

Product Spotlight



From sample to report: Chromeleon CDS end-to-end workflow for bioanalysis

Introduction

Bioanalytical studies are a fundamental part of the drug development process. They involve the quantitative measurement of compounds of interest and/or their associated metabolites in biological samples. Tandem quadrupole mass spectrometry coupled with high-performance liquid chromatography (HPLC MS/MS) is primarily used for compound detection, though more recently there is a shifting trend towards the use of high resolution accurate mass (HRAM) MS as therapeutic products become more complex in nature and the drive for greater accuracy intensifies.

The Thermo Scientific™ Chromeleon™ Chromatography Data System (CDS) workflow for bioanalysis provides a complete software solution for today's modern laboratory.

One software platform

There is only one software package to learn, which provides control, data acquisition, and data processing for LC and MS instrumentation to simplify training and provide familiarity to the end-user while delivering real productivity gains for any bioanalytical environment.



Leverage gold-standard compliance features for MS

Chromeleon CDS is designed to meet current and future regulatory requirements for chromatography and MS users including GLP, GMP, and 21 CFR Part 11 coverage. It provides centralized administration with easy-to-implement technical controls and comprehensive audit trails with object versioning for full traceability and easy side-by-side comparisons. The same features to support compliance are extended to MS data acquisition, processing and instrument tuning.

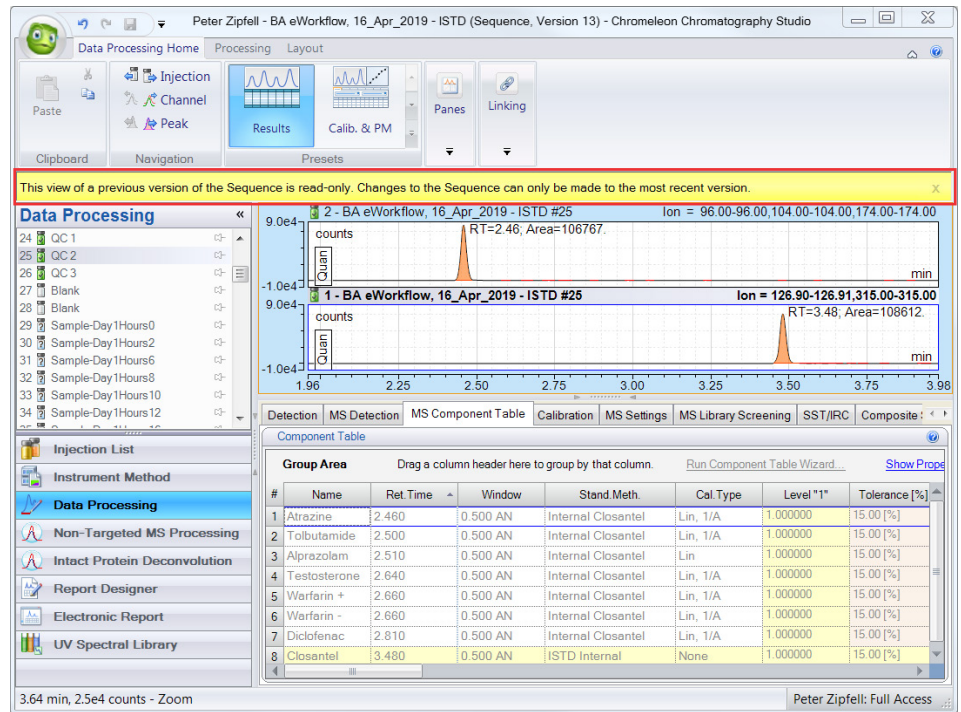


Figure 1. Opening any object in the data audit trail provides a visual assessment to simplify audit trail review

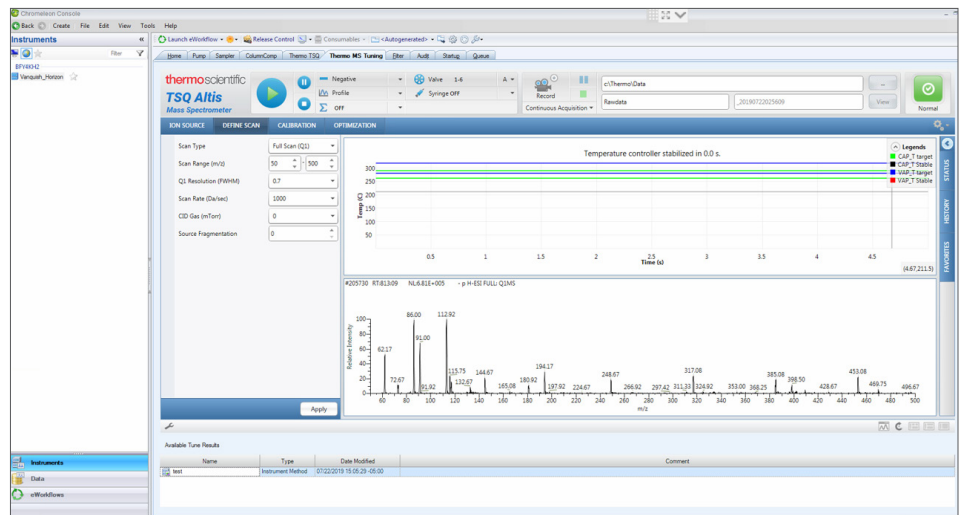


Figure 2. Privilege-controlled, compliant tune application accessed from within Chromeleon CDS

Fully integrated MS and MS/MS functionality

Chromleon Software delivers data processing features and report templates specifically devised for bioanalysis and MS that are rich in functionality, easy to define, and display clear results. These elements deliver an interactive solution for any quantitative analysis, while enhancing the user experience with an intelligent, yet functional design.

Figure 3. MS Detection settings can be applied to a whole sequence, specific injection or specific component

Figure 4. Built-in report template for bioanalysis

| Injection Details (QC Samples) | | | | | | | | | |
|--------------------------------|------|--------------------|-----------------|------------------|---------------------------------|------------------------------|------------|-------------|----------------------|
| No. | Name | Theo. Amt ng/mL | Amount ng/mL | Amount % Diff | Analyte Peak Area counts*min | ISTD Peak Area counts*min | Area Ratio | Level Check | Record Modified ? |
| 24 | QC 1 | 5.0 | 4.8 | -4.24 | 926 | 1558 | 0.59 | Pass | No |
| 25 | QC 2 | 10.0 | 8.1 | -19.10 | 1779 | 1773 | 1.00 | Fail | No |
| 26 | QC 3 | 50.0 | 48.4 | -3.17 | 9104 | 1516 | 6.01 | Pass | No |
| 89 | QC 1 | 5.0 | 5.3 | 5.74 | 994 | 1516 | 0.66 | Pass | No |
| 90 | QC 2 | 10.0 | 10.1 | 0.66 | 1965 | 1573 | 1.25 | Pass | No |
| 91 | QC 3 | 50.0 | 46.2 | -7.62 | 9055 | 1580 | 5.73 | Pass | No |
| 154 | QC 1 | 5.0 | 5.1 | 2.69 | 1047 | 1644 | 0.64 | Pass | No |
| 155 | QC 2 | 10.0 | 9.8 | -2.42 | 1856 | 1533 | 1.21 | Pass | No |
| 156 | QC 3 | 50.0 | 52.0 | 4.04 | 9667 | 1498 | 6.45 | Pass | No |

Figure 5. Report table showing QC tolerance and a clear pass/fail indication

Smart tools to streamline MS workflows

Automated sequence creation with eWorkflow™ procedures minimizes errors and allows any user, regardless of experience, to run routine MS analyses accurately and reproducibly. They are the fastest way from sample to result bringing significant time savings to your routine analysis.

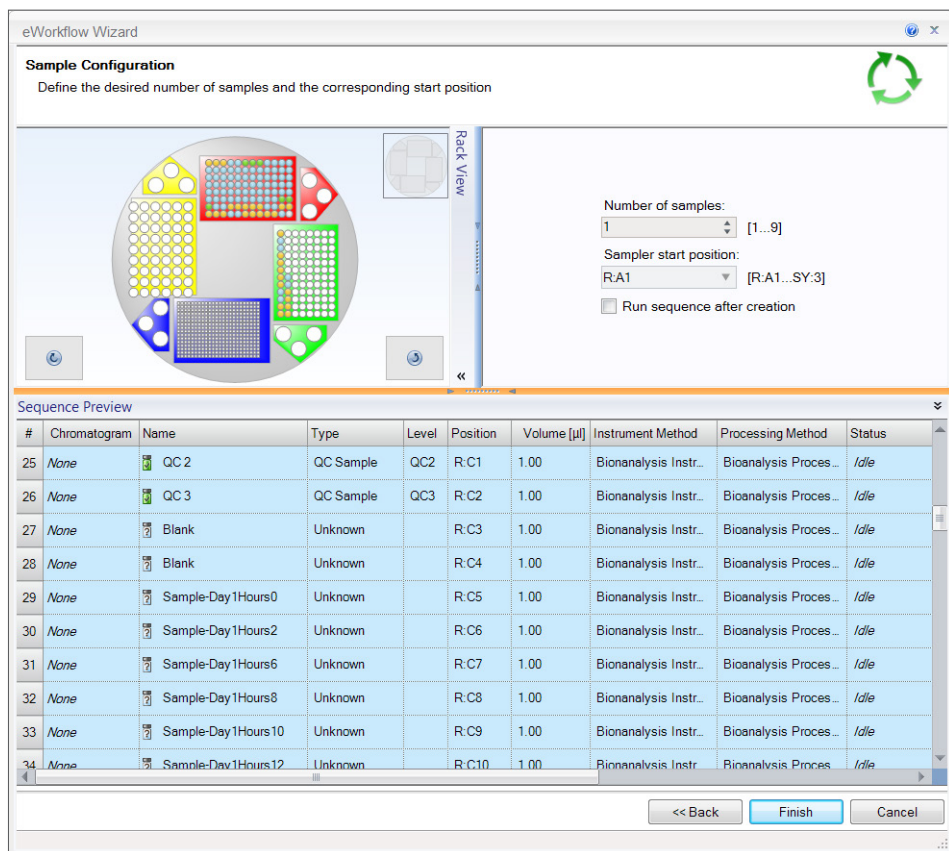


Figure 6. Starting an eWorkflow procedure—simply select how many samples to analyze, and the sequence is populated from predefined rules and templates

SmartLink is a feature that reduces the complexity of handling large MS datasets with pre-defined component-centric templates for easy data assessment. Streamline the process of data review with a tiled orientation of multiple components by injection or by peak.



Figure 7. Calibration standard quantitation ions across a sequence for a specific component per injection

Bring mass spectrometry to the enterprise

A networked CDS can expand the capabilities for bioanalysis with a solution that is scalable from workstation to a global network through seamless user experience, optimum security through central data storage, and industry-leading network failure protection. Remote access to instruments and data ensures that users are no longer required to be in the laboratory in order to control the mass spectrometer or process and review the data.

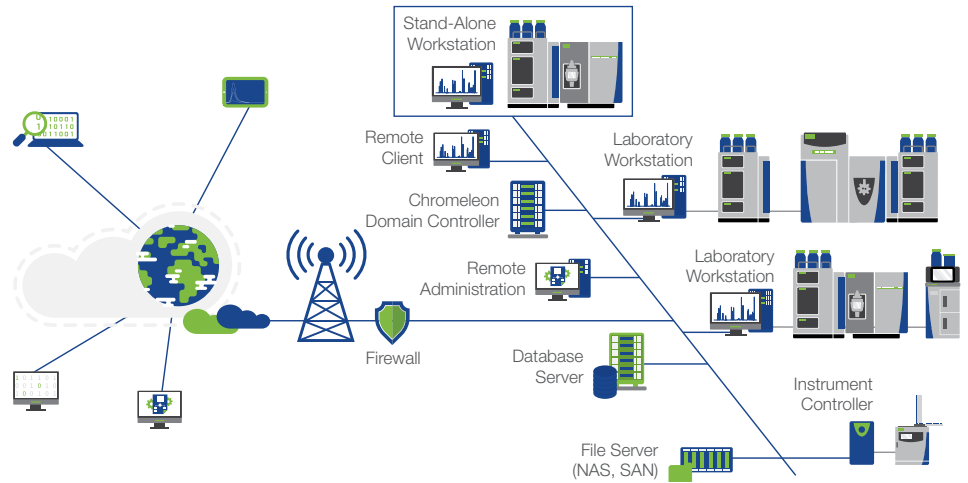


Figure 8. Network scalability—stand-alone to a global network with secure central data storage

Chromeleon CDS Software and Watson LIMS

Harmonization and automation of the complete bioanalysis workflow is achieved thanks to the out-of-the-box, bi-directional Chromeleon CDS and Thermo Scientific™ Watson™ LIMS Software gateway. By utilizing eWorkflow procedures, compliance is ensured throughout the entire workflow from study management, sample tracking, all the way through to the reporting of results.

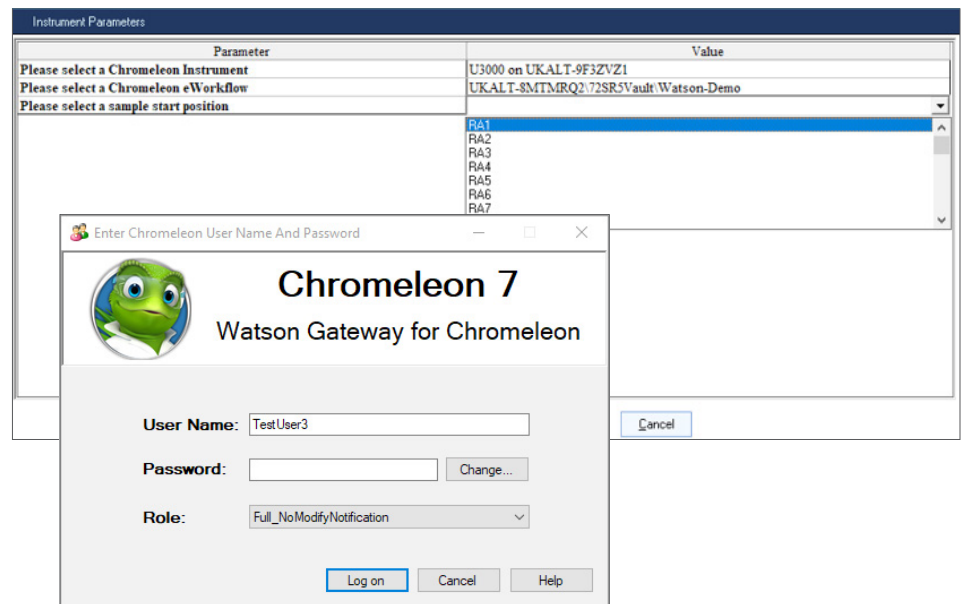
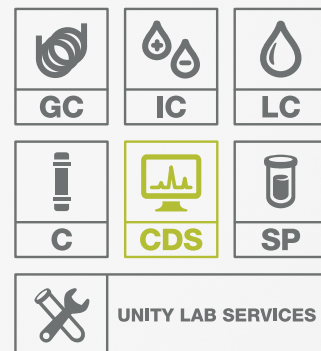


Figure 9. Watson LIMS Gateway for Chromeleon CDS Software—easy sequence creation

The collective power of chromatography

One CDS to do it all

From workstation to global deployment, Chromeleon CDS seamlessly scales to any business, from research through development to QC. Delivering proven productivity gains and straightforward compliance, Chromeleon software provides a unique unification of workflows for chromatography and mass spectrometry analysis. It's cloud-ready software that does it all, backed by a product team dedicated to keeping you one step ahead of the next regulatory or market change. With the largest portfolio of chromatography solutions, we remain a steadfast and committed partner in your endeavor to improve the world around us.



Join the Chromeleon CDS community to future proof your investment:
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