
SCIEX OS Software

For the Echo[®] MS+ System with the ZenoTOF 7600 System

Feature Guide



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Acquisition with an Echo[®] MS+ System

1

This section supplies information about the use of the SCIEX OS software to acquire acoustic ejection-mass spectrometry (AEMS) data. The section gives descriptions of the MS method and AE method parameters, batches, batch calibration, and system preparation.

MS Method

Source and Gas Parameters

The Echo[®] MS probe on the OptiFlow Turbo V ion source operates with the open port interface (OPI) on the Echo[®] MS+ system to aspirate, nebulize, and ionize samples and then supply the samples to the ZenoTOF 7600 mass spectrometer. A narrow range of source and gas parameters is recommended for this workflow.

Figure 1-1 Source and Gas Parameters

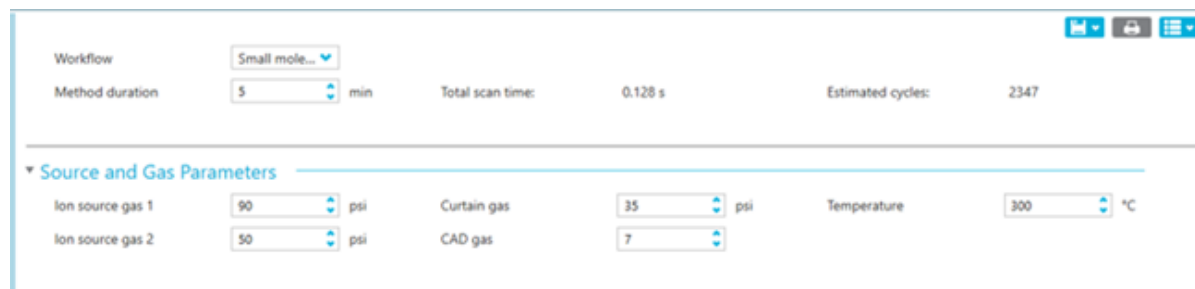


Table 1-1 Source and Gas Parameters

Parameter	Comments
Ion source gas 1 (psi)	Set the pressure for ion source gas 1. Ion source gas 1 pulls the carrier solvent from the OPI port to the ion source. Set to 90. Lower values might cause leaks in the OPI.
Ion source gas 2 (psi)	Set the pressure for ion source gas 2. This gas dissolves the carrier solvent in the ion source. Optimize the Ion source gas 2 (psi) value for the composition and flow rate of the carrier solvent. A starting value of 50 is recommended.

Table 1-1 Source and Gas Parameters (continued)

Parameter	Comments
Curtain gas (psi)	Set the pressure for the gas for the Curtain Gas interface. This gas helps prevent contamination of the ion optics. Use the highest possible value that does not decrease sensitivity. Higher values decrease contamination with a small decrease in signal intensity.
CAD gas	Set the pressure in the collision cell. For TOF MS experiments, set to 7 for collisional cooling of the ions. For TOF MS/MS experiments, optimize the CAD gas value for fragmentation of the analyte ions.
Temperature (°C)	Optimize the temperature for the composition and flow rate of the carrier solvent. A starting value of 300 is recommended. Temperature settings more than 400 are not recommended. High temperatures can decrease the life of the electrode and can also cause lower sensitivity for thermally labile compounds.

Parameters for TOF MS Experiments

Figure 1-2 TOF MS Parameters

The screenshot shows a software interface for configuring TOF MS parameters. The 'Experiment' dropdown is set to 'TOF MS'. The parameters are as follows:

Parameter	Value	Unit
Polarity	Positive	
TOF start mass	100	Da
TOF stop mass	1000	Da
Accumulation time	0.1	s
Spray voltage	4500	V
Declustering potential	80	V
DP spread	0	V
ITC mode	Dynamic	
Collision energy	10	V
CE spread	0	V
ITC	0	

Table 1-2 TOF MS Parameters

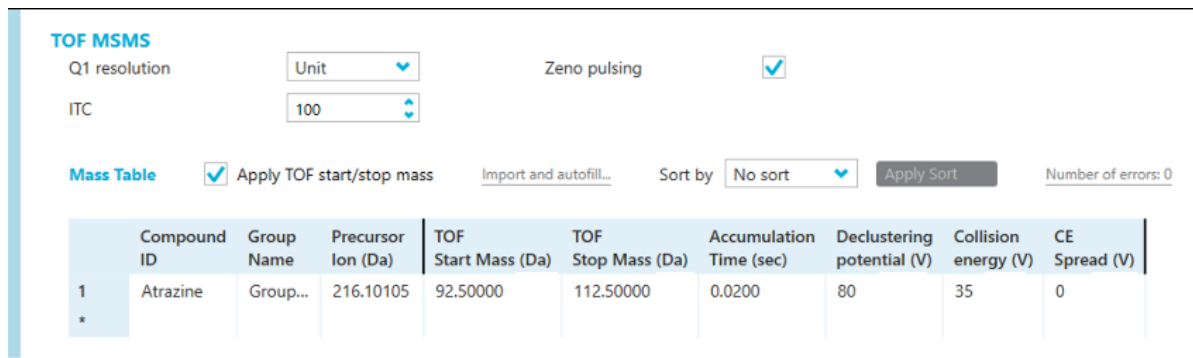
Parameter	Comments
Polarity	Identify the ionization mode. Select Positive or Negative . Polarity switching is not available.
TOF start mass (Da)	Identify the mass at the start of the target mass range. The TOF start mass (Da) must be less than the TOF stop mass (Da) .
TOF stop mass (Da)	Identify the mass at the end of the target mass range. The TOF stop mass (Da) must be more than the TOF start mass (Da) .
Accumulation time (s)	Identify the time that is required for the mass spectrometer to acquire one TOF MS spectrum. A starting value of 0.08 is recommended.

Table 1-2 TOF MS Parameters (continued)

Parameter	Comments
Spray voltage (V)	Identify the voltage to be applied to the probe electrode. Optimize the spray voltage for the composition and flow rate of the carrier solvent. To maximize the life of the electrode, do not use a value more than 4500.
Declustering potential (V)	Identify the voltage to be applied at the orifice to minimize the formation of ion clusters. Different compounds might have different optimum declustering potential (DP) values. The DP value is used for the full mass range.
DP spread (V)	Type a value for the DP spread (DPS). Together with the Declustering potential (V) , this parameter controls the DP that is applied to the ions. The DP is increased gradually from a low value of DP – DPS to a high value of DP + DPS.
ITC mode	Select Dynamic or Fixed . In dynamic mode, the ion flow is continuously monitored and automatically adjusted to prevent damage to the detector. In fixed mode, the user sets a value in the ITC field. Dynamic mode adds 27 ms to the cycle time, to monitor the ion flow before the start of the experiment. Note: Dynamic mode is only available for TOF MS experiments.
Collision energy (V)	Identify the voltage to be applied in the collision cell. In TOF MS experiments, a low value is used to move ions through the collision cell without fragmentation.
CE spread (V)	This parameter is not usually used in TOF MS experiments.
ITC	Identify the percentage of ions that will go into the mass spectrometer. When fixed mode is in use, monitor the ion intensity. Start with a low value and increase the value in small increments until the signal strength gets to the required minimum. If the expected ion intensity is not known, then use dynamic mode. Consistent high ion intensity or short periods of very high ion intensity can cause permanent damage to the detector. Note: This parameter is applicable when ITC mode is set to Fixed .

Parameters for MRM^{HR} Algorithm Experiments

Figure 1-3 MRM^{HR} Algorithm Parameters



The screenshot shows the MRM^{HR} Algorithm Parameters interface. It includes the following elements:

- TOF MSMS:** Q1 resolution (Unit), ITC (100), and Zeno pulsing (checked).
- Mass Table:** Apply TOF start/stop mass (checked), Import and autofill..., Sort by (No sort), Apply Sort, and Number of errors: 0.
- Table:** A table with columns: Compound ID, Group Name, Precursor Ion (Da), TOF Start Mass (Da), TOF Stop Mass (Da), Accumulation Time (sec), Declustering potential (V), Collision energy (V), and CE Spread (V). The first row shows Atrazine with a precursor ion of 216.10105, TOF Start Mass of 92.50000, TOF Stop Mass of 112.50000, Accumulation Time of 0.0200, Declustering potential of 80, Collision energy of 35, and CE Spread of 0.

Table 1-3 MRM^{HR} Algorithm Parameters

Parameter	Comments
Q1 resolution	Identify the resolution of the Q1 quadrupole. Select Unit , Open , Low , or High . Unit supplies a Q1 mass selection of approximately ± 0.7 Da. Open and Low supply a wider Q1 mass selection. High supplies a narrower Q1 mass selection.
ITC	Identify the percentage of ions that will go into the mass spectrometer. In MRM ^{HR} algorithm experiments, this parameter is usually set to 100 to maximize analyte sensitivity.
Zeno pulsing	Select to enable Zeno pulsing. Zeno pulsing is a unique feature of the ZenoTOF 7600 mass spectrometer. When activated, this feature makes the duty cycle better and increases signal strength.
Apply TOF start/stop mass	Select to set the TOF mass range manually. If this option is not selected, then a default mass range of 20 Da centered on the specified fragment ion is used.
TOF Start Mass (Da)	Identify the mass at the start of the target mass range. The TOF Start Mass (Da) must be less than the TOF Stop Mass (Da) .
TOF Stop Mass (Da)	Identify the mass at the end of the target mass range. The TOF Stop Mass (Da) must be more than the TOF Start Mass (Da) .
Accumulation Time (sec)	Identify the time that is required for the mass spectrometer to acquire one TOF MS/MS spectrum. A starting value of 0.01 is recommended.
Declustering potential (V)	Identify the voltage to be applied at the orifice to minimize the formation of ion clusters. In MRM ^{HR} algorithm experiments, declustering potential is identified for each row in the transition table.

Table 1-3 MRM^{HR} Algorithm Parameters (continued)

Parameter	Comments
Collision energy (V)	Identify the voltage to be applied in the collision cell. In TOF MS/MS and MRM ^{HR} experiments, this voltage breaks the precursor ions into fragments. Optimize collision energy (CE) to maximize the intensity of a fragment.
CE Spread (V)	Identify the CE spread (CES). Together with the Collision energy (V) parameter, this parameter controls the CE that is applied to the precursor ion in a Product Ion scan. The CE is increased gradually from a low value (CE – CES in positive polarity) to a high value (CE + CES in positive polarity).

AE Method

The AE method supplies the settings used for operation of the Echo[®] MS+ system.

Figure 1-4 AE Method: Standard

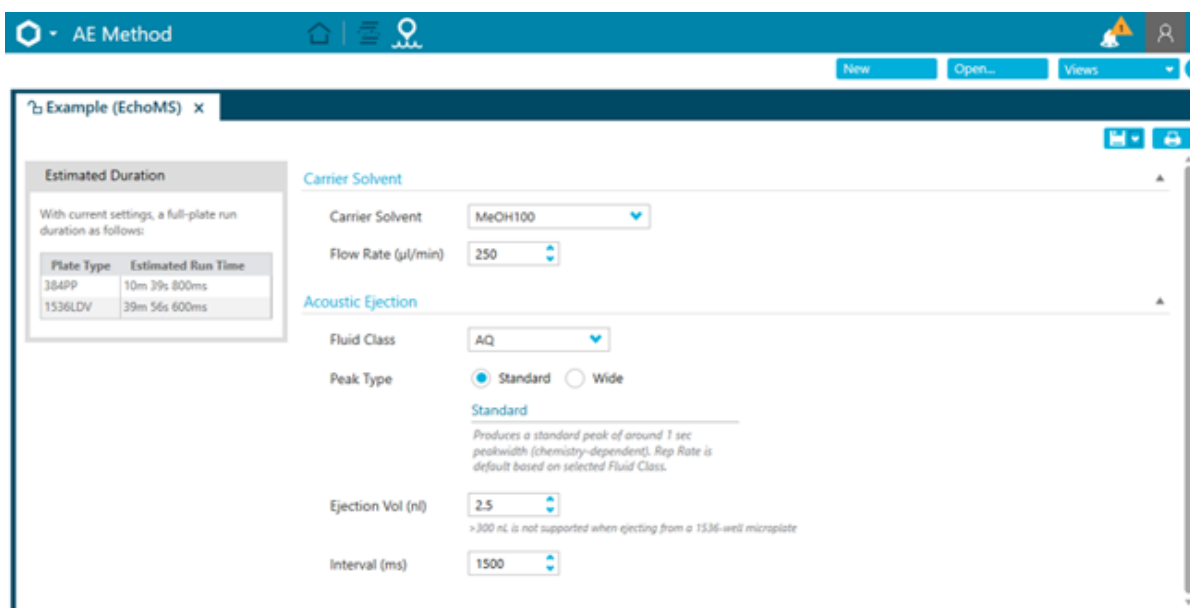


Figure 1-5 AE Method: Wide

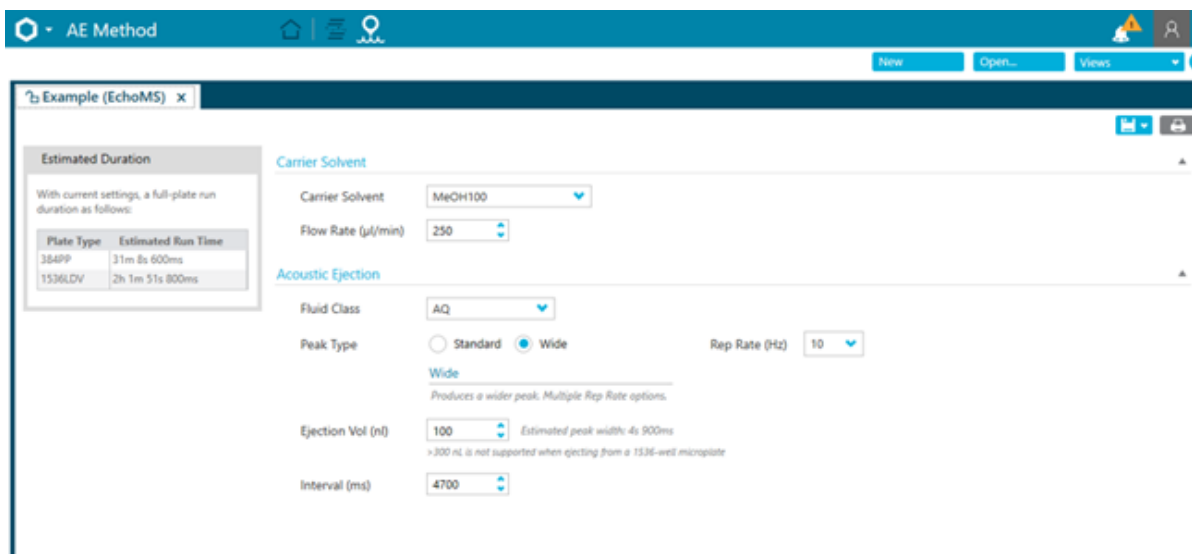


Table 1-4 AE Method Parameters

Parameter	Description
Estimated Duration	Shows the expected duration of the plate run time, calculated with the Interval (ms) and other factors that have an effect on the run time. The estimated duration is supplied for both 384-well and 1,536-well plates. The calculation does not include equilibration or batch calibration time.
Carrier Solvent	Select the value that is most closely related to the carrier solvent in use. The list contains mixtures of the most common carrier solvents: methanol (MeOH), acetonitrile (ACN), and water (H ₂ O).
Flow Rate (µL/min)	Optimize the flow rate for the system. The electrode and the composition of the carrier solvent have an effect on the optimum flow rate. If the electrode or the composition of the carrier solvent changes, then this value must be optimized again.

Table 1-4 AE Method Parameters (continued)

Parameter	Description
Fluid Class	<p>Select the sample matrix that is in the sample well. Different options are available for different plate types. Options include the following:</p> <ul style="list-style-type: none"> • AQ (Aqueous): Used for aqueous solutions. • SP (Surfactant): Used for solutions with a low surface tension, such as aqueous solutions with surfactants, for example Triton X-100, or organic-aqueous mixtures. This option is only available for 384-well plates. This option cannot be used with 1536-well plates because of the sample evaporation that occurs during analysis. • DMSO (Dimethyl sulfoxide): Used for solvents that contain between 70% and 100% DMSO.
Peak Type	<p>Select Standard or Wide mode.</p> <ul style="list-style-type: none"> • Standard: The AE system ejects droplets very quickly to make a narrow peak. • Wide: The user can identify the rate of droplet ejection to make peaks that are wider than in standard mode. Wider peaks supply more data points across the peak and support longer cycle times in the MS method. Wide peak mode is applicable to multidroplet ejections only.
Ejection Vol (nL)	<p>Identify the total volume of the sample to be dispensed by the Echo[®] MS+ system, in increments of 2.5 nL.</p> <hr/> <p>Note: The system ejects droplets of 2.5 nL.</p> <hr/> <p>When the Peak Type is Wide, the minimum value for Ejection Vol (nL) is 5.</p>
Interval (ms)	<p>Identify the time between sample ejections. The software uses the Rep Rate (Hz) and Ejection Vol (nL) to calculate a minimum Interval (ms).</p>
Rep Rate (Hz)	<p>Identify the droplet ejection repeat (rep) rate, in Hz. Ejection Vol (nL) and Rep Rate (Hz) control the widths of the peaks.</p>

Batch

Figure 1-6 Batch

Note: The following columns are not applicable to the analysis of data acquired with an Echo[®] MS+ system, and can be hidden with the **View** option: **Rack Type**, **Rack Position**, **Plate Position**, and **Injection Volume (µL)**.

Table 1-5 Batch Columns

Column Name	Description	Field Value Requirements
Sample Name	The name of the sample	Less than 252 characters. Note: During post-acquisition splitting of the data, the well position is added to the start of the sample name: for example A1-Sample1.
MS Method	The name of the MS method	Select an MS method from the list for the active project. Note: The same MS method must be used for all samples in the batch.
AE Method	The name of the AE method	Select an AE method from the list for the active project. Note: The same AE method must be used for all samples in the batch.
Plate Type	384PP or 1536LDV	Only one Plate Type can be used in a batch. Only plates from Beckman Life Sciences that are qualified for use with an Echo [®] MS+ system can be used with the Echo [®] MS+ system.

Table 1-5 Batch Columns (continued)

Column Name	Description	Field Value Requirements
Well Position	384PP: A1 to P24 1536LDV: A1 to AF48	A Well Position can only be sampled once for each row.
Sample Type	Blank, Standard, Double blank, QualityControl, Solvent, and Unknown	Sample type information is saved in the data file and can be used during processing.
Data File	The name of the file to which the acquired data is saved	All data acquired by a batch must be kept in the same Data File . Note: The same data file must be used for all samples in the batch.
Processing Method	The name of the method that will be used for automatic processing after acquisition is completed.	The processing method must be compatible with the MS method used to acquire data. Note: The same processing method must be used for all samples in the batch.
Results File	The name of the file to which the processed results are saved	Results files are kept in the <code>Results</code> subfolder of the active project. Note: The same Results file must be used for all samples in the batch. Note: Use a different Results file for each batch. We do not recommend that the Results files be used more than once. Note: If a target list file is used, then the Results file is saved in <code>txt</code> format. If a target list file is not used, then two Results files are saved, in <code>txt</code> and <code>qsession</code> format.

Table 1-5 Batch Columns (continued)

Column Name	Description	Field Value Requirements
Marker Well	Marker well: True Other wells: False (default)	Select only one Marker Well in each batch. Select a well with contents that supply a sufficiently strong MS signal for barcode recognition during data splitting. If the peak shape has excessive tailing, then data splitting might not occur.
Target List	The name of the Target List file, with the <code>CSV</code> extension	(Optional) Identify the Target List file. If the file is not in the <code>Batch</code> folder for the active project, then include the full file path. Refer to the section: Target Lists .

Automatic Calibration (Optional)

If automatic calibration is used, it must be done at the start of the batch. Calibration cannot be done between samples.

The calibrant delivery system (CDS) is used to calibrate the ZenoTOF 7600 system when it is configured with the Echo[®] MS+ system.

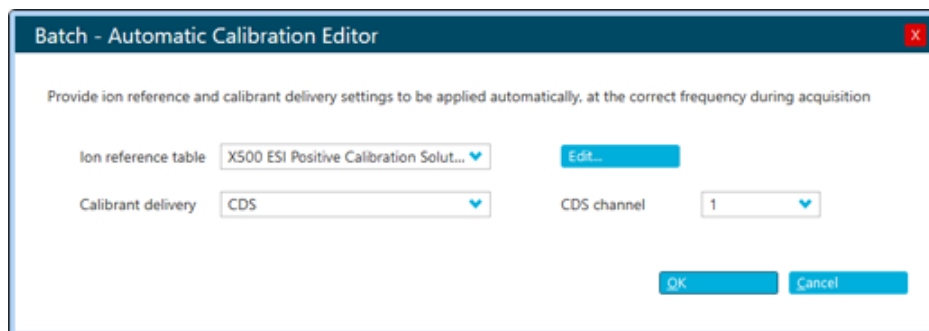
The user can select the applicable ion reference table and edit the table for the contents of the CDS reservoir and the specific calibration ions required.

To do automatic calibration at the start of the batch, select the **Auto-Calibrate** check box.

The calibration occurs in two phases:

- Cal: Initial CDS calibration, with the selected ion reference table
- Cal Phase 2: Equilibration, which removes traces of the CDS solution

Figure 1-7 Batch - Automatic Calibration Editor Dialog



Output File Configuration (Optional)

Use the `EchoExportColumnConfig.xml` file to customize the format of the Results text files path in which the output files will be written, the columns to be included in the output file, and the order of the columns.

The default `EchoExportColumnConfig.xml` file is in the `SCIEX OS Data/common-project-area` folder. To change the settings, edit this file, or make and edit a copy of the file in the project folder or the `Quantitation Results` folder for the project.

Note: Three templates are available in the `SCIEX OS Data\common-project-area\Echo MS\Example Export Column Configuration` folder:

- `EchoExportColumnConfig-1`
- `EchoExportColumnConfig-CompoundQC`
- `EchoExportColumnConfig-Intact`

Table 1-6 Elements in the Output File

Element	Description
Path	Identify the path to which the output file will be saved. Multiple paths can be specified to save multiple copies of the output file. <hr/> Note: A copy of the Results file is saved in the <code>Quantitation Results</code> folder for the project. <hr/>
Order	Identify the order for the column in the output file. Type a unique number for each column. Type 0 for the first column.
Visible	Identify if the column is included in the output file. Type <code>true</code> to include the column. Type <code>false</code> to exclude the column.

System Preparation

For MRM^{HR} algorithm and information-dependent acquisition (IDA) experiments where different ions are monitored for different wells, to make sure that the correct ions are monitored for each well, the software requires the time between droplet ejection and detection (transfer time). The transfer time is calculated and saved every time data splitting occurs.

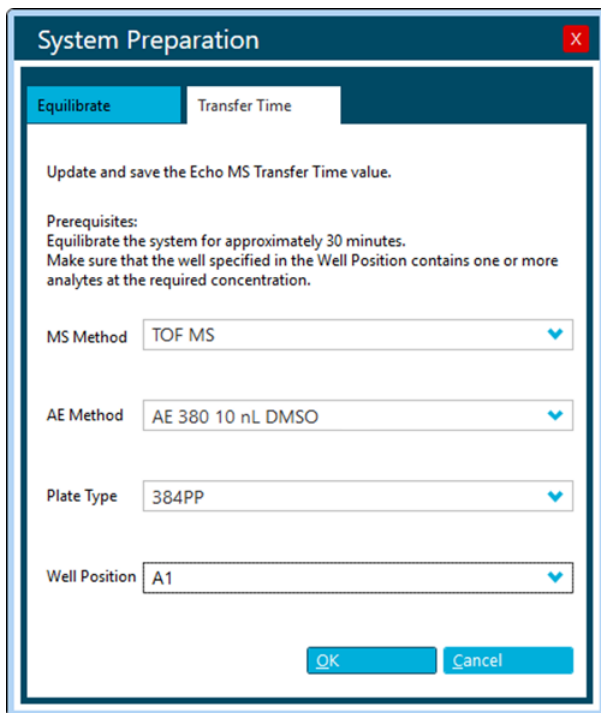
If the system has not operated recently, or if the electrode or carrier solvent has been changed, then the system runs a short batch to calculate the transfer time. Before the batch to calibrate the transfer time is run, make sure that the time for system equilibration has been a minimum of 30 minutes.

To calibrate the transfer time, do this:

1. Open the Status panel.
2. Click **Equilibrate**.

The System Preparation dialog opens.

Figure 1-8 System Preparation Dialog: Transfer Time Tab



3. Open the Transfer Time tab, and then use the following table complete the fields:

Table 1-7 Transfer Time Tab

Field	Description
MS Method	Select an MS method from the list for the active project. Any MS method can be used to adjust the transfer time. A TOF MS method usually gives the best result.

Table 1-7 Transfer Time Tab (continued)

Field	Description
AE Method	<p>Select the AE method that will be used for acoustic ejection-mass spectrometry (AEMS) analysis from the list for the active project. The AE method makes sure that the transfer time is calibrated correctly for the sample transfer conditions in the AEMS analysis. Make sure that the value for Ejection Vol (nL) in the selected method is sufficient to supply a strong signal that is almost the same as the intensity of the marker well.</p> <hr/> <p>Note: Adjust the transfer time before a different AE method is used.</p> <hr/>
Plate Type	<p>Select a plate that is applicable to the Echo® MS system. Options include the following:</p> <ul style="list-style-type: none"> • 384PP • 1536LDV
Well Position	<p>Identify the position of a well that contains a sample concentration that will give a significant signal in the mass spectrometer. A marker well is recommended. Options include the following:</p> <ul style="list-style-type: none"> • 384PP: A1 to P24 • 1536LDV: A1 to AF48

4. Click **OK**.

A batch with 15 samples is automatically created and submitted. After the batch completes, the new transfer time is calculated and saved as a system default.

Usually, a batch used with the Echo® MS+ system acquires one analyte or set of analytes for all of the samples. If a different target analyte must be specified for each row, column, or well position, in MRM^{HR} algorithm workflows, for example, then a target list must be used. For TOF MS data, the target list identifies the analytes of interest for each well, and this information is used during processing of the data. A target list can also be used to identify the analytes of interest in MRM^{HR} algorithm and IDA experiments during acquisition. The analyte information in the target list is used to update the MS method during acquisition.

The target list is a `CSV` file. The file contains analyte information that can be used in the following areas:

- For the analyte information for processing of TOF MS experiments
- For the analyte information for mass reconstruction of intact proteins and large biomolecules
- In the transition table for MRM HR experiments
- In the inclusion list for IDA experiments

To use a target list, do these procedures:

- [Create a Target List](#)
- [Configure Project Default Settings](#)
- [Create an MS Method to Be Used as a Template](#)
- [Create a Processing Method to Be Used as a Template](#)

Create a Target List

Each row of a target list file contains mass information for a single well and compound. Multiple rows can contain the same compound. Multiple rows can contain the same well position.

Note: Example target lists for different workflows are available in the `SCIEX OS Data\common-project-area\Echo MS\Example Target List` folder.

- Create a target list file in `CSV` format, and then save it in the `Batch` subfolder of the folder for the project where it will be used.

Note: Make sure that the text, capitalization, and spacing in the field names are the same as in the following table.

Target Lists

Table 2-1 Field Names in the Target List File

Field	Description
Well	Identify one well position in each row, with no spaces. Available values include the following: <ul style="list-style-type: none">• 384PP: A1 to P24• 1536LDV: A1 to AF48
Transfer Time Tolerance	Identify the number of seconds to be added to adjust the start and end of the monitoring window for a sample. This parameter is used in workflows, such as the following, where different transitions are monitored for different well positions: <ul style="list-style-type: none">• MRM^{HR} workflows where transitions are monitored by well• IDA workflows where inclusion lists are monitored by well The transfer time tolerance can be negative, but the absolute value of the transfer time must not be more than half of the ejection interval used in the AE method.
Offset	Identify the number of seconds that the scheduled acquisition window will be moved around a possible peak position. A positive value moves the window to the right. A negative value moves the window to the left.
Group	Identify the applicable group name for the compound.
Name	Identify the Compound ID of the compound.
IS Name	Identify the name of the internal standard to be used for quantitation calculations for the compound. Only one internal standard can be used for each compound.
IS	Identify if the compound is an internal standard. Available values include the following: <ul style="list-style-type: none">• True• False
Formula	Identify the elemental formula for the compound. Peptides can have single-letter amino acids and modifications. To identify specific isotopes, include the weight of the isotope, such as [2H], [18O], or [15N], in square brackets before the symbol. For example, identify heavy water (D2O) as [2H]2O.
Adduct/Charge	If a formula is specified, then identify the adduct and charge state, such as [M+H] ⁺ or [M+H] ⁻ . All adducts supported in the Analytics workspace of the SCIEX OS software are supported in target lists.

Table 2-1 Field Names in the Target List File (continued)

Field	Description
Comment	Supply more information for the row entry. As many as 128 characters can be used.
Precursor Mass (Da)	Identify the mass of the precursor ion. The applicable range is from 5 to 2,250, with as many as 5 decimal places.
TOF Start Mass (Da)	Identify the mass at the start of the target mass range for a TOF MS/MS experiment. The TOF Start Mass (Da) must be less than the TOF Stop Mass (Da) . This parameter is used if Apply TOF start/stop mass is selected in the MS method to be used as a template.
TOF Stop Mass (Da)	Identify the mass at the end of the target mass range for a TOF MS/MS experiment. The TOF Stop Mass (Da) must be more than the TOF Start Mass (Da) . This parameter is used if Apply TOF start/stop mass is selected in the MS method to be used as a template.
Fragment Mass (Da)	Type the fragment mass to be used in the processing method. The default scan range for a TOF MS/MS method is 20 Da, ± 10 Da from the specified fragment mass. Note: If Apply TOF start/stop mass is selected in the MS method to be used as a template, then the TOF Start Mass (Da) and TOF Stop Mass (Da) set in the target list are used as the TOF MS/MS scan range.
Accumulation Time (sec)	Adjust the accumulation time of the target transition to optimize the total scan time. The accumulation time is the time required for the mass spectrometer to acquire one TOF MS/MS data point. The accumulation time has an effect on the number of points across a peak. The applicable range is from 0.005 to 50. Typical values are from 0.01 to 0.100.
Declustering potential (V)	Identify the voltage to be applied to the orifice to minimize the formation of ion clusters. The declustering potential (DP) can be specified for each row of the transition table. The applicable range is from 0 to 300. Note: DP spread (V) is set in the MS method.
Collision Energy (V)	Identify the voltage to be applied to the collision cell. Collision energy (CE) is usually optimized to maximize the intensity of a fragment. The applicable range is from 0 to 150.

Table 2-1 Field Names in the Target List File (continued)

Field	Description
CE Spread (V)	<p>Identify the value to be used to increase the CE gradually. Together with the Collision Energy (V) parameter, the CE spread (CES) parameter controls the CE that is applied to the precursor ion in a Product Ion scan.</p> <p>For example, in positive polarity, the CE is increased gradually from CE – CES to CE + CES.</p> <p>The applicable range is from 0 to 150.</p>
Fragmentation Mode	<p>Identify one of the following fragmentation modes:</p> <ul style="list-style-type: none"> • CID: In collisional-induced dissociation (CID) mode, fragment ions are made by vibrational excitation of the precursor ion caused by collisions with gas molecules in the Q2 collision cell. • EAD: In electron-activated dissociation (EAD) mode, the precursor ions in the EAD cell are exposed to electrons to cause dissociation of the precursor ion to fragment ions. • EAD (conventional trapping): Conventional trapping is an EAD mode that is most applicable for academic studies of reaction kinetics. EAD mode supplies more control of the load time and reaction time (electron irradiation duration) steps. In EAD mode, these steps are optimized to occur at the same time, which increases the sensitivity approximately two times. In EAD (conventional trapping) mode, these steps are done consecutively. Selected precursors are introduced in the EAD cell for a specified load time, the electron beam is applied for a specified reaction time, and then products are ejected from the EAD cell. <hr/> <p>Tip! If accurate and predictable control of the reaction time is required, then use EAD (conventional trapping) mode.</p>
Electron KE (eV)	<p>Identify the electron kinetic energy (KE) of the irradiating electron beam. The electron KE is the same as the DC bias between the electron source and the electron-activated (EA) rod electrodes in the electro-activation dissociation (EAD) cell. This parameter is applicable when Fragmentation Mode is set to EAD or EAD (conventional trapping).</p>

Table 2-1 Field Names in the Target List File (continued)

Field	Description
ETC (%)	<p>Identify the electron transfer coefficient (ETC). This parameter controls the fraction of electrons let into the EAD cell. The range is from 0% to 100%. The parameter is applicable when Fragmentation Mode is set to EAD or EAD (conventional trapping).</p> <hr/> <p>Tip! To use the type of precursor species that is analyzed and the product ions that are acquired to control the type of EAD reaction, use this parameter.</p> <hr/>
EAD RF (Da)	<p>Identify a value between 0 Da and 300 Da. This parameter controls the RF level to keep precursor and fragment ions in the EAD cell.</p> <hr/> <p>Note: To detect product ions with a higher <i>m/z</i>, increase EAD RF (Da). The detection of product ions with a lower <i>m/z</i> might decrease.</p> <hr/>
Reaction time (ms)	<p>Identify the reaction time for electron irradiation. In EAD mode, this parameter also controls the load time.</p> <hr/> <p>Tip! If precursor consumption is not sufficient after optimization of the electron beam current, then increase the reaction time.</p> <hr/>
Time Bins to Sum	<p>Identify the number of data points to be added together. The range for small molecules or peptides is 4 to 6. The start value for intact protein analysis (> 20 kDa) is 40.</p>
Channel 1 to Channel 4	<p>Identify the analog-to-digital converter (ADC) channels. Each channel counts ions. If all four of the channels are selected, which is the default value, then all four of the channels are added together for the total ion count.</p>
Expected MW (Da)	<p>Mass Reconstruction workflow: Identify the expected molecular weight for the component, in Da.</p>
m/z Range for XIC Start (Da)	<p>Mass Reconstruction workflow: Identify the start mass for the XIC range.</p>
m/z Range for XIC Stop (Da)	<p>Mass Reconstruction workflow: Identify the end mass for the XIC range.</p>
Reconstruction Start Mass (Da)	<p>Mass Reconstruction workflow: Identify the mass at which reconstruction will start, in Da.</p>

Table 2-1 Field Names in the Target List File (continued)

Field	Description
Reconstruction Stop Mass (Da)	Mass Reconstruction workflow: Identify the mass at which reconstruction will stop, in Da.

Configure Project Default Settings

For all workflows, if a processing method will be used as a template for autotriggered processing, then configure the project default settings to optimize peak integration over the full analysis. Different ejection volumes and peak widths in the AE method require different values for the processing parameters.

The information in the project default settings is saved in the processing method to be used as a template.

Note: When the project default settings are changed in the Analytics workspace, the changes are not used for saved processing methods. To apply the changes, update the project default settings, and then create a new processing method. The new processing method will use the updated project default settings. Use this new processing method for autotriggered processing.

1. In the Analytics workspace, click **Projects > Project default settings**.

Figure 2-1 Quantitative Processing Window

Project Default Settings

Quantitative Processing

Set Project wide defaults for quantitative processing method parameters

Method Defaults

Signal to Noise Algorithm: Relative Noise

Integration Defaults

Integration Algorithm: Summation

Retention Time (RT)

XIC width: 0.02 Da

Expected RT: 0.000 min

Integration

S/N Integration Threshold: 1

Gaussian Smooth Width: 0.5 points

Summation Window: 1.5 sec

Noise % for Baseline: 10.0 %

Recentering: 0.00 sec

Adjust endpoints to local minima

Units & Calibration Defaults

Units & Calibration Defaults

Concentration units: []

Regression parameter: Area

Regression type: Linear

Weighting type: 1/x

Apply to current project Use for new projects in current data root [More Projects...](#) [Apply](#) [Close](#) [Help](#)

2. Configure the parameters.

For detailed descriptions of the parameters, refer to the document: *SCIEX OS Help System*.

3. Click **Apply**.
4. Click **Close**.

Create an MS Method to Be Used as a Template

- In the MS Method workspace, create an MS method to be used as a template. Refer to the document: *SCIEX OS Help System*.
 - For TOF MS experiments, create an MS method that has the applicable source and gas parameters and TOF MS experiment parameters.
 - For MRM^{HR} experiments, create an MS method that has the applicable source and gas parameters, TOF MS experiment parameters, and TOF MS/MS experiment parameters, such as the Q1 resolution, ITC, and Zeno pulsing settings.

Note: The Mass Table information, such as **Compound ID**, **Group Name**, **Precursor Ion**, **TOF Start Mass (Da)** and **TOF Stop Mass (Da)** or **Fragment ion (Da)**, **Accumulation time (s)**, **Declustering potential (V)**, **Collision energy (V)**, and **CE spread (V)**, is in a target list file. This information replaces information in the MS method to be used as a template, and thus supplies a well-based processing method for TOF MS experiments and both acquisition and processing methods for TOF MS/MS experiments.

Create a Processing Method to Be Used as a Template

The information in the target list file and the project default settings replaces the information in the processing method that is used as a template. Refer to the section: [Configure Project Default Settings](#).

- In the Analytics workspace, create a processing method. Refer to the document: *SCIEX OS Help System*.

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