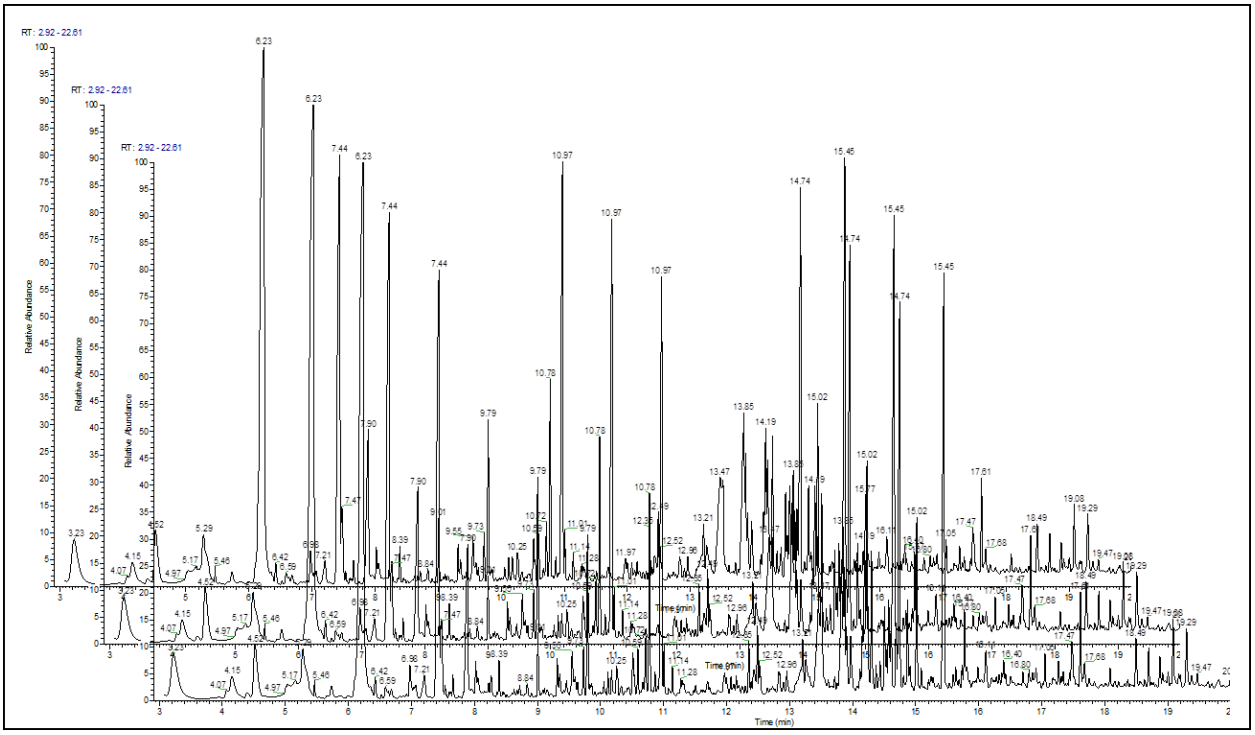
Axel Semrau®

MSChromSearch



Product Information

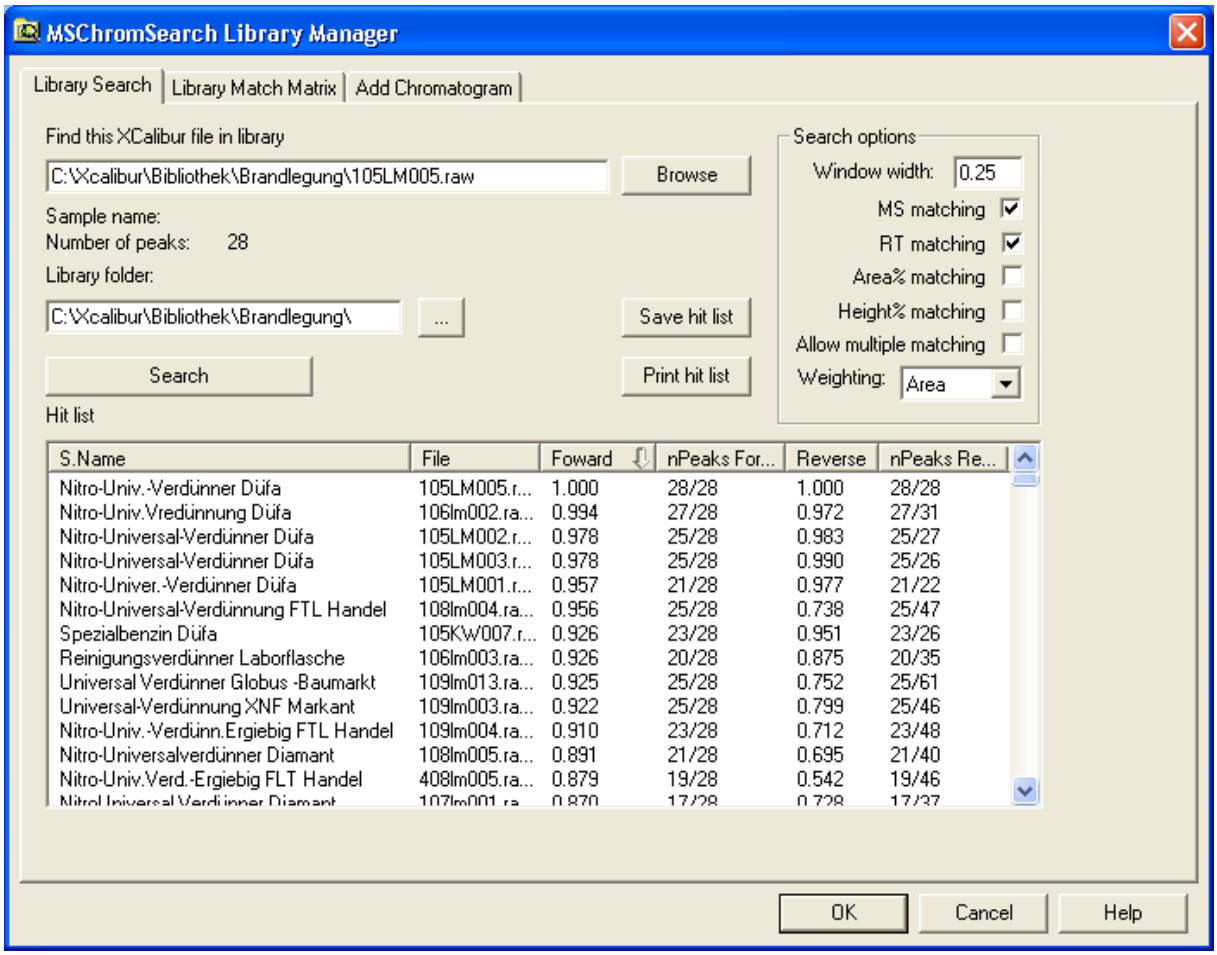


Figure 1: Overview of the software.

Software for automatic chromatogram comparison

Recognizing chromatograms

A frequent task in chromatographic analytics is to compare chromatograms with each other. Commonly, this is done visually, supported by diverse tools of evaluation systems, e.g. overlay functions.

The result of whether two chromatograms resemble each other or not is always subjective and user-dependent. There is no numeric or even limit value for the match of chromatograms as for example similar to the libraries of mass spectra.

When comparing GC/MS chromatograms in order to find matches or differences between separate analyses the user has to compare single measuring points, additionally to the TIC. If this is done manually by the user, it becomes a very time-consuming and cumbersome task evaluate every single peak. That way, a comparison of a chromatogram with a database which consists of several hundreds of chromatograms is almost impossible.

Here, MSChromSearch comes into play. The software allows the user to automatically compare a chromatogram with a data base of chromatograms. In the process, the user defines if mass spectra, retention times or intensities should be used as comparison criteria. Certainly, any desired combination of these parameters may be chosen as a basis for comparison. The drift of retention times as a results of an aging column or changing hardware etc. can be compensated by determining and considering retention indices.

The first step when using MSChromSearch is the analysis of the chromatograms to be compared with the help of an evaluation method of the data system. Thereby, peak and spectra information are obtained. The data system Xcalibur® for example creates these data using a Processing Method. During that method all chromatographic peaks are determined and stored in a file, together with the corresponding data such as retention time, mass spectrum and normalized intensity.

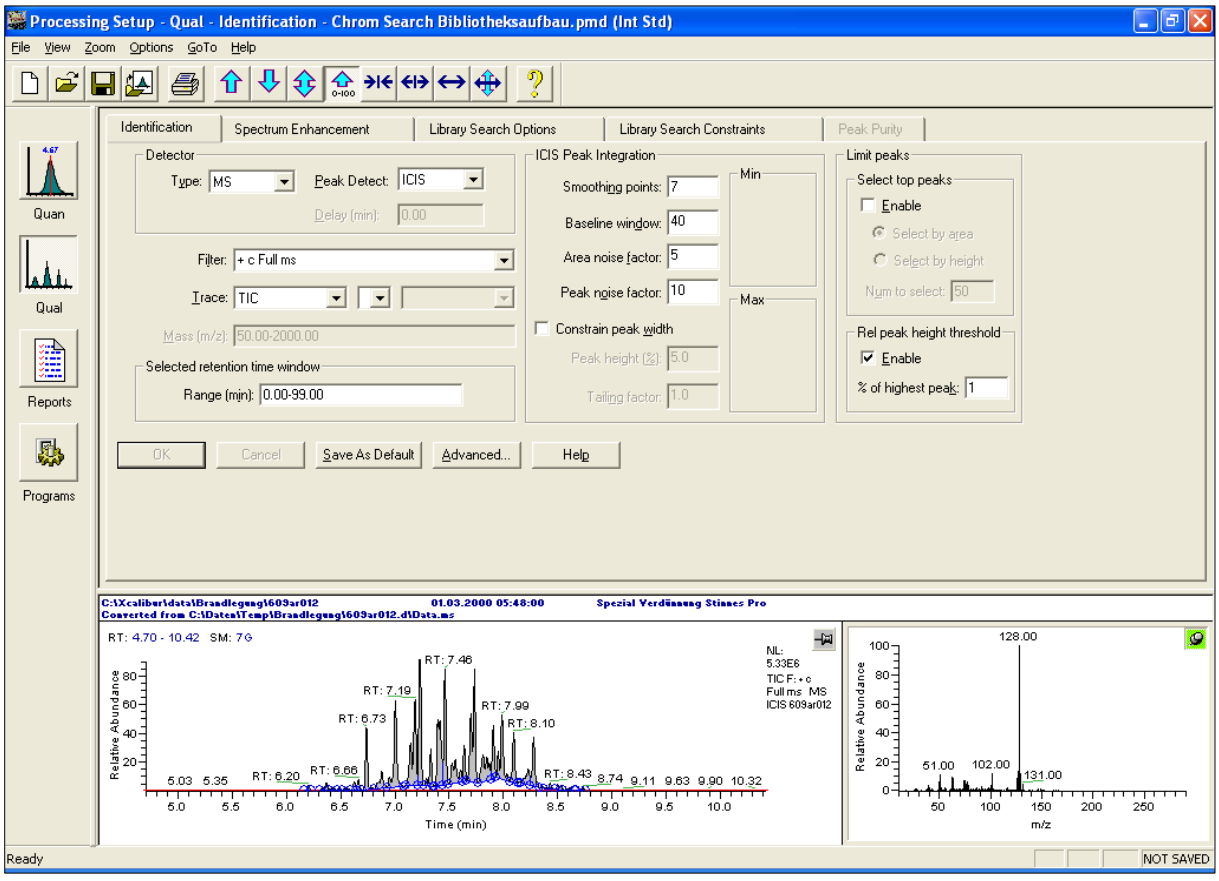


Figure 2: Processing Method by Xcalibur® for the analysis of chromatograms.

During the search, MSChromSearch compares these data with the corresponding data of chromatograms from the data base and calculates a fit value. The fit value indicates how well the searched chromatograms fits to the chromatograms in the data base. MSChromSearch generates a ranking in which the chromatograms from the data base are sorted by their degree of matching.

Of course, the list may be printed out or exported to a *.csv file which may be read directly using Excel. The user may click right to open the sample and the library chromatogram in the associated data system, e.g. Qual Browser by Xcalibur®, and process the data further.

By creating a comparative matrix or an overview table, the analysis of differences between a sample chromatogram and a library chromatogram is possible as well. In both the chromatogram comparison is performed peak by peak and thus allows for conclusions regarding the similarity of single peaks. To simplify the comparison, differences between single chromatograms are visualized by a figure or table.

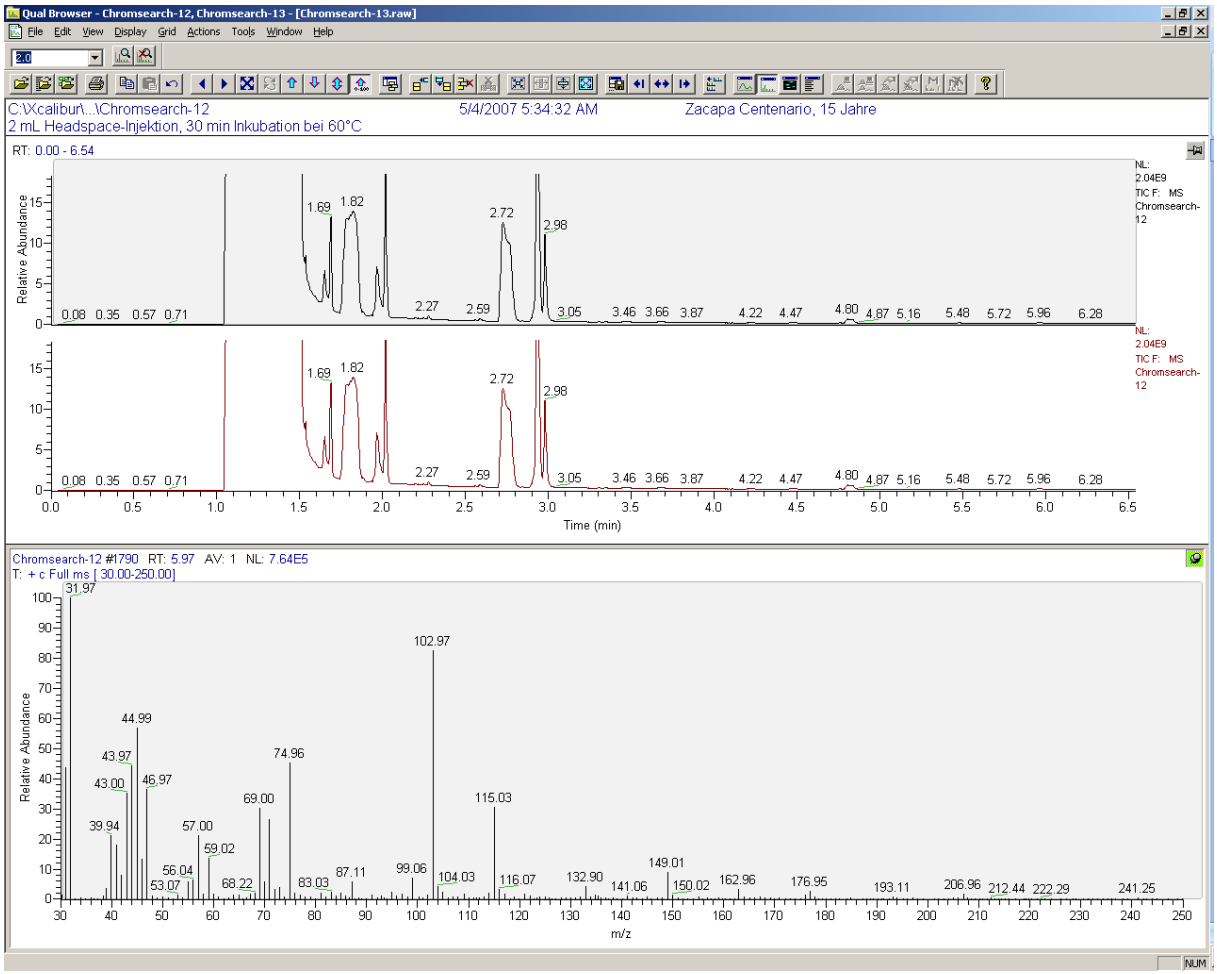


Figure 3: Overlay function in the Qual Browser by Xcalibur®.

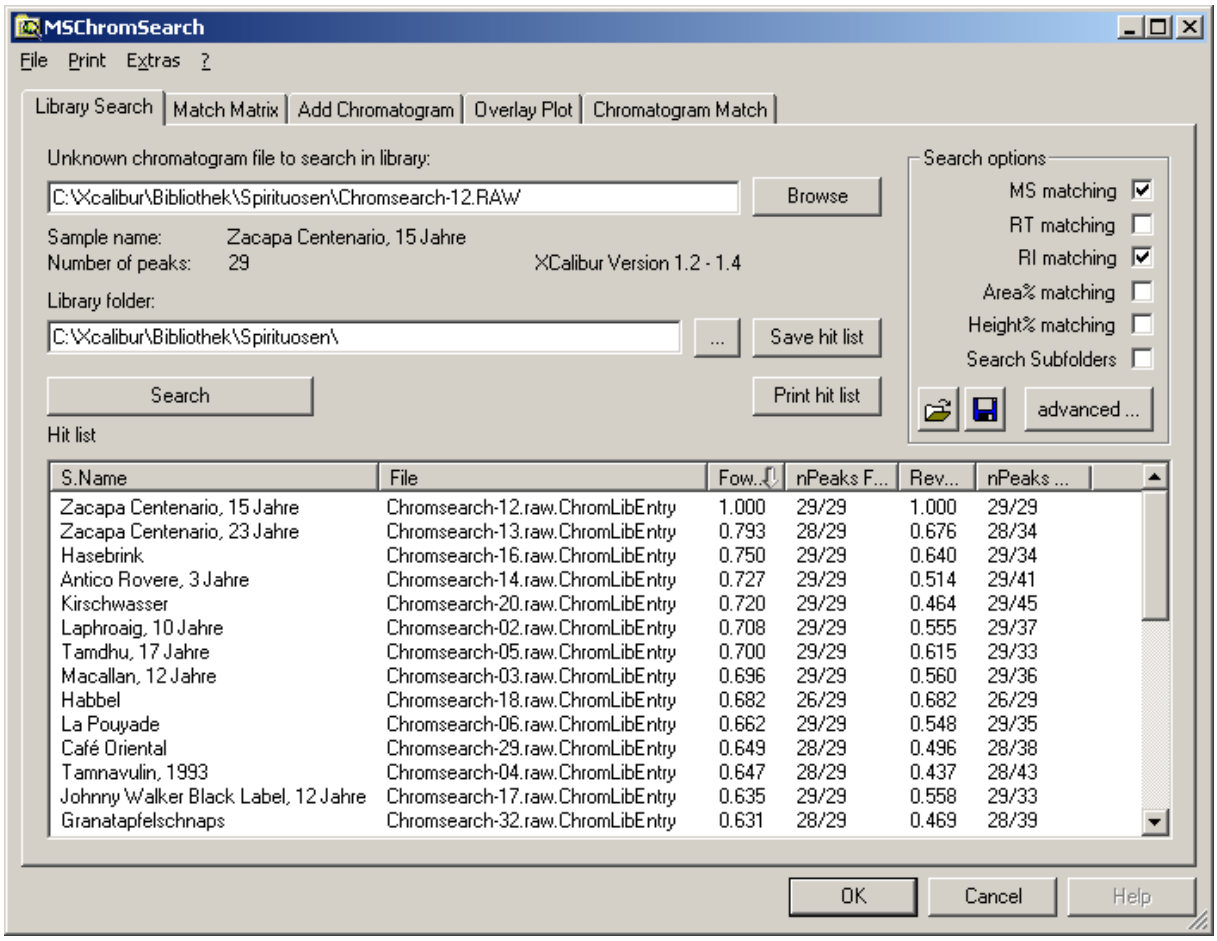
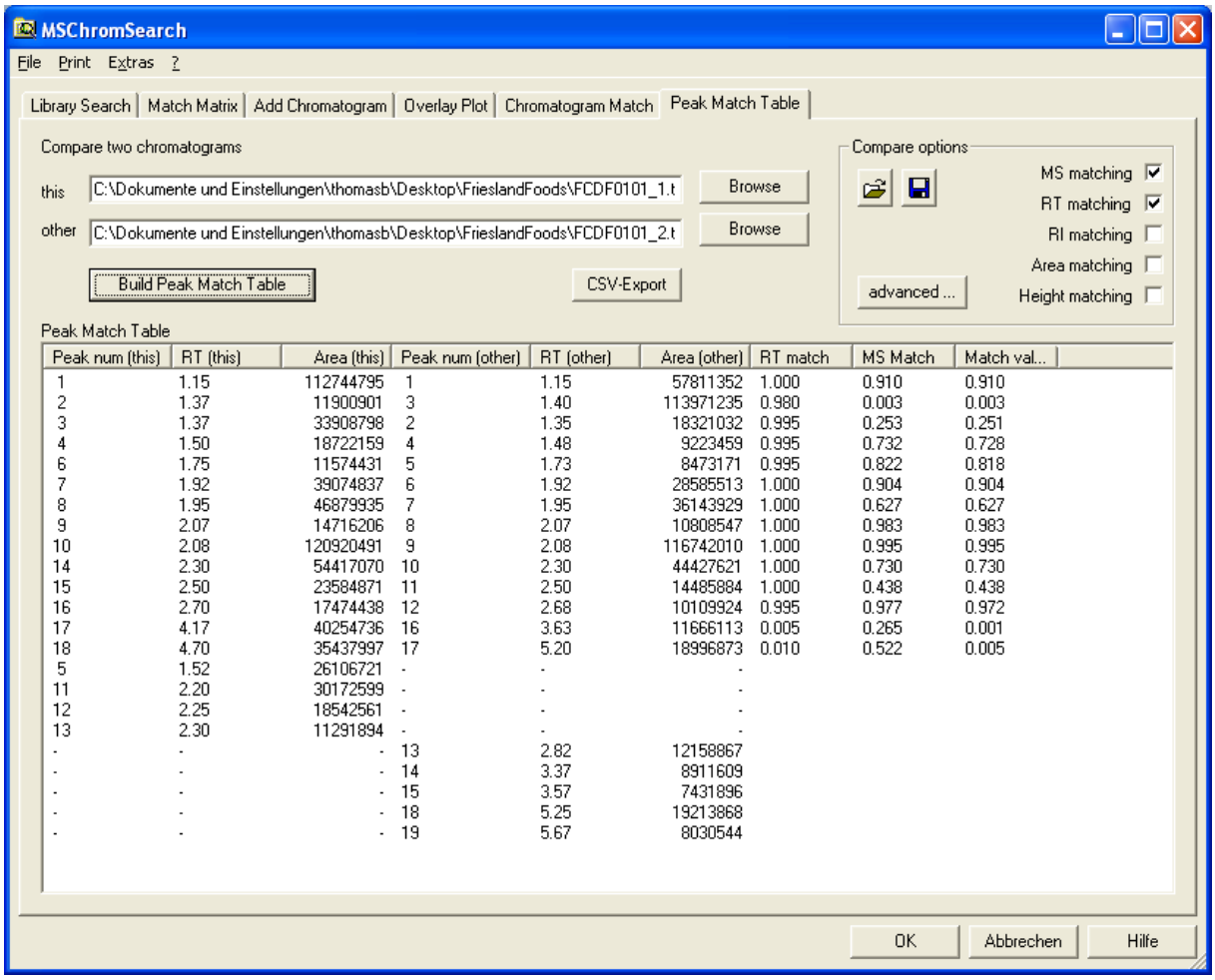


Figure 4: Hitlist by MSChromSearch.

The comparison using MSChromSearch can be performed fully automated after every chromatographical run, provided that the data system permits opening programs. Then, no action by the user is required. The results are automatically saved and/or printed out.

Components, that should have no influence on the search results (e.g. derivatization agents, septum peaks etc.) may be defined within the search options using their spectra and thereby excluded from the run. It is also possible to restrict the search to certain substances, defined by their mass spectra.



Peak num (this)	RT (this)	Area (this)	Peak num (other)	RT (other)	Area (other)	RT match	MS Match	Match val...
1	1.15	112744795	1	1.15	57811352	1.000	0.910	0.910
2	1.37	11900901	3	1.40	113971235	0.980	0.003	0.003
3	1.37	33908798	2	1.35	18321032	0.995	0.253	0.251
4	1.50	18722159	4	1.48	9223459	0.995	0.732	0.728
6	1.75	11574431	5	1.73	8473171	0.995	0.822	0.818
7	1.92	39074837	6	1.92	28585513	1.000	0.904	0.904
8	1.95	46879935	7	1.95	36143929	1.000	0.627	0.627
9	2.07	14716206	8	2.07	10808547	1.000	0.983	0.983
10	2.08	120920491	9	2.08	116742010	1.000	0.995	0.995
14	2.30	54417070	10	2.30	44427621	1.000	0.730	0.730
15	2.50	23584871	11	2.50	14485884	1.000	0.438	0.438
16	2.70	17474438	12	2.68	10109924	0.995	0.977	0.972
17	4.17	40254736	16	3.63	11666113	0.005	0.265	0.001
18	4.70	35437997	17	5.20	18996873	0.010	0.522	0.005
5	1.52	26106721	-	-	-			
11	2.20	30172599	-	-	-			
12	2.25	18542561	-	-	-			
13	2.30	11291894	-	-	-			
-	-	-	13	2.82	12158867			
-	-	-	14	3.37	8911609			
-	-	-	15	3.57	7431896			
-	-	-	18	5.25	19213868			
-	-	-	19	5.67	8030544			

Figure 5: Tabular comparison between two chromatograms.

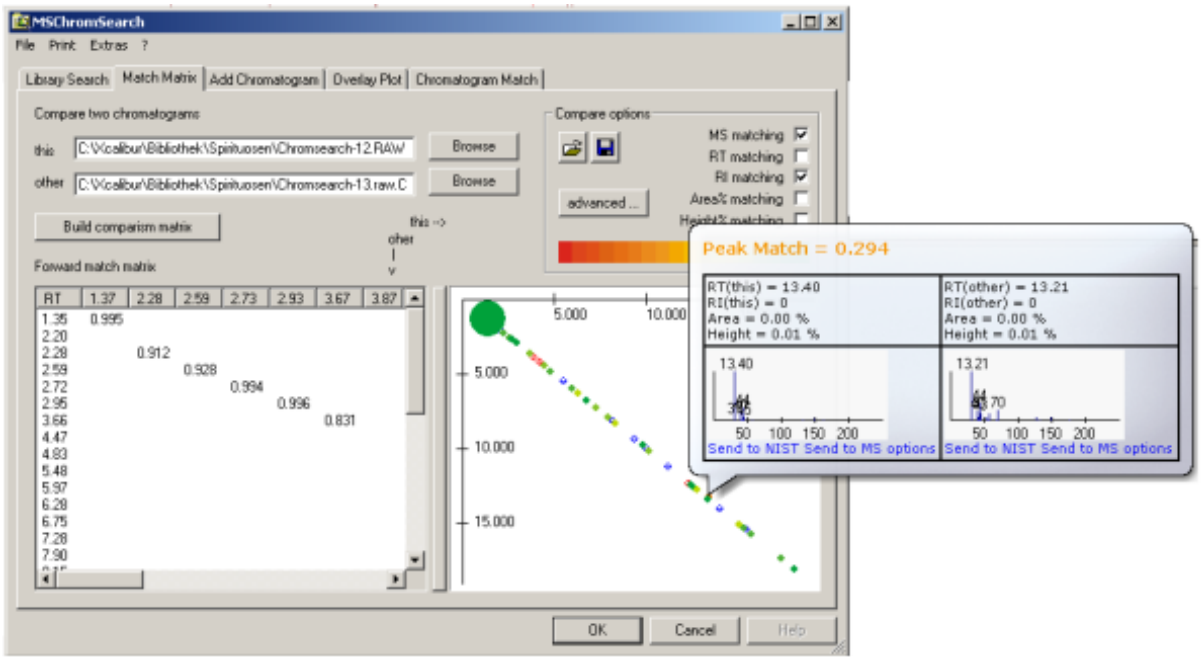


Figure 6: Comparative matrix of two chromatograms.

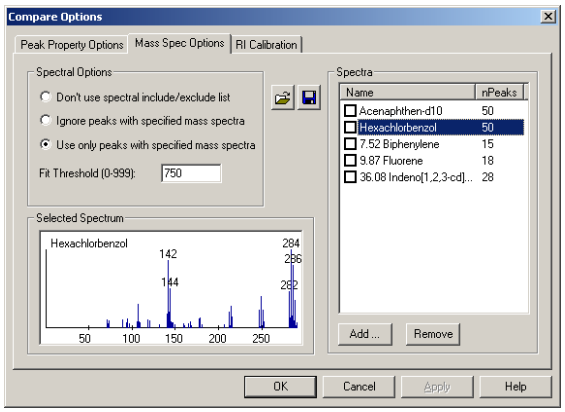


Figure 7: Mass spectra option for targeted definition of substances.

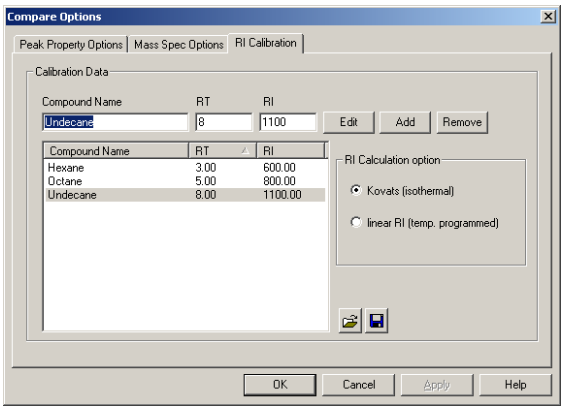


Figure 8: RI calibration data to compensate for RT fluctuations.

In order to make the application of MSChromSearch not only compatible with Xcalibur® data, there is an interface available to HP Chemstation and to the freely available GC/MS data system AMDIS.

AMDIS enables reading and evaluation GC/MS chromatograms from devices of different manufacturers. The software is available from the internet for free.

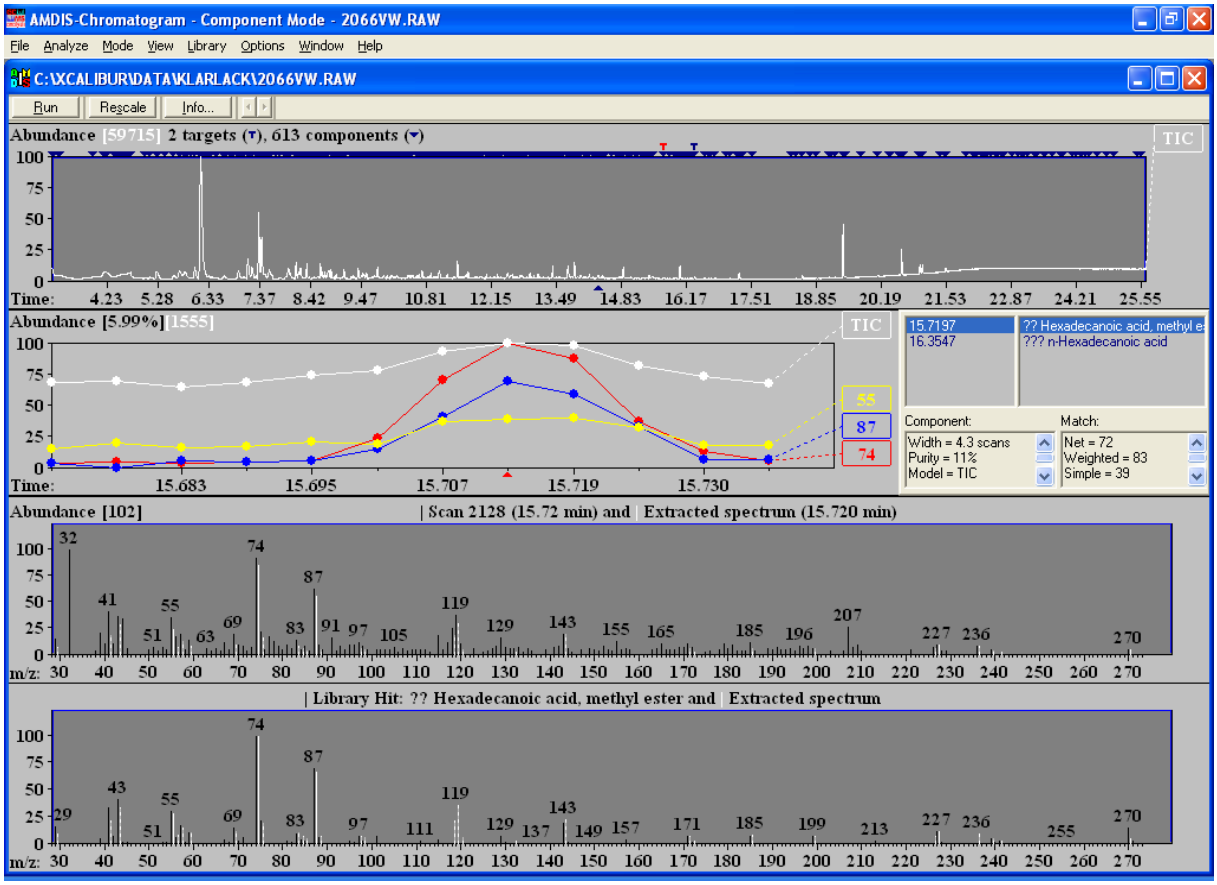


Figure 9: Pyrolysis chromatogram, analyzed by AMDIS.

System Requirements

Standard Computer

- Operating system Windows XP SP3 or Windows 7
- Processor (recommended): 2 GHz multi-core system or better
- Disk space (recommended): 4 GB

Data Systems

- Xcalibur® Version 1.2 and higher
- Chrom Perfect 5.5.3 and higher
- Agilent Chemstation
- Varian MS Workstation, Shimadzu, Bruker, Perkin Elmer, Finnigan Ion-Trap and more (via AMDIS)

Update Service

All updates of MSChromSearch which are released within one year after purchase are available for free.

Note: For MSChromSearch there is a German and an English manual available.

Subject to technical changes

MSChromSearch is a product by Axel Semrau®

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