Scripts User Guide

Analyst Software

RUO-IDV-05-0270-F

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Contents

Foreword 1

Note: This guide contains the scripts for all instruments and different software versions. To determine which scripts the software version installed on your instrument supports, refer to the Analyst software release notes.

Audience

This guide is intended for customers and Field Service Employees (FSEs).

Note on Use

Scripts make the access to and use of the Analyst software easier. In regulated and controlled operations, do not use scripts to replace traditional processes and workflows. For example, do not use scripts to create methods, to make sure that system performance and data quality is satisfactory, or to create reports.

Scripts 2

This document explains how to install and use Analyst software scripts. It also provides an overview of the uses of each script and how to uninstall a script, if required.

Note: This guide contains the scripts for all instruments and different software versions. To determine which scripts the software version installed on the instrument supports, refer to the document: *Release Notes* for the Analyst software.

Install or Uninstall Scripts

Some scripts are automatically installed when the Analyst software is installed.

The remaining scripts are available in the Scripts folder.

Scripts must be installed to use them. Refer to the section: Install a Script.

Install a Script

1. Do one of the following:
   - Browse to the `C:\Program Files (x86)\Analyst\Scripts` folder on the computer.
   - Browse to the `Extras\Scripts` folder on the software DVD, if available, or in the unzipped software web download package.
2. Open the Scripts folder.
3. Do one of the following:
   - For the sMRM Calculator script, double-click **sMRM Calculator Setup.exe**.
   - For all of the other scripts, double-click **ScriptRunner.exe**.
4. Follow the on-screen instructions to install the scripts.
   The installed scripts are available from the **Script** menu.

   Note: For some scripts, users can hold down the **Shift** key while accessing a script from the **Script** menu to view a description of the script.

Uninstall a Script

Note: Do not uninstall the DFTTracker and MRM3 Optimization scripts. If these scripts are removed, then the Analyst software must be installed again to get access to these scripts.

- To uninstall a script, do these steps as applicable:
  - For processing scripts, browse to the `<drive>:\Analyst Data\Projects\API Instrument\Processing Scripts` folder, and then delete the script dll, or, if applicable, the exe and bmp files, manually.
  - For the Create Quan Methods From Text Files, Create Text File from Quant Method, and MSServiceLog scripts, browse to the `<drive>:\Analyst Data\Projects\API Instrument\Processing Scripts` folder and then delete the script dll manually.
  - For the sMRM Calculator script, do this:
    a. Click **Start** > **Control Panel** > **Programs and Features**.
    b. Right-click **sMRM Calculator** and then click **Uninstall**.
    c. Obey the on-screen instructions.
  - For acquisition scripts, browse to the `<drive>:\Analyst Data\Projects\API Instrument\Acquisition Scripts` folder, and then delete the script dll, or, if applicable, the exe and bmp files, manually.

Add Missing Zeros

Use this script to add an intensity value of zero for the missing mass values in the spectrum. To minimize storage requirements and to show and process data faster, the Analyst software does not store or show spectral points with an original intensity of zero. If required, for example, when exporting a spectrum for subsequent processing by custom software, these data points can be added back to the spectrum.

Use the Script

- Click the spectrum and then click **Script** > **Add Missing Zeros**.
  The script addd the zero values to all missing masses in the current spectrum.

Add Normalized ADC Traces

Use this script to overlay the active chromatogram or chromatograms with normalized ADC data from a corresponding data file. Run the script when a pane containing one or more chromatograms is active in Explore mode. There might be a time region selected in a trace. If no selection is made, then the entire chromatogram is overlayed.

If the wiff file contains several ADC traces, then all of them will be shown.

Note: If the data in the active pane came from several samples, then the ADC data for the sample corresponding to the first data set, not the active data set, is shown.

Use the Script

- Do one of the following:
  - Click **Script** > **AddNormalizedADC.**
  - To view the script description and add ADC data to an active Explore pane, hold the **Shift** key down and click the script.

Analyst 1.2 Peak Finder Parameters

The Analyst software uses an improved version of Peak Finder for better peak detection and ion abundance measurement. When the Peak Finder algorithm is used to analyze wiff files that were acquired using the Analyst software, then use this script to set the peak finder algorithm parameters.

Note: This script is installed automatically when the Analyst software is installed. There is no separate installation program for it.

Tip! Browse to the `Analyst Data\Projects\API Instrument\Processing Scripts` folder and make sure that the Analyst12PeakFinderParams.dll is present.

Use the Script

1. Click **Script** > **Analyst12PeakFinderParams.**
   The Analyst 1.2 Peak Finder Algorithm Parameter dialog opens.
2. To activate the Analyst 1.2 version of Peak Finder, select the **Use Analyst 1.2 peak finder algorithm for Analyst 1.2 files** check box.
3. Do the following:
   - In the **Intensity Threshold (%)** field, type the value, as a percentage, of the minimum intensity required to distinguish between noise and peak.
   - In the **Centroid Height (%)** field, type the value, as a percentage, to be used by the centroiding algorithm to find the peak and to determine the centroid *m/z* value at this percentage height.
   - In the **Centroid Peak Width (min)** field, type the minimum value, in ppm, to be used by the centroiding algorithm to find the peak width and to determine the centroid *m/z* value at this width.
   - In the **Centroid Peak Width (max)** field, type the maximum value, in ppm, to be used by the centroiding algorithm to find the peak width and to determine the centroid *m/z* value at this width.

- In the **Centroid Merge Distance (amu)** field, type a value, in amu, to be used to determine whether two centroid peaks should be merged in to one. If two peaks are within this tolerance, then they are merged.
- In the **Centroid Merge Distance (ppm)** field, type a value, in ppm, to be used to determine whether two centroid peaks should be merged in to one. If two peaks are within this tolerance, then they are merged.

4. Click **OK**.
5. To return to the Analyst 1.4.1 Peak Finder algorithm, clear the **Use Analyst 1.2 peak finder algorithm for Analyst 1.2 files** check box.

Change All Methods

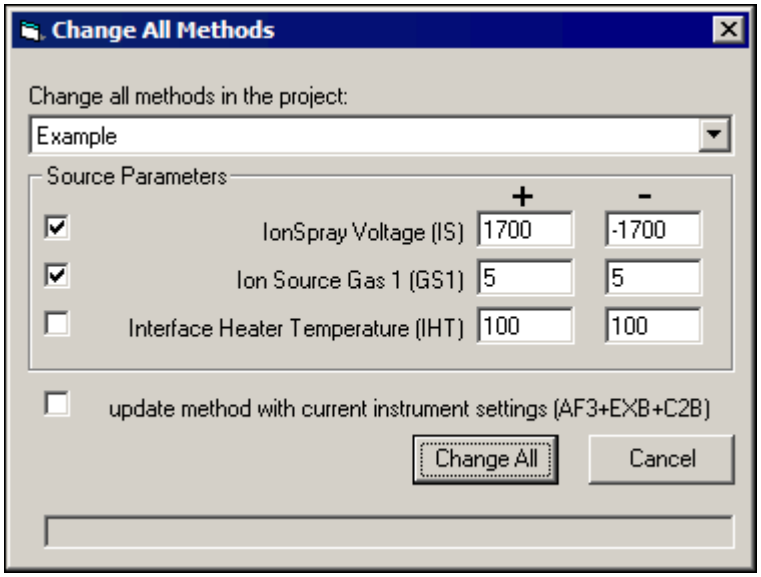
It is often necessary to change the ion source conditions of a method. This script modifies every method in a selected project with new values for IonSpray Voltage (IS), Ion Source Gas 1 (GS1), and Interface Heater Temperature (IHT).

Note: This script is used with any QTRAP® system. It is not used by QSTAR systems.

Use the Script

1. Click **Script** > **ChangeAllMethods**.

Figure 2-1 Change All Methods Dialog



2. Select a project containing the methods to be modified.
3. Select the parameters to be changed.

If the parameter is not in the method file, then it is ignored.

4. Type a value for positive experiments.
5. Type a value for negative experiments.
6. Select the **update method with current instrument settings** check box to change the **AF3**, **EXB**, and **C2B** parameters for all of the methods in the selected project.
7. Click **Change All**.

Convert Methods

Use this script to convert methods from one type of instrument to another. The script converts the method to the currently active hardware profile, using appropriate values for each parameter. Only the ion source- and compound-dependent parameters for mass ranges and experiments are shown.

The Convert Methods script automatically optimizes mass ranges and, in addition to single period, single experiment methods, converts multiple periods, multiple experiments, and IDA criteria.

Install the Script

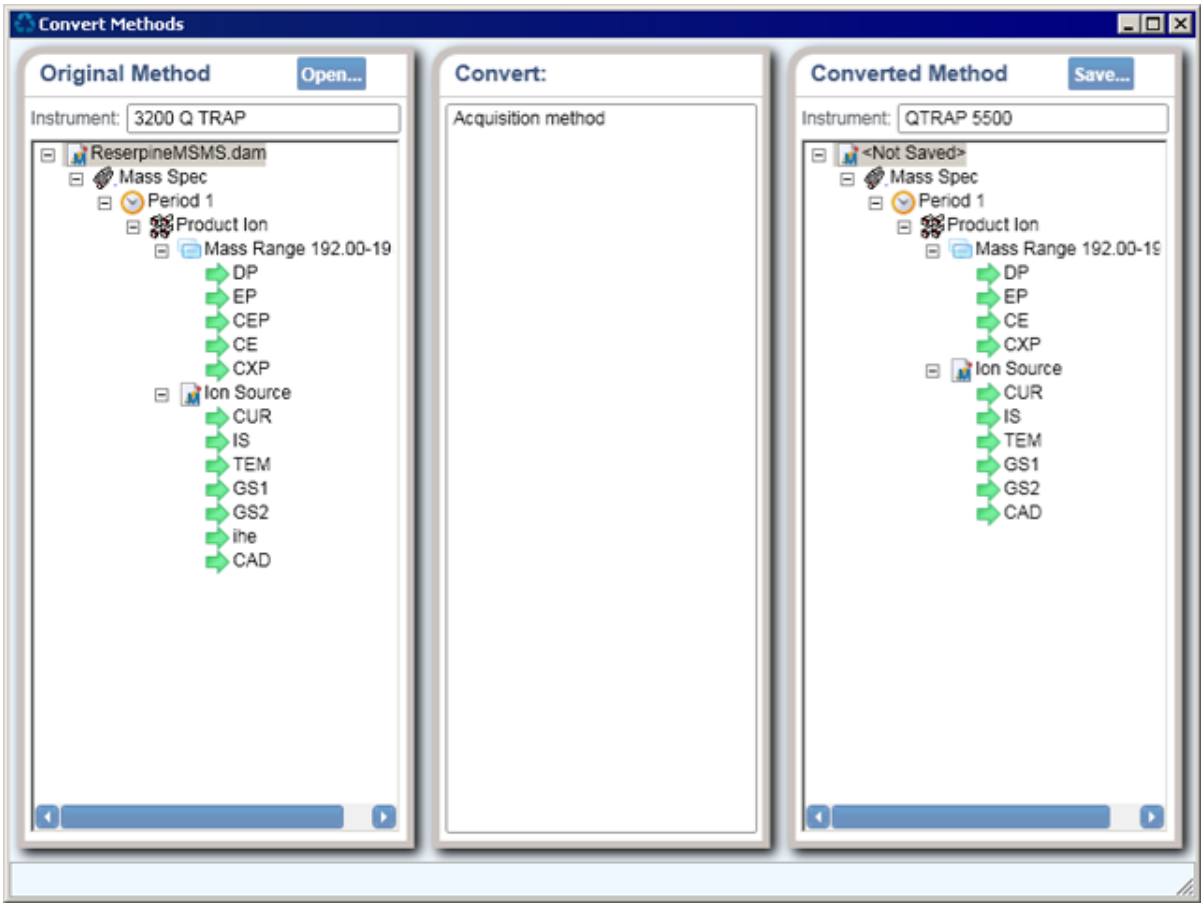
1. Browse to the `C:\Program Files (x86)\Analyst\Scripts\Convert Methods` folder and then double-click **Convert Methods Setup.exe**.
2. Obey the on-screen instructions.

Use the Script

Make sure a hardware profile is active.

1. Click **Script** > **Convert Methods.**

Figure 2-2 Convert Methods Dialog



2. Click **Open**, browse to the method to be converted, and then click **Open**.
   The Method Converter dialog shows the instrument name of the original method.
3. Click **Save**, type a name for the converted method, and then click **Save**.

Create Quantitation Methods and Text Files

The Create Text File From Quan Method script exports a quantitation method to a tab-delimited text file. The Create Quan Method From Text Files script imports the information contained in a tab-delimited text file to a Quantitation Method File (qmf). Currently, the Build Quantitation Method component in the Analyst software does not support this functionality.

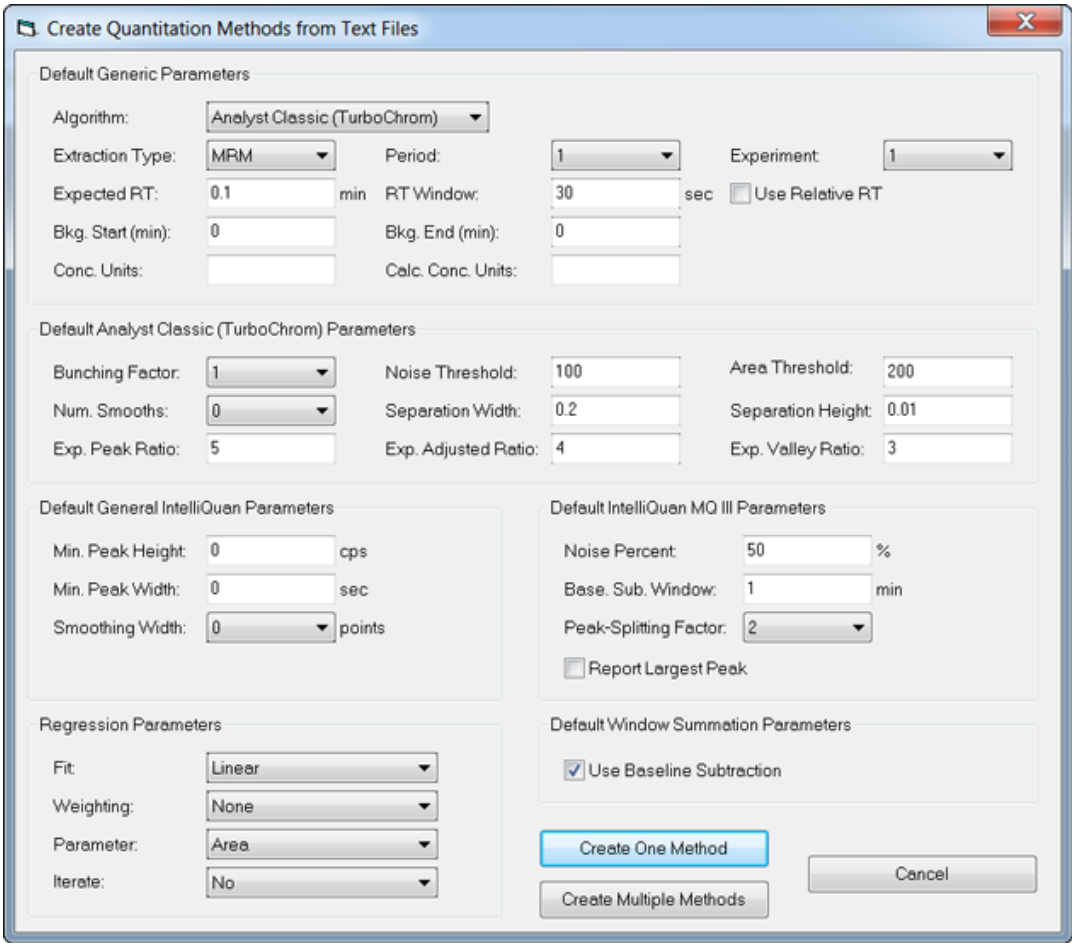
The Create Text File from Quan Method script creates a text file representation of a quantitation method file. A column for each required field is created in the text file if the **Export all columns** check box is selected. If the check box is not selected, then the script generates the text file with columns only for the fields where the field value is not the same for all peaks.

The Create Quan Method From Text Files script specifies default values for any of the non-required fields in the text file such as integration algorithm or regression parameters. For more information, refer to the section: Text File Format .

Use the Create Quan Methods From Text Files Script

1. Click **Script** > **Create Quan Methods From Text Files**.

Figure 2-3 Create Quantitation Methods from Text Files Dialog



2. Use the parameters in the Default Generic Parameters section to create a quantitation method. The **Algorithm**, **Extraction Type**, **Period**, and **Experiment** fields are not available in the Analyst software. Set the following parameters as required:

   - From the **Algorithm** list, select a peak-finding algorithm. The Window Summation algorithm sums all the intensities in the retention threshold and will not find any peaks.
   - From the **Extraction Type** list, select the type of data that will be integrated.

- From the **Period** and **Experiment** lists, select the period number and experiment number.

The Default Analyst Classic Parameters, Default General IntelliQuan Parameters, Default IntelliQuan MQ III Parameters, and the Default Window Summation Parameters groups contain the parameters that are used by the algorithm selected in the **Algorithm** field.

Note: The **Smoothing Width** field in the Default General IntelliQuan Parameters group is half the smoothing width.

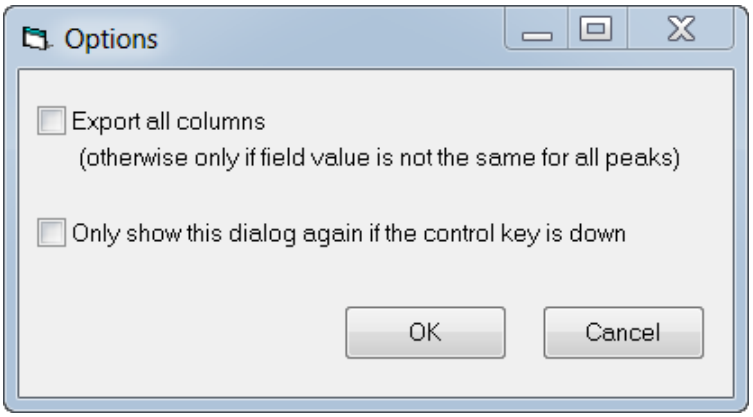
3. Select the **Use Baseline Subtraction** check box to have the Window Summation algorithm sum the intensities to the horizontal line at the minimum intensity of the data points within the summation window, as opposed to summing down to the intensity zero.
4. In the Regression Parameters section, select the regression information.
   The information specified here is applied to every analyte peak. Unlike the previous parameters, it is not possible to indicate this information in the text files. Therefore, the same regression parameters are applied to all analytes. For a full description of the parameters, refer to the document: *Help*.
5. To create one quantitation method, click **Create One Method**, browse to the text file that will be used to create the quantitation method, and then click **Open**.
   A quantitation method qmf file with the same file name as the txt file is created if the text file is in the correct format and contains the required columns. The created quantitation method is stored in the `Quantitation Methods` folder under the current working project in the Analyst software, regardless of the location of the text file.
6. To create multiple methods from multiple text files, click **Create Multiple Methods**, browse to the folder where the text files are located, and then click **OK**.

   A quantitation method qmf file with the same file name as the txt file is created for each individual text file in that folder if they are in the correct format and contain the required columns. The created quantitation methods are stored in the `Quantitation Methods` folder under the current working project in the Analyst software, regardless of the location of the text files.

Use the Create Text File from Quan Method Script

1. Create and save a quantitation method in the Analyst software.
2. Click **Script** > **Create Text File from Quan Method.**

Figure 2-4 Options Dialog



3. Select the **Export all columns** check box and then click **OK**.
4. Browse to and then select the quantitation method (qmf) file.
5. **Navigate** to and then select the location of the text file.
   The script generates the text file with all columns. If the **Export all columns** check box was not selected in step 3, then the script only generates the text file with columns for the fields where the field value is not the same for all peaks.

Text File Format

The text files used to create the quantitation methods (Create Quan Methods from Text Files) and generated from the methods (Create Text File from Quan Method) are in the following format:

- Separate the various fields with tab characters and end each line with a carriage return or line feed character.
- The first row of the file should contain column headings. All of the columns shown in the following table marked as Required must be present. The remaining columns are optional. The actual order of the columns is not important.
- Each subsequent line should contain the information as shown in the table for either one analyte or an internal standard peak.

Table 2-1 Text File Formats

Column Name	Required	Description
Peak Name	Yes	The name of the analyte or internal standard peak.
First Mass	Yes	For MRM data, the Q1 mass for the peak. For full-scan data, the starting mass for the XIC to integrate. For Q1 MI or Q3 MI data, the mass.

Table 2-1 Text File Formats (continued)

Column Name	Required	Description
Second Mass	Maybe	This field is required when integrating full-scan or MRM data, but not for Q1 MI or Q3 MI data. For MRM data, this is the Q3 mass for the peak. For full-scan data, it is the ending mass for the XIC to integrate.
Extraction Type	No	The type of data to integrate. If present, this should be one of: 0 - MRM data 1 - Q1 MI or Q3 MI data 2 - full-scan data
Is IS	No	Specifies whether the current peak is an internal standard or an analyte. TRUE if the peak is an internal standard. Otherwise, FALSE. If this column is not present, then all peaks defined are assumed to be analytes. **Note**: Internal standard peaks should be defined first in the text file before any analyte peaks that use that IS.
IS Name	No	For analyte peaks, specifies the name of the corresponding internal standard (if any). If a given analyte will not use an internal standard, then leave the contents of this field empty. For internal standard peaks themselves, the contents of this field are ignored.
Period	No	The period number for the peak (from 1 to the number of periods in the data).
Experiment	No	The experiment number for the peak (from 1 to the maximum number of experiments in the period).
Use Relative RT	No	For analyte peaks that are using an internal standard, specifies whether or not the expected retention time is relative to that of the IS. TRUE if so. Otherwise, FALSE. The contents of this field are ignored for other peaks, but must still contain either TRUE or FALSE.
Conc Units	No	The concentration units.
Calc Conc Units	No	The calculated concentration units.

Table 2-1 Text File Formats (continued)

Column Name	Required	Description
Bkg Start	No	Start time, in minutes, for the peak background. This parameter does not affect the peak integration in any way, however, it does affect how the noise, and hence S/N, is calculated.
Bkg End	No	End time, in minutes, for the peak background.
Expected RT	No	The expected retention time, in minutes, from 0 to 1666.
RT Window	No	The retention time window, in seconds, from 1 to 1000.
Algorithm	No	Specifies which peak-finding and integration algorithm should be used. If present, this should be one of: 0 - Analyst Classic (TurboChrom) 1 - IntelliQuan - IQA II (Automatic) 2 - IntelliQuan - MQ III 3 - Window Summation
Bunching Factor	No	(TurboChrom algorithm) The bunching factor for the peak, from 1 to 100.
Num Smooths	No	(TurboChrom algorithm) The number of smooths, from 0 to 10.
Noise Threshold	No	(TurboChrom algorithm) The noise threshold, from 1-6 to 19.
Area Threshold	No	(TurboChrom algorithm) The area threshold, from 1-6 to 112.
Separation Width	No	(TurboChrom algorithm) The separation width, from 0 to 5.
Separation Height	No	(TurboChrom algorithm) The separation height, from 0 to 1.
Exp Peak Ratio	No	(TurboChrom algorithm) The exponential peak ratio, from 1 to 16.
Exp Adjusted Ratio	No	(TurboChrom algorithm The exponential adjusted ratio, from 2 to 16.
Exp Valley Ratio	No	(TurboChrom algorithm) The exponential valley ratio, from 1 to 16.

Table 2-1 Text File Formats (continued)

Column Name	Required	Description
Min Height	No	The minimum allowed peak height, from 0 to 116, when using the IntelliQuan algorithm.
Min Width	No	(IntelliQuan algorithm) The minimum allowed peak width, from 0 to 116, in seconds.
Smooth Width	No	(IntelliQuan algorithm) The half-width of the Savitzky-Golay smoothing filter, from 0 to 20.
MQ III Noise Percent	No	(IntelliQuan algorithm) The noise percentage when the MQ III option is used. This should be an integer from, 0 to 100.
MQ III Baseline Sub Window	No	(IntelliQuan algorithm) The baseline subtraction window, from 0 to 10 minutes, when the MQ III option is used.
MQ III Peak Splitting Factor	No	(IntelliQuan algorithm) The peak-splitting factor, from 0 to 10, when the MQ III option is used.
MQ III Use Largest	No	(IntelliQuan algorithm) Specifies whether the largest peak when the MQ III option is used, within the retention time window, or the peak whose retention time is closest to that expected is reported. TRUE to use the largest peak and FALSE to use the closest.
Summation Baseline Sub	No	(Special window summation algorithm) Specifies whether the area should be integrated to the intensity=0 line or to the intensity value of the least intense data point within the window. TRUE if area should be integrated to the intensity value of the least intense data point, otherwise, FALSE if the area should be integrated to the intensity=0 line.

The following table shows an example text file for full-scan data. The text file contains tabs between the columns and a carriage return at the end of each line.

Table 2-2 Example Text File for Full-Scan Data

Peak Name	First Mass	Second Mass	Bunching Factor
Analyte Peak 1	500.1	500.7	1
Analyte Peak 2	812	813	2

Table 2-2 Example Text File for Full-Scan Data (continued)

Peak Name	First Mass	Second Mass	Bunching Factor
Analyte Peak 3	400	401	3

The following table shows another example for MRM data. The Analyte Peak 1 is configured to use the specified internal standard and Analyte Peak 2 does not use an internal standard.

Table 2-3 Example Text File for MRM Data

Peak Name	Is IS	IS Name	First Mass	Second Mass
IS Peak 1	TRUE	—	500.1	413.2
Analyte Peak 1	FALSE	IS Peak 1	600.2	382.1
Analyte Peak 2	FALSE	IS Peak 1	400	312.1

The following table contains a mixture of full-scan and MRM data in different experiments:

Table 2-4 Example Text File for MRM Data

Peak Name	Extraction Type	Experiment	First Mass	Second Mass
Analyte Peak 1	0	1	500.1	413.2
Analyte Peak 2	0	1	600.2	382.1
Analyte Peak 3	2	2	812	813
Analyte Peak 4	2	2	400	401

Define Custom Elements

Use this script to select a custom isotope pattern when radio-labeled compounds are used. An experiment-specific element pattern is used in the data interpretation in conjunction with the Analyst software calculators or the Metabolite ID application.

The custom isotope patterns are kept together with the information from the periodic table elements in the element definition file, SAElements.ini, which is located the folder: `C:\Program Files (x86)\Analyst\bin`

In the element definition file, the custom elements must have a unique symbol and an atomic number of 104 or higher.

Notes on Use

When the script is launched for the first time, a backup copy of the SAElements.ini file is saved in the API Instrument folder. If required, the edited SAElements.ini file can be replaced with this file in the folder: `C:\Program Files (x86)\Analyst\bin`

Update the Element Definition File Successfully

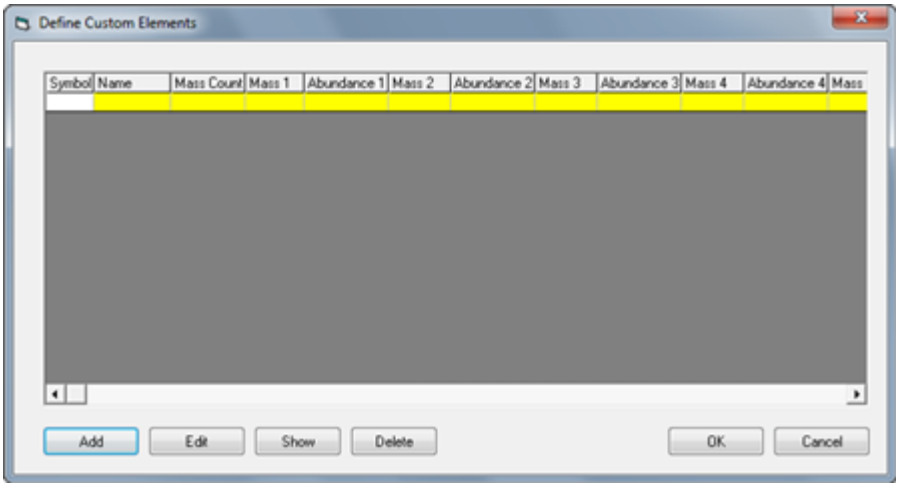
1. Do not open the SAElements.ini file in another text editor program while using the software.
2. Make sure that the file properties are set to read/write.

Edit the Define Custom Elements Table

The custom element table cannot be edited in the dialog. After the element definition file is updated, the custom elements can be used with the Analyst software calculators.

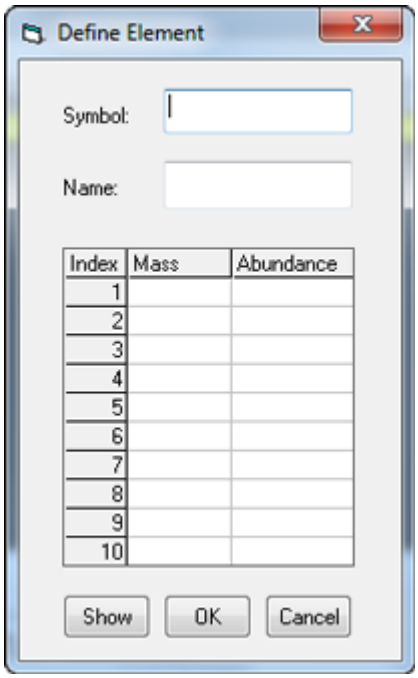
1. Click **Script** > **DefineCustomEl**.

Figure 2-5 Define Custom Elements Dialog



2. In the table, click the row containing the element.

Figure 2-6 Define Element Dialog



3. Edit the fields and then click **OK**.
4. To save the updated element definition file and exit the program, click **OK**.

View the Custom Element Symbol, Custom Element Name, and Custom Pattern

- To view the custom pattern in the mass/relative intensity graph, in the Define Custom Elements dialog, click **Show**.

  The Isotopic Distribution dialog opens.

  The total of the individual isotope abundances for an element stored in the element definition file must equal to one. Therefore, the abundances entered in the Define Element dialog are rescaled before they are added to the Define Custom Elements dialog. This Isotopic Distribution dialog cannot be edited. Zoom in on the area of interest by dragging along the corresponding X- or Y-axis region.

  The application requires the gen01.wiff example file to show custom patterns. If the gen01.wiff file is not in the Example folder in the Analyst Data\Projects folder, the software prompts the user to find this file.

Delete Others

Use this processing script to delete all panes except for the active one.

Use the Script

1. With a sample file (wiff) with multiple panes open, click a pane.
   The pane becomes the active pane.
2. Click **Script** > **DeleteOthers**.
   All of the panes except for the active one are deleted.

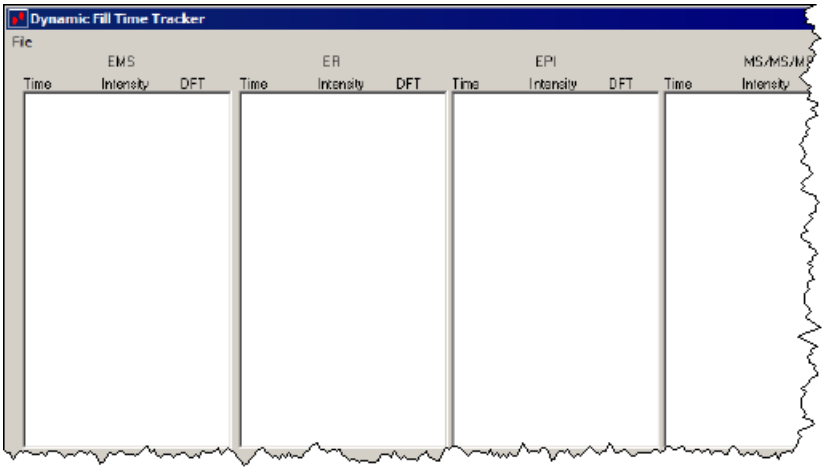
DFT Tracker

The Dynamic Fill Time (DFT) Tracker script tracks the DFT settings used during QTRAP instrument scans. Use the script to determine the optimal fill time for linear ion trap (LIT) mode to obtain high data quality over a wide dynamic range. The DFT Tracker monitors the following LIT scan types: Enhanced MS (EMS), Enhanced Resolution (ER), Enhanced Product Ion (EPI), and MS/MS/MS (MS3).

Use the Script

- Click **Script** > **DFTTracker.**

Figure 2-7 Dynamic Fill Time Tracker Dialog



DFT Tracker monitors the dynamic changes occurring during a real-time run.

The system dynamically calculates the time required to fill the linear ion trap. For abundant compounds, a short fill time reduces the space charge effects by limiting the number of ions in the ion trap. On the other hand, the longer fill time increases weak signals by allowing the ions to accumulate.

Export IDA Spectra

Use this script to export data in a format that can be searched using a third-party application. The Export IDA Spectra script exports every dependent product spectrum from an IDA (Information Dependent Acquisition) LC/MS run to a series of text files. These text files can then be submitted and searched using Sequest. The export is optimized so that any spectra in adjacent cycles with the same precursor *m/z* value are combined in a single spectrum. This optimization also applies to spectra with the same precursor but which reside in different experiments, most likely using different values of the collision energy.

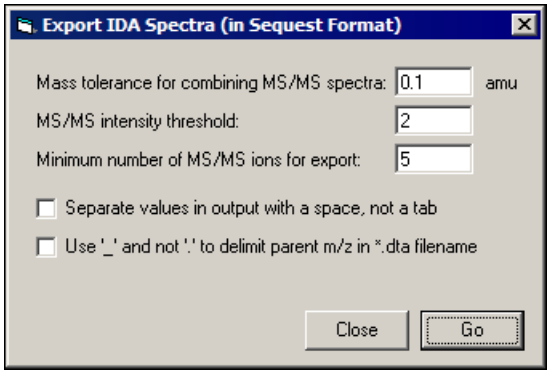
The charge state of the precursor ion is a required input. Sequest tries to automatically determine this from the isotope spacing at the precursor *m/z* value in the IDA survey spectrum. Note that while this determination is usually correct, it is not always.

Use the Script

It is assumed that the first experiment of the IDA method represents the survey spectrum and that all of the other experiments represent dependent product spectra. Therefore, this script cannot be used if there are multiple survey experiments.

1. With an IDA chromatogram in an active pane, click **Script** > **Export IDA Spectra.**

Figure 2-8 Export IDA Spectra (in Sequest Format) Dialog



2. In the **Mass tolerance for combining MS/MS spectra** field, type the tolerance to be used to determine if two precursor *m/z* values should be considered identical.

   If the precursors for two sequential product spectra differ by less than this value, then the spectra are added and a single text file is exported.

3. In the **MS/MS intensity threshold** field, type the threshold that is applied to each product spectrum after it is centroided. It is assumed that peaks below this threshold are most likely noise. Type `0` in the field to exclude a threshold.

4. In the **Minimum number of MS/MS ions for export** field, type the minimum number of ions that must be present in a product spectrum, after centroiding and thresholding, for a text file to be exported.

   If a spectrum does not contain the specified number of ions, then it is assumed that the quality of the spectrum is too low to merit exporting.

5. (Optional) To separate fields in the output files with a space character, select the **Separate values in output with a space, not a tab** check box.

   Otherwise a tab character is used. Some versions of Sequest require a space delimiter.

6. To export the text files, click **Go**.
   The Save As dialog opens.

7. Type a location and root file name for the exported text files.

   Before being exported to a text file, each of the product spectra is centroided. The cycle number range and charge state is appended to this file for each exported spectrum.

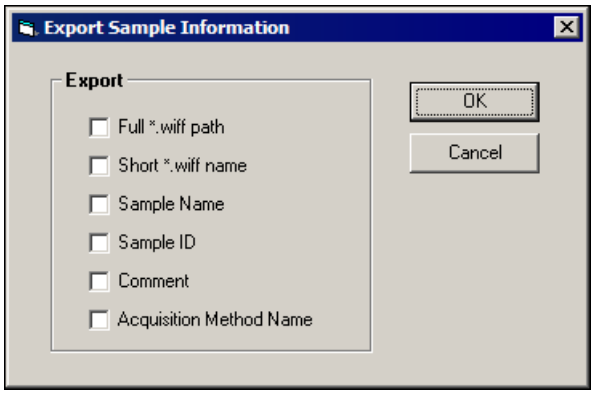
Export Sample Information

Use this script to extract sample information, such as the name, sample ID, comment, and acquisition method name for all samples in the wiff file. Define the information to be exported, and the script saves the information in an inf file located in the same folder as the wiff file.

Use the Script

1. With a chromatogram or spectrum in an active pane, click **Script** > **ExportSampleInformationFromMultipleSampleinOneWiff** while pressing **Ctrl**.

   Figure 2-9 Export Sample Information Dialog



2. Select the check boxes that correspond to the information to be exported and then click **OK**.

Export to JCamp

Use the Analyst software to export graph data to a tab-delimited text file that can be read by most applications. However, some applications require a more specific format.

Use the Export to JCAMP script to export graph data in the JCAMP format. The script works on both chromatograms and spectra. For chromatograms, depending on the number of selections made, either all of the spectral data of the chromatogram is exported, or the averaged sum of the selected regions is exported. If this script is used on a single spectrum, then only that data is exported. This script can also be attached to a batch so that the export occurs automatically after the sample is acquired.

The following table shows an overview of the operation of the script. When run interactively the exact behavior depends on the active Analyst software data.

Table 2-5 Script Operation

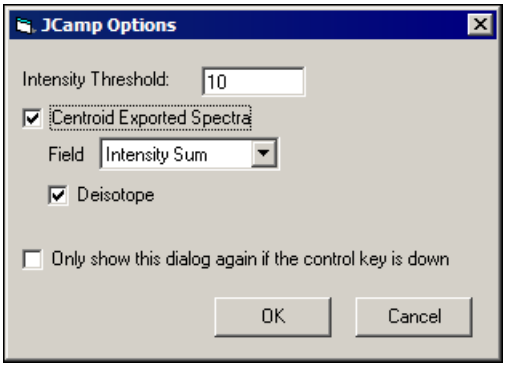
Modes	Active data	Operation
Interactive	Spectrum	The user is prompted for the name of the JCamp file and the active spectrum exported to it.
Interactive	Chromatogram with two or more selections	The user is prompted for the name of the JCamp file and an averaged spectrum corresponding to each of the selections of the chromatogram exported to it.
Interactive	Chromatogram with one or no selections	The user is prompted for the name of the JCamp file and every spectrum for the run exported to it.
Batch	N / A	The name of the JCamp file is generated by appending the sample number to the name of the wiff file and changing the extension to jdx. Every spectrum for the run is exported to the JCamp file. For multiple period/experiment data, a separate file is exported for each experiment. The period and experiment numbers are appended to the filename.

Use the Script

1. To use the Export to JCAMP do one of the following:

- With either a chromatogram or a spectrum in an active pane, click **Script** > **Export to JCAMP.**
- In the **Batch Editor** dialog, type `Analyst Data \API Instrument\Processing Scripts\Export to Jcamp.dll` in the**Batch Script** field.

Figure 2-10 JCAMP Options Dialog



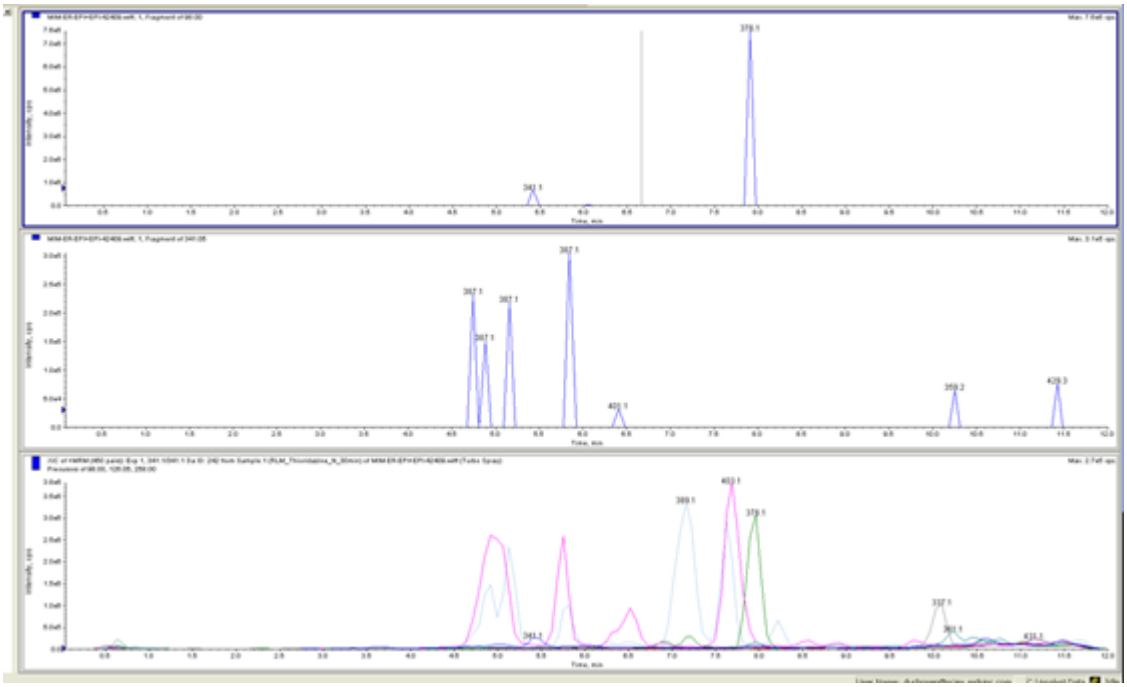
2. To select the centroiding options, do one of the following:
   - Select the **Centroid Exported Spectra** check box to centroid the spectra before exporting to the JCAMP format.
   - To show the JCAMP Options dialog only if the **Ctrl** key is pressed when the script is clicked from the **Script** menu, or when the batch is submitted to the queue, select the **Only show this dialog again if the control key is down** check box.
3. To continue processing and to export the spectra, click **OK**.
4. When prompted, type the file name of the exported JCAMP file.

   When a script is attached to the batch, the file name is automatically generated using the following format: [WiffFileName]_[Sample#]_[Period#]_[Experiment#].jdx.

IDA Trace Extractor

Use this script to review the survey data collected using Information Dependent Acquisition (IDA) based on the information in the corresponding dependent data. The script searches the MS/MS data for given neutral losses or fragments and then calculates the Extracted Ion Chromatograms (XICs) for the precursor masses, which give the specified losses or fragments. The XICs are overlaid in Explore mode and their peaks are labeled with the precursor mass. Refer to the following figure.

Figure 2-11 Characteristic Traces in Dependent Experiment and XICs of the Survey Experiment



Note: The characteristic *m/z* 387.1 detected in negative mode was converted to *m/z* 389.1 in the positive survey scan.

Use the script to do the following:

- Specify a list of expected fragments or neutral losses, in either the positive mode polarity, the negative mode polarity, or both, in terms of fragment formula or mass.
- Save the list of masses and fragments for a compound class and then load them to the settings at a later time.
- Process just a selected time region in the chromatogram.
- Show precursor (survey scan) or fragment (dependent scan) XIC traces that yield a given fragment or neutral loss.
  - From the survey scan chromatograms, the user can link to any survey scan spectra.
  - From the dependent scan traces, the user can link to any dependent scan spectra.
- Reduce the precursor XIC traces to show only peaks that have corresponding neutral losses or fragments.
- Save the precursor mass list in a text file for further processing. Build the list of precursors from a set of samples.

- Save the list of masses in a format that can be loaded to the XICfromTable script.
- Save the list of masses and peaks in a format that can be loaded to the CreateQuantMethodFromText script.

Note: The script is compatible with MRM/MIM IDA data and with the Analyst software.

Note: The script supports parallel data processing from positive and negative experiments. Multiple survey and dependent experiments of any polarity can be used.

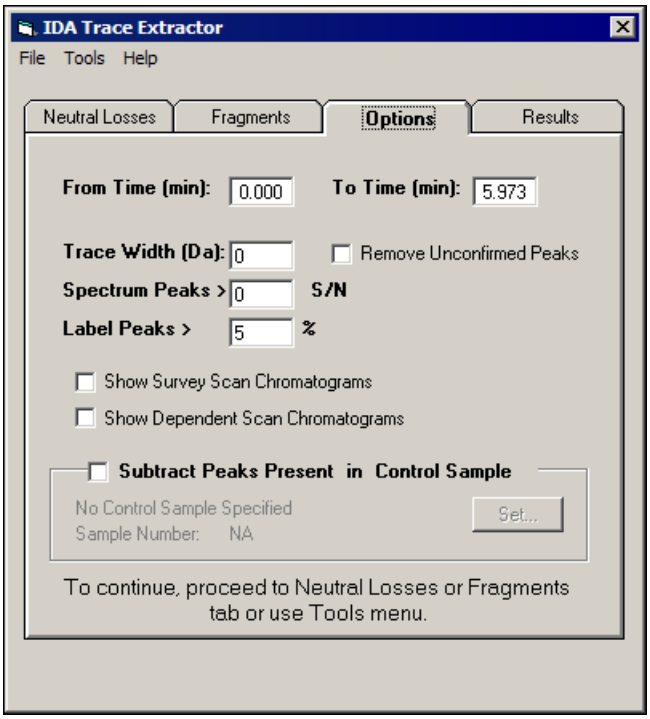
Use the Script

Note: The Analyst software version for a specific file can be shown in the **file properties** > **comments**.

Process a full chromatogram or just a selected region. Make a selection before running the script.

1. With a chromatogram (or selection) of IDA data open in an active pane, click **Script** > **IDATraceExtractor**.

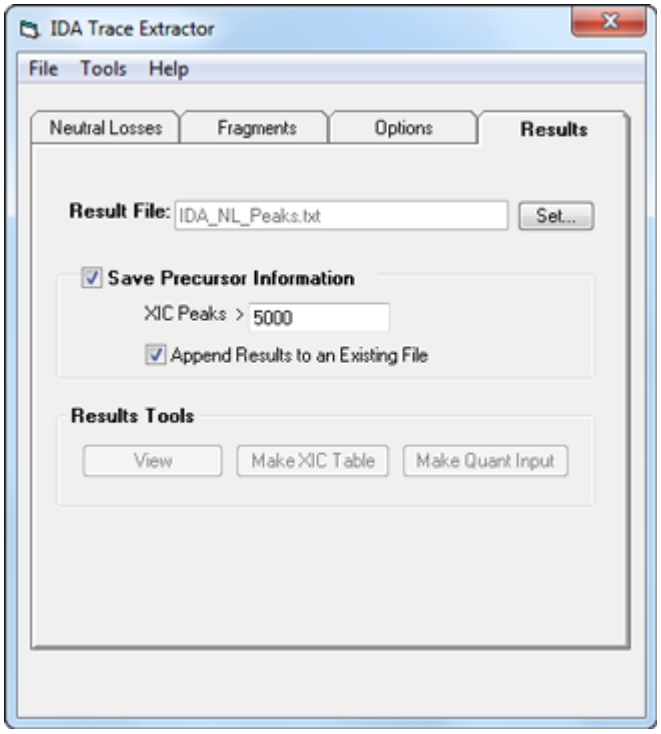
Figure 2-12 IDA Trace Extractor Dialog



2. In the Options tab, set the field values as required.
   For more information, refer to the section: IDA Trace Extractor Tabs and Menu Parameters.

3. To store the retention times and precursor masses found during processing, open the Results tab, type a file name, and then select **Save Precursor Information**.

Figure 2-13 IDA Trace Extractor Dialog: Results Tab



4. To review or enter the mass information, open the Neutral Losses or Fragments tab. Type the neutral losses and fragments as masses or chemical formulas.

   The polarity of the Neutral Loss or fragment experiment where the specified neutral loss or fragment is expected to be found can also be specified.

Figure 2-14 IDA Trace Extractor Dialog: Neutral Losses Tab

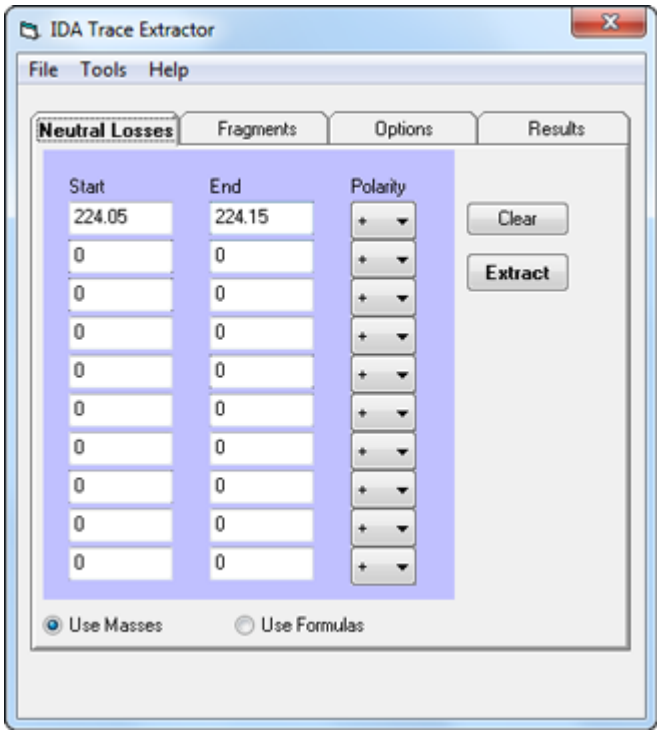
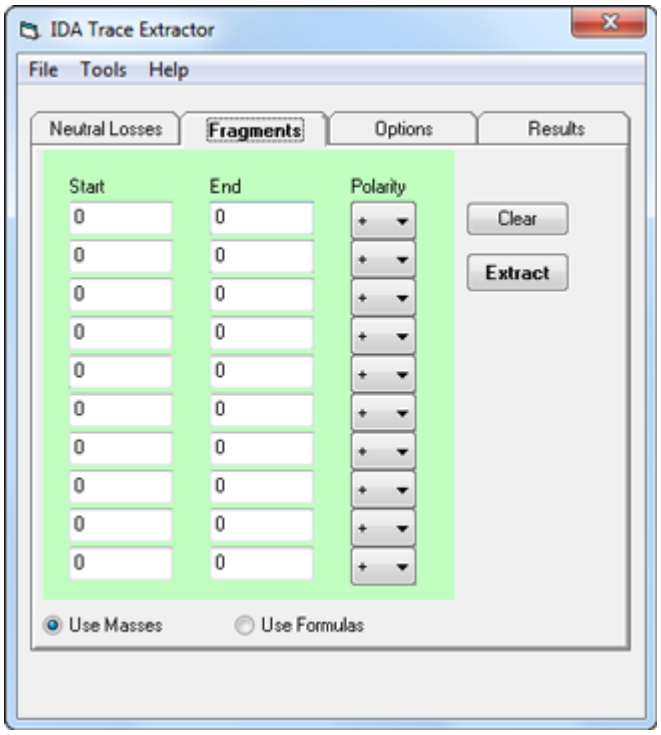


Figure 2-15 IDA Trace Extractor Dialog: Fragments Tab



5. Click **Extract** to find the survey XIC traces that give the selected neutral loss or fragment.
6. If the precursor information was saved, then the found precursor mass/time data can be converted to a compatible format using other scripts.
7. To convert the data, open the Results tab and then select the Results file. View and edit this file as required.
8. Do one of the following:
   - To make a format for the XICfromTable script, click **Make XIC Table**. The Results file is converted to a file of the same name with the suffix _XIC.
   - To make a format for the **CreateQuantMethodFromText** script on the **Precursor XICs** dialog, click **Make Quant Input**. The Results file is converted to a file of the same name with the suffix _Peaks.
9. Click **File** > **Save Settings as.**

Tip! Alternatively, previously saved settings can be used. Click **File** > **Load Settings** to open previously saved settings.

Several functions are available in the **Tools** menu. Users can start processing without switching to a specific tab.

IDA Trace Extractor Tabs and Menu Parameters

Parameters	Description
Neutral Losses Tab	
Use Masses	Select the required neutral losses as mass.
Use Formulas	Select the required neutral losses as formula.
Start	Low mass limit (From mass) for the neutral losses.
End	High mass limit (To mass) for the neutral losses.
Formula	Chemical formula of the neutral loss.
Extract	Start data processing according to the current settings.
Clear	Clear all neutral losses in the settings.
Polarity	Select the polarity of the neutral loss experiment where the specified neutral loss is expected to be found.
Fragments Tab	
Use Masses	Describe the characteristic fragments in terms of their *m/z* value.
Use Formulas	Describe the characteristic fragments in terms of their formulas.
Start	Low mass limit (From mass) for the fragment *m/z* window.
End	High mass limit (To mass) for the fragment *m/z* window.
Formula	Chemical formula of the fragment (protonated/deprotonated form).
Extract	Start data processing using the current settings.
Polarity	Select the polarity of the fragment spectrum experiment where the specified fragment is expected to be found.
Clear	Clear all fragments in the settings.
Options Tab	
From Time (min)	Start of time region to be processed.
To Time (min)	End of time region to be processed.
Trace Width (Da)	Width of XIC traces in the resulting survey scan and dependent scan chromatograms and mass tolerance window for processing if the neutral losses or fragments are specified as chemical formulas.
Remove Unconfirmed Peaks	Review all peaks in the survey XIC traces and retain only those that were validated based on the data in corresponding dependent scan.

Parameters	Description
Spectrum Peaks >	Minimum size of the diagnostic peak in a dependent scan in terms of signal to noise (lowest measurable signal).
Label Peaks >	The peak label threshold applied to the resulting survey and dependent scan chromatograms. Only the largest peak in each trace is labeled.
Show Survey Scan Chromatograms	Show XICs (original or filtered) from the survey scan that correspond to parent masses yielding specified fragment or neutral loss.
Show Dependent Chromatograms	Show neutral loss traces (one for each neutral loss) reconstructed from dependent scan data.
Subtract Peaks Present in Control Sample	Remove peaks that can be found in the control sample XICs from the survey scan chromatograms.
Results Tab	
Result File	Select the Results file (identified peak times and masses will be saved to the selected Results file).
Save Precursor Information	Write the processing results (the list of found peaks-times and masses) to the selected Results file.
XIC Peaks >	The minimum size of the peak in the survey scan to be stored in the Results file.
Append Results to an Existing File	Do not overwrite the existing Results file.
View	Open the selected Results file.
Make XIC Table	Use the selected Results file to prepare the settings file for the XIC from Table script.
Make Quant Input	Use the selected Results File to prepare an input for CreateQuanMethodFromText script.
File Menu	
Load Settings	Open previously saved script settings.
Save Settings As	Save the current script settings for future use.
Set Results File	Select the Results file (identified peak times and masses will be saved to the selected Results file).
Tools Menu	

Parameters	Description
Extract Fragments	Start data processing using the current settings.
Extract Neutral Losses	Start data processing using the current settings.
Clear Fragments	Clear all fragments in the settings.
Clear Neutral Losses	Clear all neutral losses in the settings.
Make XIC Table	Use the selected Results file to prepare the settings file for the XIC from Table script.
Make Quant Input	Use the selected Results file to prepare an input for the CreateQuanMethodFromText script.

Table 2-6 Related Scripts

Script Name	Description
Export to JCamp	Converts spectra from wiff format to JCamp format.
MSMS Methods from MW Lists	Allows lists of molecular weights obtained from text files to be used to create a series of MS/MS acquisition methods.
Multiple Batch Scripts Script	Allows multiple batch acquisition scripts to be used at the same time (the Batch Editor only allows a single batch script to be specified).
Unit Conversion	Converts from one set of concentration units to another.
Wiff To MatLab	Converts the data from a data file from the wiff format to MatLab (mat) format.

Label Selections

Use this script to add missing labels to the selected peaks in the active graph or to remove labels.

The script can be run when a pane containing a spectrum or a chromatogram is active in Explore mode, and there are one or more selections in the active pane. If neither peak mass (spectrum) nor peak retention time (chromatogram) is available, then the data will be marked with information for the selection maximum.

Note: Only font type and label color are synchronized with the automatic labels. For the best performance, synchronize the other font attributes manually in the Appearance Options dialog.

Note: Labeling spectra with centroid mass/charge state appends just the centroid mass. Labeling chromatograms with base peak ion mass or base peak ion intensity is not supported.

Use the Script

- Do one of the following:
  - To add labels to selections in the active graph, click **Script** > **LabelSelections**.
  - To view the script description and add the labels to an active Explore pane, press **Shift** while clicking **Script** > **LabelSelections**.

Label XIC Traces

Use this script when a pane containing one or more XIC traces is active in Explore mode. If no time region is selected, then the complete chromatogram is considered for processing. The script labels the largest peak in each XIC trace with mass. XIC traces with a maximum point of less than 5% of the most intense trace are not labeled. Other types of traces (TIC, ADC) in the overlay are ignored.

Note: No user settings are required for this script.

Use the Script

- Do one of the following:
  - To add labels to a selection in the active graph, click **Script** > **LabelXICs**.
  - To view the script description and add the labels to an active Explore pane, press **Shift** while clicking **Script** > **LabelXICs**.

Make Exclusion List from Spectrum

Use this script to create a text file containing all of the peaks from the active spectrum. The text file is formatted to be directly imported in the software Information Dependent Acquisition (IDA) exclusion list.

If the spectrum has been previously manually converted to a centroid spectrum, then the resulting peak list is exported directly to the exclusion text file. Otherwise, the script converts the spectrum to a centroid spectrum.

Use the Script

1. With a spectrum in an active pane, click **Script** > **Make Exclusion List from Spectrum**. The Make Exclusion List from Spectrum dialog opens.
2. In the **Exclusion List File Name** field, type the name and path of the text file.

3. If required, in the **Threshold** field, type the threshold to be applied to the centroided spectrum so that small noise peaks are not included in the exclusion list. Type `0` to not use a threshold.
4. Click **Export** to export the exclusion list using the specified parameters.

Mascot

Use this script to send either the active spectrum or all product spectra contained in the active sample, or all samples in the active data file, to the Mascot protein search engine. The script was co-developed with Matrix Science Limited, the creators of Mascot.

When sending only the active spectrum, the script can work with either MS or MS/MS data. When sending MS data, the script conducts, a peptide mass fingerprint search is conducted.

When sending all of the spectra, the script works with data acquired using two distinct types of acquisition methods: either a multiple period/multiple experiment method containing any number of product experiments or an Information Dependent Acquisition (IDA) method. For multiple period/multiple experiment data, the script calculates one spectrum for each experiment by averaging all of the spectra acquired for the experiment. For IDA data, the script uses all of the dependent product spectra, combining adjacent spectra with the same parent mass and charge state.

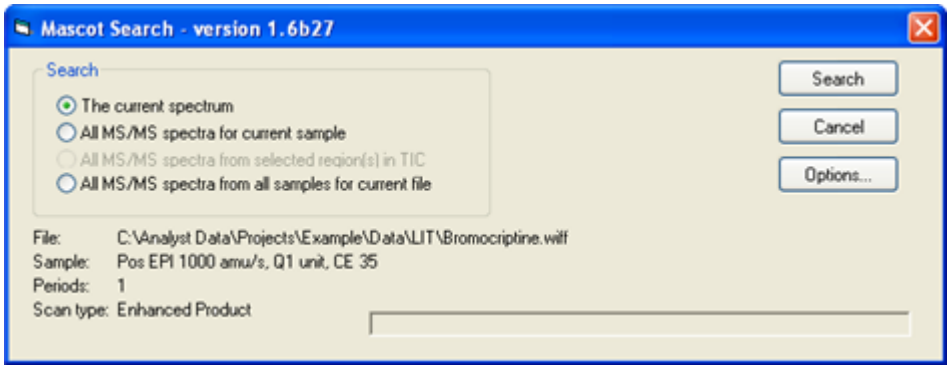
If only one spectrum is being sent to Mascot, then make sure that a centroided spectrum is active in the Analyst software before running the script. If all of the spectra contained in a sample are being sent, then the TIC for the sample should be active.

Use the Script

1. With a centroid spectrum in an active pane, click **Script** > **Mascot.**

   The **File**, **Sample**, **Periods**, and **Scan** type IDA data fields are read-only and show information about the active sample.

   Figure 2-16 Mascot Search Dialog

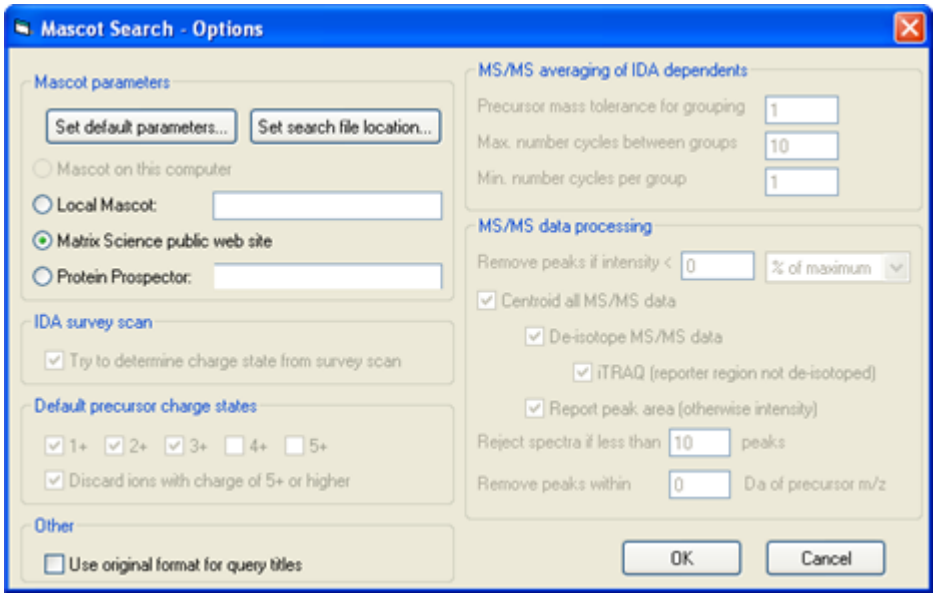


2. In the Search section, do one of the following:

- If the active pane is a centroid spectrum (either MS or MS/MS), then click **The current spectrum** to search this spectrum on its own. Select this option only if the spectrum was converted to a centroid spectrum using the **Centroid** command on the **Explore** menu.
- If the active pane contains MS/MS data, then click **All MS-MS spectra for current sample** to perform a single search using all of the spectra for the sample.
- If the active pane contains MS/MS data and also contains a selected region, then click **All MS-MS spectra from selected region in TIC** to perform a single search using only the spectra from this region. This option can help to speed the generation of the search input if only a portion of the run is known to contain useful data.
- If the active pane contains MS/MS data and the associated data file contains more than one sample, then click **All MS-MS spectra from all samples for current file** to perform a single search using all MS/MS spectra from all samples in the data file.

3. To open the Mascot search form and populate it with the appropriate information, click **Search**. If all product spectra contained in the sample are being searched, then this might take some time and a progress bar is shown. After the Web form opens, click **Start Search**.
4. To set the search options, click **Options**.

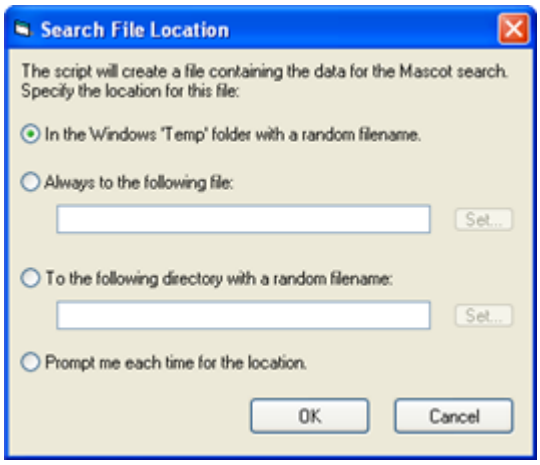
Figure 2-17 Mascot Search-Options Dialog



Tip! To show the Mascot search form defaults Web page, click **Set default parameters**.

5. To set where the text file used as input to Mascot is located, click **Set search file location**, select one of the following options and then click **OK**.

Figure 2-18 Search File Location Dialog



- To save the file in the Windows temporary folder with a random but unique file name, click **In the Windows 'Temp' folder with a random filename**.
- To always write to a specific file, overwriting the file for every search, click **Always to the following file**. To navigate to the folder, click **Set**.
- To create the file with a random but unique filename in the specified directory, click **To the following directory with a random filename**. To browse to the folder, click **Set**.
- To be prompted to save every time a search is performed, click **Prompt me each time for the location**.

In the Default precursor charge states section when searching only the current spectrum, values here are not available. The precursor charge state should be set manually using the resulting Mascot web form. When searching product spectra for an IDA run, the charge state is automatically determined by the script. The values specified here are not used unless the charge state could not be automatically determined or the **Try to determine charge state from survey scan** check box is not selected. When searching product spectra for a multiple period or multiple experiment LC/MS run, the script always considers the specified charge states for each product spectrum.

This option is only required for those using an older Mascot software version that does not accept charge states greater than 5. If one of these older versions is being used, then make sure that the **Discard ions with charge of 5+ or higher** check box is selected in the Default precursor charge states group. Some versions of the Mascot search engine cannot accept ions with a charge state of 5 or higher and show a warning for each ion exceeding this limit.

6. To use the default precursor charge states as is, clear the **Try to determine charge state from survey scan** check box. Otherwise, the script tries to determine the charge state by examining the isotope spacing in the survey spectrum, and for Analyst software data, it uses the charge state determined by the MS Acquisition Engine. The charge state is saved to

the data file. If this check box is selected but the charge state determination fails, then the default charge states are used.

7. In the MS/MS averaging of IDA dependents section, edit the parameters that pertain to the calculation of the product ion spectra for an IDA run.

   - The **Precursor mass tolerance for grouping** field is used to combine adjacent product spectra in a single spectrum if two spectra have precursors with the same charge state and the same MW within this tolerance.
   - In the **Max. number cycles between groups** field, spectra are not combined if the number of cycles between spectra with the same *m/z* value and charge state is greater than the specified value. Use this option to keep spectra with significantly different retention times separate.
   - In the **Min. num cycles per group** field, type the minimum number of spectra that need to be combined for the result to be kept.

   Note: If the dynamic exclusion IDA option was used, then set this value to 1.

8. In the MS/MS data processing section, select parameters that pertain to the filtering of product ion spectra.

   - **Remove peaks if intensity <** — Removes peaks that are less than either a specific count or a specific percent of the maximum peak intensity of the spectrum.
   - **Centroid all MS/MS data** — To centroid the MS/MS spectra before sending them to Mascot for searching, select this check box. It is recommended that this centroid option be enabled.
   - **De-isotope MS/MS data** — If the centroid option is used, then indicate whether isotope peaks should be removed from the MS/MS spectra before they are sent to Mascot by selecting this check box. It is recommended that this option be enabled.
   - **Report peak area (otherwise intensity)** — Uses the area of the peak. Otherwise, it uses the intensity at the apex.
   - **Reject spectra if less than 'n' peaks** — Eliminates a spectrum if it contains unreasonably few peaks after combining adjacent spectra (if used) and centroiding (if used).
   - **Remove peaks within 'n' Da of precursor m/z** — Sets a window around the precursor ion *m/z* and then removes any peaks within that window.

9. In the Other section, select **Use original format for query titles** if a third-party protein quantitation application is being used and if the original title format should be used.

10. To show the Mascot search form defaults Web page, click **Set default parameters**. Edit the defaults so that they do not need to be manually reset every time a search is submitted. After changing the parameters, click **Save defaults as cookie** to close the Web page.

Mass Defect Filter

The identification of drug metabolites in biological fluids with low concentrations from a total ion chromatogram (TIC) is challenging because of significant interferences from endogenous species. A technique of filtering the data based on the mass defect of the parent drug and a small tolerance value has been used to decrease the amount of interference. Using this technique helps in the identification of phase I and phase II metabolites.

The Mass Defect Filter script filters either a TIC or a spectrum using this technique. Only those data points in the spectrum whose centroid mass is within the tolerance range of the mass defect of the precursor ion applied at that nominal mass are kept. All other points are excluded. Summing the intensity for each spectrum generates the TIC. A further filtering based on absolute mass can also be applied.

A new graph of the filtered TIC or spectrum is shown below the current graph.

Use the Script

1. With either a spectrum or a TIC active, click **Script** > **Mass Defect Filter**.
   The Mass Defect Filter Settings dialog opens.
2. In the **Parent Formula** field, type the formula for the parent ion. The **Nominal Mass** and **Mass Defect** fields are automatically updated.
3. If the parent formula is unknown, then type values in the **Nominal Mass** and **Mass Defect** fields.
4. In the **Mass Defect Tolerance (+/-)** field, type the tolerance value.
5. If required, type a value in the **Resolution Factor** field. The **Resolution Factor** further filters the data by keeping only the centroid values whose resolution is greater than or equal to it.
6. If required, to allow the mass defect to be applied differently at each nominal mass in the spectrum, click the **Use Dynamic Mass Defect Calculation** check box.
   If the check box is cleared, then a constant value of the mass defect is added to each nominal mass.
7. In the Mass Range Parameters section, select the **Use Mass Range Filter** check box to set the mass range parameters.
   Only masses in the spectrum between **Start Mass** and **Stop Mass** inclusively are retained.
8. To start processing, click **OK**.

Merge MRM

Use this script to add all of the experiment data from the method to be merged to the base method. Both methods should have only one period and one experiment. The script does not

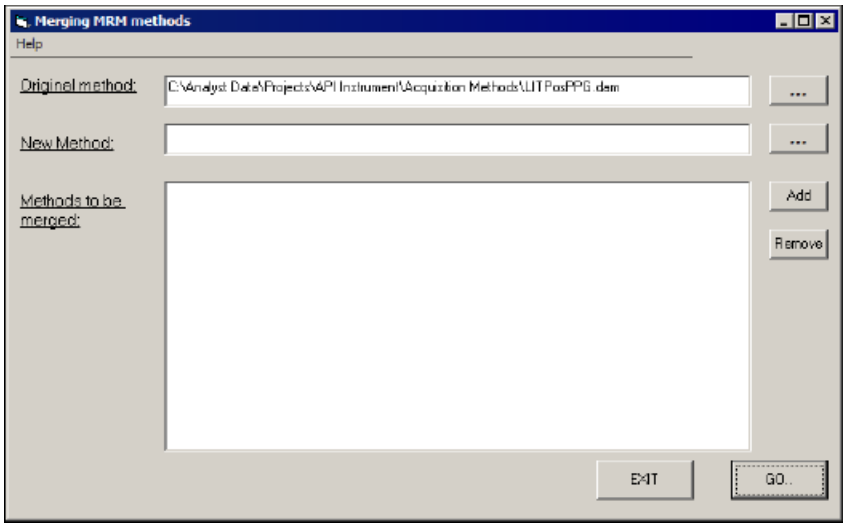
limit the number of mass ranges in an experiment. All mass ranges are saved to the base method.

This script can be used to merge multiple final methods created by cCompound optimization. After the methods are merged, the LC information can be modified, if necessary, to reflect the analysis conditions.

Use the Script

1. Click **Script** > **Merge MRM.**

Figure 2-19 Merging MRM methods Dialog



2. To browse to the original acquisition method file or template, click the button to the right of **Original method**.
3. To specify the name and location of the merged acquisition method file, click the button to the right of **New Method**, type the name of the method, and then click **Open**.
4. To add an acquisition method to the list of methods to be merged, click **Add** to the right of **Methods to be merged**. To remove a method from the list, click **Remove**.
5. (Optional) If both methods were created using Compound Optimization, then select the **Update MRM compound ID from the file name** check box to populate the compound ID column with the compound name in the merged method.
6. To add all the mass ranges from the selected methods, click **Go**.

MRM3 Optimization Script

Use this script for quantitation analysis on QTRAP systems to provide increased specificity and, therefore, improved detection when quantifying analytes in complex matrices. This script is

designed to generate an optimal MS3 acquisition method by infusion. The script performs the following optimization steps:

- Confirm precursor mass
- Optimize transmission to collision cell
- Determine the major fragment ions
- Optimize the Collision Energy (CE) for each fragment ions
- Perform MS3 scans on each fragment ion
- Optimize Excitation Energy (AF2) for all MS3 scans
- Generate a report
- Save all data and acquisition methods

The script can also be used in qualitative applications to generate collections of MS/MS and MS3 spectra for compounds in a semi-automated way (that is, one compound at a time).

MRM3 Optimization Window Overview

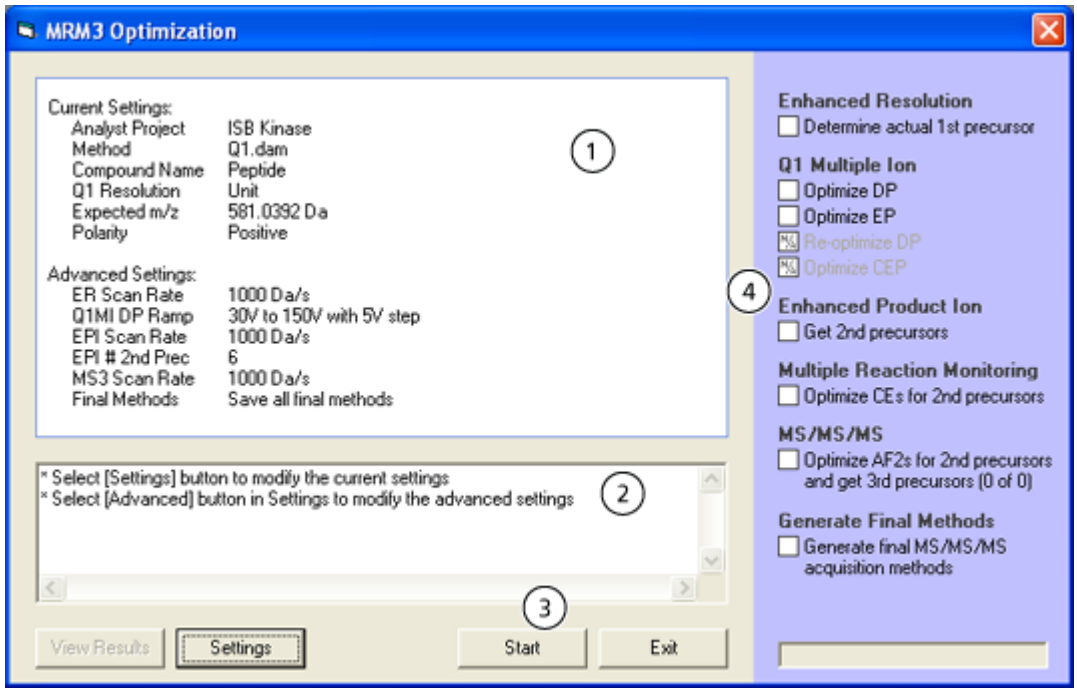
Use the controls in the MRM3 Optimization window to navigate. The window also shows the optimization results as they are generated. The following is an overview of the various sections in this window.

Table 2-7 MRM3 Optimization Window

Field	Description
Status Window	When the script is first started, this window shows the current optimization settings that will be used for optimization. When the optimization is started, spectral information is shown in this window.
Log File	Shows the results found during optimization in text format. Each entry found in this section is also added to the generated Log.txt file.
Overall Progress	Shows the overall optimization progress.
Main Controls	Contains all of the main functions associated with the setting and execution of the optimization process.

- Click **View Results**, to open and review the file using Microsoft Notepad. After the optimization is completed, a Results.txt file is automatically generated and saved.
- Click **Settings** to open a window to type compound information required for the optimization process.
- Click **Start** to initiate the optimization process. During optimization, this button is renamed to **Abort**, which can be clicked to stop the optimization process.

Figure 2-20 MRM3 Optimization Window



Item	Description
1	Status pane
2	Log file
3	Main controls
4	Overall progress

Set the Preferences

The Settings dialog opens automatically every time the script is launched.

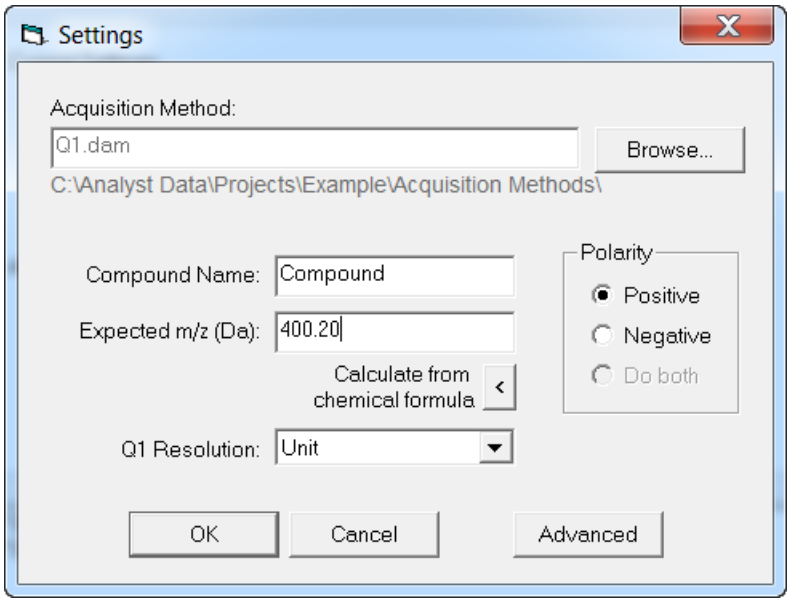
1. Click **Browse** to browse to the starter acquisition method. This method contains the source conditions to be used for the optimization.
2. In the **Compound Name** field, type a descriptive compound name. This name is used as a prefix to all of the acquisition methods and data files generated.
3. In the **Expected m/z (amu)** field, type the expected mass-to-charge ratio (*m/z*) for the compound. If the *m/z*values of the compound is not known, then click **Calculate from chemical formula** to calculate it from the chemical formula of the compound. Refer to the section: Calculate *m/z*.
4. In the **Q1 Resolution** field, select a Q1 Resolution to be used for MS/MS and MS3.

5. In the **Polarity** group, click a polarity, which can differ from the starter method. The **Do both** option is currently not supported.
6. To modify some of the settings used by the optimization process, click **Advanced**. Refer to the section: Use the Advanced Settings Dialog.
7. To verify and use the updated settings, click **OK**.

Use the Script

1. Build a starter acquisition method if one does not already exist. The starter method should be a Q1 acquisition method created in Manual Tune and should contain the source conditions required for the tuning process because these are not optimized by the script.
2. Save the method in the `Acquisition Methods` folder of the required project where all generated files will be saved.
3. Click **Script** > **MRM3 Optimization**.

Figure 2-21 Settings Dialog



4. Enter the compound information required for the optimization process and then click **OK** on the Settings dialog.
5. To initiate the optimization process, click **Start** in the MRM3 Optimization window.

Calculate *m/z*

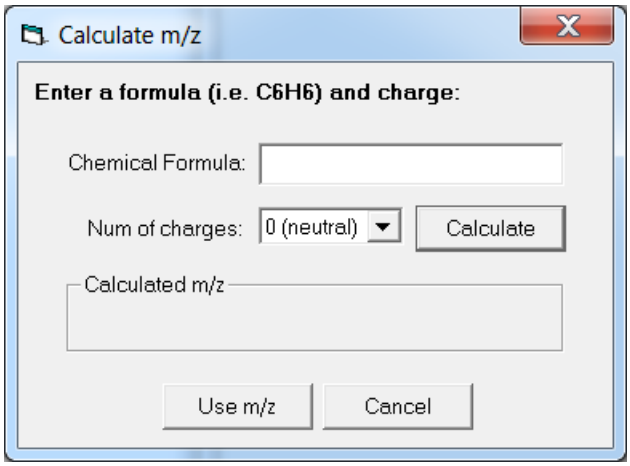
The *m/z* calculator is accessed through the Settings dialog.

1. In the MRM3 Optimization window, click **Settings**.

The Settings dialog opens.

2. Click **Calculate from chemical formula**.

Figure 2-22 Calculate m/z Dialog



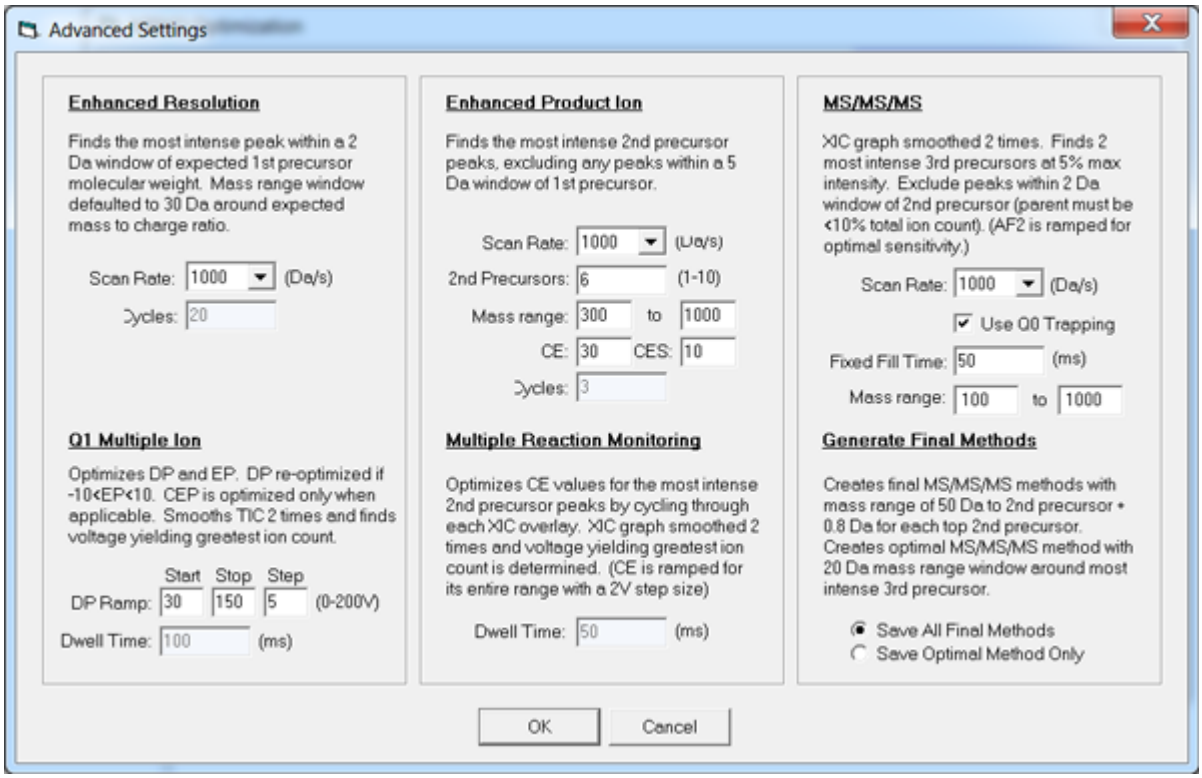
3. In the **Chemical Formula** field, type the chemical formula of the compound. Use capital letters for elements. The chemical formula for peptides is also entered in this dialog.
4. In the **Num of charges** field, click the number of charges.
5. To calculate the *m/z* for the entered chemical formula and charge, click **Calculate**.
6. To close the calculator and update the **Expected m/z (amu)** field in the Settings dialog with the calculated *m/z*, click **Use m/z**.

Use the Advanced Settings Dialog

In this dialog, a description for each of the optimization steps is provided. Some of the settings can be modified to customize the optimization.

1. In the MRM3 Optimization window, click **Settings**.
   The Settings dialog opens.
2. Click **Advanced**.

Figure 2-23 Advanced Settings Dialog



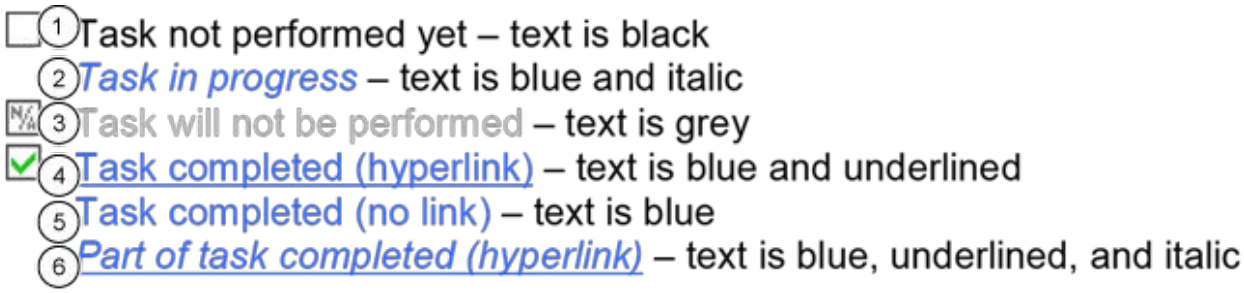
3. In the **Scan Rate** fields in the Enhanced Resolution, Enhanced Product Ion and MS/MS/MS groups, select a scan rate for **ER**, **EPI**, and **MS3**.
4. In the **Q1 Multiple Ion** group, in the **DP Ramp** fields, type the declustering potential (DP) range for optimization. The range is expressed in absolute values and the appropriate polarity is automatically applied based on the selection made in the Settings dialog.
5. In the **Enhanced Product Ion** group, do the following:
   - In the **2nd Precursors** field, type the maximum number of second precursors (fragment ions) used for MS3 optimization. Type a number between 1 and 10.
   - In the **Mass range** field, type a mass range for the second precursors that will be selected for MS3 optimization.
   - In the **CE** field, type a collision energy value and in the **CES** field, type a collision energy spread value that will provide a good MS/MS spectrum from which fragment ions can be selected.
6. To generate all of the final MS3 methods for each second precursor and the optimal MS3 method for quantitation analysis, in the **Generate Final Methods** group, click **Save All Final Methods**. Click **Save Optimal Method Only** to save only the optimal MS3 method (most sensitive for quantitation).

7. Click **OK** to accept the updated Advanced Settings.

Optimization in Progress

When the optimization is started, Manual Tune in the Analyst software is automatically stopped. While the script is running, all of the functions in the software can still be used. A Log.txt file is also updated as each part of the optimization procedure is completed. To stop the script at any time, click **Abort**. Refer to the following figures for examples of the script. In the Overall Progress section, the Checklist images and text fonts represent different statuses that are described in the following section.

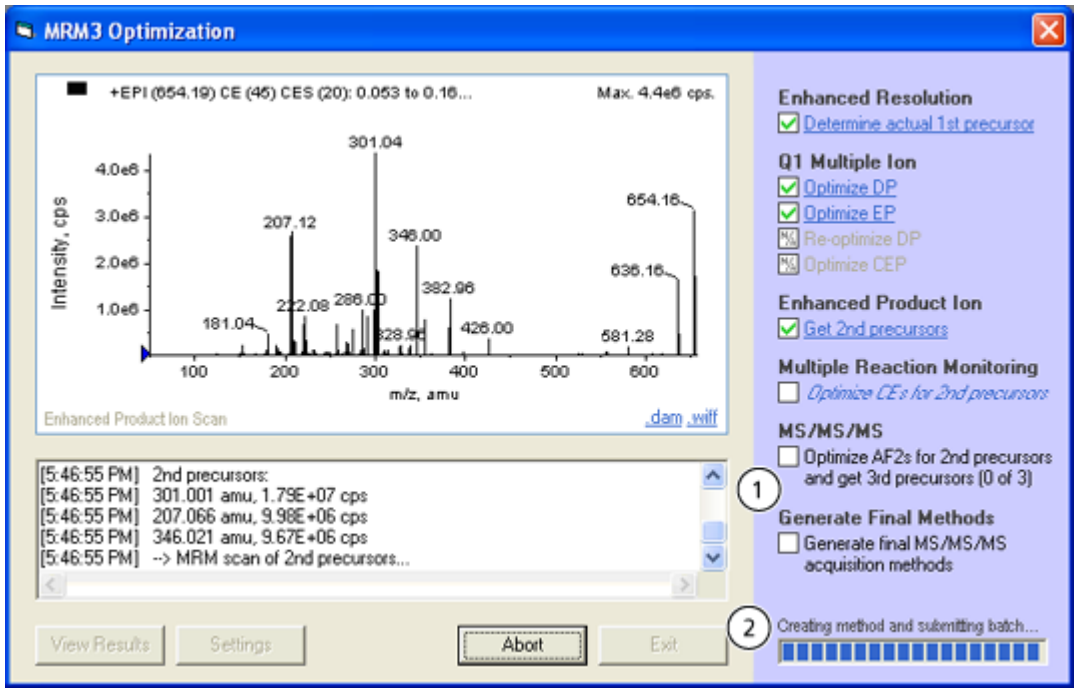
Figure 2-24 Status Examples



Item	Description
1	Tasks not performed yet - text is black
2	Task in progress - text is blue and italic
3	Task will not be performed - text is blue and underlined
4	Task completed (hyperlink) - text is blue and underlined
5	Task completed (no link) - text is blue
6	Part of task completed (hyperlink) - text is blue, underlined, and italic

When the text is underlined, click it like a web page hyperlink and the corresponding spectrum or chromatogram is shown. The text found under MS/MS/MS also shows the MS3 scan number that is being performed because it is possible to have between 1 and 10 scans. The Overall Progress section also includes a Message area. In this area, a progress bar shows the current step progress. Above the progress bar, various messages are shown such as the time and other statuses for the current optimization step.

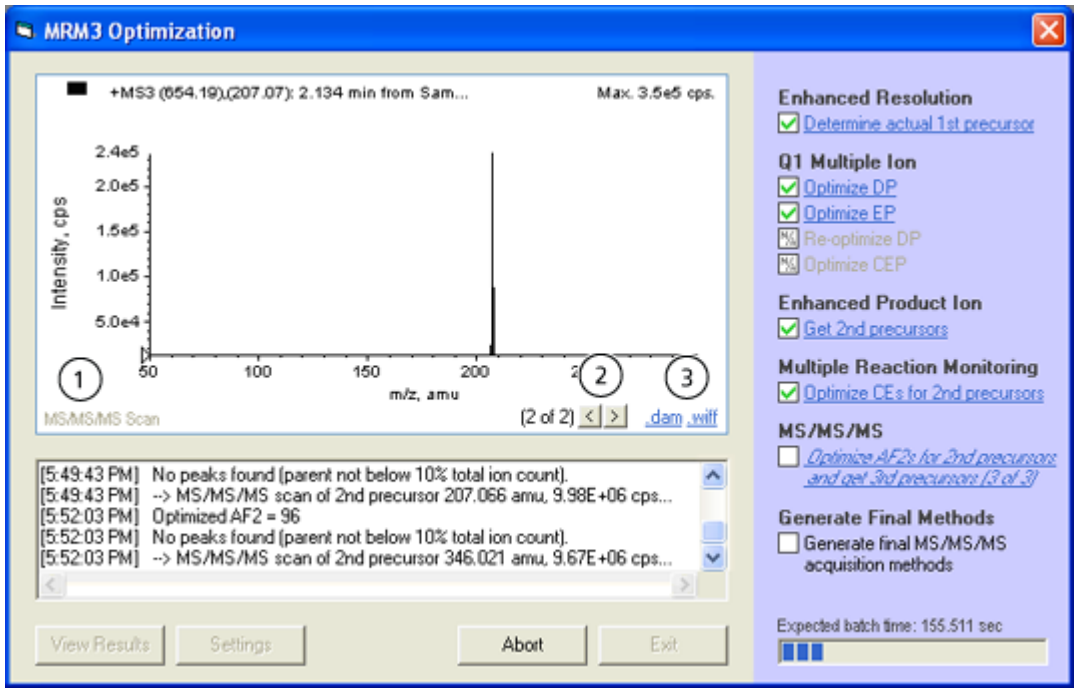
Figure 2-25 MRM3 Optimization Window After an EPI Scan



Item	Description
1	Checklist
2	Message

In the spectral status window, the previously generated spectrum or chromatogram is shown. When one of the checklist items is selected, the corresponding graph is shown. The scan type name indicates which scan is currently being shown. For each completed step, it is possible to open the acquisition method (dam) or data file (wiff) associated with the graph shown. If an MS/MS/MS scan is shown, then use the buttons to cycle through the different MS3 scans.

Figure 2-26 MRM3 Optimization Window During an MS3 Scan



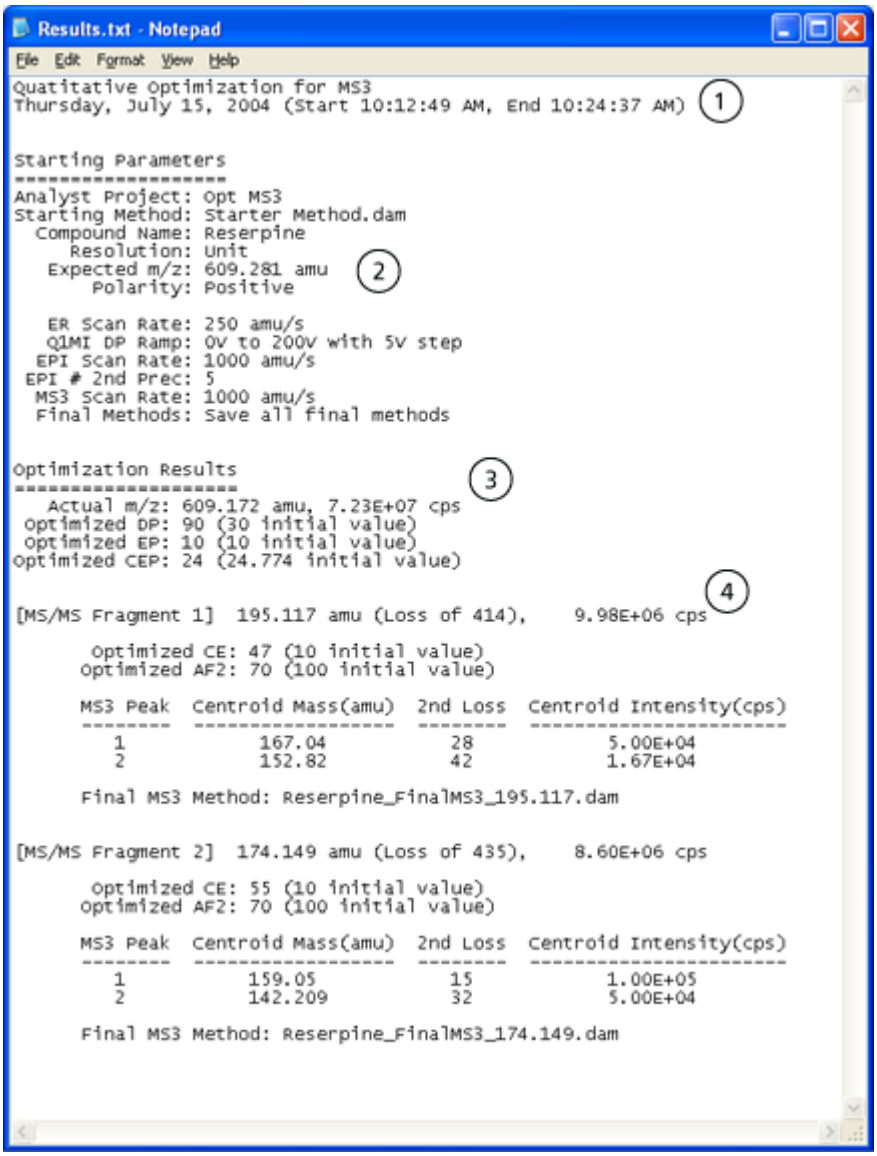
Item	Description
1	Scan type
2	Buttons to cycle through different MS3 scans
3	Links

Optimization Complete

When the quantitative optimization for MS3 is completed or stopped, a Results.txt file is generated. This file is automatically opened in Microsoft Notepad. Click **View Results** from the MRM3 Optimization window to view the file. The various parts of the Results.txt file are described below.

- **Time and Duration**: Shows the date and time duration of optimization.
- **User Starting Conditions**: Shows the settings and Advanced Settings in this section.
- **Optimization Conditions Found**: Shows the optimal conditions found during the ER and Q1MI scans.
- **MS3 Fragments Found and Associated Losses**: Shows the fragments and optimal conditions (collision energy and excitation energy) as well as associated losses found for the EPI scan and MS3.

Figure 2-27 Optimization Report



Item	Description
1	Time and duration
2	User starting conditions
3	Optimization conditions found
4	MS3 fragments found and associated losses

All of the generated acquisition methods have a descriptive file name in the format [supplied compound name] + [scan type] + [*m/z*] + dam. These methods are saved in the same folder as the starter acquisition method.

All of the data, Log.txt, and Results.txt files are saved in a Data subfolder that is created in the same project as the starter acquisition method. The subfolder has the format [supplied compound name] + OptMS3 + ([date], [time]). The data files have the format [supplied compound name] + [scan type] + [*m/z*] + wiff.

Detailed Description of Script Logic: Initialization

This section describes each phase of the optimization process. All scans are performed with the number of scans to sum set to 3.

Before performing any optimization scans, the MRM3 Optimization script performs the following initialization steps. If an error occurs during any of these steps, the script stops the optimization process.

1. Make sure that the Analyst software is running.
2. Load the starter acquisition method to determine if it is valid and to check the device type.
3. Create a new `Data` subfolder to store the wiff files.
4. Create the Log.txt file.

Enhanced Resolution Scan

This step confirms the mass of the ion used for optimization. The ER scan is performed for 20 cycles at the specified scan rate. The most intense peak within ± 1 amu of the expected first precursor *m/z* value is then selected. As in the Analyst software, this scan is performed with a 30 amu mass range around the specified *m/z* value. For multiply charged species, the C12 ion is determined in this step.

Q1 Multiple Ion Scan

This step optimizes transmission of the ion of interest up to the collision cell. This is performed using a Q1 MI scan. The script first optimizes the DP parameter by performing the scan at the specified DP ramp. Optimize the EP parameter by ramping it from 1 V to 12 V (–12 V to –1 V for negative mode), with 0.5 V step. If the optimal EP is less than 10 V (greater than –10 V for negative mode), then DP is re-optimized. The CEP parameter is also optimized by ramping from 0 V to 100 V (–100 V to 0 V for negative mode) with 2 V step. In determining the optimal voltage, graphs are smoothed two times and the voltage yielding the greatest ion count is used. Dwell Time for each scan is set to 100 ms.

Enhanced Product Ion Scan

This step selects the fragment ions that will be used for MS3 optimization. This is performed using an EPI scan for three cycles at the selected scan rate. Specify an optimal CE for

the compound to be analyzed. If the optimal CE is unknown, then specify a CES value so that a range of CE settings are used. The most intense second precursor peaks are then found, excluding any peaks within ± 2.5 amu window of first precursor. The number of second precursors to use is selected in the Advanced Settings. The mass range from which the second precursors are selected is specified by the user.

Multiple Reaction Monitoring Scan

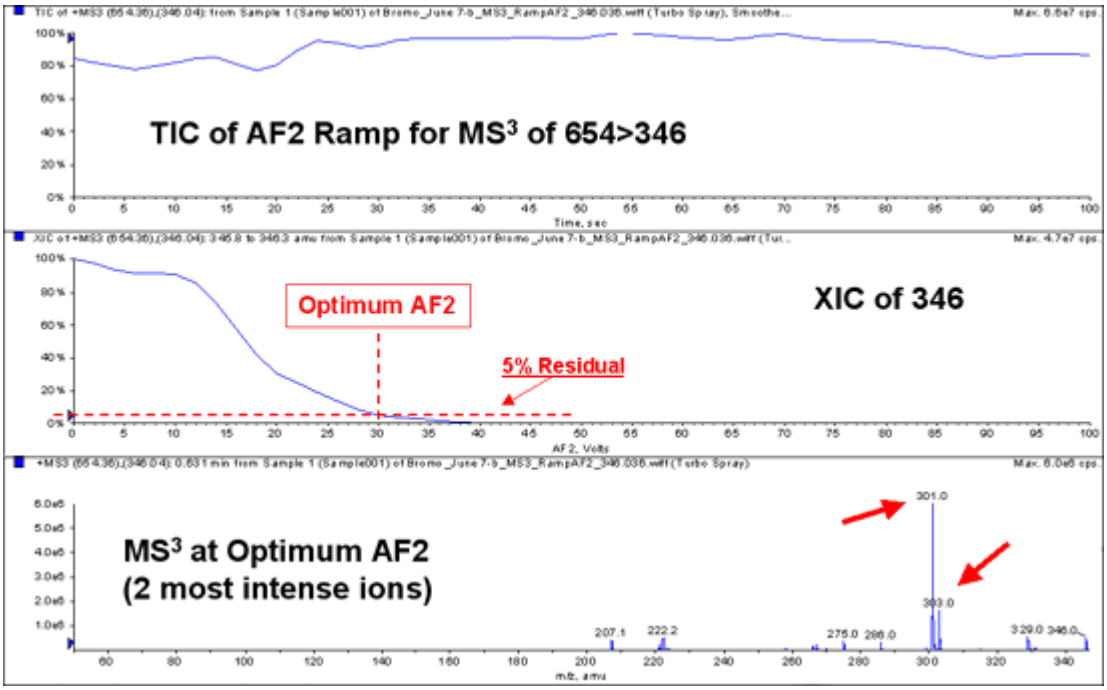
This step optimizes the collision energy for each of the fragment ions selected from the EPI scan. This is performed using MRM scans. Use CE ramps of 5 to 130 V (–130 to –5 V in negative mode) with 2 V step and Dwell Time of 50 ms. Each overlaid graph is then smoothed two times and the voltages yielding the greatest ion count are used as the optimal CE values.

MS/MS/MS (MS3) Scan

The script performs an MS/MS/MS (MS3) scan for each chosen second precursor at the specified scan rate and with an AF2 ramp of 0 to 100 V with 2 mV step for both polarities. The fill time of the scan is set, and Q0trapping can be turned on for maximum sensitivity if required. The lower limit of the mass range for the MS/MS/MS (MS3) scan can be specified, and the upper limit is second precursor + 5 amu.

The generated graphs are smoothed twice and the optimal AF2, as shown in the following figure, is obtained when the residual intensity of the second precursor (based on XIC) is at 5% of its maximum intensity. The spectrum at this AF2 value is then used to find the two most intense second-generation fragment ions, excluding peaks within ± 1 amu of the second precursor. If the second precursor *m/z* value is greater than 10% of the total ion count, then no fragments from that spectrum is used. This condition exists because if the second precursor *m/z* value is greater than 10%, then there is insufficient fragmentation.

Figure 2-28 How AF2 is Determined



Generate Final Methods

After the optimization scans are performed, the script generates the final MS/MS/MS methods. If the **Save Optimal Method Only** option is clicked in the Advanced Settings dialog, then only an optimal MS/MS/MS method with ± 10 amu around the most intense second generation fragment ion is created. If the **Save All Final Methods** option is clicked, then the optimal method as well as an MS/MS/MS method for each of the top second precursors are created using a mass range from the user-defined lower limit to an upper limit of (second precursor + 5) amu.

MS3 Quant Optimization Script

The MS3 Quant Optimization script has been replaced by the MRM3 Optimization script. Users who have upgraded from earlier versions of the Analyst software might still have this script installed. The MS3 Quant Optimization has not been tested with the Analyst software, version 1.6.3 or later. Use the MRM3 Optimization script instead.

MSServiceLog Script

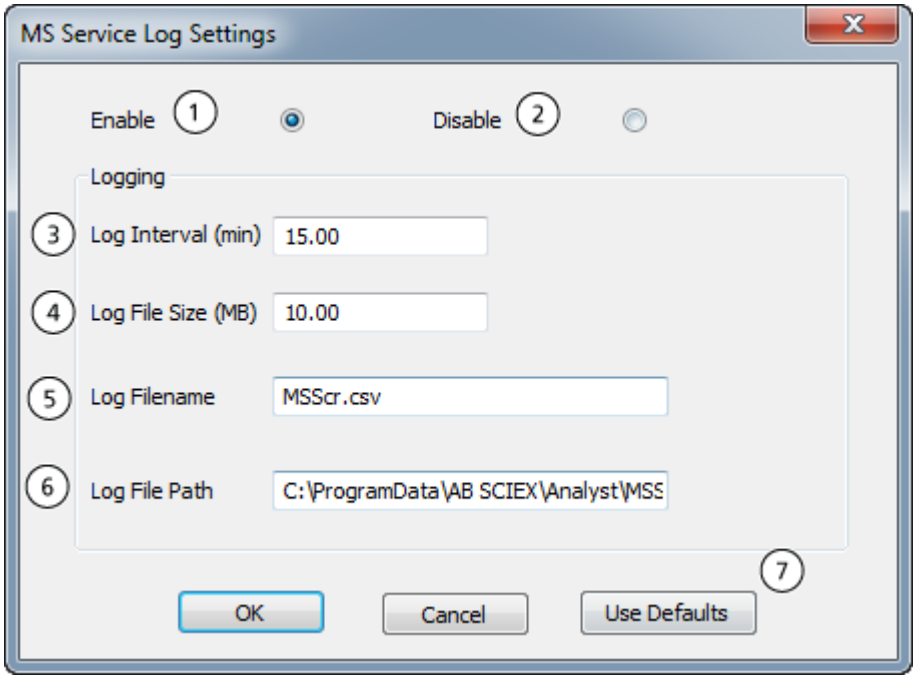
By default, readbacks from a mass spectrometer are recorded in the MS Service log file. Use the MSServiceLog script to turn off the recording of the readbacks or to start recording the readbacks from the instrument in the MS Service log file. The MSServiceLog script is only applicable to the SCIEX 3500,SCIEX 4500 systems, SCIEX 5500 systems, SCIEX 5500+ systems, SCIEX 6500 systems, and SCIEX 6500+ systems.

The MSServiceLog script can be used without an active hardware profile but any changes made to the MS Service log settings take effect only after the hardware profile is reactivated.

Use the Script

1. Deactivate the hardware profile.
2. Click **Script** > **MSServiceLog**.

Figure 2-29 MS Service Log Settings Dialog



Item	Name	Description
1	**Enable**	Select to start recording the readbacks from the mass spectrometer to the MS Service log file using the MSServiceLog script.
2	**Disable**	Select to turn off the recording of the readbacks from the mass spectrometer to the MS Service log file using the MSServiceLog script.
3	**Log Interval (min)**	Specify how frequently, in minutes, the readbacks from the mass spectrometer will be recorded to the MS Service log file. The default value is 15 minutes and the allowed range is from 1 minute to 1440 minutes.

Item	Name	Description
4	**Log File Size (MB)**	Specify the size of the log file. The default size is 10 MB, and the allowed range is 1 MB to 1000 MB. There can be up to two log files: • The current log file, where the readbacks from the instrument are recorded. • The archived log file. When the current log file reaches the specified size, it is archived with an predefined archive filename, and a current log file is created to record the readbacks with the log file name specified in the MS Service Log Settings dialog.
5	**Log Filename**	Specify a name for the log file. The accepted file extensions are csv, txt, or log.
6	**Log File Path**	Specify the location where the log file is stored. Make sure that the new location is created inside the default location `C:\ProgramData\ABSCIEX\Analyst\MSServiceLog`.
7	**Use Defaults**	Click to revert to the preset values in all the fields in the dialog.

3. Click **Disable** to turn off the recording of the readbacks in the MS Service log file.
4. Click **Enable** to start recording the readbacks from the mass spectrometer to the MS Service log file.
5. To change the values in other fields in the MS Service Log Settings dialog, refer to the figure: Figure 2-29.
6. Click **OK** the apply the changes.

Multiple Batch Scripts

Use this script to attach multiple acquisition scripts to a single batch that is submitted to the queue. These acquisition scripts are used to immediately process the data either after a sample completes or after the batch completes. In the Analyst software, only one script can be submitted with a batch, but sometimes it is convenient to run two or more scripts to perform two or more different types of processing.

Use the Scripts

1. When creating a batch, in the **Batch Script** field, browse to the script.

After the batch is submitted to the queue, the following dialog opens in which the additional acquisition scripts can be attached.

Figure 2-30 Multiple Batch Scripts Script Dialog

2. To attach an additional script to this batch, click **Add Script** to browse to the acquisition script.
3. To remove a script, click the script and then click **Remove Selected**.
4. Clear the **Only show this dialog again if the control key is down** check box to show this dialog when submitting the batch.
5. Click **Run** to attach all of the acquisition scripts to the batch.

Open in Workspace

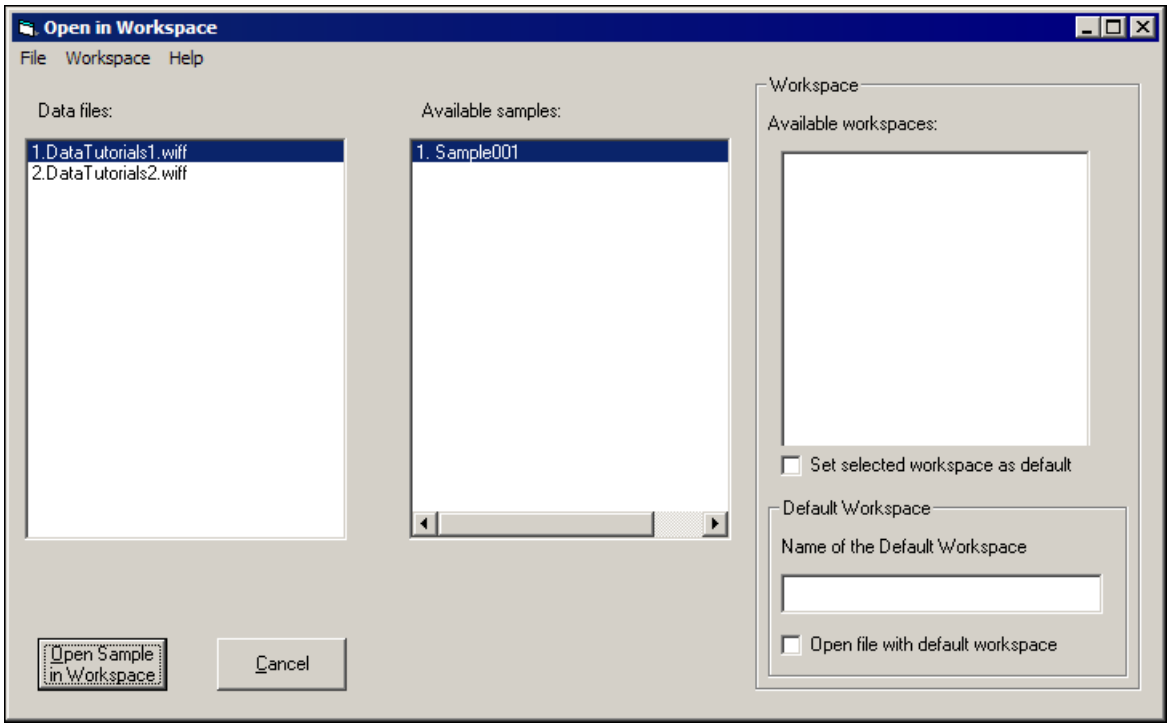
Use this script to open a sample in a previously created workspace. This script loads the previous workspace and shows the sample in the same layout as specified in the saved workspace. It is not possible to create a workspace that specifies pane arrangements so that any sample can be opened in the workspace with the same pane arrangements. For more information on workspaces, refer to the online *Help*.

Use the Script

1. Click **Script** > **OpeninWorkspace**.

   The Open in Workspace dialog is shown with the current working project data folder loaded in the **Data files** list.

Figure 2-31 Open in Workspace Dialog



2. To select a data file from another project, click **File** > **Open Data File.**
3. In the **Data files** list, click a data file.
   All of the samples in the selected data file are shown in the **Available samples** list.
4. After choosing the sample, select a workspace in the **Available workspaces** list.

Tip! To select a different workspace, click **Workspace** > **Open Workspace**.

5. To set a default workspace to be used every time this script is run, select the **Set Selected Workspace As Default** check box.
6. To open the sample, click **Open Sample in Workspace**.

Known Issues and Limitations

The Open in Workspace script is for the presentation of graphs only. The script cannot handle data lists that are saved in the workspace. If the workspace contains data lists, then a Type Mismatch error is shown. If this error occurs, save the workspaces with the graphs only and then, after loading the workspace, create the necessary data lists.

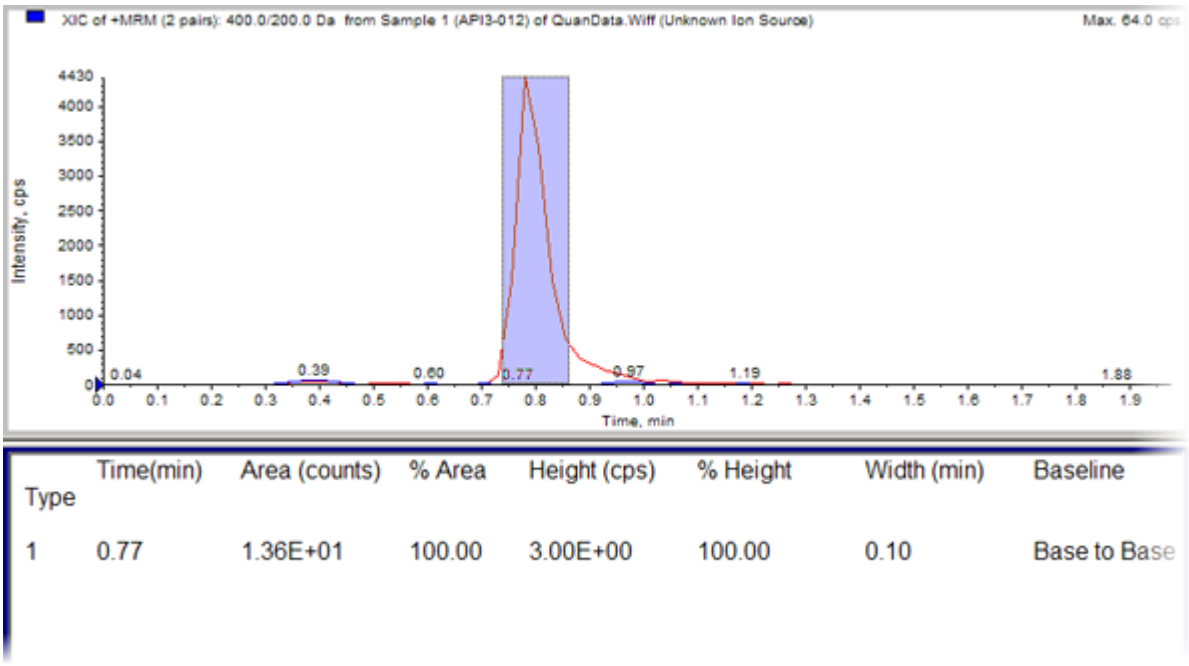
Peak List from Selection

Use this script to determine the peak data for a selected region or regions in the chromatogram. The % area and % height listed relate to peaks in the selection. The peaks are listed in a text pane below the active chromatogram. The peak definition is shown in the chromatogram. For more information, refer to the figure: Figure 2-32.

Use the Script

1. To process the data, make one or more selections in the chromatogram and then select the script from the menu.
2. Do one of the following:
   - To run the script, click **Script** > **PeakListFromSelection**.
   - To view the script description, and get the peak list, press **Shift** while clicking the script.

Figure 2-32 Data Processing with the PeakListFromSelection Script



Type	Time(min)	Area (counts)	% Area	Height (cps)	% Height	Width (min)	Baseline
1	0.77	1.36E+01	100.00	3.00E+00	100.00	0.10	Base to Base

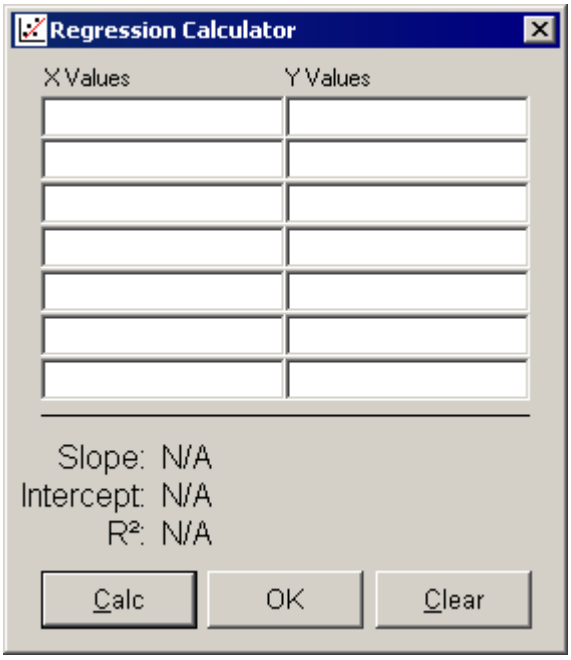
Regression Calculator

Use this script to calculate the slope, y intercept, and r values for each mass/speed dependent parameter.

Use the Script

1. Click **Script** > **Regression Calculator.**

Figure 2-33 Regression Calculator Dialog



2. Type data in pairs of X and Y co-ordinates.
3. After entering two or more pairs, to get the Slope, Intercept, and R^2 value, click **Calc**.
4. To delete the values for X and Y co-ordinates, click **Clear**.
5. To exit the application, click **OK**.

Remove Graph Selections

Use this script to clear a selected area in the graph. For example, the graph selection line can be cleared from the graph.

Use the Script

- To remove selections from the graph, click **Script** > **RemoveGraphSelections**.

Repeat IDA Method

Use this script on an acquisition computer. It opens the acquisition method for the data file and updates the exclusion list with the masses and times that have been acquired. The method is saved under the same name.

Use the Script

1. In Explore mode, open an IDA data file.
2. Click **Script** > **RepeatIDAMethod**.
3. To keep the previous exclusion list, press the **Ctrl** key while clicking the script.

Savitzky-Golay Smooth

In the Analyst software, a graph can be smoothed in **Explore** mode using one of the smoothing algorithms from the **Explore** menu: Moving Average Smooth (shown as **Smooth** under **Explore** menu) or a **Gaussian Smooth**.

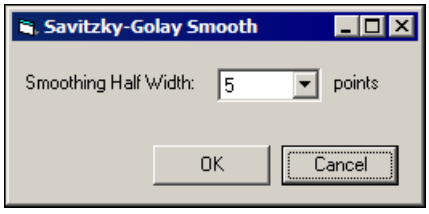
Alternatively, if the Savitzky-Golay Smooth script is installed, then a graph in **Explore** mode can be smoothed using the Savitzky-Golay Smooth algorithm from the **Script** menu. The active graph in the Analyst software is replaced by the smoothed graph.

If the IntelliQuan integration algorithm is used in **Quantitate** mode, then the Savitzky-Golay smooth algorithm is used. The Savitzky-Golay Smooth script smooths a graph in **Explore** mode in the same way as when data is smoothed in **Quantitate** mode using IntelliQuan integration algorithm.

Use the Script

1. With the peaks of interest selected in the active spectrum, click **Script** > **Savitzky-Golay Smooth.**

   Figure 2-34 Savitzky-Golay Smooth Dialog

2. In the **Smoothing Half Width** field, to set the half-width for smoothing the data. The total width is twice this value plus one.

   This parameter is the same as the smoothing parameter used with the IntelliQuan algorithm in the Analyst software.
3. To perform the smoothing, click **OK**.

Selection Average and Standard Deviation

Use this script to calculate the average intensity and standard deviation of a selection in a graph for both spectral and chromatographic data. The graph is labeled with both the average and standard deviation of the selection.

Use the Script

- Select either an active spectrum or an active chromatogram and then click **Script** > **Selection Average and StdDev** script.
  The graph is labeled with the average and standard deviation of the selection.

Known Issues and Limitations

This script works only once for each graph. Use the following procedure to run the script on the same graph more than once.

1. Copy the graph to a new pane and then click **Explore** > **Duplicate Data** > **Same Window**.
2. Make a selection in the new graph pane and then run the **Selection Average and StdDev** script again.

Send to ACD SpecManager

This script is similar to the Export to JCamp script. However, instead of prompting for the name of the JCamp file, the script exports the spectra to a temporary file and then sends them directly to the ACD SpecManager application. There is no need to open this temporary file directly.

Use the Script

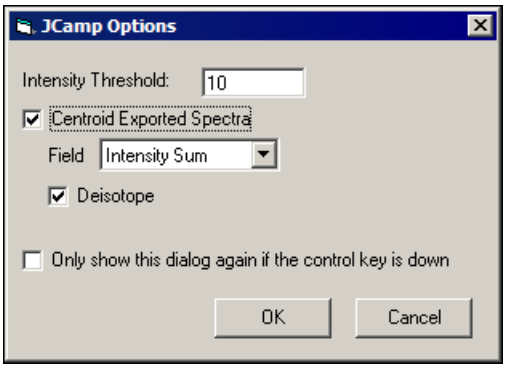
The first time the script is run, the software prompts the user to locate SpecManager. The user is not prompted again unless **Ctrl** is pressed while the script is clicked.

Note: This script cannot be used with batch acquisition.

Prerequisites
• The SpecManager software must be installed.

1. With either a chromatogram or a spectrum in an active pane, click **Script** > **Send to ACD SpecManager**.
   The JCamp Options dialog opens. If the user is interactively processing a single spectrum active in the Analyst software, then these options do not apply.

Figure 2-35 JCamp Options Dialog



2. To centroid the exported spectra, select the **Centroid Exported Spectra** check box.
   This option reduces the size of the exported JCamp file.
3. To select the threshold to be applied to the exported spectra, in the **Threshold** field, type a value. To not use a threshold, type `0` in the Intensity **Threshold** field.
4. Select the **Only show this dialog again if the control key is down** check box to have the JCAMP Options dialog open if **Ctrl** is pressed when the script is selected from the **Script** menu or when the batch is submitted to the queue.
5. Click **OK** to continue processing and to export the spectra.
   These values are used as defaults until they are changed.

Note: To close the dialog without making any changes, click **Cancel**. In the case of interactive use, canceling the dialog also stops the export operation. However, in the case of batch operation, the batch is still acquired and JCamp files is exported using the original parameters.

Signal-to-Noise Using Peak-to-Peak

The Analyst software calculates the signal-to-noise ratio by taking the standard deviation of all of the chromatographic data points between the specified background start and background end times.

Use this script to calculate the signal-to-noise ratio for the active chromatogram. The script subtracts the average background signal from the selected peak and then divides the subtracted signal by the peak-to-peak noise level. It then differentiates the noise and peak regions based on the maximum intensities of each region. Upon completion, the active chromatogram is labeled with the signal-to-noise ratio.

Use the Script

- With a noise region and the peak of interest selected in the active chromatogram, click **Script** > **S-to-N**.

The signal-to-noise ratio is calculated and the graph is labeled.

Tip! To remove the labels, press **Ctrl** while clicking the script.

Related Scripts

S_NstdDevQS: Calculates the signal-to-noise value with a method that uses the standard deviation of the noise regions.

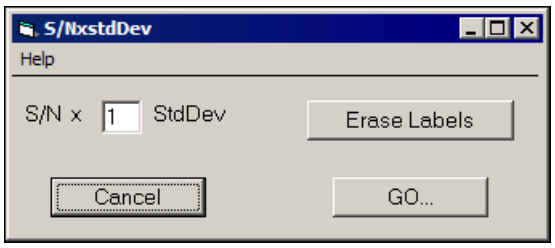
Signal-to-Noise Using Standard Deviation

Use this script to calculate the signal-to-noise ratio of chromatographic peaks and label them. The script requires two regions to be selected on the chromatogram: a selection/region containing the noise region and a selection/region containing the peak of interest. The script determines which region contains the peak and the noise based on maximum intensities in each selection. It subtracts the average background signal intensity from the peak signal intensity and then divides the subtracted signal by a user-specified factor multiplied by the standard deviation of the noise region.

Use the Script

1. With a noise region and the peak of interest selected in the active chromatogram, click **Script** > **S_NstdDevQS**.
   The S/NxstdDev dialog opens.

   Figure 2-36 S/NxstdDev Dialog

2. To erase any labels current on the active chromatogram, click **Erase Labels**.
3. To calculate the signal-to-noise ratio and label the graph, click **Go**.

Related Scripts

Signal-to-Noise Using Peak-to-Peak: Calculates the signal-to-noise for an active chromatogram. The background subtracted signal is divided by the peak-to-peak noise level.

sMRM Calculator

Use the sMRM Calculator script for a visual representation of a Scheduled MRM (sMRM) algorithm acquisition method. The script uses four graphs to show an overview of the MRM transition, its concurrency, its projected cycle time, and the dwell time to be applied to it. Refer to the figure: Figure 2-38. To achieve a suitable arrangement of the transitions over the run time, change the parameter values, such as **Maximum Dwell**, **Minimum Dwell**, **Target sMRM Cycle Time** or **Target sMRM Scan Time**, **Window Width**, **MRM Pause Time**, and **Settling Time**, in the script dialog. The four graphs are updated accordingly. Repeat this process until the required arrangement of the transitions is achieved.

Note: If **Target Cycle Time** is selected in the original method, then it cannot be changed to **Target Scan Time** in the script dialog. If **Target Scan Time** is selected in the original method, then it cannot be changed to **Target Cycle Time** in the script dialog.

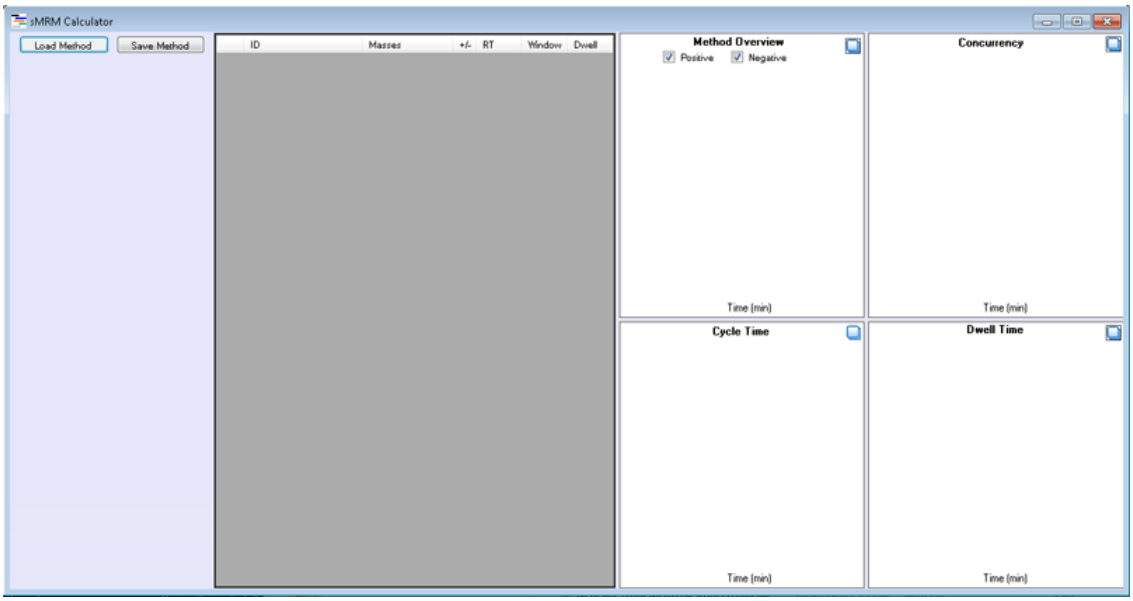
Note: The **Settling time** option can only be modified for SCIEX 5500+ systems and SCIEX 6500+ systems in the sMRM Calculator script dialog.

Use the Script

Prerequisites
• Make sure that the Analyst software is open and a hardware profile is activated. • Make sure that a Scheduled MRM (sMRM) algorithm acquisition method is already created.

1. Click **Script** > **sMRM Calculator**.
   The **sMRM Calculator** dialog opens.

Figure 2-37 sMRM Calculator Dialog



2. Click **Load Method** to select an existing Scheduled MRM (sMRM) algorithm acquisition method.
   The **Open** dialog opens.

Note: Only an acquisition method that contains Scheduled MRM (sMRM) algorithm experiments and for the active mass spectrometer in the currently selected project can be opened in the sMRM Calculator script. Only the details for Scheduled MRM (sMRM) algorithm experiments are shown. The non-Scheduled MRM (sMRM) algorithm experiments are labeled as not Scheduled MRM (sMRM) in the script.

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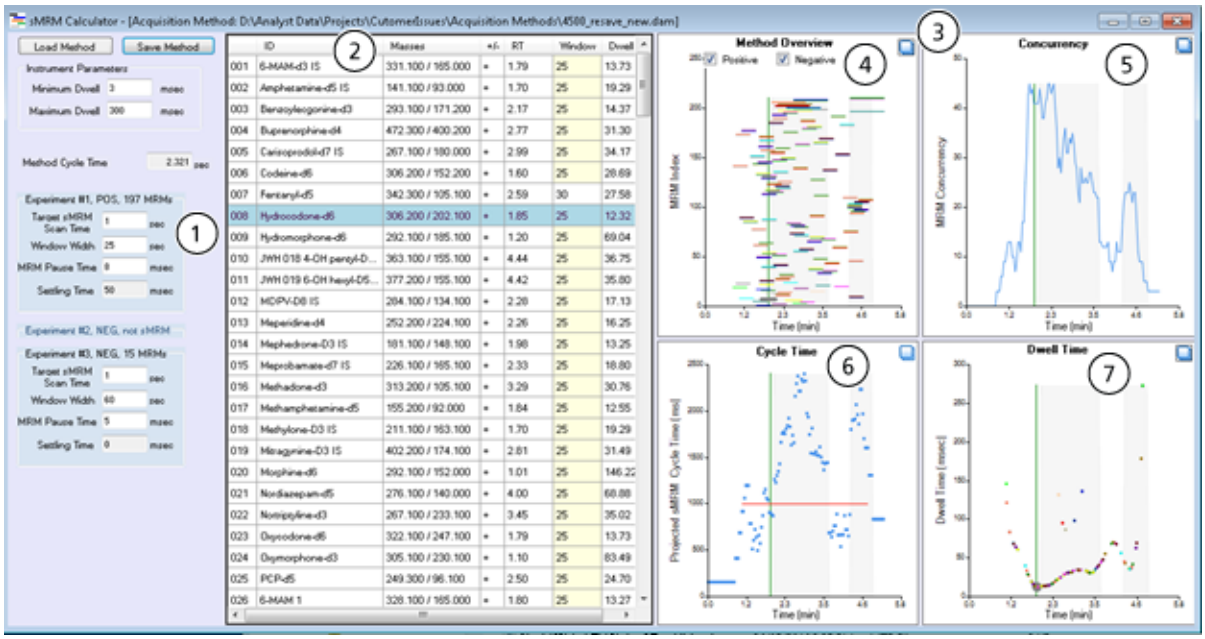
3. Select the Scheduled MRM (sMRM) algorithm acquisition method and then click **Open**.

   The selected acquisition method opens in the **sMRM Calculator** dialog. The file path of the open acquisition method file is shown in the title of the dialog.

Figure 2-38 Acquisition Method Opened in the sMRM Calculator Dialog



Item	Description
1	The left pane contains instrument and Scheduled MRM (sMRM) algorithm parameters. The parameters shown in this pane change depending on the acquisition method opened. If the arrangement of the transitions is not suitable in the four graphs in the right pane, then change the editable parameters and settings in the left pane. The affected columns in the table and the graphs are updated accordingly. The parameter values can be modified within the allowable range until a suitable arrangement of transitions is achieved. For example, if the value in the **Target sMRM Scan Time** field is changed, then the dwell time is recalculated and updated in the table, and the graphs are also updated accordingly. For example, if the value in the **Windows Width** field is changed, then this value is updated in the **Window** column for all of the transitions that use this global setting. The dwell time for all of the transitions is recalculated and updated in the table. The graphs in the right pane are also updated accordingly. For transitions with their own detection window settings in a Scheduled MRM (sMRM) Pro algorithm acquisition method, updating the global setting **Window Width** in the left pane does not update the values in the **Window** column for these transitions in the table. **Note:** The fields that show as grey in the left pane are not editable and the value cannot be changed.

Item	Description
2	The index, compound ID, Q1 and Q3 masses, polarity, window width, retention time, and dwell time are shown in the middle pane. The default view is in order by index number. To rearrange the view based on the information in the other columns, click the title of one of the seven columns: **index**, **ID**, **Masses**, **+/-**, **RT**, **Window**, and **Dwell**. The middle pane refreshes, showing the information sorted in the alphanumerical or numerical order of the selected column. For methods for SCIEX 3500 systems, SCIEX 4500 systems, SCIEX 5500 systems, SCIEX 5500+ systems, SCIEX 6500 systems, and SCIEX 6500+ systems, the window width for all transitions in that Scheduled MRM (sMRM) algorithm experiment can also be edited in the table. The dwell time in the table and the graphs in the right pane are updated accordingly. Editing the window width in the table converts a Scheduled MRM (sMRM) algorithm acquisition method to a Scheduled MRM (sMRM) Pro algorithm acquisition method. **Note:** The window width that uses the global setting from the left pane has a yellow background. After the window width in the table is manually modified for an individual transition or if it already uses the advanced window width that is specific for its transition, then the background color for that cell changes to white.
3	The right pane shows all of the Scheduled MRM (sMRM) algorithm transitions contained in the loaded Scheduled MRM (sMRM) algorithm acquisition method graphically as four different types of graphs. • The selected MRM transition in the table is depicted by the green vertical line in the graphs. • The light grey areas in the graphs represent the retention time zones where there is polarity switch in each cycle. • Tool tips in each graph show X- and Y-values for the transition under the cursor. For the Method Overview and Dwell Time graphs, the compound ID is also shown in the tool tips. • Clicking an MRM transition in the Method Overview graph selects that transition in the other three graphs and the table.
4	The first graph, Method Overview, shows all of the transitions and the detection window of each transition. The X-axis shows the retention time. The Y-axis shows the MRM index number, which is the order in which the transitions were entered in the method.

Item	Description
5	The second graph, MRM Concurrency, shows the retention time on the X-axis and the MRM transition concurrency at each retention time on the Y-axis.
6	The third graph, Projected sMRM Cycle Time, plots the projected cycle time over retention time. The red line represents the **Target Cycle Time**, if it is used. If the **Target Scan Time** is used, then the value of the red line is the sum of the **Target sMRM Scan** time of all of the Scheduled MRM (sMRM) algorithm experiments in the method. **Note:** More data points are expected for transitions for which the **Projected sMRM Cycle Time** is much lower than the **Target Cycle Time** or the sum of the **Target Scan Time** (where the red bar is). Fewer data points are expected for transitions for which the **Projected sMRM Cycle Time** is much higher than the **Target Cycle Time** or the sum of the **Target Scan Time** (where the red bar is).
7	The fourth graph shows the dwell time for each transition at its retention time. The X-axis shows the retention time. The Y-axis shows the dwell time to be applied.

4. Change the parameter values as required to optimize the method to achieve a better distribution of the **Projected sMRM Cycle Time**.
5. Click **Save Method**.
   The **Save Method File** window opens.

   The changes to the method can be saved in the original acquisition method or can be saved as a new acquisition method. If the changes are saved to the original acquisition method, then the original parameter values are overwritten by the new values.
6. Type a new file name or select the original method and then click **Save**.
7. Open the saved acquisition method in the **Acquisition Method Editor** to view the new changes.

   If the original method was open in the **Acquisition Method Editor**, then the method must be closed and opened again.
8. Click the **X** in the upper-right corner of the **sMRM Calculator** dialog to close the dialog.

Split Graph Script

Use this script to split a spectrum or chromatogram in to a specified number of panes. Each resulting pane shows a proportional fraction of the total mass (or time) range. For example, if a spectrum showing a mass range of 100 Da to 400 Da is split in three, then the original spectrum

shows a range of 100 Da to 200 Da, the second (new) spectrum shows 200 Da to 300 Da, and the third (new) spectrum shows 300 Da to 400 Da. The intention is to allow the maximum possible number of peaks to be labeled for subsequent printing.

Use the Script

1. With either a chromatogram or a spectrum in an active pane, click **Script** > **SplitGraph**.

   Tip! Press **Ctrl** while opening the script to specify the number of panes to create.

   Note: Make sure that the mass (or time) range for splitting is shown. If necessary, dock the graph to make sure that the whole graph can be seen.

2. Do one of the following:

   - The current version of the XICfromTable script can process a maximum of 25 XIC mass ranges. If **Ctrl** is pressed while the script is clicked, a dialog opens prompting the user to select the number of panes to create. The preset value is four.
   - If the **Ctrl** key is not pressed, then the last number typed in the dialog is used.

Subtract Control Data from Sample Data

Use this script when the sample data of interest are in the active graph. The data can be any spectrum, TIC, or ADC trace. The script determines the data type, retrieves the corresponding data from the control file, and then shows the subtracted data in a graph.

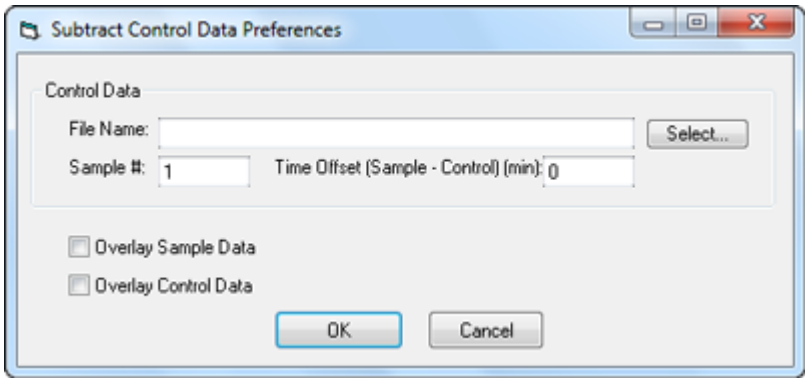
Select to overlay the subtracted data with sample data or control data.

Use the Script

1. To process the data with current preferences, click **Script** > **SubtractControlData**.
2. If the script is being run for the first time then do one of the following:

   - To view the script description, set the processing preferences, and then obtain the subtracted data, press **Shift** while clicking the script.
   - To update the processing preferences and then obtain the subtracted data, press **Ctrl** while clicking the script.

Figure 2-39 Subtract Control Data Preferences Dialog



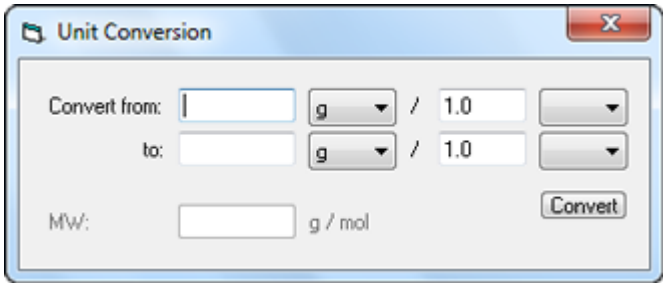
Unit Conversion

Use this processing script to convert from one set of concentration units to another.

Use the Script

1. Click **Script** > **Unit Conversion.**

Figure 2-40 Unit Conversion Dialog



2. In the **Convert from** field, type the concentration and units to be converted.
3. If the conversion is from a weight-based concentration (for example, g/L) to a molar-based concentration (for example, mol/L), then in the **MW** field, type the molecular weight of the component.
4. In the **to** field, type the unit.
5. To perform the conversion, click **Convert**.
   The calculated values are shown in the **to** field.
6. To retrieve these values, press **Ctrl +C** to select and copy them to the clipboard. These values can then be pasted in another application.

Wiff to MatLab

Use this script to extract the data from a wiff file and create the following matrices in a MatLab file: Data, Masses, Wavelengths, Scans, and Filename. For more information about these matrices, refer to the table: Table 2-8. This MatLab file can then be included in a MatLab script and used to compute and show the results.

Although the Analyst software can be used to perform various data manipulations, use this specialized script, Wiff to MatLab, for data computations. The Analyst software cannot extract data from a wiff file and then store it in a file that can be read and interpreted by MatLab.

In addition to exporting the mass spectral data, this script can also export data from a diode array detector (DAD).

The script will create a single MatLab mat file for each sample to be translated. Depending on the type of mass spectra data and the user options, the script can create data in two different formats:

- The first format saves the intensities in a matrix of size (number of masses) × (number of scans). There is therefore an entry in the matrix for every mass that was scanned and every spectrum. This is the default format for quadrupole spectra and the format that is always used for diode array data.
- The second format is sparse or compressed and allows data points that have an intensity of zero to be omitted. Depending on the number of such data points in the original wiff sample, this can potentially greatly reduce the size of the MatLab file. This format uses a matrix of size 2 × (total number of (mass, intensity) pairs). The first row represents masses and the second row the intensities. A given number of initial columns corresponds to the first spectrum, a given number of following ones to the second spectrum, and so forth. Each (sparse) spectrum is essentially stored end-to-end.

A separate vector is written, which can be used to determine the starting and ending position of any given spectrum in this matrix. This vector contains the one-based index of the start of a given spectrum. The end for a given spectrum can be determined by subtracting one from the start of the following spectrum (except for the very last spectrum, which is determined by the size of the above-mentioned matrix).

The first format is the default format for quadrupole spectra and is always used for diode array data. The second (sparse) format is always used for TOF (time-of-flight) data and can optionally be used for quadrupole data.

The actual names of the various matrices are specified using the Options dialog described later in this document.

Use the Script

1. With a chromatogram in an active pane, click **Script** > **Wiff to MatLab**.

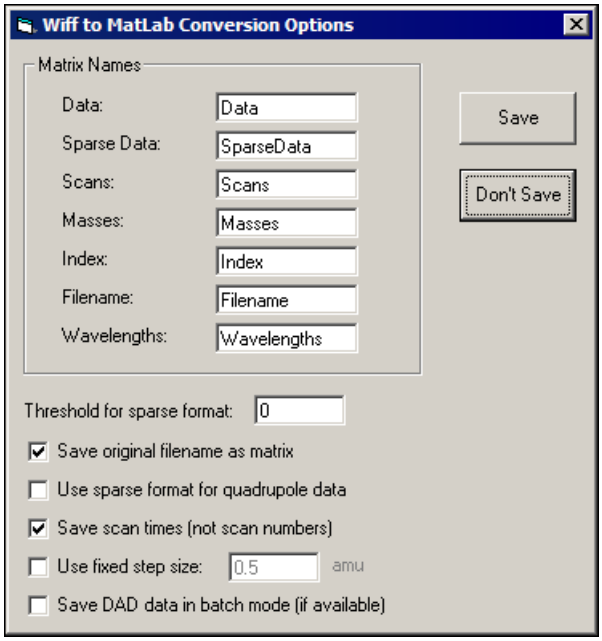
Tip! This script can be attached to a batch. Select this script using the Batch Editor.

If the chromatogram is associated with mass spectral data (TIC, XIC), then MS data is exported to the MatLab file. If the chromatogram is associated with diode array data (TWC, XWC), then DAD data is exported.

2. (Optional) To change the conversion options, open the Wiff to MatLab Conversion Options dialog by pressing the **Ctrl** key while clicking the script.

   Otherwise, the options previously specified are used.

Figure 2-41 Wiff to MatLab Conversion Options Dialog



3. In the **Matrix Names** fields, type the names of the matrices that the script produces. It is recommended that these names be kept as the default values.
4. In the **Threshold for sparse format** field, type a value that will be used to reduce the size of the output MatLab file. For the sparse format only, only (mass/intensity) pairs with intensity larger than the specified value are written.

   If the **Save original filename as matrix** field is selected, then the script creates and populates the Filename matrix.
5. To have the quadrupole spectra saved in the sparse format, select the **Use sparse format for quadrupole data** check box.

Note: TOF spectra are always saved in the sparse format and that diode array data is always saved in the non-sparse format.

If the **Save scan times (not scan numbers)** field is cleared, then the script populates the Scans matrix with the time in seconds for each scan. Otherwise, the Scans matrix is populated with the scan numbers.

6. In the **Use fixed step size** field, type the step size of the data to extract. If this field is cleared, then the acquisition step size is used.
7. To populate the wavelengths matrix with the DAD data when the script is attached to a batch, select **Save DAD data in batch mode (if available)**.
8. To save these settings and continue processing the data, click **Save**.
9. To discard any changes made to the settings, click **Don't Save**. Data processing will continue after this is clicked.
10. To automatically generate a MatLab file for every sample submitted as part of a batch run in the Batch Editor, click **Select Script** to select the script before submitting the batch to the queue. The script should be located in the Processing Scripts subproject of the API Instrument project.

    A MatLab file is created for every different experiment for each sample in the batch. The MatLab files are placed in the same location as the data files and will have the same names with the wiff extension replaced by mat. However, the index of the sample within the wiff file are appended. In addition, for samples acquired using acquisition methods containing more than one experiment, the period and experiment number are appended to the MatLab filename.

    For example, if a data file is called test.wiff and contains two samples, then the MatLab files are called:

    - test-1.mat
    - test-2.mat

    If the acquisition method contained one period and two experiments, then four MatLab files are generated, two for each sample:

    - test-1(1,1).mat
    - test-1(1,2).mat
    - test-2(1,1).mat
    - test-2(1,2).mat.

    If the data file contains diode array data and the **Save DAD data in batch mode (if available)** check box is selected, then an additional file with the sample index and (DAD) is created. For the previous example, files called test-1(DAD) and test-2(DAD).mat are created.

Known Issues and Limitations

When attaching this script to a batch, make sure that the Acquisition Queue window is open before submitting the batch. This window must be open until the acquisition has completed to make sure that the script is working properly.

Related Scripts

Export to JCamp: Converts spectra from wiff format to JCamp format.

Table 2-8 Matrix Definitions

Matrix	Dimensions	Type	Descriptions
Data	Number of masses (or wavelengths) × number of scans	Float	The raw intensities for all of the spectra.
SparseData	2 × total number of (mass, intensity) pairs	Double	The raw masses (first row) and intensities (second row) for all spectra. This matrix is used only with the sparse format.
Masses	Number of masses × 1	Float	The actual *m/z* values scanned by the instrument. This matrix is only present when exporting MS data.
Wavelengths	Number of wavelengths × 1	Float	The actual wavelengths acquired by the diode array detector. This matrix is present only when exporting DAD data.
Index	1 × number of scans	Long	N/A
Scans	1 × number of scans	Float	The retention times (in seconds) or the scan numbers for the spectra.

Table 2-8 Matrix Definitions (continued)

Matrix	Dimensions	Type	Descriptions
Filename	1 × length of filename	Text	This optional matrix specifies the filename of the original data file.

XIC from BPC

Use this script to retrieve the list of base peak masses and overlay the corresponding extracted ion chromatograms (XICs) in an Explore pane below the active pane. Run the **XIC from BPC** script after selecting a time region of interest in a chromatogram. The largest peak in each XIC trace are labeled with its mass if it is greater than 5% of the most intense XIC peak.

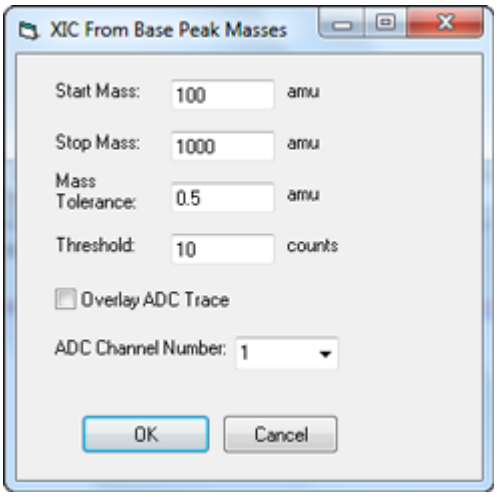
Use the Script

Users can optionally select to overlay the XIC traces with an ADC trace. The ADC trace will be normalized to the most intense XIC trace.

- Select the time region of interest in a chromatogram and do one of the following:

To do this	Do this ...
Process the data with current preferences	Click **Script** > **XIC from BPC**.
View the script description, set the processing preferences, and then obtain the overlaid XIC traces	a. Press **Shift** and then click **Script** > **XIC from BPC**. The XIC from Base Peak Masses QS Description dialog opens. b. Click **Continue**. The XIC From Base Peak Masses dialog opens. Refer to the figure: Figure 2-42.
Update the processing preferences and then obtain the overlaid XIC traces	Press **Ctrl** and then click **Script** > **XIC from BPC**.

Figure 2-42 XIC From Base Peak Masses Dialog



After processing starts, a progress bar indicates the current step. When processing is completed, a new pane with overlaid XIC traces is the active pane. To use the Cycle Overlays feature when it is unavailable, change the active pane in the software to a different pane and then reselect the overlaid XIC pane.

XIC from Table

Use this script to create or read start and stop masses from a file. The file must two columns separated by a tab. The first column must contain the start mass and the second column the stop mass.

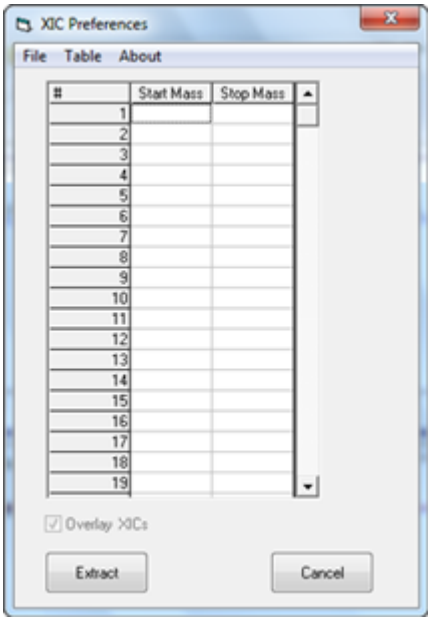
When working with full scan data, the software can show an Extracted Ion Chromatogram (XIC) for a subset of the scanned mass range. If the subsets are repeatedly used on different data, then it is often convenient to store the subsets of the mass range, consisting of a start and stop mass, in an external file and have the Analyst software generate an XIC based on this file.

The script generates the requested XICs either as one XIC per pane or with all of the XICs overlaid in one pane from the current Total Ion Chromatogram (TIC).

Use the Script

1. With a TIC open in an active pane, click **Script** > **XIC_from_table**.

Figure 2-43 XIC Preferences Dialog



2. Using the grid in the dialog, type the mass ranges to be extracted in an XIC.

Tip! To populate the grid from a text file, click **File** > **Open** and then browse to the text file.

3. (Optional) To save the current information in the grid to a file, click **File** > **Save As**.
4. (Optional) To clear the grid of all entries, click **Table** > **Clear**.
5. (Optional) To overlay all of the XICs in a single pane, select **Overlay XICs** check box.
6. (Optional) To create all of the specified XICs, click **Extract**.
7. To close the dialog and close the script, click **Cancel**.

Known Issues and Limitations

- If XIC start/stop masses are not loaded from a text file, then the maximum number of mass pairs that can be typed is 25. If XIC start/stop masses are loaded from a text file, then an unlimited number of start/stop mass pairs can be specified.
- Because of the limited space on most monitors, select the **Overlay XICs** check box when more than six XICs will be created.

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