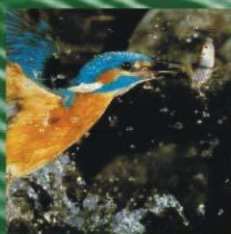


MSChromSearch 3.0

Software for fully automatic comparison of chromatograms.

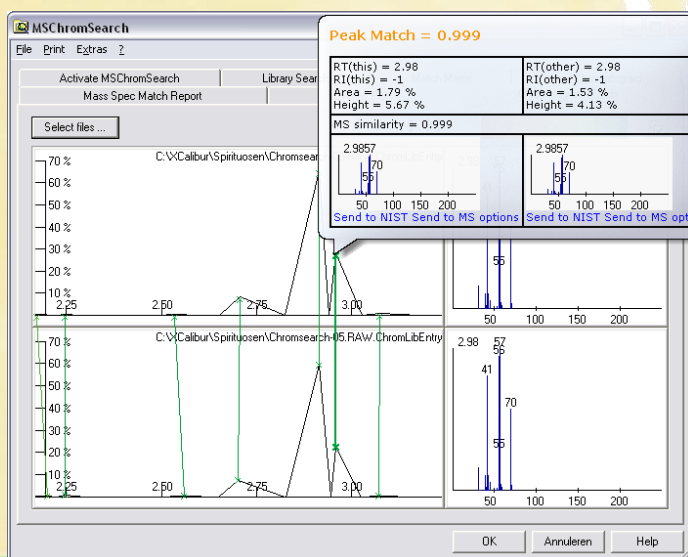
Users are regularly faced with the task of comparing chromatograms from GC/MS systems or analog detectors. Currently this is usually done visually and is thereby rather subjective. In addition, it is almost impossible to deal with larger numbers of complex chromatograms based on visual comparison.



This is exactly where MSChromSearch comes in: MSChromSearch compares a chromatogram with a library of other chromatograms, similar to a library search in a mass spectrum library. The user can select between mass spectra, retention times, retention indices, and/or peak intensity data. From the selected data a "fit value" is calculated as a measure for the match between two chromatograms. Chromatograms that were found are listed in the form of a hit list based on the fit value. MSChromSearch enables comparison of a chromatogram with several hundred chromatograms within a very short time.

In addition, two chromatograms from different data systems can be compared in detail in order to obtain information about interrelationships or deviations. The software can be used in pyrolysis applications for identification of organic solids, for comparison of volatile components to determine the cause of a fire or in quality control for good/poor comparison of samples.

MSChromSearch saves a tremendous amount of time (just think how long a visual comparison of several hundred chromatograms would take), and offers an objective numerical value for the match between two chromatograms.



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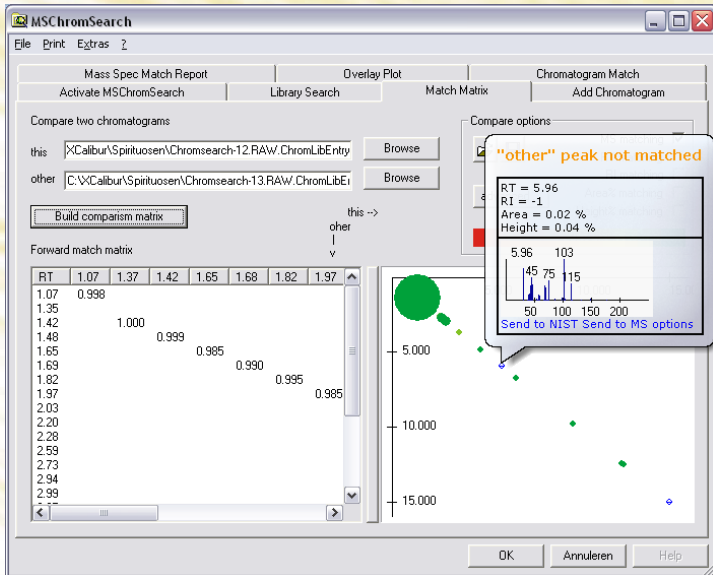
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ATAS GL
GL Sciences Company

New useful functions have been added in Version 3.0:

- New module for reading Agilent Chemstation files
- New overlay module enables superposition of any number of chromatograms from different data systems
- New "Chromatogram Match" module offers detailed comparison of two chromatograms and their spectrums and a NIST search option
- Chromatogram search in subfolders allows building structured chromatogram libraries
- Comprehensive Online help
- Mass spectrum import from NIST and other programs Inclusion of LC/MS chromatograms
- With MSChromSearch 3.0 retention indices can now also be used for comparison



Comparative matrix of two chromatograms with one highly differing peak (Peak Match)

Hit list

S.Name	File	Fow. f.	nPeaks	F...	Rev...	nPeaks...
Laphroaig, 10 Jahre	Chromsearch-02.RAW.ChromLibEntry	1.000	28/28	1.000	28/28	
Macallan, 12 Jahre	Chromsearch-03.RAW.ChromLibEntry	0.945	27/28	0.980	27/27	
Tandru, 17 Jahre	Chromsearch-05.RAW.ChromLibEntry	0.940	28/28	0.877	28/30	
Tannavulin, 1993	Chromsearch-04.RAW.ChromLibEntry	0.933	28/28	0.816	28/32	
Kirschwasser	Chromsearch-20.RAW.ChromLibEntry	0.880	28/28	0.724	28/34	
Johnny Walker Black Label, 12 Jahre	Chromsearch-17.RAW.ChromLibEntry	0.863	27/28	0.895	27/27	
Antico Rovere, 3 Jahre	Chromsearch-14.RAW.ChromLibEntry	0.841	28/28	0.765	28/30	
Hasebrink	Chromsearch-15.RAW.ChromLibEntry	0.841	28/28	0.905	28/26	
La Poujade	Chromsearch-06.RAW.ChromLibEntry	0.833	26/28	0.897	26/26	
Bacardi Black	Chromsearch-11.RAW.ChromLibEntry	0.803	26/28	0.865	26/26	
Habbel	Chromsearch-18.RAW.ChromLibEntry	0.791	26/28	0.852	26/26	
Granatapfelschnaps	Chromsearch-32.RAW.ChromLibEntry	0.768	28/28	0.741	28/29	
Zacapa Centenario, 23 Jahre	Chromsearch-13.RAW.ChromLibEntry	0.762	23/28	0.928	23/23	
Berentzen Winterapfel	Chromsearch-30.RAW.ChromLibEntry	0.743	28/28	0.520	28/40	

List of results with numerical values for the dimension of conformance

MSChromSearch is a product of Axel Semrau®



a total analytical solution

