

Advantages of the ACQUITY QDa Detector in the Medicinal Chemistry Laboratory



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GOAL

To demonstrate 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.

BACKGROUND

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.

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.

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 confirm the identity and purity of their synthetic reactions right next to their synthesis.



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THE SOLUTION

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.

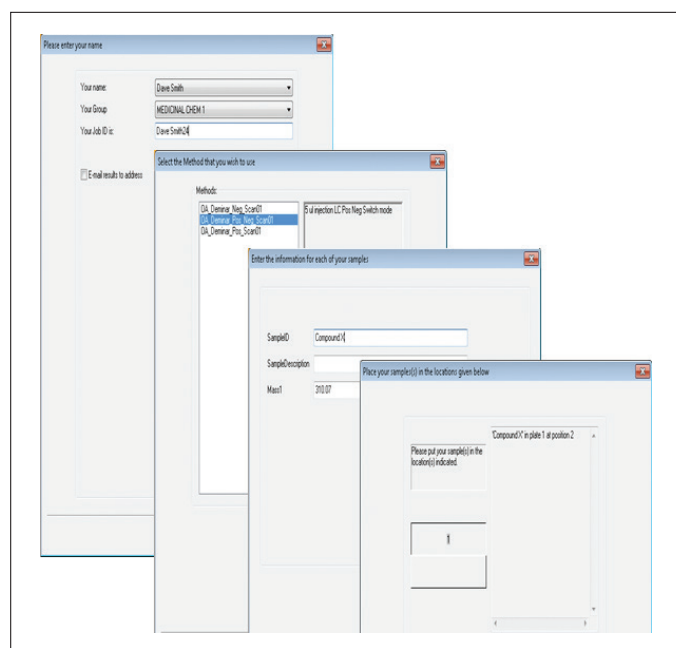


Figure 1. Sample submission workflow for a medicinal chemist.

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.

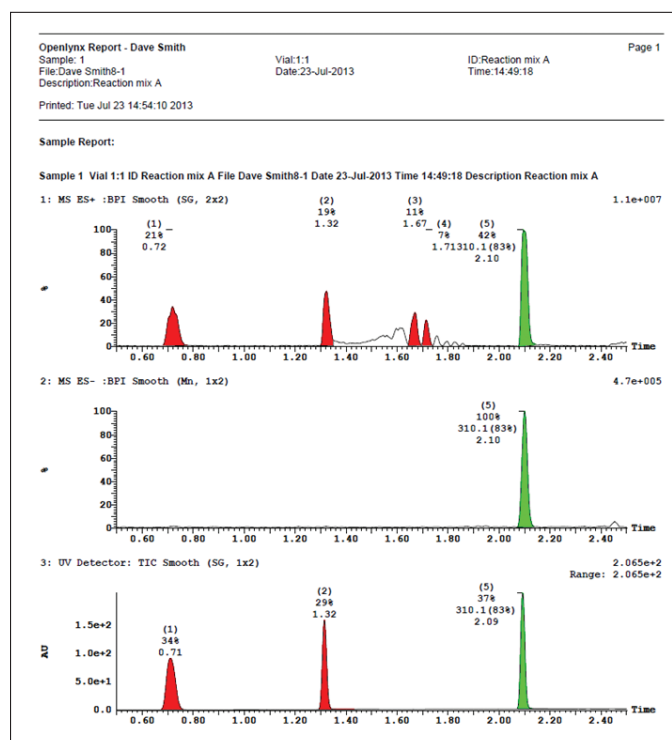


Figure 2. A typical simplified report example showing the medicinal chemist has synthesized the right reaction product and the percentage purity.

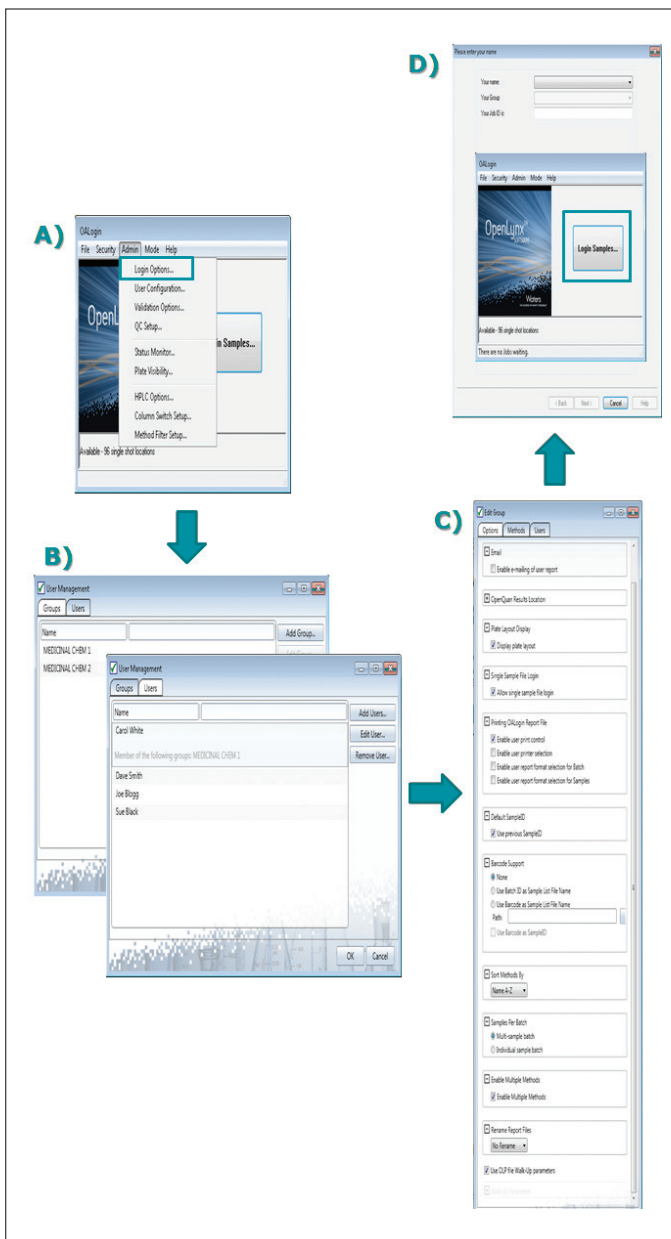


Figure 3. The User Management dialog box in Open Access OpenLynx Software.

SUMMARY

By combining an ACQUITY UPLC System with the ACQUITY UPLC PDA and ACQUITY QDa detectors on MassLynx OpenLynx Open Access Software, Waters has streamlined the workflow of medicinal chemists with a complete package for the rapid chromatographic separation and confirmation of identity of reaction products from a chemical synthesis.

Waters

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