Integrating the Agilent 7500 ICP-MS into a Laboratory Information Management System

Technical Information

ICP-MS

June 2002

Author

Steven M. Wilbur
Agilent Technologies
Bellevue, WA 98006
USA

Abstract

Integrating the ICP-MS instrument into the Laboratory Information Management System (LIMS) can greatly simplify the task of managing large amounts of data while eliminating the necessity for manual data entry and transcription of results. As a result of the automation of information flow, together with the automated QC checks built into a typical LIMS, electronic chain-of-custody is maintained and Good Automated Laboratory Practices (GALP) are adhered to.

Background

Inductively coupled plasma mass spectrometry (ICP-MS) is a high throughput elemental analytical technique that can generate an immense amount of data in a short time. The need to accurately track large numbers of samples from sample receipt through final reporting, while maintaining strict quality control and adhering to the requirements of Good Automated Laboratory Practices (GALP) necessitates integrating the ICP-MS instrument into the Laboratory Information Management System (LIMS). Such integration eliminates the need for redundant sample-related data entry, with the associated possibility for error, and also maintains an electronic chain of custody for each sample, from receipt through to final report.

Sample information such as sample name, source, date received and analysis requested is entered into the LIMS at the time of sample receipt. This can be accomplished either manually, by barcode scanning, or a combination of both. Samples for common analyses with similar turn-around time requirements can be automatically batched into sample analysis groups by the LIMS.

The instrument laboratory is notified of the receipt of a sample group so that instrument time may be scheduled. The sample preparation laboratory is also notified of the receipt of the sample analysis groups. Sample preparation information such as date prepared, initial and final weight or volume, spike, duplicate and dilution is electronically added to the sample analysis group by the prep lab. The instrument laboratory is then notified via the LIMS that the samples have been prepared and are ready for analysis. After sample analysis, the data is reviewed for QA/QC compliance and the approved data batch is uploaded to the LIMS for archival and final reporting.

Implementation

For these steps to function, the ICP-MS instrument computer must be capable of bi-directional communication with the LIMS computer(s). Most commonly, this is accomplished by networking the ICP-MS computer with the LIMS computer(s) through either a local area network (LAN) or a wide area network (WAN). Serial communication via a modem and telephone is also possible, though typically much slower and less robust. A number of industry standard network strategies are available, some client-server based, some peer to peer, and most can be interconnected as necessary. In this example, it is assumed that the LIMS utilizes Microsoft networking running on a Windows based server. A UNIX based network server would behave almost identically. The client in either case is the ICP-MS computer (ChemStation) which operates under Microsoft Windows and uses Microsoft networking to communicate with the server.

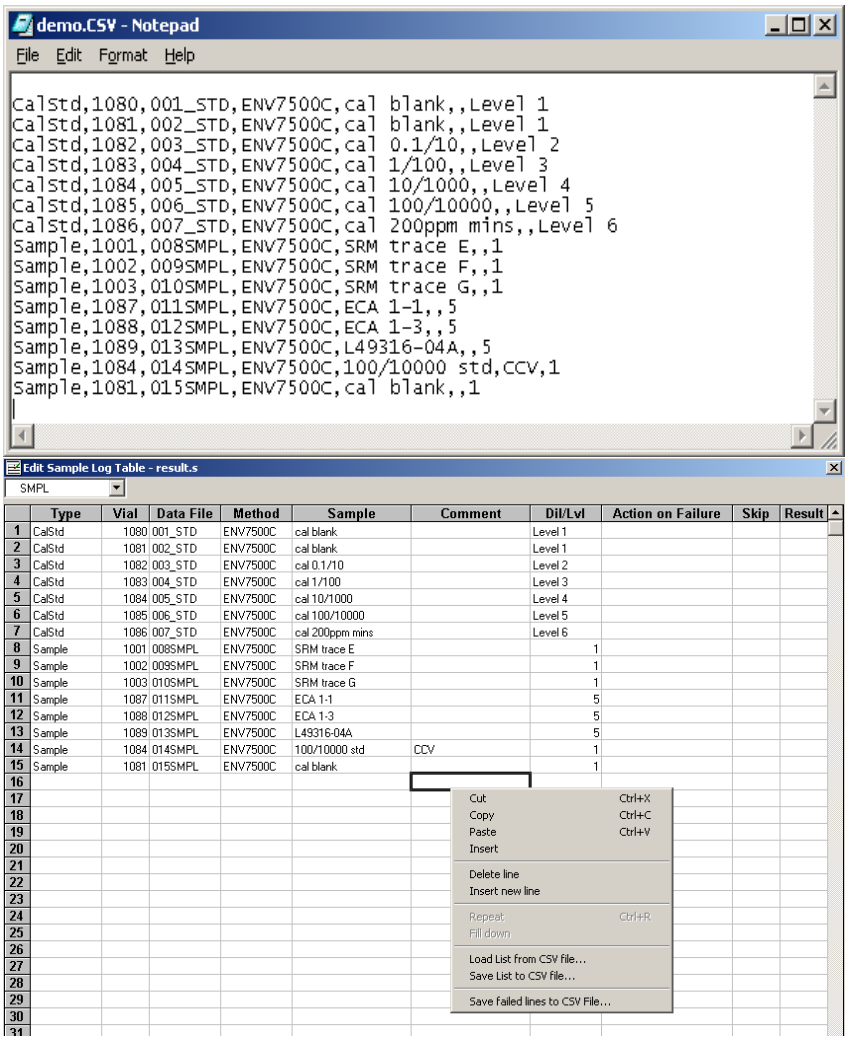
In order for information to flow *through* the ICP-MS ChemStation, the ChemStation must import sample and batch information directly from the LIMS, correctly analyze the associated samples and supply the results to the

LIMS in a format which is easily processed by the LIMS. There should also be a mechanism for data review by the ICP-MS analyst to ensure that only data of acceptable quality is reported. This review can occur either at the level of the ChemStation or at the level of the LIMS.

The Agilent 7500 ChemStation is capable of importing a sample list in a simple comma-separated-value (CSV) file format. This file format is easily created by any LIMS system. It can also be created by a simple spreadsheet program such as Microsoft Excel. This file contains one sample per line and includes sample type, ALS vial position, data file name, method, sample name, comments, dilution factor etc. The actual structure of the file must contain 10 columns separated by commas. Not all information must be included, but empty columns must be delimited by a comma. An example of such a file is shown on the right. In this example, the last three columns, relating to QC actions, are not used. The figures depict a CSV file containing several standards and samples and the sequence resulting from the import of the list into the ICP-MS ChemStation sequence editor.

In this example the dilution factors were automatically calculated by the LIMS from initial and final weights and volumes, entered by the prep lab. Other information was supplied by the receiving area at the time of sample receipt and logging. In addition to sample specific information that is typically different for each batch of samples, calibration and QC information, which doesn't vary for a particular analysis type, will also be required. This information is supplied in the form of a QC template sequence into which the specific sample batch information is inserted. The Agilent Intelligent Sequence editor allows the user to store template sequence components and select from these components to build a final sequence for a particular sample batch.

After sequence creation and sample analysis, the data must be reviewed for quality and completeness and then prepared for final reporting and archiving. This is most easily accomplished using the Agilent ChemStation QC report and online report review capabilities.



Any out-of-control conditions are automatically flagged and corrected where possible. If necessary, reruns are performed and acceptable data is transferred to the LIMS. This process may take any of a number of forms depending on the requirements of the individual laboratory. The laboratory may choose to transfer the data from multiple samples to the LIMS in a single batch – either from a spreadsheet or database. This is accomplished using either the built-in Reporting Database functionality of the ICP-MS ChemStation or the FileView batch result compiler, which is included with the ICP-MS software. In this case each sample is added to a spreadsheet either as part of the method during sequencing, or as a post-sequence batch process after data review.

Alternatively, the laboratory may prefer to transfer the sample data to the LIMS as individual sample reports. This may also be performed automatically during sequencing or in a batch mode after data review. In this case, it is usually desirable to format the sample report in such a way that the LIMS can easily access the relevant information for each sample. This formatting can be accomplished in either of three simple ways:

1) Use the Agilent custom reporting features of the ChemStation to format the report file.

2) Use the powerful ChemStation Macro language to create specialized reporting macros.

The second choice is more powerful, flexible and runs faster, but requires

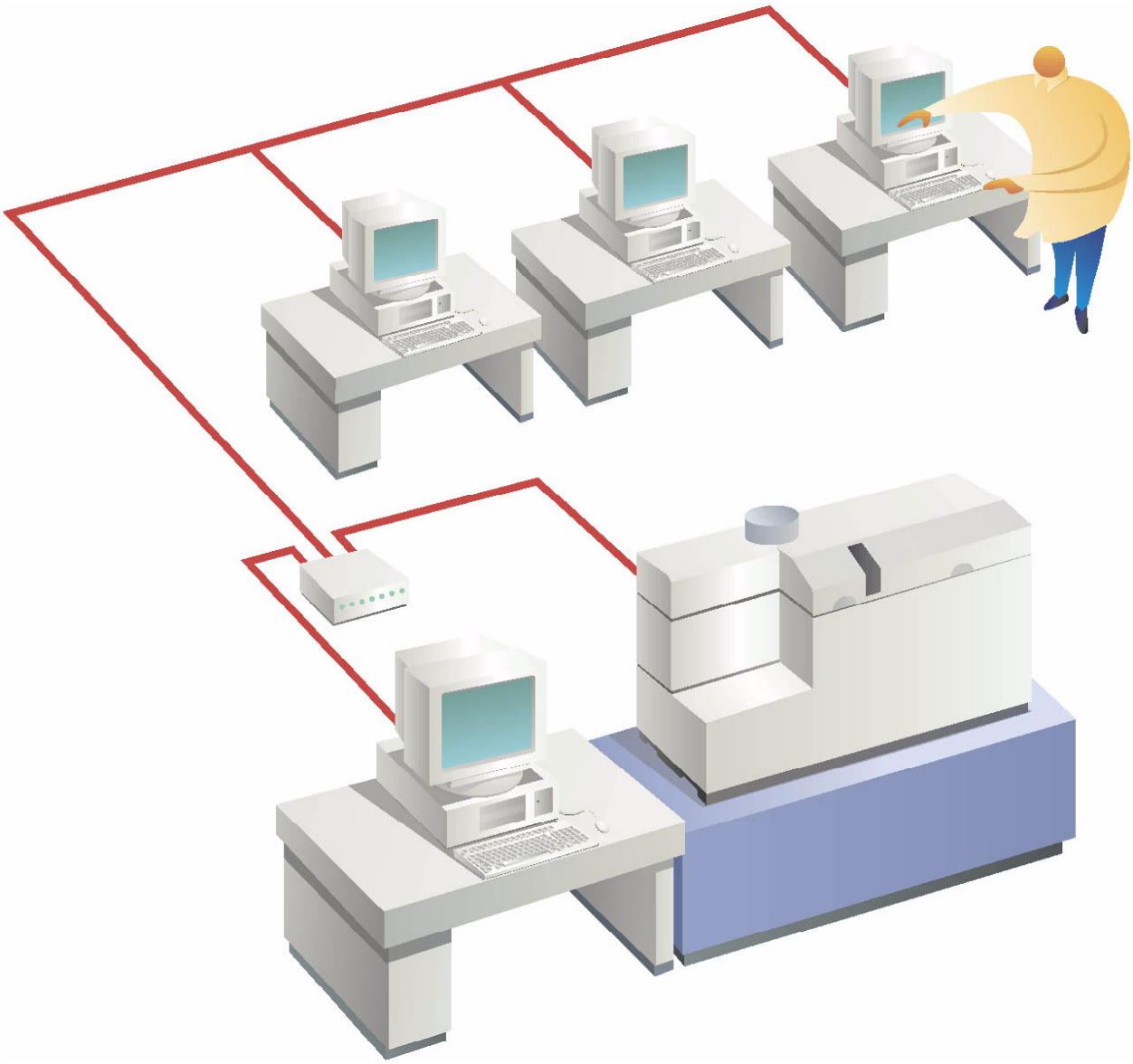


Figure 1: Typical client-based network configuration depicting information flow from sample logging through final reporting and data archival to a remote server drive. Network connections are also depicted.

some macro programming to implement.

3) Use built-in functions of the LIMS to create a report parser which locates the desired records in the standard quant or QC reports and compiles them into a format for input into the LIMS

It is this stage that can save the user the most time. Some users have reported one to two day reductions in sample turn-around time simply by automating data transfer from the ChemStation to the LIMS. This time reduction is realized through elimination of manual data entry into the LIMS and through elimination of the tedious task of manually checking for transcription errors. Furthermore, the capability for the analyst to quickly review QC compliance *before* uploading data reduces the need to re-upload out-of-control data, saving even more time.

While every LIMS implementation is different, the fact that the Agilent ICP-MS ChemStation uses built-in, industry-standard networking hardware and software minimizes difficulties in network connectivity. In addition, powerful and flexible connectivity tools simplify both the import of sample information and export of sample and quality assurance data to the LIMS.

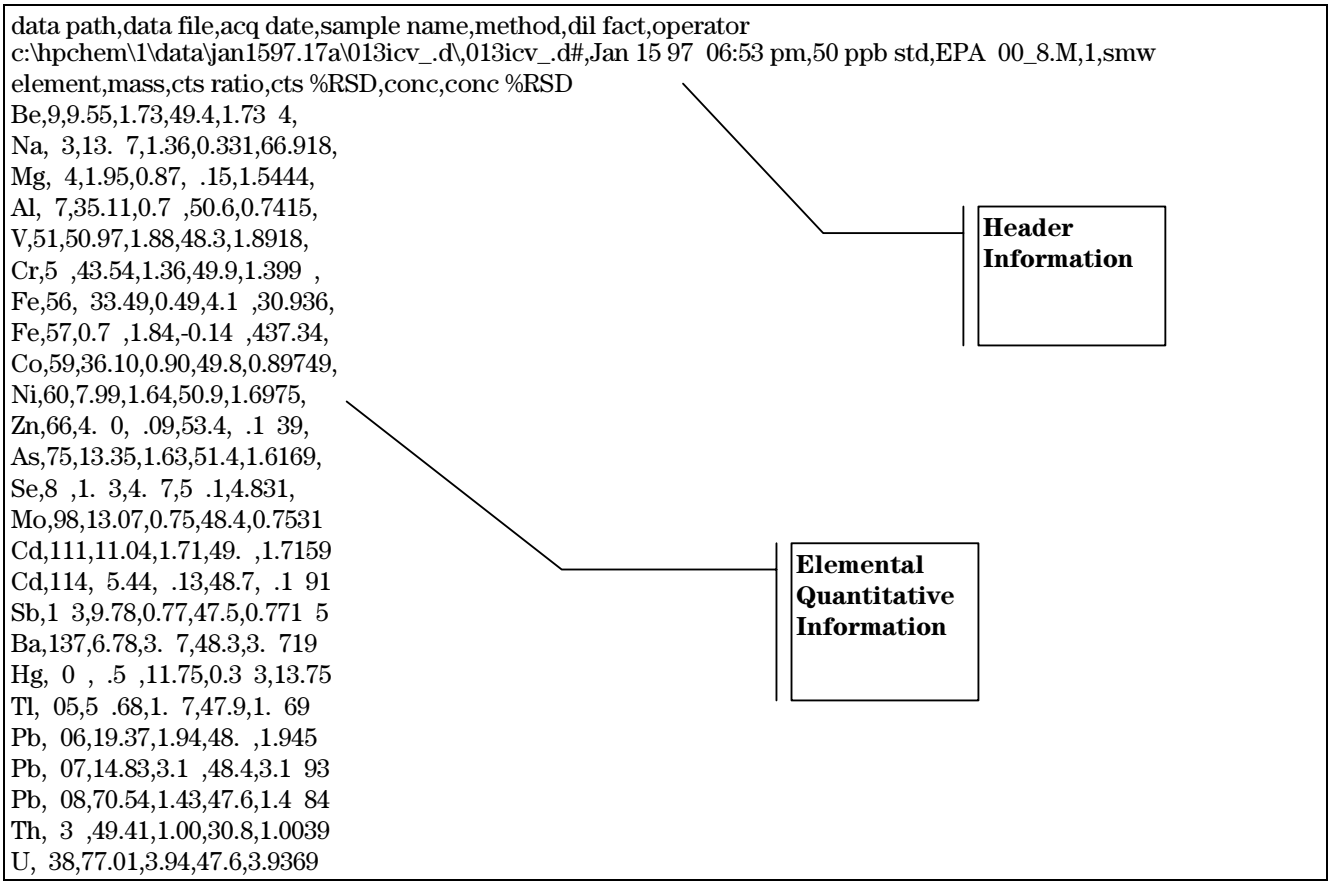


Figure 2: Example of a single sample LIMS output file in .CSV format. Lines 1 and 3 are column headers for ease of reading by humans only. Header information is stored in line 2 and element information in lines 4-28 in this example.

For More Information

For more information on our products and services, visit our Web site at www.agilent.com/chem/icpms

Printed 6/2002
Publication number: 5988-7025EN

Agilent Technologies