



Intelligent functionality: Unique CDS software features for GC-MS spectral library searching

Thermo Scientific Chromeleon 7.2 Chromatography Data System

Thermo Scientific™ Chromeleon™ 7 Chromatography Data System (CDS) software uses intelligent functionality to simplify chromatography processes—whether for a single instrument or a large enterprise. With the latest version, 7.2, Chromeleon CDS is the first software to include control, data processing and reporting for MS instruments—combining all the benefits of Chromeleon CDS with the possibilities of the Thermo Scientific MS portfolio.



Thermo Scientific™ ISQ™ Series GC-MS systems

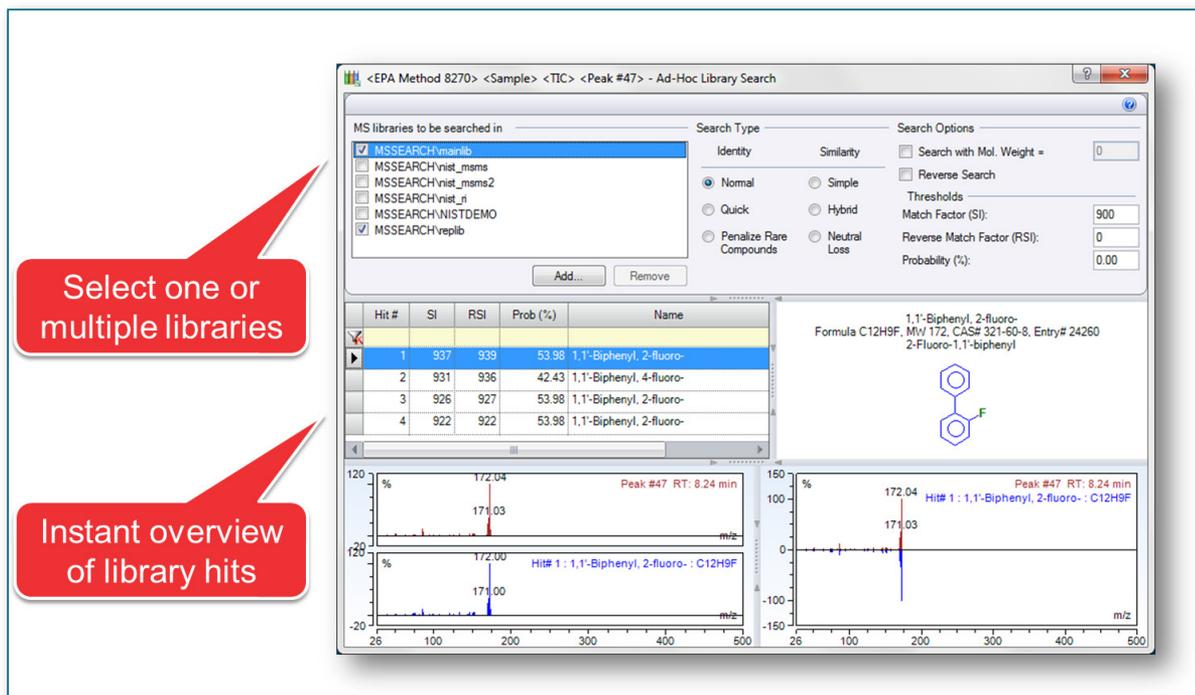
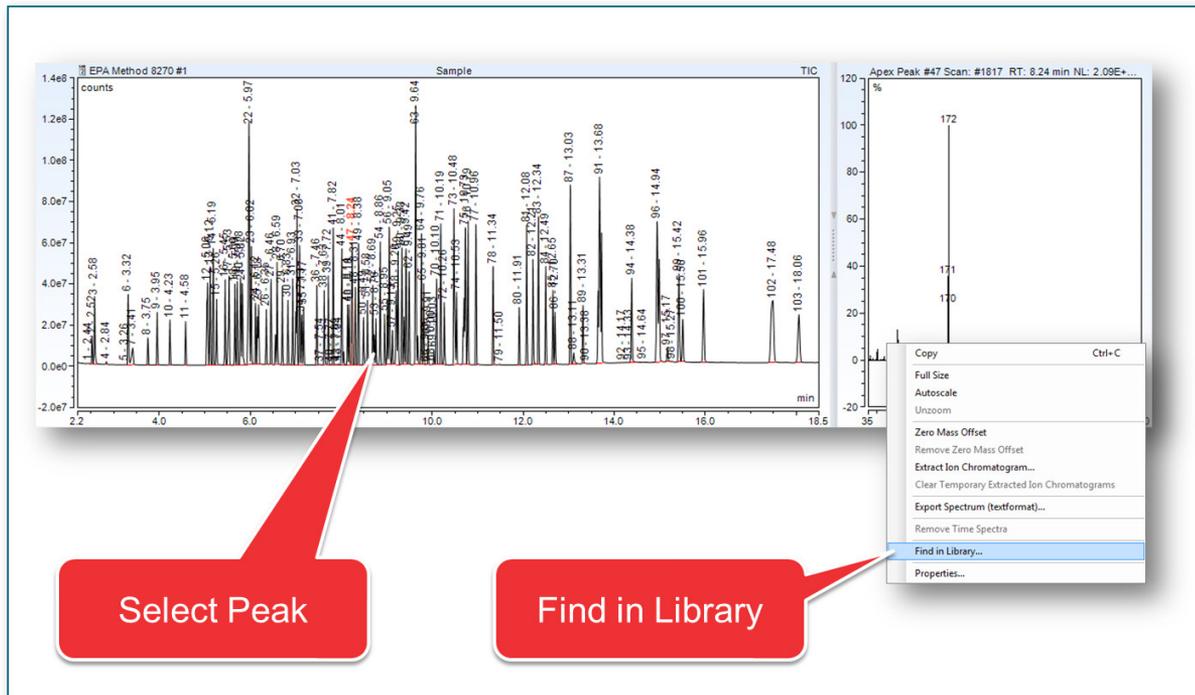


Thermo Scientific™ TSQ™ 8000 Series GC-MS systems



Spectral library search in multiple libraries

When acquiring full scan MS spectra in a GC-MS run, the acquired MS spectra of unknown peaks are often compared against various libraries for component identification. Checking the spectrum of an unknown peak against each of the libraries can be a time-consuming, manual process, especially when a chromatogram contains many peaks. With Chromeleon CDS, this process is automated and minimizes manual interactions while maximizing analyst time.



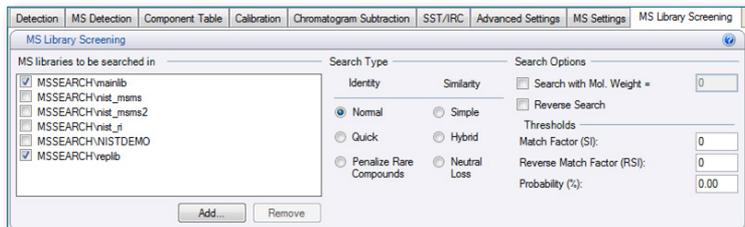
Select one or multiple libraries

Instant overview of library hits



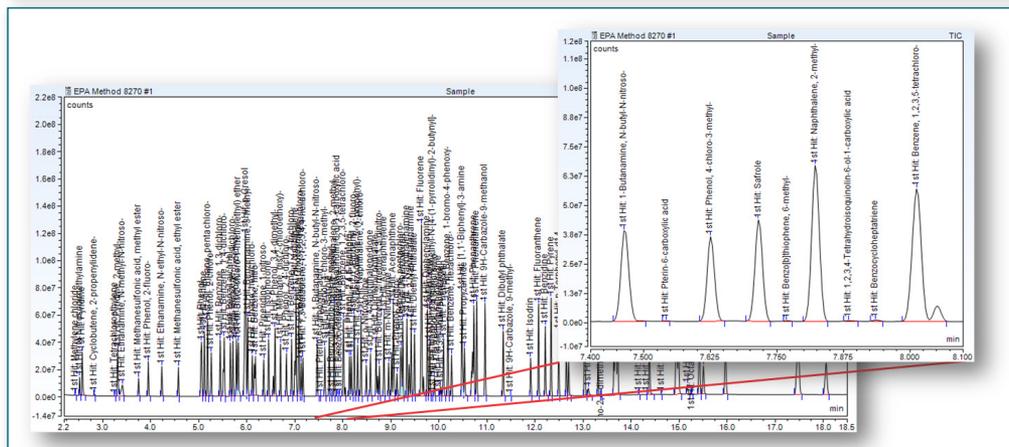
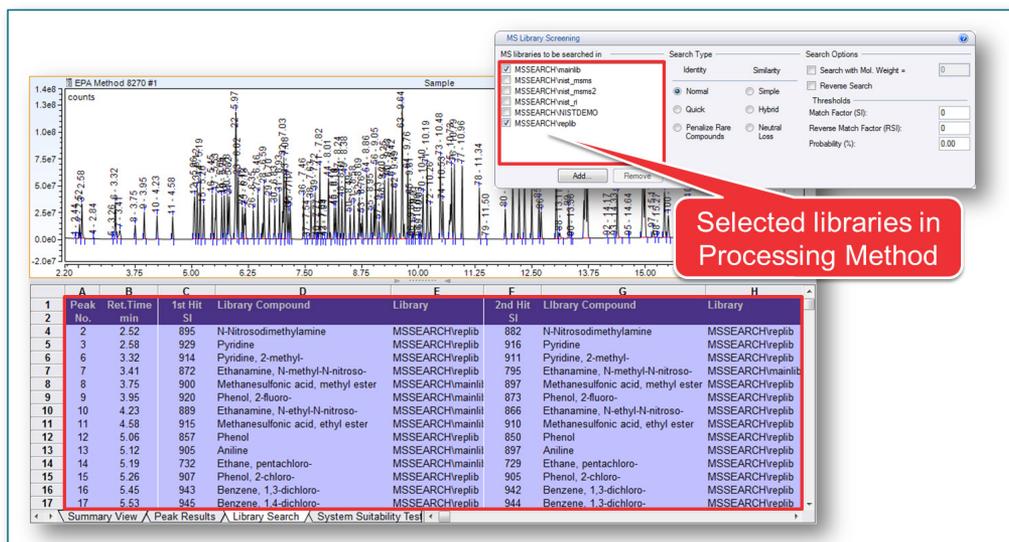
Multiple libraries—automatic search

It is possible to set up the library search in the processing method. This ensures a library search is always performed instantly, on all peaks in a chromatogram. This applies to ALL injections using the same Processing Method, even if those injections have never been looked at before the results haven't been reviewed.



Instant library search results

In the processing method, one or more of the MS spectral libraries can be easily selected. When this is done, an instant overview of spectral library search results for all peaks in the chromatogram is given in a table below the chromatogram. It is even possible to add library search results to the peak label directly on the chromatogram for an even simpler overview. It is then possible to open data files that have not previously been reviewed and see tentative hits labeled on the peaks. Data files that have not previously been reviewed can be opened and automatically have tentative hits labeled on the peaks.



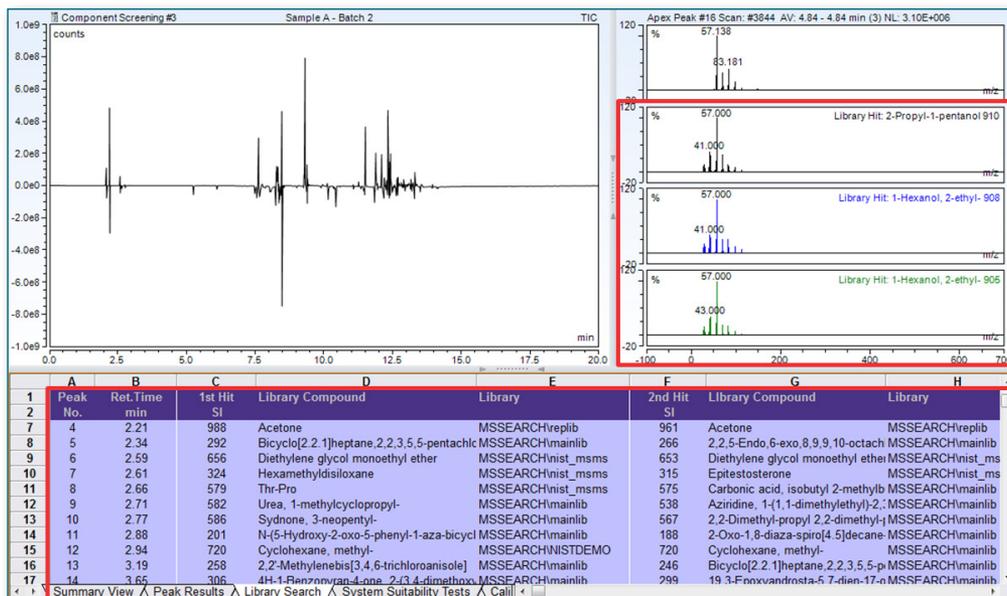
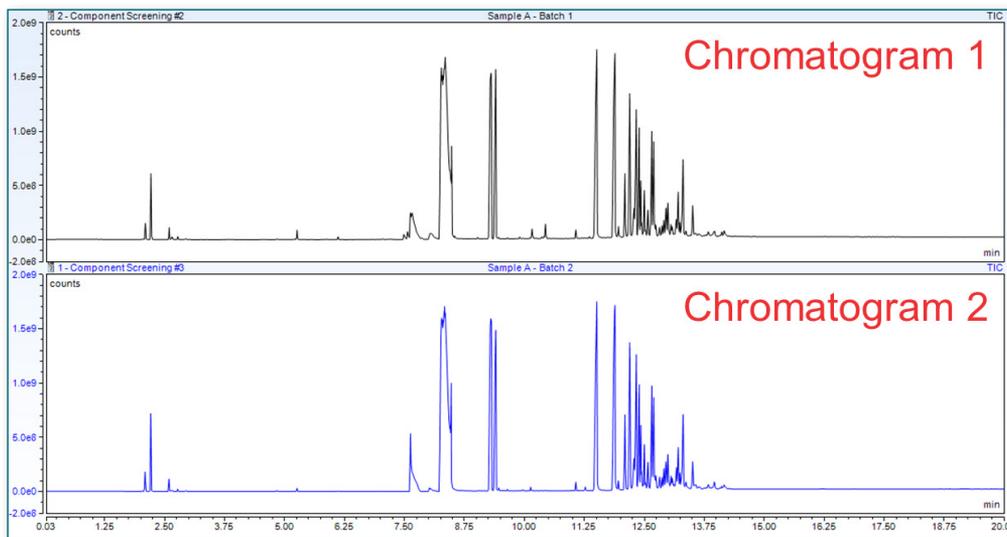


Library searching on result chromatograms

When performing an MS library search, sometimes not all of the peaks in the chromatogram may be of interest. Chromleon CDS has a built-in option to automatically subtract chromatograms:

- Subtract a blank to eliminate matrix peaks
- Subtract a fixed injection to show differences between chromatograms

The library search can be performed on the resulting chromatogram, giving valuable information about the differences in the two initial chromatograms – an automated way of chromatogram handling, saving time!



Find out more at thermofisher.com/chromleon

ThermoFisher
SCIENTIFIC