thermoscientific

Designed for MS

Thermo Scientific Chromeleon 7.2 Chromatography Data System

Thermo Scientific™ Chromeleon™ 7.2 Chromatography Data System (CDS) is the first CDS that supports Mass Spectrometry (MS) instrument control and data processing with all main front-end separation techniques (GC, IC, LC) in an enterprise (client/server) environment. Chromeleon 7.2 CDS delivers full control for many Thermo Scientific™ MS systems, including tuning and instrument calibration.

Thermo Scientific™ ISQ™ EC Single Quadrupole Mass Spectrometer

Thermo Scientific™ ISQ™ Series GC-MS systems

Thermo Scientific™ TSQ™ 8000 Series GC-MS systems

Thermo Scientific™ TSQ™ Triple Quadrupole LC-MS systems

Thermo Scientific™ Exactive™ Series Orbitrap™ LC-MS systems

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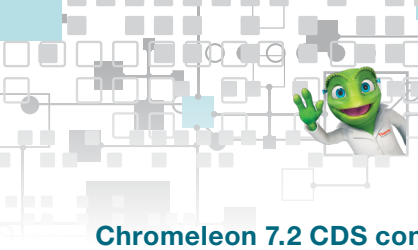
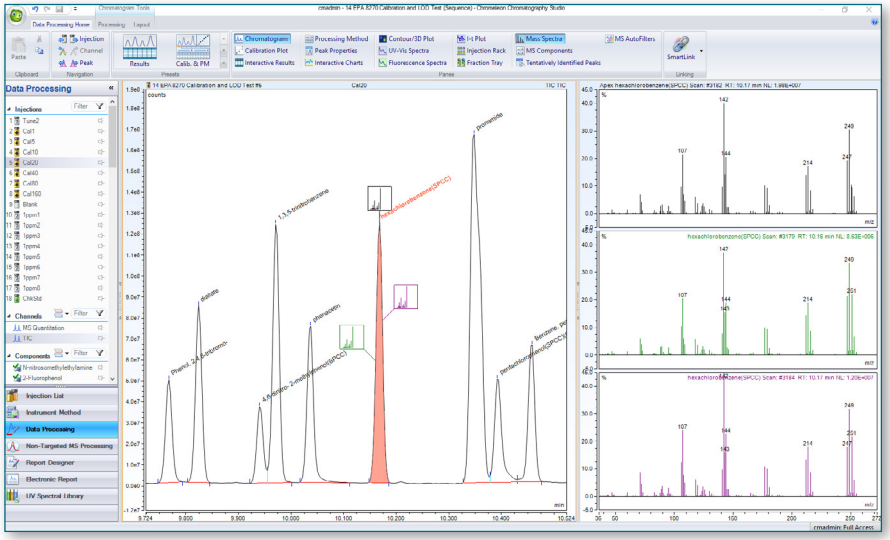
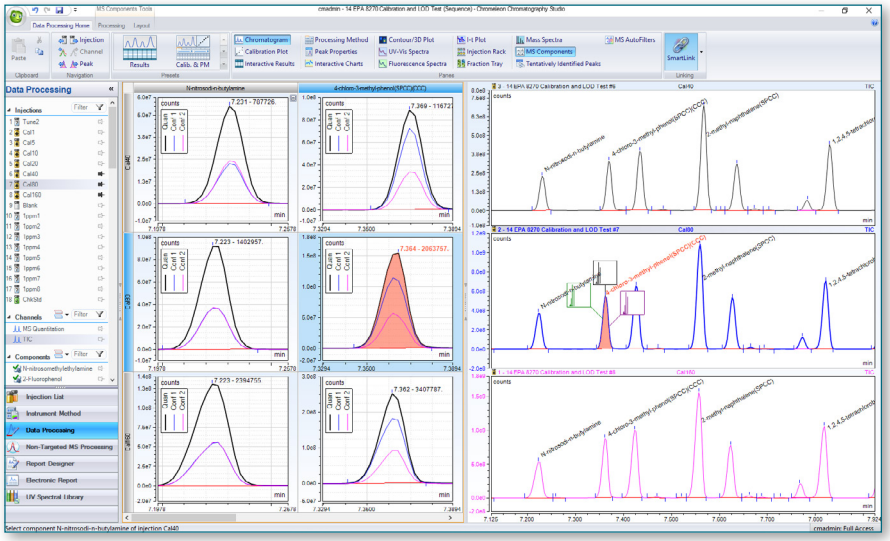


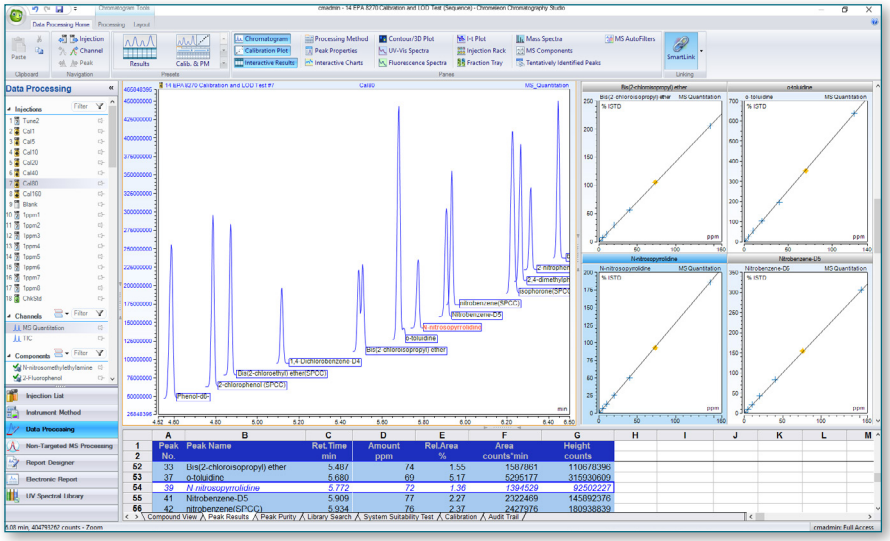
Chromeleon 7.2 CDS contains the necessary MS-specific data views, data processing, and reporting capabilities to streamline your chromatography and MS quantitation workflows in one application.



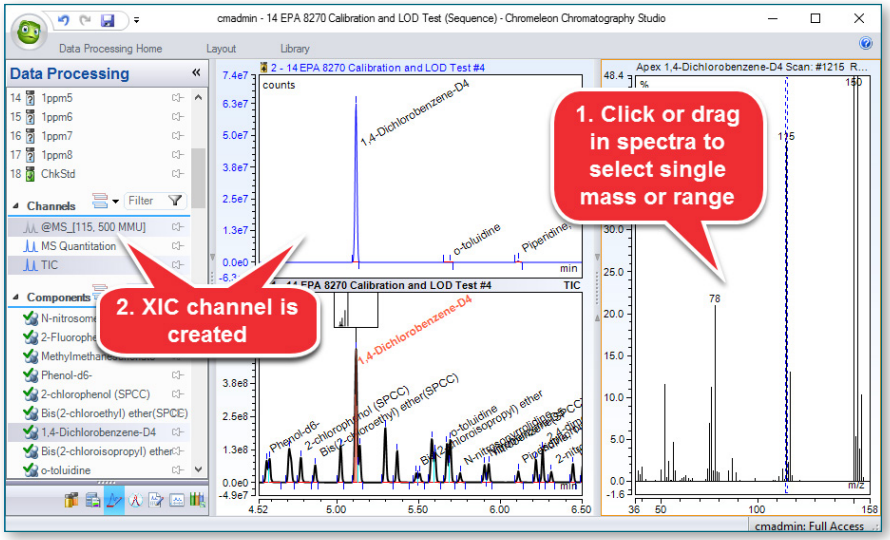
Chromatography Studio display of the Total Ion Chromatogram (TIC) and Mass Spectra plots.



Component-centric views with simultaneous visualization of both quantitation and confirmation ions (injections in rows, components in columns).

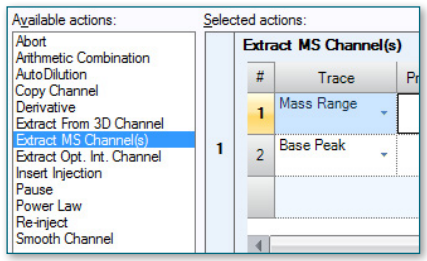


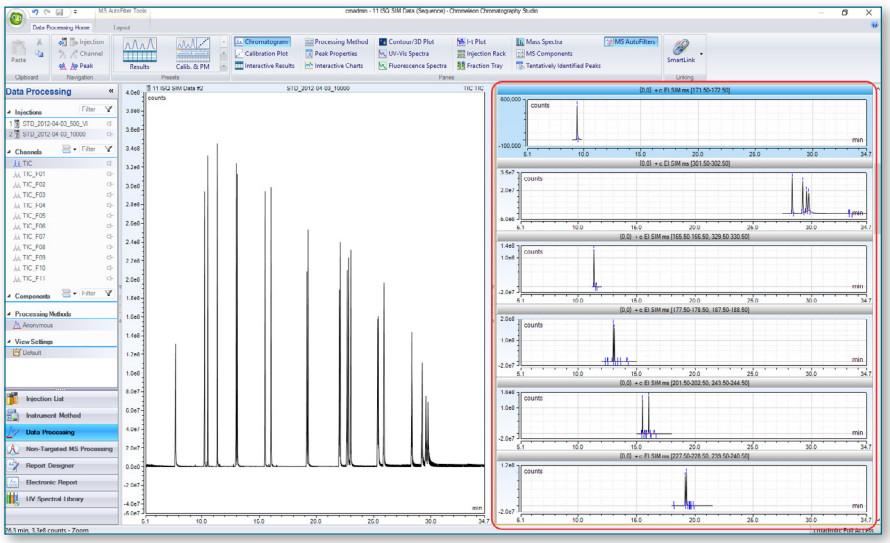
The MS Quantitation channel provides an overlaid view of all Extracted Ion Chromatograms (XICs) with easy manual or automatic extraction of XICs.



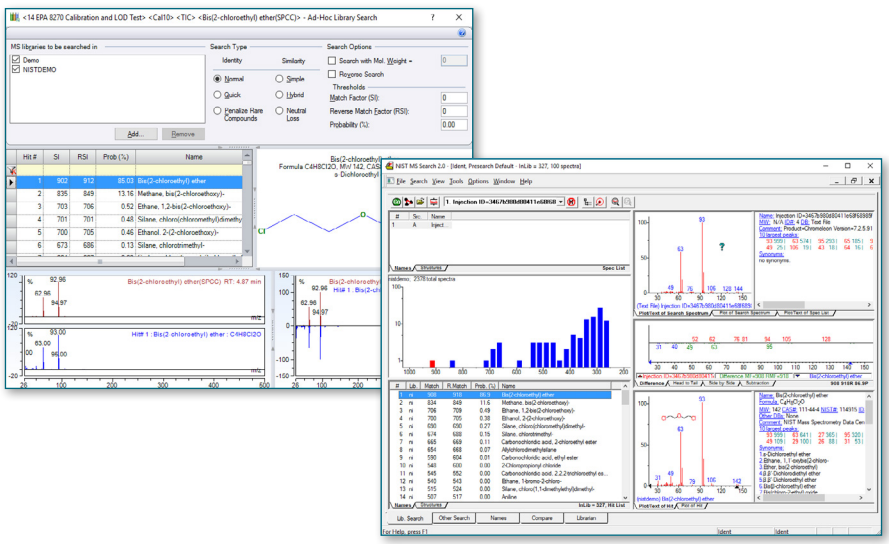
Simple graphical extraction of XICs is done by selecting a mass or dragging a range in the spectra plot. The temporary XIC channel can be retained, altered or discarded as required.

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



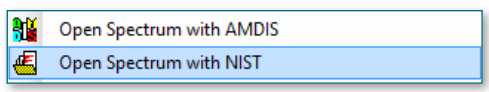


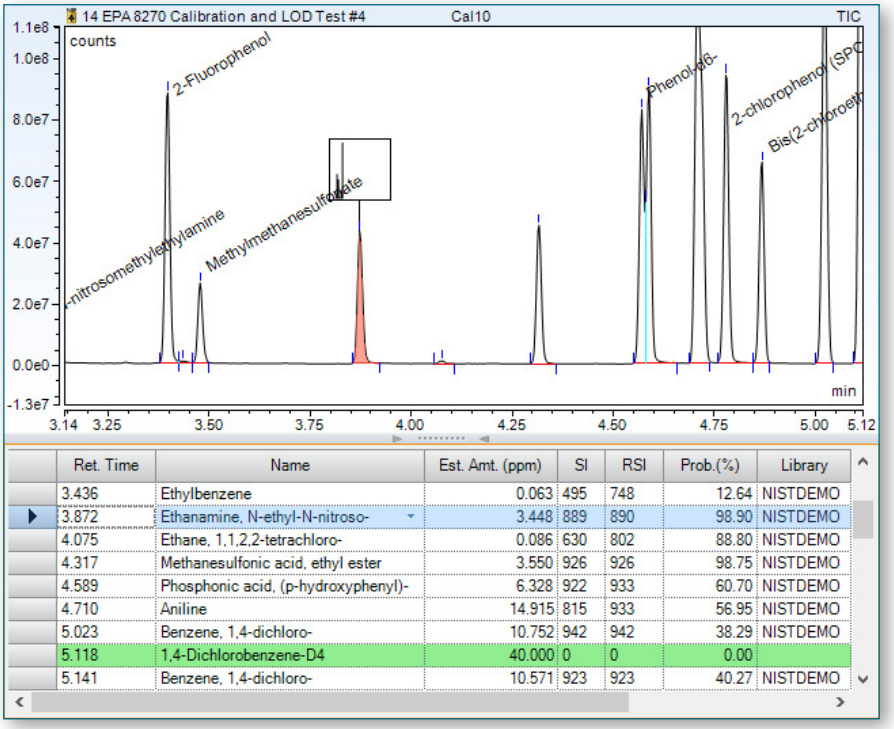
The AutoFilters Pane automatically previews all filters acquired for the selected injection(s) in a tiled, scrollable pane. A simple right click quickly creates a new channel for the selected filter.



To aid compound identification, you can use NIST (National Institute of Standards and Technology) libraries for spectral library screening and ad-hoc library searches.

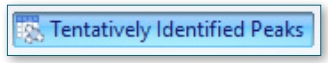
You can export raw data or spectra directly to the NIST and AMDIS (Automated Mass Spectral Deconvolution and Identification System) applications for compound identification.



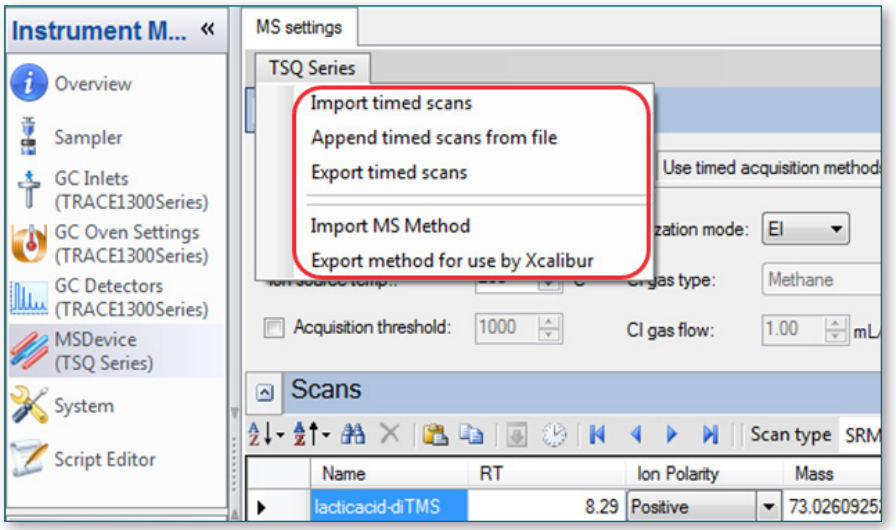


Ret. Time	Name	Est. Amt. (ppm)	SI	RSI	Prob.(%)	Library
3.436	Ethylbenzene	0.063	495	748	12.64	NISTDEMO
3.872	Ethanamine, N-ethyl-N-nitroso-	3.448	889	890	98.90	NISTDEMO
4.075	Ethane, 1,1,2,2-tetrachloro-	0.086	630	802	88.80	NISTDEMO
4.317	Methanesulfonic acid, ethyl ester	3.550	926	926	98.75	NISTDEMO
4.589	Phosphonic acid, (p-hydroxyphenyl)-	6.328	922	933	60.70	NISTDEMO
4.710	Aniline	14.915	815	933	56.95	NISTDEMO
5.023	Benzene, 1,4-dichloro-	10.752	942	942	38.29	NISTDEMO
5.118	1,4-Dichlorobenzene-D4	40.000	0	0	0.00	
5.141	Benzene, 1,4-dichloro-	10.571	923	923	40.27	NISTDEMO

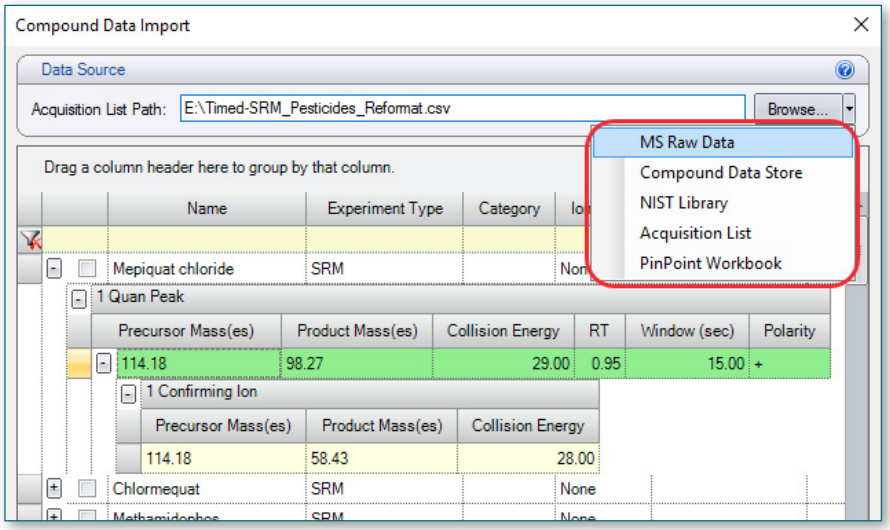
To further help with unidentified peaks, the Tentatively Identified Peaks function automatically names unidentified peaks in the injection based on library search results. The concentration of these peaks is estimated based on the nearest internal standard peak.



Chromeleon 7.2 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.



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™ PinPoint™ software workbooks, MS raw data headers, NIST library searches or acquisition lists (.csv format).

Chromeleon CDS also supports both AutoSIM and AutoSRM for GC-MS method setup. These are standalone applications for optimizing either ISQ series SIM (Selected Ion Monitoring), or TSQ 8000 series SRM (Selected Reaction Monitoring), scan filters for a collection of compounds to achieve the best overall selectivity and signal-to-noise response.

MS-based reporting objects and consolidated report tables catering for multiple traces and large data sets allow users to quickly and easily evaluate and report MS data.

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.				
131	PCB#156	6964.78	n.a.	n.a.	n.a.	n.a.	17091.02	19454.74	14612.81				
217	PCB#126	12138.98	n.a.	n.a.	n.a.	n.a.	12304.00	14606.28	n.a.				
244	PCB#153	267.00	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	24712.58				
304	PCB#188	3888.39	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.				
313	PCB#170	3220.40	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.				

The integration table can be set up to show results for all channels collected during an injection.

No. TIC	Peak Name TIC	Area counts*min TIC	Area counts*min Highest Response	Channel 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

The integration table can also set up to use the channel with the highest response for each component in the injection.

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**

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