



# Chromeleon CDS for MS

Complete Compliant Control

# Chromeleon CDS for MS

Thermo Scientific™ Chromeleon™ Chromatography Data System (CDS) is the first CDS that combines separation (GC/IC/LC) and Mass Spectrometry (MS) in an enterprise (client/server) environment.

Chromeleon CDS support for MS uses native 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 challenges in the analytical laboratory.

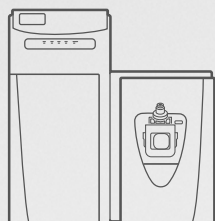
By extending Chromeleon software beyond chromatography into MS, you can now streamline your chromatography and MS quantitation workflows in one application enabling you to use your MS like any other routine detector.



## >>> Chromeleon CDS plus Mass Spectrometry Brings...



+



### ...control



- Full, native control of more than 25 MS instruments including High-Resolution Accurate Mass (HRAM)
- Supports all acquisition modes including tuning and calibration
- Remote networked instrument control with real-time status viewing, method and run control, and data processing and reporting



## Key benefits

- Reduced training effort for your lab staff – one single software package instead of several
- One set of methods, one set of reports and one central location for chromatography and MS data
- 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
- Spreadsheet-based, easily customizable, flexible and powerful reporting
- Centralized data storage with the prevention of data loss during a network outage through secure XVault infrastructure
- Remote instrument control and data processing with no compromise in performance

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



### ...compliance



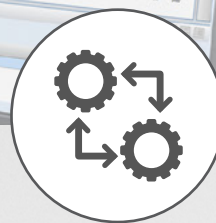
- Full 21 CFR Part 11 and GxP compliance-readiness for data acquisition, processing, and reporting
- Compliant tuning available for single and triple quadrupole MS instruments
- Take advantage of comprehensive compliance tools provided by Chromeleon CDS.



### ...MS tools



- Multiple MS-specific data views including TIC, mass spectra, quantitation channel, component traces, and XICs
- Component-centric data processing
- SmartLink to simplify working with large data sets
- Consolidated report tables for multiple traces and large data sets

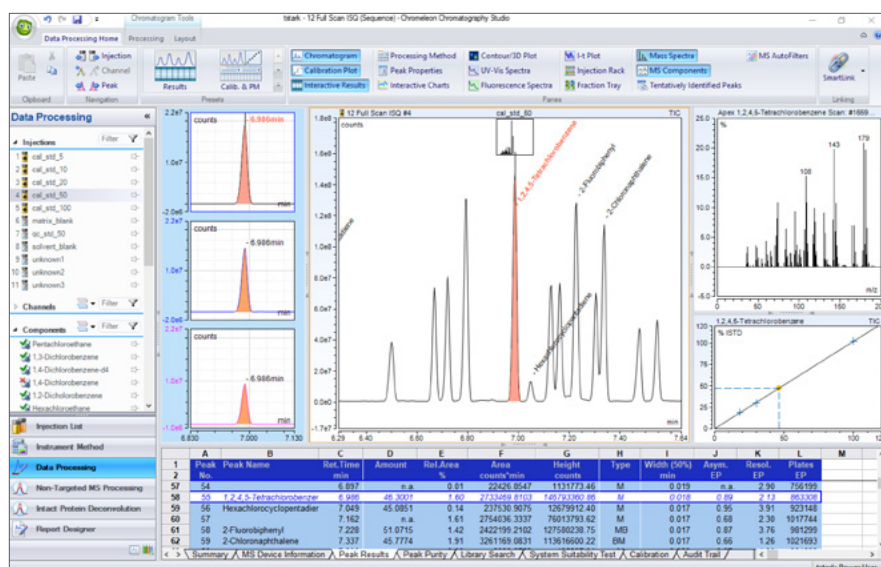


### ...connectivity

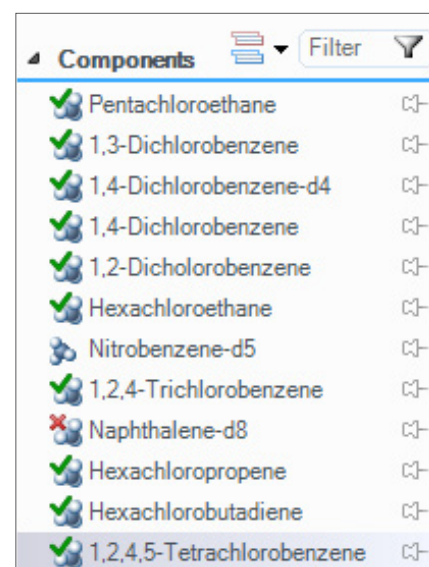
- Seamless import, processing, and reporting of Thermo Scientific™ Xcalibur™ RAW data
- Easy import of Thermo Scientific™ BioPharma Finder™ workbooks for fast method creation
- Export to Thermo Scientific™ Compound Discoverer™ software for unknown identification and elucidation of biological pathways

# Specific features for MS data

- MS-specific data views 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 Genesis and ICIS 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 and report MS data
- Remote instrument access and data processing with centralized data storage
- Seamless import and central processing and reporting of Xcalibur .RAW data
- Import of Biopharma Finder workbooks for fast method creation
- Export .RAW data for sharing with qualitative applications such as Compound Discoverer
- Import, process, and report MS data from third party software via CDF/netCDF/AnDI/AIA files



Chromatography Studio provides TIC (center) with Mass Spectra plot (right) and MS Components view for XICs including Quantitation and Confirming peaks (left).



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



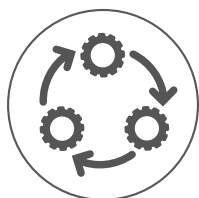
### Compliance

Leverage Chromeleon software's gold standard GxP and 21 CFR Part 11 compliance for your MS instrument and data. Compliant instrument tuning and control, more than 150 user privileges, secure log-on, audit-trail documentation covering all actions in the software and full version control for method creation, are provided as standard. Chromeleon CDS makes it easier to achieve, maintain, and demonstrate compliance.



### SmartLink

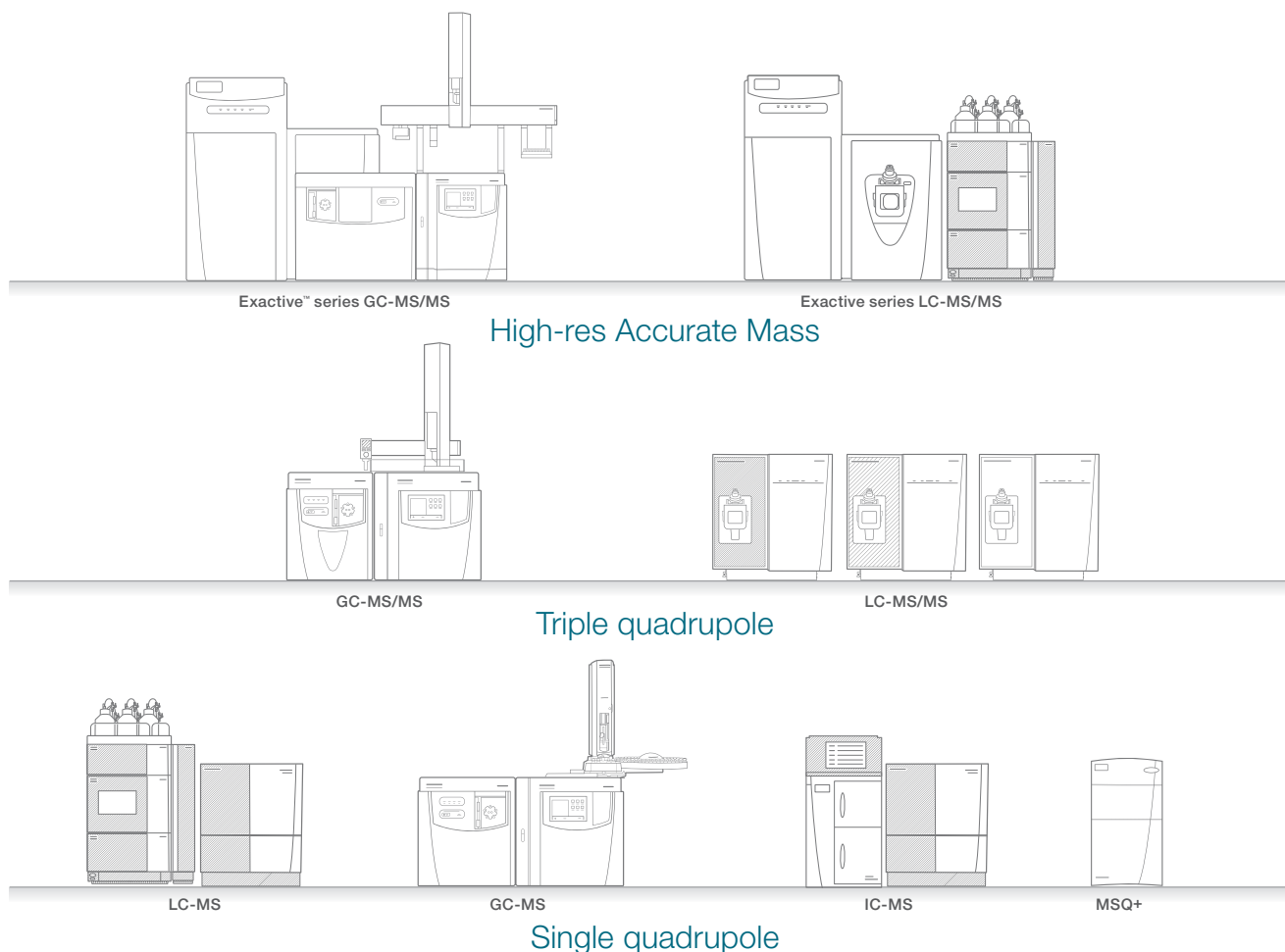
By linking the active Chromatography Studio panes to the chromatogram, data evaluation becomes simple. Calibration plots, interactive charts, and reports are linked to the active chromatogram displaying only data relevant to the current zoom or selected peaks, providing the analyst with all the information needed for fast, easy data evaluation.



### eWorkflow Procedures

Chromeleon CDS eWorkflow™ procedures capture all the unique aspects of a chromatography or MS workflow and enable you to realize significant productivity improvements in your 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 your chromatography and MS instrumentation.

## Chromeleon CDS controls over 25 Thermo Scientific™ MS instruments





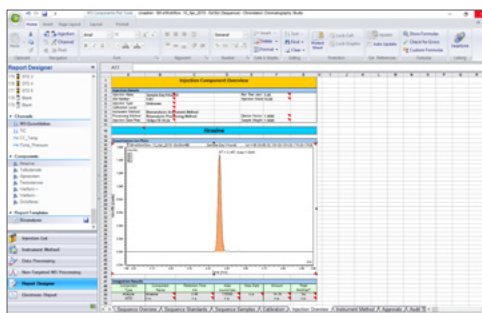
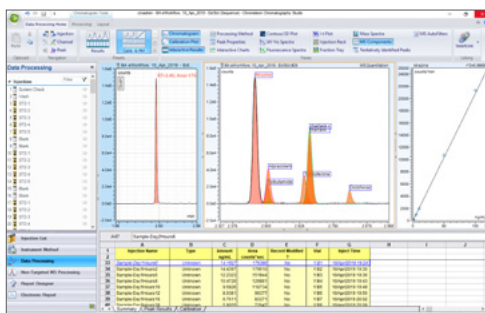
# Compliant bioanalysis

## 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

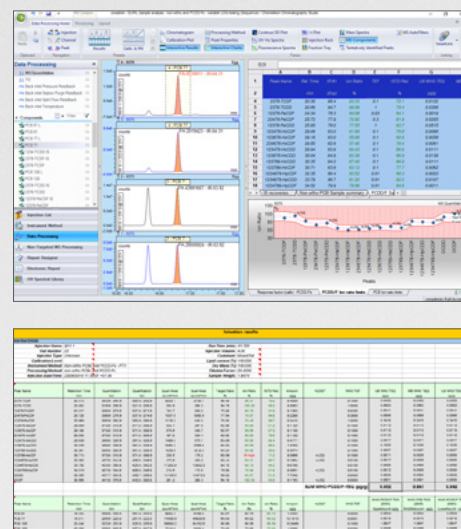


Chromeleon CDS provides a compliant bioanalysis workflow from acquisition, through data processing, to the final report

## 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 designed to handle advanced internal standard methodologies, 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:

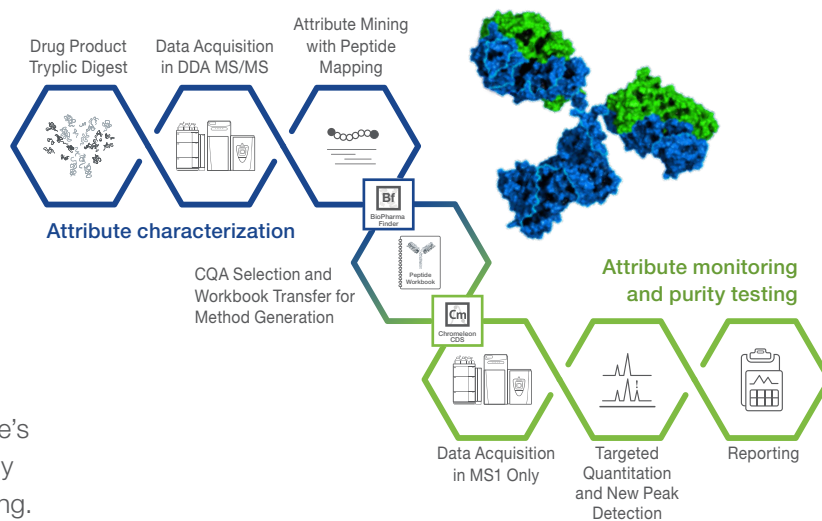
- Ensures high-quality results using two algorithms optimized for isotopically resolved (Xtract) and unresolved data (ReSpect)
- Deconvolutes isotopically unresolved data, across a wide mass range with unsurpassed speed
- Produces highly accurate results, even for low-abundance proteins
- Features an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



## Simplify your Biopharma QC 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, compliant characterization and monitoring of peptides and allows potential critical quality attributes to be monitored throughout every stage of the drug development process.

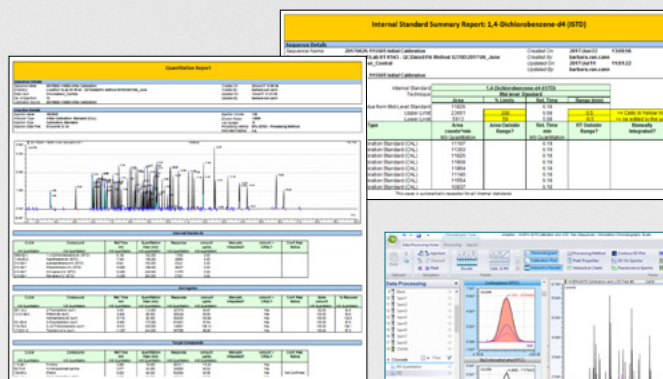
The workflow package leverages Chromeleon software's compliance capabilities from data acquisition, to quality attribute quantitation, new peak detection, and reporting.



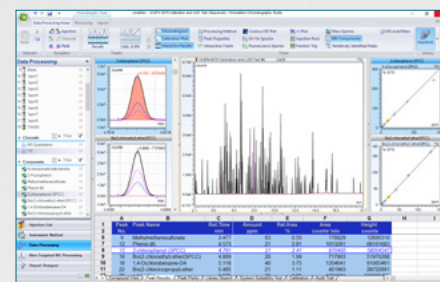
# Environmental analysis

## Easy determination of (semi)volatiles 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 (U.S.) Environmental Protection Agency (EPA) guidelines for the determination of semi-volatile organic compounds in many types of solid waste matrices, soils, air-sampling media, and water samples.



Faster creation of environmental reports – create reports in just three mouse clicks





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