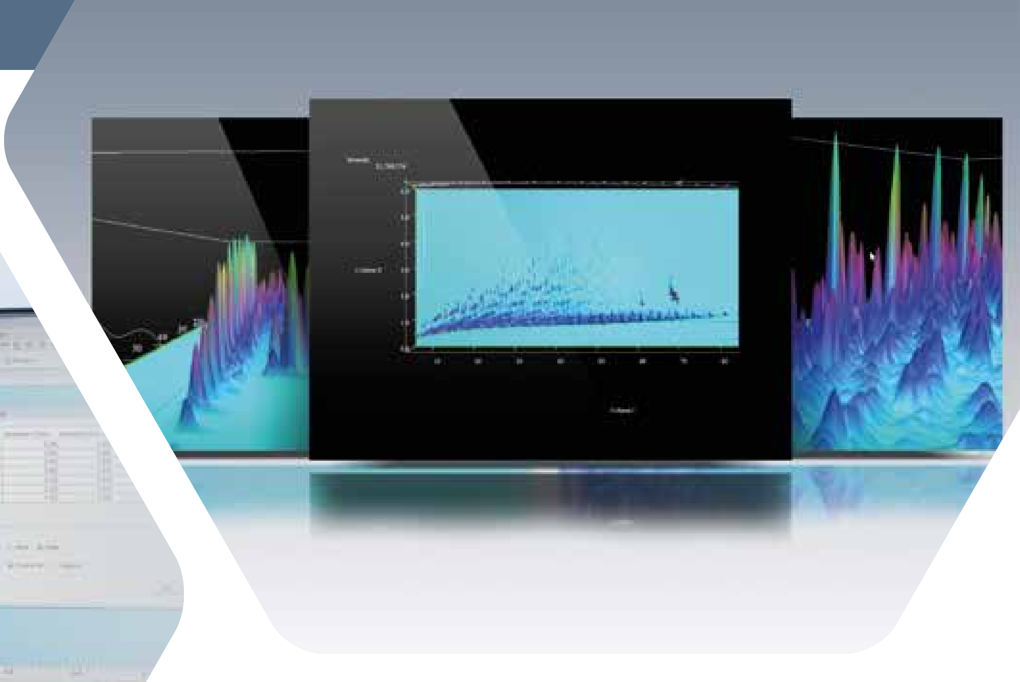
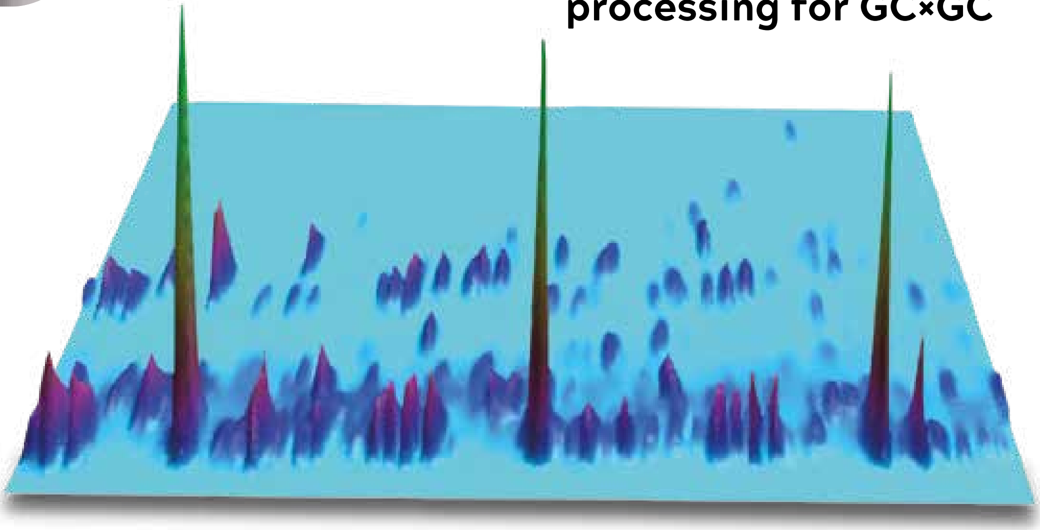


GC Image

Software for Multidimensional Chromatography

GC IMAGE SOFTWARE

Dynamic and efficient data processing for GC×GC



INSTRUMENTS
ANALYTICAL SOLUTIONS

GC Image is a powerful and dynamic software developed to handle GCxGC data. The complexity and information density typical of two-dimensional separations require advanced, high-performing software. The GC Image software package answers these needs and allows visualizing, processing, and analysing 2D data with a rich variety of tools and functionalities. Key features include excellent versatility, support for various data formats, and high flexibility.

GC Image offers intelligent and versatile data processing capabilities ranging from the most basic routine operations - integration, spectral search, quantification - to advanced tools for multi-sample class comparison. Dedicated interfaces enable qualitative and quantitative automated workflows capable of meeting all analytical needs.

A UNIVERSAL PLATFORM

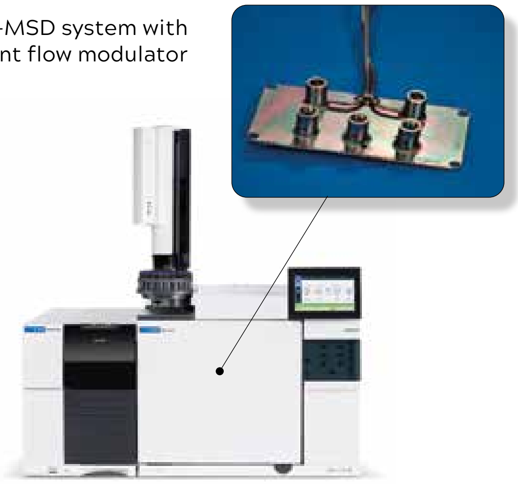
GC Image is a universal software package developed to ensure maximum flexibility. It is possible to import and process numerous data formats to guarantee compatibility with diversified instrumental platforms based on different modulators or detectors. Supported detector types include:

- Universal detectors such as FID and TCD
- Selector detectors (SCD, ECD, VUV and more)
- Mass spectrometers based on different operating principles:
  - Scan-based systems (quadrupole)
  - Time-of-Flight (TOF), including high-and low-resolution QTOF systems.

GC Image Software is available in two versions:

- **GC Image GC×GC Edition** for use with the most common detectors, including low-resolution mass spectrometers.
- **GC Image GC×GC-HRMS Edition** which supports all data formats of the standard version plus high-resolution mass spectrometry.

GCxGC-QTOF system with ZOEX thermal modulator



GCxGC-MSD system with Agilent flow modulator

ADVANCED FLEXIBILITY AND PERFORMANCE

The software package includes three components:

- **GC Image**
  for visualization, method development, analysis, and reporting of individual chromatograms.
- **GC Project**
  for automated processing of multiple chromatograms (*batch processing*).
- **Image Investigator**
  for automated and interactive multivariate analysis of multi-sample datasets for sample classification, fingerprinting, and marker compound discovery.

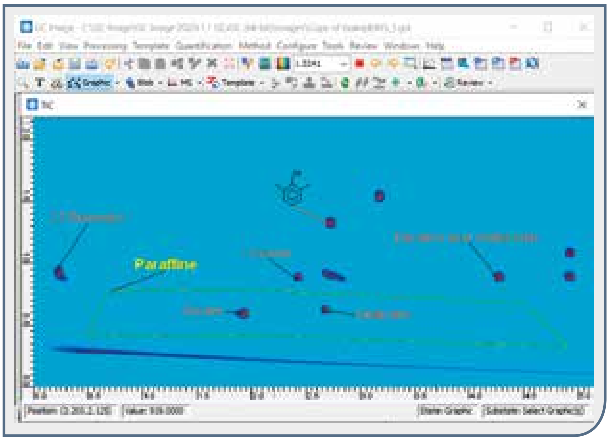
The synergy between these interfaces facilitates automated qualitative and quantitative workflows for targeted analysis and untargeted screening.

The functions offered range from the most basic yet essential operations to advanced processing tools. These include:

- Image creation (colour plot) - import, colorization
- Visualization - Multi-projection axes view, 3D view
- Baseline correction and peak integration
- Library search for compound identification
- Smart templates based on two-dimensional peaks and geometrical areas for interactive determination of target compounds and groups of interest
- Calibration curves and quantification
- Image comparisons
- Scripting to filter and extract chromatographic and spectral features (CLIC expressions)
- Automated, interactive multi-sample comparison, clustering, and marker identification.

Main screen

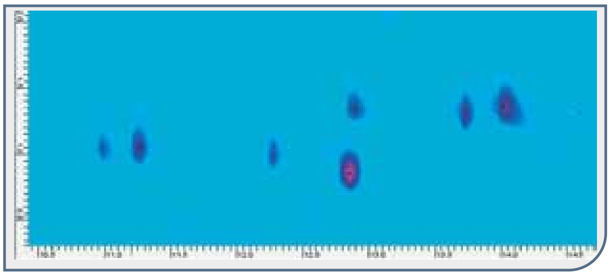
Drop-down menus and a set of icons provide quick and intuitive access to tools and functions. It is possible to switch with a simple click between different modes to manage blobs, spectra, and graphics that can be readily drawn for swift and easy determination of chromatographic areas related to chemical classes.

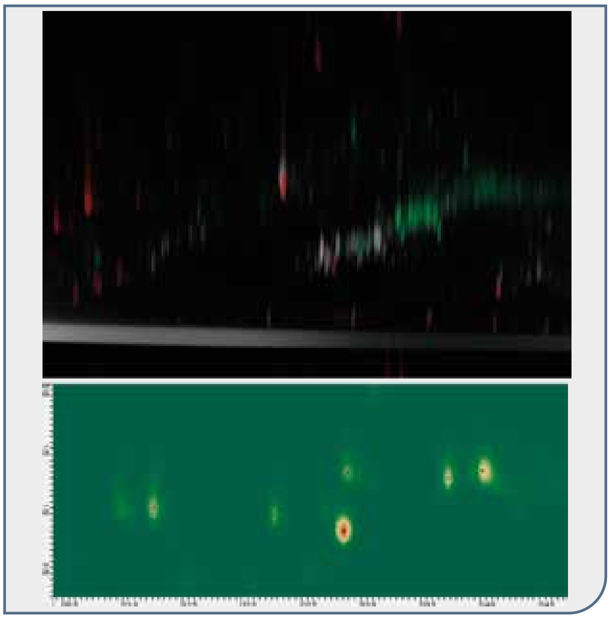


Colourization

It is possible to choose among a variety of pre-defined colour palettes to optimize visualization as desired.

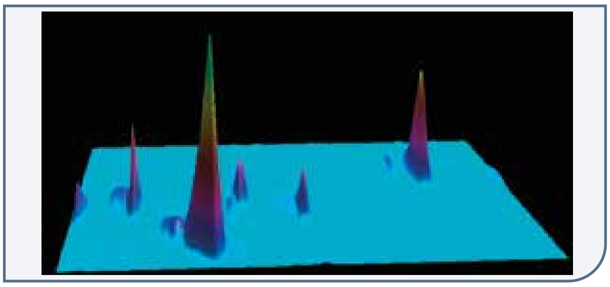
In addition, user can create, save, and export their own customised colour schemes.

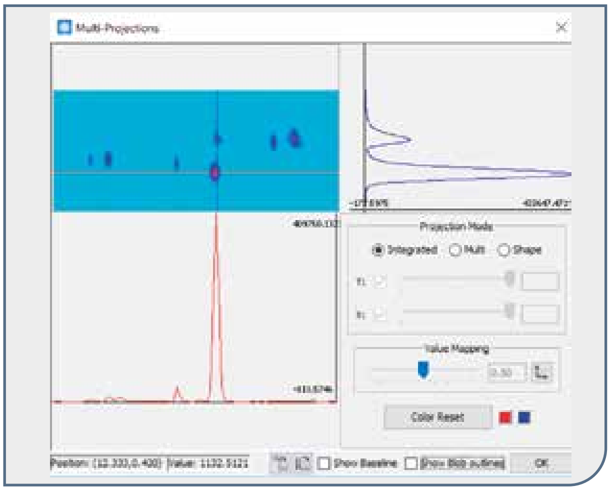




Visualization 3D, multi-projections

Multiple visualization modes enable the exploration of the chromatographic profile and two-dimensional peaks in a dynamic fashion.





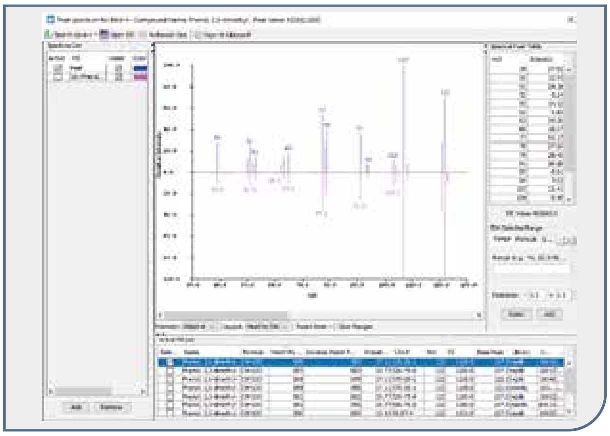
Projection Mode: ● Integrated ○ Multi ○ Shape

Position: (12.333,0.400) Value: 1132.5121

☐ Show Baseline ☐ Show Blob outlines

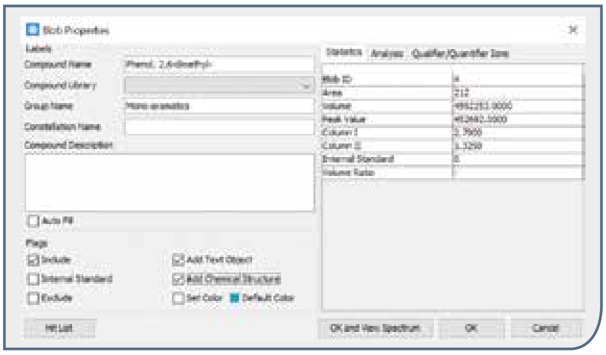
MS spectra library search

MS spectra can be searched against commercial and customized libraries. Search parameters and criteria can be tuned by the operator to maximize the reliability of the identification process.



Blob metadata

Information linked to the two-dimensional peaks (name, group, quantifier ion etc.) can be visualized and modified. Transfer of this metadata into other chromatograms is enabled by smart templates.



Compound Name: Phenol, 2,6-dimethyl-
Compound Library:
Group Name: Mono-aromatics
Constellation Name:
Compound Description:

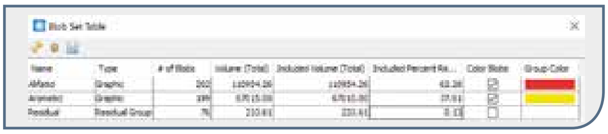
☐ Auto Fill

Flags
☑ Include
☐ Internal Standard
☐ Exclude
☑ Add Text Object
☑ Add Chemical Structure
☐ Set Color ■ Default Color

Blob ID	[illegible]
Area	212
Volume	[illegible]
Peak Value	[illegible]
Column I	[illegible]
Column II	[illegible]
Internal Standard	0
Volume Ratio	

Blob table and blob set table

Readily customized tables summarize quali-/quantitative chemical information for peaks and groups. It is possible to export as .xls or .csv data files.



Name	Type	# of Blobs	Volume (Total)	Included Volume (Total)	Included Percent Ra...	Color Blobs	Group Color
Alifatic	Graphic	202	110954.26	110954.26	48.26	☑	🟥
Aromatic	Graphic	199	67015.00	67015.00	37.61	☑	🟨
Residual	Residual Group	76	210.61	210.61	[illegible]	☐	

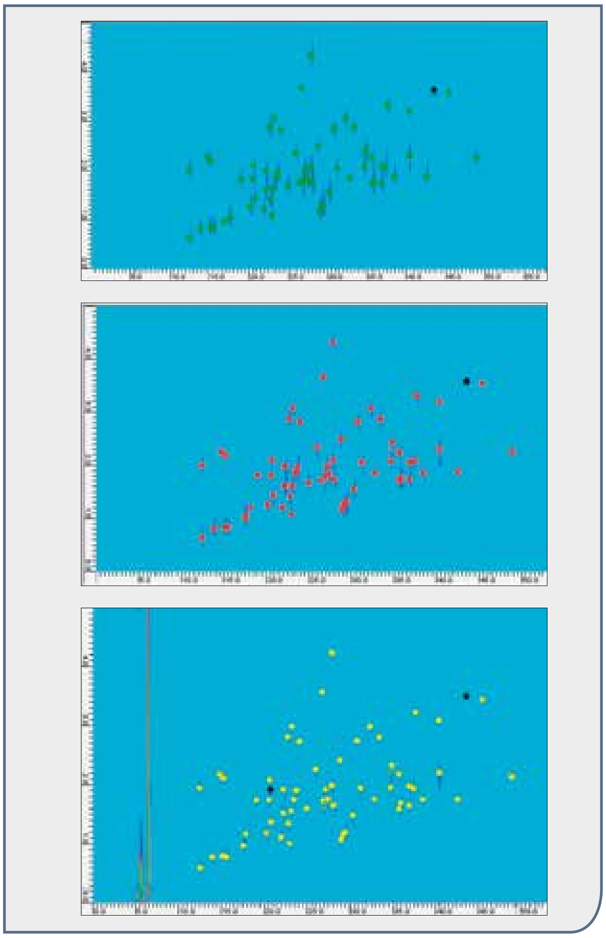
Templates

Templates define chromatographic pattern in terms of peaks and areas, including the corresponding metadata (name, group, quantifier ion etc.). This information can be searched for and recognised in subsequent images by means of a smart, interactive process. In case of positive match, metadata are seamlessly transferred to the new image.

Transfer of a chromatographic pattern and corresponding information for a standard allergens mix acquired with thermal modulation (Zoex) and parallel detection.

Images refer to two MS signals obtained with a BenchTOF-Select™ instrument with Tandem Ionization (SepSolve) - at 70 and 12 eV, respectively - and a FID detector.

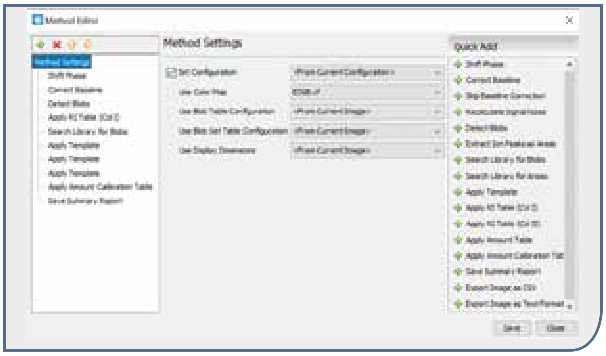
The workflow includes identification through the MS channel to build a detailed and accurate pattern for the targets. Information is transferred to the FID signal channel for robust quantification by means of smart algorithms that use global pattern transformation to adapt to different elution conditions.



Aknowledgment: Chiara Cordero, Elena Gabetti, Carlo Bicchi, Philippe Merle, Emilie Belhassen (2019). GC×GC with parallel detection by FID and TOF MS featuring tandem ionization: extra-dimensions for great flexibility in fragrance allergens profiling. In: 43rd International Symposium on Capillary Chromatography & the 16th GCxGC Symposium. Fort Worth, Texas, USA Editors: Daniel W. Armstrong and Kevin A. Schug, Fort Worth, Texas, USA, 12-17 May 2019.

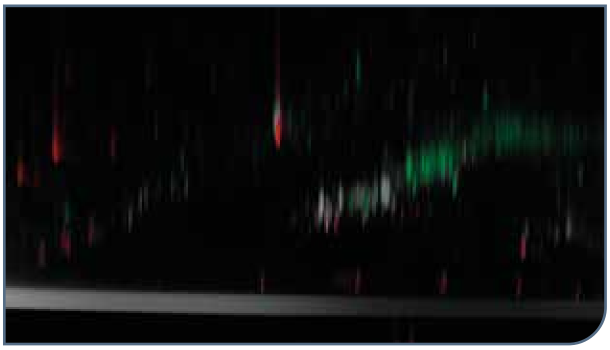
Method development

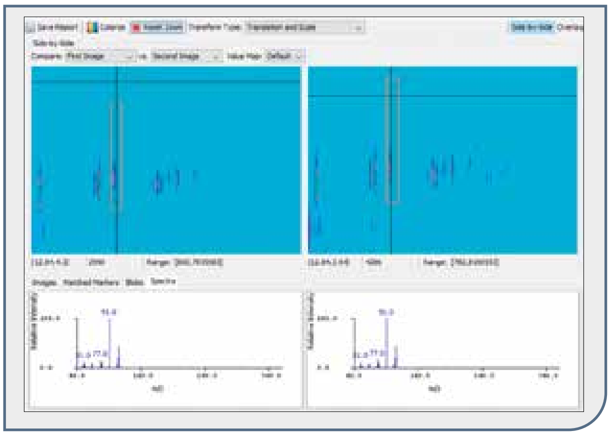
An interactive interface allows quick and accessible method development. The individual steps of interest are simply added with a few clicks.



Visual comparison tools
Differential Image, Pair View

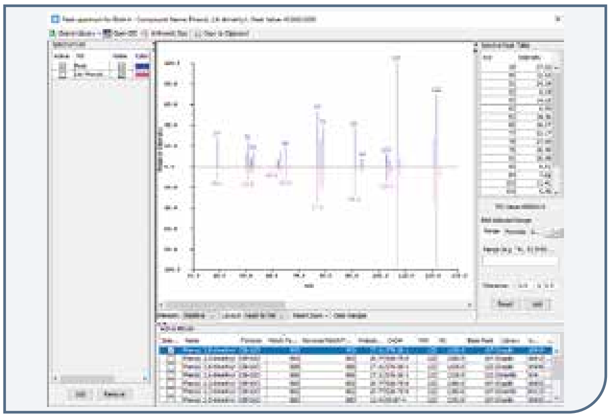
Easy yet effective comparison of the 2D profiles is enabled by multiple tools. These include Side-by-Side visualization and the possibility to create differential images between two overlaid chromatograms, where colorized pixels represent signal intensity for the sample compared to the reference image.





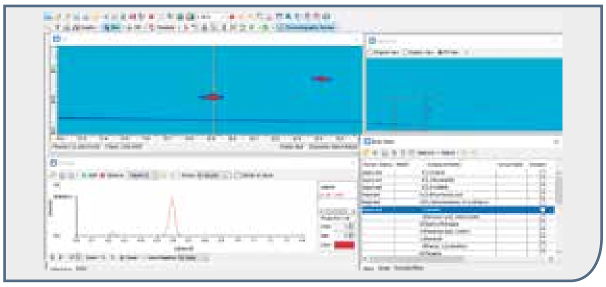
Reliable quantification

Dedicated workflows are available to build calibration curves for peaks or areas. Tables and calibration methods can be created, saved and exported for quantification and reporting of individual or multiple images.



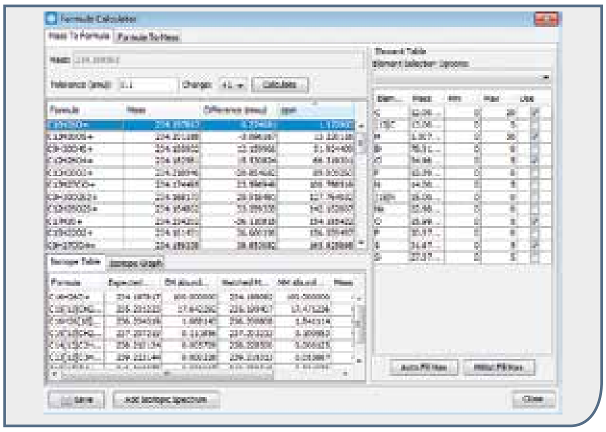
Results overview

Results can be reviewed through pre-defined multi-window interfaces for a quick, at-a-glance overview of chromatographic or spectral features. It is possible to customize layout to meet specific needs.



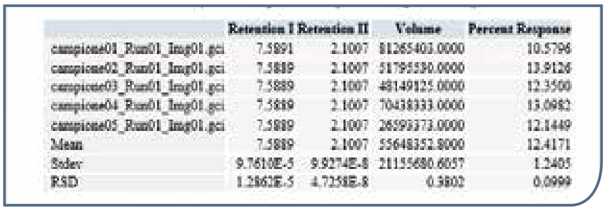
GC Image GC×GC-HRMS Edition

This version offers tools for high-resolution mass spectrometry, such as a formula generator to link accurate mass data to formulas, with full control over elemental composition and isotopic profile evaluation.



GC Project

Automated data processing and comparative reporting for multiple runs for a quick overview of sequences.



	Retention I	Retention II	Volume	Percent Response
campione01_Run01_Img01.gci	7.5891	2.1007	81265403.0000	10.5796
campione02_Run01_Img01.gci	7.5889	2.1007	51795530.0000	13.9126
campione03_Run01_Img01.gci	7.5889	2.1007	48149125.0000	12.3500
campione04_Run01_Img01.gci	7.5889	2.1007	70438333.0000	13.0982
campione05_Run01_Img01.gci	7.5889	2.1007	26593373.0000	12.1449
Mean	7.5889	2.1007	55648352.8000	12.4171
Stdev	9.7610E-5	9.9274E-8	21155680.6057	1.2405
RSD	1.2862E-5	4.7258E-8	0.3802	0.0999

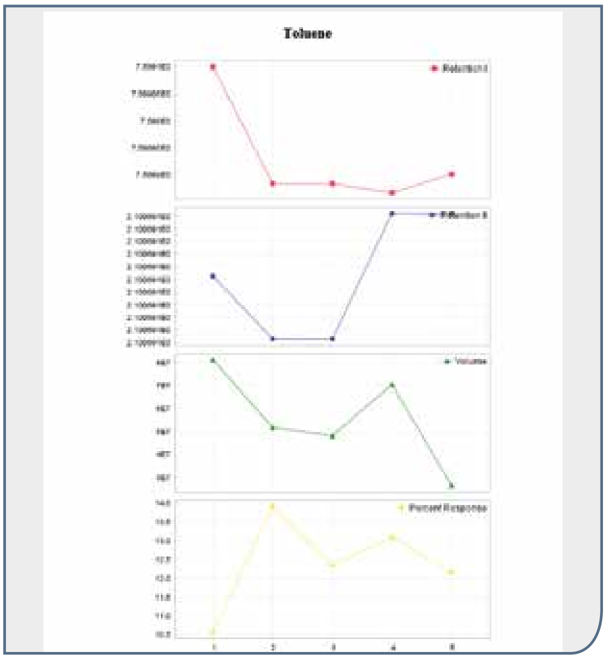
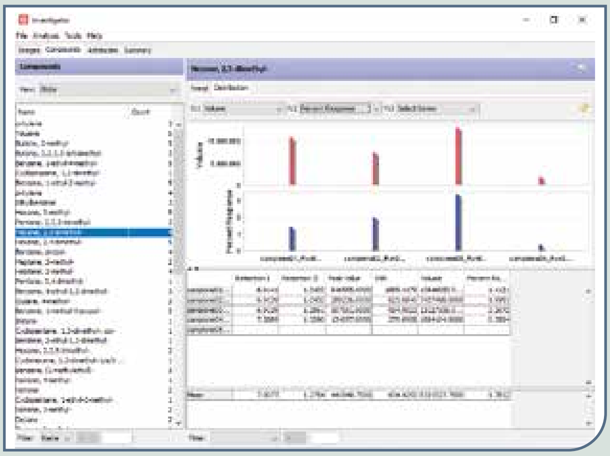


Image Investigator

Interactive multi-sample analysis with visual and statistical tools. The user can examine chromatograms focusing on components or attributes of interest. The interface enables the creation of trend plots, clusterization (PCA) and marker discovery based on statistical analysis.



Contact us for a demonstration or a personalized quote!

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SRA Instruments SpA: Via alla Castellana 3 - 20063 Cernusco S/N (MI) Italy - Ph. +39 02 9214 3258 - info@srainstruments.com
SRA Instruments SaS: 210 rue des Sources - 69280 Marcy l'étoile France - Ph. +33 4.78.44.29.47- info@sra-instruments.com