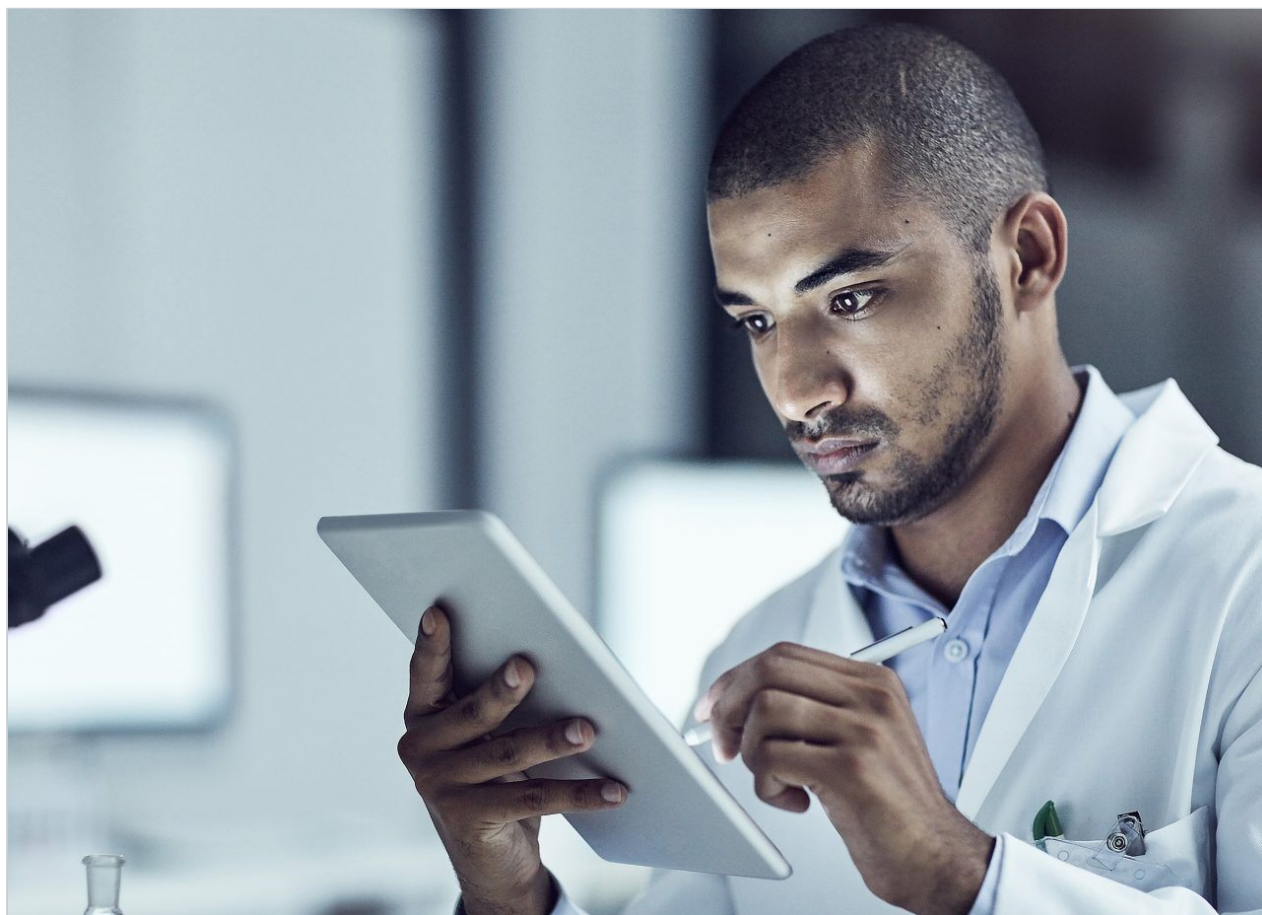




OpenLynx Open Access and Software Tools for Managing an Open Access Laboratory Environment

Waters Corporation



This is an Application Brief and does not contain a detailed
Experimental section.

Abstract

Maximum efficiency is essential for LC-MS labs challenged by throughput requirements and the management of data from a variety of systems and users. Analyzing routine samples and returning the results to chemists can easily consume an analyst's entire day, leaving them with little time to focus on tasks that require their expert attention. Walk-up open access systems allow chemists to analyze their own samples, freeing up analysts' time for more challenging analyses without compromising the quality of the final results.

The Waters OpenLynx Open Access Application Manager for MassLynx Software offers the power of chromatography and mass spectrometry to chemists who are not analytical instrumentation specialists. To minimize the learning curve for instrument operation, OpenLynx Open Access leads chemists through sample submission, method selection, and reporting options. The system is maintained by a system administrator who predefines the system configuration, available experimental methods, processing criteria, and reporting options. By allowing chemists to submit their own samples, routine analyses can be performed more efficiently, leaving instrumentation experts more time to focus on advanced analyses.

Introduction

Open access LC/UV, LC-MS , LC-MS/MS , and GC-MS

The OpenLynx Open Access Application Manager is designed to allow chemists to walk up to a terminal and log in samples onto an instrument, while inputting the minimum of information needed for the sample run. OpenLynx Open Access allows the system administrator to maintain control over the open access systems and to track the performance of each system. It also facilitates batch processing and reporting of results.

OpenLynx Open Access offers comprehensive capabilities:

- Simplified sample submission process – A single page login or a step-by-step, wizard-enabled process allows users to enter their name and sample information, and select pre-determined experimental methods and processing criteria
- Exact mass measurement utilization – For use with the appropriate mass spectrometers
- Summary report generation – Reports are automatically printed, emailed, and viewed via the OpenLynx

browser, containing sample found/not found information, purity, probable elemental composition (with exact mass MS), chromatograms, and spectra

- Walk-up optimization of MS /MS methods and quantification of compounds of interest – Combines OpenLynx Open Access with QuanOptimize and QuanLynx Application Managers
- Advanced search – Spectral library generation and searching
- Automation of routine system administration tasks – Through the use of OpenLynx Open Access Toolkit (OA Toolkit)

Results and Discussion

Software Setup

Defining parameters

OpenLynx Open Access allows remote users to run samples on the acquisition computer. For OpenLynx Open Access users to be successful, the administrator defines (via the OpenLynx method) the sample information that users must provide when running samples. An intuitive OA Login setup wizard simplifies the system configuration and administration workspace to include only the analytical features the administrator uses.

The administrator selects the fields that appear when remote users log in samples using OpenLynx Open Access via the Walk-up tab of the OpenLynx method (Figure 1). They can designate fields as mandatory so that login will not proceed unless the remote users enter values for these fields. They can also define upper and lower limits for the value of numeric fields. In addition, the administrator can define the format for text that remote users enter in text fields.

Default.olp - OpenLynx

File Edit View Help

Quality Control | MS Process | Spectrum Test

Walk-up | MS+ Data | MS- Data | DAD Data | Instrument

Description:
10 ul injection LC

Input Fields:
-None-

Edit Fields

Maximum Samples: 1

Priority Process: ☐

Night Time Process: ☐

HPLC File: ☐

Time of Analysis (mins): 0

Create Failed Samples File: ☐

Acquisition:

MS Tune: Default

MS Method: Default

Inlet Method:

Injection Volume (ul): 10.000

Pre-Run Method: None-

Post-Run Method: None-

Switch Method: None-

Fraction Method: None-

Loop Mode: ☐ LoopTime (mins): 0.00

For Help, press F1

NUM

Figure 1. OpenLynx method showing some of the OpenLynx Open Access input fields.

Setting options for users

Using the administrator mode of OpenLynx Open Access, the administrator defines how users login samples via a number of options (Figure 2). Login setup ranges from changing the window appearance to allowing

users to create their own user name. Notification of users via email can be enabled, as can barcode support. OA Login can be configured for use with either OpenLynx (sample processing) or AutoPurify (fraction processing).

QALogin Options

Mode of operation
☒ OpenLynx ☐ AutoPurify

Default Job Identifier
Base Job name:
Next Job number:
☒ Allow user to change job identifier

Default Data File Name
☐ Use Sample ID for file name
☐ Use Incremental File Naming
Base File Name:
Increment Number:

E-Mail
☐ Enable e-mailing of user report

QuantLynx Results Location
☐ Enable directory specification

Plate Layout Display
☒ Display Plate Layout

Login Screen Appearance
Title Bar Text:
Login Button Text:
Batch Identifier Text:
User Name:
☒ Allow user to create own user name
Single Sample File Login:
☐ Allow single sample file login
Printing of QALogin Report File:
☐ Enable User Print Control
Barcode Support:
☐ Use Batch ID as Sample List File Name
Path:
Sort Methods By:

OK Cancel

Figure 2. Administrator-set OpenLynx Open Access options.

Setting file options

The administrator sets several file options. These include specifying the location where the OpenLynx methods, OpenLynx status file, and HPLC files are located. The administrator can set which methods are visible to users, along with the format needed for the text fields.

Configuring quality control runs

The administrator can configure OpenLynx to check that the LC and MS instrumentation are working correctly, thus ensuring the consistency of the data. The quality control feature (Figure 3) allows users to run a standard and have it compared to the results of the same standard that was run at an earlier time. Values that can be used to confirm system operational performance include peak retention time, peak area, the presence of specific masses or wavelengths, and spectral intensity.

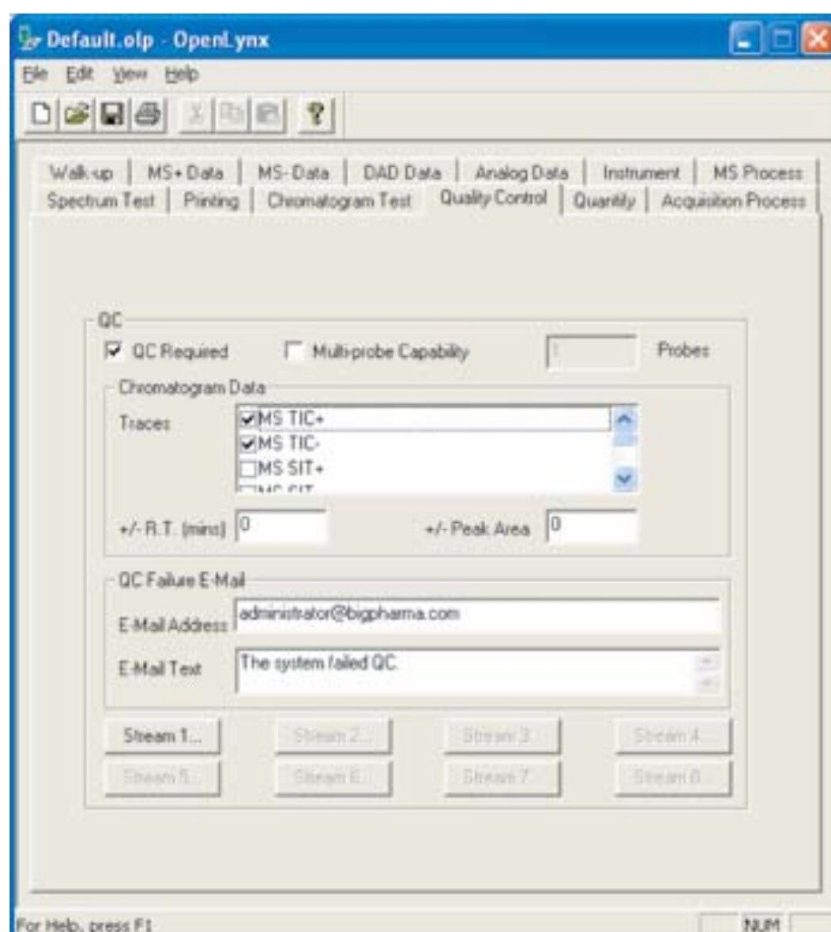


Figure 3. OpenLynx Open Access quality control options.

Before a QC comparison can be run to check the system, there must be an OpenLynx method that contains

the expected results from a standard. The QC run acquires data from a sample with a known retention time and peak intensity and then compares the results to the values defined in the OpenLynx method.

OpenLynx Open Access Toolkit (OA Toolkit)

OpenLynx OA Toolkit allows the creation and administration of OpenLynx Open Access users. It can push user information to OpenLynx Open Access PC s across the same network, as well as gather existing OpenLynx Open Access user information from OpenLynx Open Access PC s. It can create new project directories for the OpenLynx Open Access users and can move the resulting project data (such as raw data files) as it is created. The software can monitor numerous instrument PC s, providing on-the-fly information about their status as well as the status of their batch queues – all from a central location. It ensures confidence in analytical results with password protection for open access users.

The OpenLynx OA Toolkit includes the following key features:

- Administration Tool (Figure 4) – Enables an administrator to create and manage all OpenLynx Open Access users from a single PC , and replicates that information to multiple OpenLynx Open Access PC s and Acquisition PC s
- OA Toolkit Service – Runs in the background on one or more Acquisition PC s, monitors sample batches submitted by OpenLynx Open Access users that were uploaded from the Administration Tool
- Remote Status Monitor (Figure 5) – Enables any user to monitor the status of Acquisition PC s and their batch queues from a single PC

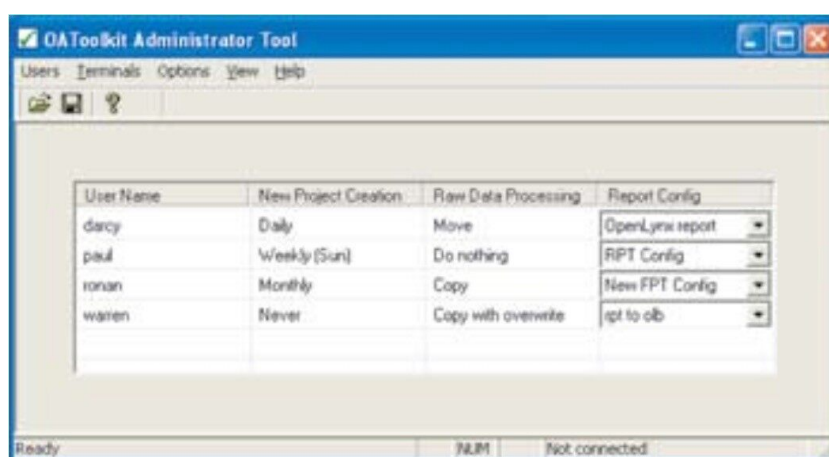


Figure 4. OpenLynx Toolkit Administrator Tool.

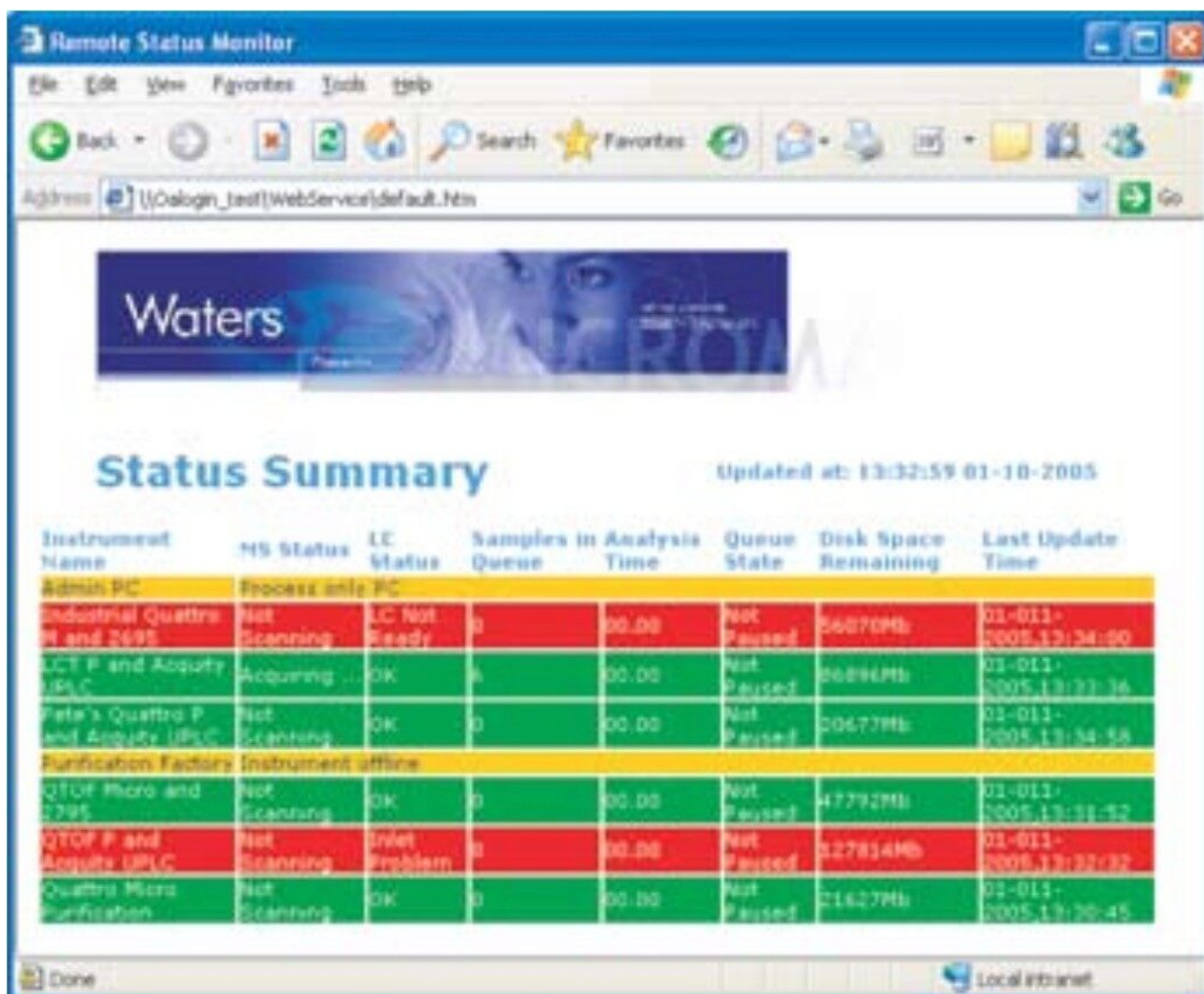


Figure 5. Remote Status Monitor.

Additionally, the OpenLynx OA Toolkit Service:

- Relocates data produced during the processing of an OpenLynx Open Access user's batch of samples
- Creates new project folders in which to store the processing data on a timed basis
- Converts report files to different formats (XML, HTML, or text)

Logging Samples

Login samples window

Running samples using OpenLynx Open Access (Figure 6) involves entering sample information to correctly identify the samples and loading the samples into the autosampler. The methods available to the users

depend on selections made by the administrator.

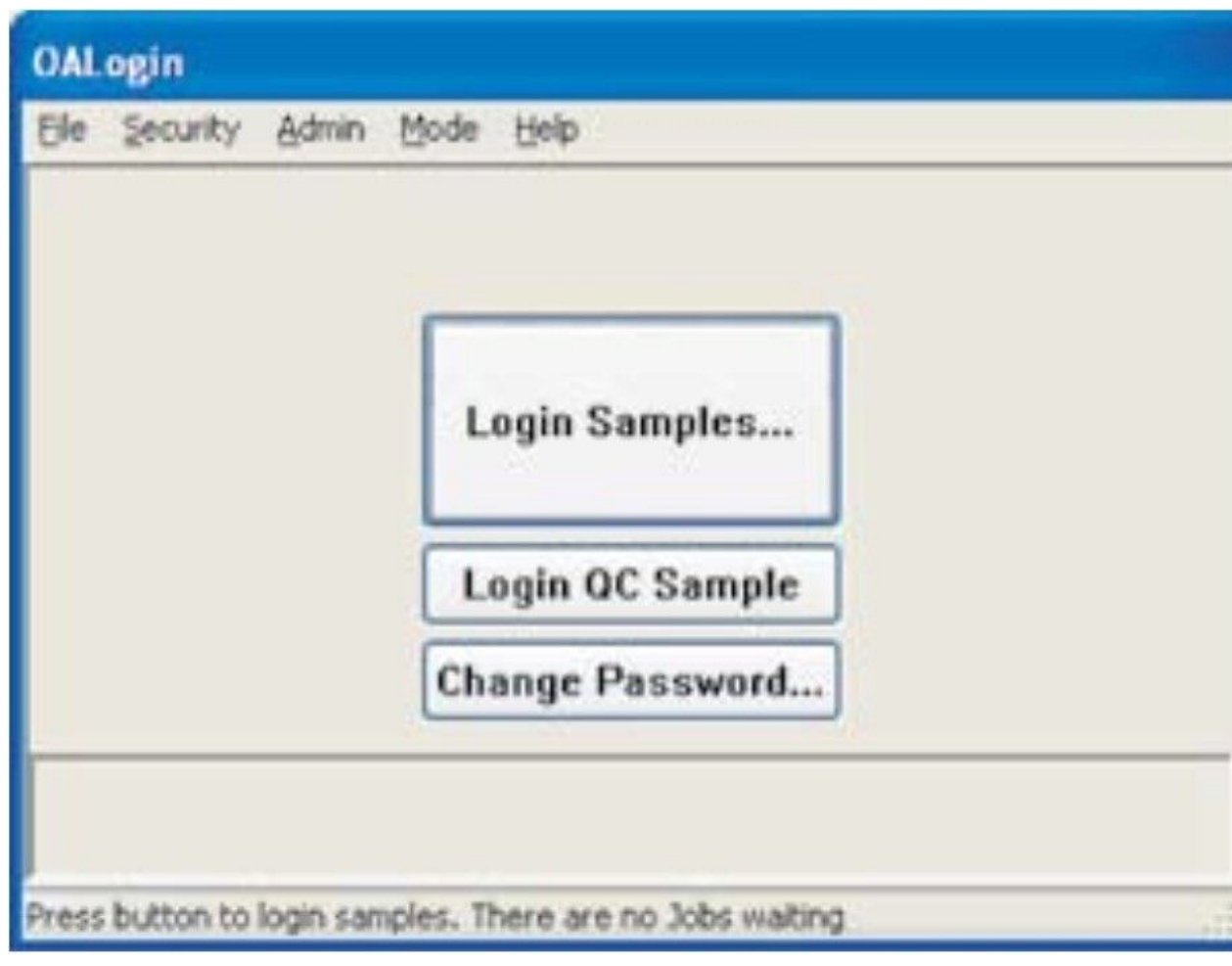
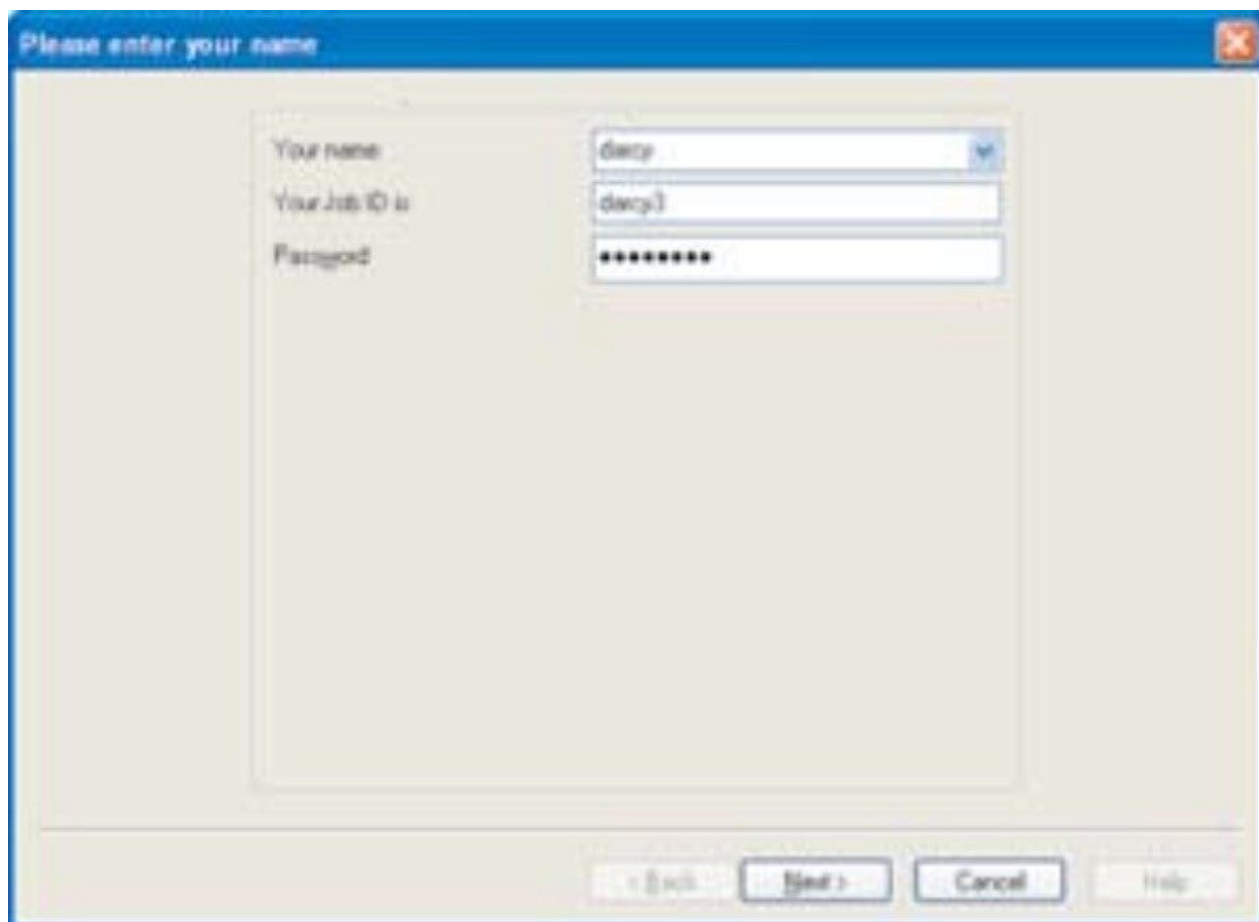


Figure 6. OpenLynx Open Access window.

If the administrator enables user passwords (using OpenLynx OA Toolkit), the user must enter their designated password before they can login samples (Figure 7). If they enter an incorrect password, an error message appears and they cannot continue until the correct password has been entered.



Please enter your name

Your name: darcy

Your Job ID is: darcy3

Password: *****

Back Next > Cancel Help

Figure 7. Entering user password.

Single-page log-in vs. wizard

OpenLynx Open Access displays the wizard for sample login by default. However, the administrator can allow OpenLynx Open Access users to use a single-page dialog box (Figure 8) for “single shot” samples. Users can enter multiple samples in this way. OpenLynx Open Access views the samples logged in as a single job.

The screenshot shows a software window titled "DMLogin" with a blue header bar. Below the header, there are two tabs: "Sample" and "Security", with "Security" being the active tab. The "Login Information" section contains four input fields: "User Name" (containing "New User"), "Job ID" (containing "New User"), "Method" (containing "DM200"), and "Description" (containing "200 ul injection LC"). Below these fields is a checkbox labeled "E Mail Results to Address". The "Sample Details" section contains six input fields: "Vial", "SampleID", "SampleGroup", "Man1", "Man2", and "VialLength1". At the bottom of the window, there is a status bar that says "Press button to login samples. There are no jobs waiting." and a button labeled "Login Samples".

Figure 8. Single-page dialog box.

The single-page login contains most of the selections on the wizard pages (Figure 9) necessary to schedule samples. The benefit of the single-page login is the speed of entering information for a single sample in a single dialog box, rather than through a wizard. This wizard is beneficial when logging in larger sample sets.

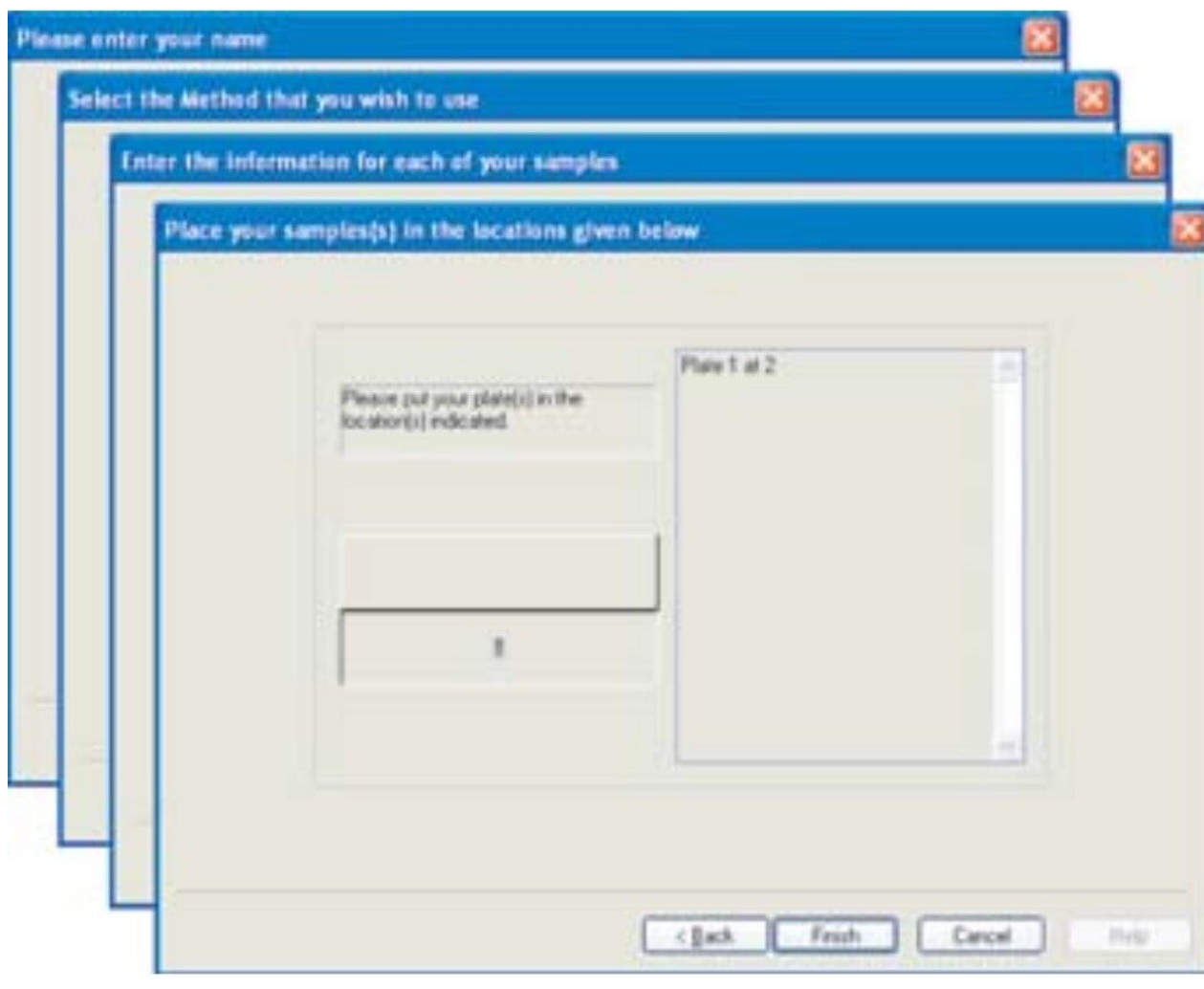


Figure 9. With the wizard, walk-up users enter their name, choose a method, enter sample information, and place the sample in the autosampler.

Loading samples into the autosampler

There are two ways to load samples into the autosampler. The system administrator designates each plate in the autosampler as either "single shot" or "whole plate" login. If a plate is designated for single shot login, the user enters data for their samples manually or imports data from a tab-delimited text file. OpenLynx assigns available positions for the samples on existing plates. If a plate is designated for whole plate login, the user prepares data in a spreadsheet or as a text file and imports it into OpenLynx Open Access. This is useful if the user needs to run a large number of samples in one run. OpenLynx reserves the entire plate for samples and the user selects the sample locations.

Typically, a system with multiple plates will have both single shot and whole plate login available.

Processing Samples

Processing data automatically

The administrator determines how OpenLynx processes the Open Access results. To configure OpenLynx Open Access to process data automatically, the administrator must create an OpenLynx method that defines the processing parameters.

The administrator must define the integration parameters for the type of data they want to process:

- MS + data – For positive ions (total ion chromatogram (TIC), base peak intensity (BPI), and mass chromatograms)
- MS – data – For negative ions (TIC , BPI , and mass chromatograms)
- Analog data – For up to four channels of analog chromatograms
- DAD data – For total absorbance chromatogram (TAC), BPI , and wavelength chromatograms

Specifying how peak detection occurs involves selecting the integration algorithm and parameters that control peak detection, enabling smoothing (if desired), and setting the smoothing parameters and setting threshold values.

When setting the integration and peak detection parameters (Figure 10), the administrator can specify which integration algorithm (standard or ApexTrack) to use; how the baseline will be treated for valleys, peak tailing, and drift; and how peak separation for fused peaks and shoulders will be handled. By enabling smoothing, noise will be decreased by filtering data points. Smoothing types include Savitzky-Golay and mean. The threshold values are set for one or more of the four threshold parameters: relative and absolute height and relative and absolute area. This option is used to remove peaks whose height or area is less than a specified percentage of the highest peak.

In addition to acquiring and processing data, quantitation and optimization can be performed through OpenLynx Open Access.

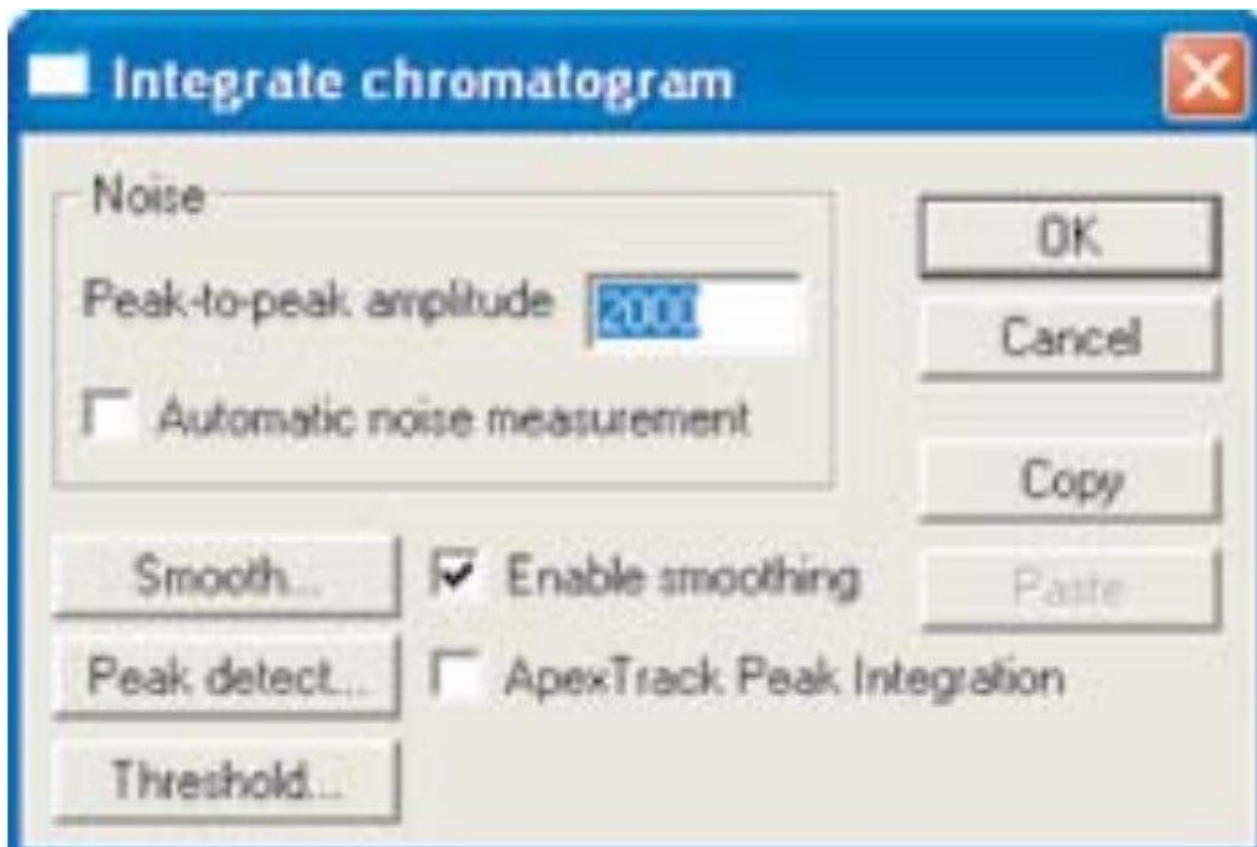


Figure 10. Chromatogram integration window.

Performing quantitation

Open Access quantitation is a way for the user to run quantitation analysis through OpenLynx Open Access (Figure 11). OpenLynx stores the conditions required for a particular quantitation analysis in an OpenLynx method. OpenLynx Open Access users select the OpenLynx method during login.

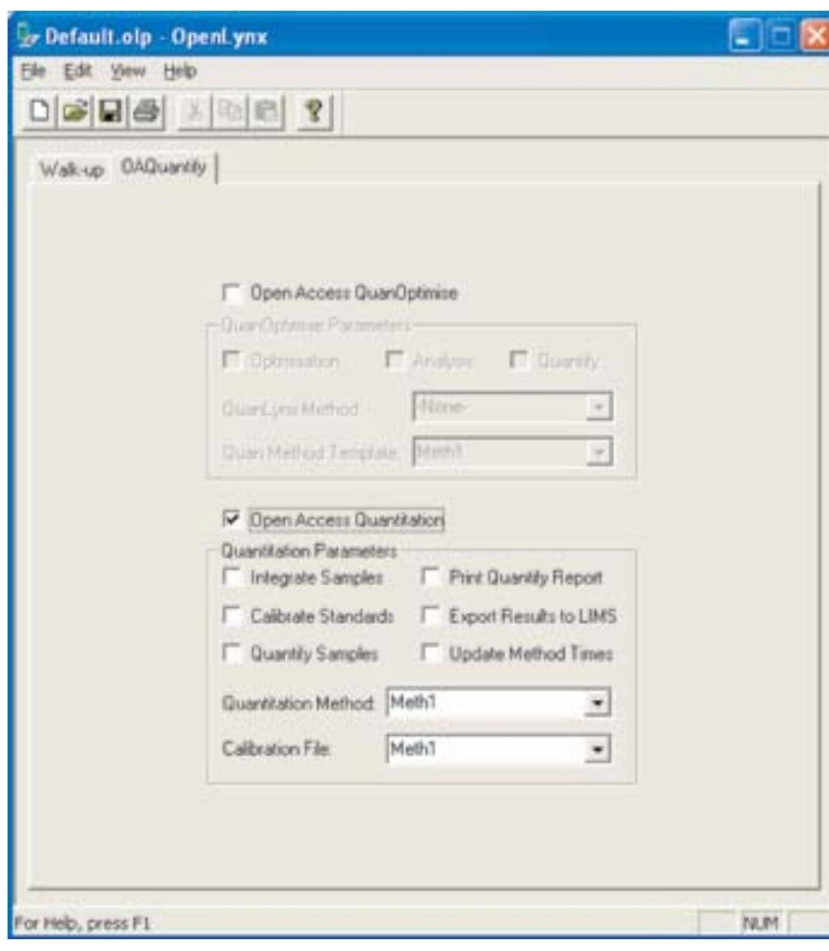


Figure 11. Open Access quantitation parameters.

Using Open Access quantitation, OpenLynx Open Access users can quantify the results as data are acquired. The processing steps available include:

- Integrating samples
- Quantitating samples
- Calibrating standards

Using QuanOptimize with OpenLynx Open Access

The optional QuanOptimize optimizes the acquisition and quantitation parameters for a particular experiment. Open Access QuanOptimize (Figure 12) generates MS and MS/MS parameters by optimizing the cone voltage, parent ion, and collision energy parameters. QuanOptimize then takes these MS methods and performs automated acquisition and processing using processing methods developed on the fly. It can quantify these results using specified methods. This technique is useful for high throughput screening.

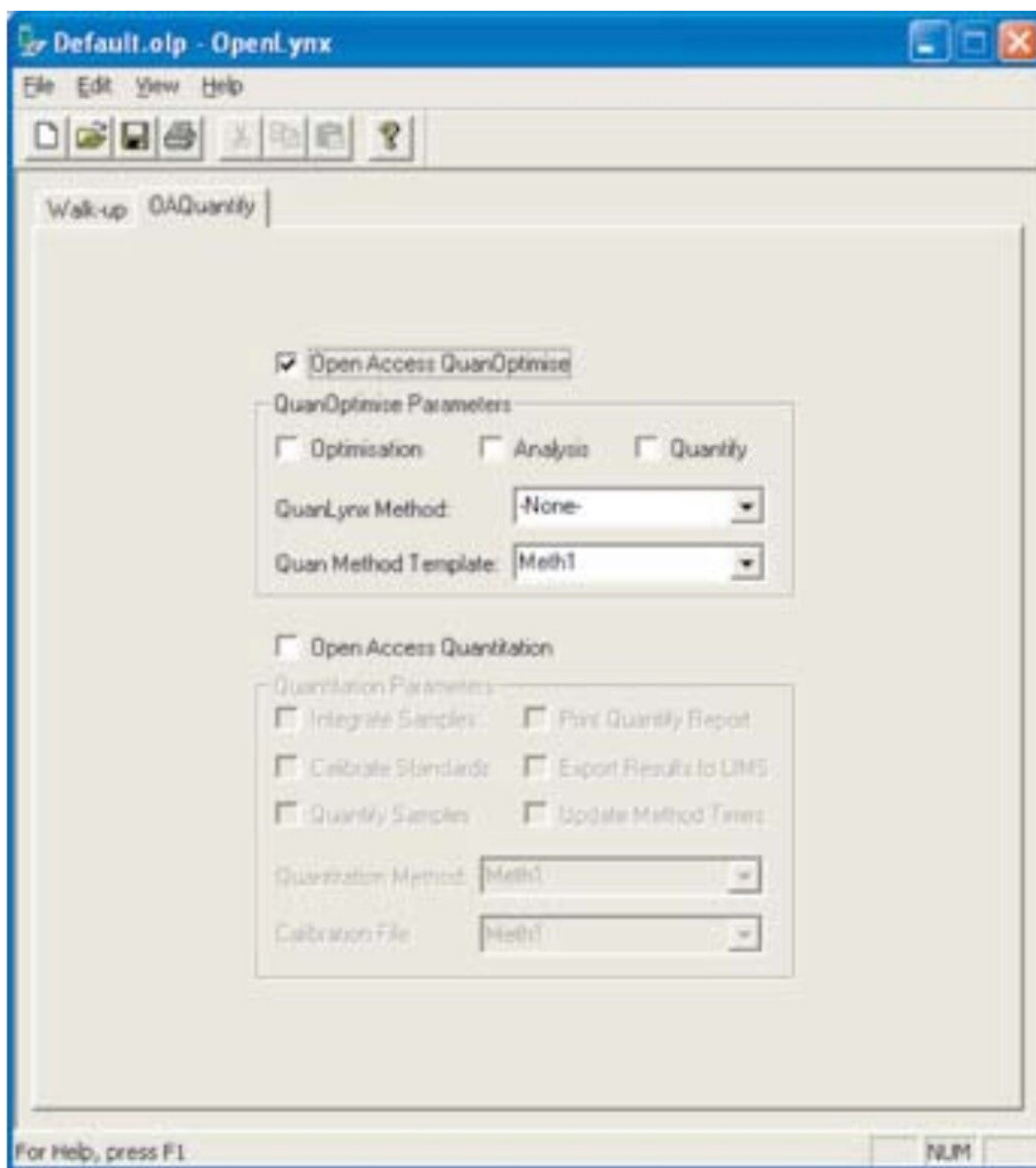


Figure 12. Open Access QuanOptimize parameters.

Reporting

Results reporting

Reporting in Open Access systems is facilitated by the OpenLynx Application Manager. OpenLynx can report

results using a flexible array of printed reports or through a results browser.

The standalone OpenLynx browser (Figure 13) is an interactive tool for viewing OpenLynx results and can be run on any windows PC without requiring a full MassLynx installation. Chemists can use the browser on their desktop PC to view the results (.rpt file format) that had been automatically emailed to them at the end of OpenLynx processing.

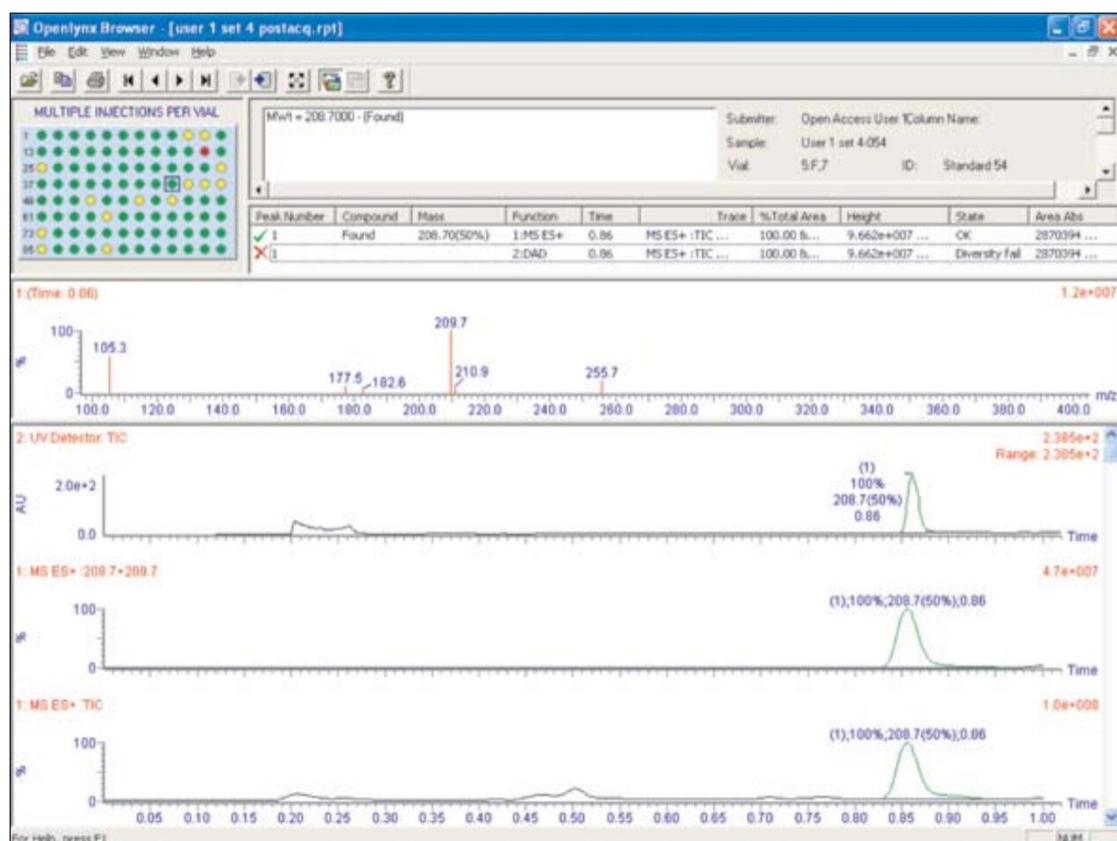


Figure 13. OpenLynx browser.

The OpenLynx browser presents a summary of results as a colorcoded (found/not found/tentative) map for easy visualization of analysis results. Chemists can access and review the data supporting any found/not found/tentative assignment by simply pointing and clicking on the sample location of interest. Chromatograms, spectra, sample purity, peak height, peak area, retention time, and other information can easily be reviewed within the browser.

Printing and distributing reports

OpenLynx creates an OpenLynx browser report file (.rpt) after it finishes a run and processes the data. This file resides in the OpenLynx Open Access\Reportdb folder. The file is named with the job number followed by

the extension .rpt when the user logs in to OpenLynx. OpenLynx report files may be exported in .txt, .tab, .csv, and .xml formats.

The administrator can configure OpenLynx Open Access so remote users can find the reports that OpenLynx generates after running samples. Information such as where to store reports and what print report format to use can be specified.

Conclusion

The OpenLynx Open Access Application Manager provides comprehensive, easy, and flexible open access walk-up LC/UV, LC-MS, LC-MS/MS, and GC-MS systems operation management for laboratories that have chemists with varying levels of instrumental analysis experience. With customizable batch processing and results review to support the large amounts of data resulting from high throughput analyses, a highly productive environment is ensured for high-volume laboratories.

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