[product solution]

Waters

Waters Open Access Systems

Powerful sample analysis for everyone

YOUR LAB WILL THRIVE WITH THE ACCESSIBILITY OF OPEN ACCESS UPLC

Maximum efficiency is essential for analytical laboratories that are constantly challenged to increase throughput and deliver results to research chemists in pharmaceutical discovery.

In a walkup environment, Waters' specialized software enables chemists with varying levels of instrument knowledge to perform routine analysis on a variety of chromatography systems. Waters Open Access UPLC[®] systems allow chemists to simply walk up to a system, log in their sample, place the sample in the instrument as instructed, and walk away to retrieve results at their desk by email or printout – with minimal wait time.

A variety of Waters systems, including ACQUITY UPLC[®] and ACQUITY UPLC H-Class, can be used for open access. The instrument combines with application-specific software for intuitive and versatile operation, with fast and robust analyses using ELS, UV, or MS detection for nominal and exact mass measurements.

Waters Open Access systems for UPLC/MS are built around the OpenLynx[™] Open Access Application Manager for MassLynx[™] Software, which brings the power of chromatography and mass spectrometry to chemists who are not analytical instrumentation specialists.

STREAMLINING OPEN ACCESS LAB TASKS WITH SPECIALIZED SOFTWARE

- Set up the system with OpenLynx Open Access
- Manage users with OAToolkit
- Log in samples with OALogin
- Optimize system performance with Remote Status Monitor and IntelliStart[™]
- View results by email, printout, or in the OpenLynx browser
- Make information more accessible with NuGenesis[®] SDMS

So simple, samples analyze themselves

- Quickly run singleshot samples
- Select the right method using a software wizard
- Versatile configurations streamline LC, LC/MS, and purification applications
- Data delivered in easy-to-read reports



The ACQUITY UPLC System with a Sample Organizer for analyzing plates of samples in a walkup environment.

BRINGING EFFICIENCY TO OPEN ACCESS LABORATORIES

The OpenLynx Open Access Application Manager is software that is designed to allow chemists to walk up to a terminal and log in samples onto an instrument, while inputting a 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 Application Manager for MassLynx Software allows chemists to analyze their own samples and to run system QC samples.





FOR THE SYSTEM ADMINISTRATOR: STREAMLINED CONTROL OF USERS AND DATA

OAToolkit is an OpenLynx Open Access feature that increases the flexibility and ease-of-use of Open Access systems by automating system management tasks. The system administrator manages users from a central computer, remotely assigning detailed configuration information and attributes for each user and then exporting that information to the available instruments. New project directories can be created on a per-user basis and the administrator can prompt the resulting project data, such as raw data files or reports, to automatically move into that directory as it is created. With this automated file-saving process for data and results, users can access their results faster while the data is secured from a system failure. OAToolkit can also convert reports to other formats, facilitating their entry into data systems.

FOR THE CHEMIST: WALK UP, LOG IN SAMPLE, GET RESULT

OpenLynx Open Access is ideal for laboratories whose chemists have varying levels of experience operating analytical instruments. Users simply enter their name, select a predetermined experimental method and processing criteria, and then enter some basic sample information. The software displays a wizard for sample login by default. Chemists also have the choice of using a single-page dialog box to log in single-shot samples, and even multiple samples can be entered as a singleshot. Both task-driven interfaces have all the functionality necessary to submit the sample for analysis. 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. The step-by-step wizard is beneficial when logging in larger sample sets.

Login Informati	on						
Your Name:	Darcy	~	Job ID:	Darcy48			
Your Group:	Automation	~	Description	10 ul injection LC			
🗹 E-Mail Resu	Its to Address:	darcy_shave@waters.com	Print OALo	Print OALogin Report			
			🖳 Change Pr	inter	OpenLynx_UNIFY 7.1	Printe	
			🔽 Select Bat	ch ORS file	C:\MassLynx\SummaryReport.ors		
			🗹 Select San	nple ORS file	C:\MassLynx\SampleReport.ors		
C1 20_80 base C1 50_50 acid C1 50_50 base C1 5_95 acid C1 5_95 base C2 20_80 acid C2 20_80 base C2 50_50 acid		C ≥ 20,000 +	nu site site d te				
Sample Details			10				
SampleID	CE4 007 4F	0.0 44					

With OpenLynx OALogin, selecting multiple methods and receiving comprehensive results is streamlined.

Open Access Software connects chemists with multiple ACQUITY UPLC Systems



Managing a networked flow of laboratory data, from monitoring systems to delivering results, using OpenLynx OAToolkit.

OPTIMIZING SYSTEM PERFORMANCE

To ensure that your Open Access lab is continually operating at peak performance, Waters has two on-board software packages to oversee instrument operation, Remote Status Monitor for LC instruments and IntelliStart for LC/MS instruments.

Remote Status Monitor actively monitors Waters LC instruments. Status information can be viewed and interrogated in a browser, allowing chemists to to quickly see which instruments have the shortest wait times. When the user is ready to log in a sample, they can also see the queues already running on that instrument. Remote Status Monitor allows administrators to determine if any instruments are down, and to oversee solvent levels. Each solvent reservoir and waste container is identified in the Solvent Monitor console and email notification is available to alert the administrator when a warning level has been reached.

IntelliStart Software provides a simple and automated system check procedure to ensure that a Waters LC/MS system is operating properly, reducing the burden of complicated setup. The software allows an inexperienced user to run a full QC check of the whole system: simply run a standard and compare it to results of the same standard that was run at an earlier time. Values that can be used to confirm that the system is operating correctly include peak retention time, peak area, the presence of specific masses or wavelengths, and spectral intensity. Regular automated system checks save downtime by detecting problems as early as possible.

RESULTS AT YOUR FINGERTIPS

Reporting for Waters Open Access Systems is also performed by OpenLynx Open Access. Results and reports are available in a variety of formats, from printed copies, to pdfs, to viewing in a browser on the chemist's office PC without requiring MassLynx installation. The browser presents a summary of results as a color-coded map – highlighting found, not found, and tentative information – for easy visualization of the analytical results. Chemists can quickly access and review the data supporting an assignment by simply 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.

Status Summary			Updated at: 13:33:13 26-07-2010					
Instrument Name	MS Status	LC Status	Samples in Queue	Queue State	Last Update Time			
GCT	Instrument offline for maintenance							
MassLynx PC	Process only PC							
Purification System 1	Acquiring	ок	4	Not Paused	26-07- 2010,10:45:12			
Purification System 2	Acquiring	ок	12	Not Paused	26-07- 2010,10:45:12			
SQD 1	Acquiring	ок	8	Not Paused	26-07- 2010,10:45:12			
SQD 2	System Idle	Inlet Problem	8	Not Paused	26-07- 2010,10:45:12			
SQD 3	Acquiring	ок	6	Not Paused	26-07- 2010 10:45:12			

Remote Status Monitor provides oversight of the status of the workflow queue.



IntelliStart checks the system to ensure it is operating properly.

BETTER ACCESS TO INFORMATION THROUGHOUT YOUR ORGANIZATION

System administrators can use OpenLynx's OAToolkit to not only manage users and systems, but to make the results and reports accessible to designated groups or contacts within an organization. Waters NuGenesis Scientific Data Management System (SDMS) significantly extends the availability of this information. SDMS automatically captures and catalogs diverse data generated by instruments, scientists, and outside sources in a centralized data warehouse, offering excellent integration with a multitude of research applications. With SDMS you can find and repurpose information, from reports to chemical structures, with traceable, hyperlinked access to the source data that generated that information. Robust tools allow you to export that information to business applications and share it with collaborators anywhere in the world.

NO MATTER YOUR APPLICATION, OUR OPEN ACCESS SYSTEMS ARE READY TO RUN

Quaternary UPLC

Many labs allow users to run their samples with a variety of solvents, modifiers, and columns to quickly determine the best separation conditions, for example in method scouting. For this application, the ACQUITY UPLC H-Class System with



a Column Manager is optimal. The quaternary pumping system allows the user to switch between solvents and modifiers, to automate the formulation of mobile phase gradients, and with the addition of the Column Manager, to utilize up to six columns.

The quaternary ACQUITY UPLC H-Class System with the Column Manager and single quadrupole detector.

Binary UPLC

For labs that use just a few methods and do not need the flexibility of quaternary solvent blending, such as in compound confirmation, the binary ACQUITY UPLC System is the perfect choice. This proven, reliable technology simultaneously improves laboratory productivity, efficiency, and throughput. For labs with the need for larger sample capacities or high throughput such as in library screening, the Sample Organizer is recommended.

Open bed UPLC

For Open Access labs that need to further extend productivity and capacity, the Open Architecture UPLC System includes a flatbed Sample Manager – an industry-standard autosampler that is familiar to chemists who prefer to add their sample vials or well plates to an open bed rather than having to access a sample rack position inside a system. With an EverFlow[™] Valve, the system reliably operates at high pressures over an extended lifetime.



This solution is ideal for analyses such as compound verification, fraction purity checks, and final product analysis.

Open access quantitation

Pairing an ACQUITY UPLC System with the tandem quadrupole Xevo® TQ-S System and OpenQuan™ Software allows users who do not have expertise with mass spectrometry to submit sample batches for MS/MS quantitation, while Open Access QuanOptimize™ automatically develops MRM methods.

Open access exact mass

Combining UPLC and Xevo® G2 Tof, Open Access Exact Mass allows non-expert MS users to submit samples and receive a report outlining the most likely chemical formulas for their compound.

Open access purification

For labs that provide preparative LC or purification capabilities in an open access environment, Waters' easy-to-use systems and

software allow samples to be run with unattended system operation. This improves productivity by enabling chemists to focus on their results rather than on the instrument.



AutoPurification System.

Open access biopharmaceutical characterization

The ability to acquire and process UPLC and UPLC/MS data for proteins, peptides, and other biomolecules in a walk-up, open access environment empowers non-analytical scientists to obtain quicker turnaround for routine biomolecule analyses, and analytical groups to streamline routine analytical processes.



ACQUITY UPLC with Xevo G2 QTof.

UPLC Open Architecture System with the 2777 Sample Manager.



Waters



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