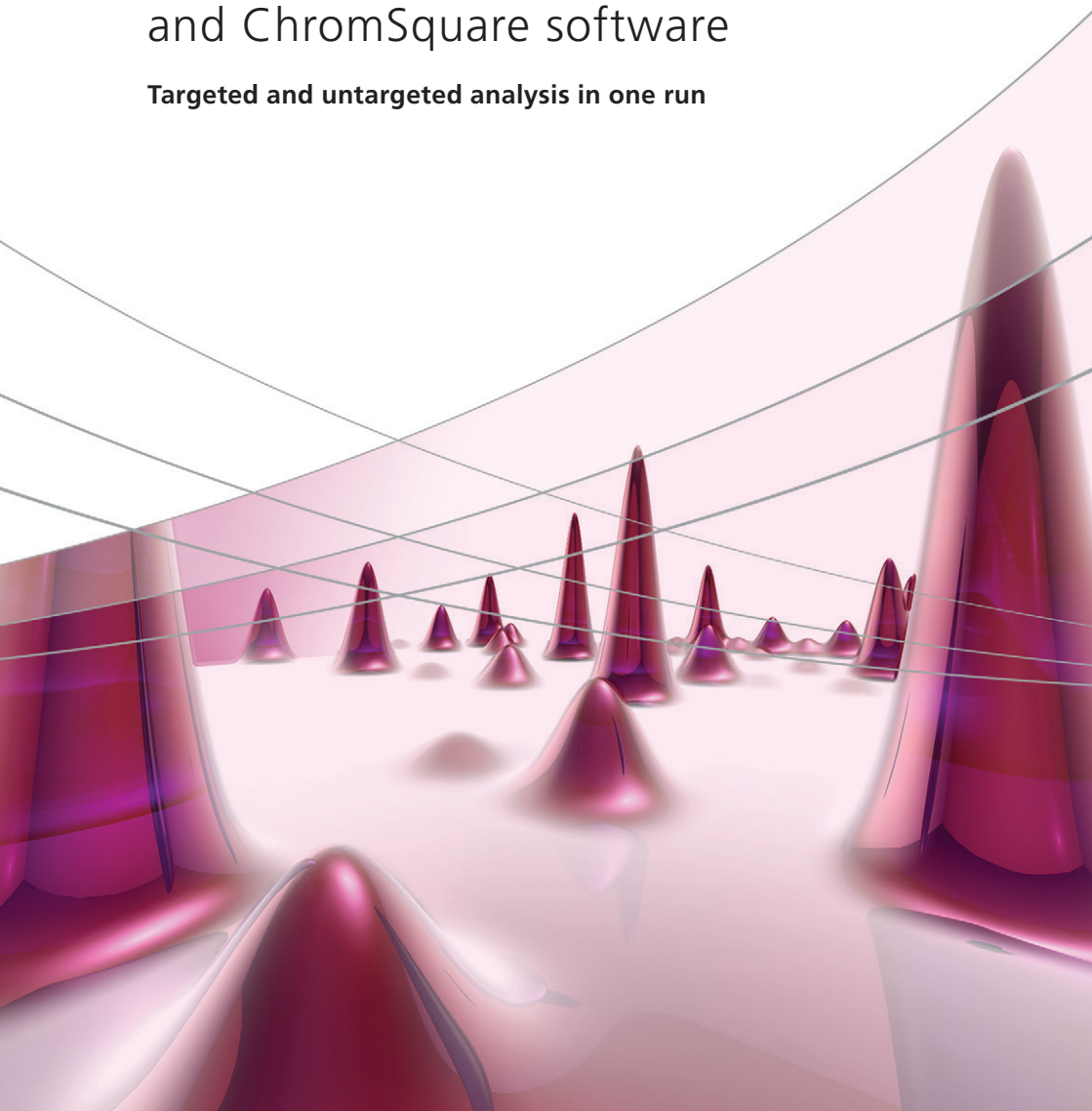
SHIMADZU
Excellence in Science

SEG-A-105

A complete solution using GCxGC/MS with GCMS-QP2020 and ChromSquare software

Targeted and untargeted analysis in one run



For various industries: in-depth insights with just a click

Shimadzu's ChromSquare software solution meets the needs of qualitative and quantitative GCxGC/MS. It provides easy-to-use data handling in Comprehensive Chromatography applications and gives in-depth insights of the sample at any point in the process. At a glance, the user interface shows contour plot, chromatogram and spectra in one window.

ChromSquare and GCxGC/MS with the GCMS-QP2020 provide a complete solution for food, environmental, flavour & fragrance industries as well as the chemical industry.

ChromSquare and GCMS-QP2020: a perfect match

Targeted and untargeted analysis in one run

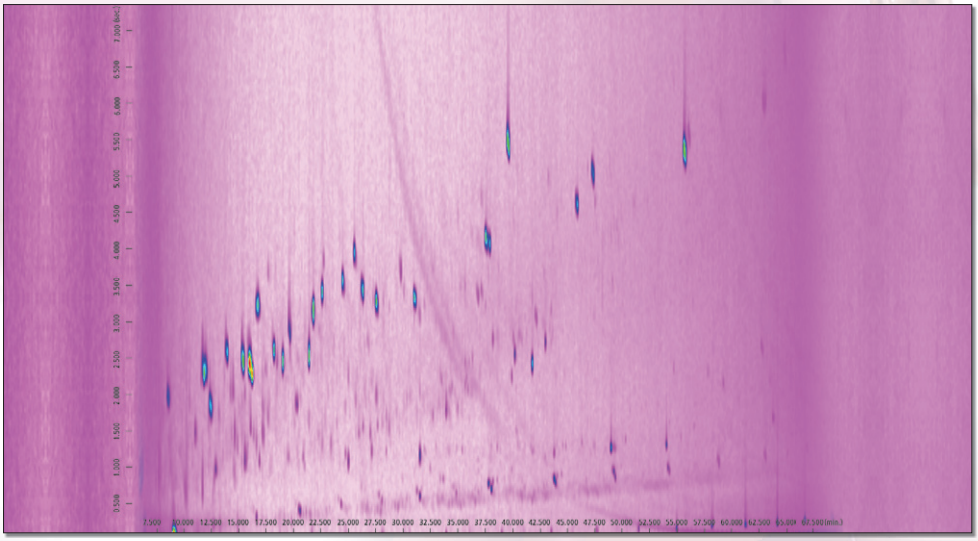
During quality control procedures in the production of consumer goods, a sample of a lot is taken and checked for compounds which define the quality of the product. Although the manufacturer is usually aware of the ingredients the product consists of, additional compounds may have accidentally been included during production. After just one analytical run, the ChromSquare software determines known (targets) and unwanted, unknown compounds (untargeted signals).

As coelution cannot be predicted in such a situation, the best chromatographic separation is needed in order to obtain the complete data set in one run. This is particularly important in environmental analysis and many other fields, and even more so in consumer safety applications regarding food ingredients. The target compound list here is defined by EU authorities.

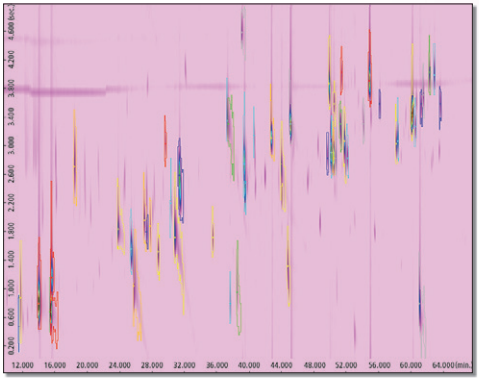
The example of matrix water: Comprehensive Chromatography and ChromSquare at work

Whether drinking or waste water, as well as the known contaminants depending on the local situation, an analysis of the untargeted compounds is also necessary. Chromatographic resolution is very important in this context.

The largest peak capacity in chromatography is achieved by comprehensive techniques, e.g. GCxGC/MS. Usually in comprehensive GCxGC, an orthogonal set of columns is used, i.e. an unpolar phase column and a polar phase column are connected to each other. The mass spectrometer operated in scan mode allows the use of different libraries for qualitative analysis.



Contour plot of contaminants in river water



Contour plot of perfume

GCxGCMS with thermal modulation using the cryo modulator (Zoex cooperation, USA) refocuses the peaks eluting from the first dimension and releases them into the second. Peaks reaching the detector show widths at the base of around 200 to 300 msec depending on the diameter of the second column. For quantitative precision, each modulated peak should be recorded with 8 to 10 scans. This means that 33 to 50 scans per second are necessary with a mass range covering the application.

At high acquisition speeds, the GCMS-QP2020 single quadrupole mass spectrometer enables 50 or 33 spectra/sec over a mass range of 310 u or 450 u respectively due to the patented ASSP (Advanced Scanning Speed Protocol, patented US6610979) function. Consequently, the interscan delay time is very small, and the scanning speed of the quadrupole is 20,000 u/sec maximum without skewing of the spectra in comparison to libraries.

In GCxGC/MS, typically 3 or more peaks are related to one compound separated by the modulation frequency. Data evaluation therefore needs extra software, e.g. ChromSquare for targeted and untargeted analysis.

The example of flavour & fragrance analysis: contour plot of a perfume

The signals are integrated and the blobs are assembled from peaks taking the modulation time difference in a first step and in addition checking the similarity of spectra taken from the modulated peaks. The ChromSquare software enables choosing of various ways to average spectra over the peaks with subsequent baseline subtraction.

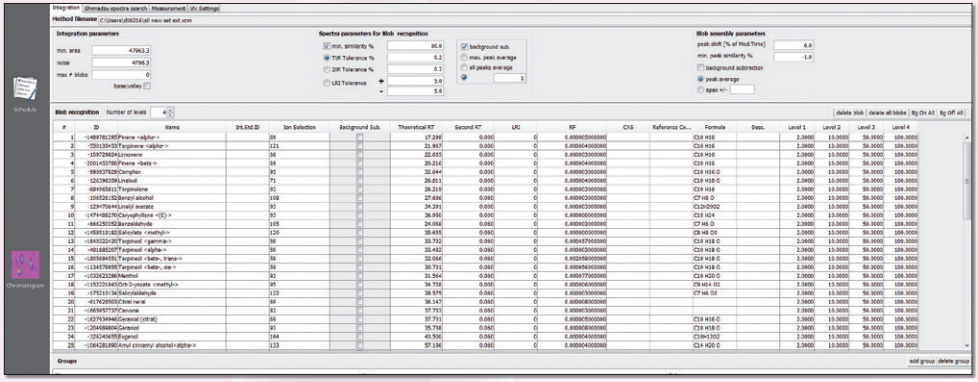
Easy definition of target compounds

ChromSquare enables easy definition of target compounds as the data set is integrated with a subsequent library search. Only the targeted blobs have to be selected and added to the ChromSquare method file. With this operation, the compounds and the baseline corrected spectra together with the two dimensional retention times and linear retention indices (as selection option) are stored within the method. The method tab of ChromSquare containing the extended list of potential allergens (see IFRA) is shown on the right.

ChromSquare supports method matching

Once the method is created with ChromSquare, it can be applied to process a series of samples. Spectra and retention times of the targets stored in the method are compared with the relevant blobs in the samples. Two criteria have to be fulfilled:

- the retention times should be within specified limits
- the spectra of the target blobs in the sample are compared with those stored in the method, and the similarity index must be larger than a given value (blob recognition).



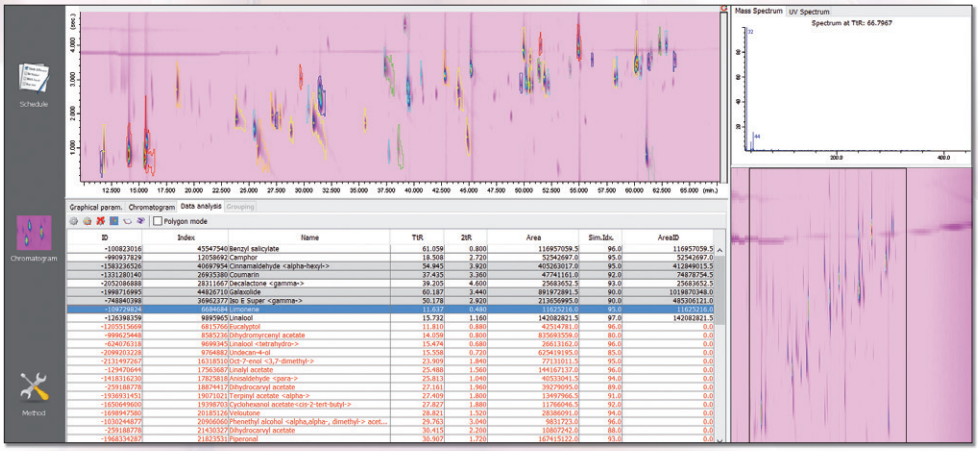
Method tab with 59 potential fragrance allergens

In addition to being able to import data from GCMSsolution directly, ChromSquare can also use GCMSsolution mass spectra search technology.

Selection of up to five libraries

All blobs in a sample are integrated, and the blobs not identified by the method are specified to be unknown. A subsequent library search can be performed and the unknowns may be identified according to the libraries used. Up to five libraries can be selected, e.g. the FFNSC3 for natural and synthetic compounds while the targets method identification remain unchanged. The resulting peak table contains the method related blobs (targets black) and blobs which are identified by the library search process (untargeted). As example, a part from the peak table is shown. Names in black are targets, while names in red are untargeted identified blobs.

Combination of the GCxGC/MS system with the GCMS-QP2020 single quadrupole mass spectrometer and ChromSquare provides a powerful tool for analysis of complex samples of all kinds as well as targeted and untargeted analysis in one run.



Target and untargeted blobs in the result table

For more information regarding GCMS-QP2020, ChromSquare software or application support please contact us:

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