Data acquisition and integration, storage, archiving, and reporting of raw data – all in one central database

Current bioanalytical LC-MS/MS workflows require the use of multiple software packages to track samples, acquire and process data, create reports and archive studies. Managing multiple separate databases adds significant time, cost, and complexity to drug development. Until now, no laboratory information management system managed the bioanalytical workflow from beginning to end.

With the introduction of the TSQ Module™ for Thermo Scientific Watson LIMS, data from the entire bioanalytical workflow can now reside in a single database, significantly increasing lab efficiencies. The combination provides tighter regulatory control – from method development through data archiving. Data review, processing, reporting, and archiving is under the control of Watson LIMS, where security and audit functionality are easily managed. Together, Watson LIMS, the TSQ Module, and Thermo Scientific TSQ Series mass spectrometers form the most comprehensive, fully integrated solution for regulated bioanalytical laboratories.

Watson LIMS is the foremost bioanalytical LIMS relied upon by 18 of the top 20 pharmaceutical companies as well as leading CROs worldwide. Watson is a highly specialized, protocol-driven software application designed to support drug metabolism and pharmacokinetic (DMPK) studies in drug discovery and development. Pharmaceutical companies and CROs that standardize on Watson LIMS can count on secure data transmissions, regulatory compliance, reliable audit trails and improved time to market.
TSQ Module

Data acquisition, integration, archiving, and Watson Run List View

Run lists are created in Watson and can be directly submitted over the network to the TSQ Module on any configured TSQ Series mass spectrometer for data acquisition. The run list contains all information for the instrument to acquire data, such as the LC/MS method and the well position. If a user’s rights allow the run list to be edited on the instrument side, the changes are captured by the audit trail and sent back to Watson. This view shows a list of runs that could be submitted to any local or remote TSQ Series instrument on the network, allowing lab managers to balance workloads among global resources.

Run Manage Queue

On the instrument side, the Run Manage Queue shows the runs that have been submitted from Watson to this instrument. The user can select the order in which the runs are analyzed on the TSQ Series MS. A status shows for each run — submitted, acquiring, pending, or stopped. Runs can be sent back to Watson and resubmitted to another instrument anywhere on the network. The flexibility allows the lab manager to distribute the workload among the instruments.

TSQ Module Highlights

Simplified workflow
The TSQ Module provides a simple, easy-to-use instrument interface for acquiring data and managing runs submitted from Watson, and for real-time viewing of data. The batches submitted to the TSQ Module directly from Watson contain all of the information needed to generate data.

XML data support for future-proofing studies
The data acquired with the TSQ Module is sent directly to the Watson database in an XML format. Studies in this format can be opened in any future versions of Watson. Old software versions need not be maintained to open historical data, simplifying data management. Study data can be de-archived for regulatory review in the future, if required.

One data set, and data processing in Watson
The coupling of data acquisition and processing with core Watson functionality enables easier sample tracking and management, data review, processing, and reporting — saving significant time and money by eliminating the need for the manual verification processes required when maintaining two data sets.
Watson security safeguards the single database
Data review, processing, reporting, and archiving are controlled in a single database where security and audit functionalities are easily managed.

Reporting
Reports can now include chromatograms from data processed directly in Watson. Audit trails track changes throughout a study, maintaining a record and making reporting to regulatory authorities easier.

A single database of record
With Watson LIMS directly acquiring data from the Thermo Scientific TSQ Series mass spectrometer, peak integration, storage, archiving, and reporting of raw data is all done in one central database.

Run list
The Manage Run View displays the Watson run list that was sent to the TSQ Module. If permissions allow, the TSQ Module user can edit vial position, injection volume and add a comment. All edits are logged in the audit trail and sent back to Watson when the run is completed. To start data acquisition, the user clicks the Run button in this TSQ Module window.

Real-time display
During data acquisition, status of the analyte intensity and retention time can be monitored in real-time. When acquisition is complete, sample data in XML format is transferred automatically and securely to Watson over the network for processing and storage. No sample data is retained on the instrument PC. XML sample data stored in Watson is the only copy of the data, making Watson the single database of record. This eliminates the need for independent data backup procedures for each data acquisition workstation, further simplifying the workflow.
Run Review Window

Since the XML data is now stored in Watson, data processing such as peak detection, integration, and regression can be done directly in Watson. This means there is only a single set of results, eliminating the time-consuming manual verification process required when having duplicate sets of data. When using the TSQ Module, all study raw data (XML), results, chromatograms, audit trail, and reports are archived together in a single database.

The Run Review window is exclusive to Watson LIMS systems with the TSQ Module enabled.

Watson Reporting with Chromatograms

The FDA requires that at least 20% of representative chromatograms are reported. Previously, instrument software was required to generate the chromatograms. Now, all reports including chromatograms are easily generated directly within Watson. This new Watson capability eliminates the need for two separate sets of reports in two separate databases.