MS OPERATIONS

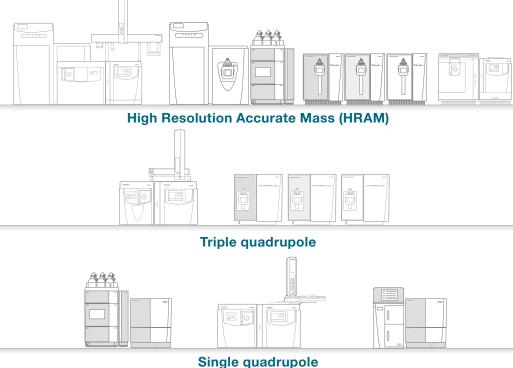
Product Spotlight



Designed for MS

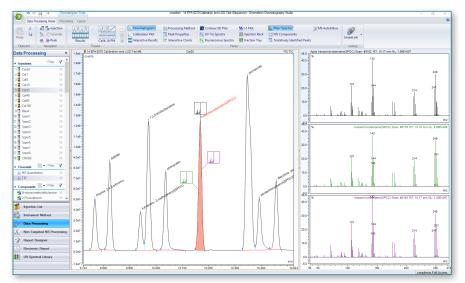
Thermo Scientific™ Chromeleon™ Chromatography Data System (CDS) is the first CDS that combines all separation and detection techniques, including mass spectrometry (MS), into a single compliance-ready enterprise (client/server) environment. Chromeleon CDS delivers full control for most Thermo Scientific™ MS systems, including compliant tuning and instrument calibration.

Chromeleon CDS controls over 35 Thermo Scientific MS instruments

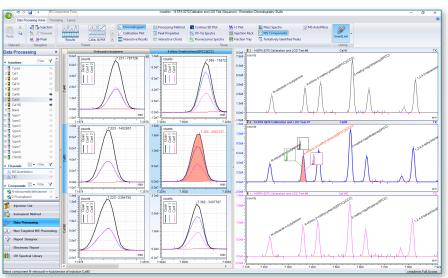




Chromeleon CDS delivers the necessary MS-specific data views, data processing, and reporting capabilities to streamline your chromatography and MS quantitation workflows in one application.



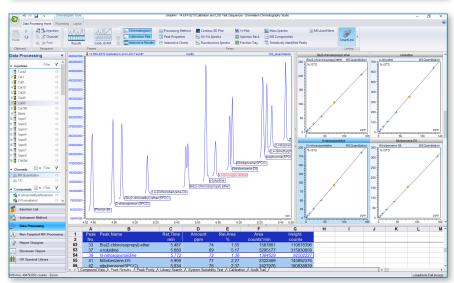
Chromatography Studio display of the Total Ion Chromatogram (TIC) and Mass Spectra plots.



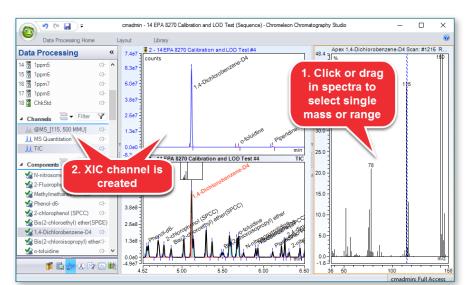
Component-centric views with simultaneous visualization of both quantitation and confirmation ions. Smartlink allows you to visualize all the information needed for fast, easy data evaluation (for example, injections in rows with components in columns).



Component confirmation indicators provide clear identity status, simplifying data review. Confirmation criteria can be set on a component by component basis.

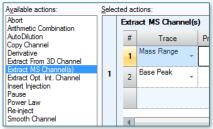


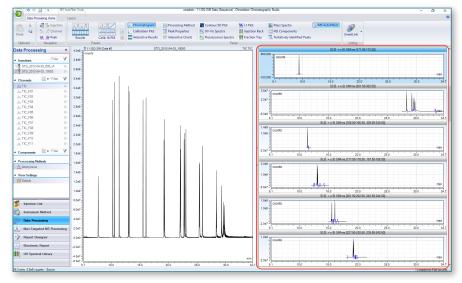
The MS Quantitation channel provides an overlaid view of all Extracted Ion Chromatograms (XICs) with easy manual or automatic extraction of XICs.



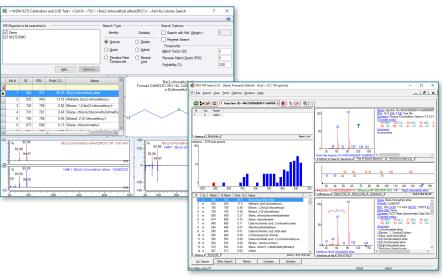
Simple graphical extraction of XICs is achieved by selecting a mass or dragging a range in the spectra plot. The temporary XIC channel can be retained, altered or discarded as required.

Intelligent Run Control can automatically extract unlimited XICs either unconditionally or based on the results of the just-acquired injection.



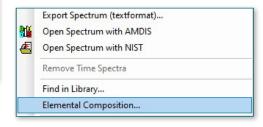


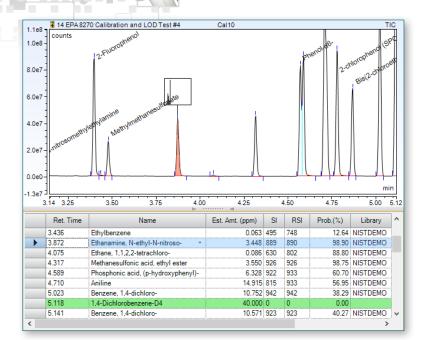
The AutoFilters Pane automatically previews all filters acquired for the selected injection(s) in a tiled, scrollable pane. A simple right click quickly creates a new channel for the selected filter.



To aid compound identification, you can use NIST (National Institute of Standards and Technology) libraries for spectral library screening and ad-hoc library searches. You can also create your own libraries within Chromeleon CDS.

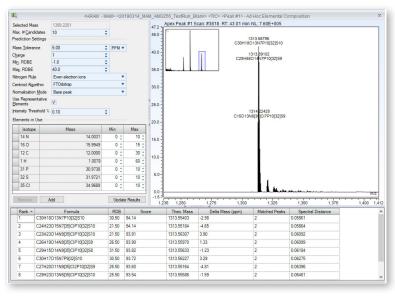
You can export raw data or spectra directly to the NIST and AMDIS (Automated Mass Spectral Deconvolution and Identification System) applications for compound identification and view Elemental Composition when working with HRAM data.





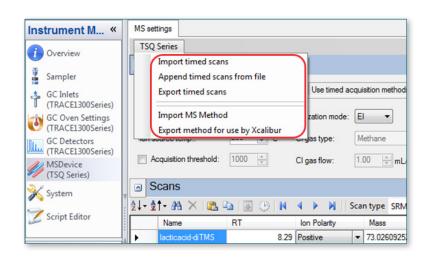
To further help with unidentified peaks, the Tentatively Identified Peaks function automatically names unidentified peaks in the injection based on library search results. The concentration of these peaks is estimated based on the nearest internal standard peak.

Tentatively Identified Peaks



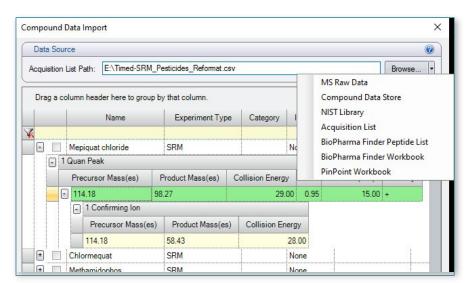
There is also the ability to view and determine the chemical formulas of ions with the Elemental Composition feature. Display formulas on the MS plot for any HRAM data.

Chromeleon CDS streamlines analysis setup, simplifying processing method creation while ensuring synchronization with the instrument method.



Easily import and export component scan events in both the instrument method and the processing method to ensure synchronization of names, retention times and windows and scan event information.

Supporting for example, both AutoSIM and AutoSRM for GC-MS method setup. These are standalone applications for optimizing either ISQ series SIM (Selected Ion Monitoring), or TSQ series SRM (Selected Reaction Monitoring) scan events, which can seamlessly be imported into Chromeleon CDS.



Directly import information into your component table including component name, retention time and window, quantitation and confirming ions, CAS number and chemical formula.

Import from predefined compound data stores e.g., Thermo Scientific™ TraceFinder™ software, Thermo Scientific™ BioPharma Finder™ software, Thermo Scientific™ PinPoint™ software workbooks, MS raw data headers, NIST library searches or acquisition lists (.csv format).

Chromeleon CDS offers a fully customizable spreadsheet-based Report Designer.

Integration Results													
No.	Peak Name Area												
		counts*min											
TIC	TIC	TIC	TIC_F01	TIC_F02	TIC_F03	TIC_F04	TIC_F05	TIC_F06	TIC_F07	TIC_F08	TIC_F09	TIC_F10	TIC_F11
1	PCB#18	65532.06	83971.06	53723.76	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.
14	PCB#28	79797.65	104873.21	68275.51	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.
15	PCB#33	77186.91	107441.73	66747.11	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.
27	PCB#52	22333.79	n.a.	n.a.	28060.53	20123.99	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.
46	PCB#95	15384.05	n.a.	n.a.	n.a.	n.a.	16229.40	18804.83	n.a.	n.a.	n.a.	n.a.	n.a.
70	PCB#70	11805.59	n.a.	n.a.	23790.64	639.98	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.
131	PCB#156	6964.78	n.a.	n.a.	n.a.	n.a.	17091.02	19454.74	14612.81	7891.28	n.a.	n.a.	n.a.
217	PCB#126	12138.98	n.a.	n.a.	n.a.	n.a.	12304.00	14606.28	n.a.	n.a.	n.a.	n.a.	n.a.
244	PCB#153	267.00	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	24712.58	6895.64	n.a.	n.a.	1.32
304	PCB#188	3888.39	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	5757.50	2258.66
313	PCB#170	3220.40	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	4771.49	2534.16

MS-based reporting objects and consolidated report tables catering for multiple traces and large data sets allow users to quickly and easily evaluate, filter, and report MS data. Flexible reporting options enable customized reports and calculations to be created within Chromeleon CDS, eliminating the need to transfer data to an external spreadsheet and, thus, eliminating the risk of human error.

The integration table can be set up to show results for all channels collected during an injection. Or set up to display the channel with the highest response for each component in the injection.

Built in report templates are also available with automatic print and export options following analysis.

No.	Peak Name	Area	Area	Channel
		counts*min	counts*min	
TIC	TIC	TIC	Highest Response	Highest Response
1	PCB#18	65532.06	83971.06	TIC_F01
14	PCB#28	79797.65	104873.21	TIC_F01
15	PCB#33	77186.91	107441.73	TIC_F01
27	PCB#52	22333.79	28060.53	TIC_F03
46	PCB#95	15384.05	18804.83	TIC_F06
70	PCB#70	11805.59	23790.64	TIC_F03
131	PCB#156	6964.78	19454.74	TIC_F06
217	PCB#126	12138.98	14606.28	TIC_F06
244	PCB#153	267.00	24712.58	TIC_F07
304	PCB#188	3888.39	5757.50	TIC_F10
313	PCB#170	3220.40	4771.49	TIC_F10

By extending Chromeleon CDS beyond chromatography into MS, it is now possible to streamline chromatography and MS quantitation workflows within a single software package and use your MS like any other routine detector.

Find out more at thermofisher.com/chromeleon

