

Built for **mass spectrometry.**
Built for **compliance.**
Without compromise



Compliance-ready
mass spectrometry

Chromeleon CDS for MS

Thermo Scientific™ Chromeleon™ Chromatography Data System (CDS) software is the first CDS that combines all separation and detection techniques, including mass spectrometry (MS), into a single compliance-ready enterprise (client/server) environment.

Chromeleon CDS support for MS uses Thermo Scientific™ MS drivers for instrument control and provides the necessary MS-specific data views, data processing, and reporting capabilities. This merges the benefits of Chromeleon CDS with our leading MS instrumentation and application expertise for a superior answer to the productivity and regulatory challenges in the analytical laboratory.

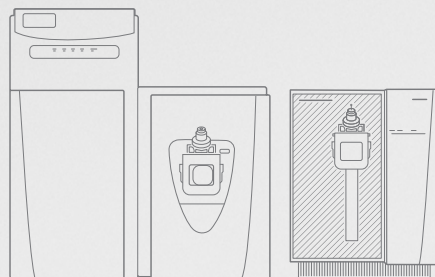
By extending Chromeleon software beyond chromatography into MS, you can now streamline your chromatography and MS quantitation workflows in one application enabling you to use your MS like any other routine detector.



>>> Chromeleon CDS plus Mass Spectrometry brings...



+



...control



- Full, native control of more than 30 MS instruments including High-Resolution Accurate Mass (HRAM) systems
- Supports the majority of acquisition modes, including tuning and calibration
- Work remotely with real-time status viewing, method and run control, data processing, and reporting

Key benefits

Chromeleon CDS delivers superior MS data processing and automation capabilities, boosting your overall lab productivity.

- A comprehensive suite of MS productivity tools including MS Autofilters, Tentatively Identified Peaks, Compound Data Import, and System Suitability Tests (SST) with Intelligent Run Control, targeted peptide mapping, and intact mass deconvolution capabilities
- Data security through automated data backup and centralized storage
- Full 21 CFR Part 11 and GxP compliance-readiness for data acquisition, processing, and reporting
- One set of methods, one set of reports and one central location for your chromatography and MS data, enabling the prevention of data loss during a network outage through secure XVault™ infrastructure
- Spreadsheet-based, easily customizable, flexible and powerful reporting
- Reduced training effort for your lab staff—one single software package instead of several



...compliance



- Full 21 CFR Part 11 and GxP compliance-readiness for data acquisition, processing, and reporting
- Compliant tuning available for the latest HRAM, single and triple quadrupole MS instruments
- Take advantage of comprehensive compliance tools provided by Chromeleon CDS

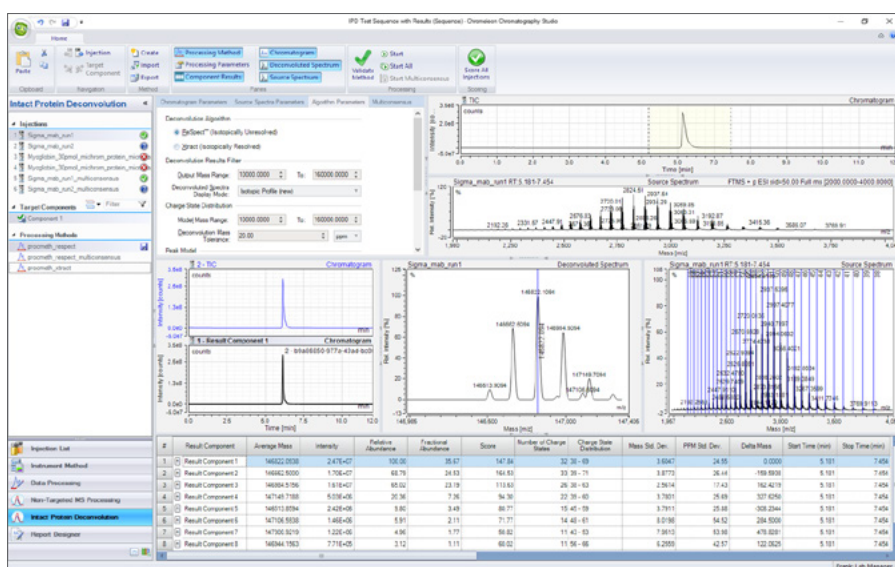


...connectivity

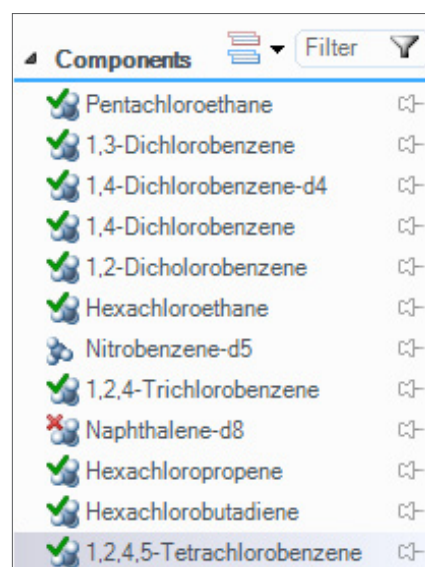
- Seamless import, processing, and reporting of Thermo Scientific™ Xcalibur™ RAW data
- Easy import of Thermo Scientific™ BioPharma Finder™ workbooks for fast method creation
- Export to Thermo Scientific™ Compound Discoverer™ software for unknown identification and elucidation of biological pathways
- Export to multiple third-party packages for additional processing capabilities

Specific features for MS data

- MS-specific data view for live MS channels and for post-acquisition channels such as Total Ion Chromatogram, Mass Spectra, MS component traces, MS quantitation channel, and Extracted Ion Chromatogram
- MS data processing on a component-by-component basis using MS-specific detection algorithms alongside the quantitative tools and integration options provided by Chromeleon CDS
- Consolidated report tables cater for multiple traces and large data sets allowing users to quickly and easily evaluate, report, and filter MS data
- Streamlined data security and retrieval through remote instrument access, data processing, and centralized data storage
- Seamless import and central processing and reporting of Xcalibur data, plus MS data from third-party software via CDF/netCDF/AnDI/AIA files
- Streamline targeted peptide mapping or intact mass deconvolution within a compliance-ready environment with direct import of processing methods from BioPharma Finder workbooks
- Export data for additional data processing or interrogation using applications such as Compound Discoverer



Chromeleon CDS provides all standard MS data processing and visualization tools plus others like intact protein deconvolution.



Component-centric processing with component confirmation indicators.



MS Quantitation channel (right) shows all XICs with SmartLink enabled for the MS Components pane (left).

Additional features for MS



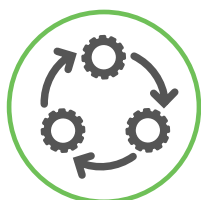
Compliance

Leverage Chromeleon software's gold standard GxP and 21 CFR Part 11 compliance for your MS instrument and data. Compliant instrument tuning and control, with secure log-on, audit-trails covering all actions and full version control, are provided as standard. Chromeleon CDS makes it easier to achieve, maintain, and demonstrate compliance.



SmartLink

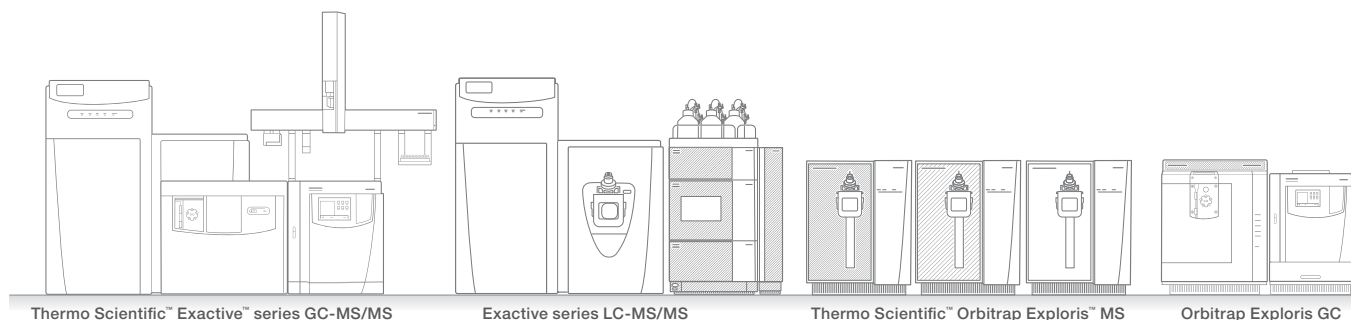
Speed through your data processing by linking the active Chromatography Studio panes to the data currently viewed. Calibration plots, interactive charts, and reports are linked to the active data view displaying only information relevant to the current zoom or selected peaks, streamlining easy data evaluation.



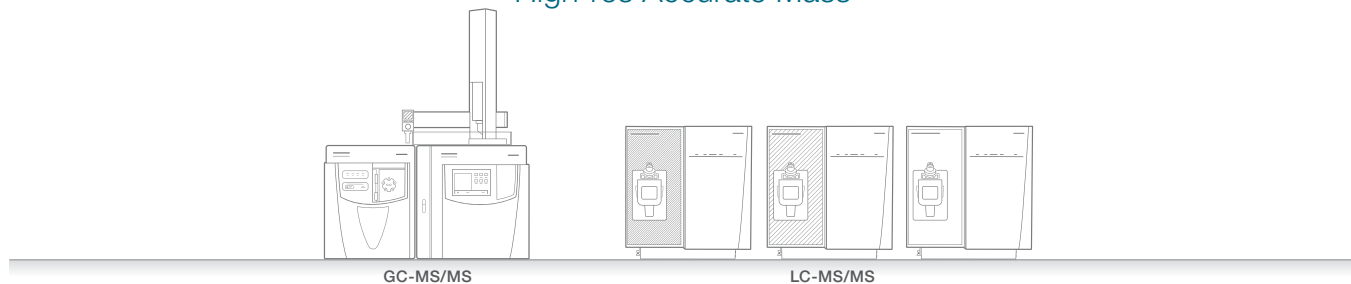
eWorkflow Procedures

Chromeleon eWorkflow™ procedures capture all the unique aspects of a chromatography or MS workflow and enable significant productivity improvements in routine analyses while ensuring that procedural rules and guidelines are followed accurately. With as little as two mouse clicks, any user can create and run analyses on all chromatography and MS instrumentation.

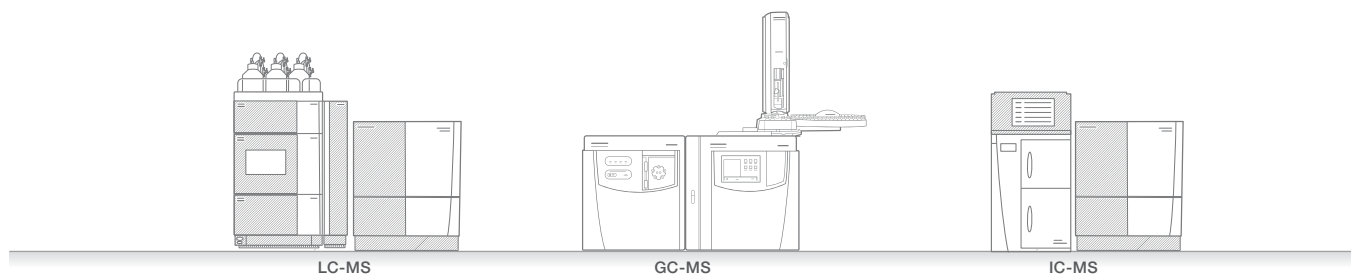
Chromeleon CDS controls over 30 Thermo Scientific™ MS instruments



High-res Accurate Mass



Triple quadrupole



Single quadrupole

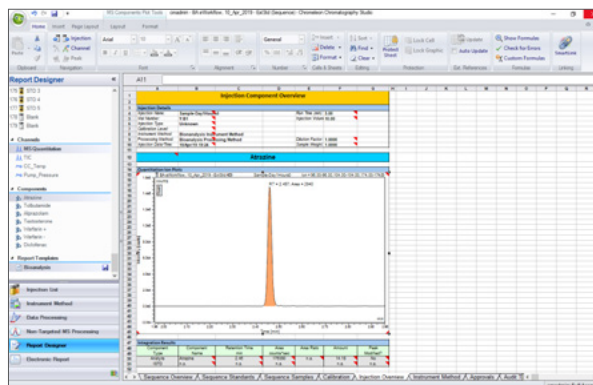
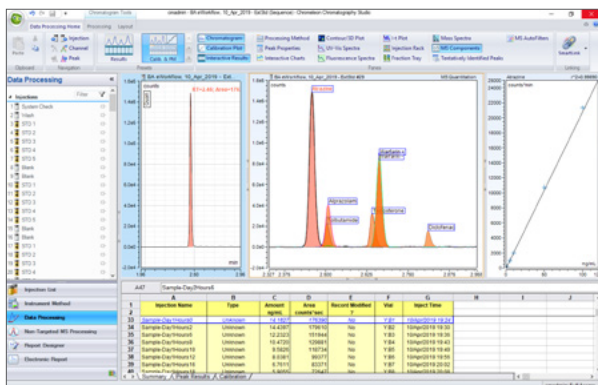
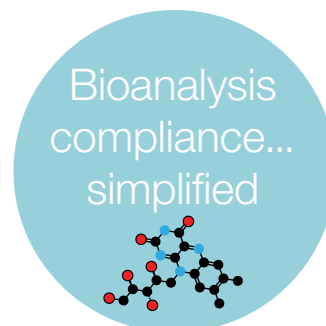
Compliant bioanalysis

Make compliance an advantage in bioanalysis

Bioanalytical studies involve the quantitative measurement of a compound (drug) and/or associated metabolites in biological fluids, such as blood, plasma, serum, urine, or tissue extracts. This typically requires multiple software platforms for the chromatography and MS instruments. Additionally, the requirement to meet evolving regulatory guidelines means that bioanalysis is coming under closer scrutiny throughout every stage of the workflow where the traceability, accuracy, and integrity of data is vital. Chromeleon CDS addresses these challenges, providing a compliant, single software, end-to-end solution for bioanalysis

Complete, compliant workflow solution for bioanalysis:

- Simplified compliance with extensive audit trails
- Out-of-the-box end-to-end workflow: LIMS and CDS
- Secure network data acquisition and processing
- Seamless instrument control with compliant MS tune
- Bi-directional digital exchange with Thermo Scientific™ Watson™ LIMS
- Built-in functionality for business continuity and data archival
- Eliminate analysis errors with eWorkflow procedures



Chromeleon CDS provides a compliant bioanalysis workflow from acquisition, through data processing, to the final report.

Dioxin and PCB analysis

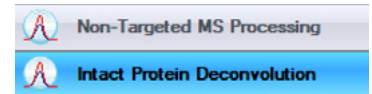
Advanced internal standard techniques for pollutant quantitation

The complicated matrices found in many environmental, food, and other testing areas give rise to the need for advanced use of internal standards. Dioxins and PCBs are persistent organic pollutants and are routinely monitored in food, air, water, and soil samples. This analysis uses isotope dilution mass spectrometry (IDMS) with surrogate standards and associated syringe standards with variable amount values. As an integral part of the Thermo Scientific™ Dioxin Analyzer workflow, Chromeleon CDS provides built-in capabilities which include extensive sample reporting templates with ¹³C-labelled standards recovery, ion ratio, sum parameters, and LOQ flagging, allowing the CDS to automatically perform the calculations, eliminating the need to perform them outside the software.



Chromeleon CDS enables advanced calibration, processing and reporting techniques for dioxin and PCB analysis

Protein analysis



Confidently characterize and monitor without compromise

Chromeleon CDS streamlines the analysis and quantitation of intact proteins. The Intact Protein Deconvolution (IPD) process identifies multiple charge states created during the MS ionization process and groups them to render a composite, unionized mass spectrum of the compound. The Chromeleon CDS IPD workflow is based on BioPharma Finder software, but is tightly integrated with the compliance, reporting, and other functionality of Chromeleon software.

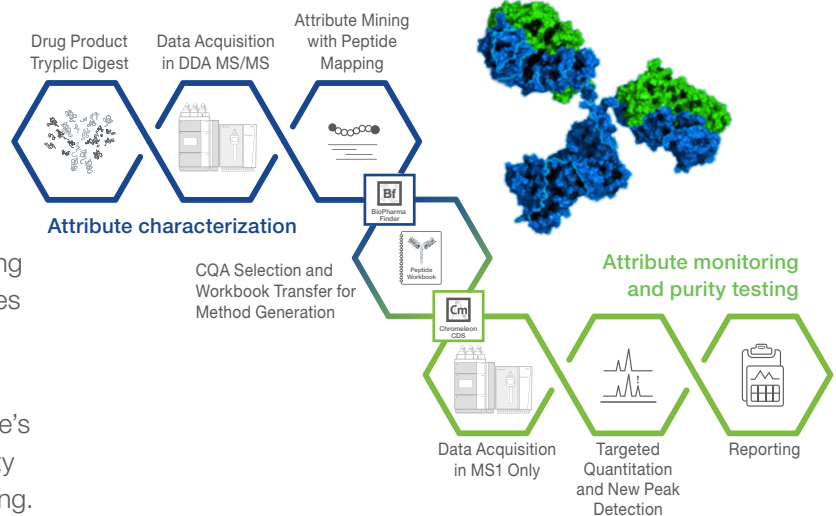
High-throughput, high-confidence results:

- Ensures high-quality results using two algorithms optimized for isotopically resolved (Xtract) and unresolved data (ReSpec™)
- Deconvolutes isotopically unresolved data, across a wide mass range with unsurpassed speed
- Produces highly accurate results, even for low-abundance proteins
- Features an easy-to-use, workflow-driven interface

Simplify your BioPharma product quality analysis with a single verified workflow

Chromeleon CDS is an integral part of the Thermo Scientific™ HR Multi-Attribute Method (HR-MAM). This powerful, high-resolution mass spectrometry-based integrated workflow delivers easy, compliance-ready characterization and monitoring of peptides and allows potential critical quality attributes to be monitored throughout every stage of the drug development process.

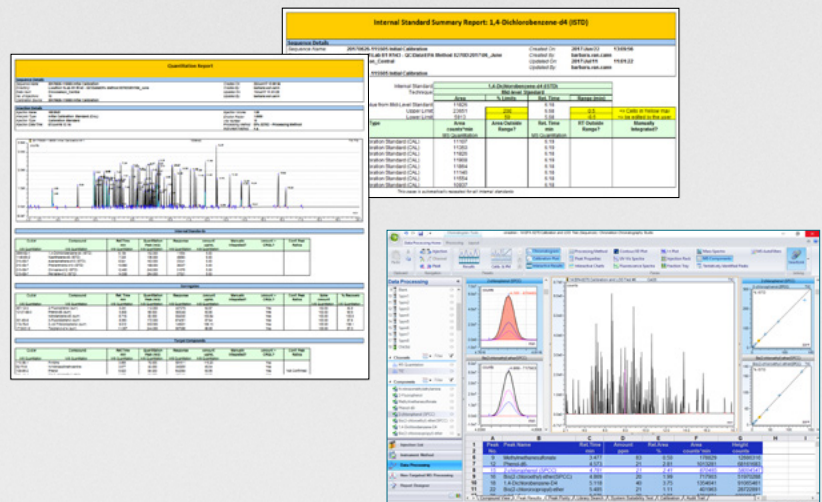
The workflow package leverages Chromeleon software's compliance capabilities from data acquisition, to quality attribute quantitation, new peak detection, and reporting.



Environmental analysis

Easy determination of semivolatile organic compounds (SVOCs) in drinking water and solid waste

Chromeleon CDS offers a fast and simple way to run analyses and create environmental reports using an integrated GC-MS workflow in accordance with the requirements of the United States Environmental Protection Agency (USEPA) guidelines for the determination of semi-volatile organic compounds in many types of solid waste matrices, soils, air-sampling media, and water samples.



“To process so many samples, it’s really nice to have a solid, unified platform for acquiring, processing, and reviewing data, which we have with Chromeleon CDS. When we perform lead selection studies, the first thing is to determine if our candidate molecules are aggregating, along with their identities. We can do that in a single experiment with native SEC(UV)-MS and Chromeleon software, and it’s a matter of seconds screening through the results.”

— Dr. Dan Bach Kristensen, Principal Scientist, Symphogen

“Setting up sequences on the LC-MS is really simple and guided through the use of eWorkflows; analysts can come in and select the relevant workflow which contains all the relevant methods which are locked down and validated, only needing to add the samples to the LC as the system automatically brackets samples.”

— Kerry Malone, Team Leader, Broughton Laboratories

“Using the enterprise version for all the instruments makes remote reviewing and approving easier. There are 23 users of our enterprise installation and our MS systems will be a part of that.”

— Trine Meiborg Sloth, Senior Technician, Analytics and Formulation, Symphogen



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