Syngistix for ICP-MS

Software setup for LA-ICP-MS analysis

User's Guide

PerkinElmer®
For the Better

Contact Information

For technical and application support, contact your PerkinElmer local office or distributor.

In Australia:

PerkinElmer
Lvl 2, Bldg C, Tenancy A, 211 Wellington Road,
Mulgrave, VIC 3170
AUSTRALIA

Tel +61 1800 066776
Email ausales.aes@perkinelmer.com

Last updated 1/03/2023


PerkinElmer®
For the Better

Contents

Getting Started

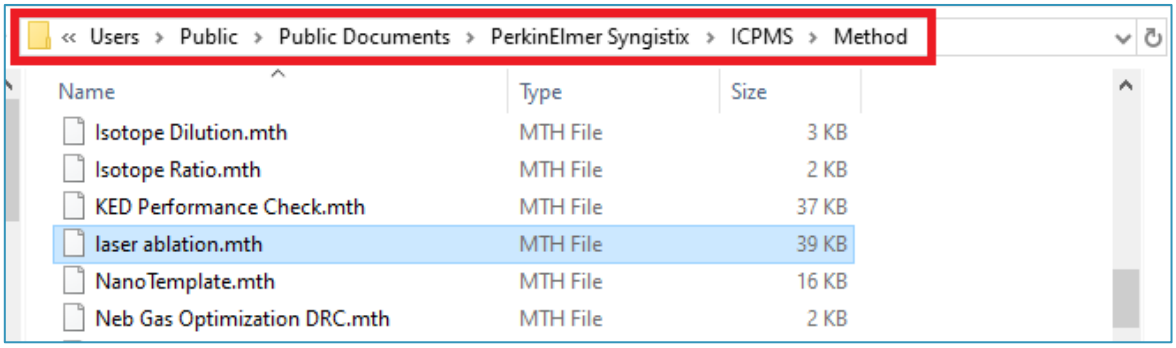
Files Required During an Analysis

During a determination, several 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
- A **Dataset** for storing the raw data from the analysis

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:



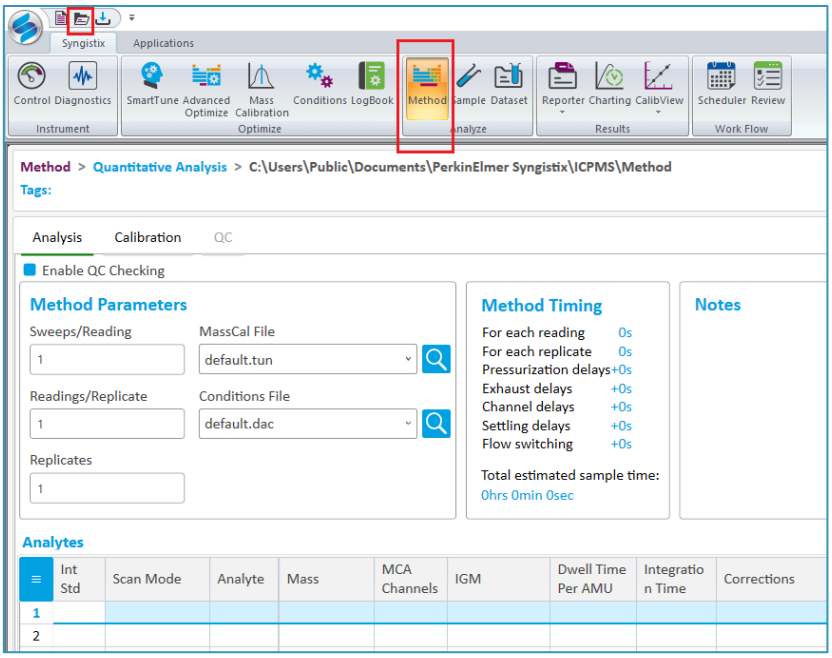
The laser ablation method template is a **Quantitative Analysis** method that includes the necessary attributes to perform data acquisition and data retrieval during LA-ICP-MS analysis. This template is provided to support consistent implementation of LA-ICP-MS methods across systems and operators.

Method Setup

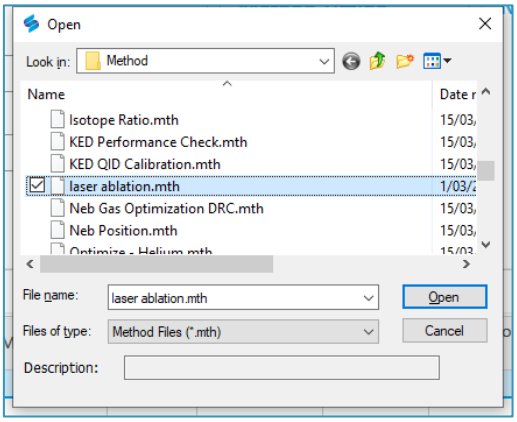
Follow the steps below to set up a method for LA-ICP-MS analysis using the provided template.

Alternatively, create a new **Quantitative Analysis** method and configure the method's settings as described below.

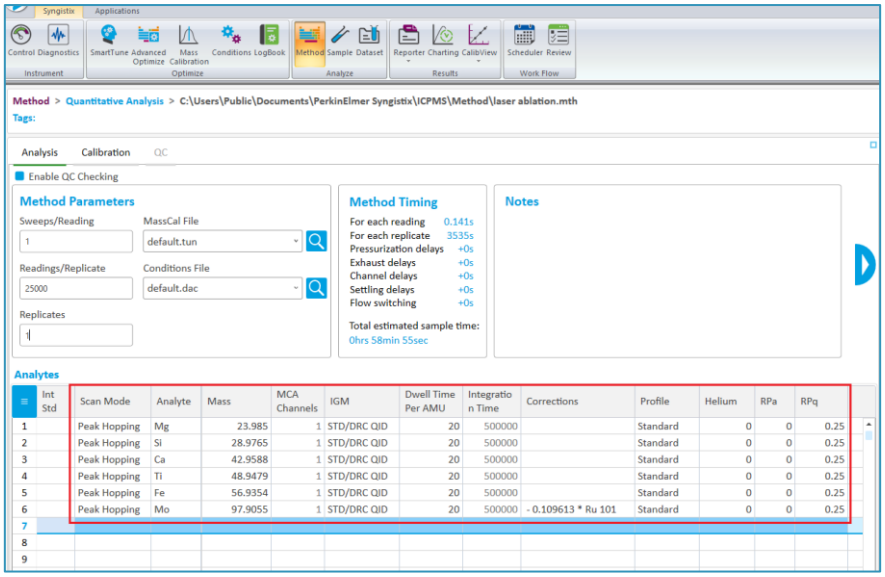
1. Go to the **Method** screen and then click on the *Open file* icon in the top left corner.



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

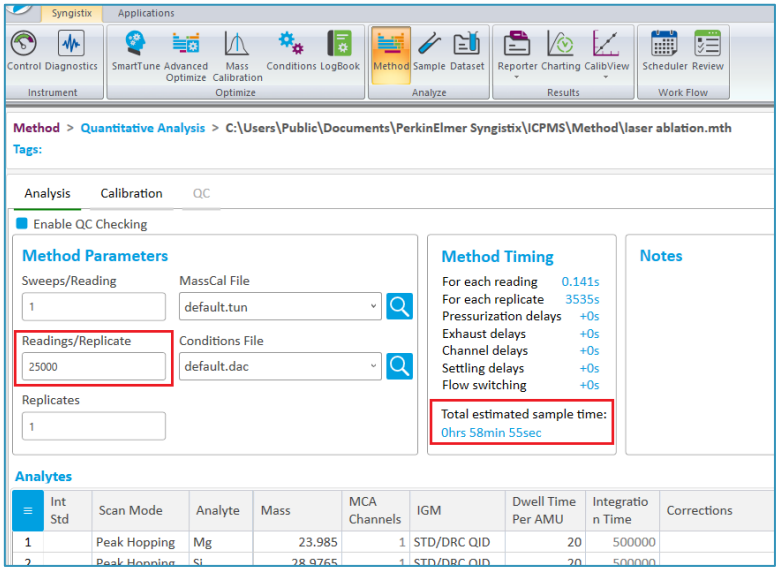


3. On the Method window, use the Analytes table to specify the isotopes you want to measure, as well as the specifics about the measurement timing conditions, such as Dwell Time for each isotope. See the Method Development section of the Software Reference Guide* for detailed descriptions of all Method parameters.



	Int Std	Scan Mode	Analyte	Mass	MCA Channels	IGM	Dwell Time Per AMU	Integration Time	Corrections	Profile	Helium	RPa	RPq
1		Peak Hopping	Mg	23.985	1	STD/DRC QID	20	500000		Standard	0	0	0.25
2		Peak Hopping	Si	28.9765	1	STD/DRC QID	20	500000		Standard	0	0	0.25
3		Peak Hopping	Ca	42.9588	1	STD/DRC QID	20	500000		Standard	0	0	0.25
4		Peak Hopping	Ti	48.9479	1	STD/DRC QID	20	500000		Standard	0	0	0.25
5		Peak Hopping	Fe	56.9354	1	STD/DRC QID	20	500000		Standard	0	0	0.25
6		Peak Hopping	Mo	97.9055	1	STD/DRC QID	20	500000	- 0.109613 * Ru 101	Standard	0	0	0.25
7													
8													
9													

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



	Int Std	Scan Mode	Analyte	Mass	MCA Channels	IGM	Dwell Time Per AMU	Integration Time	Corrections
1		Peak Hopping	Mg	23.985	1	STD/DRC QID	20	500000	
2		Peak Hopping	Si	28.9765	1	STD/DRC QID	20	500000	

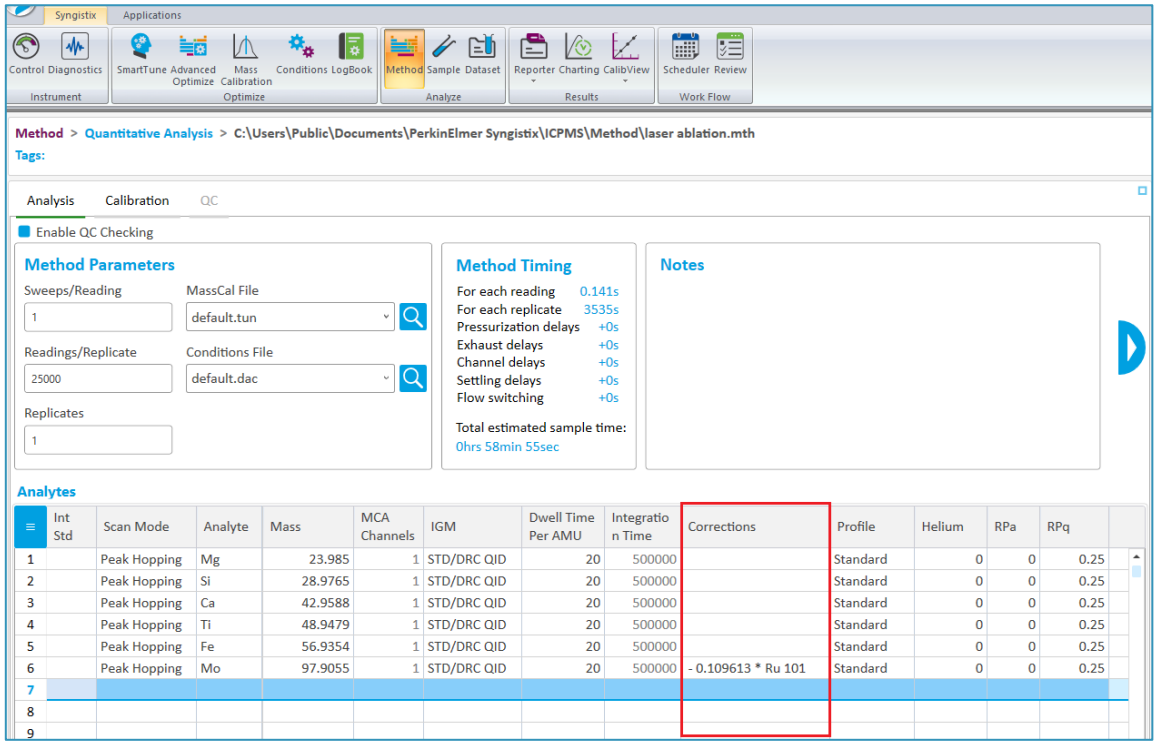
* To view the Software Reference Guide:

1. On the **Syngistix ball menu**, click **Help > Software Reference Guide**. The *Software Reference Guide* opens in another window.
2. 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.

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.

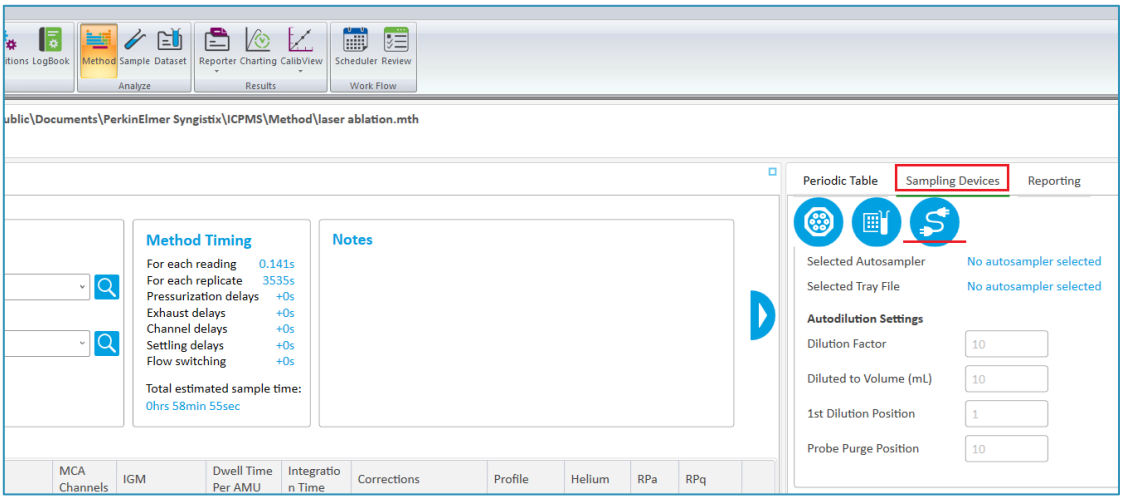
5. Check the entries on the Corrections column and make sure to remove any correction equation you don't wish to apply.



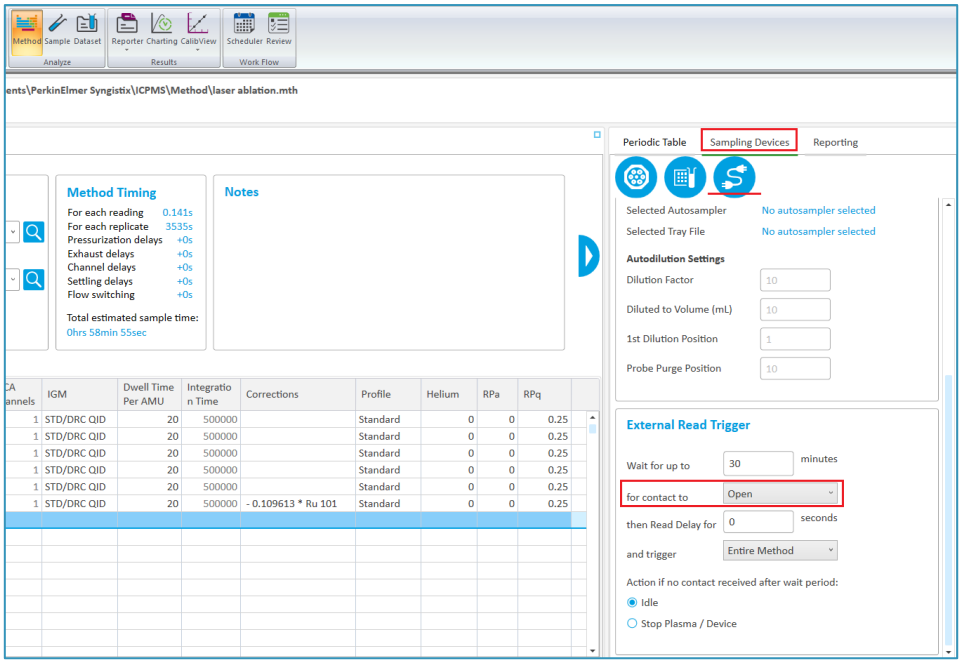
NOTE: INTERFERENCE CORRECTIONS IN LA-ICP-MS

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 the Analytes list in your method.

6. On the Sampling Devices tab, click on the External Trigger icon to activate the External Read Trigger pane.

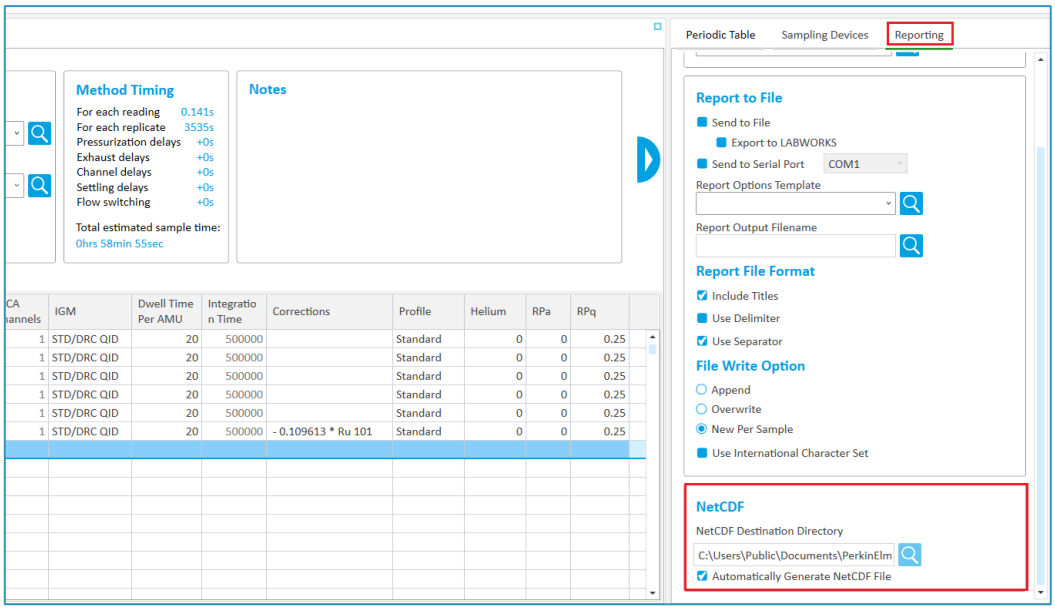


7. The **External Read Trigger** pane can be found at the bottom of the Sampling Devices panel. The external sampling device (i.e., your laser ablation system) must send a contact closure or opening signal to the NexION ICP-MS instrument before the ICP-MS starts measuring. Here you can select the type 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.

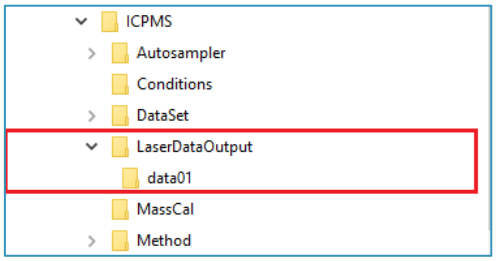


8. Use the Reporting tab to export the LA-ICP-MS results as NetCDF files. Select the **Automatically Generate NetCDF File** checkbox.

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



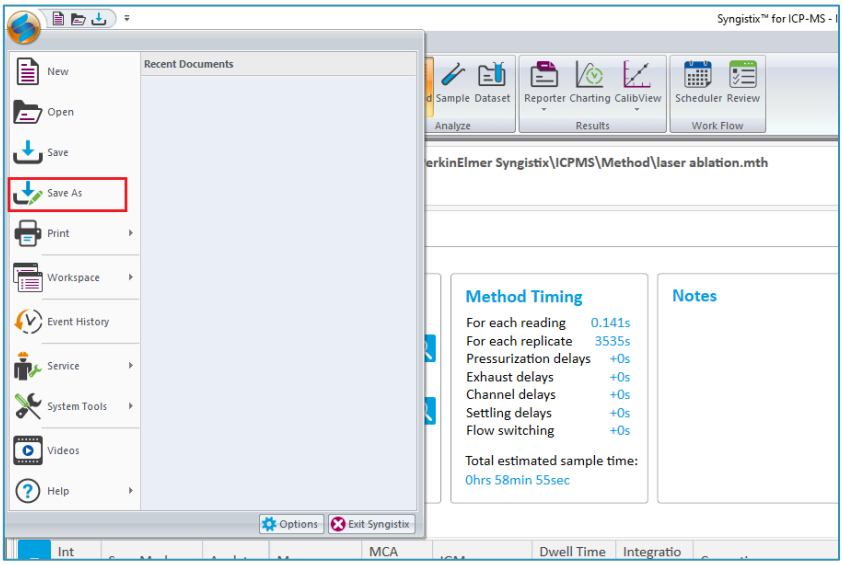
9. Use the **Browse** icon to select the destination directory for the results. The software will automatically export the data as a **NetCDF** file after each sample is run.



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.

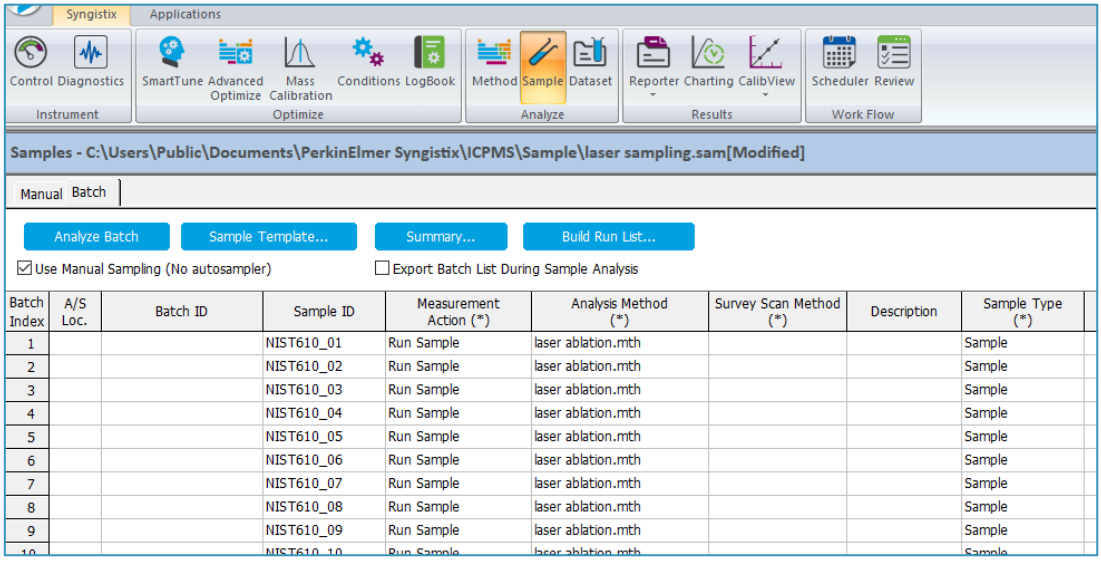


Create a Sample File

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 main sampling control interface of your NexION ICP-MS.



Batch Index	A/S Loc.	Batch ID	Sample ID	Measurement Action (*)	Analysis Method (*)	Survey Scan Method (*)	Description	Sample Type (*)
1			NIST610_01	Run Sample	laser ablation.mth			Sample
2			NIST610_02	Run Sample	laser ablation.mth			Sample
3			NIST610_03	Run Sample	laser ablation.mth			Sample
4			NIST610_04	Run Sample	laser ablation.mth			Sample
5			NIST610_05	Run Sample	laser ablation.mth			Sample
6			NIST610_06	Run Sample	laser ablation.mth			Sample
7			NIST610_07	Run Sample	laser ablation.mth			Sample
8			NIST610_08	Run Sample	laser ablation.mth			Sample
9			NIST610_09	Run Sample	laser ablation.mth			Sample

Follow the steps below to set up your analysis sequence:

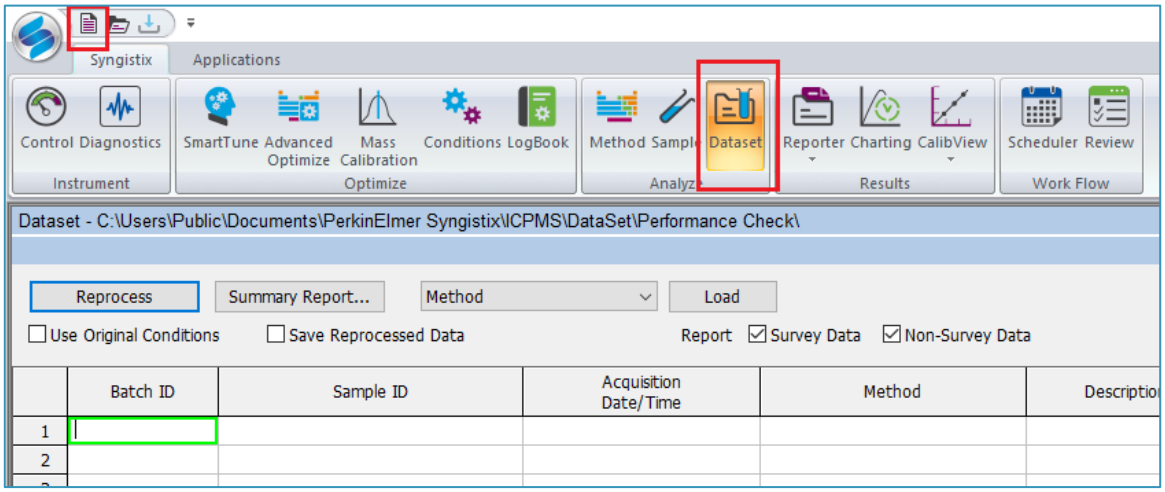
1. Select the User **Manual Sampling (No autosampler)** checkbox.
2. Enter a unique **Sample ID** for each laser ablation spot or traverse. You can also copy and paste the Sample ID information from a text or Excel file or use the **Sample Template…** window to automatically generate unique Sample IDs 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

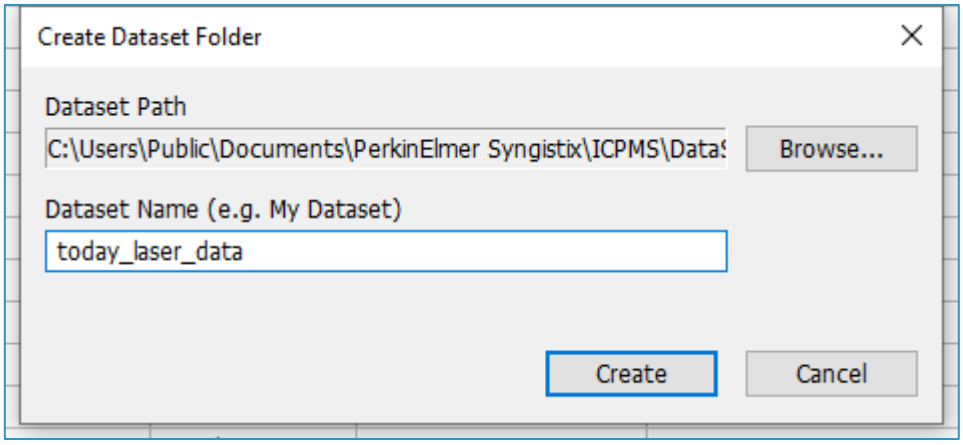
Syngistix stores the raw data acquired after each analysis within the open dataset. The data for each sample analysis is saved as an individual data file, with the complete series of measurements in the dataset constituting a folder on the hard disk of your computer.

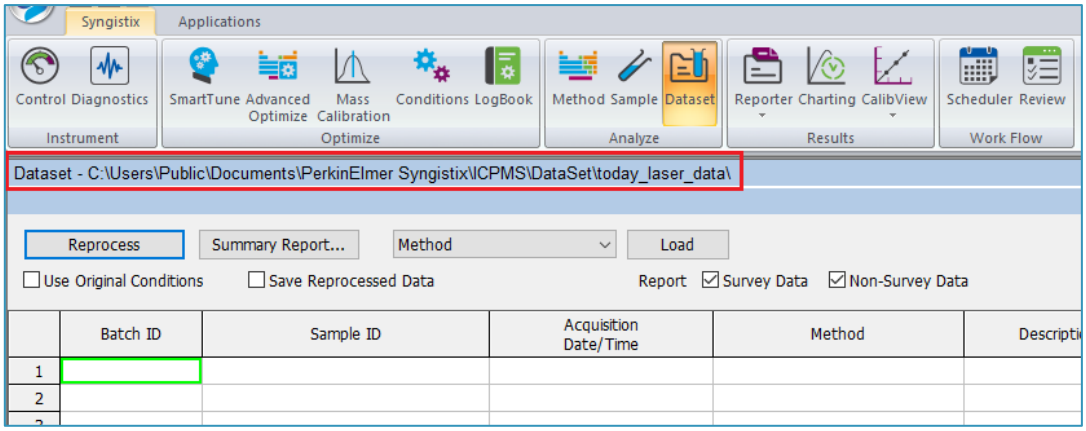
The software creates the individual file names using the Sample ID entered on the Sample panel. Each sample file is generated using the parameters specified in your method, for example the number of readings acquired, measured mass, dwell time per mass, etc..

1. To create a new dataset, go to the **Dataset** panel and then click on the **Create a new file** icon found in 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 data acquired during a run, and to reprocess acquired data (see Exporting Existent Data for more details). Only the raw data files are stored within a dataset.

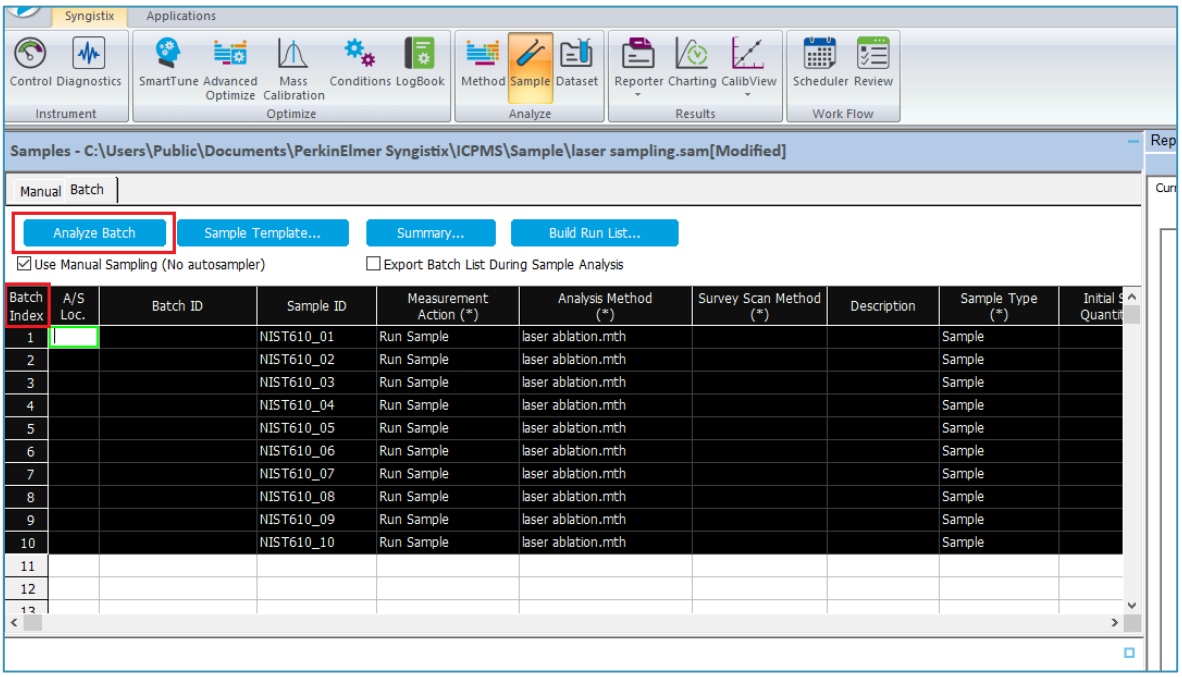
NOTE:

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 Bacth** to initiate the analysis sequence. Syngistix will wait for the external trigger coming from the laser ablation system to start data acquisition.



Exporting Existent Data

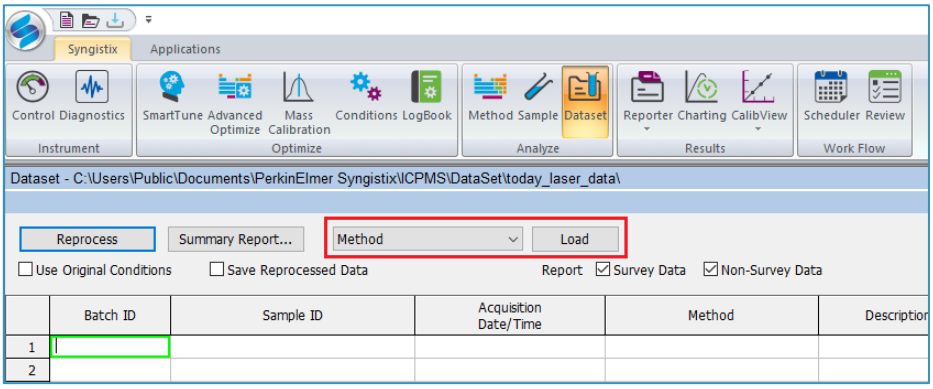
You can use Syngistix to reprocess export previously acquired data.

This can be useful in many circumstances. For example, if you find after a determination that the incorrect reporting options were selected in your method (**Method – Reporting Tab**), you can reprocess the data using a modified version of the method which includes the **Automatically Generate NetCDF File** selection.

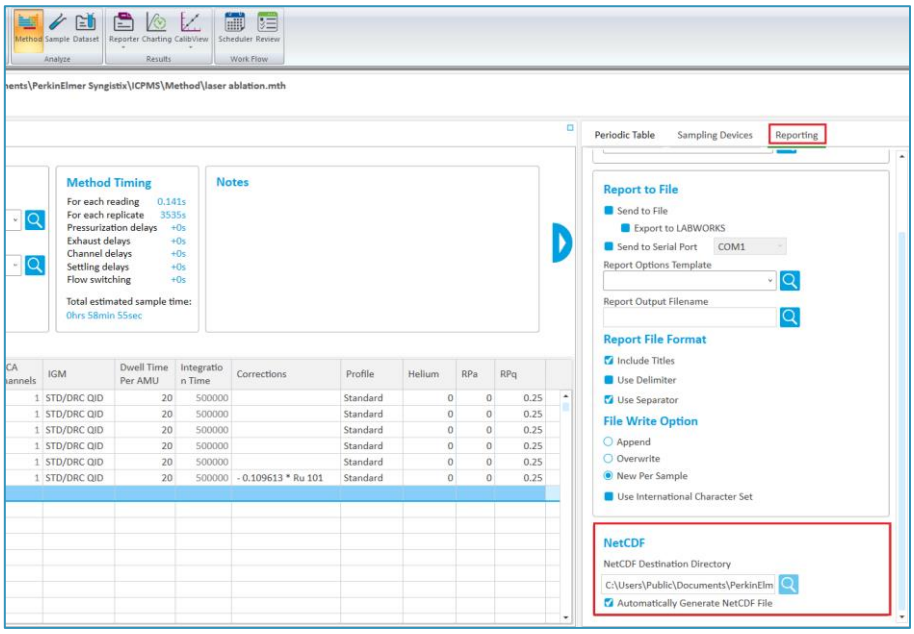
The reprocessing function uses the reporting options specified in the active method. Note that reprocessing does not alter the acquired data; you can view the original results at any time using the Dataset panel.

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 – Reporting tab** and select the **Automatically Generate NetCDF File** checkbox. Use the **Browse** icon 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**.