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OpenLynx Application Manager: Quality Control Confidence for Open Access Systems

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

Abstract

This application brief focuses on the Quality Control capability of the Waters OpenLynx Application Manager for MassLynx 4.1.

Benefits

Extremely efficient and user-friendly method of automatically running periodic open access system evaluations

Introduction

Trusting in Your Results

Combinatorial chemistry programs generate hundreds of samples a day that require product confirmation and purity assessment. In these environments, easy, and expeditious analysis protocols are essential tominimize costly sample backlogs. To keep up with these sample loads, it is often necessary for highthroughput analytical systems to operate in batch mode as close to 24 hours a day, 7 days a week as possible.

Chemists in Medicinal Chemistry laboratories continually synthesize new compounds that require purity assessment and ID confirmation by UV and MS analysis. In these laboratories, open access systems allow chemists to walk up, log in their sample for LC/UV or LC-MS analysis, and then return to other tasks while their analysis is being run.

While open access systems service chemists well, the variation in the quality of samples submitted to the system has the potential to create system performance challenges, which must then be addressed by the system administrator. Increased throughputrequirements also mean that system administrators must be made aware if their systems begin to operate outside of acceptable performance criteria.

Quality Control in OpenLynx Open Access Systems

The Quality Control capability of the Waters OpenLynx Application Manager for MassLynx 4.1 Software offers both open access system administrators and walk-up users the ability to run a simple check of the entire system to ensure optimum performance. This Quality Control feature enables administrators to be notified

when occasional system errors occur (e.g., column failure, sample precipitation, or dry solvent reservoirs).

By utilizing Quality Control in OpenLynx, users and administrators can maintain a high level of confidence in their analyses.

Results and Discussion

How Open Access QC Works

Automating QC

System performance is monitored through the use of automated quality control injections, which can be scheduled to run at a certain time, or after a defined number of batches. In addition, the manual QC function allows the initiation of a test injection when necessary. This is useful in situations where chemists wish to ensure the performance of the system before they inject their sample. OpenLynx evaluates the results of the injection of a known standard, compares it against the standard information within the OpenLynx processing methods, and determines a suitable course of action.

Openlynx Qualty Control Setup Explained

Enabling QC in the OpenLynx Method

QC checking is enabled in the OpenLynx processing method (Figure 1). The administrator defines which traces will be monitored and what the pass/fail parameters will be. When setting up the QC injection, the administrator first analyzes a QC standard to determine compound retention time(s) and peak area(s) on the system when it is functioning correctly. These parameters are defined in the Stream Parameters window (Figure 2). By right clicking on an entry in the Chromatogram Parameters box, more lines can be added, meaning more peaks can be used for QC.

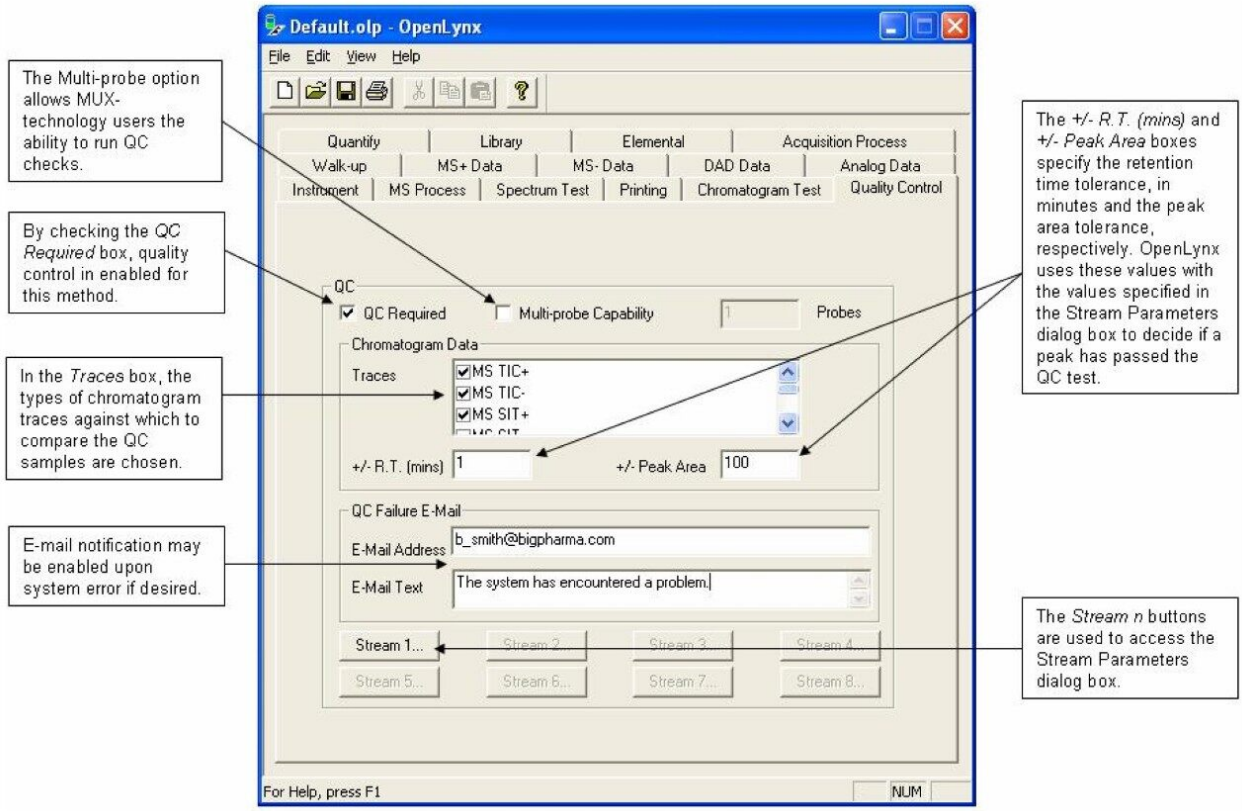

Figure 1. Defining QC parameters.

In the Intensity box, the parameters for peak height can be entered. The Mode can be either Relative % or Absolute. Relative % uses the specified Min Intensity value as a percentage relative to the base peak while Absolute uses the absolute intensity as specified in the Min Intensity field.

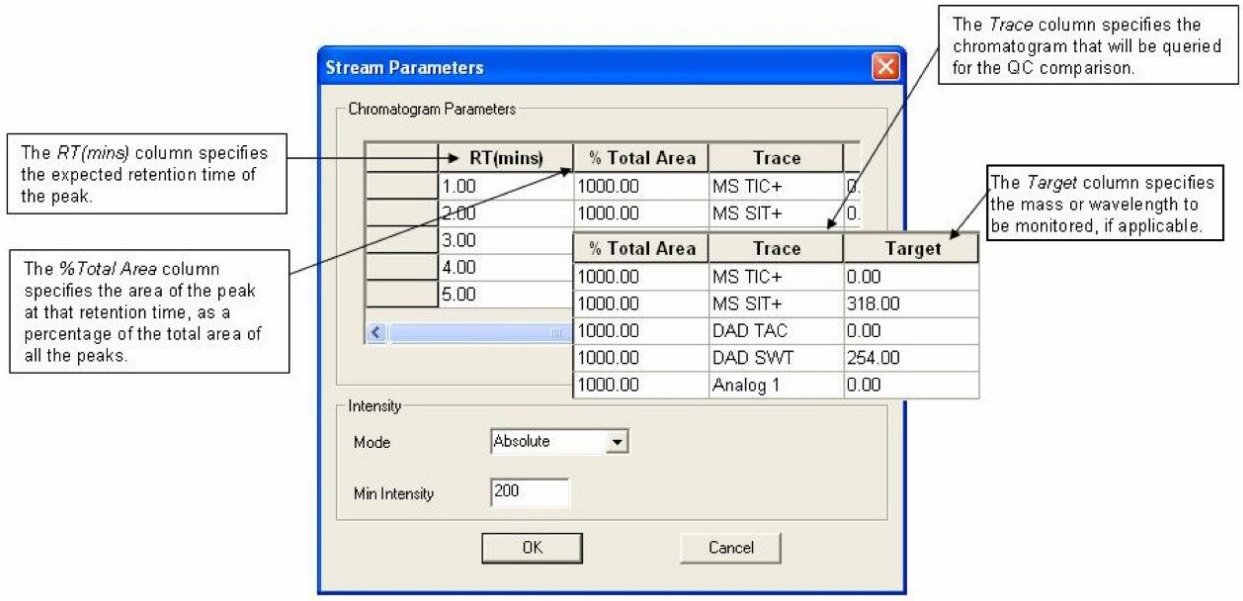

Figure 2. Stream parameters.

Enabling QC in OALogin

Quality Control must also be enabled via the OALogin page. This is done through the QC Setup option under the Admin menu. Choosing this opens the QC Options window (Figure 3).

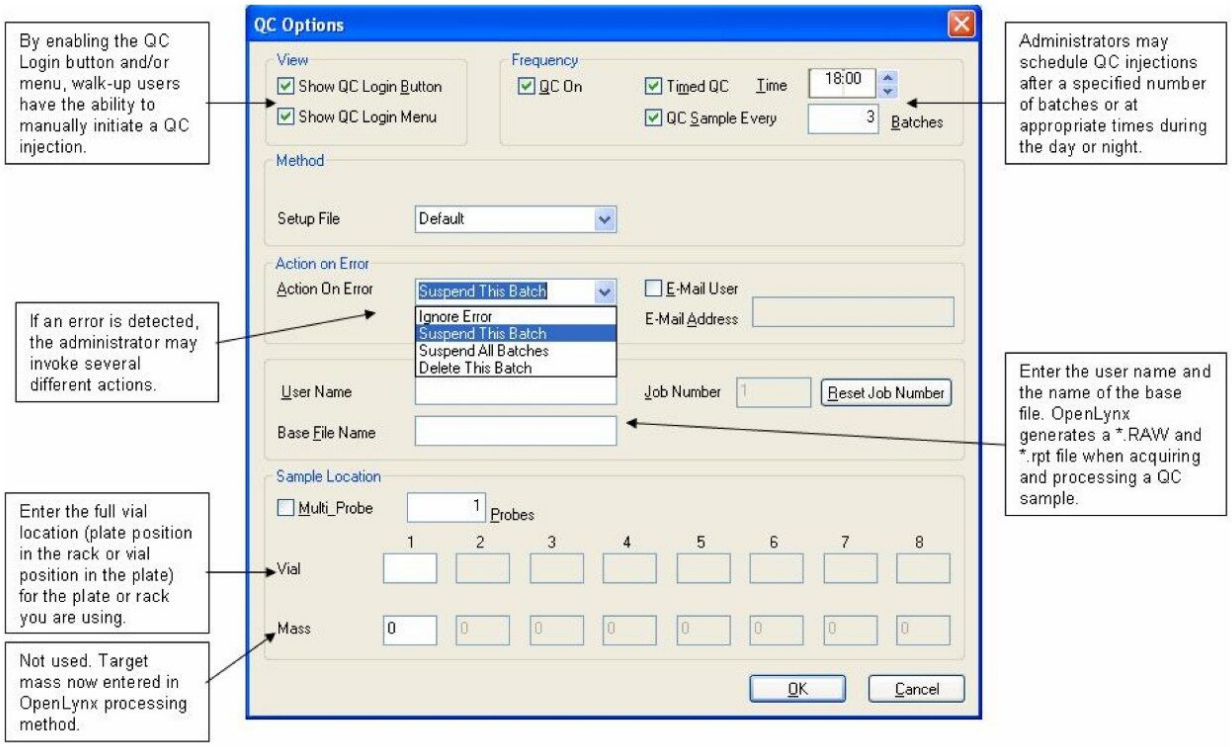

Figure 3. QC options from OALogin window.

Running QC Tests

Based on the QC settings enabled by the system administrator, performance checks will run automatically as scheduled, or walk-up users may initiate them as required. The OALogin screen (Figure 4) displays the Login QC Sample button when QC is enabled. Walk-up users can simply click on this button to queue up a QC run. If the QC sample does not meet the specified parameters, the system will take the chosen action and, if enabled, an e-mail notification will be sent to the administrator.

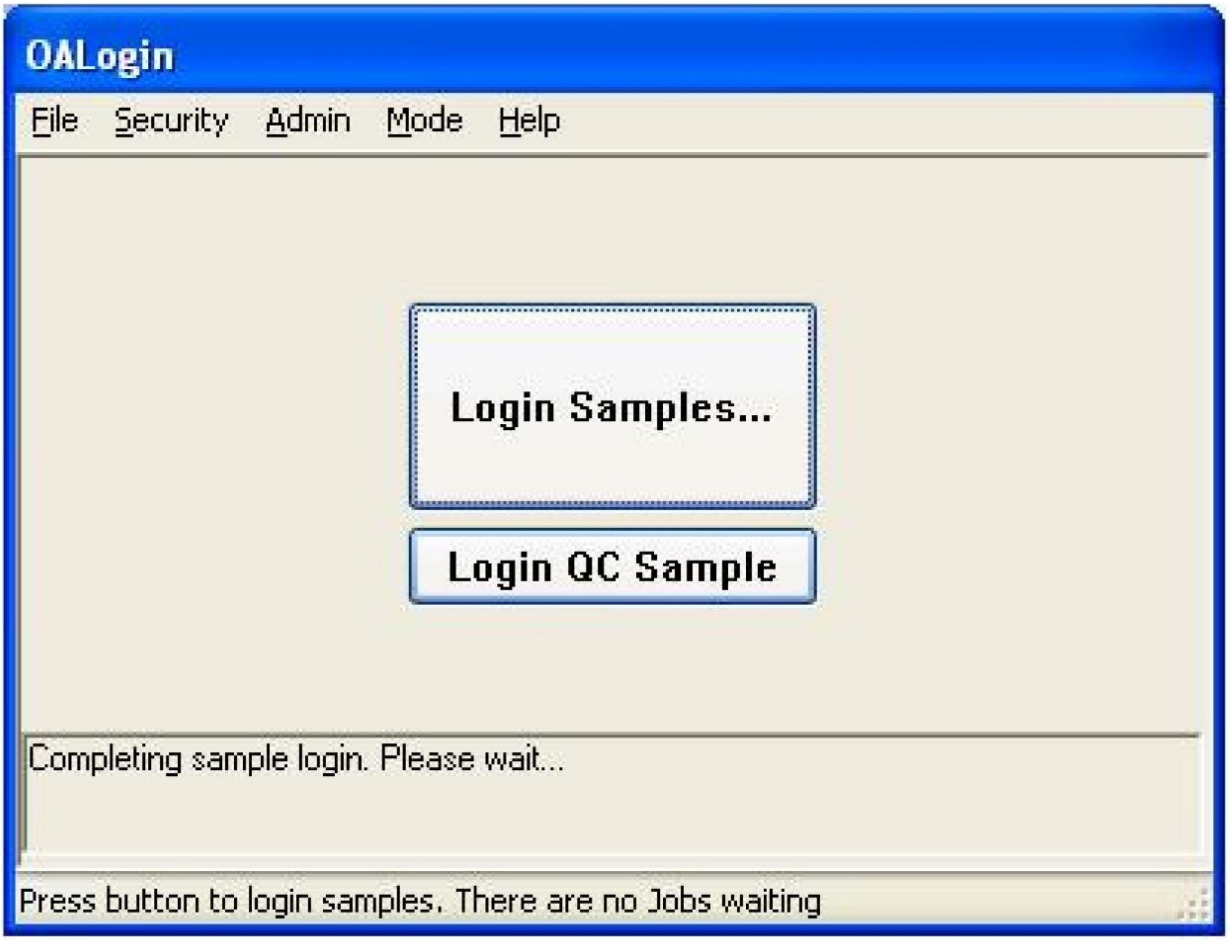

Figure 4. OALogin window with QC login option.

Viewing QC Results

Results from scheduled or user-initiated quality control checks are presented in the familiar OpenLynx browser (Figure 5). If the peak is not found or the retention time, peak area, or peak intensity fall outside the administrator-defined tolerances, the quality control sample fails. This is indicated by a red well in the browser and described in the Sample Summary area.

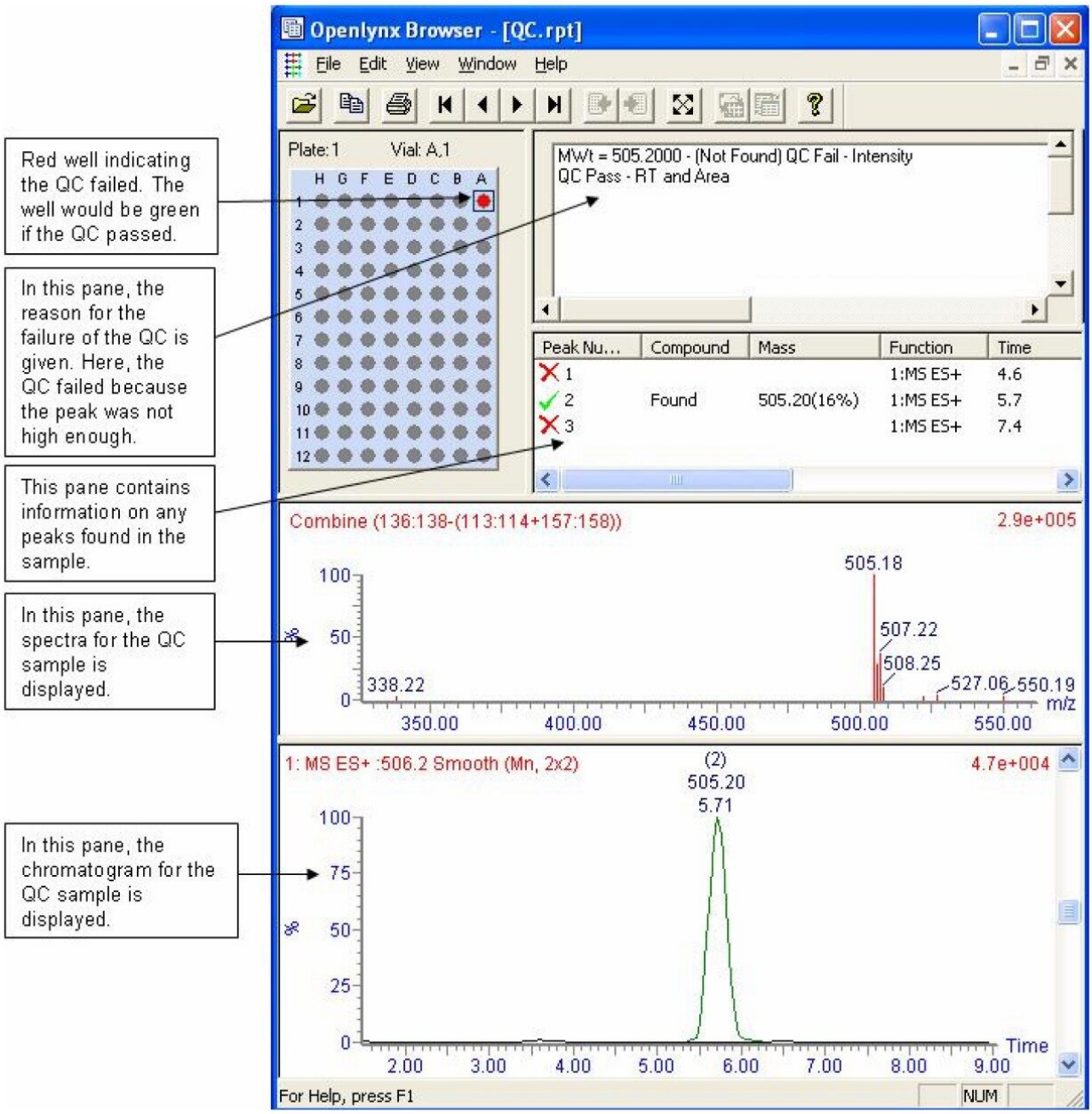

Figure 5. OpenLynx browser showing a failed QC sample.

Conclusion

Increased Confidence in Your Results

The Quality Control feature of the OpenLynx Application Manager for MassLynx Software is an extremely efficient and user-friendly method of automatically running periodic open access system evaluations. The software affords the administrator the knowledge that the system is always functioning optimally. The Quality Control feature also gives chemists confidence in their analysis, by allowing a simple yet comprehensive system check before running their precious samples.

Waters Open Access Suite of Solutions

Waters Open Access Systems give chemists the ability to analyze their own samples close to the point of production by simply walking up to the LC-MS system, logging their samples, placing their samples in the system as instructed, and walking away. As soon as the analysis is completed, sample results are e-mailed or printed as desired. Easy system configuration and setup is enabled through a System Administrator, determining login access, method selection, and report generation privileges.

Waters Open Access Systems provide the most comprehensive and powerful user-friendly solutions available on the market today. With versatile combinations of robust and reliable HPLC injectors, solvent delivery modules, column chemistries, MS technologies and informatics capabilities, Waters has a solution to suit every laboratory's specific needs.

Waters ACQUITY UPLC System with the Waters Micromass LCT Premier Mass Spectrometer.

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MassLynx MS Software <https://www.waters.com/513662>

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