

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

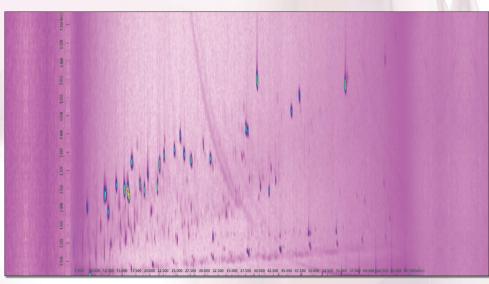
During quality control procedures in the production of consumer goods, a sample of a lot is taken and checked for compounds which define the quality of the product. Although the manufacturer is usually aware of the ingredients the product consists of, additional compounds may have accidentally been included 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

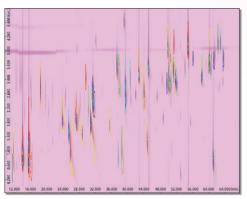
The example of matrix water: Comprehensive Chromatography and ChromSquare at work

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 Chrom-Square, 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).

	Integrati	on parameters	8	Spectra parameters for Blob recognition						Blob assembly	parameters					
	min, area 47943.3 Holise 4796.3 min, if 3 lobis 0				min. similarity %	80.0	✓ background sub. ✓ mex. peak surrage ✓ all peaks average				peak shift (% o	(Med.Time)	6.0			
					TIR Tolerance %	0.2			min, peak similarity %			urby %	-1.0			
					© 2/R Tolerance % © LRI Tolerance #	0.2				background subtraction						
7																
						5.0				@ peak average						
					-	5.0			© spec +/-							
	Still recognition Tumber of levels 4(5)															
		D Same	Drt.Std.ID	Ion Selection	Reciground Sub.	Theoretical RT	Second RT	URI	RF	CIS	Reference Co Formula	Dept.	Level 1	Level 2	Level 3	Level 4
	1	-1489781295/Pinere valoher?	69		P1	17.296	0.000	el.	0.000005000000		C10 H16		2,0000	10,0000	50.0000	109,0000
	2	-550135453 Terpinere <elphe></elphe>	12			21.957	0.000	0	0.0000040000000		C10 H36		2,0400	19,0000	50,0000	109,0000
	3	-109729824 Limonene	58			22,635	0.000	0	0.000003000000		C10 H36		2,0000	19,0000	59,0000	109,0000
	4	-2001453700 Pinere <bets-></bets->	69			20.216	0.000	0	0.000004000000		C10 H36		2,0000	19,0000	58.0000	100.0000
	5	-990937829 Comphor	95			32.644	0.000	0	6.600603000000		C10 H16 C		2,0000	10,0000	58.0000	100.0000
	6	-126290359 Lineled	71			26.811	0.000	0	0.000004000000		C10 H18 O		2,0400	10,0000	58,0000	109,0000
	7	-604965811 Terpinalene	93		P	26.219	0.000	0	0.000003000000		C10 H16		2,0400	19,0000	58.0000	109,0000
	8	-106526152 Benzyl alcohol	100	3		27,636	0.060	0	6.600003000000		C7 H3 O		2,0000	19,0000	58,0000	100.0000
	9	-129470644 Linalyl acetate	93			31.391	0.000	0	0.000003000000		C12I-2002		2,0000	10,0000	58,0000	108,0000
	10	-1474488270 Caryophyllone <(E) >	93		E	36.950	0.000	0	0.00000000000		C15 H24		2.0000	19,0000	58.0000	109.0000
	11	-666250052 Berzaldshyde	105			24,068	0.060	0	6.600603000000		C7 HS O		2,0000	10,0000	58.0000	100.0000
	12	+0459519082 Salicylate < methyl->	120)		35.655	0.060	0	0.000000000000		CB H3 O3		2,0000	10.0000	58,0000	109.0000
	13	-1840322420 Terpined <gamma-></gamma->	50			33.732	0.060	0	6.600457000060		C10 H3B O		2.0000	19.0000	58.0000	109.0000
	14	-491885207 Terpined <alpha->-</alpha->	50		E) :	33,412	0.060	0	0.000003000000		C10 H18 O		2,0000	10,0000	58.0000	100.0000
	15	-1805684551 Terpined <beta-, trans-=""></beta-,>	50			32.066	0.060	0	0.002059000000		C10 H18 O		2,0000	19.0000	58.0000	100.0000
	16	-1134579955(Terpined <beta-, de-=""></beta-,>	59		E .	30.731	0.060	0	0.000956000000		C10 H18 O		2.0000	19.0000	58.0000	109.9000
	17	-1032623286 Menthol	93			31.564	0.060	0	0.000077000000		C10 H20 C		2.0000	10.0000	58.0000	100.0000
	18	-1152221843 Oct-2-ynoate cmethyl->	05			34.728	0.000	0	0.000006000000		C9 H14 O2		2.0000	19.0000	58.0000	109,0000
	10	-175210134 Salicylaldehyde	120		E)	28.575	0.060	0	0.000003000000		C7 H5 O2		2.0000	19.0000	58.0000	100.0000
	20	-617628503 Ctral neral	60			36.147	0.060	0	0.000008000000				2.0000	10.0000	50.0000	109.0000
	21	-1665957737 Carvena	82			37.713	0.060	0	0.000003000000				2.0000	10,0000	58.0000	109.0000
	22	-1627934946 Geranial (otral)	69		E	37.731	0.050	0	6.800865000080		C10 H16 O		2.0000	19.0000	50.0000	100.0000
	23	-1204989804 Geraniol	93		E .	35.738	0.050	0	0.0000080000000		C10 H18 O		2.0000	10.0000	58.0000	109.0000
	24	-326243655 Espend	164			43.510	0.050	0	0.000004000000		C16H1202		2.0000	19.0000	58.0000	100.0000
	25	-1064281890/Amyl cinnamyl alcohol <algha-></algha->	130			57.196	0.060	0	0.800804000080		C14 H20 O		2.0000	19.0000	58.0000	109.0000

Method tab with 59 potential fragrance allergens

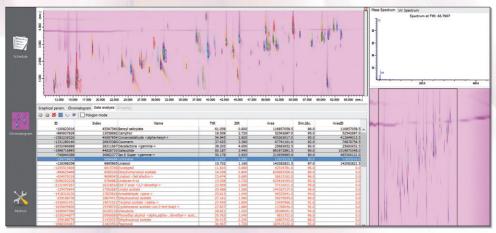
In addition to being able to import data from GCMSsolution directly, ChromSquare can also use GCMSsolution mass spectra search technology.

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:



Shimadzu Europa GmbH

Albert-Hahn-Str. 6-10 · D-47269 Duisburg

Tel.: +49 - (0)203 - 76 87-0 Fax: +49 - (0)203 - 76 66 25 shimadzu@shimadzu.eu www.shimadzu.eu