files

☐ Include .RDB files

☐ Include .WIFF files

☐ Include .ATA files

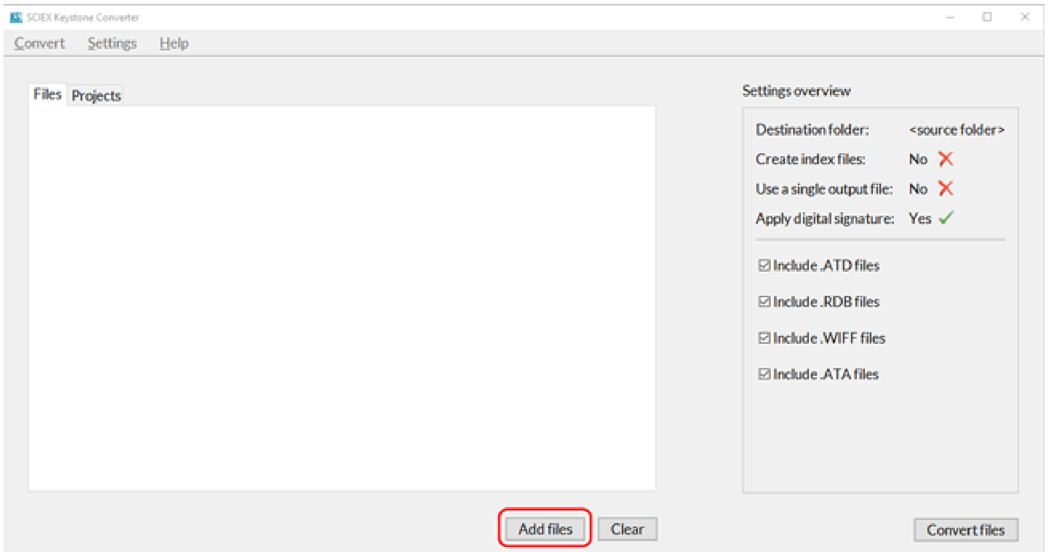
Convert a wiff File

Note: The active data root folder in the Analyst® Software must be the same data root that contains the data to be converted.

---

1. Open the Analyst® Software.
2. Click **Start > SCIEX Keystone > SCIEX Keystone Converter** to open the Keystone Converter Software.
3. Click **Convert**.
4. On the **Files** tab, click **Add files**.

Figure 3-10 SCIEX Keystone Converter: Files Tab



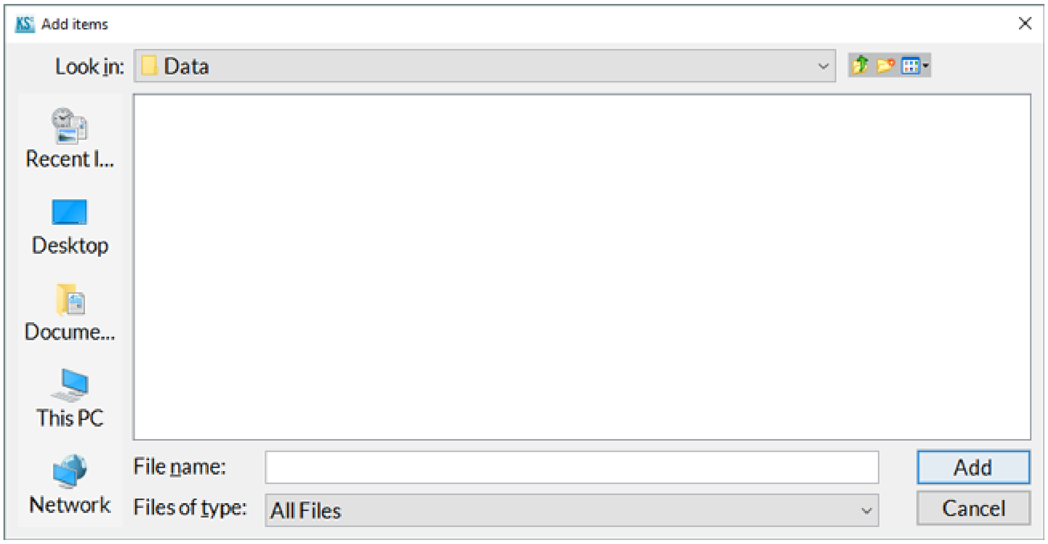
Settings overview

Destination folder: <source folder>
Create index files: No ✗
Use a single output file: No ✗
Apply digital signature: Yes ✓

☑ Include .ATD files
☑ Include .RDB files
☑ Include .WIFF files
☑ Include .ATA files

The Add items dialog opens.

Figure 3-11 Add items Dialog



Look in: Data
File name:
Files of type: All Files

5. Browse to and then select the wiff file to be converted.

Tip! Use the **Ctrl** or **Shift** key to select multiple files.

---

6. Click **Add**.

7. Select the **Include .WIFF files** check box. Refer to Figure 3-10.
8. Click **Convert files**.

   The Output file dialog opens.

   > **Note:** If a default Destination folder has been configured, then the software opens the specified folder. If a default Destination folder has not been configured, then the software automatically saves the converted files in the same location as the source files.

9. If required, type a **File name** for the converted file.

   > **Note:** If one file is being converted, then the software automatically assigns the source file name to the converted file and appends *animl* to the file name. If the **Single output file** option was selected, then a **File name** must be provided.

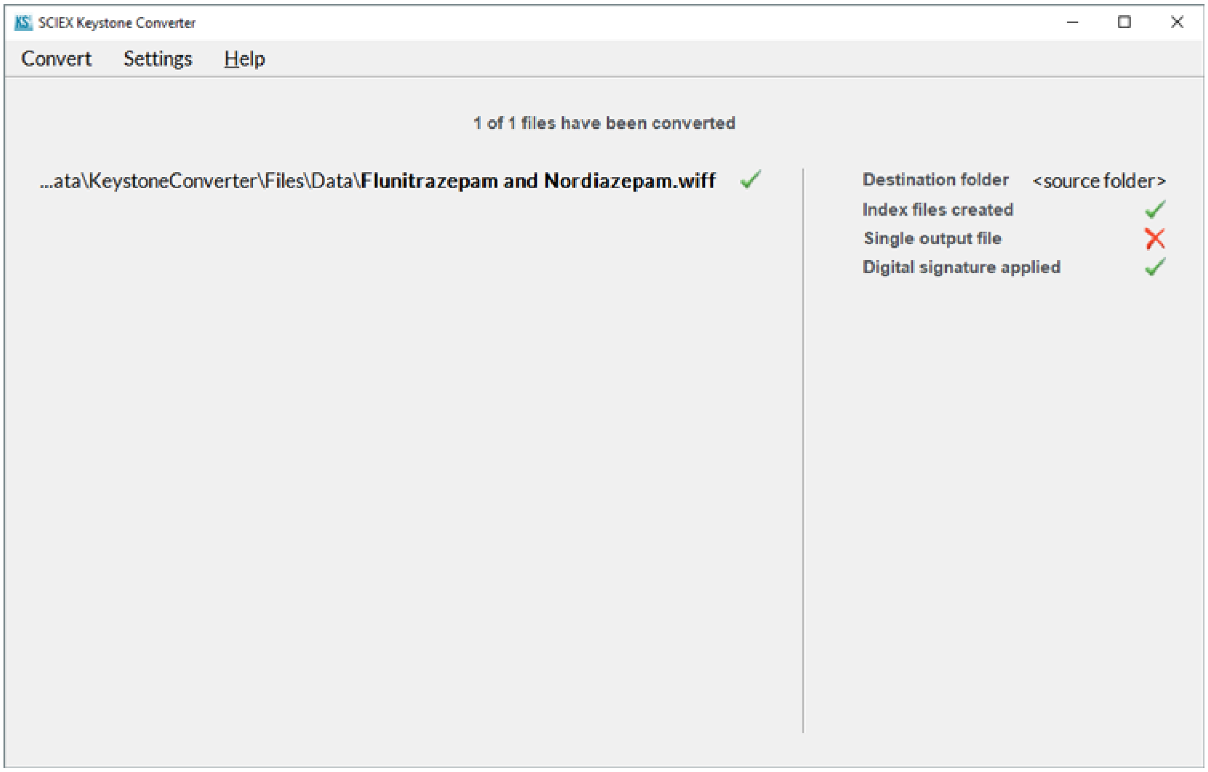
10. Click **Save**.

    The Output file dialog closes and a progress bar is shown.

11. When the conversion is complete, click **OK**.

    The dialog refreshes, showing the results of the conversion.

Figure 3-12 Conversion Status: Success



1 of 1 files have been converted

...ata\KeystoneConverter\Files\Data**Flunitrazepam and Nordiazepam.wiff** ✓

Destination folder <source folder>
Index files created ✓
Single output file ✗
Digital signature applied ✓

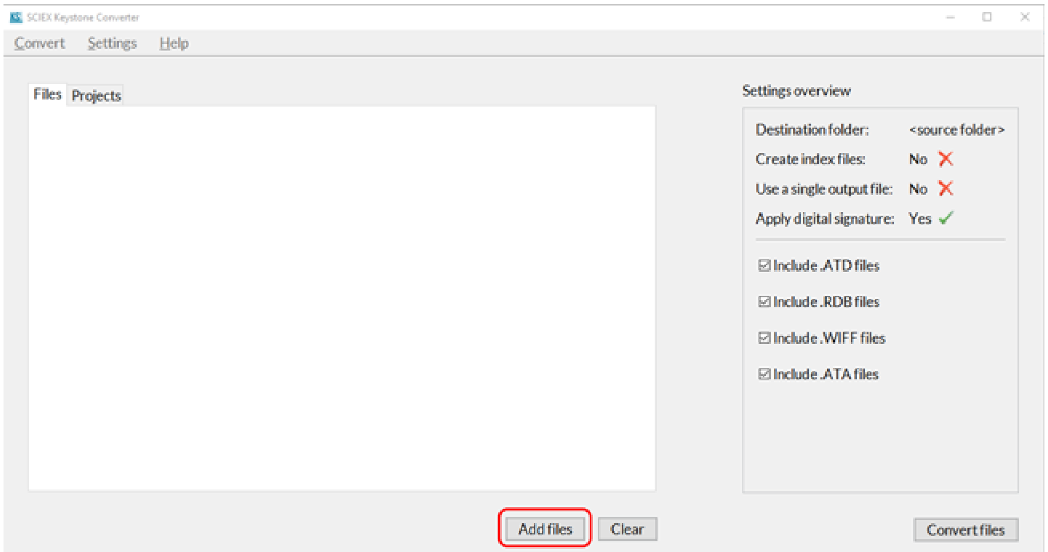
Convert an rdb File

Note: The Analyst® Software must be open to convert an rdb file.

Note: The active data root folder in the Analyst® Software must be the same data root that contains the data to be converted.

1. Open the Analyst® Software.
2. Click **Start > SCIEX Keystone > SCIEX Keystone Converter** to open the Keystone Converter Software.
3. Click **Convert**.
4. On the **Files** tab, click **Add files**.

Figure 3-13 SCIEX Keystone Converter: Files Tab

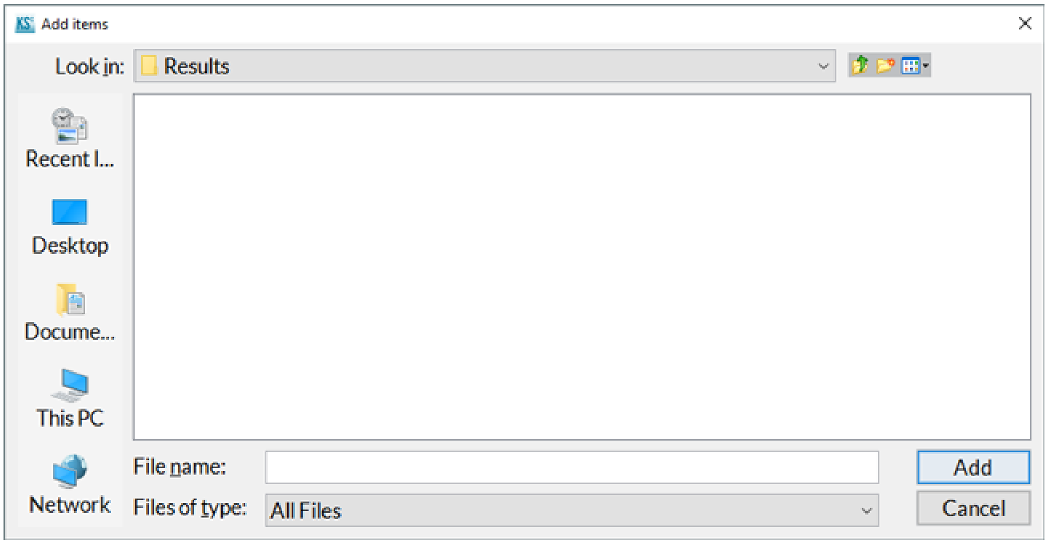


Destination folder: <source folder>
Create index files: No ✗
Use a single output file: No ✗
Apply digital signature: Yes ✓

☑ Include .ATD files
☑ Include .RDB files
☑ Include .WIFF files
☑ Include .ATA files

The Add items dialog opens.

Figure 3-14 Add items Dialog



Look in: Results
File name:
Files of type: All Files

5. Browse to and then select the rdb file to be converted.

Tip! Use the **Ctrl** or **Shift** key to select multiple files.

---

6. Click **Add**.

7. Select the **Include .RDB files** check box. Refer to Figure 3-13.

8. Click **Convert files**.

   The Output file dialog opens.

   Note: If a default Destination folder has been configured, then the software opens the specified folder. If a default Destination folder has not been configured, then the software automatically saves the converted files in the same location as the source files.

   ---

9. If required, type a **File name** for the converted file.

   Note: If one file is being converted, then the software automatically assigns the source file name to the converted file and appends *animl* to the file name. If the **Single output file** option was selected, then a **File name** must be provided.

   ---

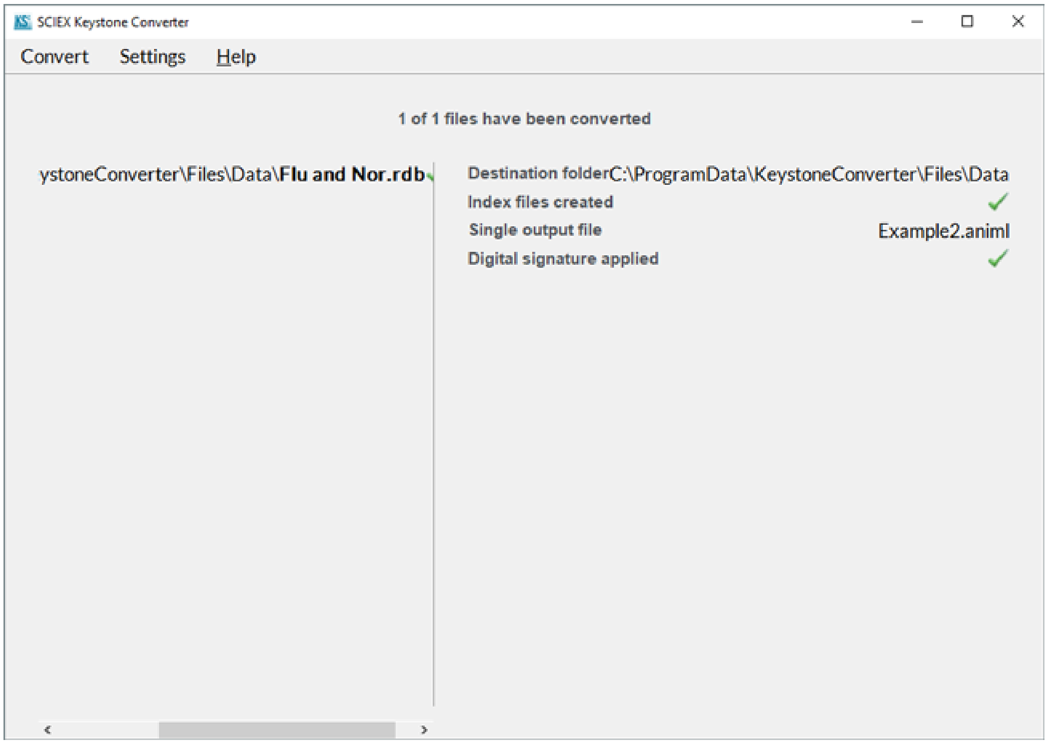
10. Click **Save**.

    The Output file dialog closes and a progress bar is shown.

11. When the conversion is complete, click **OK**.

    The dialog refreshes, showing the results of the conversion.

Figure 3-15 Conversion Status: Success



1 of 1 files have been converted

ystoneConverter\Files\Data\Flu and Nor.rdb ✓

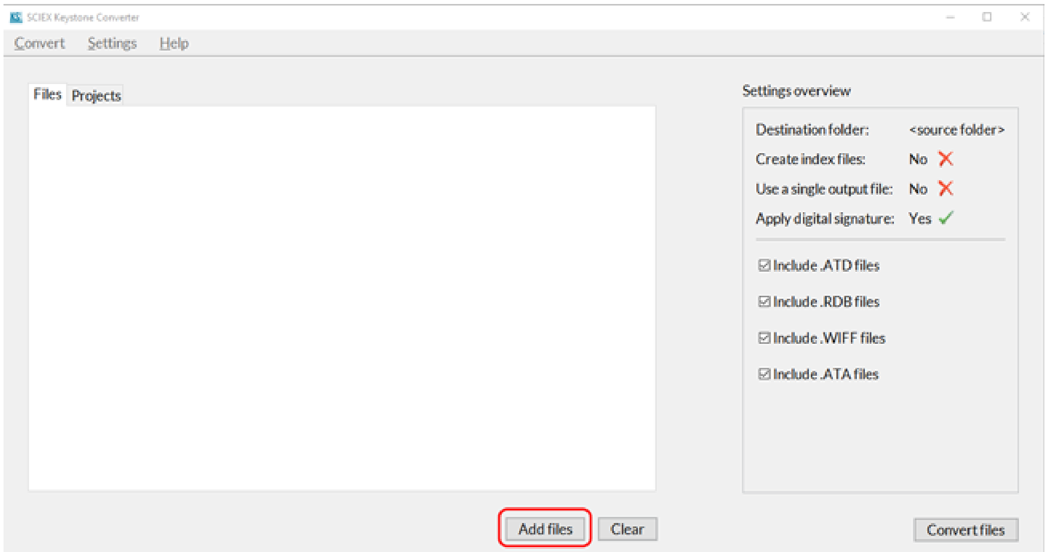
Destination folder C:\ProgramData\KeystoneConverter\Files\Data
Index files created ✓
Single output file Example2.animl
Digital signature applied ✓

Convert an ata or atd File

Note: The active data root folder in the Analyst® Software must be the same data root that contains the data to be converted.

1. Open the Analyst® Software.
2. Click **Start > SCIEX Keystone > SCIEX Keystone Converter** to open the Keystone Converter Software.
3. Click **Convert**.
4. On the **Files** tab, click **Add files**.

Figure 3-16 SCIEX Keystone Converter: Files Tab



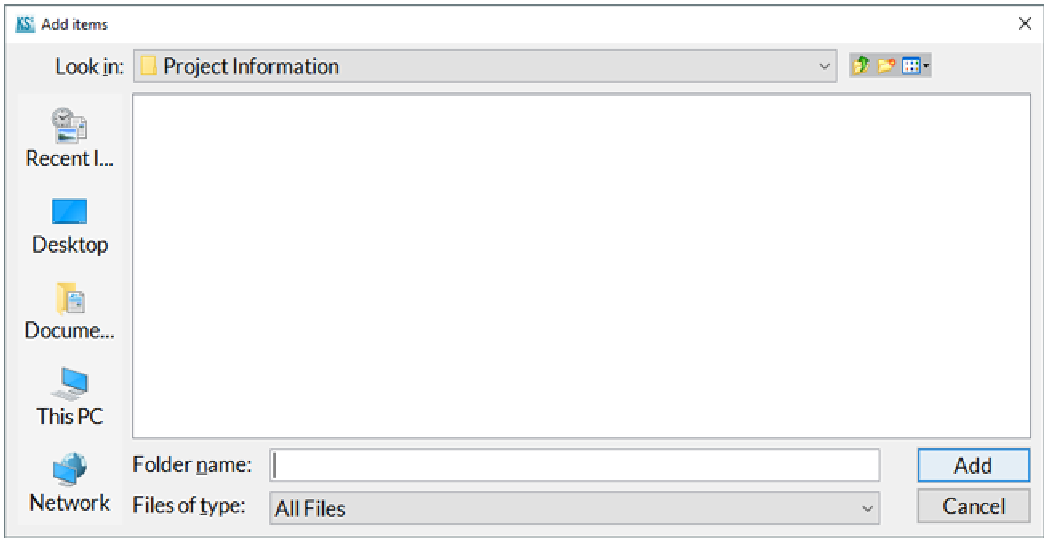
Settings overview

Destination folder: <source folder>
Create index files: No ✗
Use a single output file: No ✗
Apply digital signature: Yes ✓

☑ Include .ATD files
☑ Include .RDB files
☑ Include .WIFF files
☑ Include .ATA files

The Add items dialog opens.

Figure 3-17 Add items Dialog



Look in: Project Information
Folder name:
Files of type: All Files

5. Browse to and then select the ata or atd file to be converted.

Tip! Use the **Ctrl** or **Shift** key to select multiple files.

---

6. Click **Add**.

7. Select the **Include .ATD files** check box. Refer to Figure 3-16.

8. Click **Convert files**.

   The Output file dialog opens.

   Note: If a default Destination folder has been configured, then the software opens the specified folder. If a default Destination folder has not been configured, then the software automatically saves the converted files in the same location as the source files.

9. If required, type a **File name** for the converted file.

   Note: If one file is being converted, then the software automatically assigns the source file name to the converted file and appends *animl* to the file name. If the **Single output file** option was selected, then a **File name** must be provided.

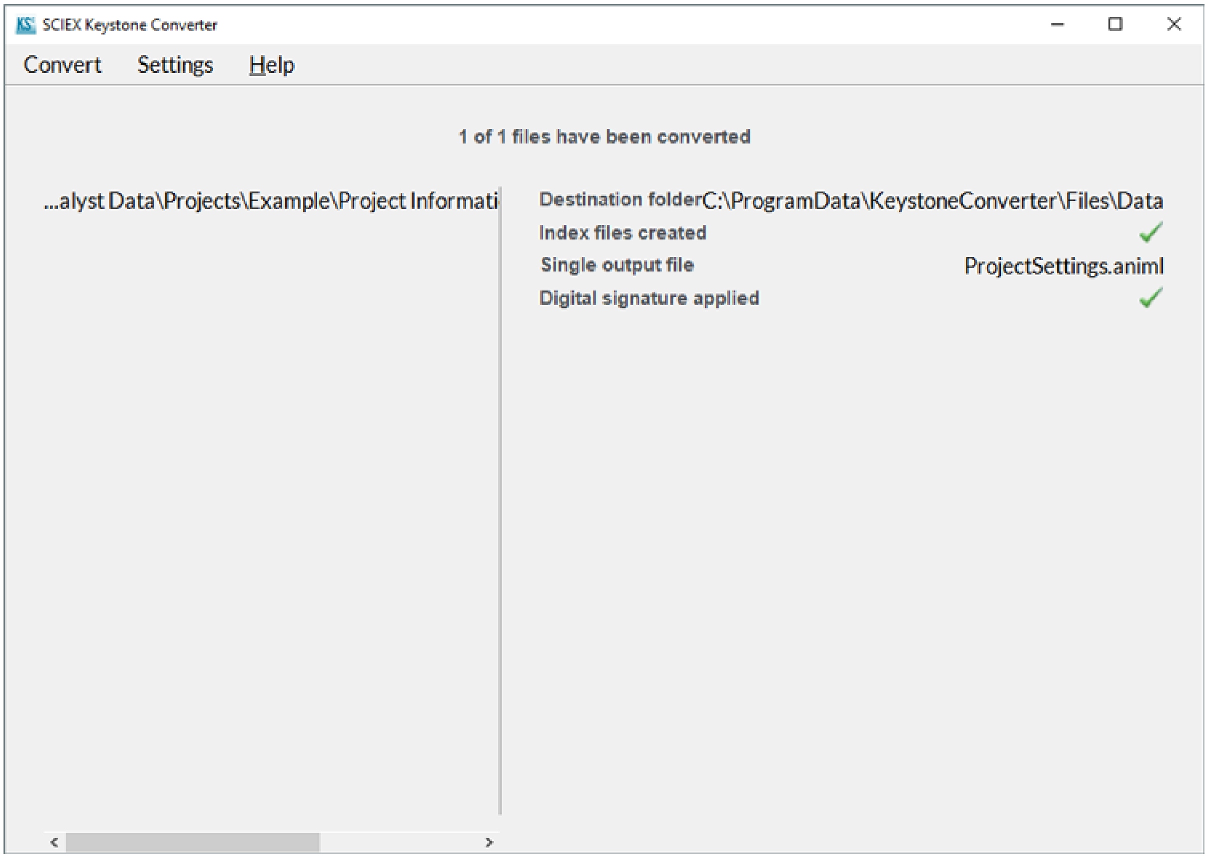
10. Click **Save**.

    The Output file dialog closes and a progress bar is shown.

11. When the conversion is complete, click **OK**.

    The dialog refreshes, showing the results of the conversion.

Figure 3-18 Conversion Status: Success



1 of 1 files have been converted

...alyst Data\Projects\Example\Project Informati

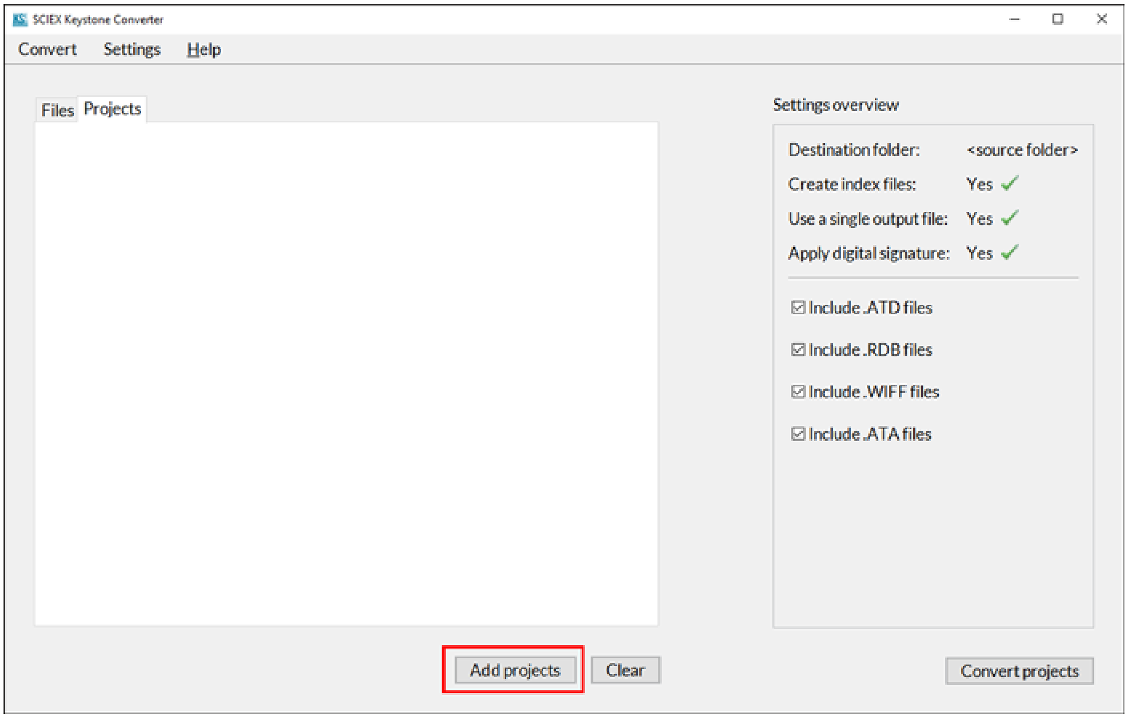
Destination folder	C:\ProgramData\KeystoneConverter\Files\Data
Index files created	✓
Single output file	ProjectSettings.animl
Digital signature applied	✓

Convert all of the Files in a Project

Note: The active data root folder in the Analyst® Software must be the same data root that contains the data to be converted.

1. Open the Analyst® Software.
2. Click **Start > SCIEX Keystone > SCIEX Keystone Converter** to open the Keystone Converter Software.
3. Click **Convert**.
4. On the **Projects** tab, click **Add projects**.

Figure 3-19 SCIEX Keystone Converter: Projects Tab

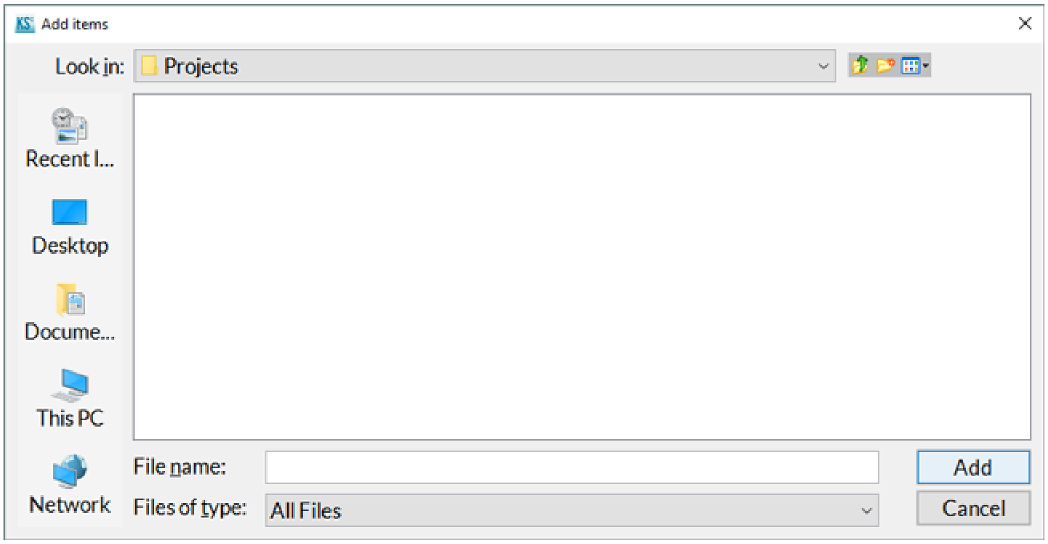


Destination folder: <source folder>
Create index files: Yes ✓
Use a single output file: Yes ✓
Apply digital signature: Yes ✓

☑ Include .ATD files
☑ Include .RDB files
☑ Include .WIFF files
☑ Include .ATA files

The Add items dialog opens.

Figure 3-20 Add items Dialog



Look in: Projects

Files of type: All Files

5. Browse to and then select the project files to be converted.

Tip! Use the **Ctrl** or **Shift** key to select multiple projects.

6. Click **Add**.
7. Select the check box for each type of file to be converted. Refer to Figure 3-19.

Note: One or more check boxes can be selected.

8. Click **Convert projects**.

   The Output file dialog opens.

Note: If a default Destination folder has been configured, then the software opens the specified folder. If a default Destination folder has not been configured, then the software automatically saves the converted files in the same location as the source files.

9. If the **Use a single output file** option has been selected, then type a **File name** and click **Save**.

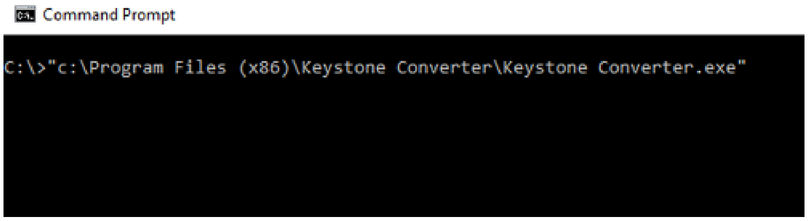
Note: If the **Use a single output file** option has not been selected, then each converted file is automatically given the same name as the source file.

Convert Data using the Command Line

1. Open the Command Prompt window.
2. Type the following command and then press **Enter**:

   <drive>:**"c:\Program Files(x86)\Keystone Converter\Keystone Converter.exe"**

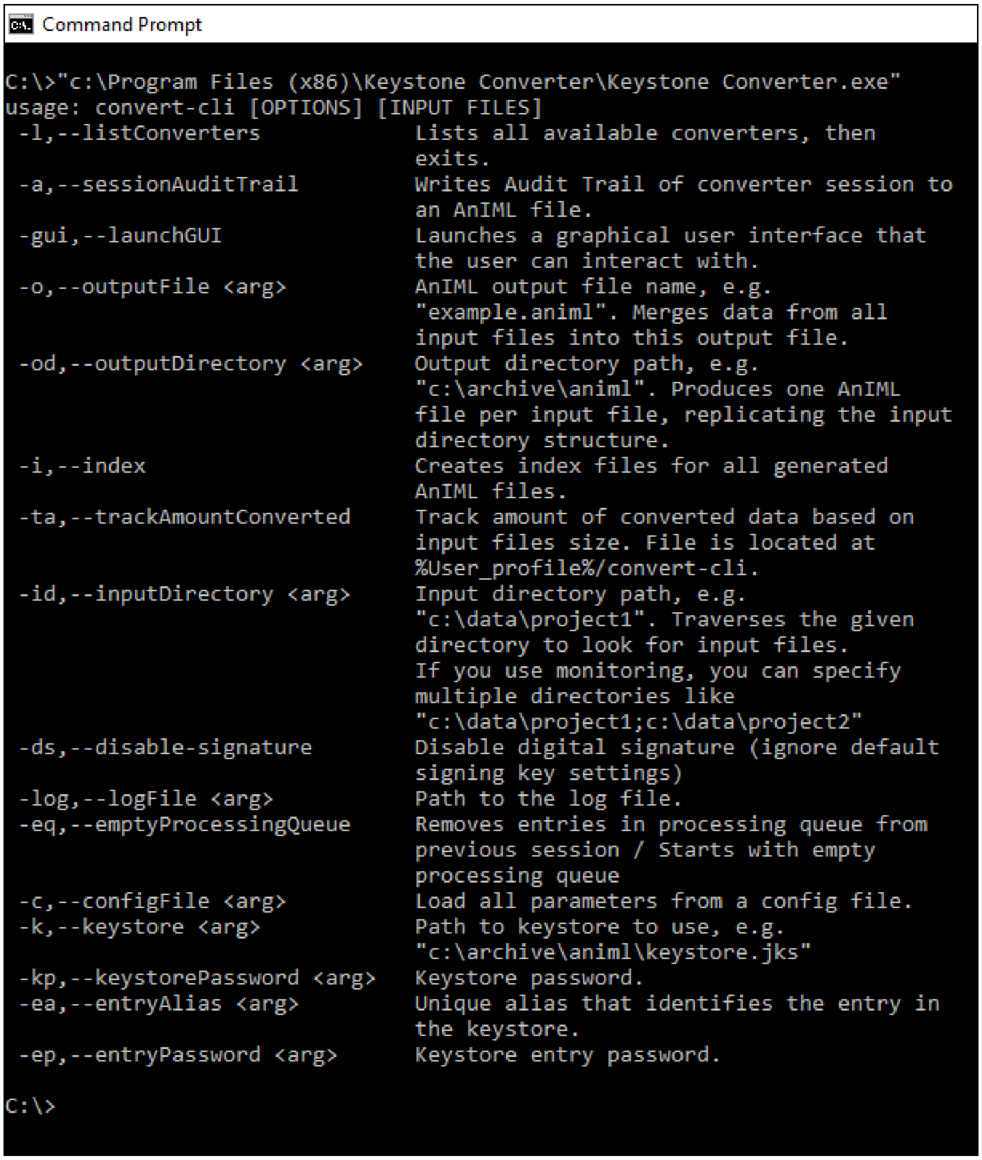
Figure 3-21 Command Prompt: Run the Executable



```
C:\>"c:\Program Files (x86)\Keystone Converter\Keystone Converter.exe"
```

Tip! To view a list of available options, type <drive>**:\"c:\Program Files(x86)\Keystone Converter\Keystone Converter.exe"** and then press **Enter**

Figure 3-22 Software Options



```
C:\>"c:\Program Files (x86)\Keystone Converter\Keystone Converter.exe"
usage: convert-cli [OPTIONS] [INPUT FILES]
 -l,--listConverters            Lists all available converters, then
                                exits.
 -a,--sessionAuditTrail         Writes Audit Trail of converter session to
                                an AnIML file.
 -gui,--launchGUI               Launches a graphical user interface that
                                the user can interact with.
 -o,--outputFile <arg>          AnIML output file name, e.g.
                                "example.animl". Merges data from all
                                input files into this output file.
 -od,--outputDirectory <arg>    Output directory path, e.g.
                                "c:\archive\animl". Produces one AnIML
                                file per input file, replicating the input
                                directory structure.
 -i,--index                     Creates index files for all generated
                                AnIML files.
 -ta,--trackAmountConverted     Track amount of converted data based on
                                input files size. File is located at
                                %User_profile%/convert-cli.
 -id,--inputDirectory <arg>     Input directory path, e.g.
                                "c:\data\project1". Traverses the given
                                directory to look for input files.
                                If you use monitoring, you can specify
                                multiple directories like
                                "c:\data\project1;c:\data\project2"
 -ds,--disable-signature        Disable digital signature (ignore default
                                signing key settings)
 -log,--logFile <arg>           Path to the log file.
 -eq,--emptyProcessingQueue     Removes entries in processing queue from
                                previous session / Starts with empty
                                processing queue
 -c,--configFile <arg>          Load all parameters from a config file.
 -k,--keystore <arg>            Path to keystore to use, e.g.
                                "c:\archive\animl\keystore.jks"
 -kp,--keystorePassword <arg>   Keystore password.
 -ea,--entryAlias <arg>         Unique alias that identifies the entry in
                                the keystore.
 -ep,--entryPassword <arg>      Keystore entry password.

C:\>
```

Note: The -od and -o options cannot be used together. The -od option writes all of the files to a new folder, using the existing name plus animl as the extension. The -o options sets the filename for one new file. This file can include a complete folder if one did not exist originally.

Renew the Keystone Converter Software License

1. Obtain a new license file from SCIEX and then save it on the desktop.
2. Browse to C:\ProgramData\KeystoneConverter\license and then delete the keystone_license.lic file.
3. Click **Start > SCIEX Keystone > SCIEX Keystone Converter** to open the Keystone Converter Software.
4. Click **Select**.
5. Browse to the Desktop, select the **keystone converter license.lic** file, and then click **Open**.

   The license selection dialog refreshes, showing the license file that was selected.
6. Click **Finish**.

   The Keystone Converter Software opens.

Keystone Viewer Software

4

View Converted wiff Files

A wiff file is the proprietary format for storage of data acquired by SCIEX mass spectrometers. The wiff file contains general information about the file, such as acquisition methods, batch, and device, as well as raw data.

Open a wiff.animl File

1. Click **Start > SCIEX Keystone > SCIEX Keystone Viewer**.
2. Click **File > Open**.

   The Open dialog opens.
3. Browse to and select the appropriate wiff.animl file and then click **Open**.

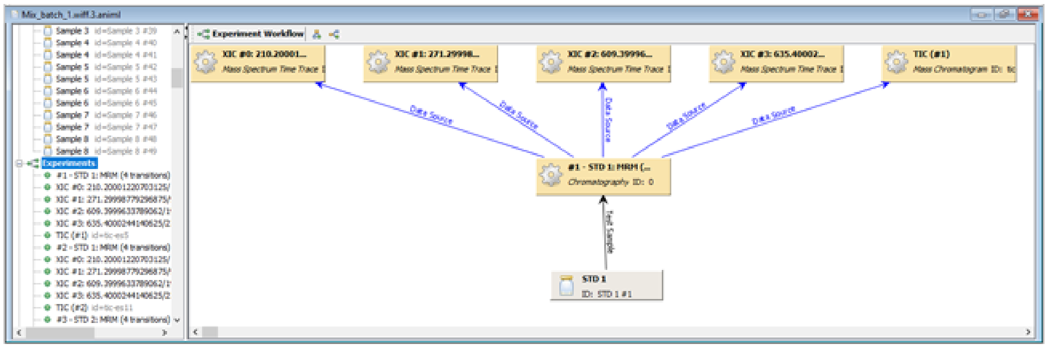
Tip! Press the **Shift** key to select multiple wiff.animl files.

View the Experiment Workflow

1. In the Navigation pane, click **Experiments**.

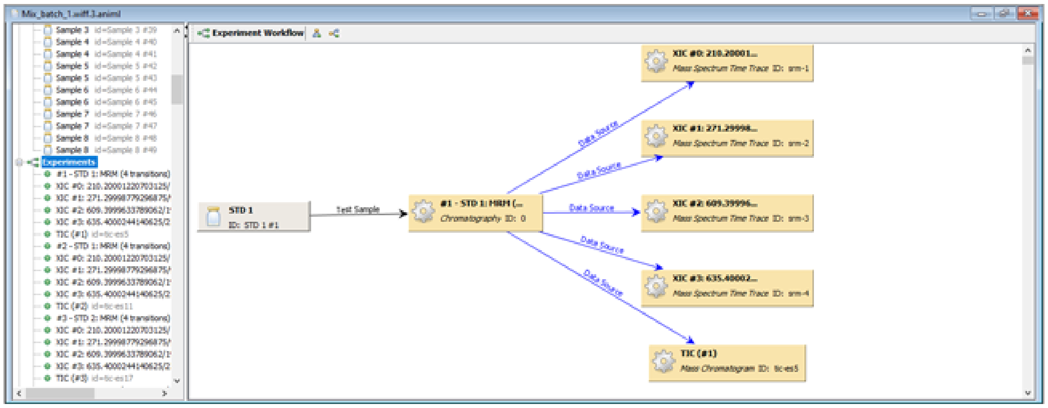
   The Experiment Workflow pane opens. By default the information is shown hierarchically.

   Figure 4-1 Hierarchical View



Tip! (Optional) To view the information horizontally, click .

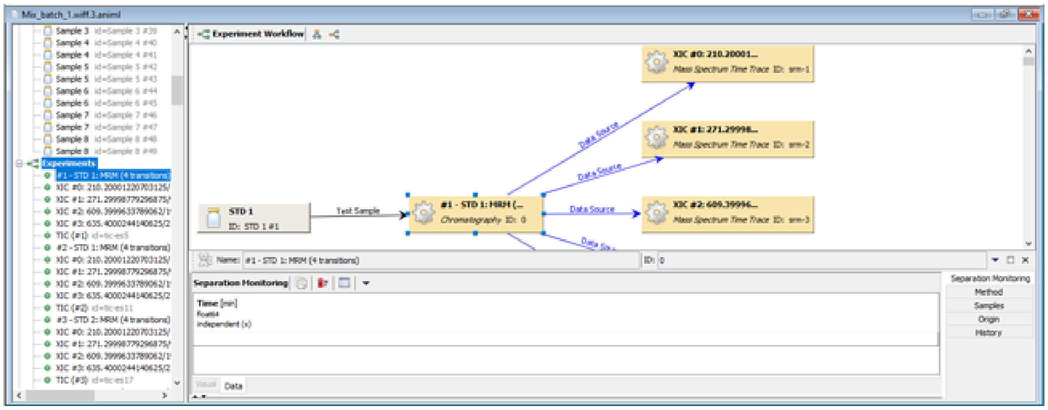
Figure 4-2 Horizontal View



---

2. Click an item to view the associated information.
    - If a sample is selected, then the corresponding sample is highlighted in the Navigation pane, and a new pane opens at the bottom of the window, showing the **Name** and the **Sample ID**.
    - If an MRM transition is selected, then the corresponding MRM entry is highlighted in the Navigation pane, and a new pane opens at the bottom of the window, showing the **Name** and **ID** of the MRM transition.

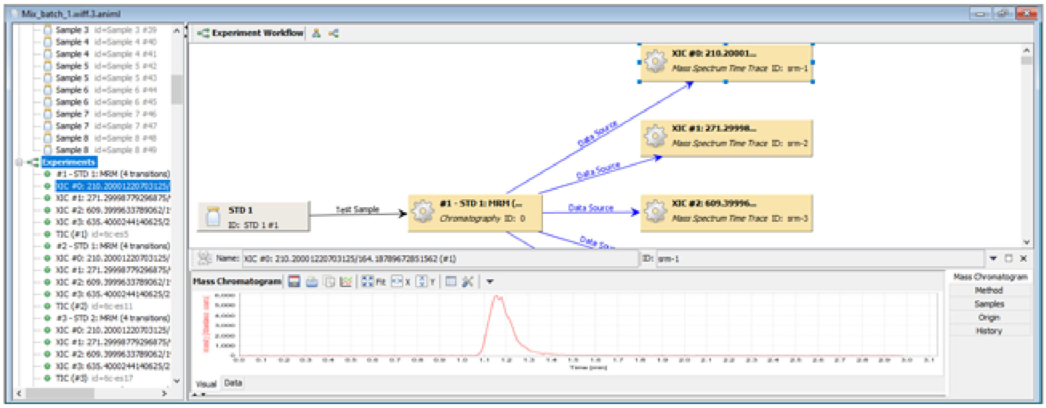
Figure 4-3 Example: MRM



Name: #1 - STD 1: MRM (4 transitions)
ID: 0

- If an XIC is selected, then the corresponding XIC entry is highlighted in the Navigation pane, and a new pane opens at the bottom of the window, showing the mass chromatogram of the selected XIC.

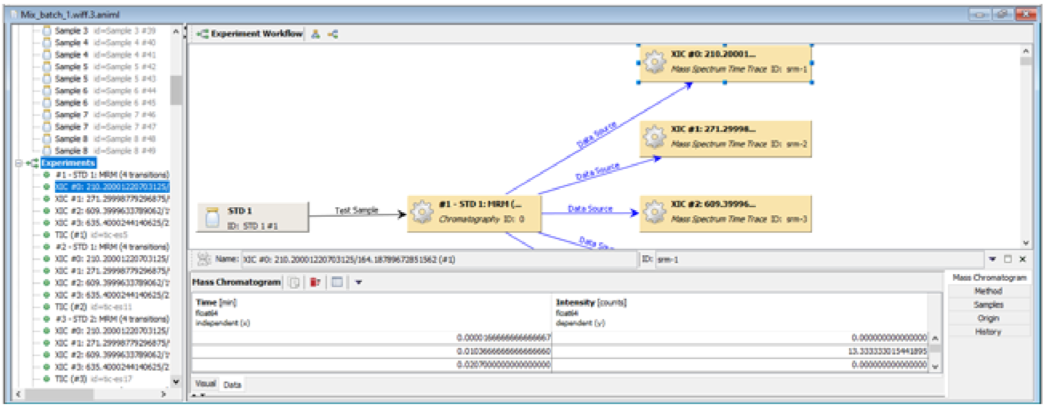
Figure 4-4 Example: XIC #0 Visual Tab



3. (Optional) Click **Data**.

   The pane at the bottom of the window refreshes, showing the **Time** (X-axis) and **Intensity** (Y-axis) values in table format.

Figure 4-5 Example: XIC #0 Data Tab



View MRM Transition Information

Prerequisite Procedures
- Open a wiff.animl File.

1. In the Navigation pane, click the **MRM** transition to be viewed.

   The pane at the right side of the window refreshes, showing the **Name** and the **ID** of the selected transition.

Figure 4-6 Example MRM Transition: Separation Monitoring

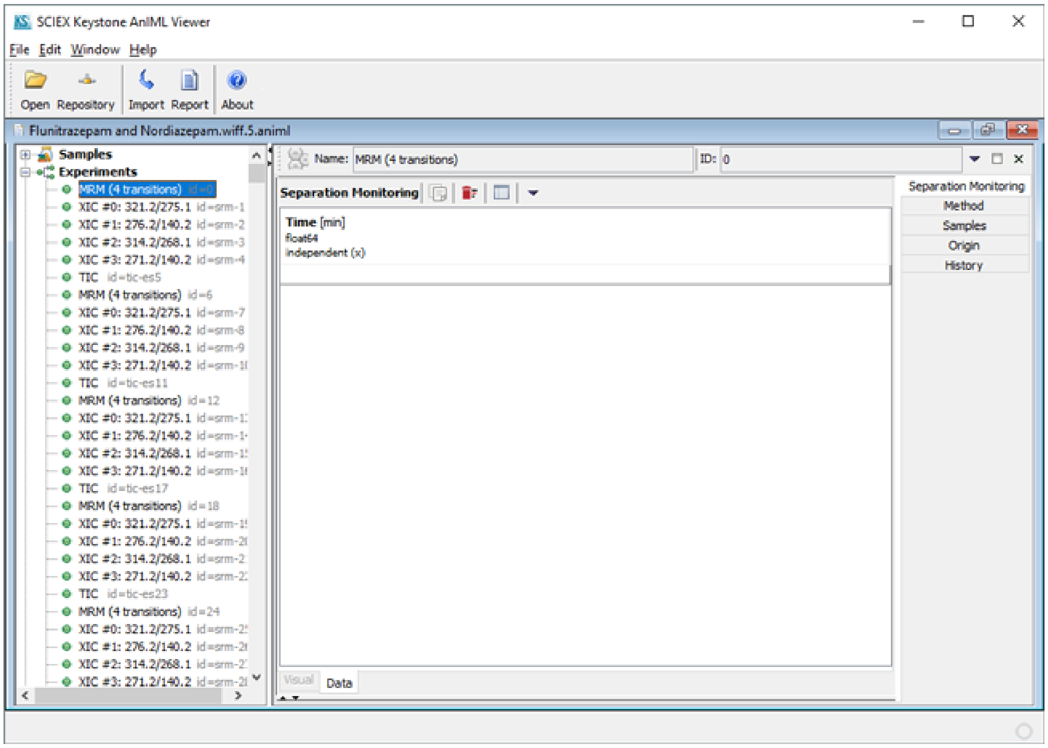


Table 4-1 Icons

Icon	Name	Description
⧉	Copy table data	Creates a copy of the table information and puts it on the computer clipboard.
🗑	Remove row	Removes the selected row from the table. **Tip!** Use the **Ctrl** or **Shift** key to select multiple rows. Changes made in the Viewer do not affect the actual file.

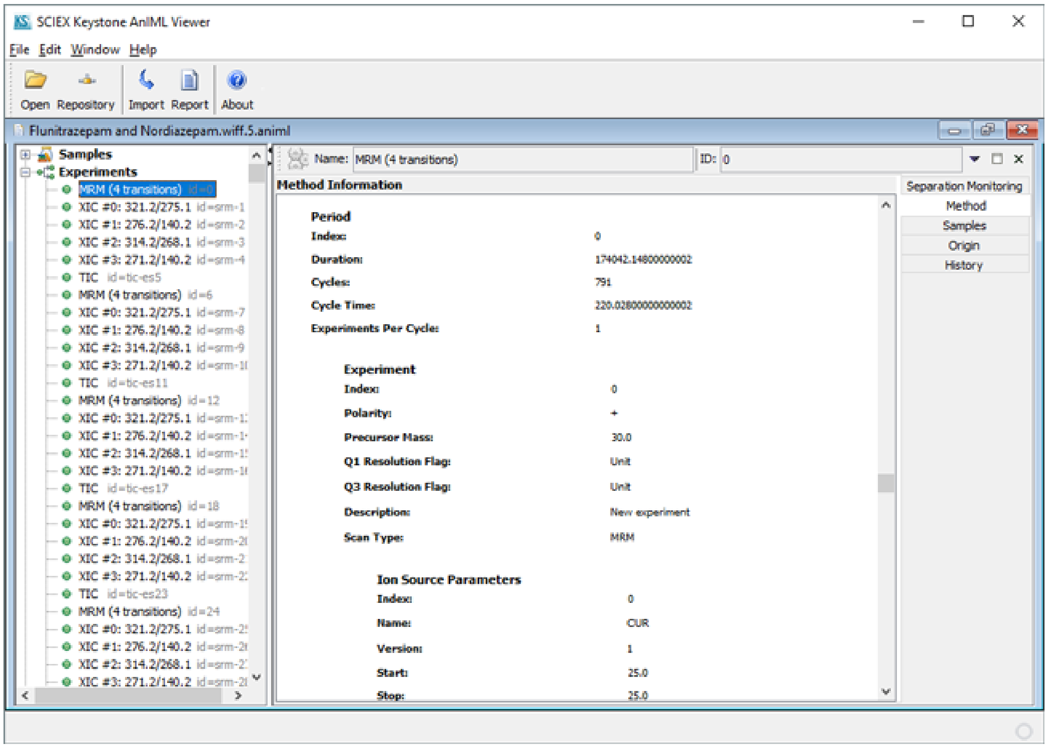
Table 4-1 Icons (continued)

Icon	Name	Description
▦	Configure visible columns	Opens a dialog that can be used to show or hide columns.
▼	Actions — Export to Excel	Exports the information to a Microsoft Excel spreadsheet.

2. To view the details of the acquisition method associated with the selected MRM transition, under Separation Monitoring in the right panel, click **Method**.

Note: This information corresponds to the File Information available using the **Explore > Show > Show File Information** option in the Analyst® Software.

Figure 4-7 Example MRM Transition: Method



Name: MRM (4 transitions)
ID: 0

Method Information

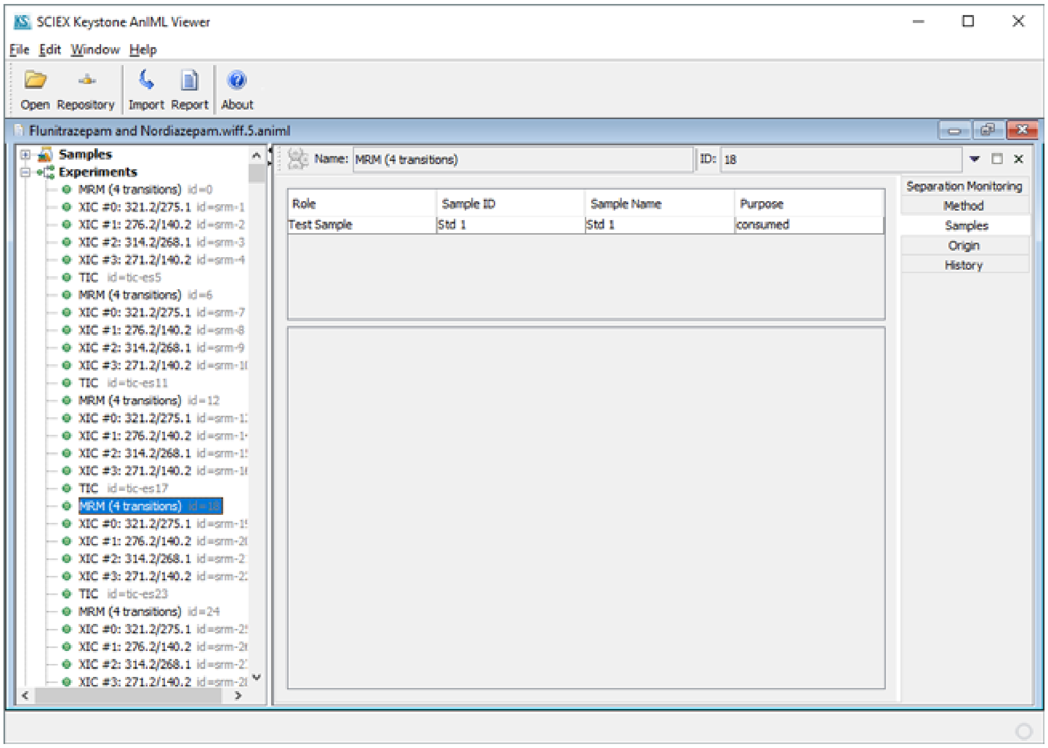
Period
Index: 0
Duration: 174042.14800000002
Cycles: 791
Cycle Time: 220.02800000000002
Experiments Per Cycle: 1

Experiment
Index: 0
Polarity: +
Precursor Mass: 30.0
Q1 Resolution Flag: Unit
Q3 Resolution Flag: Unit
Description: New experiment
Scan Type: MRM

Ion Source Parameters
Index: 0
Name: CUR
Version: 1
Start: 25.0
Stop: 25.0

3. To view the details of the sample associated with the selected MRM transition, click **Samples**.

Figure 4-8 Example MRM Transition: Samples



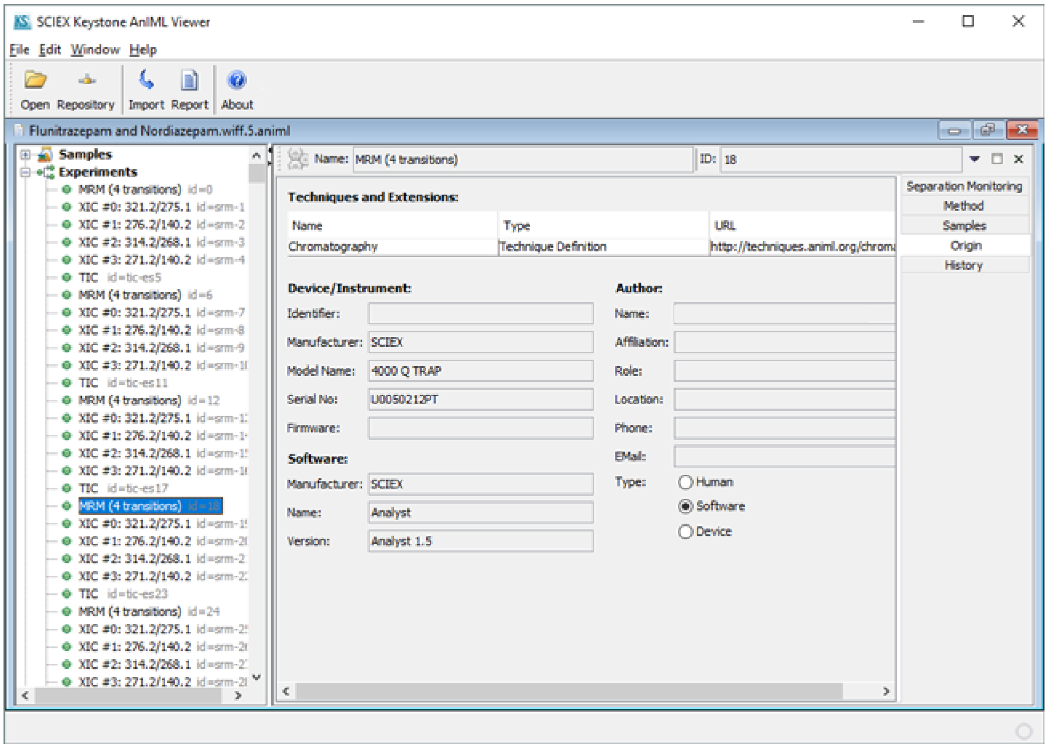
Name: MRM (4 transitions)

ID: 18

Role	Sample ID	Sample Name	Purpose
Test Sample	Std 1	Std 1	consumed

4. To view the details of the instrument and software used to acquire the data, as well as the user information, click **Origin**.

Figure 4-9 Example MRM Transition: Origin



Name: MRM (4 transitions)
ID: 18

Techniques and Extensions:

Name	Type	URL
Chromatography	Technique Definition	http://techniques.animl.org/chrom

Device/Instrument:

Identifier:
Manufacturer: SCIEX
Model Name: 4000 Q TRAP
Serial No: U0050212PT
Firmware:

Software:

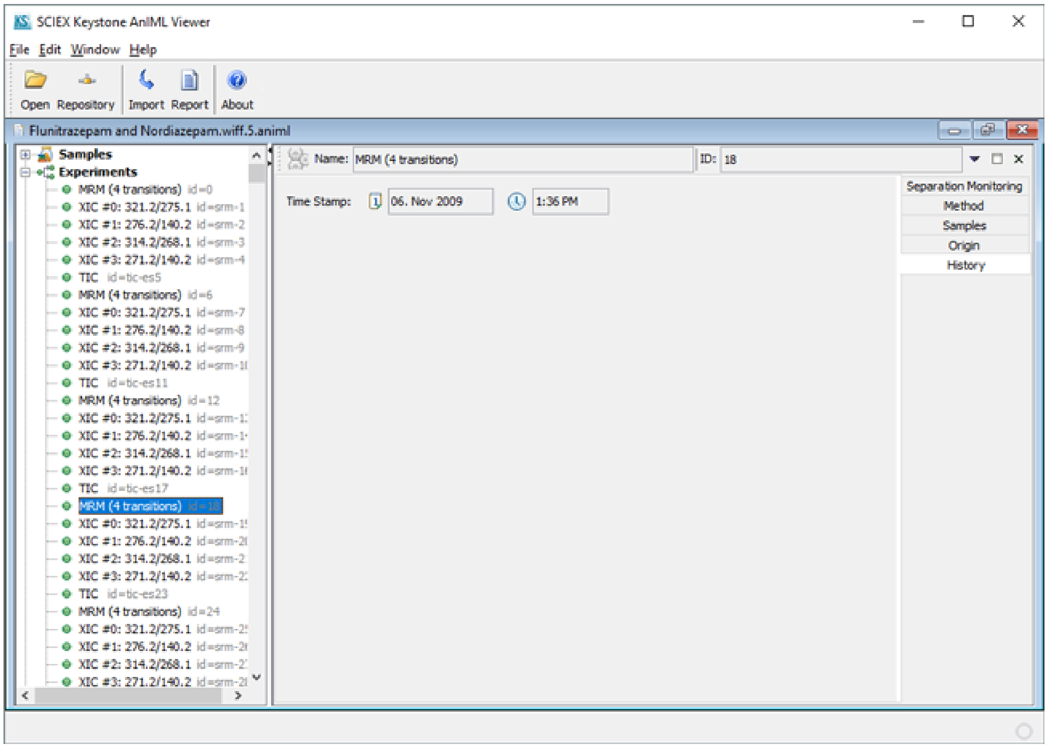
Manufacturer: SCIEX
Name: Analyst
Version: Analyst 1.5

Author:

Name:
Affiliation:
Role:
Location:
Phone:
EMail:
Type: ○ Human ● Software ○ Device

5. To view the date and time that the sample was acquired, click **History**.

Figure 4-10 Example MRM Transition: History



Name: MRM (4 transitions)

ID: 18

Time Stamp: 06. Nov 2009 1:36 PM

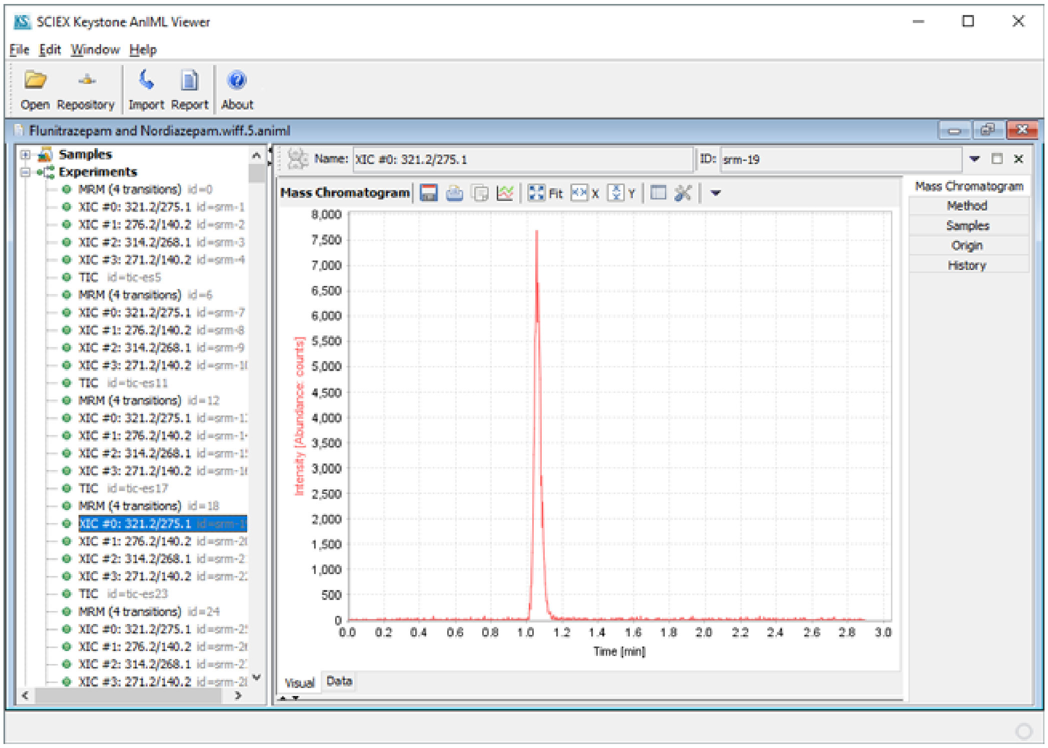
View Extracted Ion Chromatogram (XIC) Information

Prerequisite Procedures
• Open a wiff.animl File.

1. In the Navigation pane, click the **XIC** to be viewed.

   The pane at the right side of the window refreshes, showing the **Name**, **ID**, and **Mass Chromatogram** for the selected XIC.

Figure 4-11 Example: XIC #0 Visual Tab



Name: XIC #0: 321.2/275.1

ID: srm-19

Table 4-2 Icons

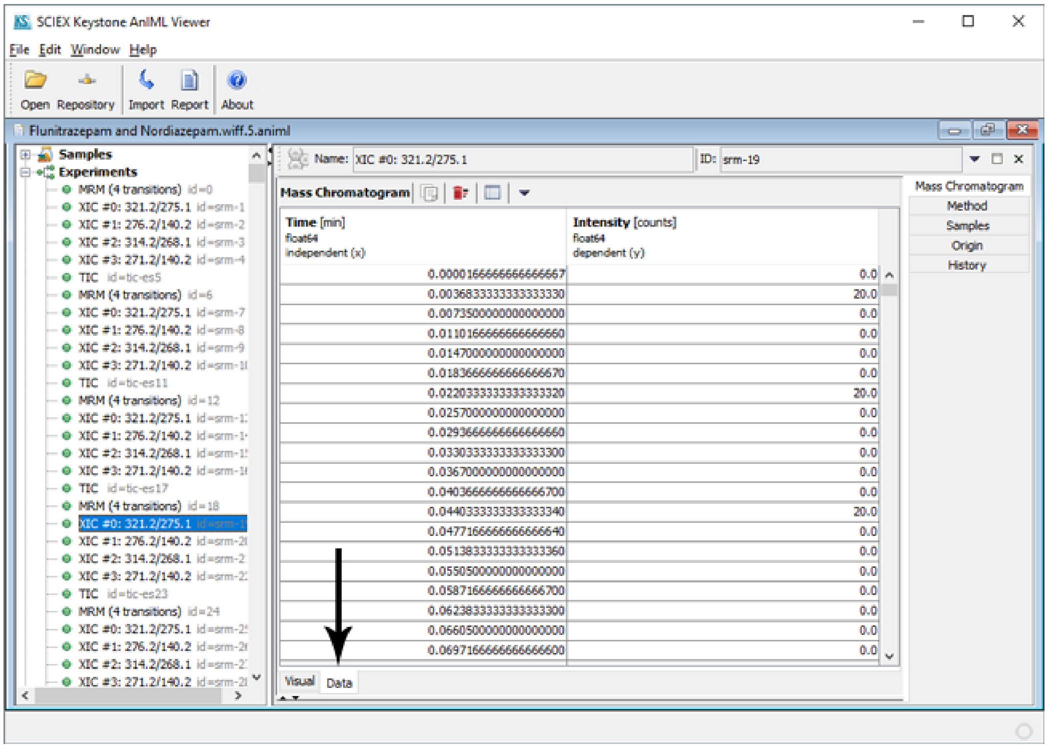
Icon	Name	Description
💾	Export image	Exports the image to a Portable Network Graphic (png) file.
🖨	Print	Prints the chromatogram to a selected printer.
⧉	Copy image	Creates a copy of the image and puts it on the computer clipboard.
📈	Add to Visualization	Adds the chromatogram to a visualization graph. Refer to Create a Visualization Graph.
Fit	Scale to fit	Returns a zoomed chromatogram to the original size.
X	Scale to fit x axis	Resizes the chromatogram to span the full X-axis.

Table 4-2 Icons (continued)

Icon	Name	Description
↕ Y	Scale to fit y axis	Resizes the chromatogram to span the full Y-axis.
▤	Configure visible series	Reorders or hides columns. Refer to Configure Visible Series or Columns.
✂	Format plot	Sets the formats of the plots. Refer to Set Chart Properties.
▼	Export to Excel	Exports the **Time** and **Intensity** values for the chromatogram to a Microsoft Excel spreadsheet.

2. Click the **Data** tab to view the **Time**, in minutes, of each peak apex and the **Intensity**, in counts per second, of each peak, in table format.

Figure 4-12 Example: XIC #0 Data Tab



Name: XIC #0: 321.2/275.1

ID: srm-19

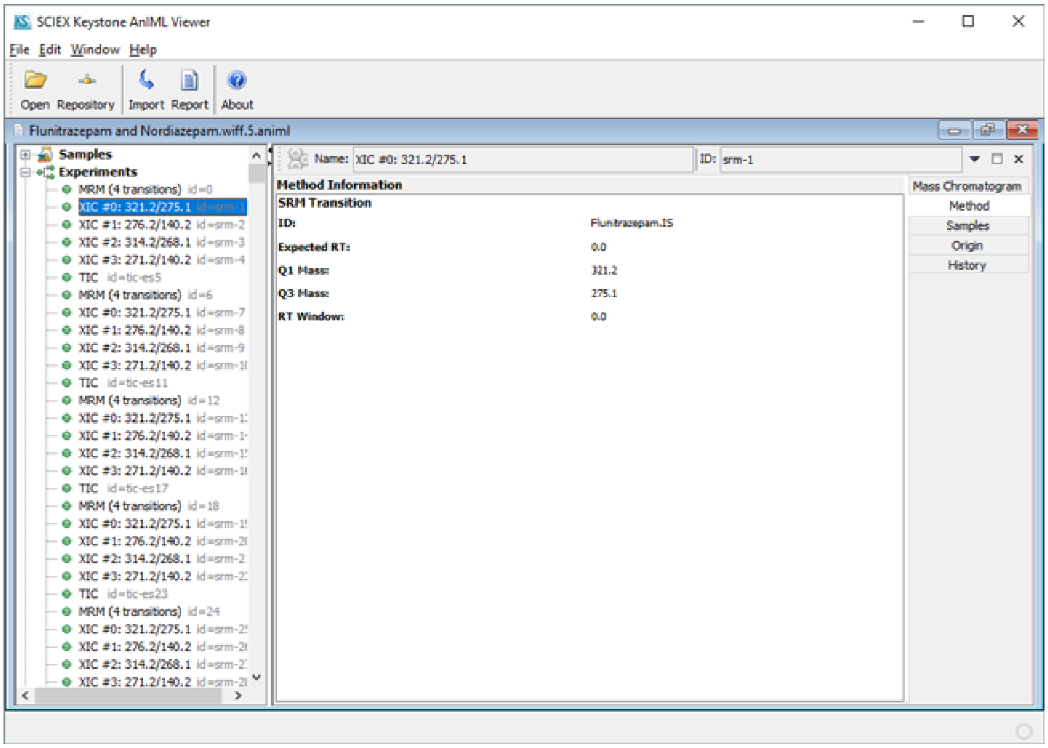
Time [min] float64 independent (x)	Intensity [counts] float64 dependent (y)
0.0000166666666666667	0.0
0.0036833333333333330	20.0
0.0073500000000000000	0.0
0.0110166666666666660	0.0
0.0147000000000000000	0.0
0.0183666666666666670	0.0
0.0220333333333333320	20.0
0.0257000000000000000	0.0
0.0293666666666666660	0.0
0.0330333333333333300	0.0
0.0367000000000000000	0.0
0.0403666666666666700	0.0
0.0440333333333333340	20.0
0.0477166666666666640	0.0
0.0513833333333333360	0.0
0.0550500000000000000	0.0
0.0587166666666666700	0.0
0.0623833333333333300	0.0
0.0660500000000000000	0.0
0.0697166666666666600	0.0

Table 4-3 Icons

Icon	Name	Description
⧉	Copy table data	Creates a copy of the table information and puts it on the computer clipboard.
🗑	Remove row	Removes the selected row from the table. **Tip!** Use the **Ctrl** or **Shift** key to select multiple rows.
▤	Configure visible columns	Refer to Configure Visible Series or Columns.
▼	Actions — Export to Excel	Exports the **Time** and **Intensity** values for the chromatogram to a Microsoft Excel spreadsheet.

3. Click **Method** to view the details of the MRM transition.

Figure 4-13 Example: XIC #0 Method



Name: XIC #0: 321.2/275.1
ID: srm-1

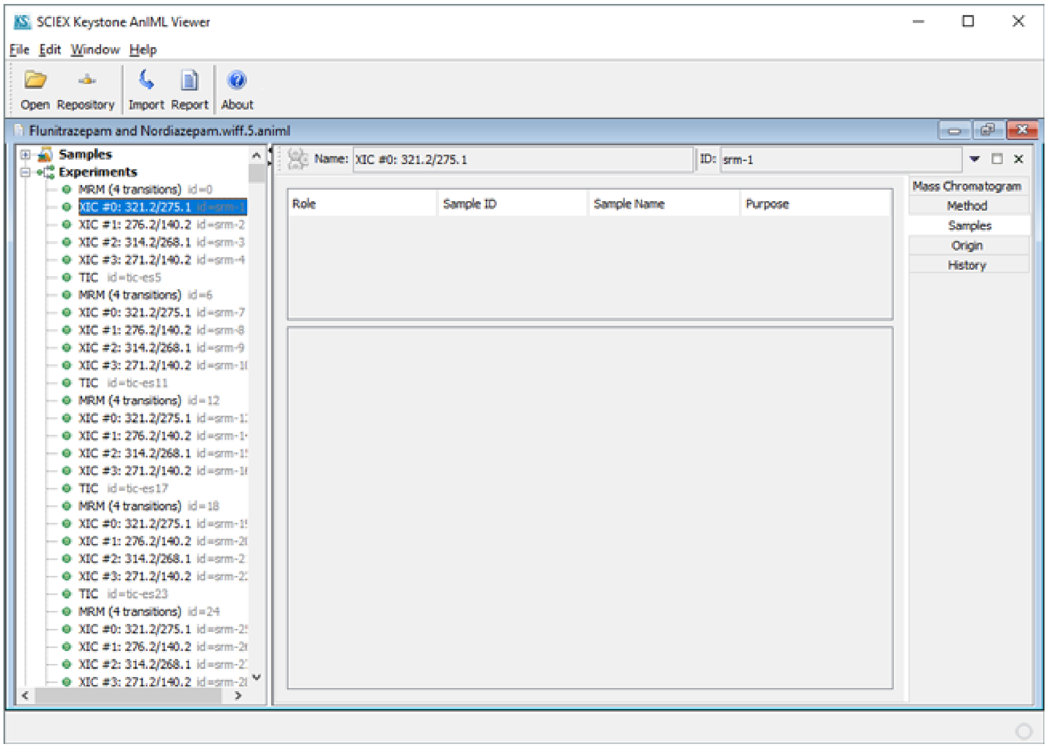
Method Information

SRM Transition

ID:	Flunitrazepam.IS
Expected RT:	0.0
Q1 Mass:	321.2
Q3 Mass:	275.1
RT Window:	0.0

4. Click **Samples** to view the details of the sample associated with the XIC.

Figure 4-14 Example: XIC #0 Samples



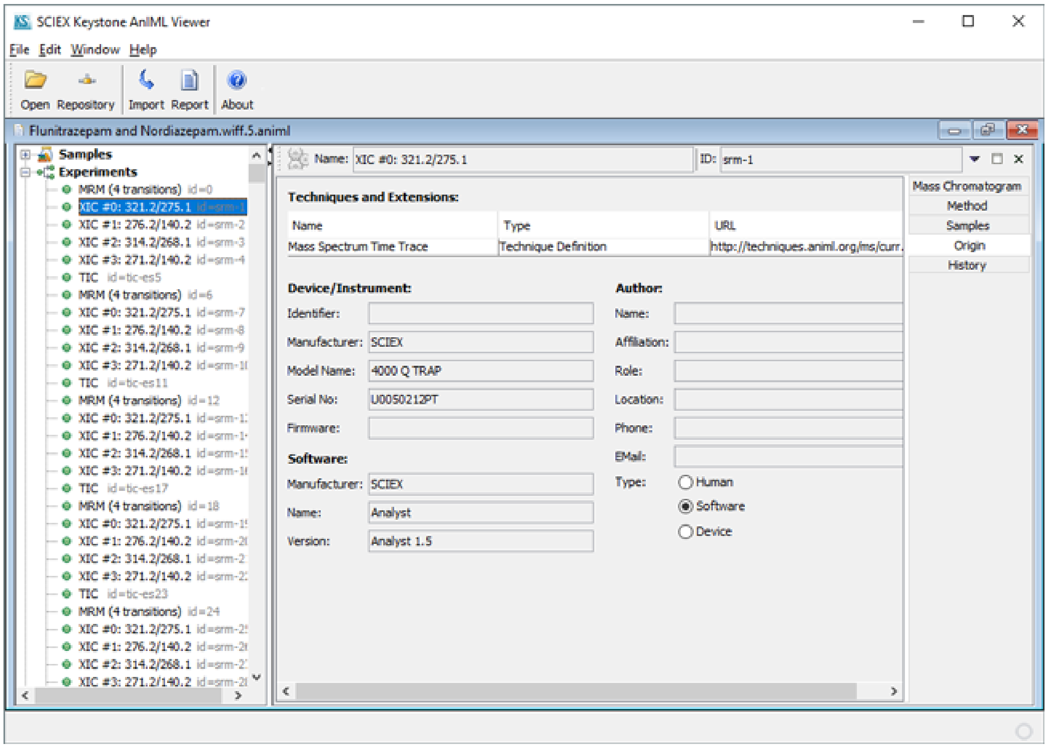
Name: XIC #0: 321.2/275.1

ID: srm-1

Role	Sample ID	Sample Name	Purpose

5. Click **Origin** to view the details of the instrument and software used to acquire the data, as well as the user information.

Figure 4-15 Example: XIC #0 Origin



Name: XIC #0: 321.2/275.1

ID: srm-1

Techniques and Extensions:

Name	Type	URL
Mass Spectrum Time Trace	Technique Definition	http://techniques.animl.org/ms/curr.

Device/Instrument:

Identifier:

Manufacturer: SCIEX

Model Name: 4000 Q TRAP

Serial No: U0050212PT

Firmware:

Software:

Manufacturer: SCIEX

Name: Analyst

Version: Analyst 1.5

Author:

Name:

Affiliation:

Role:

Location:

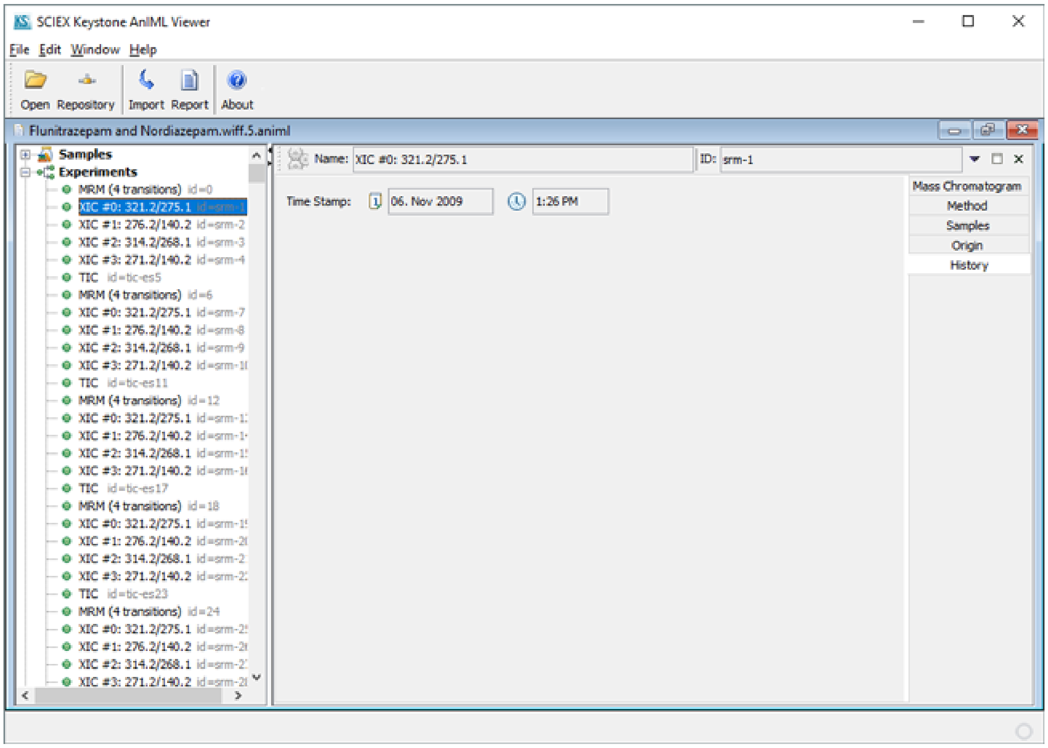
Phone:

EMail:

Type: ○ Human ● Software ○ Device

6. Click **History** to view the date and time that the sample was acquired.

Figure 4-16 Example: XIC #0 History



Name: XIC #0: 321.2/275.1

ID: srm-1

Time Stamp: 06. Nov 2009 1:26 PM

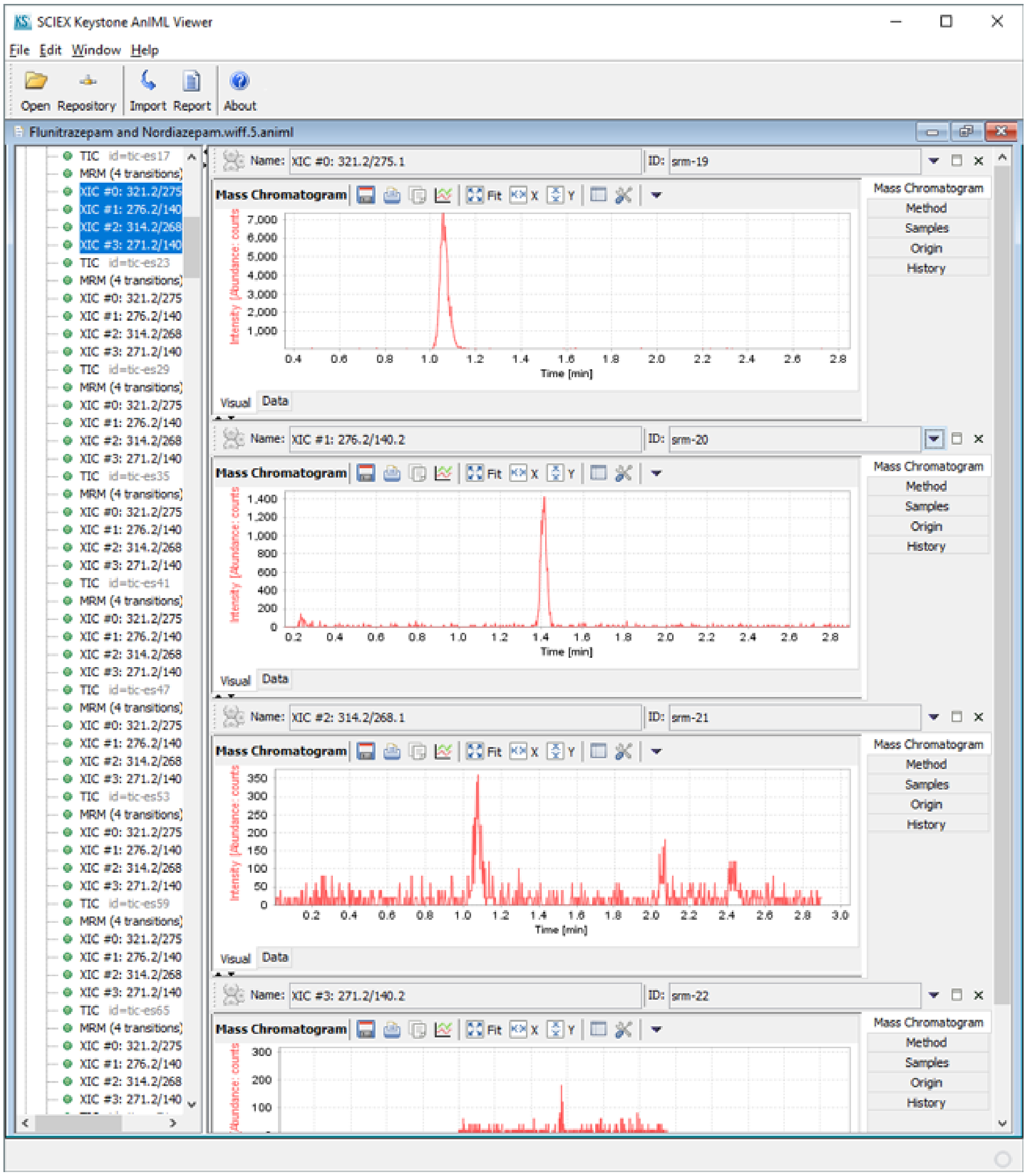
Create a Visualization Graph

Prerequisite Procedures
• Open a wiff.animl File.

1. In the Navigation pane, select two or more XICs to be viewed.

   The pane at the right side of the window refreshes, showing a mass chromatogram pane for each XIC selected.

Figure 4-17 Selected XICs



Name: XIC #0: 321.2/275.1 ID: srm-19

Name: XIC #1: 276.2/140.2 ID: srm-20

Name: XIC #2: 314.2/268.1 ID: srm-21

Name: XIC #3: 271.2/140.2 ID: srm-22

2. Click **Add to Visualization** ( ) in the first mass chromatogram pane to create the initial visualization graph.

Figure 4-18 Initial Visualization Graph

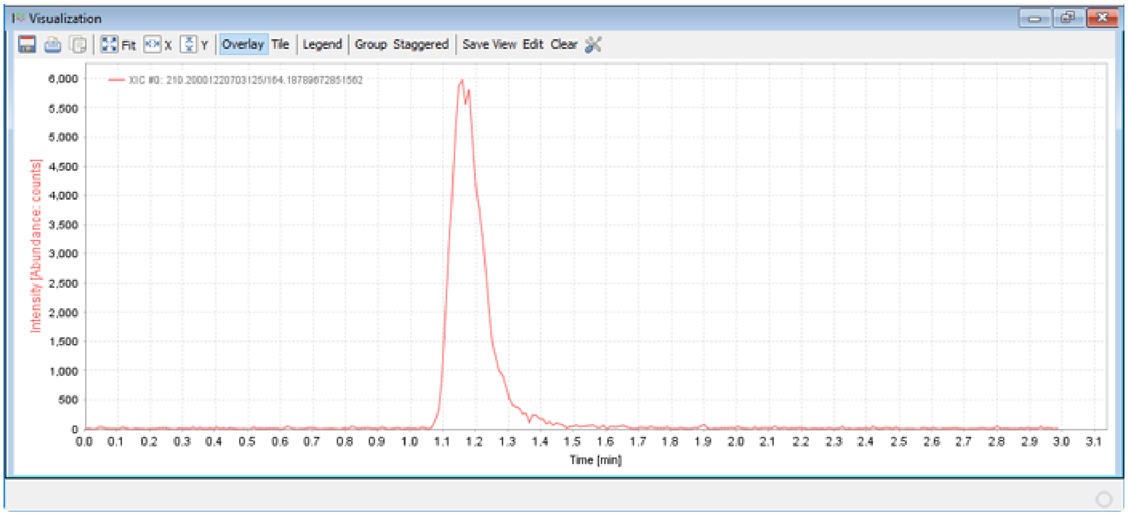


Table 4-4 Icons

Icon	Name	Description
💾	Export image	Exports the image to a Portable Network Graphic (png) file.
🖶	Print	Prints the chromatogram to a selected printer.
⎘	Copy image	Creates a copy of the image and puts it on the computer clipboard.
Fit	Scale to fit	Returns a zoomed chromatogram to the original size.
X	Scale to fit x axis	Resizes the chromatogram to span the full X-axis.
Y	Scale to fit y axis	Resizes the chromatogram to span the full Y-axis.
—	Overlay	Combines all of the selected chromatograms in one pane. The chromatograms are shown in the default **Overlay** format, each one in a different color. Refer to Figure 4-19.
—	Tile	Refer to Figure 4-20.
—	Legend	Refer to Figure 4-22.
—	Group	Refer to Figure 4-23.

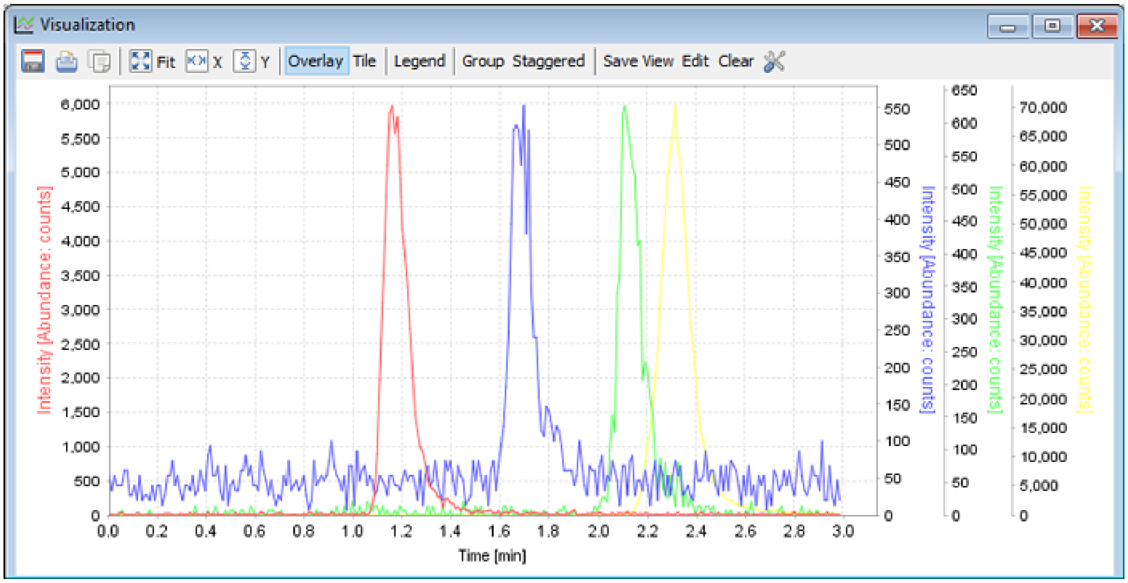
Table 4-4 Icons (continued)

Icon	Name	Description
—	Staggered	Refer to Figure 4-24.
—	Edit	Refer to Figure 4-26.
—	Clear	Removes all of the information from the visualization graph.
🛠	Format plot	Refer to Set Chart Properties.

3. Click 📈 in each mass chromatogram pane to add the required XICs to the visualization graph.

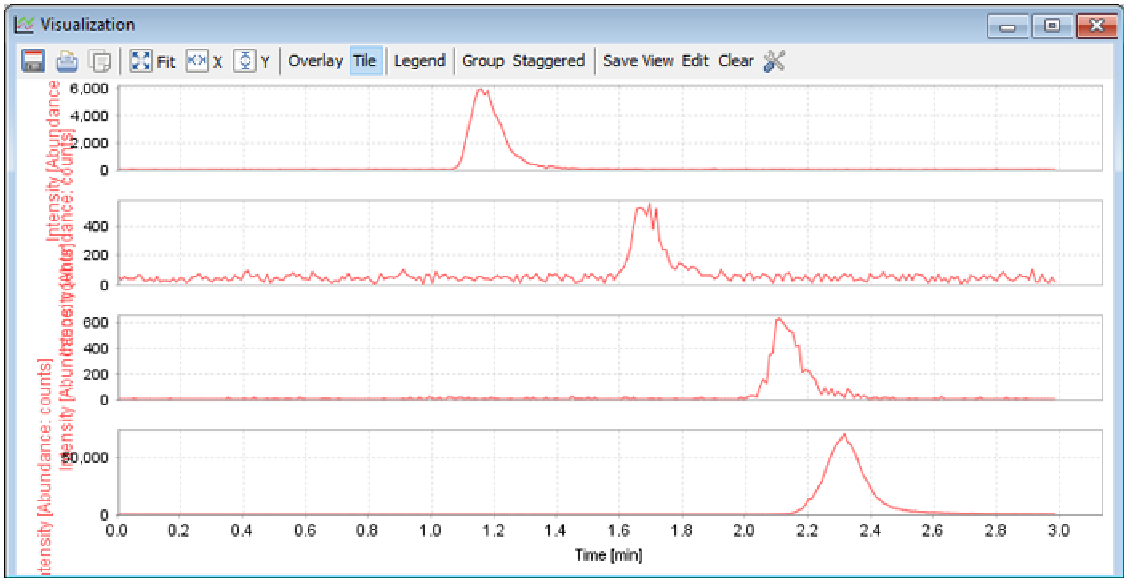
   The selected XICs are shown in the default **Overlay** format.

Figure 4-19 Visualization Graph: Overlay Format



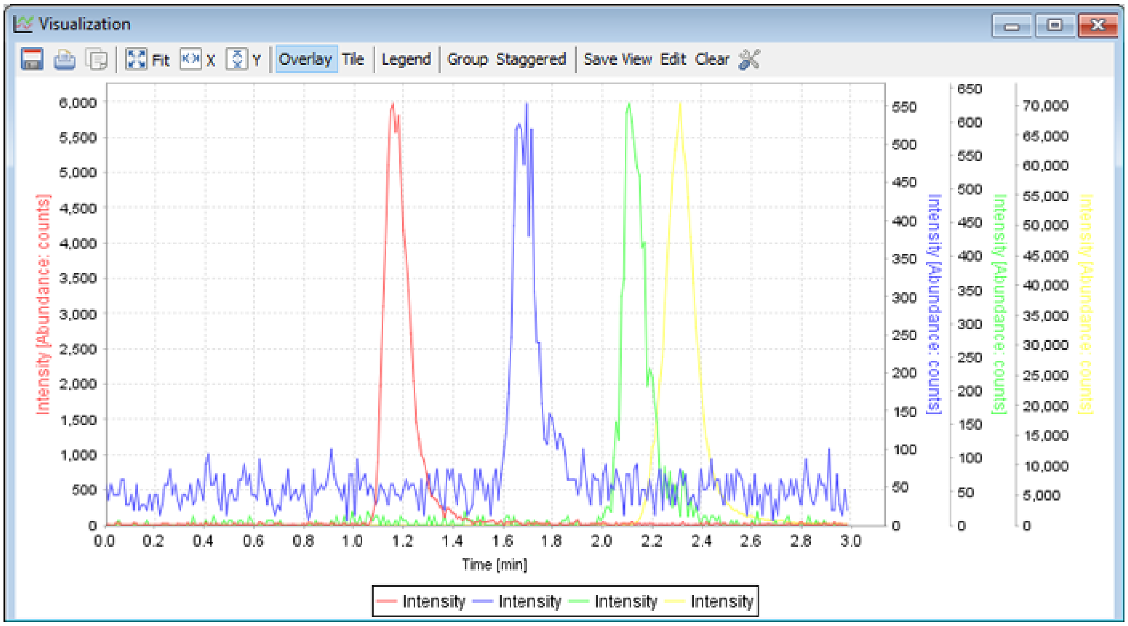
4. Click **Tile** to show all of the selected chromatograms, stacked in the pane.

Figure 4-20 Visualization Graph: Tile Format



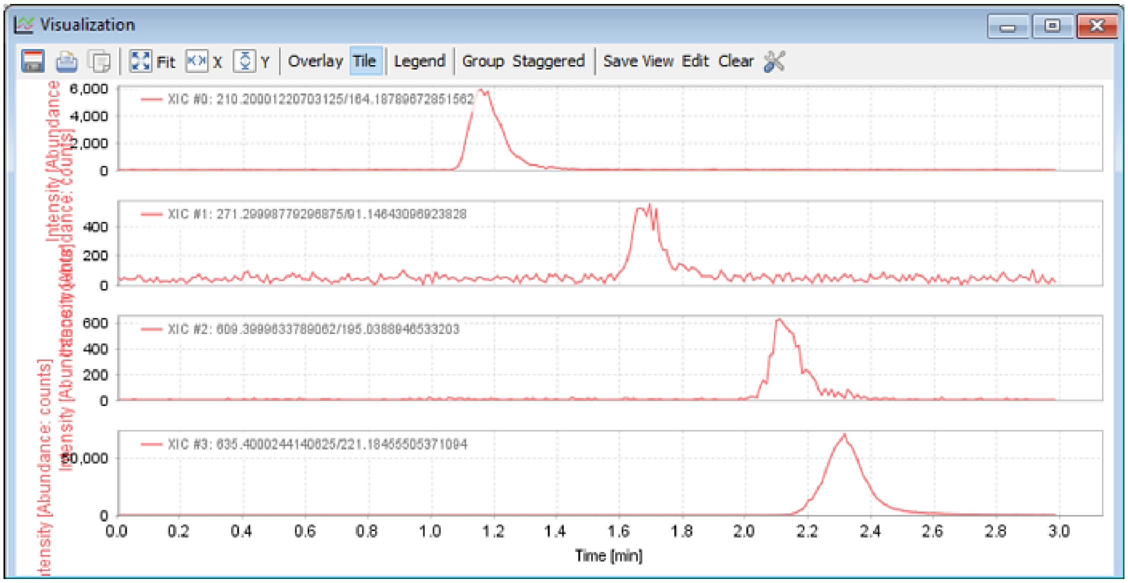
5. Click **Legend** to add an abbreviated name for the XIC to the bottom of the pane in the overlay view or to add the name of the XIC to each pane in the tiled view.

Figure 4-21 Legend: Overlay View



Tip! Mover the cursor over the legend entry to view the name of the associated XIC.

Figure 4-22 Legend: Tile View



6. Click **Group** to show all of the selected chromatograms.

Figure 4-23 Group View

7. Click **Staggered** to combine all of the selected chromatograms in one pane, in a stacked view.

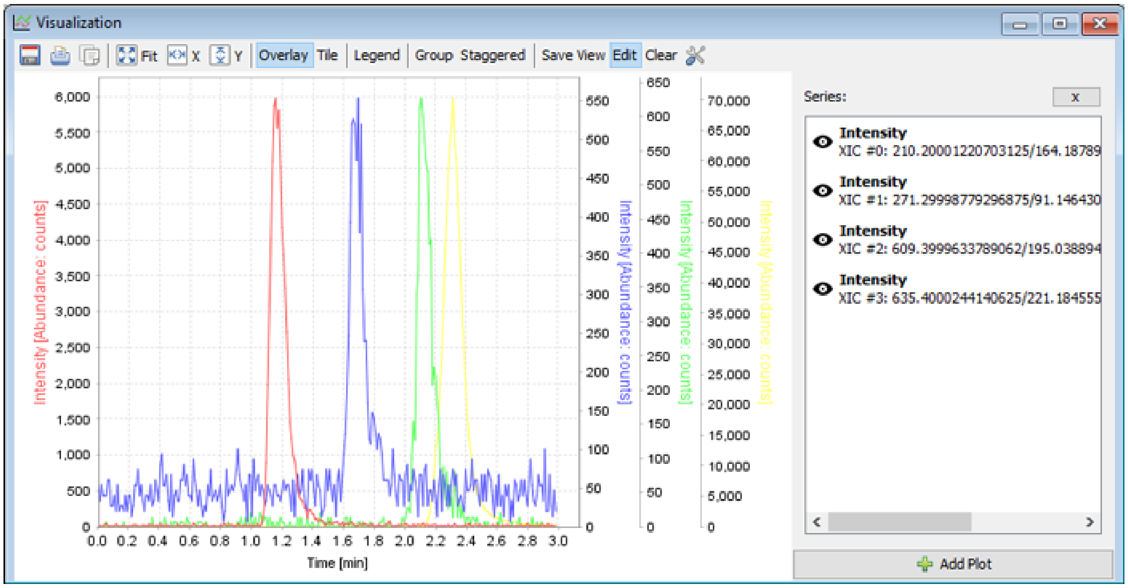
Note: The Y-axis for each chromatogram is shown, at consistent intervals.

Figure 4-24 Staggered View

8. Type a **Name** in the field provided and then click **OK**.

9. Click **Edit**.

Figure 4-25 Edit View



Intensity
XIC #0: 210.20001220703125/164.18789

Intensity
XIC #1: 271.29998779296875/91.146430

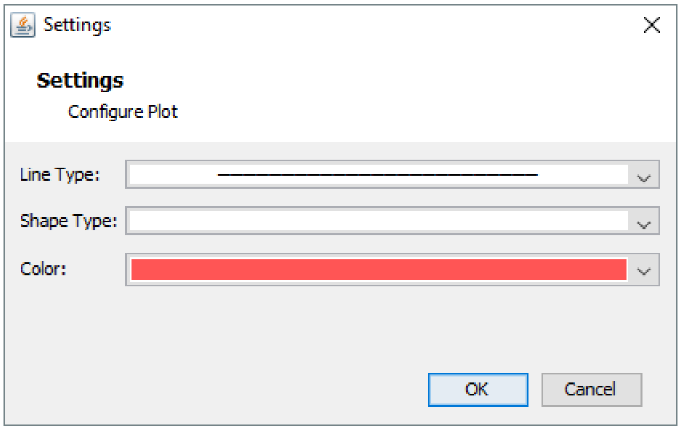
Intensity
XIC #2: 609.3999633789062/195.038894

Intensity
XIC #3: 635.4000244140625/221.184555

10. Right-click the name of an XIC and do one of the following:
    - Click **Remove** to delete the selected XIC from the view.

- Click **Configuration** and then change the settings:

Figure 4-26 Settings Dialog

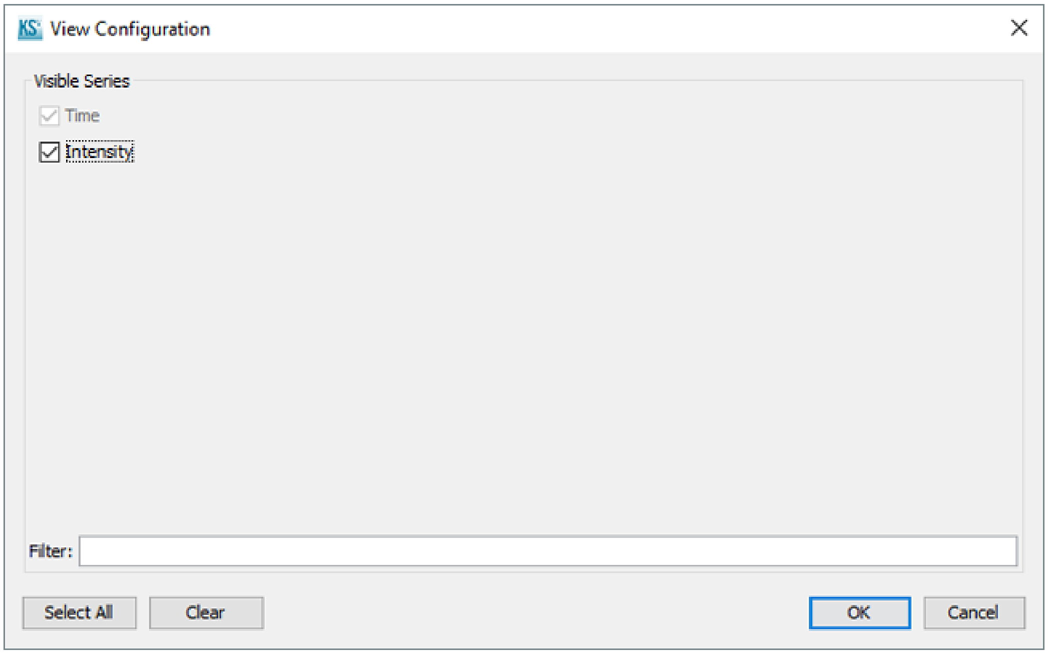


a. Change the type of the line used to draw the chromatogram.
b. Change the shape of the data points on the chromatogram.
c. Change the color of the line used to draw the chromatogram.
d. Click **OK**.

Configure Visible Series or Columns

1. Click **Configure Visible Columns** (▤).

Figure 4-27 View Configuration Dialog



2. (Optional) Clear the **Intensity** check box to hide the **Intensity** column on the Data tab.

   Note: The **Time** column cannot be hidden.

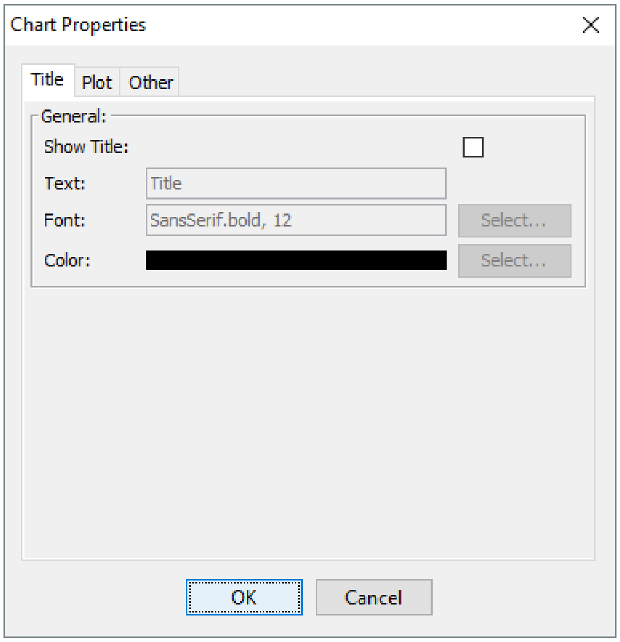
3. Click **OK**.

Set Chart Properties

Prerequisites
One of the following panes must be open: • An XIC Mass Chromatogram pane. Refer to View Extracted Ion Chromatogram (XIC) Information. • A visualization chart. Refer to Create a Visualization Graph. • A TIC Mass Chromatogram pane. Refer to View Total Ion Chromatogram (TIC) Information .

1. Click **Format plot** (🛠).

Figure 4-28 Chart Properties: Title Tab



General:

Show Title: ☐

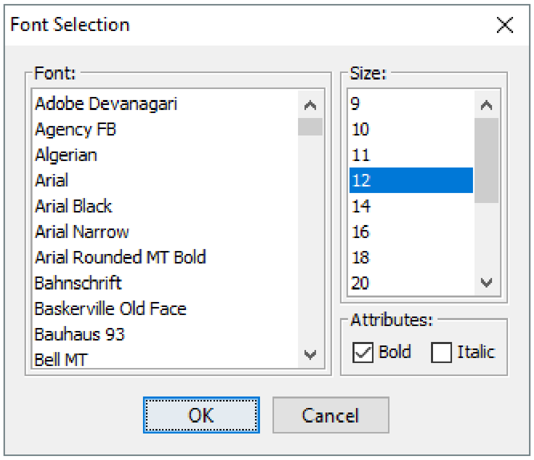
Text: Title

Font: SansSerif.bold, 12

Color: ■

2. Click the **Show Title** check box and then type a title for the chromatogram in the **Text** field.
3. Click **Select** to the right of **Font**.

Figure 4-29 Font Selection Dialog



Font:

Adobe Devanagari
Agency FB
Algerian
Arial
Arial Black
Arial Narrow
Arial Rounded MT Bold
Bahnschrift
Baskerville Old Face
Bauhaus 93
Bell MT

Size:

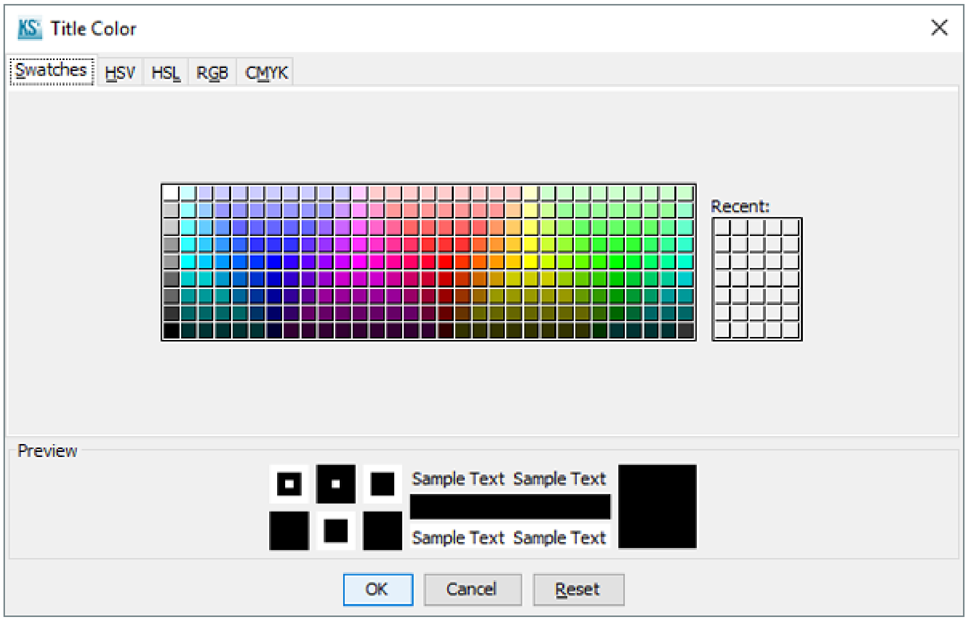
9
10
11
12
14
16
18
20

Attributes:

☑ Bold ☐ Italic

4. Select the **Font**, **Size**, and **Attributes** and then click **OK**.
5. Click **Select** to the right of **Color**.

Figure 4-30 Title Color Dialog

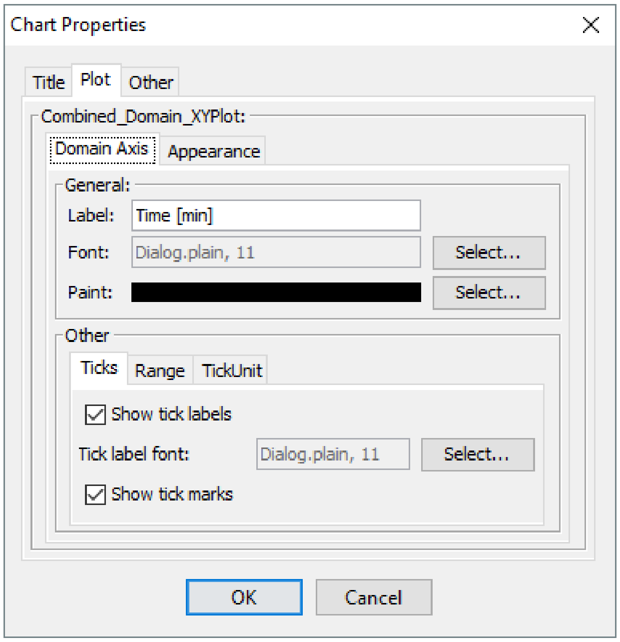


6. Select the appropriate color on the Swatches tab and then click **OK**.

7. Click the **Plot** tab.

   The tab opens to the default Domain Axis tab.

Figure 4-31 Chart Properties: Domain Access



Label: Time [min]

Font: Dialog.plain, 11

☑ Show tick labels

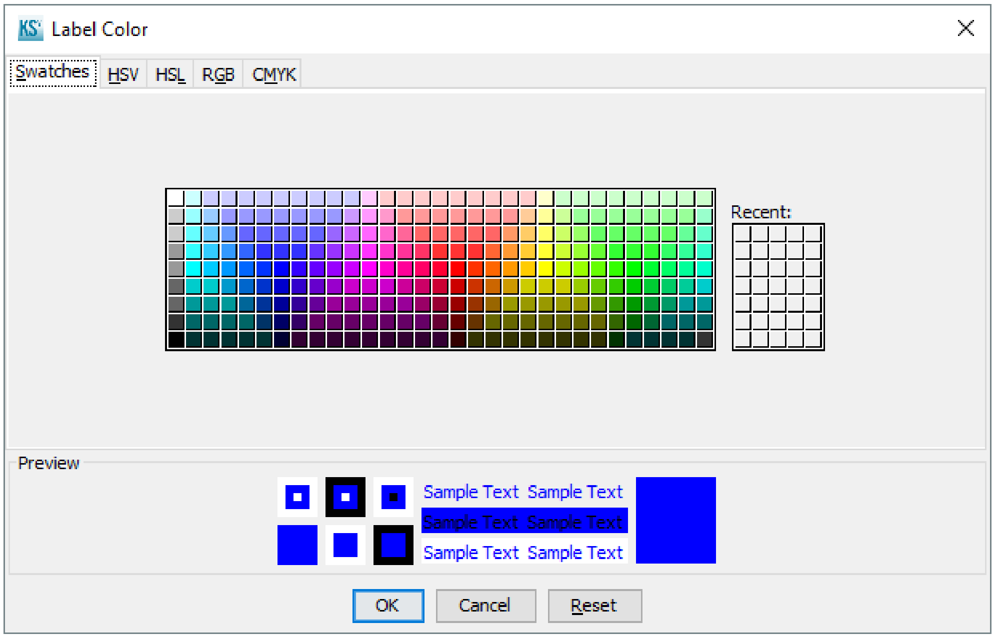
Tick label font: Dialog.plain, 11

☑ Show tick marks

8. In the **General** section, type the new **Label** for the X-axis.
9. Click **Select** to the right of **Font**.

   Refer to Figure 4-29.
10. Select the **Font**, **Size**, and **Attributes** and then click **OK**.
11. Click **Select** to the right of **Paint**.

Figure 4-32 Label Color Dialog



12. Select the appropriate color on the **Swatches** tab and then click **OK**.

13. In the **Other** section, on the Ticks tab:

Figure 4-33 Other Section: Ticks Tab

☑ Show tick labels

Tick label font: Dialog.plain, 11

☑ Show tick marks

- Select the **Show tick labels** check box to show the units of measure on the X-axis.

  Note: This option is selected by default.

- Clear the **Show tick labels** check box to remove the units of measure from the X-axis.
- Click **Select** to the right of **Font**. Refer to Figure 4-29. Select the **Font**, **Size**, and **Attributes** and then click **OK**.

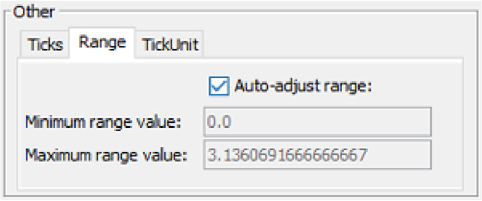
- Select the **Show tick marks** check box to show the unit of measure indicators on the bottom of the X-axis.

  Note: This option is selected by default.

- Clear the **Show tick marks** check box to remove the unit of measure indicators from the bottom of the X-axis.

14. In the **Other** section, on the Range tab, set the options:

Figure 4-34 Other Section: Range Tab



☑ Auto-adjust range:

Minimum range value: 0.0

Maximum range value: 3.1360691666666667

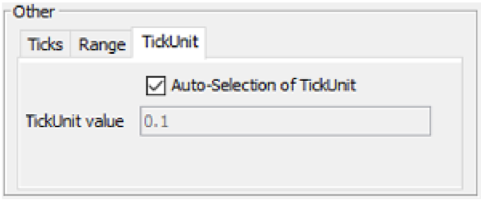
- Select the **Auto-adjust range** check box to enable the software to automatically set the **Minimum range value** for the units of measure on the X-axis to 0.0 and to set the **Maximum range value** to 3.1360691666666667.

  Note: This option is selected by default.

- Clear the **Auto-adjust range** check box to manually adjust the minimum and maximum range values for the units of measure on the X-axis. Type the appropriate values in the **Minimum range value** and **Maximum range value** fields provided and then click **OK**.

15. In the **Other** section, on the TickUnit tab, set the options:

Figure 4-35 Other Section: TickUnit Tab



☑ Auto-Selection of TickUnit

TickUnit value 0.1

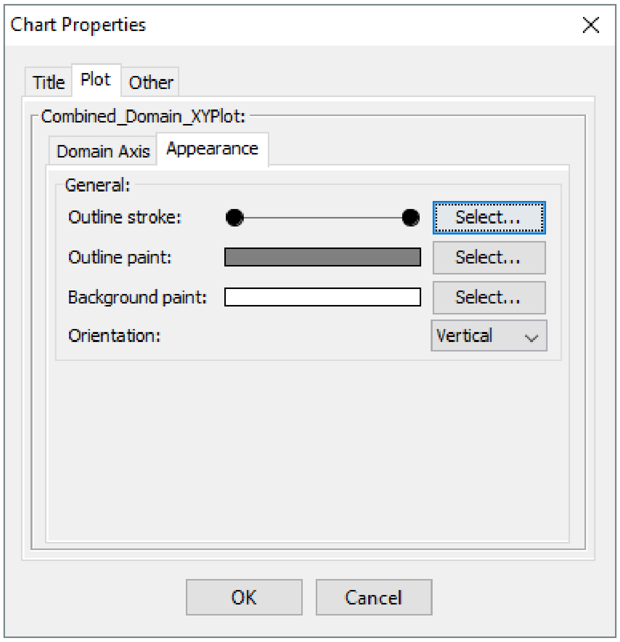
- Select the **Auto-Selection of TickUnit** check box to enable the software to automatically set the **TickUnit value** to 0.1 to increment each unit of measure on the X-axis by 0.1.

  Note: This option is selected by default.

- Clear the **Auto-Selection of TickUnit** check box to manually adjust the incremental amount for the units of measure on the X-axis. Type the appropriate value in the **TickUnit value** field provided and then click **OK**.

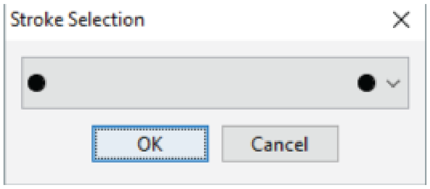
16. Click the **Appearance** tab.

Figure 4-36 Plot Tab: Appearance



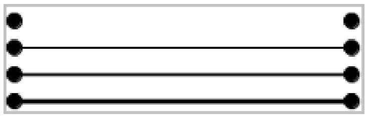
17. Click **Select** to the right of **Outline stroke**.

Figure 4-37 Stroke Selection Dialog



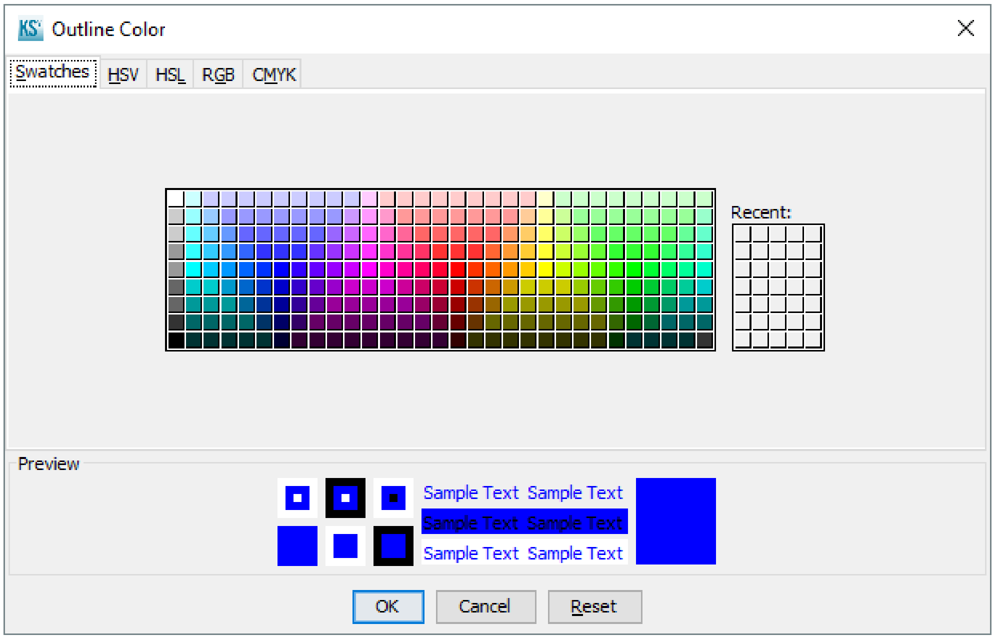
18. Select the appropriate stroke type from the options provided and then click **OK**.

Figure 4-38 Stroke Type Options



19. Click **Select** to the right of **Outline point**.

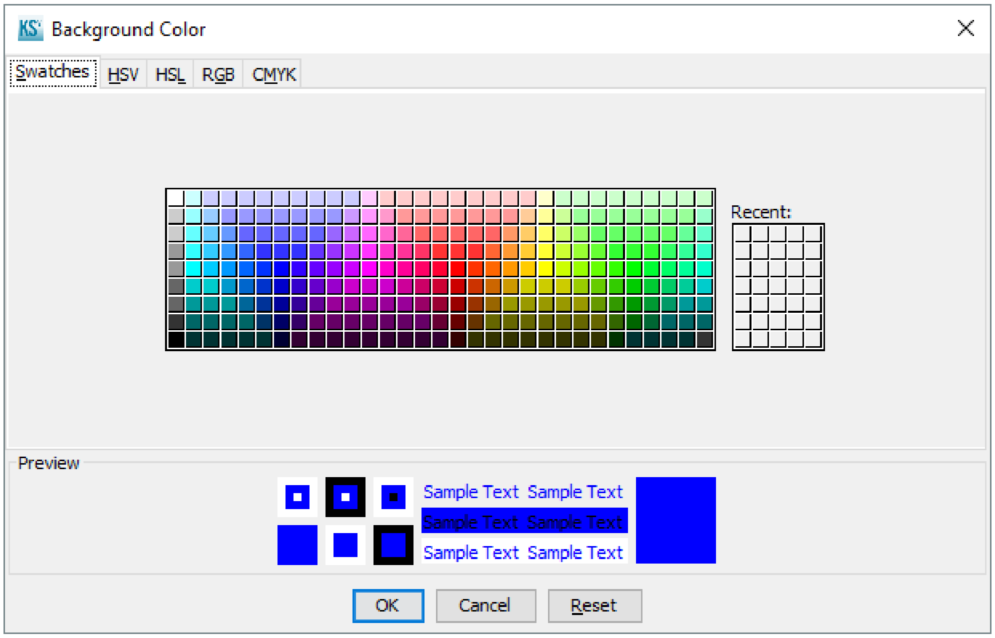
Figure 4-39 Outline Color Dialog



20. Select the appropriate color on the Swatches tab and then click **OK**.

21. Click **Select** to the right of **Background paint**.

Figure 4-40 Background Color Dialog

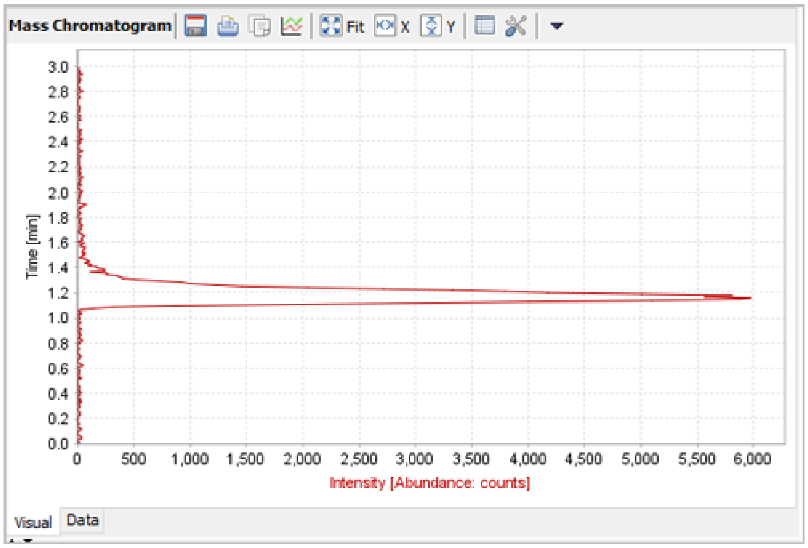


22. Select the appropriate color on the **Swatches** tab and then click **OK**.

23. Select **Horizontal** to the right of **Outline stroke** and then click **OK**.

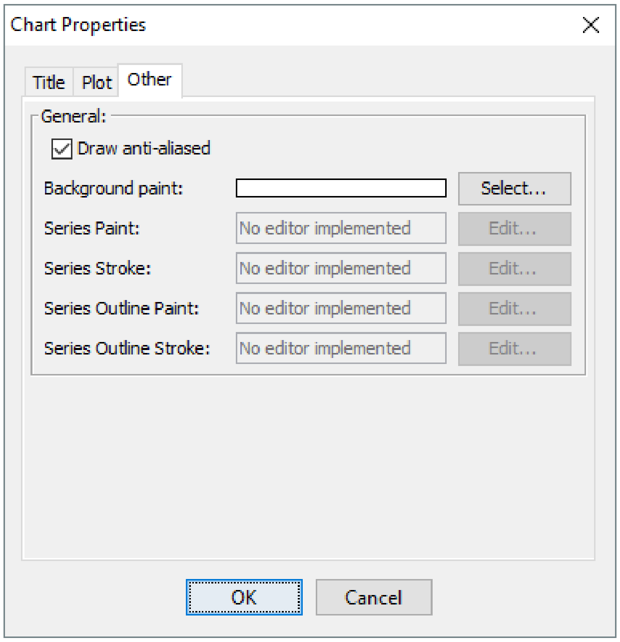
    The **Time** axis is shown vertically and the **Intensity** axis is shown horizontally.

Figure 4-41 Horizontal Orientation



24. Click the **Other** tab.

Figure 4-42 Other Tab



☑ Draw anti-aliased

Background paint:

Series Paint: No editor implemented

Series Stroke: No editor implemented

Series Outline Paint: No editor implemented

Series Outline Stroke: No editor implemented

25. Do one of the following:
    - Select the **Draw anti-aliased** check box to create a smoother version of the graph.
    - Clear the **Draw anti-aliased** check box to revert the graph.
26. Click **Select** to the right of **Background paint**. Refer to Figure 4-40.
27. Select the appropriate color on the **Swatches** tab and then click **OK**.

View Converted rdb Files

An rdb file is the proprietary format for the Results Table generated by the Analyst® Software. The Results Table is a report of each compound or potential metabolite found in a sample, presented in a table format.

Open an rdb.animl File

1. Click **File > Open**.

   The Open dialog opens.

2. Browse to and select the appropriate rdb.animl file and then click **Open**.

Tip! Hold down the **Shift** key to select multiple rdb.animl files.

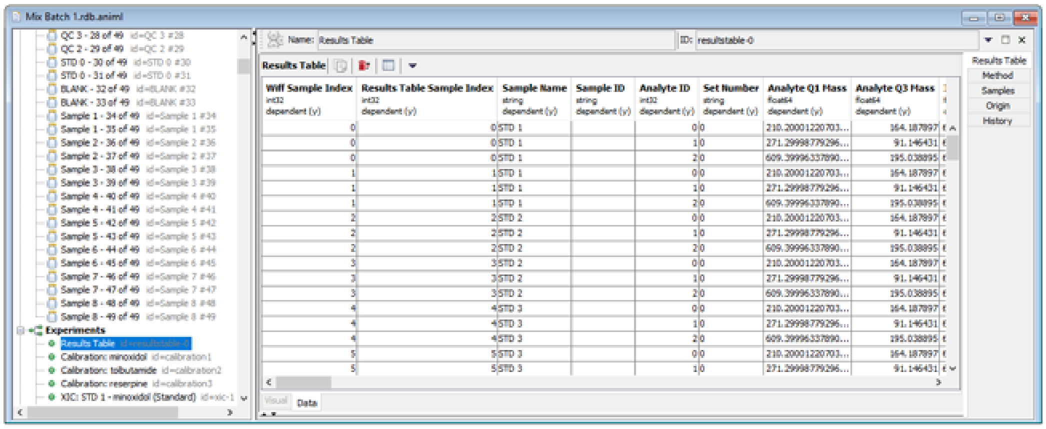
View a Results Table

Prerequisite Procedures
- Open an rdb.animl File.

1. In the Navigation pane, click the **Results Table** to be viewed.

   The pane at the right side of the window refreshes, showing the information for the selected Results Table. Only the Data tab is accessible.

Figure 4-43 Example Results Table



Name: Results Table

ID: resultstable-0

Wiff Sample Index int32 dependent (y)	Results Table Sample Index int32 dependent (y)	Sample Name string dependent (y)	Sample ID string dependent (y)	Analyte ID int32 dependent (y)	Set Number string dependent (y)	Analyte Q1 Mass float64 dependent (y)	Analyte Q3 Mass float64 dependent (y)
0	0	STD 1		0	0	210.20001220703...	164.187897
0	0	STD 1		1	0	271.29998779296...	91.146431
0	0	STD 1		2	0	609.39996337890...	195.038895
1	1	STD 1		0	0	210.20001220703...	164.187897
1	1	STD 1		1	0	271.29998779296...	91.146431
1	1	STD 1		2	0	609.39996337890...	195.038895
2	2	STD 2		0	0	210.20001220703...	164.187897
2	2	STD 2		1	0	271.29998779296...	91.146431
2	2	STD 2		2	0	609.39996337890...	195.038895
3	3	STD 2		0	0	210.20001220703...	164.187897
3	3	STD 2		1	0	271.29998779296...	91.146431
3	3	STD 2		2	0	609.39996337890...	195.038895
4	4	STD 3		0	0	210.20001220703...	164.187897
4	4	STD 3		1	0	271.29998779296...	91.146431
4	4	STD 3		2	0	609.39996337890...	195.038895
5	5	STD 3		0	0	210.20001220703...	164.187897
5	5	STD 3		1	0	271.29998779296...	91.146431

Table 4-5 Icons

Icon	Name	Description
🗐	Copy table data	Creates a copy of the table information and puts it on the computer clipboard.
🗑	Remove row	Removes the selected row from the table. **Tip!** Use the **Ctrl** or **Shift** key to select multiple rows.

Table 4-5 Icons (continued)

Icon	Name	Description
▤	Configure visible columns	Refer to Configure Visible Columns.
▾	Actions — Export to Excel	Exports the information to a Microsoft Excel spreadsheet. Hidden columns are exported.

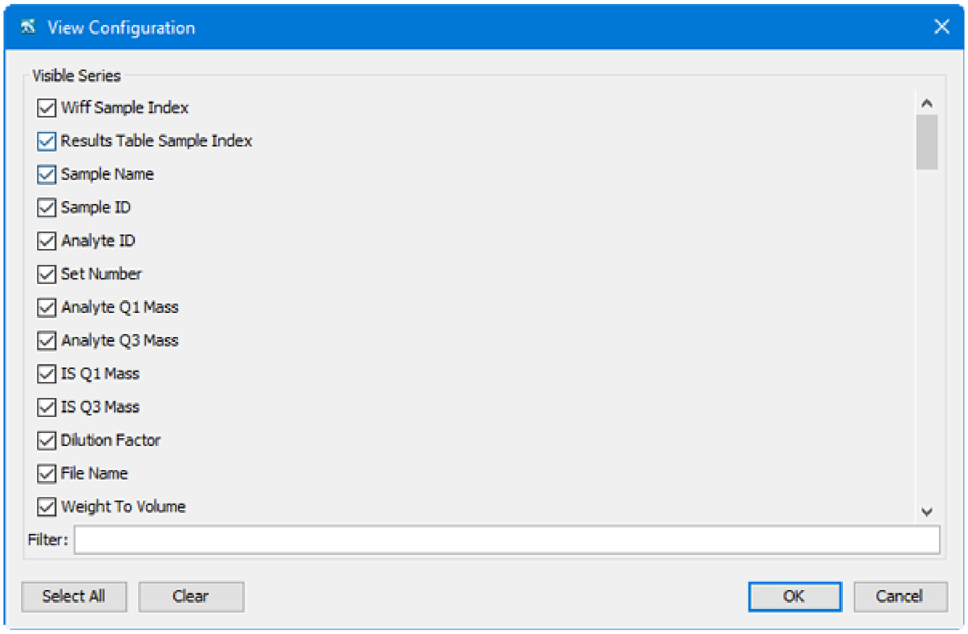
2. Click **Method** to view the method information.
3. Click **Samples** to view the details of the samples associated with the Results Table.
4. Click **Origin** to view the details of the instrument and software used to acquire the data, as well as the user information.
5. Click **History** to view the date and time that the Results Table was generated.

Configure Visible Columns

Columns in the Results Table can be reordered or hidden. The order of columns does not persist from session to session. In addition, if columns are hidden after they have been reordered, then the order of the shown columns reverts back to the original order.

1. To hide columns, click **Configure Visible Columns** (▤).

Figure 4-44 View Configuration Dialog



Visible Series

☑ Wiff Sample Index
☑ Results Table Sample Index
☑ Sample Name
☑ Sample ID
☑ Analyte ID
☑ Set Number
☑ Analyte Q1 Mass
☑ Analyte Q3 Mass
☑ IS Q1 Mass
☑ IS Q3 Mass
☑ Dilution Factor
☑ File Name
☑ Weight To Volume

Filter:

2. (Optional) Clear the check box beside each column to be hidden.

   Tip! Click **Clear** to clear all of the check boxes. Use the **Filter** field to minimize the number of columns shown for selection.

3. Click **OK**.
4. To reorder columns, click the column header and drag the column to the new location.

View Converted Audit Trail Files

Each workstation has one Instrument Audit Trail. It records events such as additions or replacements to the mass calibration resolution tables, system configuration changes, security events, and entries in the Instrument Maintenance Log. For computers not directly connected to a mass spectrometer, the Instrument Audit Trail records only security events. The Instrument Audit Record has a file extension of atd.

Each project has a Project Audit Trail. It records events such as the creation, modification, and deletion of projects, data, quantitation methods, acquisition methods, batch, tuning, Results Table, and report template files, as well as module opening, closing, and printing events. The Project Audit Record has a file extension of atd.

The Audit Trail is comprised of three modules: Instrument, Project, and Results Table Audit Trail. The Instrument Audit Trail captures user log on, log off, settings changes and so on, and is stored as an atd file in the Project Information folder for the API Instrument project. The Analyst® Software Project Audit Trail captures module access, file creation, printing, and so on, and is stored as an atd file in the Project Information folder of the project. The Results Table Audit Trail capture events related to the creation and modification of the Results Table and is stored with the Results Table.

When the Instrument and Project Audit Trails reach 1000 entries the Audit Trail is archived as a time and date-stamped ata file. The Results Table Audit Trail has no limit on the number of entries.

Both ata and atd Audit Trail files can be converted to the AnIML format.

Open an ata.animl or atd.animl File

1. Click **File > Open**.

   The Open dialog opens.

2. Browse to and select the appropriate ata.animl or atd.animl file and then click **Open**.

   Tip! Hold the **Shift** key to select multiple ata.animl or atd.animl files.

View Total Ion Chromatogram (TIC) Information

Prerequisite Procedures
• Open a wiff.animl File.

1. In the Navigation pane, click the **TIC** to be viewed.

   The pane at the right side of the window refreshes, showing the **Name**, **ID**, and **Mass Chromatogram** for the selected TIC.

Figure 4-45 Example TIC – Visual Tab

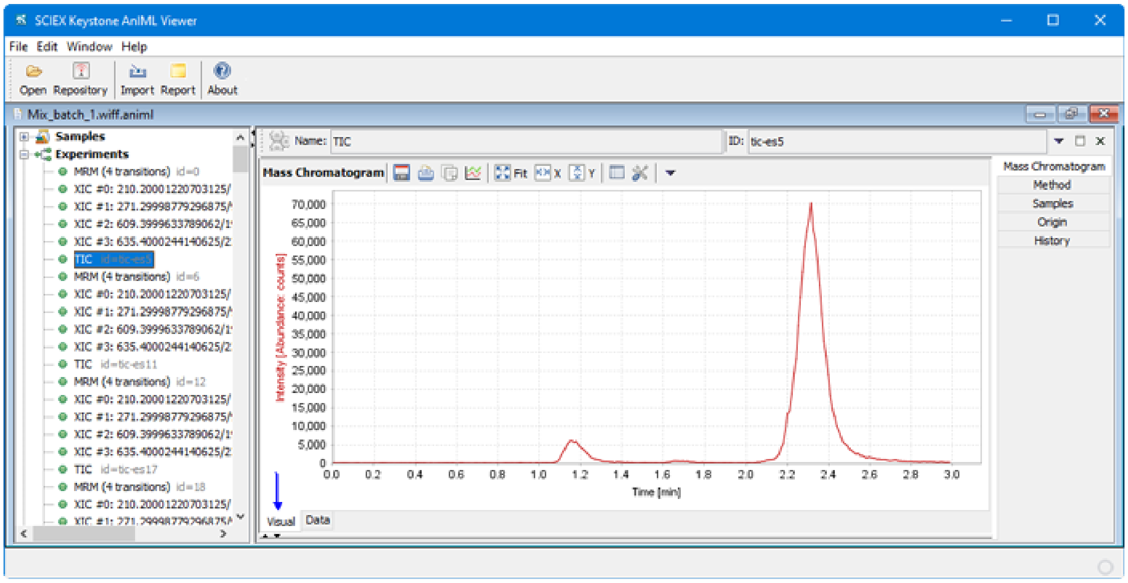


Table 4-6 Icons

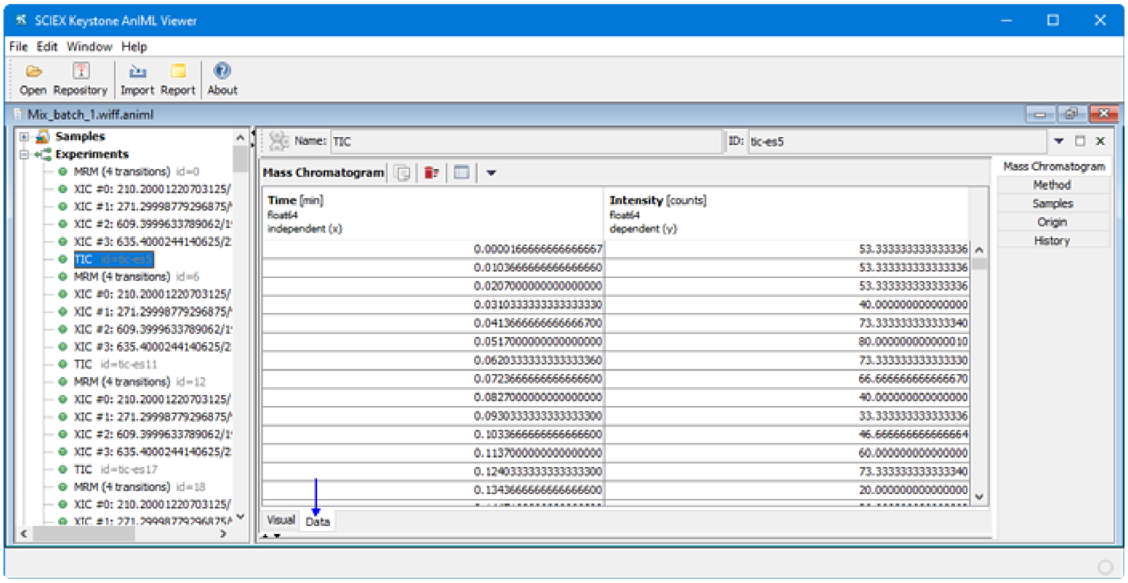
Icon	Name	Description
💾	Export image	Exports the image to a Portable Network Graphic (png) file.
🖨	Print	Prints the chromatogram to a selected printer.
⧉	Copy image	Creates a copy of the image and places it on the computer clipboard.
📈	Add to Visualization	Adds the chromatogram to a visualization graph. Refer to Create a Visualization Graph.

Table 4-6 Icons (continued)

Icon	Name	Description
Fit	Scale to fit	Returns a zoomed chromatogram to the original size.
X	Scale to fit x axis	Resizes the chromatogram to span the full X-axis.
Y	Scale to fit y axis	Resizes the chromatogram to span the full Y-axis.
▤	Configure visible series	Refer to Configure Visible Series or Columns.
✂	Format plot	Refer to Set Chart Properties.
▼	Export to Excel	Exports the **Time** and **Intensity** values for the chromatogram to a Microsoft Excel spreadsheet.

2. Click the **Data** tab to view the **Time**, in minutes, of each peak apex and the **Intensity**, in counts per second, of each peak, in table format.

Figure 4-46 Example TIC - Data Tab



Name: TIC

ID: tic-es5

Mass Chromatogram

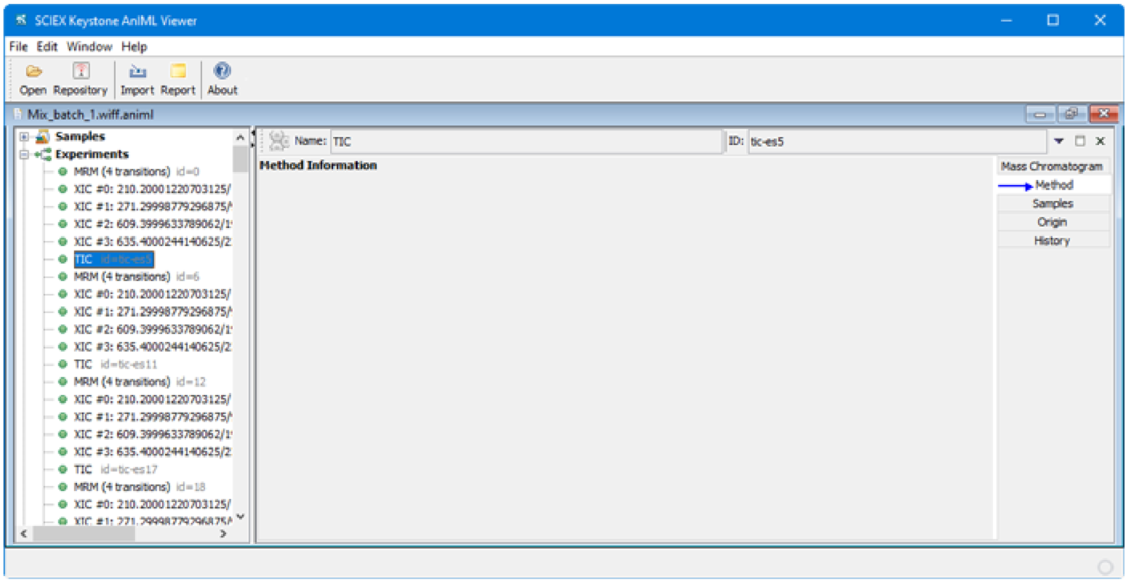
Time [min] float64 independent (x)	Intensity [counts] float64 dependent (y)
0.0000166666666666667	53.333333333333336
0.0103666666666666660	53.333333333333336
0.0207000000000000000	53.333333333333336
0.0310333333333333330	40.000000000000000
0.0413666666666666700	73.333333333333340
0.0517000000000000000	80.000000000000010
0.0620333333333333360	73.333333333333330
0.0723666666666666600	66.666666666666670
0.0827000000000000000	40.000000000000000
0.0930333333333333300	33.333333333333336
0.1033666666666666600	46.666666666666664
0.1137000000000000000	60.000000000000000
0.1240333333333333300	73.333333333333340
0.1343666666666666600	20.000000000000000

Table 4-7 Icons

Icon	Name	Description
⧉	Copy table data	Creates a copy of the table information and places it on the computer clipboard.
🗑	Remove row	Removes the selected row from the table. Use the **Ctrl** or **Shift** key to select multiple rows.
▤	Configure visible columns	Refer to Configure Visible Series or Columns.
▼	Actions — Export to Excel	Exports the **Time** and **Intensity** values for the chromatogram to a Microsoft Excel spreadsheet.

3. Click **Method** to view the details of the method associated with the TIC.

Figure 4-47 Example TIC – Method

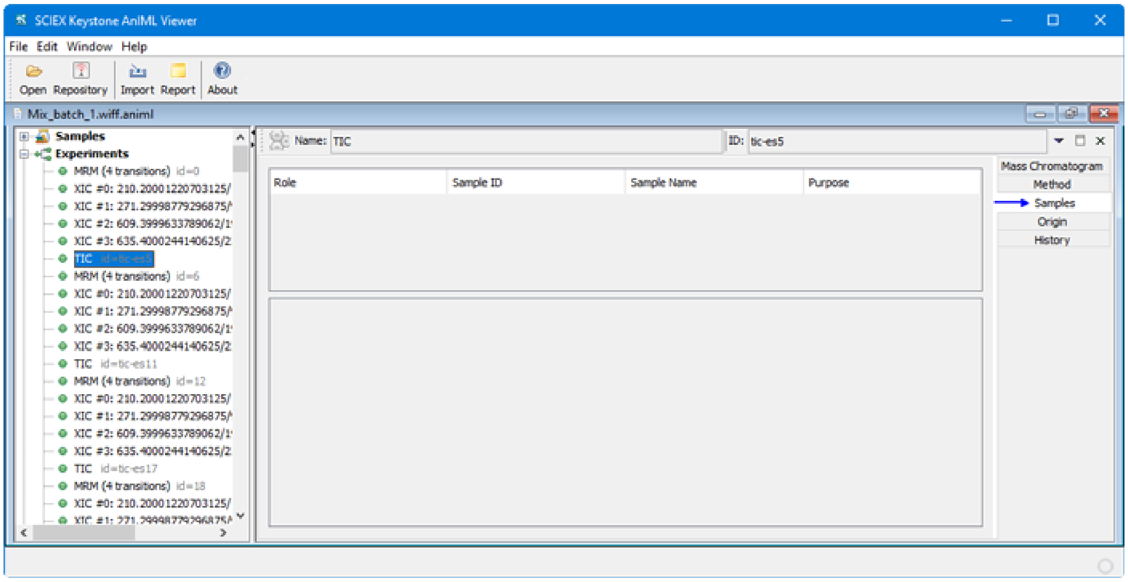


Name: TIC

ID: tic-es5

4. Click **Samples** to view the details of the sample associated with the XIC.

Figure 4-48 Example TIC – Samples

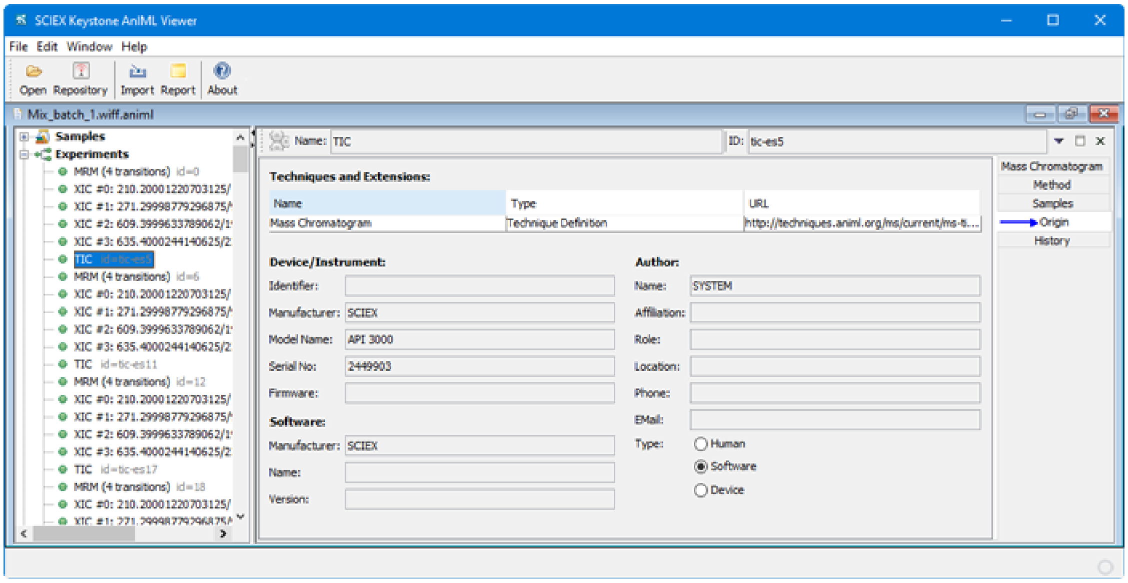


Name: TIC
ID: tic-es5

Role	Sample ID	Sample Name	Purpose

5. Click **Origin** to view the details of the instrument and software used to acquire the data, as well as the user information.

Figure 4-49 Example TIC – Origin



Name: TIC
ID: tic-es5

Techniques and Extensions:

Name	Type	URL
Mass Chromatogram	Technique Definition	http://techniques.animl.org/ms/current/ms-t...

Device/Instrument:

Identifier:
Manufacturer: SCIEX
Model Name: API 3000
Serial No: 2449903
Firmware:

Software:

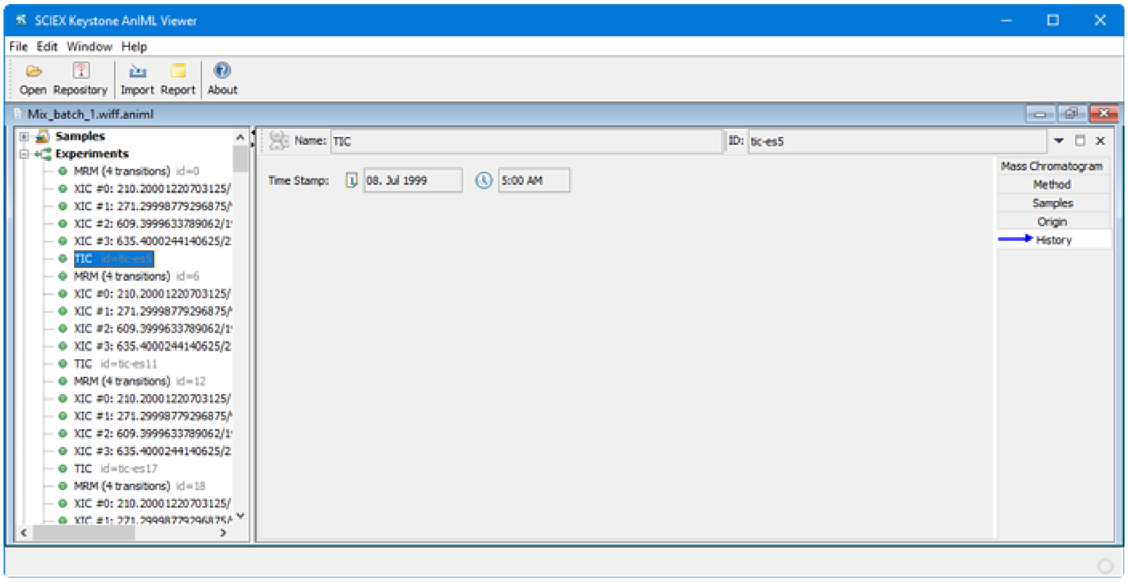
Manufacturer: SCIEX
Name:
Version:

Author:

Name: SYSTEM
Affiliation:
Role:
Location:
Phone:
EMail:
Type: ○ Human ● Software ○ Device

6. Click **History** to view the date and time that the sample was acquired.

Figure 4-50 Example TIC – History



Name: TIC
ID: tic-es5
Time Stamp: 08. Jul 1999 5:00 AM

View Audit Trail Generated by the Keystone Converter Software

The time and date stamps are in the Audit Trail records in UTC format. When the files are opened, they are converted to the local time and shown in the right panel.

1. Open the Keystone Viewer Software.
2. Click **File > Open** and then browse to the file location.
3. Select the appropriate animl file.

Tip! Hold the **Shift** key to select multiple animl files.

---

4. In the left panel, click **Audit Trail**.
5. Scroll to the Audit Trail at the end of the file.

Renew the Keystone Viewer Software License

1. Obtain a new license file from SCIEX and then save it on the desktop.

2. Browse to C:\ProgramData\KeystoneViewer\license and then delete the **keystone_license.lic** file.
3. Click **Start > SCIEX Keystone > SCIEX Keystone Viewer** to open the Keystone Viewer Software.
4. Click **Select**.
5. Browse to the desktop, select the **keystone viewer license.lic** file, and then click **Open**.

   The license selection dialog refreshes, showing the license file that was selected.
6. Click **Finish**.

   The Keystone Viewer Software opens.

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