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Application Note

Advantages of the ACQUITY QDa Detector in the Medicinal Chemistry Laboratory

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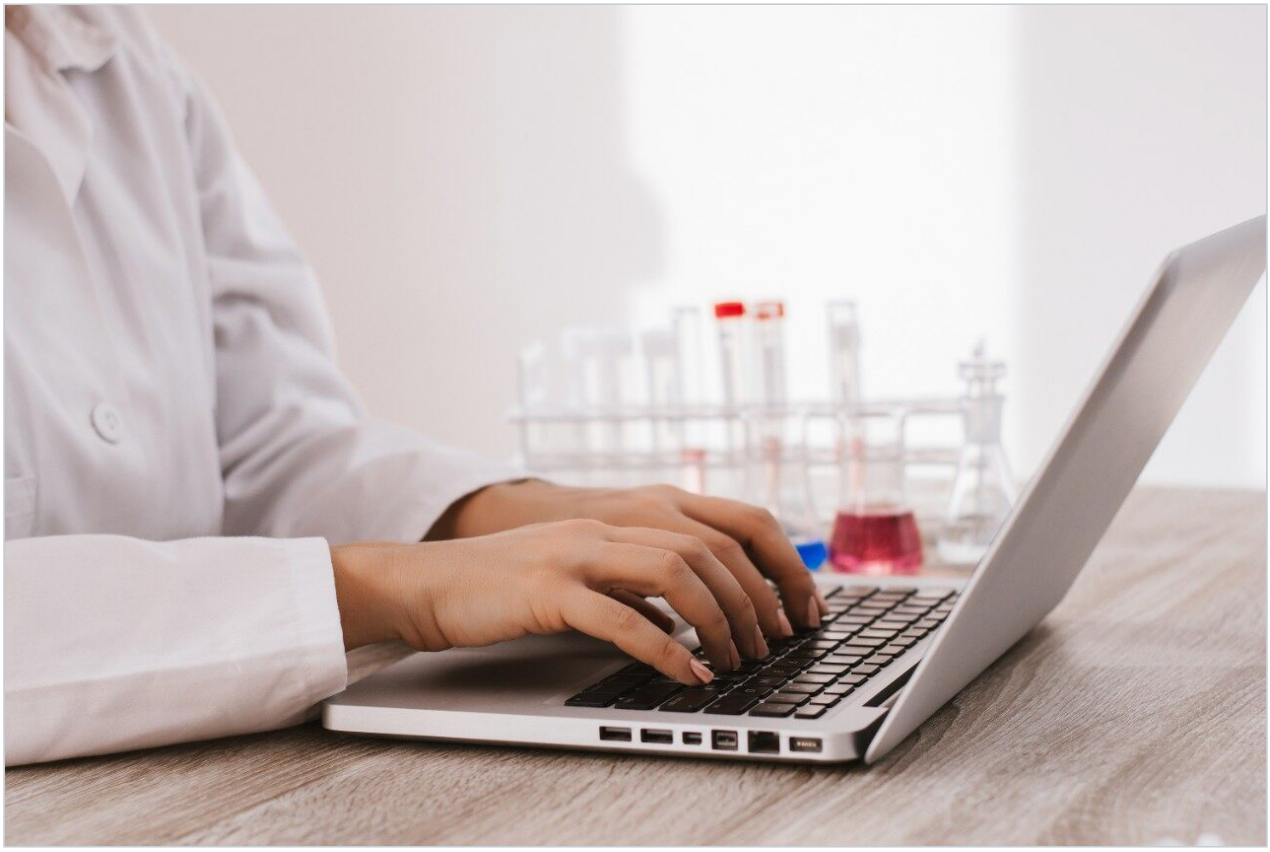


This is an Application Brief and does not contain a detailed Experimental section.

Abstract

This application brief demonstrates the benefits of utilizing MassLynx 4.1 Software with OpenLynx Open Access Application Manager in conjunction with an ACQUITY UPLC System and the ACQUITY QDa Detector in a medicinal chemistry laboratory.

Benefits

By combining UV and mass detection with open access software in a synergistic UPLC system, medicinal chemists can rely on rapid chromatographic separation and confirmation of the identity of reaction products in a chemical synthesis.

Introduction

There has been a growing demand in the pharmaceutical industry to improve and accelerate the drug development process. This has resulted in new working practices being introduced into all stages of the drug discovery and development process, with goals to ensure quality, drive efficiency, and increase productivity.

Since about 1995, medicinal chemists have been able to analyze more than 100,000 samples a year by liquid chromatography/mass spectrometry (LC-MS) to monitor synthetic reactions and investigate the structure or purity of new chemical entities. One technology that has enabled this high workload is MassLynx Software's OpenLynx Open Access. This tool provides chemists with fully automated workflows that lead them through sample submission, method selection and reporting options.

The ACQUITY QDa Detector is a mass detector that has been designed to work synergistically with a separation system. Its mass detection capabilities are built around the needs of analytical scientists who routinely perform chromatographic assays. The mass spectral information combines seamlessly into the same workflow as an LC analysis, providing more complete separation characterization by confirming the identity of components. By combining an ACQUITY UPLC System with ACQUITY UPLC PDA and ACQUITY QDa detectors in an open access environment, medicinal chemists can to confirm the identity and purity of their synthetic reactions right next to their synthesis.

Results and Discussion

In this example, we demonstrate the UPLC analysis of a typical synthetic reaction mixture using our open access tools along with UV and mass detection.

- The medicinal chemist logs in and enters the molecular mass of the reaction product (310 Da in this example, Figure 1). The medicinal chemist places the reaction mixture in a specified vial location.
- The report is emailed directly to the medicinal chemist (Figure 2). Highlighted in green is the important information: the ACQUITY QDa Detector confirms that the required product (310 Da) has been successfully synthesized.
- The percentage purity is determined by the ACQUITY UPLC PDA Detector.

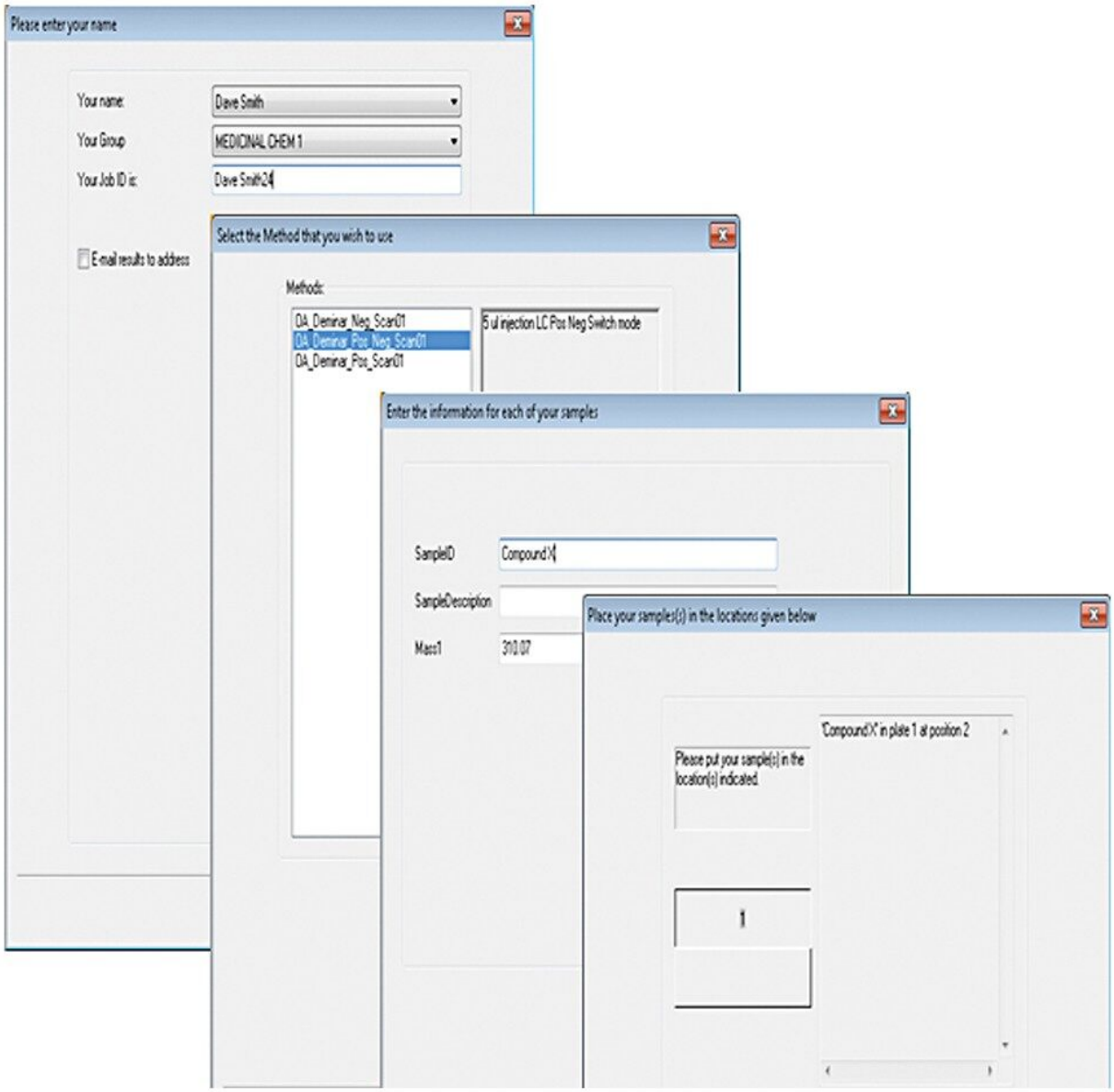


Figure 1. Sample submission workflow for a medicinal chemist.

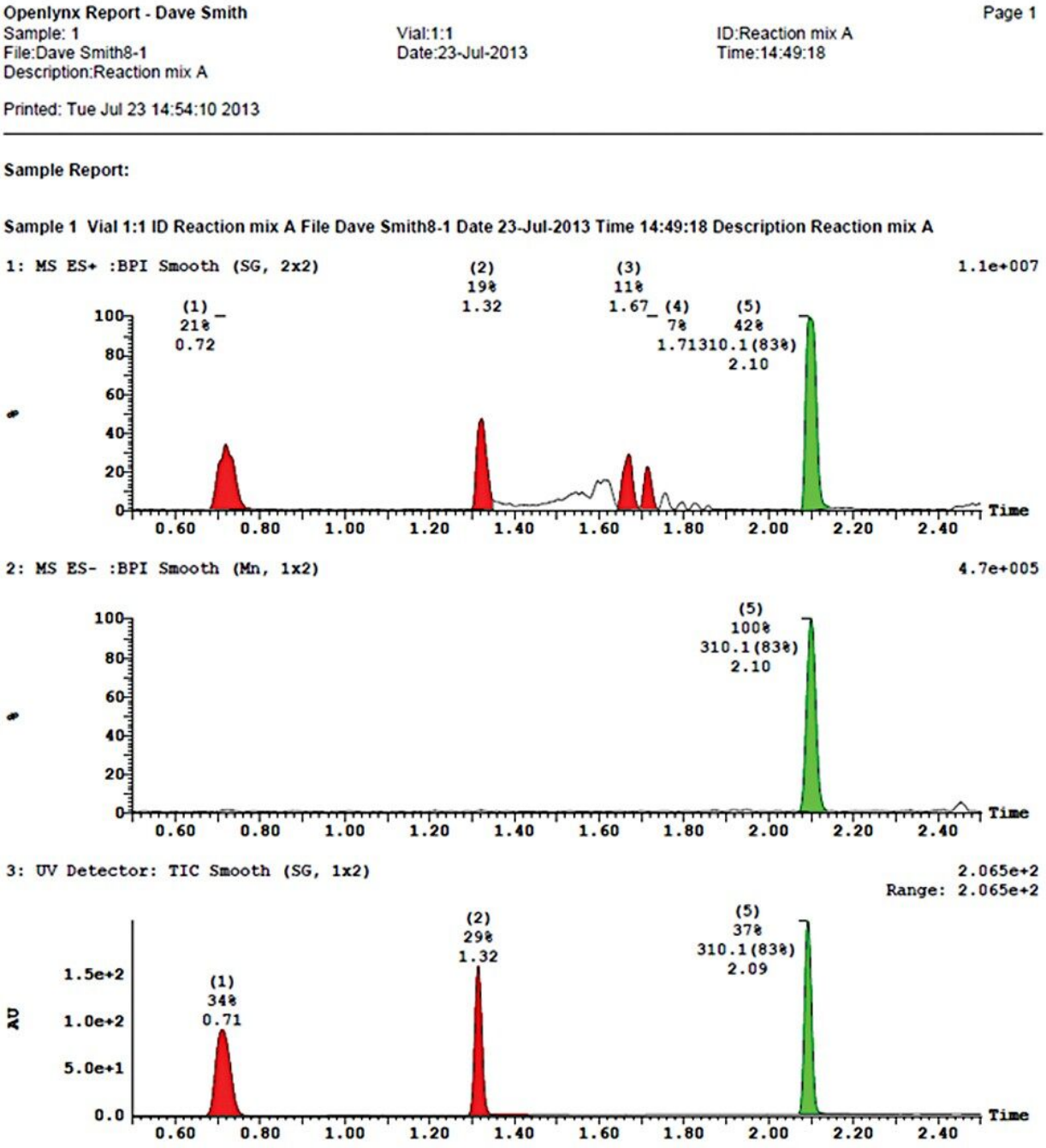


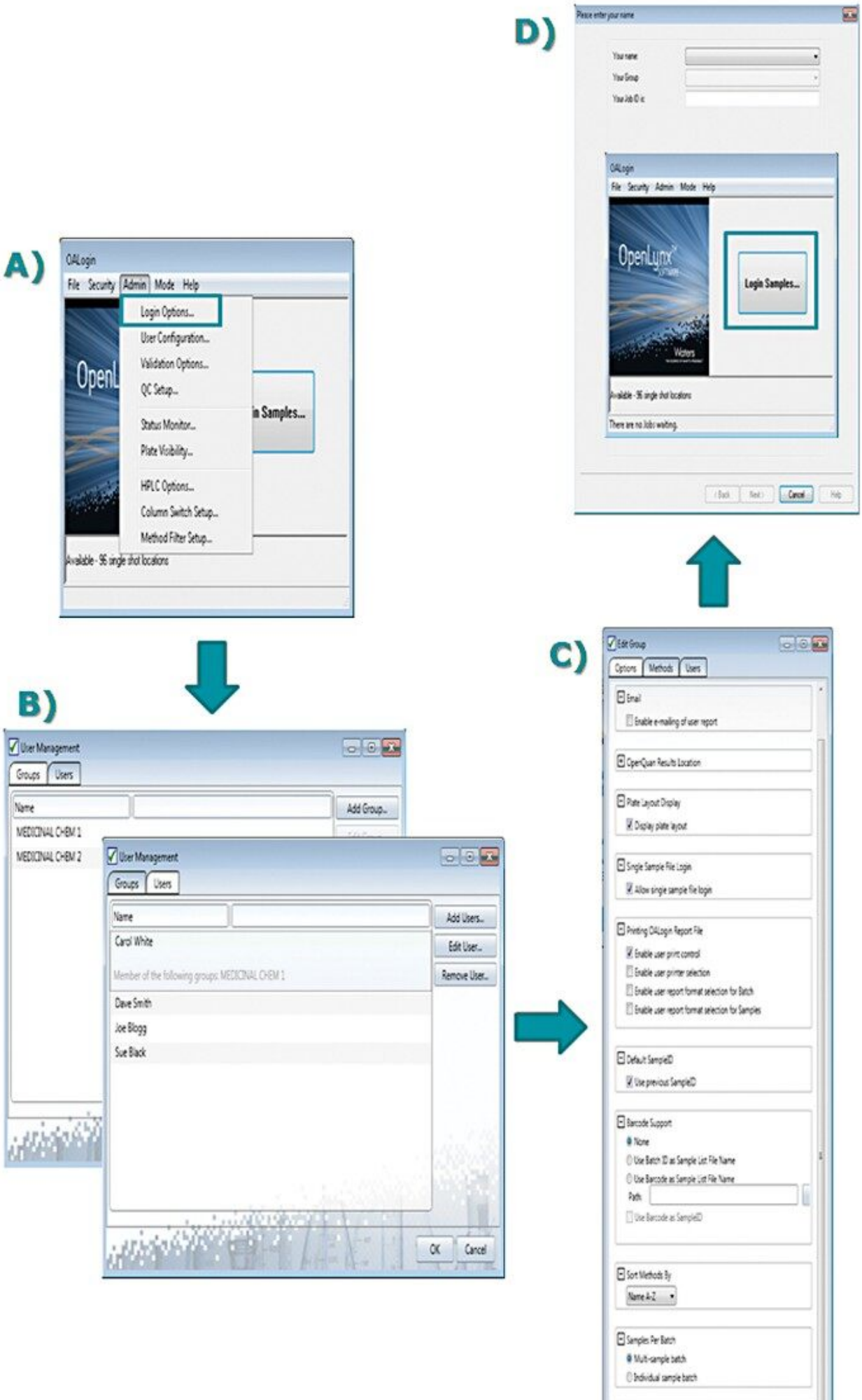
Figure 2. A typical simplified report example showing the medicinal chemist has synthesized the right reaction product and the percentage purity.

Managing use of this open access environment is straightforward:

- In OpenLynx Open Access, administrator management has been simplified with the addition of a User

Management dialog box (see Figures 3A and 3B). The administrator can now define groups and assign users to these groups.

- As seen in Figure 3C, the options for each group address email, plate layout display, single sample file login, OALogin report file printing, sample ID format, barcode support, methods order, and walk-up parameters available, as well as the ability to enable multiple methods per sample and to rename report files.


A)
OALogin
File Security Admin Mode Help
Login Options...
User Configuration...
Validation Options...
QC Setup...
Status Monitor...
Plate Visibility...
HPLC Options...
Column Switch Setup...
Method Filter Setup...
Available - 96 single shot locations
B)
User Management
Groups Users
Name
Add Group...
MEDICINAL CHEM 1
MEDICINAL CHEM 2
Add Users...
Edit User...
Remove User...
Carol White
Member of the following groups: MEDICINAL CHEM 1
Dave Smith
Joe Blogg
Sue Black
OK
Cancel
C)
Edit Group
Options Methods Users
Email
Enable e-mailing of user report
OpenQuan Results Location
Plate Layout Display
Display plate layout
Single Sample File Login
Allow single sample file login
Printing OALogin Report File
Enable user print control
Enable user printer selection
Enable user report format selection for Batch
Enable user report format selection for Samples
Default SampleID
Use previous SampleID
Barcode Support
None
Use Batch ID as Sample List File Name
Use Barcode as Sample List File Name
Path
Use Barcode as SampleID
Sort Methods By
Name A-Z
Samples Per Batch
Multi-sample batch
Individual sample batch
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Please enter your name
Your name
Your Group
Your Job ID is:
OALogin
File Security Admin Mode Help
OpenLynx
Waters
Login Samples...
Available - 96 single shot locations
There are no Jobs waiting.
Back
Next
Cancel
Help