

## Thermo Scientific TSQ Module for Watson™ LIMS



### 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.**



# DATA ACQUISITION, INTEGRATION, ARCHIVING, AND

## 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 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 #	Run Name	Run Type	Run Date	Analyst	Acq. Date	Acq. Time	Instrument	Instrument ID	Biological Sample	Assay	Assay ID	Assay Description	Run Description	Report File Name
1	Created by Instrument	INSTRUMENT	05-Apr-2009		05-Apr-2009	12:00:00	Thermo Scientific TSQ Vantage	Thermo Scientific TSQ Vantage	Plasma					
2	Completed	INSTRUMENT	05-Apr-2009		05-Apr-2009	12:00:00	Thermo Scientific TSQ Vantage	Thermo Scientific TSQ Vantage	Plasma					
3	Completed	INSTRUMENT	05-Apr-2009		05-Apr-2009	12:00:00	Thermo Scientific TSQ Vantage	Thermo Scientific TSQ Vantage	Plasma					
4	Completed	INSTRUMENT	05-Apr-2009		05-Apr-2009	12:00:00	Thermo Scientific TSQ Vantage	Thermo Scientific TSQ Vantage	Plasma					
5	Completed	INSTRUMENT	05-Apr-2009		05-Apr-2009	12:00:00	Thermo Scientific TSQ Vantage	Thermo Scientific TSQ Vantage	Plasma					
6	Completed by Instrument	INSTRUMENT	05-Apr-2009		05-Apr-2009	12:00:00	Thermo Scientific TSQ Vantage	Thermo Scientific TSQ Vantage	Plasma					
7	Completed by Instrument	INSTRUMENT	05-Apr-2009		05-Apr-2009	12:00:00	Thermo Scientific TSQ Vantage	Thermo Scientific TSQ Vantage	Plasma					
8	Completed by Instrument	INSTRUMENT	05-Apr-2009		05-Apr-2009	12:00:00	Thermo Scientific TSQ Vantage	Thermo Scientific TSQ Vantage	Plasma					
9	Completed by Instrument	INSTRUMENT	05-Apr-2009		05-Apr-2009	12:00:00	Thermo Scientific TSQ Vantage	Thermo Scientific TSQ Vantage	Plasma					
10	Completed by Instrument	INSTRUMENT	05-Apr-2009		05-Apr-2009	12:00:00	Thermo Scientific TSQ Vantage	Thermo Scientific TSQ Vantage	Plasma					
11	Completed by Instrument	INSTRUMENT	05-Apr-2009		05-Apr-2009	12:00:00	Thermo Scientific TSQ Vantage	Thermo Scientific TSQ Vantage	Plasma					
12	Completed by Instrument	INSTRUMENT	05-Apr-2009		05-Apr-2009	12:00:00	Thermo Scientific TSQ Vantage	Thermo Scientific TSQ Vantage	Plasma					
13	Completed	INSTRUMENT	05-Apr-2009		05-Apr-2009	12:00:00	Thermo Scientific TSQ Vantage	Thermo Scientific TSQ Vantage	Plasma					
14	Completed by Instrument	INSTRUMENT	05-Apr-2009		05-Apr-2009	12:00:00	Thermo Scientific TSQ Vantage	Thermo Scientific TSQ Vantage	Plasma					
15	In Progress (1 of 4) Sample Processed	VALIDATION	05-Apr-2009		05-Apr-2009	12:00:00	Thermo Scientific TSQ Vantage	Thermo Scientific TSQ Vantage	Plasma					Validation Study
16	Submitted by Instrument	VALIDATION	05-Apr-2009		05-Apr-2009	12:00:00	Thermo Scientific TSQ Vantage	Thermo Scientific TSQ Vantage	Plasma					Validation Study Method Validation Study
17	Submitted by Instrument	VALIDATION	05-Apr-2009		05-Apr-2009	12:00:00	Thermo Scientific TSQ Vantage	Thermo Scientific TSQ Vantage	Plasma					Validation Study Method Validation Study
18	Submitted by Instrument	VALIDATION	05-Apr-2009		05-Apr-2009	12:00:00	Thermo Scientific TSQ Vantage	Thermo Scientific TSQ Vantage	Plasma					Validation Study Method Validation Study
19	Submitted by Instrument	VALIDATION	05-Apr-2009		05-Apr-2009	12:00:00	Thermo Scientific TSQ Vantage	Thermo Scientific TSQ Vantage	Plasma					Validation Study Method Validation Study
20	Submitted by Instrument	VALIDATION	05-Apr-2009		05-Apr-2009	12:00:00	Thermo Scientific TSQ Vantage	Thermo Scientific TSQ Vantage	Plasma					Validation Study Method Validation Study
21	Submitted by Instrument	VALIDATION	05-Apr-2009		05-Apr-2009	12:00:00	Thermo Scientific TSQ Vantage	Thermo Scientific TSQ Vantage	Plasma					Validation Study Method Validation Study
22	Submitted by Instrument	VALIDATION	05-Apr-2009		05-Apr-2009	12:00:00	Thermo Scientific TSQ Vantage	Thermo Scientific TSQ Vantage	Plasma					Validation Study Method Validation Study

### 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.

Status	URL	Database	Run Name	External ID	Acquisition Date	Assay Date	Description	Extractions Date	Analyst	Observations
Pending	http://localhost	ACT	Sample_182		4/18/2009 1:24:2	4/18/2009 12	Method Valid...	4/18/2009 12:00:00	Signed	Pr...
Pending	http://localhost	ACT	Sample_182		4/18/2009 1:24:3	4/18/2009 12	Method Valid...	4/18/2009 12:00:00	Signed	Pr...
Acquiring	http://localhost	ACT	Sample_182		4/18/2009 1:15:3	4/18/2009 12	Method Valid...	4/18/2009 12:00:00	Signed	Pr...
Submitted	http://localhost	ACT	Sample_182		4/18/2009 1:15:3	4/18/2009 12	Method Valid...	4/18/2009 12:00:00	Signed	Pr...
Submitted	http://localhost	ACT	Sample_182		4/18/2009 1:15:3	4/18/2009 12	Method Valid...	4/18/2009 12:00:00	Signed	Pr...
Submitted	http://localhost	ACT	Sample_182		4/18/2009 1:15:3	4/18/2009 12	Method Valid...	4/18/2009 12:00:00	Signed	Pr...
Submitted	http://localhost	ACT	Sample_182		4/18/2009 1:24:3	4/18/2009 12	Method Valid...	4/18/2009 12:00:00	Signed	Pr...

# REPORTING – ALL IN ONE CENTRAL DATABASE

## 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.

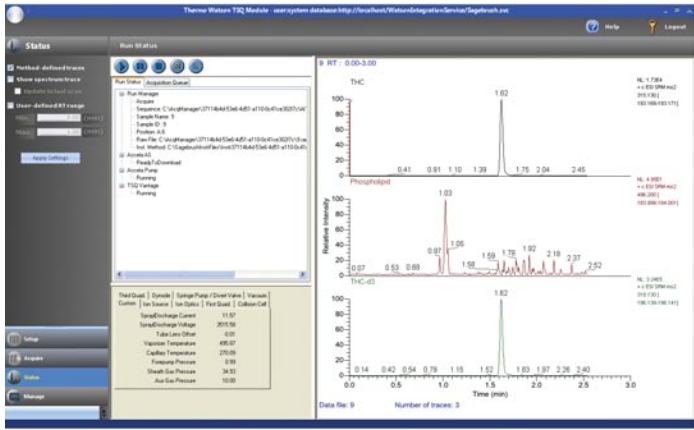
## A single database of record

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

Sample ID	Level	Vial Pos	Inj Volume
CONTROL BLANK	2	Q 99M 125	1.81
QC	3	Q 99M 125	1.81
QC	4	Q 99M 200	1.81
QC	5	Q 99M 200	1.81
CONTROL BLANK	6	Q 99M 1	1.81
CONTROL BLANK	7	Q 99M 1	1.81
QC	8	Q 99M 1	1.81
QC	9	Q 99M 1	1.81
QC	10	Q 99M 2.5	1.82
QC	11	Q 99M 2.5	1.82
CONTROL BLANK	12	Q 99M 2.5	1.82
STANDARD	13	Std 0.200	1.82
STANDARD	14	Std 0.500	1.82
STANDARD	15	Std 1.000	1.82
STANDARD	16	Std 5.000	1.82
STANDARD	17	Std 25	1.82
STANDARD	18	Std 75	1.82
STANDARD	19	Std 125	1.82
STANDARD	20	Std 200	1.82
STANDARD	21	Std 300	1.82
STANDARD	22	Std 400	1.82
STANDARD	23	Std 500	1.82
CONTROL BLANK	24	Std 500	1.84
CONTROL BLANK	25	Std 500	1.84
QC	26	Q 99M 1	1.84
QC	27	Q 99M 1	1.84
QC	28	Q 99M 1	1.84
QC	29	Q 99M 1	1.84
QC	30	Q 99M 1	1.84
QC	31	Q 99M 1	1.84
QC	32	Q 99M 1	1.84

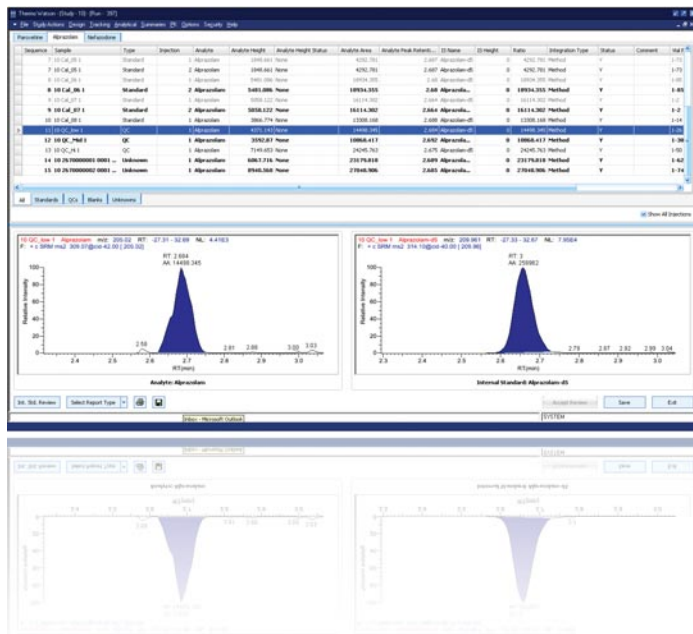
## Run list

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.



## 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.

## 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.

