Samples and Batches

A batch is a collection of information about the samples that you want to analyze. Samples are usually grouped into sets to make it easier for you to submit them. Grouping your samples into a set also reduces the amount of data you must manually enter. A set can consist of a single sample or multiple samples. All of the sets in a batch use the same hardware profile; however, samples in a set can have different acquisition methods. Batches link together the following information:

- **Sample information such as name, ID, and comment**
- **Autosampler location (rack information)**
- **Acquisition methods**
- **Processing method or script (optional)**
- **Quantitation information (optional)**
- **Custom sample data (optional)**
- **Set information**

Topics in this section:

Working with Samples and Batches

A single sample or multiple samples make up a set. A batch consists of one or more sets. You can only create and submit a batch from a workstation that is connected to a mass spectrometer.

Topics in this section:

Setting Queue Options

You can set the queue conditions before you begin a batch or sample.

1. **Click Tools > Settings > Queue Options.**

   The Queue Options dialog appears.
2. **To change the default values for any of the queue options, click in the relevant area and type the new value.**
3. **Click OK.**

Creating a Batch

Note: The following procedure does not give specific details for all steps. For details of each step, click the links.

Before you begin, review and set the queue options, if required.

1. **On the Navigation bar, under Acquire, double-click Build Acquisition Batch.**

   The Batch Editor window appears.

2. **On the Sample tab, in the Set field, type the name of the set and then click Add Set.**
3. **Click Add Samples to add samples to the new set**

   The Add Sample dialog appears.

4. **In the Sample name section, in the Prefix field, type a name for the samples in this set.**
5. **To add incremental numbering to the end of the sample name, select the Sample number check box.**
6. **If you have selected the Sample number check box, in the Number of digits field, type the number of digits to include in the sample name. For example, if you type 3, the sample names would be samplename001, samplename002, samplename003.**
7. **In the Data file section, in the Prefix field, type a name for the data file that will store the sample information.**
8. **If you want the set name to be part of the data file name, select the Set name check box.**
9. **Select the Auto Increment check box to increment the data file names automatically.**

   Note: The data for each sample can be stored in the same or separate data file. The names of the data file will have numerical suffixes starting from 1.

10. **In the Sub Folder field, type a name for the sub folder.**

    The folder is stored in the Data folder for the current project. If you leave the sub folder field blank, the data file will be stored in the Data folder and a sub folder will not be created.

11. **In the New samples section, in the Number field, type the number of new samples that you want to add and then click OK.**

    The sample table fills with the sample names and data file names.

12. **In the Vial Position column, enter the location of the vials.**

    Tip: Fill Down and Auto Increment options are available in the right-click menu after you select a single column heading or several rows in a column.

13. **In the Acquisition group, select an acquisition method from the list.**
14. **If you want to select different masses for individual samples, select the Use as Template check box and then enter the mass ranges in the columns that appear.**
15. **If you want to select different methods for each sample, click the Use Multiple Methods check box, and then in the Acquisition Method column that appears, specify a method for each sample.**
16. **If required, in the Quantitation group, select a quantitation method or click Quick Quant to create a quantitation method.**
17. **If you want to run a script on the batch, click Select Script and then locate a script file.**
18. **(Optional) If you did not set the vial positions in the sample table, then on the Locations tab, select sample locations.**
19. **If required, on the Quantitation tab, select the quantitation information for the samples.**
20. **If required, on the Submit tab, reorder samples within the set.**
21. **To save the batch file, click File > Save.**
22. **To submit the batch to the queue, on the Submit tab, click Submit.**

    Note: The Submit button on the Submit tab is unavailable until you complete all mandatory fields. If any required batch information is missing, the Submit button is not available. Check the Submit Status box on the

Submit tab for any messages about the batch, including any missing information.

Adding Samples to a Batch

1. In the Batch Editor window, on the Sample tab, click Add Samples.

   The Add Sample dialog appears.
2. If required, in the Sample name group, type a Prefix for the samples.
3. If you want a sample number to be added to the sample name, select the Sample number check box and then in the Number of digits field, type the number of digits to include as the sample name. For example, if you type 3, the sample names will be samplename001, samplename002, and so on.
4. If required, in the Data file group, type a Prefix for the data file.
5. If you want the set name to be part of the data file name, select the Set name check box.
6. To acquire each sample to a different data file, select the Auto Increment check box.

   A number will be added to the end of the data file name and incremented with each sample added.
7. Type the number of samples you want to add, and then click OK.

Tip: To remove samples from the batch, click the row label on the left, and then click Del Samples.

Deleting Samples from a Batch

Samples are deleted from a batch on the Sample tab. If you do not want to submit a sample and do not want to delete it, you can submit selected samples only.

1. With a batch file open in the Batch Editor window, click the Sample tab.
2. Choose the set name you want to modify from the Set list.
3. Select the sample row(s) you want to remove.

Note: To select multiple rows, press and hold the Ctrl or Shift key as you select the rows.

4. Click Del Samples and then click OK to confirm deletion.

Changing the Sample Order in the Batch Editor

1. With a batch file open in the Batch Editor window, click the Submit tab.
2. Click the row number for the sample you want to reorder.
3. Using the row number, drag the row to the new location.
   A red line appears to show where the row will be inserted.

   The new sample order is saved when you switch to another tab.

Tip: If you want to update the sample order on the Sample tab to match the order on the Submit tab, when you submit the set, select the Apply New Sample Order check box.

Resubmitting a Batch

1. Open the batch file you want to resubmit in the Batch Editor window.
2. Make any changes as required to the batch.
3. If you do not want to append acquired samples to the existing file, change the location or name of the data file on the Sample tab.
4. On the Submit tab, click Submit.

(Optional) Selecting Different Masses for Individual Samples

You can select different masses for individual samples in the same batch. For example, you may want to change the mass range of a sample, change the first precursor mass for a Product Ion scan, or change the second precursor ion for an MS/MS/MS scan.

1. In the Batch Editor window, on the Sample tab, select the Use As Template check box.

   Additional columns appear in the Sample table.

2. For each sample in the Sample table, select the mass ranges or precursor mass.

(Optional) Selecting Sample Locations

On the Locations tab, you can indicate the position of the rack on the autosampler and the position of the samples on the rack.

Tip: To clear all the selected wells or vials in a rack, click .

1. In the Batch Editor window, on the Locations tab, choose an autosampler from the Autosampler list.

   The appropriate number of racks appears.

2. On the rack where you want to specify the samples, right-click, and then click a rack type.
3. To view the wells or vials for the rack type, click the rack and then click the Autosampler/Plate View button.
4. To indicate whether samples are marked by row or column, click the Row/Column Selection button. If the button shows a red horizontal line, the Batch Editor marks the samples by row. If the button shows a red vertical line, the Batch Editor marks the samples by column.
5. For each set in the batch, do the following:
   a. In the Set list, select a set.
   b. Click the sample wells or vials in the order that you want them to be analyzed. Click a selected well or vial to clear it.

Tip: To select more than one well or vial at a time, hold down the Shift key and click the first and last well or vial. The Batch Editor marks every well or vial in between.

(Optional) Selecting Quantitation Information for a Sample

1. On the Quantitation tab, select the set containing the sample.
2. In the appropriate column, select the following information for each sample:
   - Quant Type
   - Dilution Factor
   - Weight/Volume
   - If applicable, Analyte
   - If applicable, Internal Standard

Note: The appropriate Internal Standard and Standard columns appear in the Quantitation tab according to the current quantitation method.

(Optional) Submitting Part of a Batch (a sample or a set of samples)

1. With a batch file open in the Batch Editor window, click the Submit tab.
2. Select the sample rows you want to submit.

   Tip: To select multiple rows, press and hold the Ctrl key or Shift key as you select the rows.

3. Click Submit.
4. In the Acquisition dialog, click Selected samples and then click OK.

   The Submit Status column shows the status of each sample.

Selecting Quantitation Information

Use the Quantitation tab to identify the sample type and concentration information. You can select quantitation information for a batch, a set, or even a single sample.

The fields available in the Quantitation table depend on the internal standard and analyte columns in the selected quantitation method. Use the following procedures to select quantitation information for a set and a sample:

Selecting Quantitation Information for a Set

(Optional) Selecting Quantitation Information for a Sample

Selecting Quantitation Information for a Set

Use the Quantitation tab to identify the sample type and concentration information. You can select quantitation information for a batch, a set, or even a single sample.

The fields available in the Quantitation table depend on the internal standard and analyte columns in the selected quantitation method.

1. **With a batch file open in the Batch Editor window, click the Sample tab.**
2. **In the Set list, select the set you want to modify.**
3. **To create a quantitation method, click Quick Quant or to edit a quantitation method, in the Quantitation list, click a method, and then click Quick Quant.**

Creating and Using Batch Templates

You can create batch templates for use with the Batch Editor.

Topics in this section:

Creating a Batch Editor Template

Creating a Batch from a Template

Creating a Batch Editor Template

1. **Create a batch with the details you want to save in a template.**
2. **On the Sample tab, right-click and then click Save As a Template.**

   The file is saved to the Batch\Template folder of the current project.

Notes:

- **You can only save a batch template if all required data is entered. Required data includes a set, autosampler, and rack type.**
- **Only batches that have a single set can be saved as a template.**

Creating a Batch from a Template

1. **Click File > Open and then select an Acquisition Batch Template file, which has a .dat extension.**
2. **Add any additional details to the batch.**
3. **To save the batch file, click File > Save.**
4. **To submit the batch, on the Submit tab, click Submit.**

Working with Columns in the Batch Editor Table

You can show and hide columns in the tables on the Sample, Quantitation, and Submit tabs. You can add custom information to the table on the Sample tab.

Topics in this section:

Hiding or Showing a Column

Hiding or Showing a Column

1. In the Batch Editor window, right-click and then click Hide/Show Column.

   The Show Column dialog appears.
2. Select the table whose columns you want to show or hide.
3. In the Shown column, clear or select the check boxes to hide or show the columns.
4. Click OK.

Adding a Custom Column

1. On the Sample tab, in the Sample table, right-click and then click Add Custom Column.

   The Add Column dialog appears.
2. In the Column title field, type a title for the custom column.
3. In the Column type group, click the type of values for the column, and then click OK.

Deleting a Custom Column

1. On the Sample tab, in the Sample table, right-click and then click Delete Custom Column.

   The Delete Column dialog appears.
2. Click the name of the column, and then click OK.

Importing and Exporting Batch Files

You can export the information in the batch file for use with other applications such as Microsoft Excel, Microsoft Access, and LIMS. The file is exported as a tab-delimited text file and can then be edited in another application, such as Microsoft Excel. As long as it is formatted correctly, you can import the file back into the Analyst® software.

You can also create batch files in other applications and import them as long as they are formatted correctly.

Topics in this section:

Exporting a Batch File

1. Open a batch or create a new batch.
2. Click File > Export.

Importing a Batch File

1. Make sure that the batch file is formatted correctly.
2. In the Batch Editor window, click the Sample tab.
3. In the Sample table, right-click and then click Import From > File.
4. In the Files of type list, click the file type. Common file types include Microsoft Excel (*.xls), Microsoft Access (*.mdb), or comma-separated text (*.txt, *.csv).
5. Select the file to import, and then click Open.

Formatting Batch Files for Import

You can export batch files from the Analyst® software as tab-delimited text files, edit them in other applications, and then import them back into the Analyst software. You can also create batch files in other applications and import them into the Analyst software. To be imported, batch files must have ODBC drivers and must be formatted correctly. For examples of correctly formatted files, see the DABImport files in the Example/Batch folder in the Analyst Data folder.

To format a batch file for import

- **If the file is a text file, no changes in format are needed. The fields are preset to be delimited with tab characters. If you want to use another character, you must specify it using the % Delimiter= keyword.**
- **If you are editing the file in Microsoft Excel, the top-left cell, or cell A1, will contain the string "% header=SampleName". Change that string to "SampleName". Also, to make sure that the Analyst software recognizes the Excel file, rename it DABImport.xls or rename the default worksheet DABImport.**
- **If you are editing the file in Microsoft Access and have saved it as an Access database, rename the default table DABImport.**

Importing Worklists from SQL*LIMS

You can create batch files using Worklists that have been imported from SQL*LIMS. These lists have been previously created within the SQL*LIMS program, and have unique identifiers.

Note: You must have both the Analyst® software and SQL*LIMS program installed on the same system to import data.

To import a Worklist into the Batch Editor

1. **In the Batch Editor window, on the Sample tab, right-click, point to Import From, and then click SQL *LIMS Worklist.**

   The SQL*LIMS Login dialog appears.

2. **Enter a user name and password and in the Oracle host string box, type the SQL*LIMS instance, and then click OK.**

   The Sequence Worklist dialog appears.

3. **Select one of the worklists.**
4. **Select a LIMS operation. The LIMS operations listed are those currently available within the SQL*LIMS program. Each operation corresponds to a different worklist.**
5. **Select a Method from the list. The methods listed are the acquisition methods currently available within the selected Analyst software project.**
6. **In the Base file name box, type an identifier for the data files. If you leave this box blank, the default file name is Data.**
7. **Click OK.**

   A batch is created within the Batch Editor which corresponds to the imported Worklist. Two new columns appear in the Sample table: LIMS TaskID and LIMS SampleID.

Importing TaskIDs from SQL*LIMS

You can create batch files using TaskIDS that have been imported from SQL*LIMS. These lists have been previously created within the SQL*LIMS program, and have unique identifiers.

Note: You must have both the Analyst® software and SQL*LIMS program installed on the same system to import data.

To import a TaskID into the Batch Editor

1. **On the Sample tab, right-click, point to Import From, and then click SQL *LIMS TaskID.**

   The SQL*LIMS Login dialog appears.

2. **Enter a user name and password and in the Oracle host string box, type the SQL*LIMS instance, and then click OK.**

The LIMS ID dialog appears.

3. **Select an Operation from the list. The operations listed are those currently available within the SQL*LIMS program. Each operation corresponds to a different TaskID listing.**
4. **Select a TaskID from the list, and then click OK.**
5. **If the specified TaskID has replicates, the Task Replicates dialog appears. Type a Replicate number, or select Include all replicates which will expand the batch to include all replicates. Once the task replicate option is selected, click OK.**

   A batch is created within the Batch Editor which corresponds to the imported TaskID. Two new columns appear in the Sample table: LIMS TaskID, and LIMS SampleID.