

Thermo Scientific iCAP PRO Series ICP-OES and Qnova Series ICP-MS

LIMS interfacing for trace element analysis

In high throughput laboratories, analysis of thousands of samples a week is a routine requirement and any delay in getting samples prepared, sample lists created, data acquired, results validated, exported and reported costs money. In a manual data entry environment, as the number of samples climbs, so does the time taken to input sample names and related information, such as dilution factors and rack position identifiers for the sample vials. Increasing sample numbers also carry a higher risk of data entry errors, potentially leading to result misreporting and the subsequent need to re-run samples, further increasing costs and damaging the reputation of the laboratory. As laboratories have evolved to handle increasing numbers of samples, automated software solutions for efficient, accurate and reliable sample data transcription have therefore become essential. These software systems are referred to as Laboratory Information Management Systems (LIMS) and interfacing them effectively with instrumentation in the laboratory is critical. In this Product Spotlight the capabilities of the Thermo Scientific™ Qtegra™ Intelligent Scientific Data Solution™ (ISDS) software for interfacing and integrating with LIMS for trace elemental analysis instrumentation (ICP-OES and ICP-MS) from Thermo Fisher Scientific is described.

Streamlining data entry requires a process that starts with the initial arrival of samples at the laboratory. The samples then need to be booked in and allocated to the appropriate instrument according to the analysis required. Sample information can be provided in various ways, for example



as a CSV or XML data file, as digital codes (e.g., bar or QR codes) on the sample containers, as a hardcopy printout or simply written directly on the sample vessels. The first two options support a direct digital means of collating sample information while the second two require manual transcription, either into a digital form (usually as a CSV file) or entered directly into the sample list, in the instrument software. Manual data transcription is only practical when the number of samples is relatively small and, while digital codes provide a convenient way of adding sample data one at a time directly into the sample list, this approach is also impractical for large numbers of samples. High throughput laboratories, therefore, rely on sample information being provided in a digital form in preparation for importing into the sample list and this information is usually uploaded to a server location from where it can be accessed by the instrument for which the analysis is destined.

The minimum information required for any sample is its identity name or number. Calculation relevant information may also be required for importing into the sample list, such as sample weight, final volume or simply a given dilution factor. In addition, there could be comments or additional meta information provided with the samples that also need to be included in the sample run information. The complication then arises as to how the format of the information provided can be matched against the corresponding data fields in the instrument software's sample list. To enable imported sample information to be matched with the correct field in the instrument software, the Qtegra ISDS software provides a simple, user editable XML mapping file, as shown in Figure 1.

```
<?xml version="1.0"?>
- <TranslationTable>
  <!-- The column delimiter / separator used in the CSV file. -->
  <Delimiter>,</Delimiter>
  - <Item>
    <!-- 'Name' is the column name used by the LIMS. -->
    <Name>Sample_ID</Name>
    <!-- 'Translation' is the column name used by Qtegra. -->
    <Translation>Label</Translation>
  </Item>
  - <Item>
    <Name>Sample_Weight</Name>
    <Translation>Amount</Translation>
  </Item>
  - <Item>
    <Name>Final_Volume</Name>
    <Translation>Final_Quantity</Translation>
  </Item>
  - <Item>
    <Name>Batch</Name>
    <Translation>Comment</Translation>
  </Item>
  - <Item>
    <Name>Rack#</Name>
    <Translation>Rack</Translation>
  </Item>
  - <Item>
    <Name>Vial#</Name>
    <Translation>Vial</Translation>
  </Item>
</TranslationTable>
```

Figure 1. Qtegra ISDS software XML mapping file format.

As shown in the example in Figure 1, the column name for each piece of sample information in the LIMS supplied file defined in the <Name> fields in the XML mapping file is then linked to the column name in the Qtegra ISDS software sample list (Figure 2) specified in the <Translation> fields. In this example, where the LIMS file defined sample name is "Sample_ID," the mapping file pushes this information into the "Label" column in the Qtegra ISDS software sample list. The mapping file can be easily edited to ensure that the LIMS file content corresponds to additional Qtegra ISDS software headers, such as number of repeats per sample, dilution factor, etc., using the format shown in Figure 1.

	Label	Comment	Amount	Final Quantity	Rack	Vial
1	BLK	<Comment>			Standard	1
2	STD 1	<Comment>			Standard	2
3	STD 2	<Comment>			Standard	3
4	STD 3	<Comment>			Standard	4

Figure 2. Target column title entries (shown boxed in red) in the Qtegra ISDS software sample list that can be linked to LIMS data types using an XML mapping file. For reasons of clarity, not all mappable entries are displayed.

To import complete sample run lists from LIMS, Qtegra ISDS software uses a template-based approach that takes the LIMS provided CSV files through the mapping process, and automatically creates the sample list for analysis by the instrument. Through the use of supplied or user defined templates, LIMS sample information can be combined with template defined information such as QC test type and frequency.

To create a LabBook that combines LIMS and template defined information, the user simply (1) selects "Create a new LabBook from an existing Template" from the LabBooks tab in Qtegra ISDS software: (2) enters a name for the LabBook, (3) chooses the required template ("Food" in this example), (4) selects the LIMS-supplied CSV file from the folder where it has been placed by the system, and (5) the appropriate mapping file, as shown in Figure 3. A screenshot of the CSV file used for this example is presented in Figure 4. Upon clicking "Create LabBook," a Qtegra ISDS software LabBook is generated, combining the method details from the selected template and sample information from the supplied CSV file. The resulting sample list is shown in Figure 5, where based on the sample weight and final volume information from LIMS, and any additional dilution, the total dilution factor is automatically calculated by the Qtegra ISDS software.

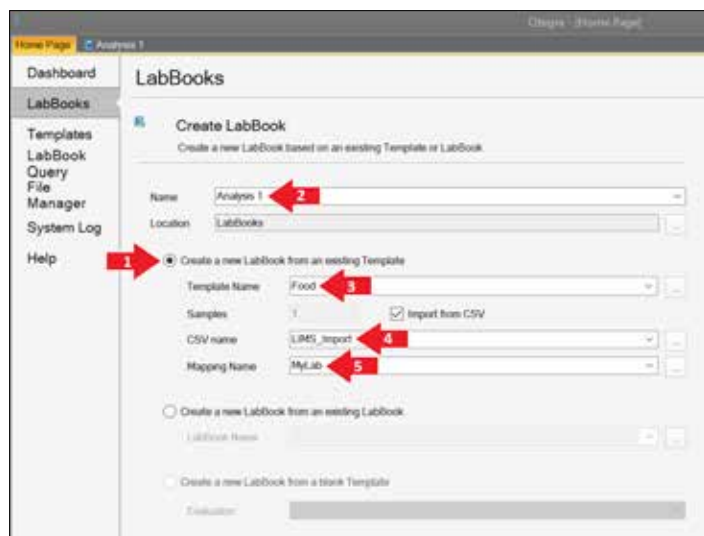


Figure 3. Importing sample information from LIMS into the Qtegra ISDS software analysis LabBook.

	A	B	C	D	E	F
1	Sample_ID	Sample_Weight	Final_Volume	Batch	Rack#	Vial#
2	Unk_1	100 mg	50 g	Salmon	1	1
3	Unk_2	110 mg	50 g	Halibut	1	2
4	Unk_3	90 mg	50 g	Halibut	1	3
5	Unk_4	105 mg	50 g	Halibut	1	4
6	Unk_5	100 mg	50 g	Salmon	1	5
7	Unk_6	110 mg	50 g	Salmon	1	6
8	Unk_7	90 mg	50 g	Halibut	1	7
9	Unk_8	105 mg	50 g	Halibut	1	8
10	Unk_9	100 mg	50 g	Halibut	1	9
11	Unk_10	110 mg	50 g	Salmon	1	10
12	Unk_11	90 mg	50 g	Salmon	1	11
13	Unk_12	105 mg	50 g	Halibut	1	12
14	Unk_13	100 mg	50 g	Halibut	1	13
15	Unk_14	110 mg	50 g	Halibut	1	14
16	Unk_15	90 mg	50 g	Salmon	1	15
17	Unk_16	105 mg	50 g	Salmon	1	16
18	Unk_17	100 mg	50 g	Halibut	1	17
19	Unk_18	110 mg	50 g	Halibut	1	18
20	Unk_19	90 mg	50 g	Halibut	1	19
21	Unk_20	105 mg	50 g	Salmon	1	20

Figure 4. Snapshot of the “LIMS_Import” CSV file used in this example.

	Label	Status	Repeats	Comment	Evaluate	Sample Type	Standard	Dilution Factor	Amount	Final Quantity	Total Dilution Factor
1	BLK		10	<Comment>	✓	BLK		1			1
2	STD 1		3	<Comment>	✓	STD	STD 1	50			50
3	STD 2		3	<Comment>	✓	STD	STD 1	10			10
4	STD 3		3	<Comment>	✓	STD	STD 1	1			1
5	ICV_QC		3	<Comment>	✓	QC	1568B RICE FLOUR	500			500
6	ICVQ_QC		3	<Comment>	✓	QC	1577 Bovine	500			500
7	CCV_QC		3	<Comment>	✓	QC	1577 Bovine	500			500
8	Unk_1		3	Salmon	✓	UNKNOWN		10	100 mg	50 g	5000
9	Unk_2		3	Halibut	✓	UNKNOWN		10	110 mg	50 g	4545 45454545455
10	Unk_3		3	Halibut	✓	UNKNOWN		10	90 mg	50 g	5555 55555555556
11	Unk_4		3	Halibut	✓	UNKNOWN		10	105 mg	50 g	4761 90476190476
12	Unk_5		3	Salmon	✓	UNKNOWN		10	100 mg	50 g	5000
13	Unk_6		3	Salmon	✓	UNKNOWN		10	110 mg	50 g	4545 45454545455
14	Unk_7		3	Halibut	✓	UNKNOWN		10	90 mg	50 g	5555 55555555556
15	Unk_8		3	Halibut	✓	UNKNOWN		10	105 mg	50 g	4761 90476190476
16	Unk_9		3	Halibut	✓	UNKNOWN		10	100 mg	50 g	5000
17	Unk_10		3	Salmon	✓	UNKNOWN		10	110 mg	50 g	4545 45454545455
18	CCV_QC		3	<Comment>	✓	QC	1577 Bovine	500			500
19	Unk_11		3	Salmon	✓	UNKNOWN		10	90 mg	50 g	5555 55555555556
20	Unk_12		3	Halibut	✓	UNKNOWN		10	105 mg	50 g	4761 90476190476
21	Unk_13		3	Halibut	✓	UNKNOWN		10	100 mg	50 g	5000
22	Unk_14		3	Halibut	✓	UNKNOWN		10	110 mg	50 g	4545 45454545455
23	Unk_15		3	Salmon	✓	UNKNOWN		10	90 mg	50 g	5555 55555555556
24	Unk_16		3	Salmon	✓	UNKNOWN		10	105 mg	50 g	4761 90476190476
25	Unk_17		3	Halibut	✓	UNKNOWN		10	100 mg	50 g	5000
26	Unk_18		3	Halibut	✓	UNKNOWN		10	110 mg	50 g	4545 45454545455
27	Unk_19		3	Halibut	✓	UNKNOWN		10	90 mg	50 g	5555 55555555556
28	Unk_20		3	Salmon	✓	UNKNOWN		10	105 mg	50 g	4761 90476190476
29	CCV_QC		3	<Comment>	✓	QC	1577 Bovine	500			500

Figure 5. Qtegra ISDS software sample run list populated with information imported from the “LIMS_Import” CSV file (Figure 4) using the “MyLab” mapping file (Figure 1).

Closing the loop with the transfer of measured sample data back to LIMS is just as straightforward in the Qtegra ISDS software. Data can be automatically reported (using flexible, user-defined templates as PDFs), exported (in CSV or XML formats) or printed, either directly after each sample is analyzed or as a complete data set once the LabBook finishes. Digitally reported or exported data can then be collected and distributed as required by the LIMS. The user can define what data from an analysis is exported/reported via the options available in the automatic export window, as shown in Figure 6. The selected data options, including instrument set and readback values, can be saved as a scheme within the automatic export window which can then be applied to any other LabBook. Figure 6 also shows that exported data can be transposed from rows to columns via the “Export sample lines as rows” check box and data such as average result, standard deviation, % RSD for each sample can be grouped as blocks with a column separator, should either of these options be required by the LIMS.

This Product Spotlight has highlighted the capabilities of the Qtegra ISDS software for importing and exporting sample data from and to LIMS for trace element analysis in high sample throughput laboratories. By providing tools for flexible and easily adaptable mapping of the LIMS sample information format to the sample list, the Qtegra ISDS software enables seamless import and export of data in digital laboratory information management system environments.

Automating the generation of sample run lists from LIMS with the Qtegra ISDS software saves significant time setting up analytical runs in the laboratory and removes the potential for transcription errors, thereby improving productivity, eliminating incorrectly entered sample re-runs and preventing delays on the delivery of final results within the laboratory or organization.

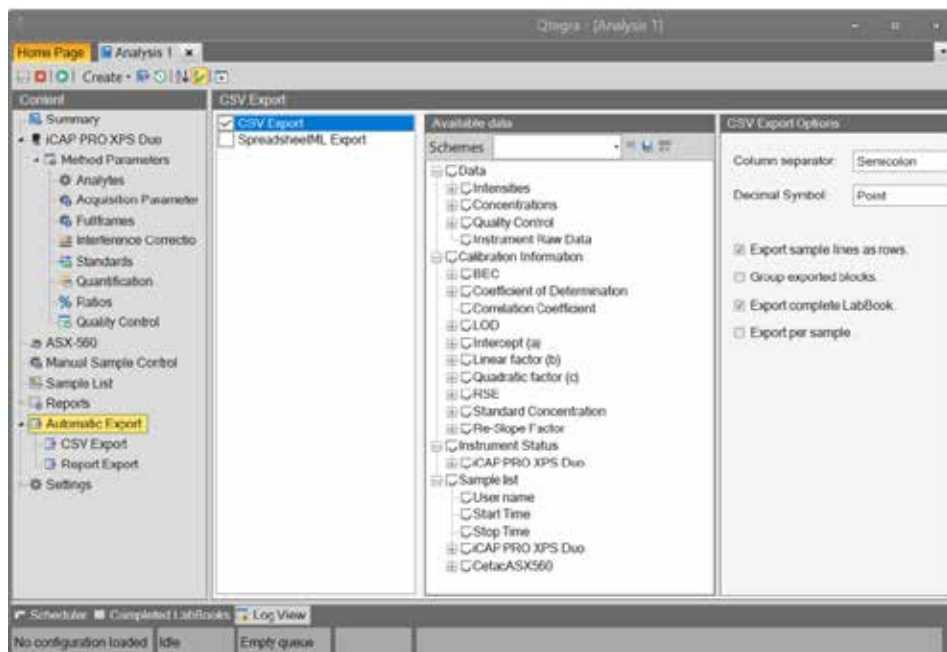


Figure 6. Data options available in the Qtegra ISDS software LabBook automatic export window.

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