

# Syngistix for ICP-MS

Software setup for LA-ICP-MS analysis

User's Guide



## Contact Information

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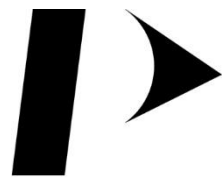
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## Getting Started

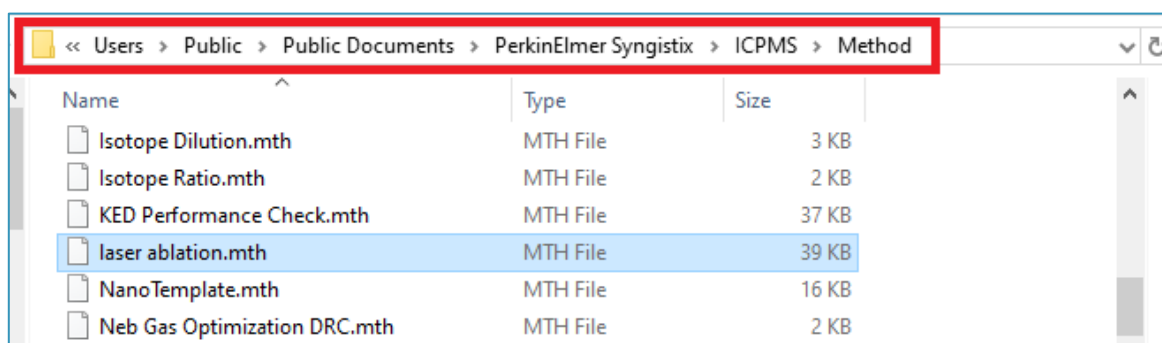
### Files Required During an Analysis

During a determination, a number of files must be open for data acquisition and processing to occur properly. These files include:

- An analytical **Method file**
- A **Sample file** containing the names of your samples and specific instructions for performing the determination
- A **Dataset** for storing the results from the determination

Included with this guide is a laser ablation method file that can be used as a template during method development. You can modify this template to suit your analysis requirements.

To use the method template, place the **laser ablation.mth** file in the **C:\Users\Public\Documents\PerkinElmer Syngistix\ICPMS\Method** folder as shown in the figure below:

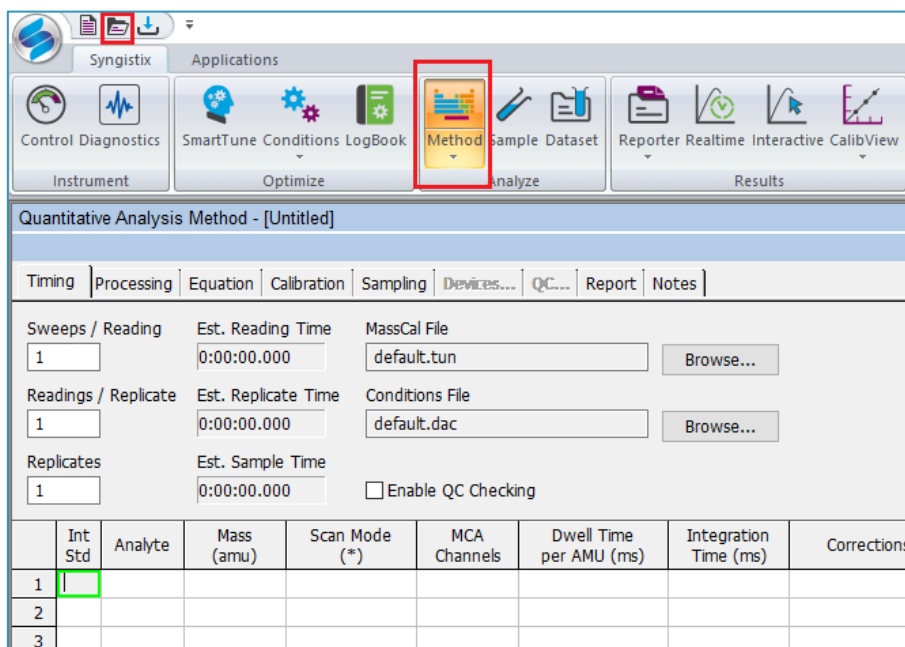


The laser ablation method template is a **Quantitative Analysis** method that includes the necessary attributes to perform data acquisition and data retrieval during LA-ICP-MS analysis. This template is provided to support consistent implementation of LA-ICP-MS methods across systems and operators.

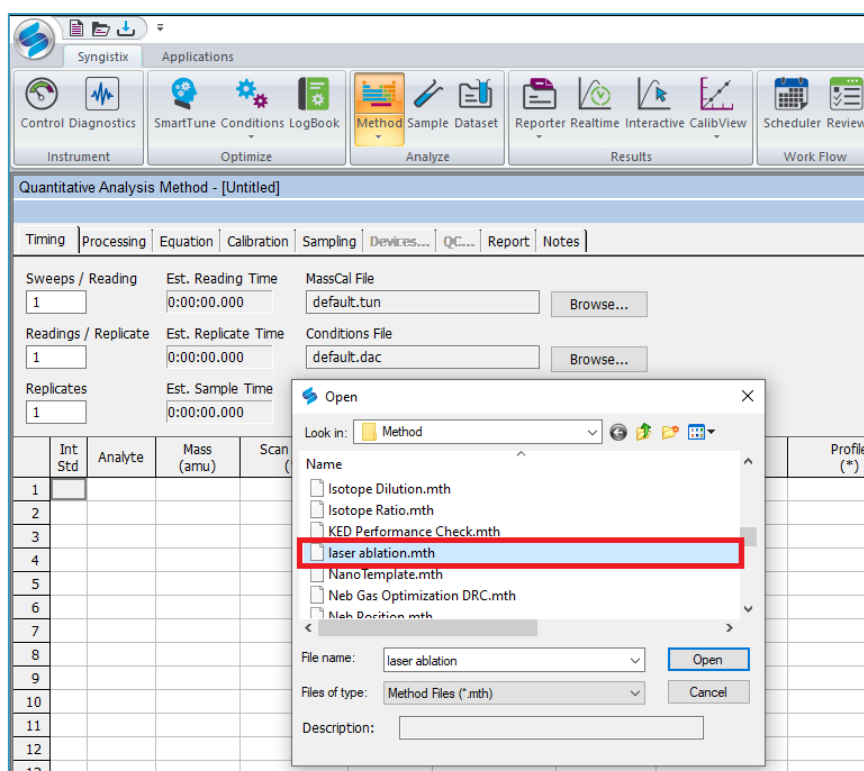
## Method Setup

Follow the steps below to set up a method for LA-ICP-MS analysis using the provided template. Alternatively, create a new **Quantitative Analysis** method and configure the method's settings as described below.

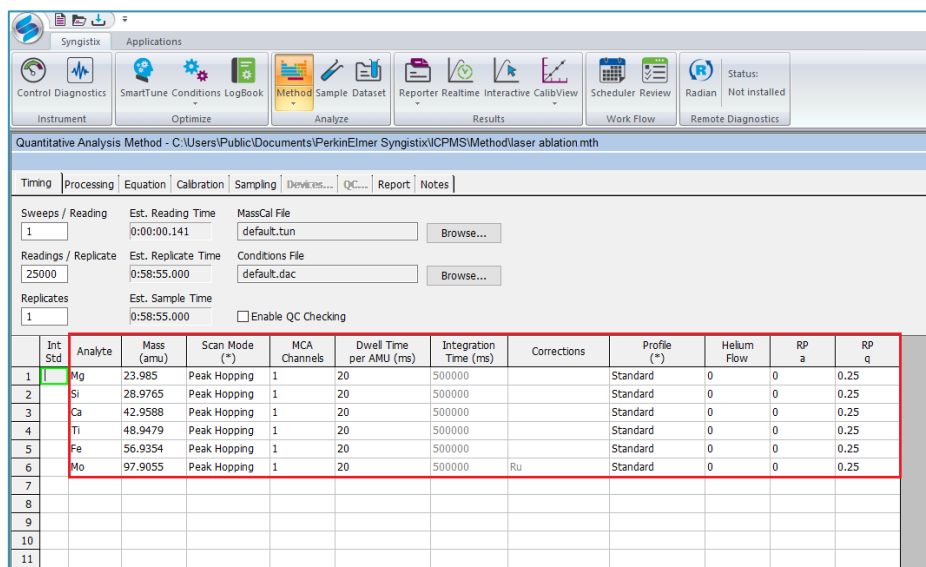
1. Go to the **Method** screen and then click on the *Open file* icon in the top left corner.



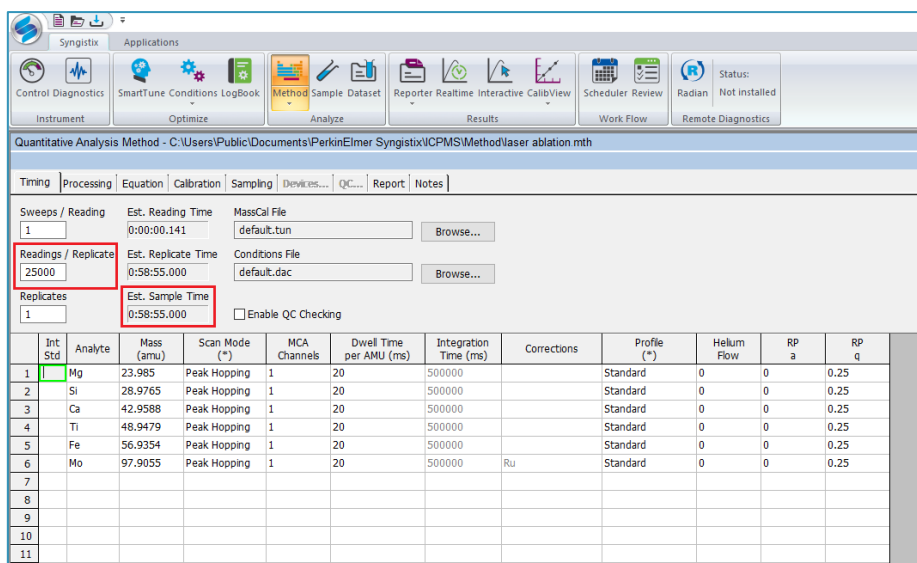
2. Browse to locate the **laser ablation.mth** file, and then click Open.



- On the Timing tab, use the Timing table to specify the isotopes you want to measure, as well as the specifics about the measurement timing conditions. See the Method Development section of the Software Reference Guide\* for detailed descriptions of all Timing table parameters.



- Adjust the number of Readings/Replicate to match the Est. Sample Time to your laser sampling time.



\* To view the Software Reference Guide

- On the **Syngistix ball menu**, click **Help > Software Reference Guide**. The *Software Reference Guide* opens in .PDF format in another window running Adobe Reader.
- The *Software Reference Guide* is a fully functional manual with a Table of Contents and detailed Index. It contains in-depth Information about the software, including software screen examples and detailed reference information. Once open, you can browse or search the guide as desired. You can also save a copy to your desktop or another location of your choosing for easy reference. In .PDF format, internal links and cross-references help you to navigate the document. However, if you prefer, the guide has also been formatted for easy printing on standard 8.5x11 letter size printer paper.

**NOTE: LASER SAMPLING**

Note that laser ablation sampling time typically includes a short (~10-15 s) gas background measurement before the main scan/spot ablation time. In the laser ablation software, set up the ablation sequence so that there is adequate time for the ICP-MS to complete data acquisition for each sample before the next sample ablation starts. This is usually done by adding a delay at the start of each laser sampling step, before the trigger is sent to the ICP-MS.

- On the Equation tab, check the entries on the Corrections column and make sure to remove any correction equation you don't wish to apply.

Quantitative Analysis Method - C:\Users\Public\Documents\PerkinElmer Syngistix\ICPMS\Method\laser ablation.mth

Timing | Processing | **Equation** | Calibration | Sampling | Devices... | QC... | Report | Notes

Isotope Information

Isotope	Mass	Abundance	Interferences
Mo 92	91.9063	14.840000	Zr, AsO
Mo 94	93.9047	9.250000	Zr
Mo 95	94.9058	15.920000	BrO
Mo 96	95.9046	16.680000	Ru, Zr, BrO
Mo 97	96.9058	9.550000	BrO
Mo 98	97.9055	9.130000	Ru, BrO

	Int Std	Analyte	Mass (amu)	Corrections	Potential Interferences
1		Mg	23.985		LiO, NaH, Ti++, Ti+, Ca++
2		Si	28.9765		SiH, CO, AlH, BO, N2
3		Ca	42.9588		CaH, MgO, CNO, AlO, BO2, Sr++, Sr+
4		Ti	48.9479		CaH, CCl, SO, PO, HSO
5		Fe	56.9354		CaO
6		Mo	97.9055	- 0.109613 * Ru 101	Ru, BrO
7					
8					
9					
10					
11					



## NOTE: INTERFERENCE CORRECTIONS IN LA-ICP-MS

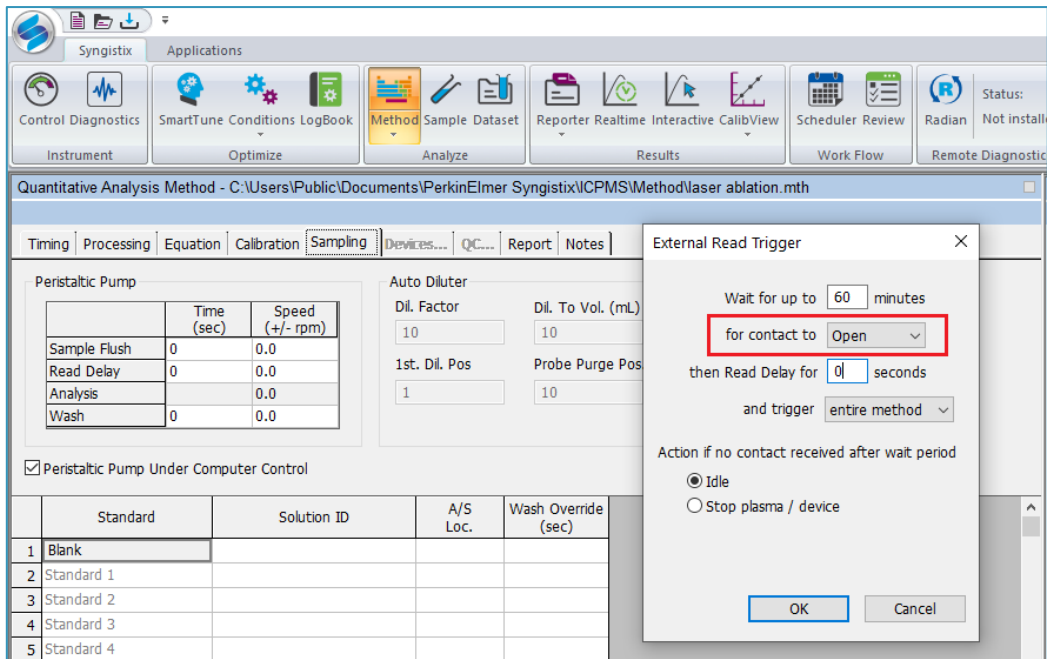
Typically in LA-ICP-MS analysis, interference corrections are applied during post-acquisition data processing using advanced LA-ICP-MS data reduction software. This requires that both, the analyte and the interfering mass proxy\*, are measured. If your LA-ICP-MS data processing software has the ability to apply (isobaric or polyatomic) interference corrections, make sure to remove any equations on the Method panel Equation tab and then add the isotope used to calculate the interference to your method (on the Timing tab).

6. On the Sampling tab, select the External option from the Sampling Device dropdown menu.

The screenshot shows the Syngistix software interface. The top menu bar includes Syngistix, Applications, and various tool icons. The main window title is "Quantitative Analysis Method - C:\Users\Public\Documents\PerkinElmer Syngistix\ICPMS\Method\laser ablation.mth[Modified]". The "Sampling" tab is active, showing a "Sampling Device" dropdown menu with "External" selected. Below the dropdown are fields for "Peristaltic Pump" (Time and Speed) and "Auto Diluter" (Dil. Factor, Dil. To Vol., 1st. Dil. Pos, Probe Purge Pos.). A table at the bottom lists standards:

	Standard	Solution ID	A/S Loc.	Wash Override (sec)
1	Blank			
2	Standard 1			
3	Standard 2			
4	Standard 3			
5	Standard 4			

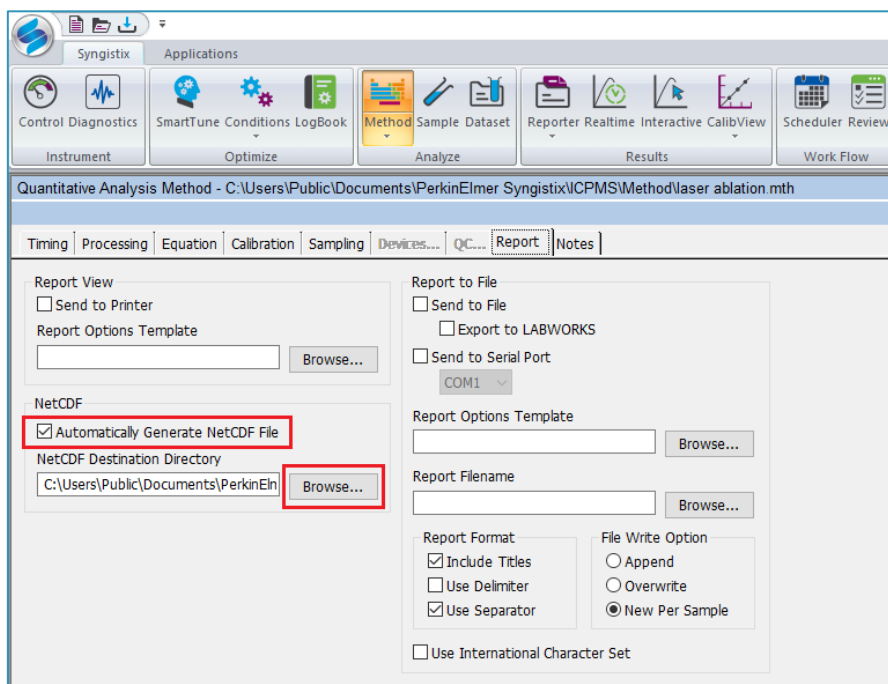
7. When you select **External**, the **External Read Trigger** dialog box appears. The external sampling device (i.e. your laser ablation system) must effect a contact closure or opening in conjunction with the ICP-MS instrument before it starts its measurements. Here you can select the type of external read trigger needed (Open or Close). Note that external devices also require a connector cable to communicate between the external sampling device and the instrument.



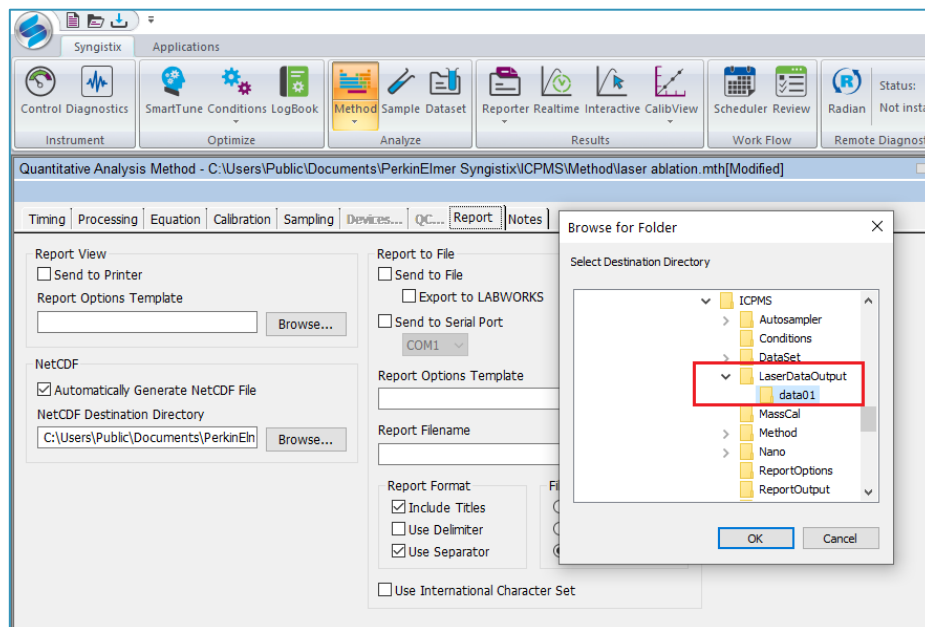
- Use the Report tab to export the LA-ICP-MS results as NetCDF files.

**NOTE:**

The NetCDF file format is supported by several commercially available LA-ICP-MS data processing software. Check with your LA-ICP-MS software provider for more information on supported file formats.



9. Use the **Browse...** button to select the destination directory for the results. The software automatically exports the data as a **NetCDF** file after each sample is run.

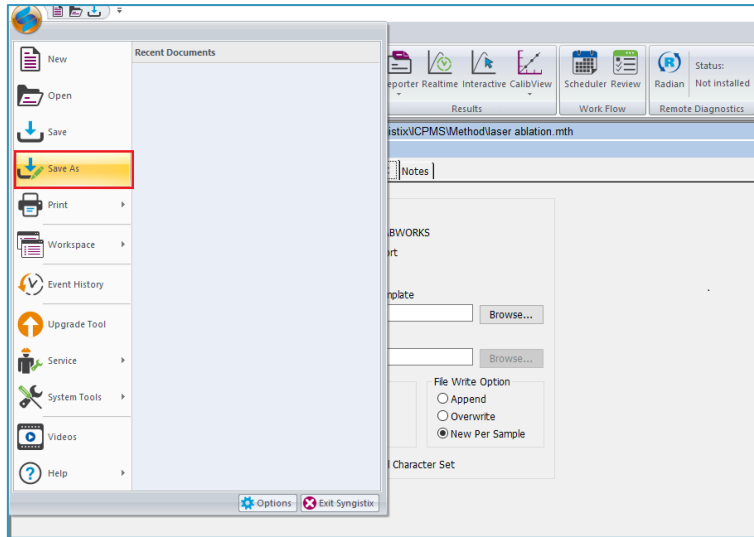


#### NOTE:

It is recommended to create a dedicated folder to store the files that are automatically exported after each analysis has been completed. In the example below, we have created a folder called **LaserDataOutput** and a subfolder called **data01**.

In the example above, all the files exported from an analytical run will be stored within **C:\Users\Public\Documents\PerkinElmer Syngistix\ICPMS\LaserDataOutput\data01**

10. On the Syngistix ball menu, select **Save As**. Enter a name for your method and then click **Save**.

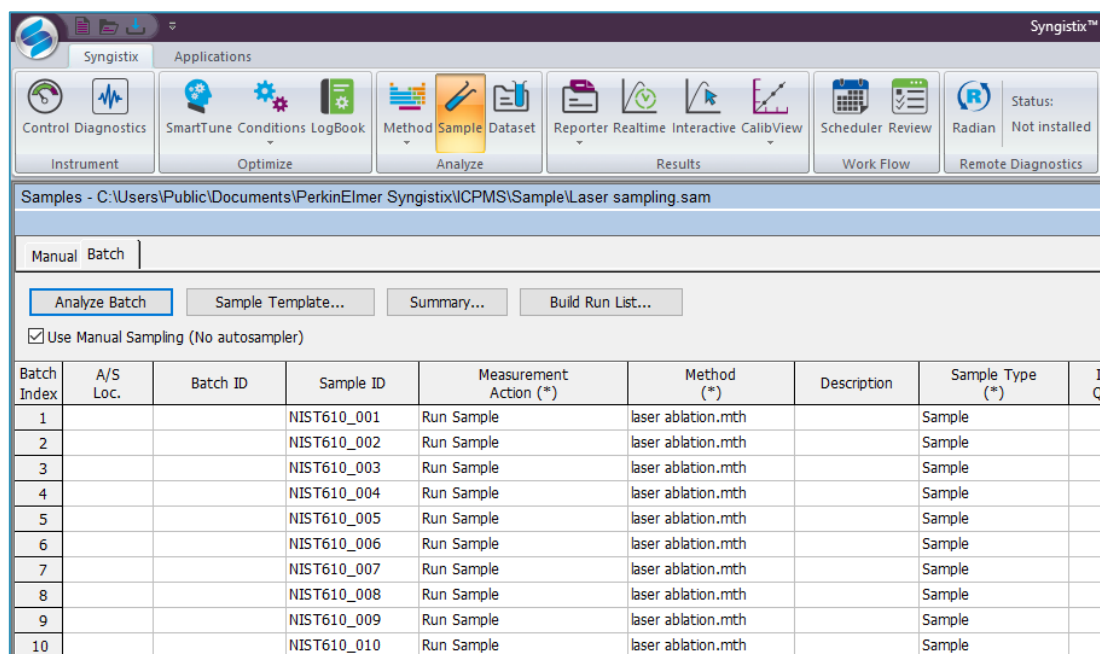


## Create a Sample File

Use the Sample panel to identify samples, control the order in which they are measured, and initiate the analysis.

### Sample Panel: Batch Tab

This tab is the primary measurement control interface on an instrument configured with a laser ablation system for sample introduction.



Batch Index	A/S Loc.	Batch ID	Sample ID	Measurement Action (*)	Method (*)	Description	Sample Type (*)	I Q
1			NIST610_001	Run Sample	laser ablation.mth		Sample	
2			NIST610_002	Run Sample	laser ablation.mth		Sample	
3			NIST610_003	Run Sample	laser ablation.mth		Sample	
4			NIST610_004	Run Sample	laser ablation.mth		Sample	
5			NIST610_005	Run Sample	laser ablation.mth		Sample	
6			NIST610_006	Run Sample	laser ablation.mth		Sample	
7			NIST610_007	Run Sample	laser ablation.mth		Sample	
8			NIST610_008	Run Sample	laser ablation.mth		Sample	
9			NIST610_009	Run Sample	laser ablation.mth		Sample	
10			NIST610_010	Run Sample	laser ablation.mth		Sample	

Follow the steps below to set up your analysis sequence:

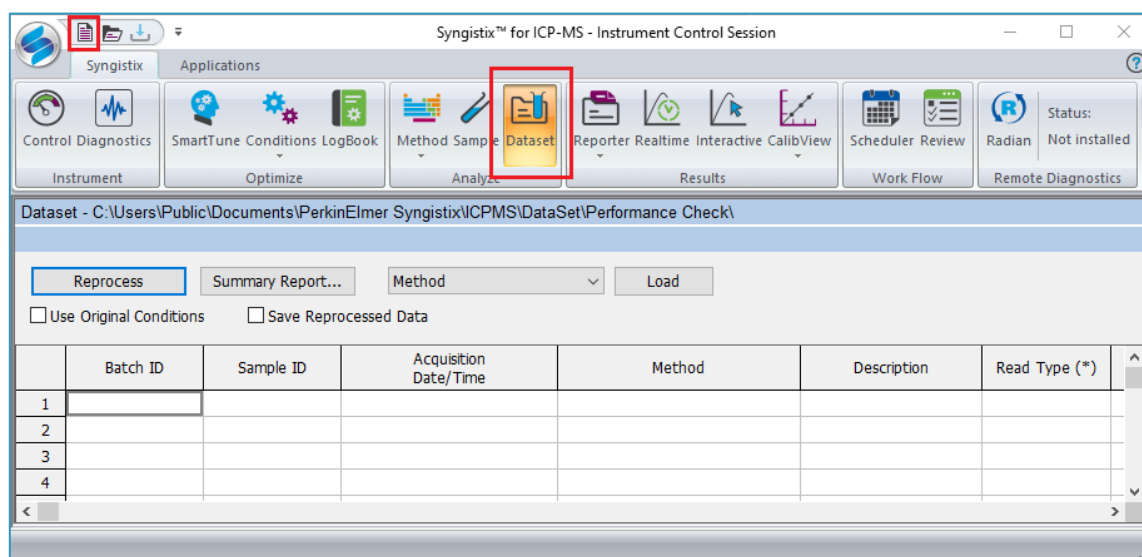
1. Select the User **Manual Sampling (No autosampler)** checkbox.
2. Enter a unique **Sample ID** for each laser ablation spot or traverse. You can also copy and paste the Sample ID information from a text or Excel file or use the **Sample Template...** window to automatically generate unique Sample IDs for you batch of samples.
3. In the **Measurement Action (\*)** field, right-click to prompt the options menu and choose **Run Sample**.
4. In the **Method (\*)** field, enter the name of your analysis method or right-click to browse for a method file.
5. Save your sample file.

## Create a Dataset

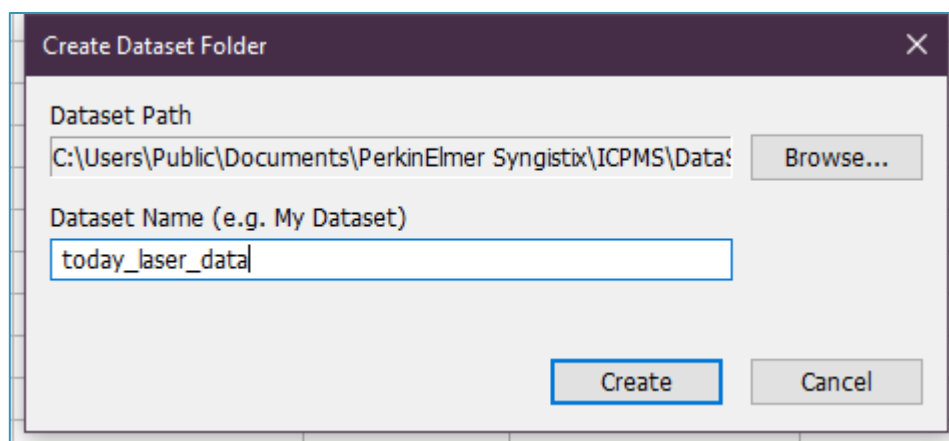
Syngistix stores the raw data acquired after each analysis within the current dataset. The data for each sample analysis is saved as an individual data file, with the complete series of measurements in the dataset constituting a folder on the hard disk of your computer.

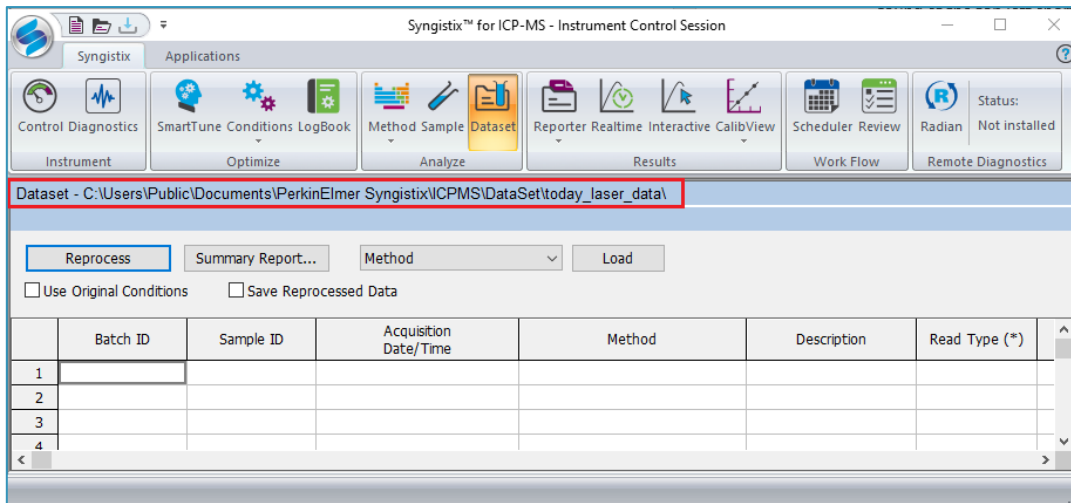
The software creates the individual file names using the Sample ID entered on the Sample panel. Each dataset file generated will be consistent with the method parameters; that is, the raw data readings acquired will match the analysis method parameters.

1. To create a new dataset, go to the **Dataset** panel and then click on the **Create a new file** icon found at the top left shortcut menu:



2. Enter a new dataset name and then click **Create**.





The **Dataset** panel displays the results of a determination; use it to review the samples run during a measurement, and to reprocess acquired data (see [Exporting Existent Data](#) for more details). Only the raw data files, which include some additional metadata to describe the properties of the raw data, are stored within a dataset.

**NOTE:**

Most advanced LA-ICP-MS data reduction software require data in NetCDF format for post-processing. These files are automatically exported after each sample analysis to the directory specified in your method. In the example above, all NetCDF files are stored within **C:\Users\Public\Documents\PerkinElmer Syngistix\ICPMS\LaserDataOutput\data01**

## Running an Analysis Batch

To start data acquisition:

1. Go to the **Sample Panel – Batch Tab**.
2. Click on **Batch Index** at the top left corner of the batch table to highlight all the samples in the batch.
3. Then select **Analyze Batch** to initiate the analysis sequence. Syngistix will wait for the external trigger coming from the laser ablation system to start data acquisition.

The screenshot displays the Syngistix™ for ICP-MS software interface. The top toolbar includes various application icons such as Control Diagnostics, SmartTune, Conditions, LogBook, Method, Sample, Dataset, Reporter, Realtime, Interactive, CalibView, Scheduler, Review, Radian, and Remote Diagnostics. The main window shows a 'Samples' panel with a 'Manual Batch' tab. Below the tab are buttons for 'Analyze Batch', 'Sample Template...', 'Summary...', and 'Build Run List...'. A checkbox labeled 'Use Manual Sampling (No autosampler)' is checked. The 'Batch Index' table is visible, with the first column highlighted in red. The table contains the following data:

Batch Index	Batch ID	Sample ID	Measurement Action (*)	Method (*)	Description	Sample Type (*)	Initial Sample Quantity (mg)	Sample Volume
1		NIST610_001	Run Sample	laser ablation.mth		Sample		
2		NIST610_002	Run Sample	laser ablation.mth		Sample		
3		NIST610_003	Run Sample	laser ablation.mth		Sample		
4		NIST610_004	Run Sample	laser ablation.mth		Sample		
5		NIST610_005	Run Sample	laser ablation.mth		Sample		
6		NIST610_006	Run Sample	laser ablation.mth		Sample		
7		NIST610_007	Run Sample	laser ablation.mth		Sample		
8		NIST610_008	Run Sample	laser ablation.mth		Sample		
9		NIST610_009	Run Sample	laser ablation.mth		Sample		
10		NIST610_010	Run Sample	laser ablation.mth		Sample		
11								



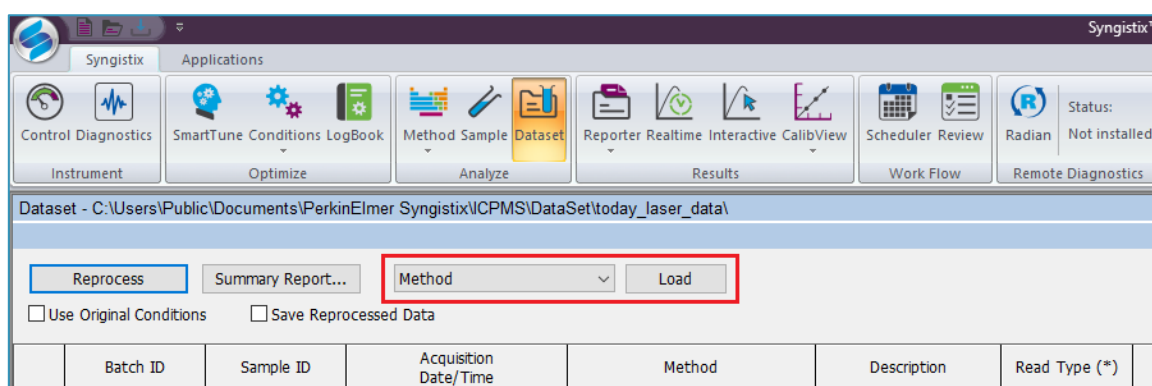
## Exporting Existent Data

You can use Syngistix to reprocess previously acquired analytical data, which can be useful in several circumstances. For example, if you find after a determination that the incorrect reporting options were selected in your method (**Method Panel – Report Tab**), you can reprocess the data using a modified method which includes the **Automatically Generate NetCDF File** option.

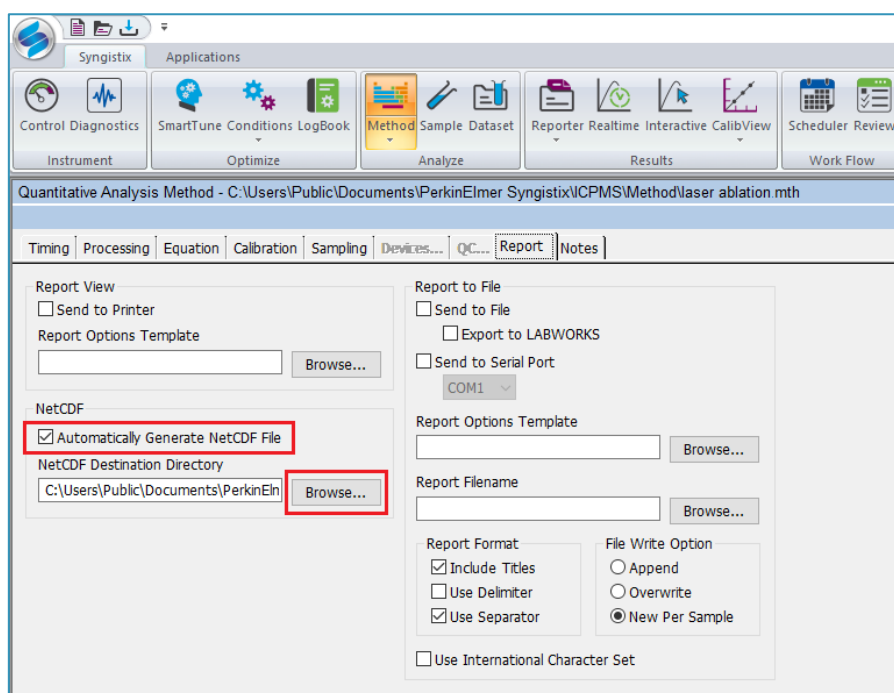
The reprocessing function uses the reporting instructions contained in the method used. Note that reprocessing does not alter the acquired data; you can view the original results at any time using the Dataset panel.

To export previously acquired data as NetCDF files:

1. Go to the **Dataset** panel and open the dataset you want to reprocess.
2. Select **Method** from the dropdown menu next to the Load button and then click **Load**.



3. Go to the **Method panel – Report tab** and select the **Automatically Generate NetCDF File** checkbox. Use the **Browse...** button to select the directory to store the NetCDF files.



4. Save the method.

5. Go to the **Dataset** panel and make sure that the “Use Original Conditions” checkbox is **NOT** selected.
6. Select the samples to reprocess and then click **Reprocess**.