Integration of GC/MSD ChemStation with OpenLAB ECM

Technical Overview

Introduction

OpenLAB Enterprise Content Manager (ECM) is a Web-based electronic library that provides a secure storage place for all electronic data. ECM allows users to collect, organize, index, store, archive, and share data of any file type, such as raw analytical instrument data, PDF reports, Microsoft (R) Office documents, or molecular drawings (Figure 1). Data and files in the system are automatically indexed, thus enabling users to quickly search for specific items and retrieve them in a meaningful context. Content within ECM is easily accessed with Microsoft Internet Explorer.

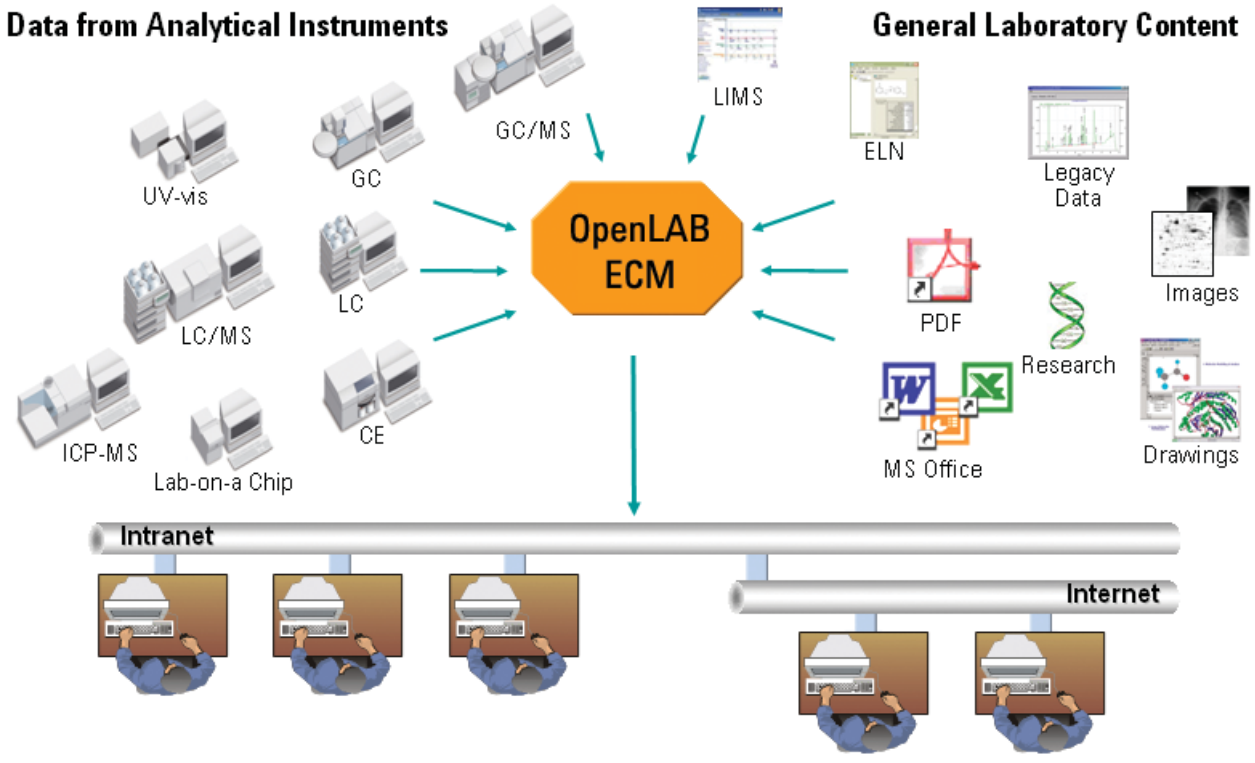

Figure 1. All data are securely stored in ECM.

Agilent Technologies

Integration of the MSD Productivity ChemStation E.00.00 with OpenLAB ECM provides your organization with the following advantages:

- Integrate common ECM functions within the GC/MSD ChemStation user interface, allowing organizations to store and organize data from multiple instruments in one central secure repository without disrupting current workflow.
- Increase productivity by making GC/MSD ChemStation data immediately available to users for review, reprocessing, and reuse with ECM's indexing and search options.
- Ensure the integrity of GC/MSD ChemStation methods, sequences, data files, and reports stored in the restricted access ECM repository.
- Maintain a traceable history of GC/MSD ChemStation methods, sequences, data files, and reports using ECM's revision-control and audit-trailing capabilities.

Data archival and retrieval is enabled seamlessly through this integration of GC/MSD ChemStation E.00.00 and ECM. Users can log on to ECM directly from the GC/MSD ChemStation. In GC/MSD ChemStation, ECM is seen as just another storage location for GC/MSD ChemStation data. Users can store data to ECM and load data from ECM as they would from the local disk drive via the special ECM save and load functionalities.

Once the data are in ECM, they are stored in full compliance with GLP, GMP, and FDA 21 CFR part 11. The GC/MSD ChemStation methods, sequences, data files, and reports are securely stored in ECM. Only authorized users have access to the system, and user privileges determine which users can alter a record or electronically sign it. PDF files in the ECM can be electronically signed. Users cannot sign electronically from the GC/MSD ChemStation. In addition, all content within ECM is under the control of a secure, computer-generated, time-stamped audit trail.

How It All Works

Integration of GC/MSD ChemStation with ECM allows users to store methods, sequences, data files, and reports into ECM directly from GC/MSD ChemStation. Users work from the familiar GC/MSD ChemStation user interface. An ECM pull-down menu is added to both the Instrument Control and Data Analysis user interfaces in the GC/MSD ChemStation. A GC/MSD ChemStation user can log directly into ECM to save methods, sequences, and data files into ECM or retrieve data from ECM for review or reprocessing on the GC/MSD ChemStation (Figure 2).

Automated and Manual Data Transfer Are Both Available

Data transfer between the GC/MSD ChemStation and OpenLAB ECM can be automatic or manual.

Uploading data to ECM is automatic if the user is logged into ECM. Uploading of all raw data file directories happens immediately after data acquisition and reprocessing. Critical instrument reports, that is the tune report, are also automatically uploaded to ECM, as well as the ancillary sequence completes, is paused, or is aborted. However, if the user did not log into ECM or cancelled out of the ECM login panel, the automatic data transfer would not happen after the data acquisition or reprocessing. The user may choose to manually transfer the data to ECM by using the Save Data File to ECM functionality in the ECM menu in the Data Analysis view. The GC/MSD ChemStation data files are always written to the local GC/MSD ChemStation file system first, then copied to ECM. Once the data are securely stored in ECM, they can be analyzed or reprocessed. For data security, any alteration to the data is audit trailed and results in a new version of the data.

For data analysis or reprocessing, users can load data from the local file system or from ECM. If local data are reprocessed, the reprocessed data will be saved into ECM automatically, assuming the user is logged into ECM, whereas the original local data remains in the GC/MSD ChemStation file system. If the data for reprocessing is loaded from ECM, the reprocessed data will be stored as a new version of the original data.

In a typical workflow, a user would load a master method and master sequence from OpenLAB ECM via the "Load Method from ECM" and "Load Sequence File from ECM" in the ECM Menu in the Instrument Control View of the GC/MSD ChemStation. The method and sequence are then copied and loaded onto the local GC/MSD ChemStation.

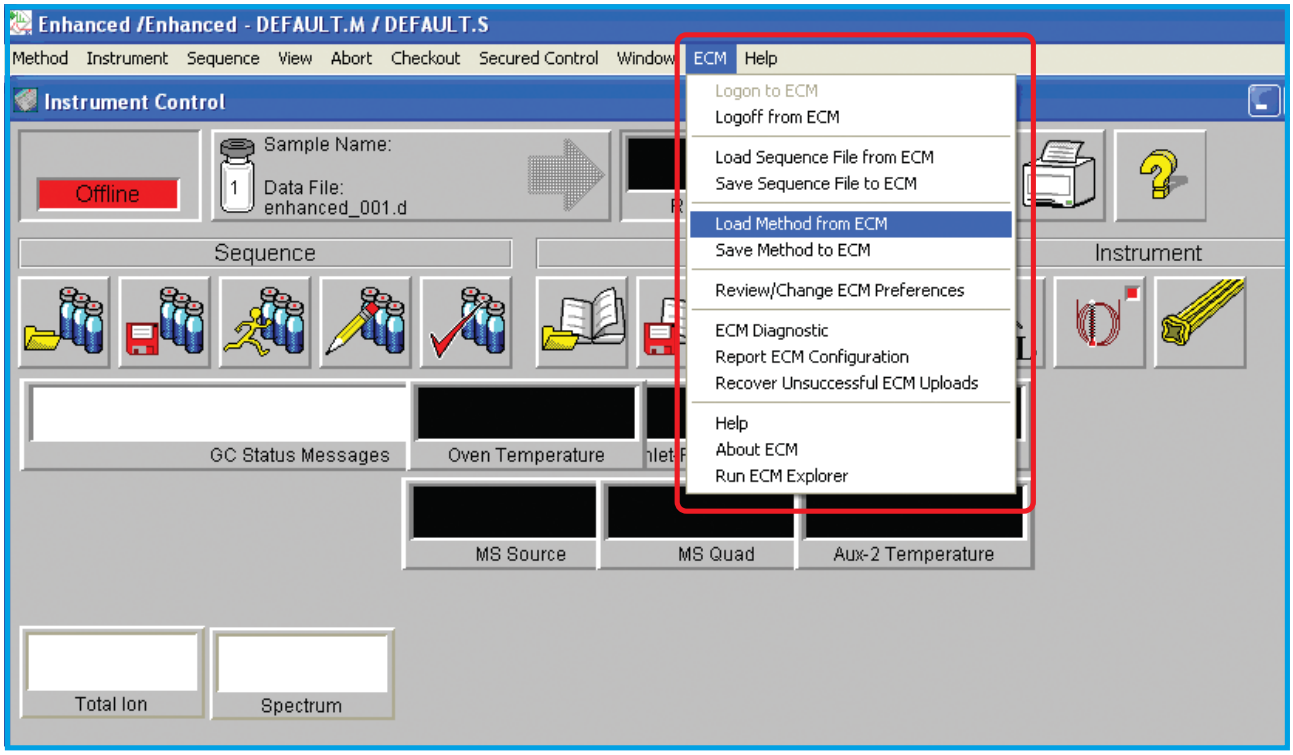

Figure 2. In the GC/MSD ChemStation Instrument Control interface, and ECM pull-down menu allows users to work with data stored in ECM.

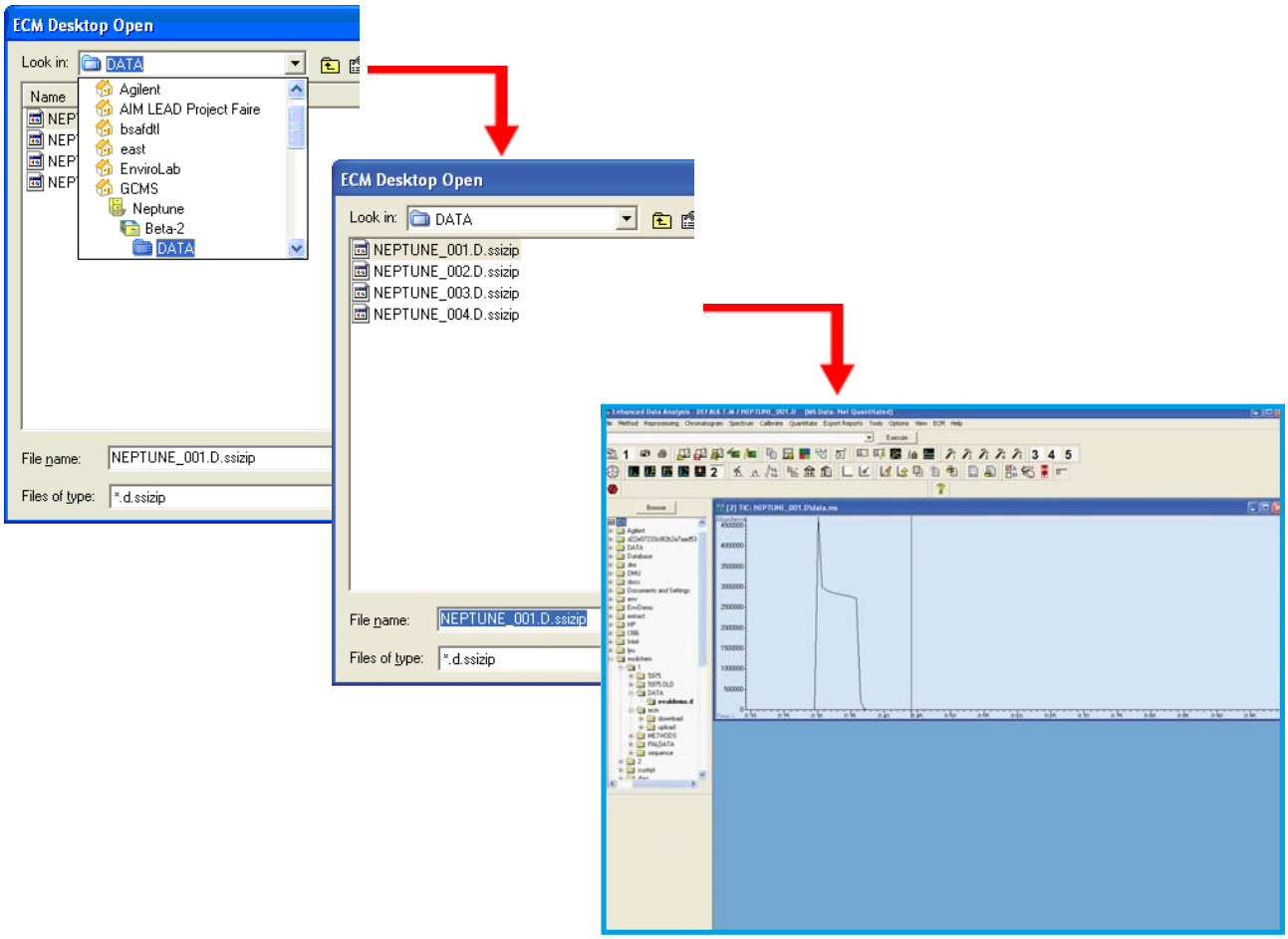

Figure 3. Load Data File from ECM copies and loads the data file from ECM onto the local GC/MSD ChemStation.

The user modifies the master method and master sequence as appropriate for data acquisition, checks the sequence parameters for completeness, and runs the sequence from the GC/MSD ChemStation. Once the acquisition is complete, the acquired data are automatically stored into the ECM repository. The user can then load the data file from ECM via the “Load Data File from ECM” in the ECM menu in the “Data Analysis View onto the local GC/MSD ChemStation.

The GC/MSD ChemStation data are stored in ECM as SSIzip files. An SSIzip file wraps the entire data set, including sequence and method information, ensuring full data integrity in ECM. A single run data file (*.d.SSIzip_ wraps the *.d file, ACQ.m, and DA.M. Once a data file or method has been placed in ECM, subsequent uploads will be returned to the same place.

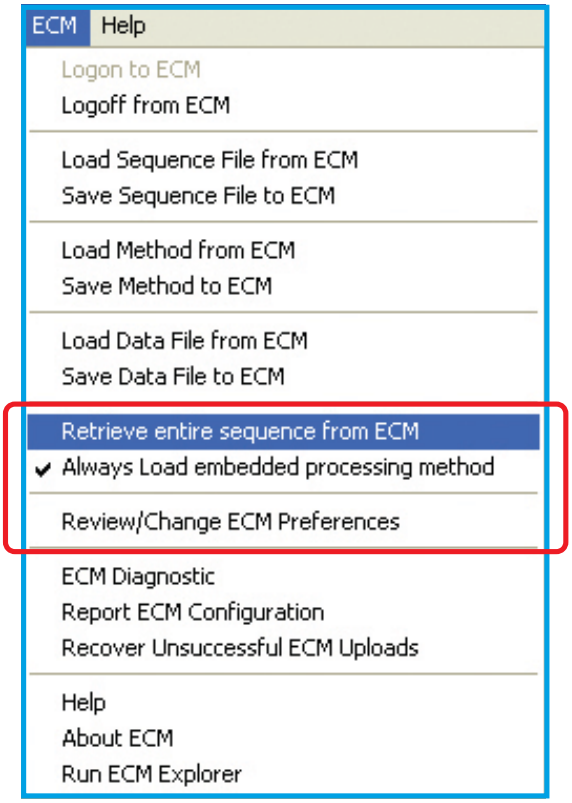

Figure 4. Additional capabilities are available from the Data Analysis ECM Menu.

ECM Diagnostic Capability

A user logged into ECM can run a diagnostic to verify fundamental capability of the Integration of GC/MSD ChemStation with OpenLAB ECM, the robustness of the network, and the availability of the OpenLAB ECM server.

Recover Unsuccessful Uploads

Integration of GC/MSD ChemStation with OpenLAB ECM is designed to be fault tolerant of the network or ECM becomes unavailable. When this occurs, the system will remember files that should have been uploaded and this menu will attempt to upload files that previously had been unable to upload successfully. If a user is not logged into ECM, no recovery of file uploads will be possible.

Additional Capabilities in Data Analysis

The ECM menu in the Instrument Control view and Data Analysis view is similar, except the Data Analysis view has the following two additional functions:

- Retrieve entire sequence from ECM. This will present a batch or sequence selection interface. Once the batch or sequence is selected, all of the data files and the final sequence file be retrieved and loaded into Data Analysis.
- Always load embedded processing method. Data files uploaded to ECM will always include embedded method for processing. This menu item specifies that the embedded method will automatically be loaded whenever a data file is loaded via Load Data File from ECM.

Data in ECM Are Organized in Clear Four-Level Hierarchy

Within ECM, data are organized in a clear four-level hierarchy of Location, Cabinet, Drawer, and Folder (LCDF), called ECM Path in the GC/MSD ChemStation. Users can either select an existing LCDF or create the LCDF structure dynamically. The naming conventions for Drawer and Folder can be dynamic, for example, the name of a

Drawer can be based on the instrument name and the name of a Folder on the operator name (Figure 5). With this setting, all data from Instrument1 would be saved into a Drawer Instrument1. Data acquired by user Joe Miller would be saved to a Folder Joe Miller, and those acquired by May Smith to a Folder Mary Smith. This organization of the data makes it easy for users to access their own data. In addition, on the ECM server, access restrictions can be set on each hierachical level. User privileges could be set, for example, to allow Mary Smith to write into her folder but prevent her from changing data in Joe Miller's folder.

Finding Data in ECM is Fast and Easy

Users can search for the data they want to review or reprocess by using the powerful search functionalities provided by ECM. GC/MSD ChemStation data stored in ECM can be indexed for a large number of keys. This indexing of the data allows users to quickly find the data they need. Searches can be started from the GC/MSD ChemStation and can be simple or detailed. The example of a simple search shown in Figure 6 retrieves all data files that contain "paracetamol" anywhere in their index. For an example of a more specific search, the Advanced Search option retrieves all GC/MSD ChemStation data files acquired by Mary Smith containing a peak named "paracetamol" at a relative amount exceeding 20% of the sample. From GC/MSD ChemStation, users can search for data files, methods (*.M.SSIzip), or sequences (*.S.SSIzip) stored in ECM. A search for data files retrieves Single Runs (*.D.SSIzip) and Sequence Data Containers (*.SC.SSIzip) generated using GC/MSD ChemStation Rev E.00.00.

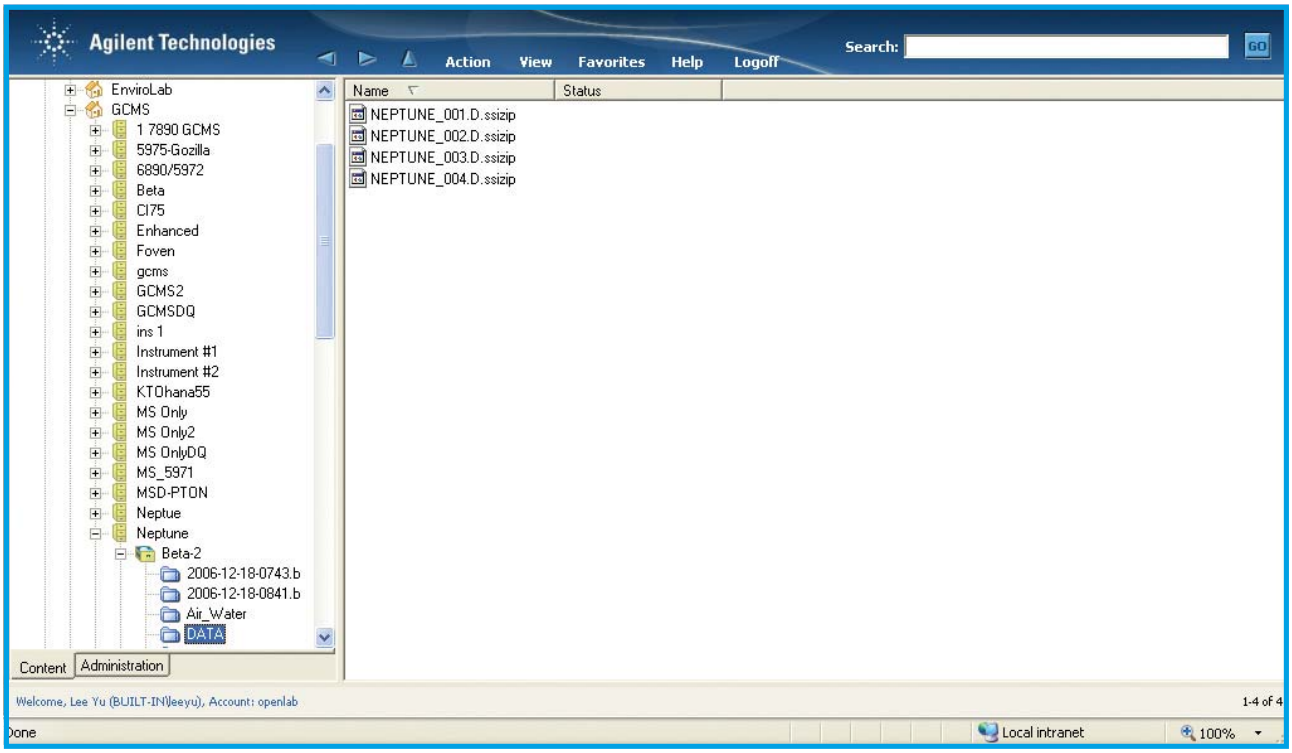

Figure 5. Data are organized in a clear four-level heirarchy of Location, Cabinet, Drawer, and Folder (LCDF), called ECM Path.

Automatically Generated PDF Reports

In addition to storing analytical raw data from the GC/MSD ChemStation into ECM, six specific reports are generated automatically in PDF format: Autotune, Tune Evaluation, Air-Water Check, Quant, Library Search, and Area Percent. The PDF reports in ECM provide a secure and revision-controlled storage of your GC/MSD ChemStation analytical reports.

Using the optional ECM PDF template extraction plug-in, PDF reports can be indexed for searching. The ECM search functionality allows users to search and retrieve GC/MSD ChemStation PDF reports from within the GC/MSD ChemStation user interface. In addition, the GC/MSD ChemStation PDF reports stored in ECM can be electronically signed using the ECM eSignature plug-in, which creates a visible eSignature on the PDF report (Figure 7).

If the OpenLAB Business Process Manager (BPM) is part of the ECM installation, any file generated can be submitted to a user-defined process. For example, the PDF reports can be part of an approval workflow requiring several parties to electronically sign off on the report. Or the GC/MSD data can be automatically evaluated for pass/fail criteria and the appropriate user notified

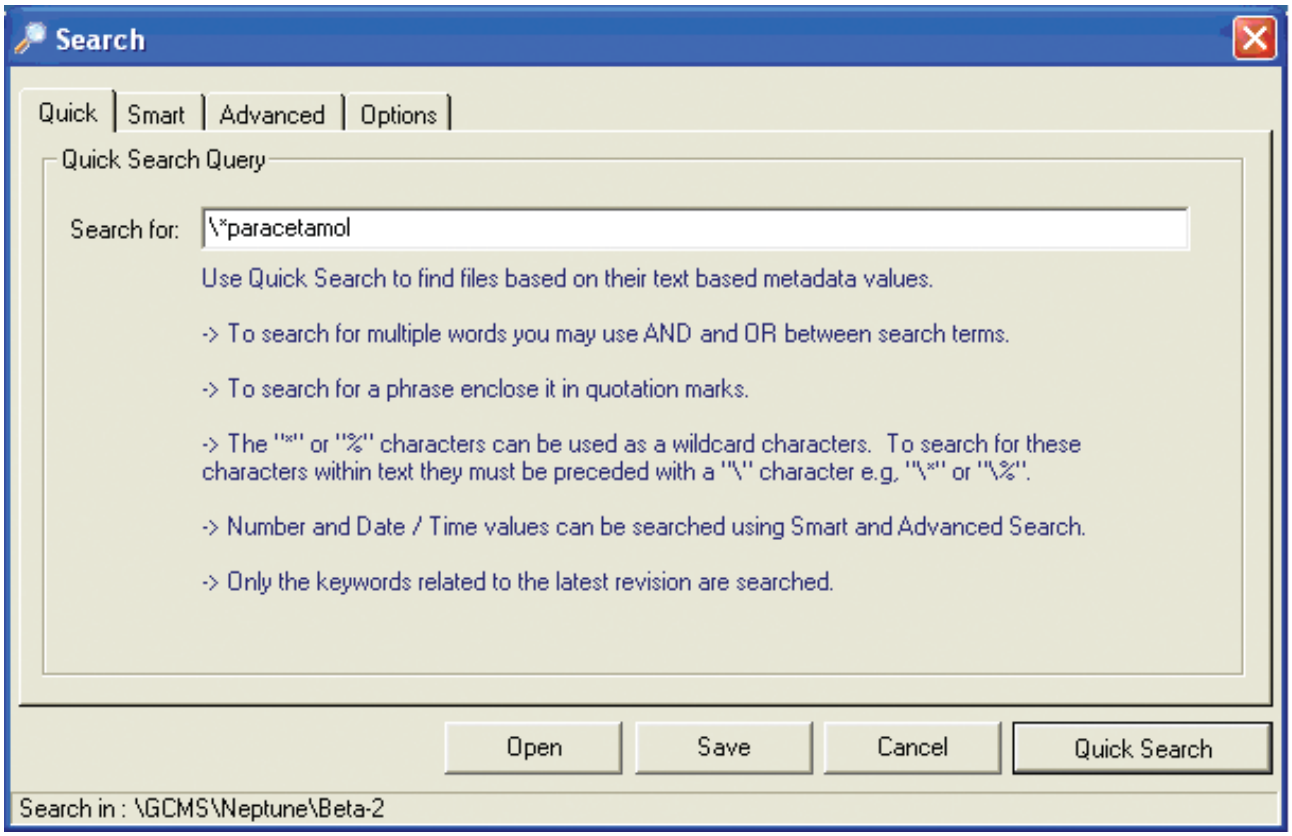

Figure 6. Searching ECM data is enabled from the GC/MSD ChemStation.

immediately in the event of either case. For more information on BPM, please refer to the Agilent Technical Overview "Business Process Management from Agilent Technologies" (publication number 5989-1668EN).

Requirements and Installation

Unless otherwise specified, integration of GC/MSD ChemStation with OpenLAB ECM applies to all application modes, that is, Enhanced Mode, EnviroQuant, DrugQuant, and Aromatics in Gasoline. However, it does not apply to G1732AA MSD Security ChemStation Software.

The client application offered by the integration of GC/MSD ChemStation with OpenLAB ECM requires:

- MSD Productivity ChemStation E.00.00 software and license
- OpenLAB ECM server (Rev. 3.2 or 3.3.1)

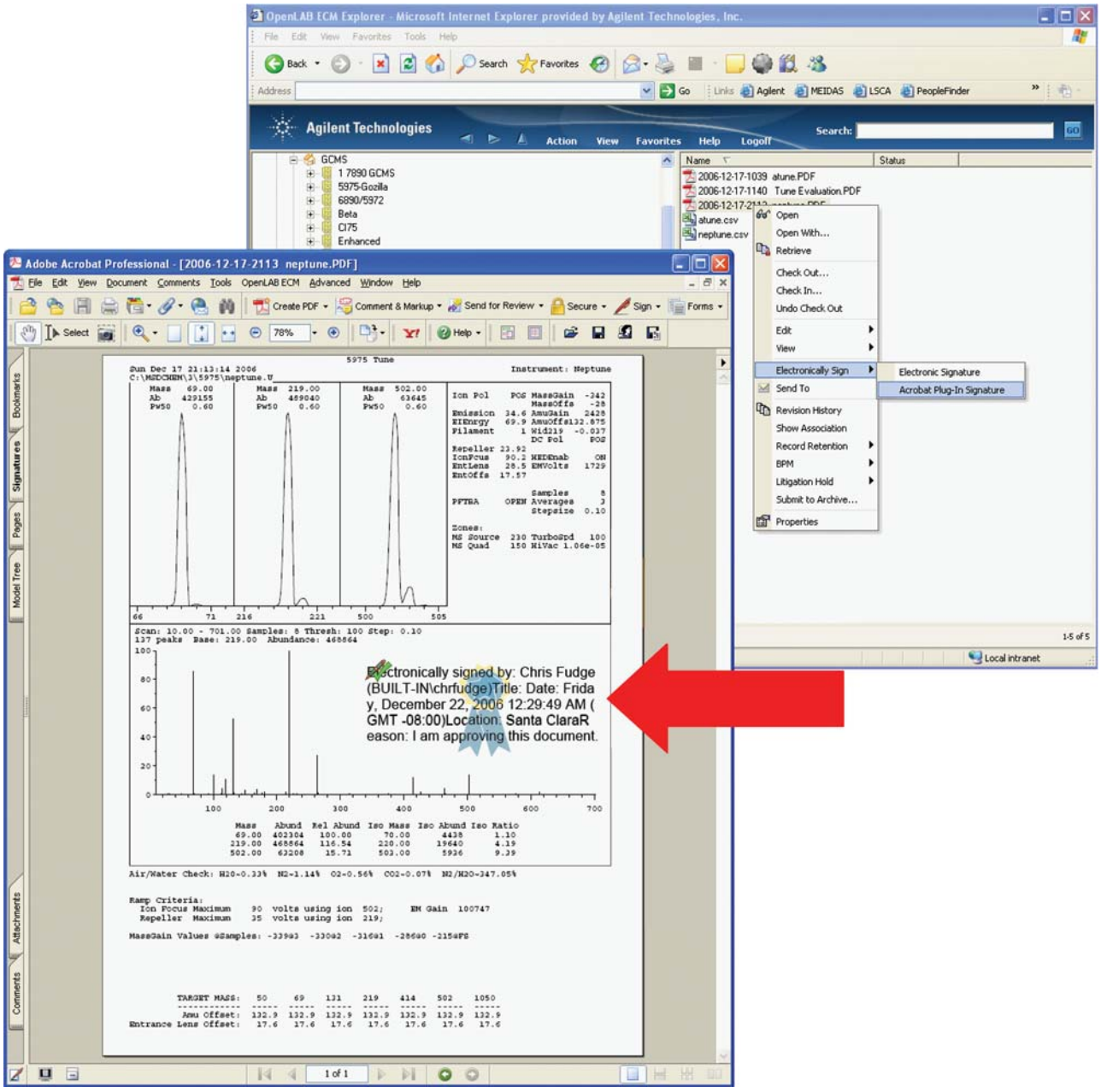

Figure 7. ECM provides visible electronic signatures for PDF documents.

- One OpenLAB ECM Web client (Rev. 3.2 or 3.3.1) and one OpenLAB ECM desktop integration per client PC
- Microsoft .Net 1.1 installed on the GC/MSD ChemStation PC
- Adobe® Acrobat® Standard or Professional Rev. 5.x, 6.x, or 7 (if PDF reports are desired)

Optional components include:

- OpenLAB BPM Client software
- OpenLAB eSignature Plug-in for Adobe Acrobat
- OpenLAB Adobe Acrobat PDF Template Plug-in

Limitations of the Integration of GC/MSD ChemStation with OpenLAB ECM

The use of other ECM client services, such as the ECM Scheduler, ECM Print Services with files created, maintained, and manipulated by the GC/MSD ChemStation, is not necessary with the Integration of GC/MSD ChemStation with OpenLAB ECM. Furthermore, GC/MSD ChemStation–ECM Integration is designed to operate with a single ECM server. Operations that move or rename GC/MSD ChemStation data within ECM are not supported.

Although the GC/MSD ChemStation will support up to four instruments per PC, only one instrument is supported when the GC/MSD ChemStation–ECM Integration is used. This restriction improves the reliability of the integration of GC/MSD ChemStation with ECM and avoids potential file management issues on both the GC/MSD ChemStation and ECM.

The GC/MSD ChemStation–ECM Integration does not support GC-only configurations or sequencing operations that acquire more than one data file, that is, dual tower operation methods.

Advantages of Integration of GC/MSD ChemStation with OpenLAB ECM

ECM allows the storage of all your data in compliance with 21 CFR part 11.

- Access to ECM is controlled. Users need to authenticate with their user name and password. Users log onto ECM from the GC/MSD ChemStation.
- Automatically store data acquired via the GC/MSD ChemStation into ECM immediately after data acquisition, thus ensuring that data generation and all changes to the data are under audit trail and version control.
- Access to the data in ECM and what each user is allowed to do with that data is controlled by user privileges.
- All data and records stored in ECM are protected. Users have no direct access to the physical files stored on a secure file server. All metadata, descriptive information for each file within the ECM, is stored in a relational database (Oracle® or Microsoft SQL Server™).
- All actions in ECM are under audit trail control.
- ECM ensures that accurate and complete copies of the data are kept, Any changes to the data result in a new version of the data file, thus ensuring data integrity and traceability.
- ECM provides electronic signatures, allowing users to sign off on data.
- Training users on the new system is straightforward because they are working from the familiar GC/MSD ChemStation.

The Complete Solution

In addition to data generated with GC/MSD ChemStation, organizations generate millions of electronic files each year, including:

- Business forms
- Corporate policies
- Design specifications
- Employee records
- Financial records
- Images
- Operating procedures
- Presentations
- Quality records
- Reports
- Data
- Spreadsheets

Clearly, a powerful way of organizing and harnessing data for easy access, retrieval, and re-use is needed in today's competitive business environment. The best solution for this "information overload" challenge is a solid enterprise content management strategy.

Storing, organizing, and protecting your company's critical electronic records are only part of the solution. Making information accessible when, where, and how you need it is what makes the

OpenLAB Enterprise Content Manager (ECM) system a powerful tool for increasing your knowledge base. The OpenLAB ECM system provides a flexible, scalable architecture designed to grow with your business. From a single-user system to a corporate-wide enterprise implementation, the OpenLAB ECM system can provide the level of data storage and protection that your company's intellectual property requires.

For More Information

Please visit the Agilent Web Site (http://www.agilent.com/chem) for the Agilent GC/MSD ChemStation and the OpenLAB ECM products.

The following documents are available for further reading:

- GC/MSD SW Specifications "MSD Productivity ChemStation Revision E.00.00 Specifications" (5989-6115EN)
- White Paper "OpenLAB ECM Technical Overview" (5989-6104EN)

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