

Creating sample set methods to acquire data manually

■ Run Samples > Samples tab

A sample set method is an ordered list of sample information and corresponding functions you create to define data acquisition. You can create or modify a sample set method by entering, modifying, and selecting sample information in the Samples table.

Requirement: To create sample sets for dissolution, you must use the Sample Set Method Wizard.

Customizing your view of the Samples table

You can adjust your view of the Samples table, for example, enlarge its size and define the columns you want to appear within it.

To customize your view of the Samples table:

1. To maximize the Samples table view, in the Navigation pane, clear View Acquisition.
2. To define the columns you want to appear in the table, click File > Apply Table Preferences, or on the toolbar, click .
3. In the Table Preferences dialog box, select the table preferences you want to use, and then click Apply.
4. Click File > Save.

To manually create a sample set method in the sample queue workspace:

1. On the Samples tab, click the Function cell in the first row of the Samples table, and then select the function that you want to perform.

Tip: Default values in many of the table's columns are based on your settings in the Customize > Defaults dialog box.

2. In each row of the table, modify the default Injection Volume, Vial, Sample name, Run Time and Processing column entries.

Important: The 2487 and 2489 UV detectors use different mechanisms to determine the run time end.

| UV detector model | Mechanism used to determine run time end |
|-------------------|---|
| 2487 | The run time (in minutes) entered into the Sample set, plus a margin of a few seconds. Doing so prevents timing issues such as whether the run starts and ends on a data point, which can affect the number of points actually collected. |
| 2489 | The number of data points. If you program 1 point per second for 10 minutes, |

| UV detector model | Mechanism used to determine run time end |
|-------------------|--|
| | <p>the ICS collects 600 data points, and ends the run after collecting the total number of points.</p> <p>If a problem occurs that prevents the detector from collecting necessary amount of data, then the ICS reports an instrument failure in the Empower message center.</p> |

Tip: Using Auto Fill can save you time and reduce the chance of name entry errors by automatically generating incremental sample names for you. An example for using the Auto Fill function is shown below:

- Click the SampleName column in the Samples table.
 - Right-click the table, and then click Auto Fill.
 - If you want to generate an incrementing prefix and/or suffix for your sample name, enter the numbers or letters in the appropriate text boxes. This feature applies to the SampleName, Label, Label Reference, Level, and Auto Additions columns.
 - Click OK, and then confirm that your samples were named as you intended.
 - Click File > Save Sample Set Method.
3. Click the Method Set/Report Method column, and then from the list, select the method set (or report method if you selected a report function for the row) you want to use for the row.
 4. To enter component information (component names, amounts, units, and so on) for a sample or standard in the table, click a sample row (or rows), and then click Components .
 5. In the Component editor, enter component information, using this table as a guide:

Columns in the Samples table

Tip: For GPC/V applications, enter information for broad standards or unknowns in the Mol Weights, K-Alphas, Moments, Distribution, or Cumulative tabs for the current sample. Your component information is saved when you save the sample set method.

Rule: To specify the units in the All Samples tab of the Components Editor, you must enter a less than sign (<) before the units. For example, to set the units to milligrams, enter "<mg". The less than sign is not necessary if you enter the units in the Current tab.

Restriction: You cannot modify any locked channels or locked vials, but you can view them.

7. Select a run mode to specify running, reporting, and/or processing actions during sample acquisition.

| Run mode | Description |
|----------|-------------|
| | |

| Run mode | Description |
|-----------------|---|
| Run Only | The software acquires data but does not process the data or print a report. |
| Run and Process | The software acquires and processes data, but does not print a report. |
| Run and Report | The software acquires data, processes the data, and prints a report. |

Tip: If you change the run mode from the Run Mode list in Run Samples while a sample set is running, the change takes effect for the currently running injection of the current sample set. If you change the run mode for a sample set in the Sample Sets table queue, the Run Mode list displays the selected run mode (when the sample set runs). You can specify run mode for individual lines of your sample sets using the Processing column of the Samples table.

- To store the sample set method for future use, click File > Save, and then in the Name box, enter a name for the sample set method, or select a name from the list of sample set methods to overwrite an existing method.

Tip: You do not need to save the sample set method to run it. Save the sample set method only if you plan to reuse it.

- Click Save.
- When required, enter a comment and your password, and then click Save.

To print the sample set method as displayed in the Run Samples table:

- On the Samples tab, right-click the table, then click Print Table.
- Modify print settings as needed, and then click OK.

Columns in the Samples table

Use the columns in this table to create or modify a sample set or sample set method. You can copy data from the last filled row to the next empty row in the table by clicking anywhere in the empty row. You can copy values down a column by using Ctrl-d.

Samples Table columns:

| Column | Description |
|--------|--|
| Vial | <p>Use this column to indicate the vial number in the autosampler or rack of samples from which a particular injection is to be made, or to indicate the injection number when using a manual injector. Run Samples automatically increments the vial number when you start a new row in the Samples table. Valid entries: 1 to 384.</p> <p>When you use a chromatographic system configured for plates:</p> <ul style="list-style-type: none"> The vial column header is labeled according to the terminology selections made in the Referencing tab when the plate type is created. |

| Column | Description |
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| | <ul style="list-style-type: none"> ■ The rows in the column reflect the referencing scheme selections made when the plate type is created (for example, 1:A,1). <p>When you use a chromatographic system configured for Dual Tower:</p> <ul style="list-style-type: none"> ■ When your Empower system is connected to a 5890S/7673S or a 6890 or 7890 GC in a Dual Tower configuration, each row in the vial column specifies both the carousel vial number <i>and</i> the tower location (front or back) from which to inject the sample. For example, an injection from vial number 2 on the front tower appears as F:2; an injection from vial number 6 on the back tower appears as B:6. Simultaneous injections are highlighted in the Samples table as identically colored pairs of rows, with one injection from the front tower and one from the back tower. |
| SampleName | <p>Use this column to specify the identifier for a sample (unknown and standard). If you do not enter an identifier, the software inserts default identifiers: Unk. for unknowns and Std. for standards.</p> <p>Tip: SampleName is a default custom field. You can rename it, change its width, or specify an identifier (used for both standards and unknowns) in your project's properties within Configuration Manager. Waters recommends that you not delete or make any additional changes to this custom field. You can use the Auto Fill dialog box to automatically add an incrementing prefix or suffix to the sample name.</p> |
| Label | <p>Use this column to label each Inject function row in the Samples table on which you want Empower software to perform a Calibrate, Quantitate, or Report function. When Empower software runs Inject function row(s) that contain a particular label in their Label column <i>and</i> then encounters a matching label in the Label Reference column of a subsequent row (one that contains a Calibrate, Quantitate, or Report function), The software performs the Calibrate, Quantitate, or Report function on all preceding rows with the matching label.</p> <p>The Label column can work alone (in the case of Intersample and Summary Custom Fields) or with the Function and Label Reference columns. You enter your own label in the Label column for a specific Inject function row or use the Sample Set Wizard to have Empower do this for you automatically.</p> <p>You can also use the Label column to create a labeled injection to perform baseline subtraction of 2D data or to perform PDA 3D blank subtraction.</p> <p>Tip: Duplicate labels are allowed in a sample set. You can also generate incrementing prefixes and suffixes for the Label, Label Reference, Level, and Auto Additions columns.</p> |
| Inj Vol (µl) | <p>Use this column to specify the volume of sample to inject for a single injection or row in a sample set.</p> <p>For GC autosamplers, injection volume is linked to the syringe size definitions for the sample set. The maximum injection volume must not exceed 50% of the syringe volume.</p> <p>If no syringe is defined, the injection volume range is not limited. If a syringe is defined, Empower error-checks for valid injection volumes based on the user-provided information in the GC Sample Set Information</p> |

| Column | Description |
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| | <p>for each tower. Use Customize > Defaults to set default syringe information for your GC.</p> <p>Tip: If your system includes a 2790/2795 Separations Module and the instrument method parameter for Loop Option (set in the General tab of the 2790/2795 Separations Module) is set to Full, the software ignores the Injection Volume in each Samples table row that contains the instrument method. Instead, the injection volume is set to the volume of the installed sample loop plus any additional overfill volume (as specified by the Full-Loop Overfill parameter).</p> |
| # of Injs | <p>Use this column to specify the number of injections you want to make from each vial.</p> |
| Function | <p>Use this column to specify the function for each row in the Samples table. There are several categories of functions including injection, processing, GPC sample definition and instrument control.</p> <p>Use these functions to define the injection process and sample type:</p> <ul style="list-style-type: none"> ■ Inject Standards – Makes an injection from the specified vials containing standards. During processing, a standard is integrated and calibrated. ■ Inject Samples – Makes an injection from the specified vials containing unknown samples. During processing, a sample is integrated and quantitated. ■ Inject Controls – Makes an injection from the specified vials containing controls. During processing, a control sample is integrated and quantitated. When processed, calculated amounts or concentrations of the control samples are compared to specified values, and % Deviation is computed. <p>Tip: You can set System Suitability limits to provide fault detection for % Deviation and/or calculated amounts or concentrations that fall outside the limits.</p> <ul style="list-style-type: none"> ■ Inject Immediate Standards – Runs the method set without triggering an autoinjector. A short Preparing for Inject status is available, during which you can make a manual injection of a standard. After this pause, the software immediately begins to collect data. Methods are run as in an Inject Standards row. This option is often used for large prep injections. ■ Inject Immediate Samples – Runs the method set without triggering an autoinjector. A short Preparing for Inject status is available, during which you can make a manual injection of a sample. After this pause, the software immediately begins to collect data. Methods are run as in an Inject Samples row. This option is often used for large prep injections. ■ Inject RF Internal Standards – Makes an injection from specified vials and processes it as an unknown, not a standard. The internal standard is quantitated and a response factor (RF) is calculated for the Standard Peak. (A Standard Peak is a peak in the sample's processing method that has an amount specified either in the sample, or the default |

| Column | Description |
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| | <p>amounts in the processing method.) The RF of the standard peak is then used to quantitate unknown peaks.</p> <p>Use these functions to process acquired data:</p> <ul style="list-style-type: none"> • The following four Summarize Custom Fields functions calculate all intersample summary custom fields when you process an acquired sample set using Run and Process, Run and Report, or background processing. Each function varies in the way it calculates result summaries, so keep these guidelines and recommendations in mind when deciding which function to use: <ul style="list-style-type: none"> ■ Summarize Custom Fields – Calculates summary results using all samples above its table row that match the custom field syntax, and stores the new summary result for each of these samples. To include all samples in the summary calculation, place the Summarize Custom Fields function at the end of the sample set. ■ Summarize Custom Fields (Exclude Faulted) – This function also calculates summary results using all samples above its table row that match the custom field syntax, but excludes from its summary calculation any faulted injections whose individual results fell outside of the system suitability limits. This function then stores the new summary result for all samples above its table row that match the custom field syntax. <p>Important: If you add more than one Summarize Custom Field function within a sample set, each subsequent function calculates summary results using all samples above its table row that match the custom field syntax, including samples above previous Summarize Custom Field function rows. However, subsequent Summarize Custom Field functions store their newly calculated summary value for all samples above their table row and above previous function rows, overwriting summary values that previous Summarize Custom Field functions stored for the samples above their table rows. The last Summarize Custom Fields function in the sample set stores its newly calculated summary result for all samples above its row in the sample set, including the samples above all previous function rows.</p> <p>Recommendation: To produce incremental summary values between groups of samples, use the Summarize Custom Fields Incrementally function or the Summarize Custom Fields Incrementally (Exclude faulted) function. When using interactive system suitability Stop on Fault, Reinjecton Fault, and so on, use these two functions because they retain the incremental summary values with the chromatographic results, whereas multiple Summarize Custom Fields functions overwrite these temporary incremental summary values each time it occurs in the sample set.</p> <ul style="list-style-type: none"> ■ Summarize Custom Fields Incrementally – Calculates summary results for all samples above this table row that match the custom fields syntax, and stores the new summary value for the samples above its row and below a previous Summarize Custom Fields Incrementally function row. |

| Column | Description |
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| | <ul style="list-style-type: none"> ■ Summarize Custom Fields Incrementally (Exclude Faulted) – This function also calculates summary results for samples above its table row, but excludes from its summary calculation any faulted injections whose individual results fell outside of the system suitability limits. This function then stores the newly determined result for all samples above its table row and below a previous Summarize Custom Fields Incrementally (Exclude Faulted) function row. ■ Clear Calibration – Clears calibration curves associated with processing methods of the specified method set (default processing method, and all processing methods in the Channels table). ■ Quantitate – Processes the unknown samples. Processing can include creating derived channels, followed by integration and quantitation of the sample data according to the specified method set. <p>Tip: If there is a standard among the specified samples, the Quantitate function processes the standard as an unknown. Use Quantitate with Inject Unknowns, Inject Standards, Labels, Label References, and the other processing functions to perform bracketing. The Quantitate function without a Label Reference instructs the software to quantitate all samples injected as unknowns from the previous rows.</p> <ul style="list-style-type: none"> ■ Calibrate – Processes the standard samples. This processing can include the creation of derived channels, followed by integration and calibration of the sample data according to the specified method set. <p>Tip: If there is an unknown among the specified samples, the Calibrate function processes the unknown as a standard. Use Calibrate with Inject Standards, Inject Unknowns, Labels, Label References, and the other processing functions to perform bracketing. The Calibrate function without a Label Reference instructs the software to calibrate all samples injected as standards from the previous rows.</p> <ul style="list-style-type: none"> ● Report - Reports the acquired data using the specified report method. ● Pause - Pauses the sample set. Sample set will remain paused until the user allows it to proceed. <p>Use these functions to define the type of GPC/V sample to be injected:</p> <ul style="list-style-type: none"> ■ Inject Narrow Standards – Makes an injection from specified vials. During processing, uses narrow integration parameters to detect and integrate the peak(s) in the chromatogram. Uses viscosity narrow integration parameters to integrate the viscometer channel data (GPCV only). Incorporates sample information and data from the integration results into a calibration curve. Creates a viscosity law plot for the calibration curve (Universal Calibration only). ■ Inject Broad Standards – Makes an injection from specified vials. During processing, uses broad integration parameters to detect and integrate the peak(s) in the chromatogram. Uses viscosity broad |

| Column | Description |
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| | <p>integration parameters to integrate the viscometer channel data (GPCV only). Incorporates sample information and data from the integration results into a calibration curve. Creates a viscosity law plot for the calibration curve (Universal Calibration only).</p> <ul style="list-style-type: none"> ■ Inject Narrow Unknowns – Makes an injection from specified vials. During processing, uses narrow integration parameters to detect and integrate the peak(s) in the chromatogram. Uses viscosity narrow integration parameters to integrate the viscometer channel data (GPCV only). Quantitates the integration results (calculates peak molecular weight) using a calibration curve. Calculates the intrinsic viscosity of the peak (GPCV only). ■ Inject Broad Unknowns – Makes an injection from specified vials. During processing, uses broad integration parameters to detect and integrate the peak(s) in the chromatogram. Uses viscosity broad integration parameters to integrate the viscometer channel data (GPCV only). Quantitates the integration results (calculates peak molecular weight averages and slice weights) using a calibration curve. Calculates the intrinsic viscosity of the distribution and peak and the branching index g' (GPCV only). <p>Use these functions to carry-out advanced control actions on instruments included in the chromatographic system and selected instrument method:</p> <ul style="list-style-type: none"> ● Equilibrate – Executes the instrument method's initial conditions, for the user-specified run time. No data collection or injections are made during equilibration. Include at least one active channel in the instrument method and a run time in the Samples table. <p>Tip: If you define a gradient pump instrument method, the initial flow conditions are maintained, but the gradient is not started.</p> <ul style="list-style-type: none"> ■ Condition Column – Executes the instrument method (including pump gradient) for the user-specified run time. No data is collected during the Condition Column function. <p>Tip: The instrument method must define a pump gradient to start the gradient. Include at least one active channel in the instrument method (of the method set) and a run time in the Samples table.</p> <ul style="list-style-type: none"> ■ Purge Inj – Instructs the Waters family of IEEE-488 autosamplers, the ACQUITY Sample Manager, and the 2690/2695 and 2690D/2695D Separations Modules to purge their autosampler fluidic lines for the user-specified run time. The purge uses the initial conditions of the instrument method specified in the associated method set. Ensure that the instrument method pump parameters specify a flow rate between 0.5 and 3.0 mL/min. Enter a run time value in the Run Time column from 6.5 to 15.0 min. <p>Tips:</p> <ul style="list-style-type: none"> ● If the instrument method has a low-pressure limit greater than zero, the software shuts down the pumps when the Purge Inj |

| Column | Description |
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| | <p>function starts. To avoid this problem, use an instrument method with a low-pressure limit of zero.</p> <ul style="list-style-type: none"> ● If you are using a 2695 system, the number you specify in the Purge Inj field is multiplied by the loop volume, the total of which is the purge volume for the system. For example, if you enter a value of 10, the system will purge for approximately 6 minutes. <ul style="list-style-type: none"> ■ Wet Prime – Instructs a 2690/2695 or 2790/2795 Separations Module to prime the fluidic lines of the instrument with solvent. ■ Purge Det – Instructs the 2410 or 2414 RI Detector to purge the flow cell for the user-specified run time. Purge Det occurs at the initial conditions of the instrument method specified in the associated method set. ■ Refresh Syringe – Instructs the 2790/2795 Separations Module or the ACQUITY Sample Manager to refill its syringe with fresh, degassed purge solvent. This function uses the number of Purge Cycles (syringe strokes) and the Purge Solvent Volume values set in the instrument method specified in the associated method set. ■ Wash Needle – Instructs the 2790/2795 Separations Module or the ACQUITY Sample Manager to wash the inject port and the outside and inside of the needle using wash solvent, then replace the wash solvent with degassed purge solvent. This function uses the Frequency (for example, Every Injection), number of Wash Cycles, Inject Port Wash Time, and Needle Wash Time values set in the instrument method specified in the associated method set. ■ Sys Prep – Instructs the 2790/2795 Separations Module or ACQUITY UPLC Sample Manager to perform system preparation during startup, including priming of the fluidic lines with solvent, refreshing the syringe, and washing the needle. Select a method set in Method Set/Report Method. In the Auto Additions column, enter a value of 1 if you do not want a solvent changeover, or enter 2 to specify a solvent changeover. <p>Use these functions to control processing and reporting of dissolution test results:</p> <ul style="list-style-type: none"> ● Dissolution Wait - Delays injection of samples or standards until the specified Dissolution Wait time (shown as Run Time in the Samples table) has elapsed. With the 2690D/2695D Separations Module, the Dissolution Wait function allows you to schedule standards or nondissolution injections just before the time of a dissolution sample transfer. <p>For example, suppose you have scheduled dissolution sample transfers at 6 hours and 9 hours and you want to run standards at 8 hours 45 minutes. If you place the Inject Standards line between the two Inject Samples lines without specifying a Dissolution Wait time, the Inject Standards function is carried out immediately after the sample transfers at 6 hours are complete. However, by inserting a Dissolution Wait time of 525 (8 hours 45 minutes), the standards are injected 15 minutes before the sample transfer at 9 hours.</p> |

| Column | Description |
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| | <p>Tip:Without a 2690D/2695D Separations Module, you can insert a Dissolution Wait function before injection of each group of samples at each transfer time. Then you can transfer the samples manually or by using a third-party dissolution apparatus just before the next set of injections is scheduled to occur.</p> <ul style="list-style-type: none"> • Compute Dissolution - Calculates the Amount Dissolved and % Dissolved for each peak specified in the Components page of the New Sample Set Method wizard (or in the Components tab of the Dissolution dialog box). The Compute Dissolution function uses the sample set method parameters Media Volume, Removed Volume, Replaced Volume, Component Names, and Claimed Amounts. In addition, the Compute Dissolution function uses the Bath, Vessel, and Transfer Times from the Transfer Times table in the Samples tab of the Dissolution dialog box. Peak amounts are calculated using normal LC processing; amount units must be consistent. <p>The Compute Dissolution algorithm:</p> <ul style="list-style-type: none"> • Calculates the amount and percent dissolved for the sample peaks you specified in the Components page of the New Sample Set Method wizard (or in the Components tab of the Dissolution dialog box) • Sequences the results for all samples (not standards) in the dissolution sample set by bath, vessel, and transfer time, in the order in which the samples were transferred . <p>Tip:The Compute Dissolution function is automatically inserted in the dissolution sample set method. This function occurs after results from one or both dissolution baths are quantitated but before a report is generated.</p> |
| Label Reference | <p>A Label Reference entry in a row of the Samples table instructs Empower software to perform the Calibrate, Quantitate, or Report function specified in that row on all previous rows containing a matching label entry in the Label column. This feature is useful when you are performing bracketing. When you enter a label in the Label Reference column, you can include wildcards (* or ?) to represent characters in the Label column as follows:</p> <ul style="list-style-type: none"> • The asterisk (*) represents one or more characters (for example, Std* specifies all labels starting with Std, including StdA, StdAB, and StdABC) • The question mark (?) represents a single character (for example, Std? specifies all labels containing Std plus one more character, including StdA, StdB, and StdC). |
| Processing | <p>Use this column to control processing and system suitability actions for rows in the Samples table by overriding the Run mode and Interactive System Suitability selections in Run Samples. The processing and system suitability options in this column are:</p> |

| Column | Description |
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| | <ul style="list-style-type: none"> ■ Don't Process or Report – Do not process, report, or print data. Used with sample set bracketing to eliminate creating multiple method sets and generating multiple results or results quantitated on the wrong calibration curve. ■ Don't Report – Process data, but do not print a report. ■ Normal – Apply the global Run mode (as selected in your method set and in the Run Mode drop-down list box) to the row. ■ Ignore Faults – Continue injections even if a fault condition is detected. This selection overrides Stop on Fault or Reinject on Fault (selected in the Interactive System Suitability list). ■ No Sys Suit – Disables System Suitability testing parameters (of the System Suitability software option) for the processing method. This selection does <i>not</i> override the selection in the Interactive System Suitability list. For example, if you select Stop on Fault in the list and specify a "must peak" in the processing method, acquisition automatically stops when the "must peak" is not found. <p>Tip: If you set the global Run mode to Run Only (in your method set and in the Run Mode list), no processing occurs, regardless of the Processing column setting.</p> |
| <p>Method Set/Report Method</p> | <p>Use this column to specify the following methods:</p> <ul style="list-style-type: none"> ● Method set to use with the associated function. ● Report method to use with the associated Report function. <p>Tips:</p> <ul style="list-style-type: none"> ● For acquisition, the method set used must contain an instrument method. ● For processing, reporting and/or exporting, the method set must also contain a processing method, report method and/or export method. ● When you specify an acquisition, control, or processing function, clicking the Method Set/Report Method column lists the method sets that are defined for the specific acquisition system. ● When you specify a Report function, clicking the Method Set/Report Method column lists available report methods. |
| <p>Run Time <i>or</i> Dissolution Wait Time (minutes)</p> | <p>Use this column to specify the length of time in minutes to collect data for a sample or to perform a function, such as Purge Detector or Condition Column, or for the Dissolution Wait function.</p> <p>Use this column in the Samples table to specify the amount of time to wait before transferring and injecting dissolution samples (Dissolution Wait) and to calculate dissolution results (Compute Dissolution).</p> <p>If the Run Time column displays the Dissolution Wait time it represents</p> |

| Column | Description |
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| | the total duration of the dissolution test (dissolution test duration + infinity test duration). |
| Data Start (minutes) | <p>Use this column to specify the time that data collection is to begin, as measured from injection time. Data Start allows you to delay start of data acquisition to control the size of the data file. Data Start is also useful for eliminating eluent fronts from the data file.</p> <p>Tip: If your laboratory is regulated, verify that the regulatory agency allows use of the Data Start parameter.</p> |
| Next Inj Delay (minutes) | Use this column to add a delay between the end of data acquisition for an injection and the start of setup for the next injection. The instrument method continues to run for the duration of the Next Inj Delay but data is not acquired. |
| SampleWeight | <p>Use this column to specify the sample weight factor by which the software (during calibration) <i>multiplies</i> the calculated amount or concentration of each standard component.</p> <p>During quantitation, Empower software divides the X value read from the calibration curve (of the standard components) by the Sample Weight value to calculate amounts and concentrations for each unknown sample.</p> <p>Tip: SampleWeight is a default custom field. You can rename it or change its width in your project's properties in Configuration Manager. However, Waters recommends that you not delete or make any additional changes to this custom field.</p> |
| Dilution | <p>Use this column to specify the dilution factor by which the software (during calibration) <i>divides</i> the calculated amount or concentration of each standard component.</p> <p>During quantitation, Empower software multiplies the X value read from the calibration curve (of the standard components) by the Dilution value to calculate amounts and concentrations for each unknown sample.</p> <p>Tip: Dilution is a default custom field. You can rename it or change its width in your project's properties in Configuration Manager. However, Waters recommends that you not delete or make any additional changes to this custom field.</p> |
| Target Mass (Da) 1-5 | <p>Use the target-mass columns to specify as many as five target masses. If the processing method includes the MS Expected Mass processing function, when you process your data, the Peaks table includes information about whether the target masses are present.</p> <p>The target masses that you specify in the sample table supersede the base mass that you specify in the processing method. Rather than reporting the base mass, for each target mass in the Samples tab the software reports any adducts that you specify in the processing method MS Expected Mass parameters.</p> |
| Peak ratio reference | Select the check box to use the sample's peak ratio as a reference value. If the processing method includes peak ratio (MS ion ratio) processing, the peak ratio of each sample must be within the tolerance, which you specify in the method, of the reference value. If you select more than one |

| Column | Description |
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| | <p>peak ratio reference in a sample set, the software processes the samples in the order specified in the sample set and applies a running average of the reference values.</p> |
| Level | <p>Use this column to identify all standards in the sample set that are to have their amounts averaged together. All vials identified with the same level label are averaged together to create a single data point in the calibration curve if the Average by Level parameter is specified in your processing method.</p> <p>The Level label of a vial appears in parentheses next to the Vial number in the Component Editor. You can enter custom values or select a Level label from a list of any labels already used in the sample set method by clicking the Level column.</p> |
| Column Position | <p>Use this column to specify the column flow direction through an optional Column Selection Valve in a 2790/2795, 2690D/2695D Separations Module, or ACQUITY Column Manager. This column is accessible only if the optional valve is installed, and only for rows where a Condition Column or Equilibrate function is selected. The available choices for this field depend on the type of installed Column Selection Valve: Three-Column, Six-Column, Column Regenerative Valve, or ACQUITY Column Manager.</p> <p>For GPC/V-LS, AutoFill lists No Change, Positions 1 through 6, and Toggle.</p> <p>Tip: By selecting No Change (the default), you automatically use the Column Position value previously set in the instrument method (specified in the Method Set/Report Method column for the current row). If you choose a value other than No Change, the Column Position set in the sample set method line overrides the setting in the instrument method so you can equilibrate and condition your column in your sample set method without creating several specific instrument methods to do so.</p> |
| Auto Additions | <p>Use this column to perform the Auto Additions function with the 2690/2695, 2690D/2695D, and 2790/2795 Separations Modules. Auto Additions makes an injection that is composed of sample from up to ten vials, one of which is the sample vial.</p> <p>The total volume of this injection must be less than the sample loop volume. You can specify a delay time to allow the sample to mix once the sample from all vials is in the sample loop.</p> <p>The Auto Additions column is also used to enter the:</p> <ul style="list-style-type: none"> ■ Flow rate when a Wet Prime is specified (2690/2695 or 2790/2795 Module). Allowed values are 0.01 to 10.0 mL/min. Default: None ■ Solvent change parameter when a Sys Prep is specified (2790/2795 Module only). Enter 1 for no solvent changeover, or 2 to specify a solvent changeover. <p>Tip: You can edit the Auto Additions column by right-clicking, and then clicking Edit Auto Additions.</p> |
| Bath (Dissolution) | <p>Use this column to specify the bath (A or B) in the dissolution system from which to make an injection. In a dissolution sample set method, the</p> |

| Column | Description |
|----------------------------------|---|
| | <p>Bath column is not editable in the Samples table unless you specify a Dissolution Wait function.</p> <p>Tip: You can edit the Bath column in Alter Samples and/or Sample Set Method Editor only if your sample set method does <i>not</i> specify a 2690D/2695D Alliance Dissolution System.</p> |
| Vessel (Dissolution) | <p>This column specifies the vessel in the dissolution bath from which a sample is to be transferred. The Vessel column is not editable in the Samples table. Specify this information in the Bath A or B Setup page of the New Sample Set Method wizard or in the Bath A or B Setup tab of the Dissolution dialog box.</p> <p>Tip: You can edit the Vessel column in Alter Samples and/or Sample Set Method Editor only if your sample set method does <i>not</i> specify a 2690D/2695D Alliance Dissolution System.</p> |
| Transfer Time (Dissolution) | <p>This column indicates the time to transfer (or draw) a dissolution sample from the bath to the autosampler for injection. Transfer Time is not editable in the Samples table. Specify this information in the Bath A or B Transfer page of the New Sample Set Method wizard or in the Bath A or B Transfer tab of the Dissolution dialog box.</p> <p>Tip: You can edit the Transfer Time column in Alter Samples and/or Sample Set Method Editor only if your sample set method does <i>not</i> specify a 2690D/2695D Alliance Dissolution System.</p> |
| RI Sensitivity (GPC/V-LS option) | <p>Use this column to specify the relative RI sensitivity of a sample (based on the ratio of the detector sensitivity value set at instrument calibration to the detector sensitivity value set in the instrument method). This factor is required to accurately calculate dn/dc or concentration from dn/dc.</p> <p>Tip: The default value for data precision in Empower 2 (build 2154) and Empower 3 is 4. The default value for this field in Empower (build 1154) was 0. To change the data precision value, right-click the RI Sensitivity column header, and then click Column Properties.</p> <p>Example: Suppose a 2410 RI Detector is calibrated at a sensitivity setting of 4. If a row in the Samples table specifies an instrument method with the 2410 sensitivity set to 16, enter 0.25 in the RI Sensitivity column of the Samples table. If a row in the Samples table specifies an instrument method with the 2410 sensitivity set to 1, enter 4 in the RI Sensitivity column of the Samples table.</p> <p>Tip: Using AutoFill, you can insert a value for the RI Sensitivity, and also set an increment value. Right-click the RI Sensitivity cell, and then click AutoFill.</p> |

Rule: In a Dissolution Samples table, you cannot edit the Vial number, Auto Additions, Bath, Vessel, and Transfer Time fields, nor can you move or delete a dissolution sample row (an Inject Sample row with a Vessel number and Transfer Time). However, you can copy, cut, and/or paste non-dissolution rows into a dissolution method. To modify dissolution parameters, click Edit > Dissolution.

Restriction: If you use default data or data from a sample set method that was not created using the template, you cannot modify the dissolution parameters.

Applying table preferences in sample tables

Use table preferences to select the columns that you want to appear in the sample tables for editing sample set methods and altering samples. Those sample tables appear in the Sample Set Method editor, Alter Sample window, and on the Samples and Running tabs in Run Samples.

Empower provides default table preferences, and you can create your own as well. The same list of table preferences applies to all of the sample tables. All users for a project can access the table preference list to temporarily adjust table preferences.

Tip: For Method Validation projects, the default table preference for each validation test displays only the fields required for that validation test.

Any keyboard or calculated custom sample fields in the sample table are present when you apply a saved table preference. You can then save the table preference with the same name or a different name if you do not want these field(s) to be visible using the table preference. To save named table preferences, you must have the Save Named Table Preferences privilege.

Tip: When you create a new project, you can copy the table preferences from an existing project by selecting to copy the preferences in the New Project wizard.

To apply a table preference to a sample table:

1. Access a sample table in one of the following ways:
 - Using the QuickStart interface:
 - From the Run Samples tab, click Sample Queue > Samples tab
 - From the Run Samples tab, click Sample Queue > Running tab
 - From the Browse Project tab, click Tools > Alter Sample or Database > Import Data (to edit sample information with imported data)
 - Using the Pro interface:
 - From the Run Samples window, click the Samples tab
 - From the Run Samples window, click the Running tab
 - From the Project window, click Tools > Alter Samples or File > Open > Sample Set Method
 - From the Validation Manager window, click Tools > Alter Sample or File > Open > Sample Set Method or File > New Sample Set
2. From the Apply Table Preferences toolbar, select the table preference you want to apply. If the Apply Table Preferences toolbar is not visible, click View > Toolbars > Apply Table Preferences.

Alternative: Click File > Apply Table Preferences, select the desired table preference, and then click Apply.

3. To save a table preference, select either File > Save Table Preferences or File > Save As Table Preferences.

Requirement: To save named table preferences, you must have the Save Named Table Preferences privilege.

Deleting table preferences

You can delete both user-created and default table preferences. When you delete a default table preference, Empower automatically restores it with the original default settings. You cannot delete the current table preference unless it is a default table preference.

Requirement: To delete named table preferences, you must have the Delete Named Table Preferences privilege.

To delete table preferences:

Click File > Delete Table Preferences, select the table preference to delete, and then click Delete.



- » Creating sample set method templates
- » Creating sample set methods for instruments with sample plates
- » Creating sample set methods from other sample set methods
- » Creating sample set methods to acquire data (using the wizard)