Syngistix for ICP-MS

Software setup for LA-ICP-MS analysis User's Guide





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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:

🔥 « Users > Public > Public Documents :	 PerkinElmer Syngistix 	> ICPMS > Method	~
Name	Туре	Size	^
Isotope Dilution.mth	MTH File	3 KB	
Isotope Ratio.mth	MTH File	2 KB	
KED Performance Check.mth	MTH File	37 KB	
laser ablation.mth	MTH File	39 KB	
NanoTemplate.mth	MTH File	16 KB	
Neb Gas Optimization DRC.mth	MTH File	2 KB	

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.

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

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	Name	Date r ^
	📄 Isotope Ratio.mth	15/03,
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	KED QID Calibration.mth	15/03,
	🗹 📄 laser ablation.mth	1/03/2
	Neb Gas Optimization DRC.mth	15/03,
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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.

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2	Peak Hopping	Si	28.9765		STD/DRC QID	20	500000		Standard	0	0		
3	Peak Hopping	Ca	42.9588		STD/DRC QID	20	500000		Standard	0	0		
4	Peak Hopping	Ti	48.9479		STD/DRC QID	20	500000		Standard	0	0		
5	Peak Hopping	Fe	56.9354		STD/DRC QID	20	500000		Standard	0	0		
6 7	Peak Hopping	Mo	97.9055	1	STD/DRC QID	20	500000	- 0.109613 * Ru 101	Standard	0	0	0.25	
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4. Adjust the number of **Readings/Replicate** to match the **Est. Sample Time** to your laser sampling time.

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^{*} 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.

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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		STD/DRC QID	20	500000		Standard	0		0.25	
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NOTE: INTERFERENCE CORRECTIONS IN LA-ICP-MS

Typically in LA-ICP-MS analysis, interference corrections are applied during postacquisition 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.

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ublic\Documents\PerkinElmer Syngistix\ICPMS\Method\laser ablation.mth			
		Periodic Table Sampling	Devices Reporting
Method Timing Notes For each reading 0.1415 For each replicate 35355 For each replicate 35355		Selected Autosampler Selected Tray File	No autosampler selected No autosampler selected
C Exhaust delays +0s Channel delays +0s Settling delays +0s Flow switching +0s Total estimated sample time:	D	Autodilution Settings Dilution Factor Diluted to Volume (mL)	10
Ohrs 58min 55sec		1st Dilution Position Probe Purge Position	1
MCA Channels IGM Dwell Time Integratio Per AMU n Time Corrections Profile Helium RPa	RPq		

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.

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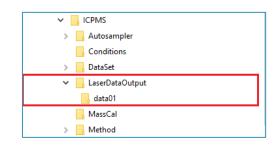
8. Use the Reporting tab to export the LA-ICP-MS results as NetCDF files. Select the Automatically Generate NetCDF File checkbox.

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.

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										Use International Character Set
										NetCDF
										NetCDF Destination Directory
										C:\Users\Public\Documents\PerkinElm

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.

	Syngistix™ for ICP-MS
New Recent Documents Image: Open Open	d Sample Dataset Analyze Reporter Charting CalibView Results Work Flow
Save	erkinElmer Syngistix\ICPMS\Method\laser ablation.mth
Print >	
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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.

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2			NIST610_02	Run Sample		laser ablation.	nth				Sample
3			NIST610_03	Run Sample		laser ablation.	nth				Sample
4			NIST610_04	Run Sample		laser ablation.	nth				Sample
5			NIST610_05	Run Sample		laser ablation.	nth				Sample
6			NIST610_06	Run Sample		laser ablation.	nth				Sample
7			NIST610_07	Run Sample		laser ablation.	nth				Sample
8			NIST610_08	Run Sample		laser ablation.	nth				Sample
9			NIST610_09	Run Sample		laser ablation.	nth				Sample
10			NIST610 10	Run Comolo		beer ablation	nth				Cample

Follow the steps below to set up your analysis sequence:

- 1. Select the User Manual Sampling (No autosampler) checkbox.
- 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:

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2									

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

Create Dataset Folder		×
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C:\Users\Public\Documents\PerkinElmer Syngistix\ICPMS\Data	Browse	
Dataset Name (e.g. My Dataset)		
today_laser_data		
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Create	Cancel	

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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 postprocessing. 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.

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Analyze Batch	Sample	Template	Summary	Build Run List				
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ch A/S ex Loc.	Batch ID	Sample ID	Measurement Action (*)	Analysis Method (*)	Survey Scan Method (*)	Description	Sample Type (*)	Initial S ^ Quantit
		NIST610_01	Run Sample	laser ablation.mth			Sample	
2		NIST610_02	Run Sample	laser ablation.mth			Sample	
		NIST610_03	Run Sample	laser ablation.mth			Sample	
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3		NIST610_08	Run Sample	laser ablation.mth			Sample	
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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.

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 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.

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- Q	Exhaust de Channel de Settling de Flow switc	eading 0.14 eplicate 353 tion delays 4 elays 4 elays 4 elays 4 hing 4 nated sample ti	11s 40s 40s 40s 40s 40s 40s	tes					D	Report to File Send to File Export to LABWORKS Send to Serial Port COM1 Report Options Template Report Output Filename Q
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	STD/DRC QID	20			Standard	0	0	0.25		Use Separator
	STD/DRC QID	20	500000		Standard	0	0	0.25		
1	STD/DRC QID	20	500000		Standard	0	0	0.25		File Write Option
1	STD/DRC QID	20	500000		Standard	0	0	0.25		O Append
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1	STD/DRC QID	20	500000	- 0.109613 * Ru 101	Standard	0	0	0.25		New Per Sample Use International Character Set
										NetCDF NetCDF Destination Directory C:\Users\Public\Documents\PerkinElm Q

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**.