



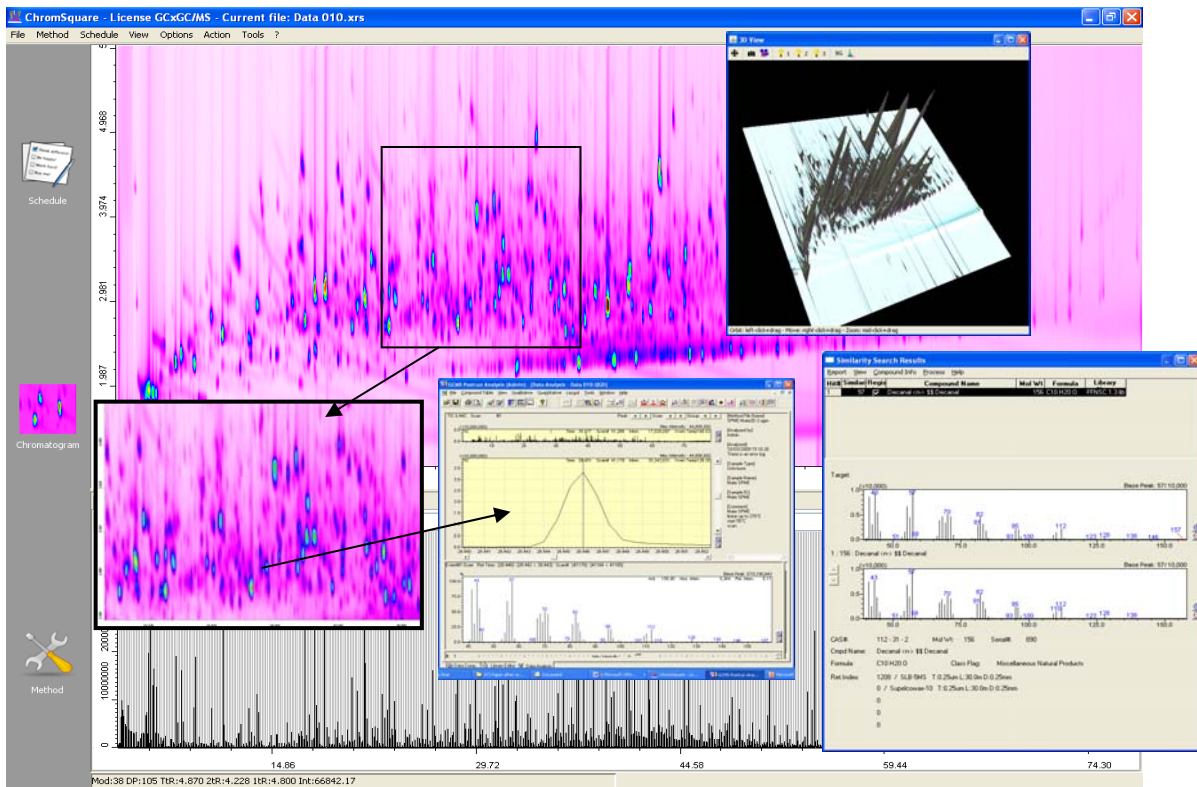
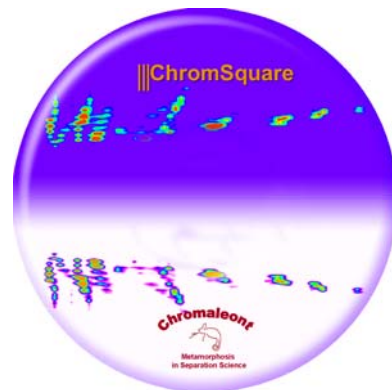
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Academic Spin-off with the
University of Messina

ChromSquare

A tool for multidimensional chromatography

Produced by
Chromaleont s.r.l.
via Industriale 143, Messina (Italy), I-98123
tel. +39 339 2620612 fax +39 090 358220
www.chromaleont.it
chromaleont@chromaleont.it

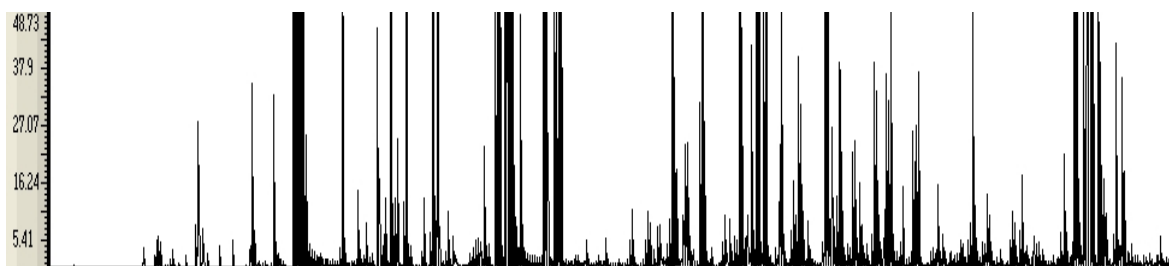


Comprehensive chromatography (LCxLC, GCxGC, LCxGC)

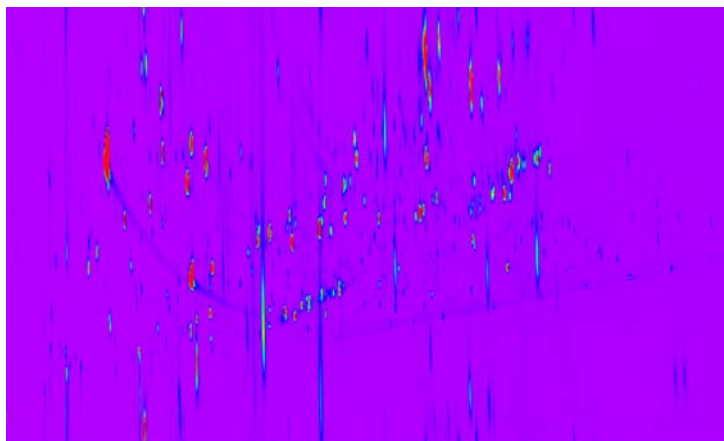
The analysis of real matrices, namely biological, food and environmental samples, poses a high demand for chromatographic methods enabling determination and identification of a large number of compounds occurring in the samples.

However, a single column does not often have sufficient separation power for the baseline separation of all components in complex samples and the extent of peak overlap is enhanced as the number of compounds increases.

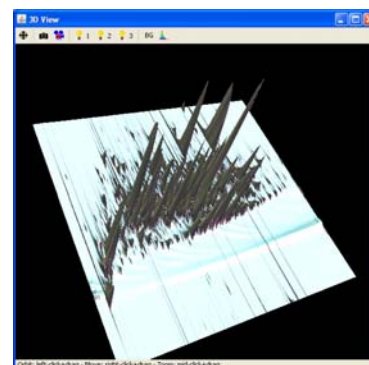
Comprehensive chromatography (LCxLC, GCxGC, LCxGC) is a powerful analytical tool when dealing with complex mixtures and it has been increasingly and successfully employed in various applications over the last two decades. In contrast with other multidimensional (MD) LC approaches, in such an approach every part of the sample is subject to two individual separation dimensions resulting in a tremendous increase in resolving power when highly orthogonal separation mechanisms are combined.



Untransformed 2D data



2D contour plot



3D View

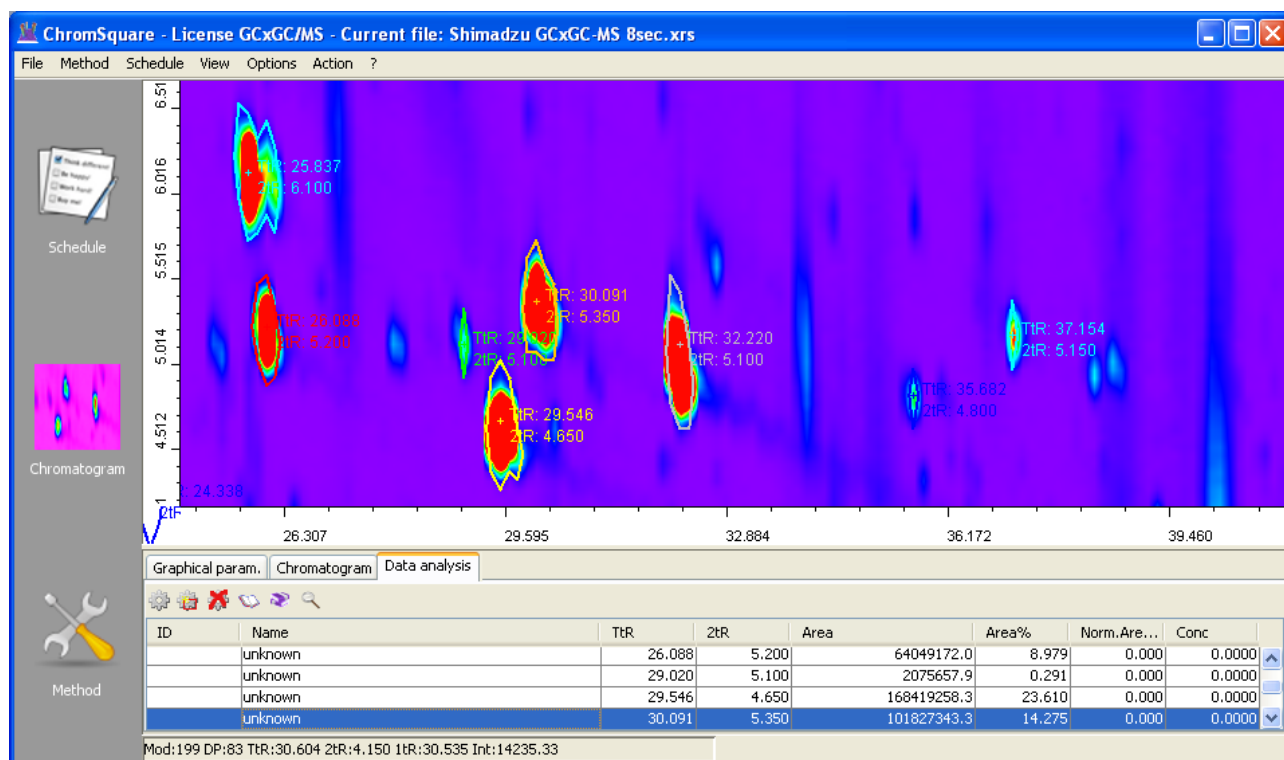


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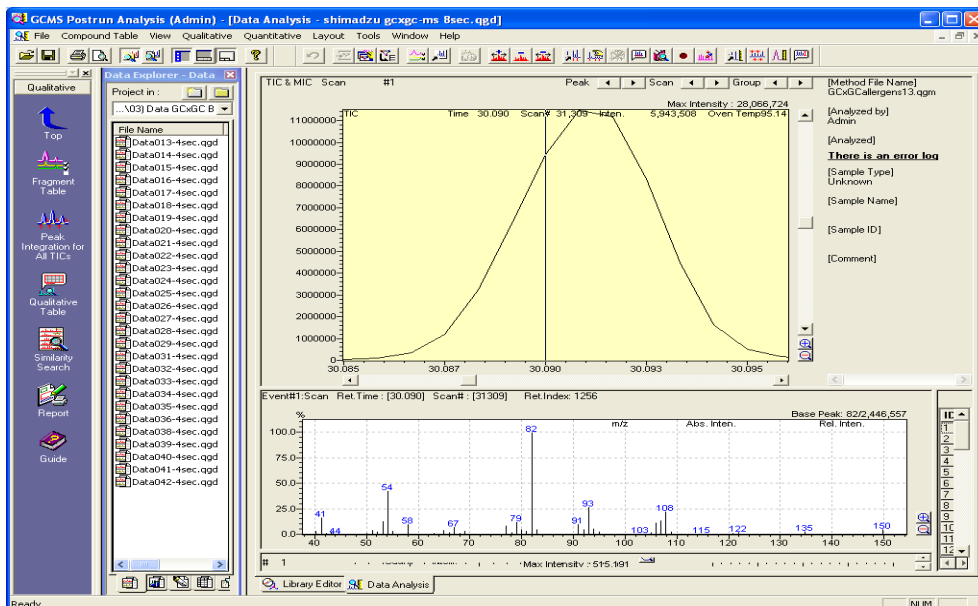
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Qualitative analyses

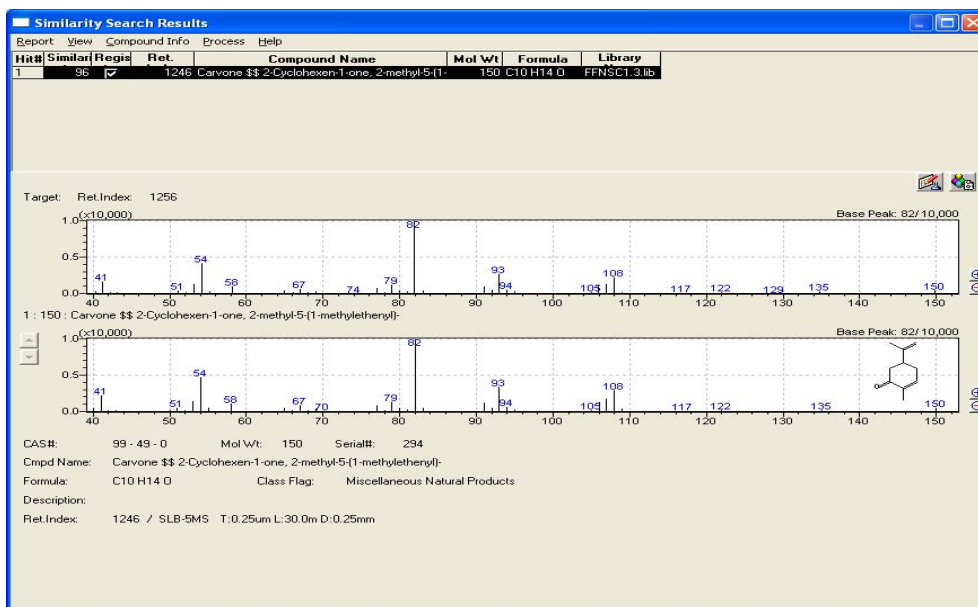
The software allows to visualize, analyze, and process data produced by comprehensive two-dimensional chromatography. By selecting a Blob in Data Analysis, the target compound is displayed (via GCMSolution or LCMSolution windows), along with the spectrum from the data point at the peak apex, and derived from the search in the GCMSolution or LCMSolution Libraries.



Search for a selected Blob in the GCMSolution software



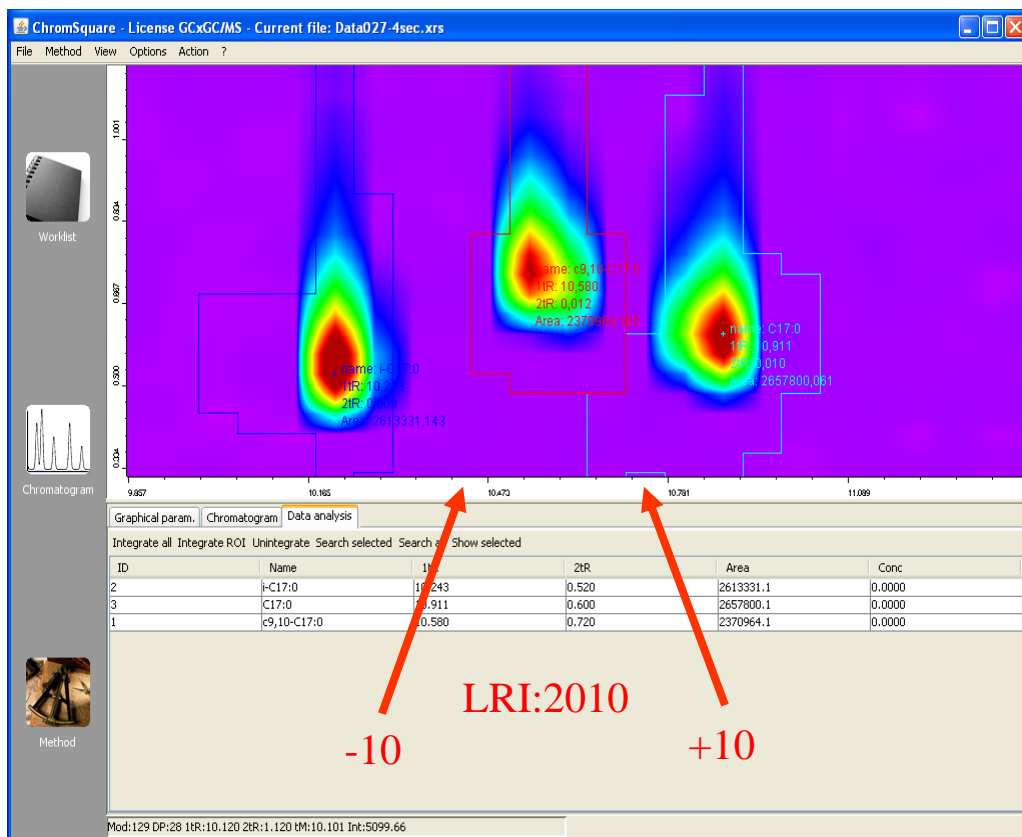
GCMS Postrun Analysis window along with the experimental spectrum, then searched in the GCMSolution Library



Spectral Similarity Search window for the selected Blob

Use of linear retention indices as a filter function during library search

The comprehensive chromatography software works with the GCMSolution software. Therefore, it is possible to perform the MS library search from the former software, through the tools of the latter one, enabling the application of a twin-filter: (1) spectral similarity, and (2) LRI range. The primary filter eliminates matches with a spectral similarity (expressed in %) lower than a minimum value set by the analyst; the other filter deletes library spectra, characterized by an LRI value outside a pre-defined range, and with respect to the LRI value of the unknown compound.



Use of an LRI filter during MS library searching

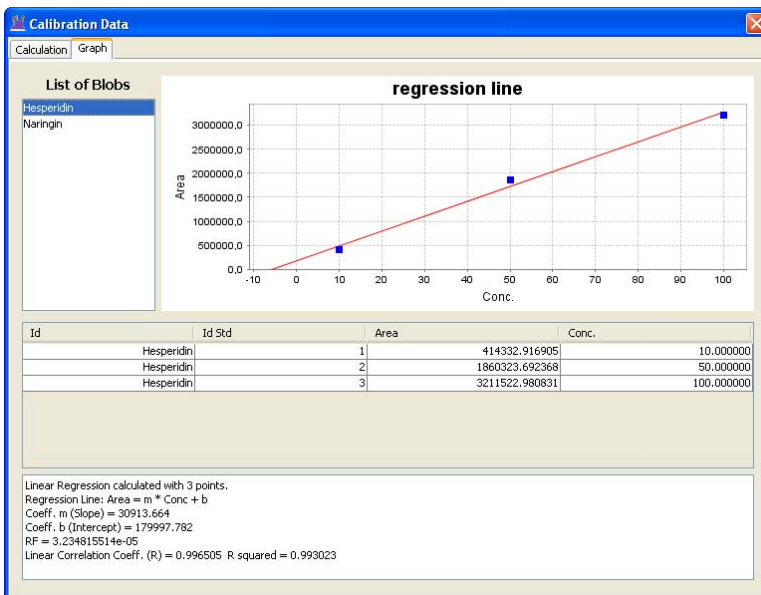


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Quantitative analyses

The software can be used to build calibration graphs by processing data analyses performed at different concentration levels for selected blobs, using pre-measured GCsolution/ LCsolution or GCMSSolution/ LCMSsolution files. When dealing with groups of Blobs IDs (a Blob ID is a group of adjacent Blobs) a similar function is available. In this case, more Blobs belonging to a given Region can be assembled and quantified by the user according to different criteria.



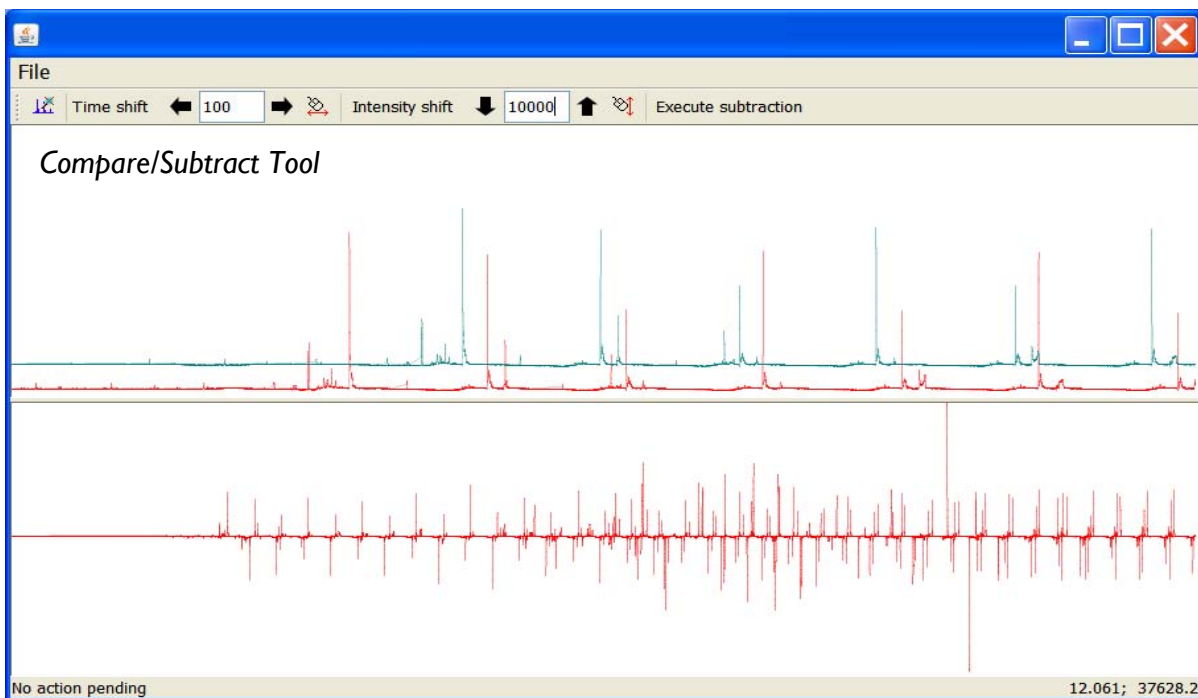
Calibration graph for
a selected standard

Correct Wrap Around

By this command the software allows to add a time interval to the start modulation time: in this way all modulations are shifted by the same time amount; the visual result is that the map will appear shifted towards the top or the bottom, with a “wrap” effect.

Comparing/Subtracting chromatograms

By a special tool (Compare/Subtract) two different chromatograms can be either superimposed or subtracted.



Ion selection

If the chromatogram under analysis is generated by a mass spectrometer, a selection of fragments can be used for quantitation instead of the total ion current data.

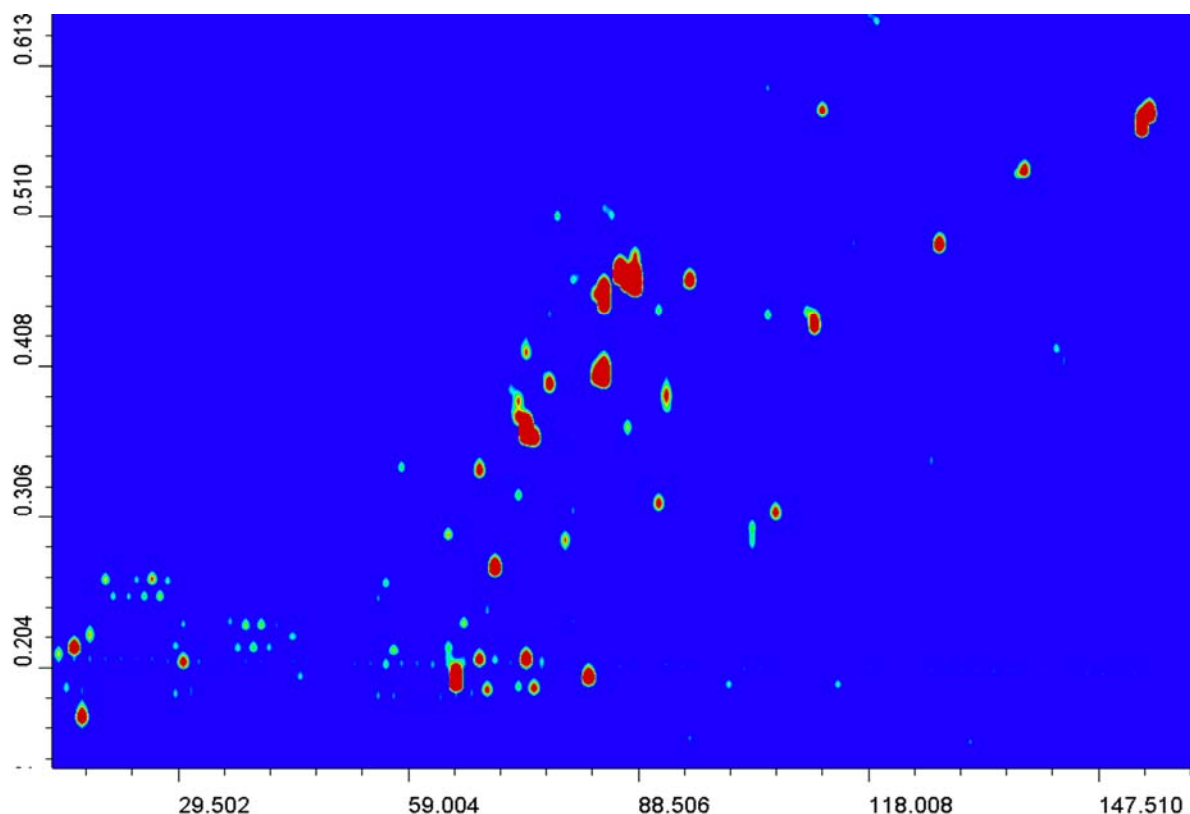


Chromaleont is a Society that offers solutions for the development of analytical instrumentation and dedicated software for chemical analysis and consulting in the field of Separation Science. The scope is therefore the development of new analytical methodologies for the analysis of complex mixtures by using innovative analytical instrumentation.

Chromaleont spin-off with the University of Messina has its office at "The Mediterranean Separation Science Foundation Research and Training Center" guest in the Dipartimento Farmacochimico of the School of Pharmacy of the University of Messina.

For information about Chromaleont, please visit our Web site at www.chromaleont.it

To contact us: chromaleont@chromaleont.it



Key contents

- Rapid and straightforward transformation of comprehensive raw chromatograms into 2D and 3D plots
- Qualitative analysis: Direct GC/LC(MS)solution library search on a selected blob.
- Quantitative analysis: Automatic construction of calibration curves from integrated blobs in the 2D plot.
- Wrap-around correction function.
- Compare/subtract function for two different chromatograms
- Ion selection function