

# Interfacing EZChrom Elite to LIMS

White Paper

## Introduction

Agilent EZChrom Elite is used in chromatography operations around the world to provide chromatography data acquisition, processing and control of gas and liquid chromatographs. EZChrom Elite provides a unified computing strategy for the laboratory allowing users to work with a variety of instruments through a uniform user interface, perform instrument control and data collection, data analysis, and centralize and report the data from those instruments.

Chromatography is often only part of a larger set of instrumentation technologies providing analytical data and results for corporate decision making. Many organizations use a Laboratory Information Management System (LIMS) to manage the vast number of samples, laboratory users, instruments, and laboratory data while maintaining the secure environment required for regulatory compliance.



**Agilent Technologies**

**Benefits of Interfacing EZChrom Elite to LIMS**

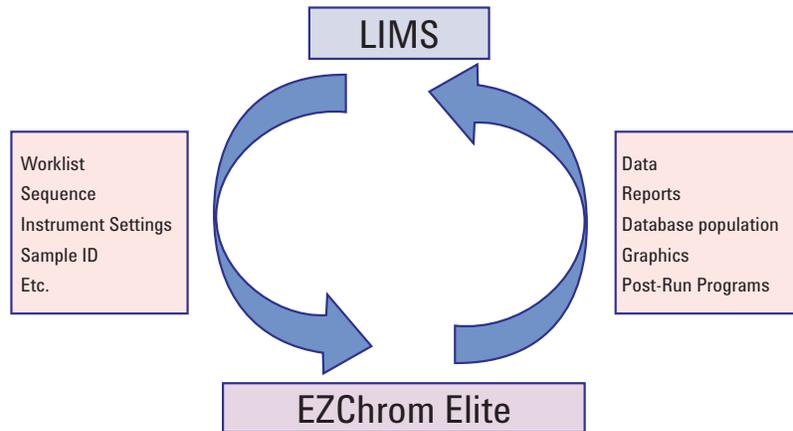
Interfacing EZChrom Elite to a LIMS allows the chromatography operations to fit seamlessly into the normal workflow of the organization. The LIMS is used to manage and organize the assignment of samples to available instruments with appropriate methods. These assignments are then automatically downloaded into EZChrom Elite. The laboratory users do not have to perform tedious data entry or worry about the possibility of errors in numeric entry including transposition of numbers or errors in decimal place. Reducing the time spent in data entry allows instrument operators to focus on the important data analysis tasks and reduces stress related to improper data entry. After the runs are completed, data, results and graphics can be automatically uploaded to the LIMS eliminating the need for the users to stand by the instruments and manually upload the data.

A LIMS and EZChrom Elite interface provides two way communications between the systems. Expert tasks such as sample identification, instrument and method assignments, and worklist generation are often performed automatically by the LIMS and then downloaded to EZChrom Elite. After the samples are processed and the data acquired, EZChrom Elite sends the results back to the LIMS for analysis, reporting and storage, all traceable by the LIMS ID#. In addition to these tasks, there may be a requirement to perform post-run calculations on the results using a post-run program. No special

programming or knowledge is required to integrate EZChrom Elite to LIMS this solution uses built-in functionality within the EZChrom Elite

user interface. The information which flows back and forth between the two systems is summarized in Figure 1 below.

**Figure 1: LIMS-EZChrom Elite Integration**



The benefits of such communication are shown in the table below.

**Table 1: Benefits of EZChrom Elite - LIMS Integration**

- Seamlessly integrate EZChrom Elite into Corporate and Laboratory Workflow
- Decrease analysis set up time by automatically downloading worklists
- Eliminate errors in data entry, such as decimal place and number transposition
- Automatically upload results to LIMS databases
- EZChrom native functionality can be used to execute post run programs to perform specialized calculations
- Automatically post results to other systems or processes
- Email results to management
- Single routine instrument interface: users do not learn and use multiple user interfaces
- Multiple levels of user access, with password permission if required (for example allowing, a super-users to configure instruments and determine acceptable method combinations)
- EZChrom standard traceability and audit features enable regulatory compliance with your LIMS

### Summary of EZChrom Elite – LIMS Interfacing Options

Three interfacing options are described in this white paper for interfacing EZChrom Elite to LIMS. Each interface offers various strengths and weaknesses as well as differing

investments of time, programming effort, and cost. The purpose of this white paper is to describe the various interfaces to EZChrom Elite.

**Table 2: EZChrom Elite - LIMS Interfacing Options**

	Key Features	How does it work?	Supplier	Time	Your Labor	Additional Software Cost
1. Agilent EZChrom Elite	Easy to use Standard and built -in to EZChrom Elite	File-based interface to import worklists and upload results. Menus available in EZChrom user interface.	Agilent	Low	Low	None
2a. Labtronics LIMSLink CDS	Connects EZChrom Elite to ANY vendor's LIMS Automatic, unidirectional upload to LIMS	Purchased from and implemented through Labtronics	Labtronics	Medium	Low	Medium
2b. Labtronics LIMSLink CDS Custom	Connects EZChrom Elite to ANY vendor's LIMS. Full featured, out-of-box connectivity	Purchased from and implemented through Labtronics with an additional software purchase from Agilent required	Labtronics and Agilent	Medium	Low	High
3. Agilent EZChrom Elite Custom Automation Toolbox SDK	Provides custom interfacing tools and External access to EZChrom Elite commands. Precisely fits EZChrom Elite into your exact workflow. Can provide a unified user interface	Enables customer user interface design and programmatic access to EZChrom Elite. Use to create interfaces to fit your exact workflow. Requires programming resources to implement	Agilent	Long	High, or hire Agilent Consultants to assist	High

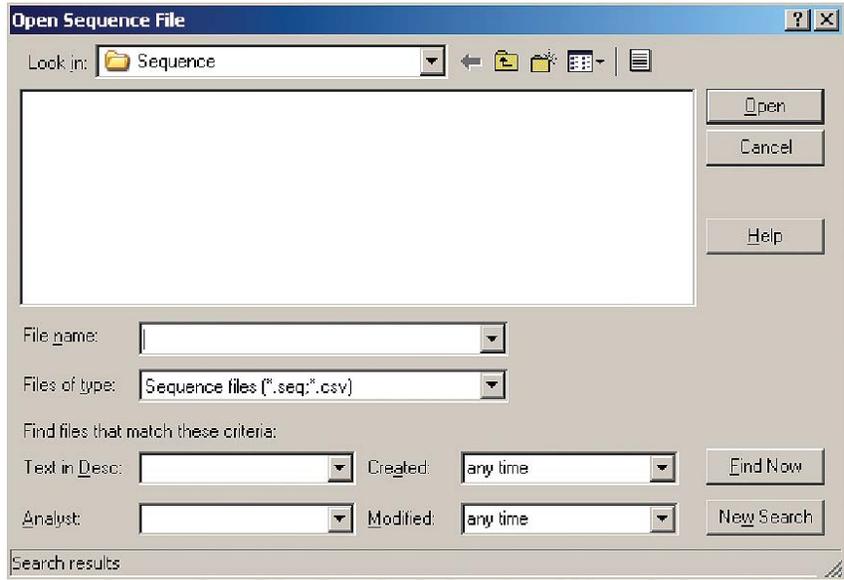
### 1. EZChrom Elite Built-in LIMS Interfacing

The easiest and most cost effective interface between EZChrom Elite to LIMS is built into the EZChrom Elite software. The user is able to utilize these functions from the already familiar EZChrom Elite user interface.

This standard, built-in functionality capitalizes the ability of all major LIMS systems to send a formatted sequence file from the LIMS to EZChrom Elite and to automatically accept data sent from EZChrom Elite into the LIMS. This provides the user with the ability to import ready made sequence tables from the LIMS. Doing so eliminates the need for the instrument user to manually enter the sample lists, data file names and other information, saving time and eliminating data entry errors (such as transposing numbers or decimal point errors).

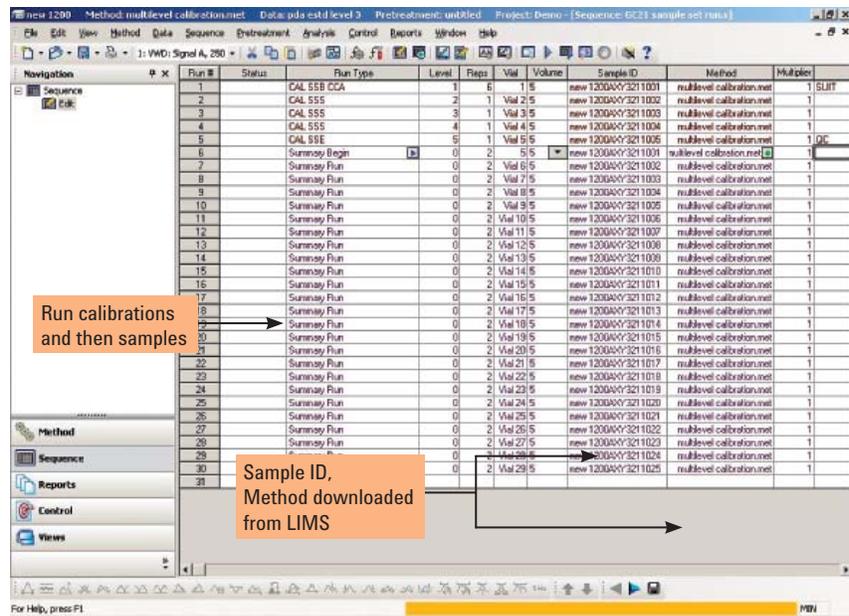
After the run, there are a wide variety of automatic export options for individual results, and complete reports including graphics in a variety of formats which can be parsed by the LIMS. In addition, there are hooks to execute post run programs to perform custom calculations or send results to management.

EZChrom Elite then imports the specified file from the LIMS with the correct sequence information including sample names, file names, valid instrument methods, etc. The instrument operator does not have to perform the tedious and error prone task of numeric sample entries and file naming. This downloaded sequence file can be in EZChrom Elite format or CSV ASCII format and is searchable. For example, a user might sort the sequence file to see which worklist is for their use or which instrument should be used. The user then just loads the samples and presses the START button to begin the runs.



**Figure 3: Automatically Download Sequence Tables**

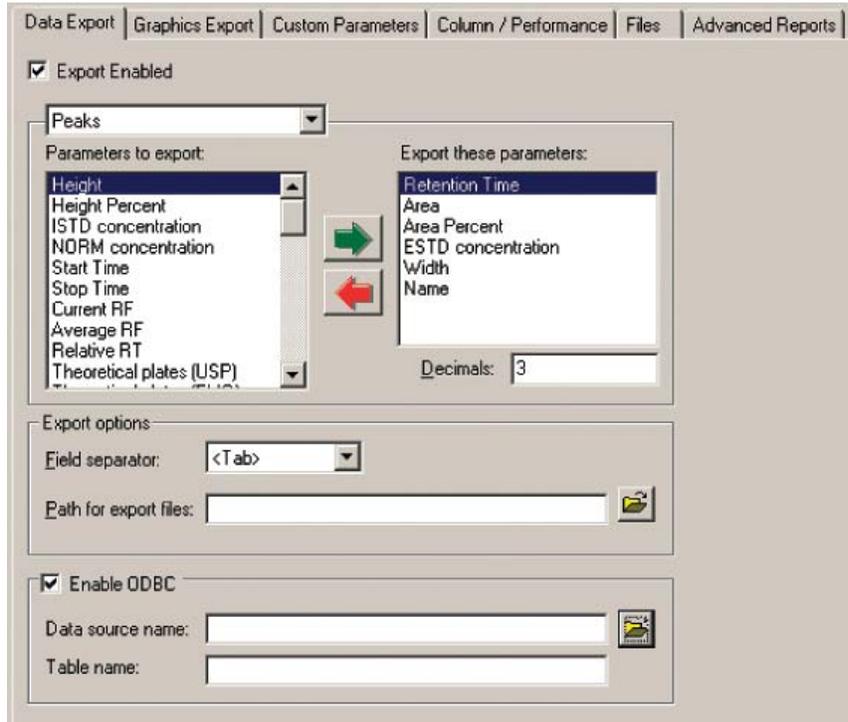
The sequence can be automatically created and formatted by the LIMS and exported as a worklist to EZChrom Elite



**Figure 4: Downloaded Sequence Table, filled in with data from LIMS**

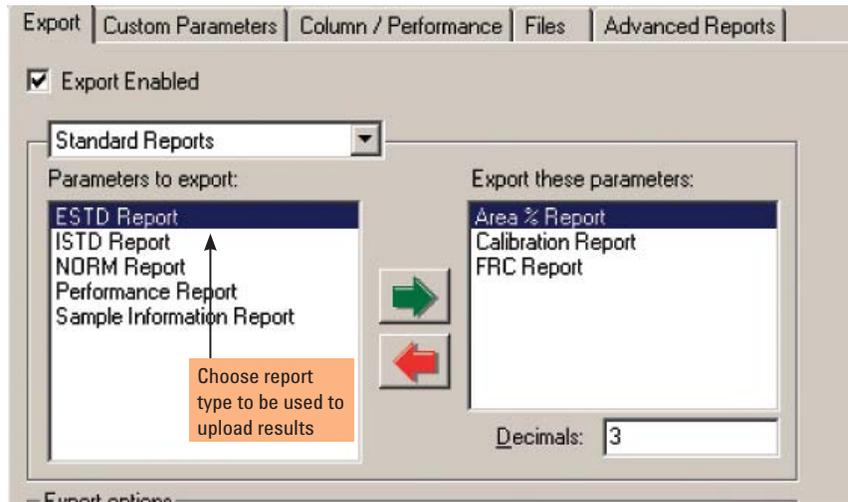
**Figure 5: Automatically Upload Results to the LIMS**

At the end of the run, EZChrom Elite can export results automatically into a variety of file formats with the necessary data separators. EZChrom Elite offers a comprehensive list of results items which can be preconfigured such as Name, Area, and Concentration as shown in the screen below. At the bottom of this screen, there is a field which enables an ODBC connection to be made which can populate the data directly into database tables at the LIMS.



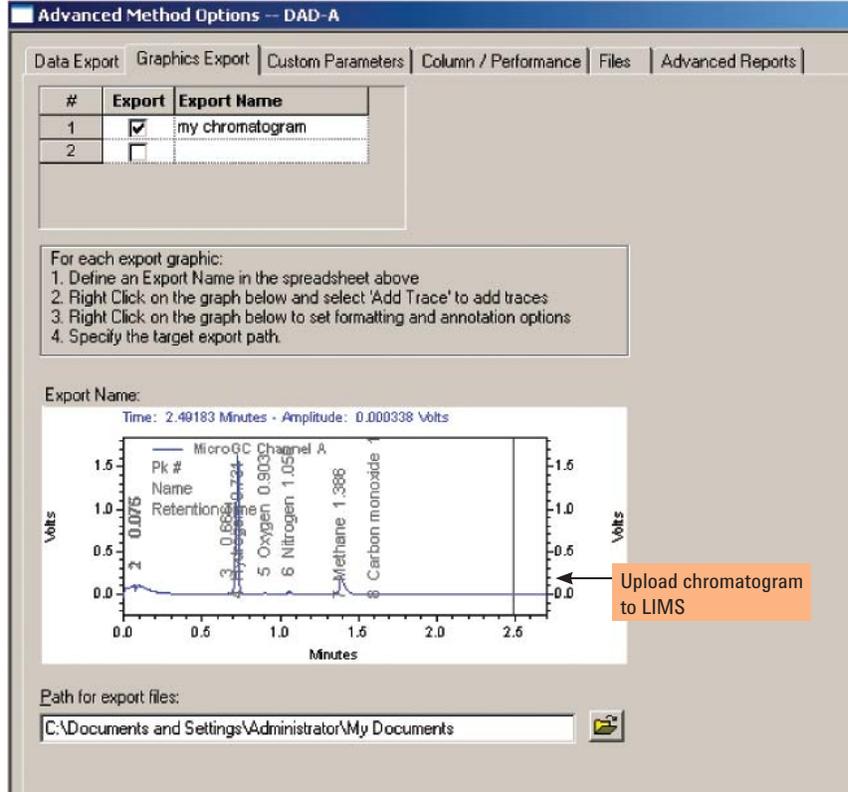
**Figure 6: Automatically Upload Reports to the LIMS**

Standard EZChrom Elite reports can be exported to the LIMS, for example an ISTD report, the Sample Information Report or the Performance report. The desired reports are selected from the pull down menu shown below. These reports are automatically uploaded to a folder monitored by the LIMS after the results are complete.



**Figure 7: Export Graphics to LIMS**

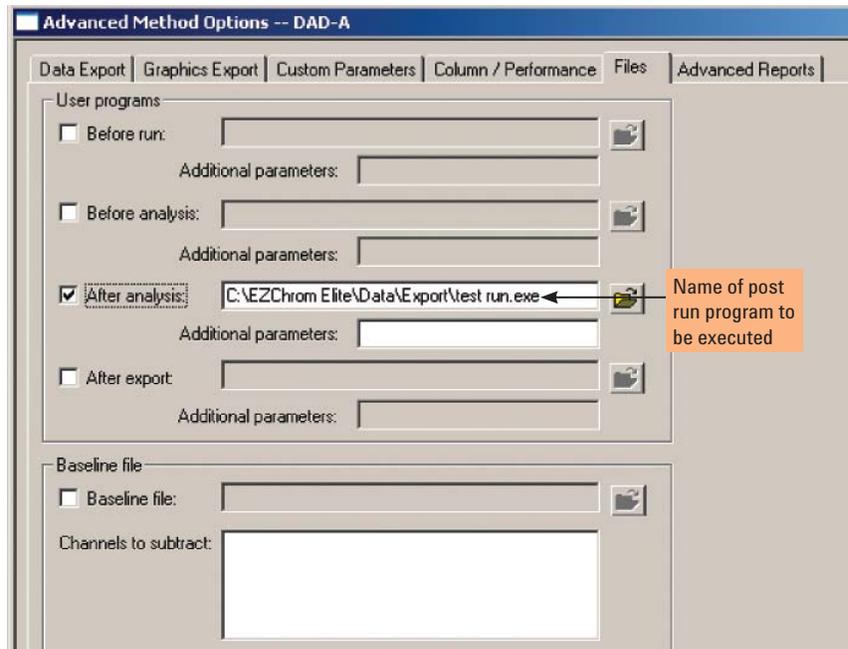
EZChrom Elite can also automatically export graphics to LIMS. For example, in the screen shown below, the chromatogram has been prepared for export to the LIMS.



**Figure 8: Automatically Execute Post-Run Programs**

EZChrom Elite can execute a variety of post run programs. For example, you might send an email to your manager with some critical results. You might hook to a Visual Basic program or an Excel macro for a customized calculation or report.

The advanced method options screen, shown below, allows you to specify which program should be run after the chromatography results are complete.



**2. Partner Integration with Labtronics LIMSLink CDS**

A second choice for interfacing EZChrom Elite to LIMS is LIMSLink CDS/EZChrom Elite product, provided by an Agilent partner, Labtronics, Inc., Guelph, Ontario, Canada. There are two ways to use LIMSLink with EZChrom Elite: the first uses LIMSLink 4.1 to provide automatic upload to any LIMS, the second provides secure, bi-directional communication between the LIMS and EZChrom Elite. This product is specifically designed to connect EZChrom Elite to "ANY Vendor's LIMS". Labtronics developed these solutions using knowledge gained from years of experience in creating CDS/LIMS interfaces; and in cooperation with Agilent and various LIMS developers.

In the first LIMSLink 4.1 solution, simple, unidirectional EZChrom Elite - LIMS connectivity is provided. For example, a petrochemical refinery implemented a solution between EZChrom Elite and a SampleManager LIMS from Thermo Scientific. A unidirectional interface allows the user to walk to up an available GC, run a sample, process it with EZChrom Elite, add LIMS sample identifier information and generate a report that is collected automatically by the LIMSLink software. The results were parsed and posted to the LIMS. In this example, 57 separate GCs using EZChrom Elite were connected to the LIMS. In this refinery, the technicians were skilled in the set up and the operation of the GCs with EZChrom Elite and therefore did not require that sequences be prepared and downloaded from the LIMS. Figure 9 illustrates this solution.

In the second, more full-featured solution using the LIMSLink CDS/EZChrom Elite Interface, a LIMS method is used to create and upload a sequence and to retrieve results. The sequence upload portion uses an intermediate ASCII file to interface with the EZChrom Elite Automation Toolbox SDK (purchased separately from Agilent). The result retrieval portion of the interface is fileless. A valid EZChrom Elite username and password is required to create a sequence and to retrieve results from the interface.

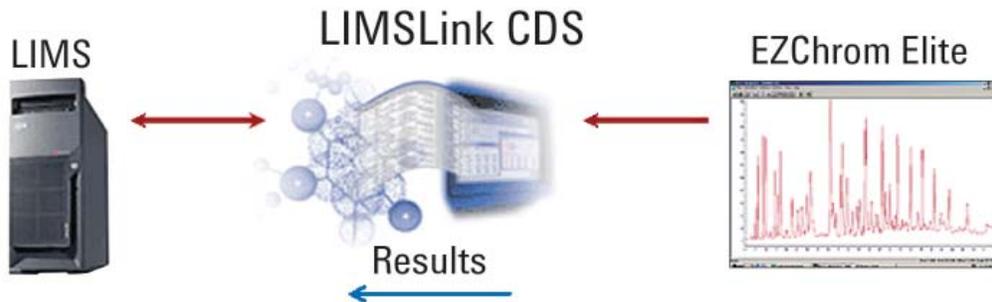


Figure 9: Uni-directional LIMSLink CDS Interface

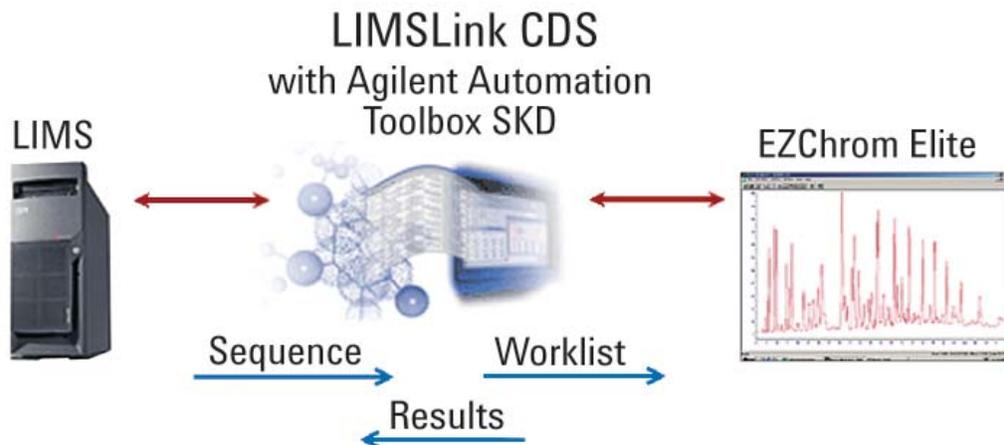
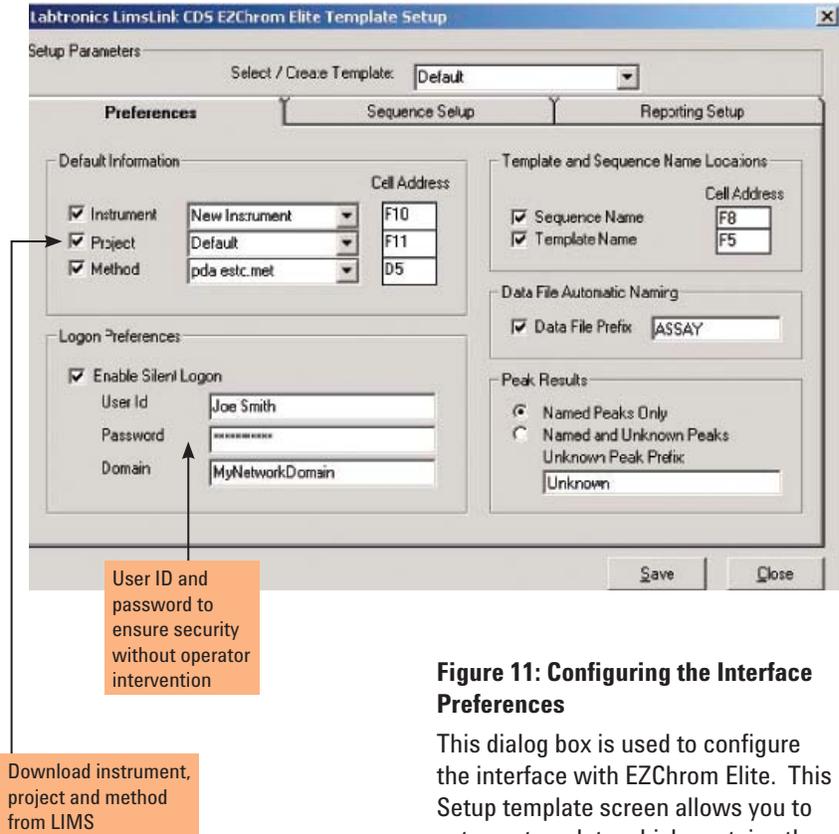


Figure 10: Bi-directional LIMSLink CDS Interface

Some of the key features of this solution include:

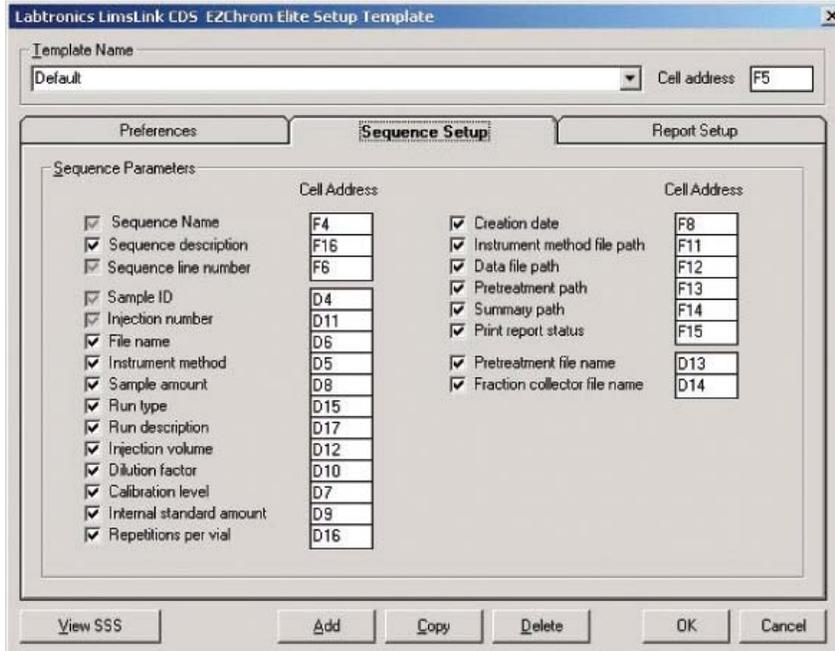
- Smart Logon Technology** allows LIMSLink CDS to automatically prompt the user to select from a full list of instruments and projects. If desired, the user can be required to enter a User ID and password to gain access to the system.
- Bi-Directional Communication** connects EZChrom Elite to the LIMS. LIMSLink CDS can use a worklist of samples from the LIMS to create a sequence for EZChrom Elite. Result data from EZChrom Elite can be collected and transferred to the LIMS without creating a file outside of either application.
- Automatic Number of Sample Vials and Naming of Results** eliminates the need for additional setup steps in the EZChrom Elite software. Both the Sample Vial numbers and parameters for the naming of the data (.dat) files can be provided from the LIMS.
- Control multiple CDS**  
One LIMSLink installation can collect data from multiple CDS Systems and report this data to LIMS with no user interaction required
- Work with many LIMS vendors**  
LIMSLink can transfer results to any LIMS.
- Powerful parser and reporting engine**  
A powerful graphic parser and reporting engine eliminates the need to write custom parsing scripts.
- Data Review**  
Users can choose to review the data in LIMSLink and then manually send the data on to LIMS.

Some examples of the workflow using the LIMSLink EZChrom Elite Interface are shown in Figures 11-13.



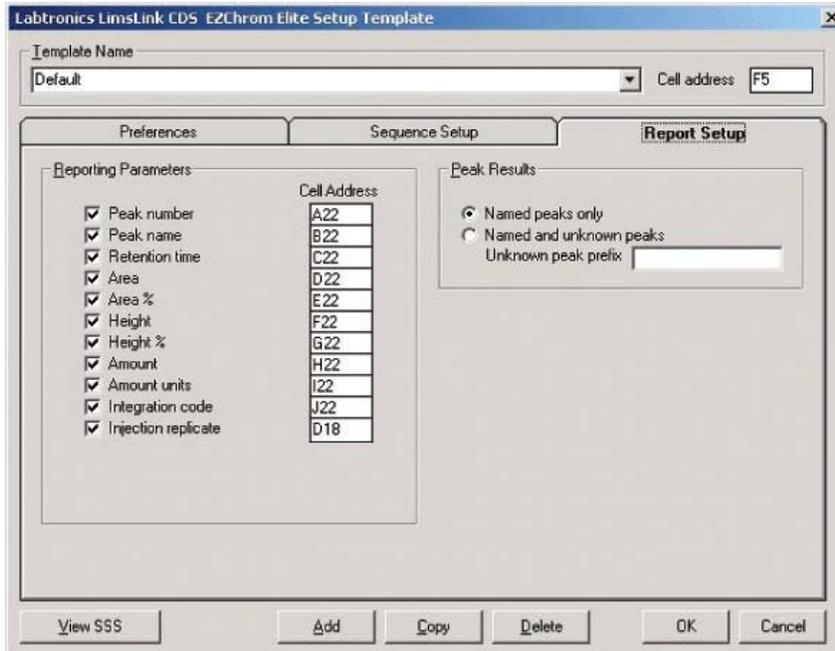
**Figure 11: Configuring the Interface Preferences**

This dialog box is used to configure the interface with EZChrom Elite. This Setup template screen allows you to set up a template which contains the instrument, project and method information. If automatic login is needed, the user id, password and domain can be set up in advance here.



**Figure 12: Setting up the Sequence**

The Sequence Setup Tab contains the parameters required to create a sequence. The user determines the sequence file content by choosing from a series of checkboxes.



**Figure 13: Setting up the Report**

The Report Setup Tab contains the parameters required when sending results from EZChrom Elite to the LIMS. Again, checkboxes are used to choose which parameters to include in the report to LIMSLink EZChrom Elite.

**Ordering**

The current interface has been implemented with EZChrom Elite version 2.8 and 3.0 for both standalone and enterprise versions. The EZChrom Elite interface requires the installation of the EZChrom Elite Automation Toolbox SDK to manage the communication between the LIMSLink CDS and EZChrom Elite.

This LIMSLink CDS/EZChrom solution is priced per instrument to be connected. Installation and consulting time is required to assure the best implementation in your laboratory. If you choose this solution, your Agilent representative can coordinate with Labtronics for implementation.

### 3. EZChrom Elite Automation Toolbox SDK for LIMS Interfacing

The third option for EZChrom Elite to LIMS integration is the optional Agilent EZChrom Elite Automation Toolbox SDK. This Toolbox enables custom user interface design and programmatic access to almost all of the commands in EZChrom Elite. The Automation Toolbox is well suited to organizations with the need for a customized LIMS interface and with a programming staff with the bandwidth and expertise to take advantage of this powerful capability. An investment of time and money will be required to make this option work, but there are unlimited capabilities with this solution. The Agilent Professional Services organization can also partner with your organization to provide additional expertise and programming resources to implement solutions using the Automation Toolbox.

Large organizations may develop and implement their own custom LIMS applications to address specific needs. These organizations can take advantage of the customization available using the Automation Toolbox to integrate EZChrom Elite into these specialized corporate LIMS solutions. The Automation Toolbox can be used to deploy “walk-up” analysis stations where EZChrom Elite can run in the background, invisible to the users. Expert users using the corporate LIMS can configure the samples, instruments, methods and decide the report formats for the results. An operator just has to review the screen, load the samples and press the start button, with no need to learn how to operate the EZChrom user interface. The user can also see the status as the experiments are in progress. After the run, data of all kinds including results, reports and graphics can be automatically exported to the LIMS without any user interaction.

### An Integration Example using the EZChrom Elite Automation Toolbox

In this example, a major chemical company wished to automate sample submission and manual data entry processes in order to improve data integrity and save on technician labor. They accomplished this by using the Automation Toolbox to integrate their EZChrom installations with the front end of their LabVantage Sapphire LIMS. The LIMS has web page capability which is used to present information to the technicians in the laboratory in a familiar format without having to learn EZChrom Elite. The workflow for this example is shown in Figure 14.

For sample submission, EZChrom Elite was downloaded predetermined configurations including instrument, project, method, factors, volumes, etc. The filenames were built in a uniform manner and fields were pre-populated with sample ID and description.

The technician in the chromatography laboratory sees a “backlog” page to view samples. After choosing samples for analysis, all of the sample information is filled in for that sample including tests, instruments, sample ID, date, method, factors, etc.

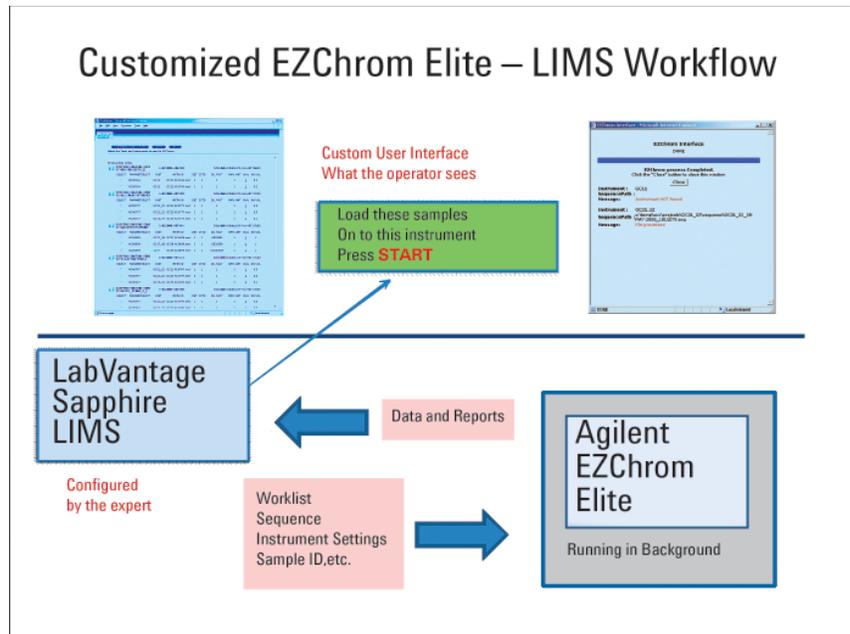
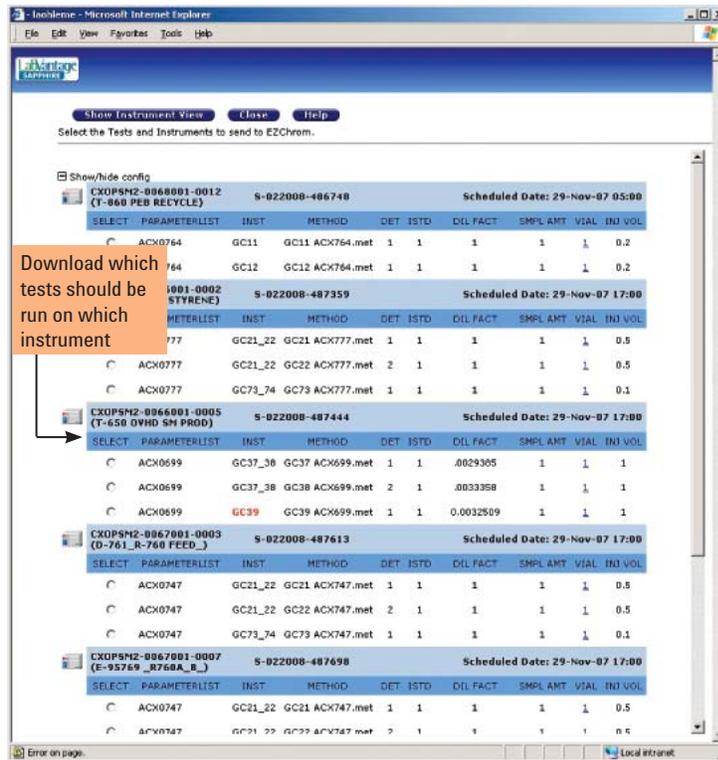


Figure 14: Example Workflow Made Possible by Automation Toolbox

Figures 15-17 illustrate some examples of the workflow using the EZChrom Elite Automation Toolbox.

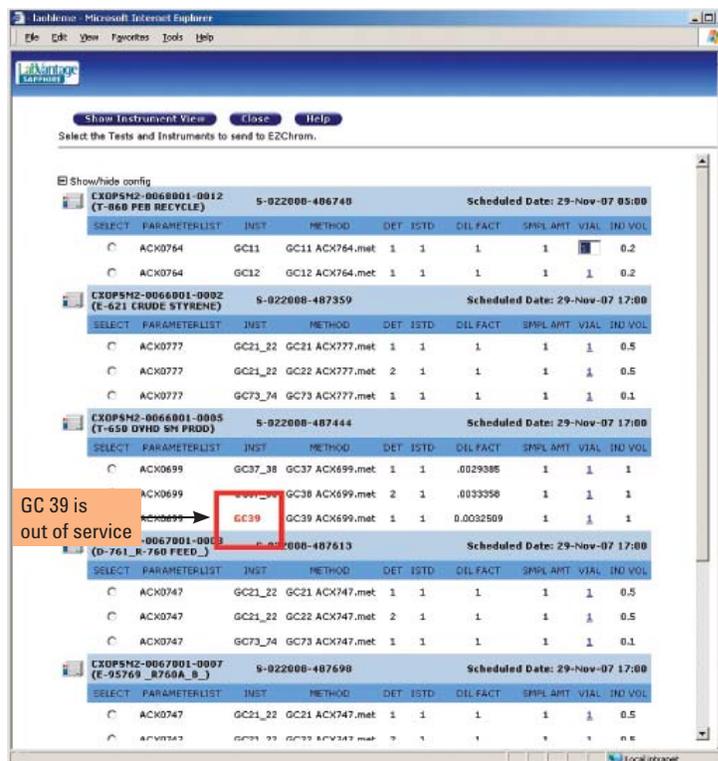
**Figure 15: Backlog View for the Technician, Sample Worklist Automatically Downloaded to EZChrom Elite**

In the example, the expert user at the LIMS system configures the instruments and the list of which samples will be run on which instruments. The worklist is downloaded automatically and presented to the technician in a familiar screen.



**Figure 16: Out of Service Instruments Shown to Technician**

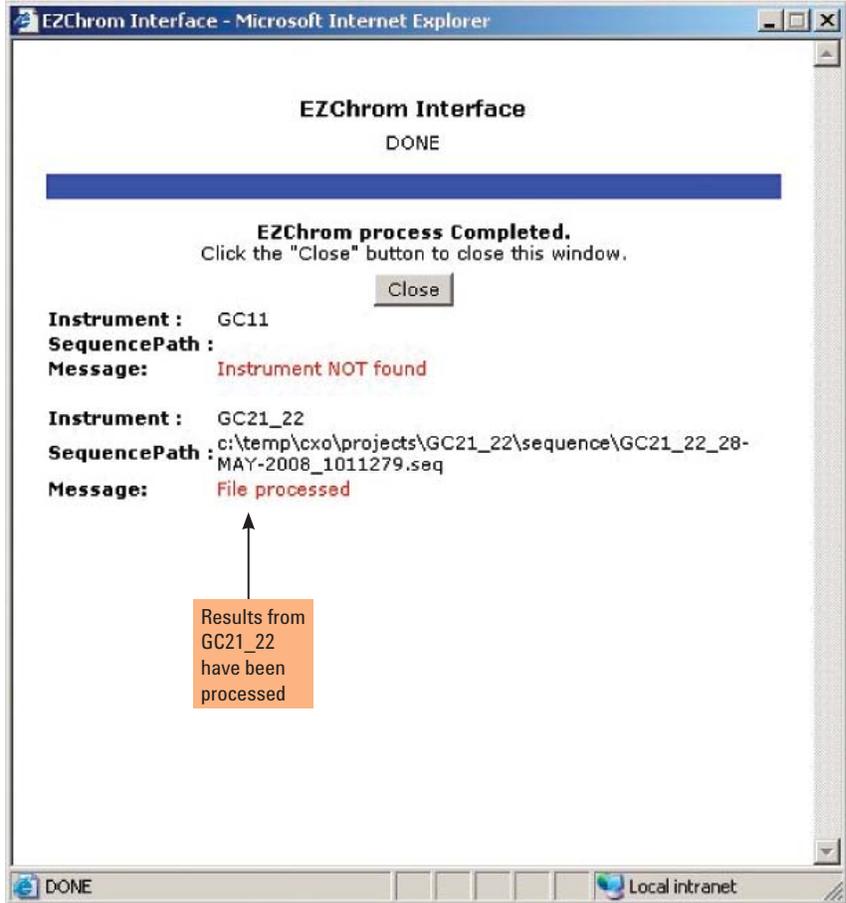
If any of the instruments are out of service, they are noted in red as shown below. The instrument may be out of service due to a calibration problem or hardware issues, for example.



**Figure 17: Technician's View of the Status**

After data acquisition, the new automation capabilities automatically transferred and populated the data fields in LIMS, again, without operator intervention.

The technician sees a custom user interface based on the corporate LIMS system design. There is no need to learn how to operate EZChrom Elite. The Automation Toolbox allows the LIMS to control remotely the EZChrom Elite system. The user sees the status screen shown below which shows that one instrument is off line and the other has completed the runs.



### Significant Savings Achieved by Minimizing User Interaction

The chemical company in this example reported a labor savings measured in multiple years resulting from 50% reduction in instrument start up time and an almost complete (<.1%) reduction in data entry error. They calculated an annualized savings of 6.4 labor years including 3.9 years for sample submission and another 2.5 years of data entry labor.

### Programming Languages Available

Using the Automation Toolbox, interfaces may be written in C++, VB or HTML for control via the intranet/internet.

### Documentation Available

The EZChrom Elite Automation Toolbox SDK includes wide variety of documentation on a number of interfaces and controls to assist programmers with automation including:

- Analog Acquisition Automation Interface
- CIODIO Automation Interface
- Elite Automation Toolbox Instructions
- Elite CS Automation
- Elite CS Graph Control
- HP1100 Automation Interface
- HPMicroGC Automation Toolkit
- OEMFolderAccess API
- PE200 Automation Interface
- Varian 8400 Automation Interface
- Waters Alliance Automation Interface

### Ordering

#### G4667AA Agilent EZChrom Elite Automation Toolbox SDK

Allows installation on 1 development machine and includes 1 run-time license for development purposes. Requires, but does not include, EZChrom Elite software. Must specify software version (3.1.7 or higher). Requires a separate technical support contract arranged directly with the Professional Services Organization.

#### G4669AA EZChrom Elite Toolbox Run-Time License

Provides components needed to run applications developed with EZChrom Elite Automation Toolbox. 1 license required per client. Must specify software version (3.1.7 or higher)

### Conclusion

Agilent EZChrom Elite can be integrated with a LIMS in three different ways. You can take advantage of the import and export capabilities built into the standard EZChrom Elite product without requiring any additional training, programming or expense. You can work with an Agilent and Agilent's partner, Labtronics, Inc., to purchase and implement the LIMSLink/EZChrom Elite product, in either a uni-direction upload or a full featured, out of the box solution (which also requires purchase of the EZChrom Elite Automation Toolbox SDK). You can purchase the EZChrom Elite Automation Toolbox SDK and either use your company's programming resources or contract with the Agilent Professional Services Organization to create and customize the LIMS interface to meet your exact needs. All of these solutions accomplish seamless integration between EZChrom Elite and your LIMS system. EZChrom Elite has been interfaced with a wide variety of LIMS solutions from many different vendors, consult with your local Agilent representative to decide which solution is the best for your LIMS and your

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