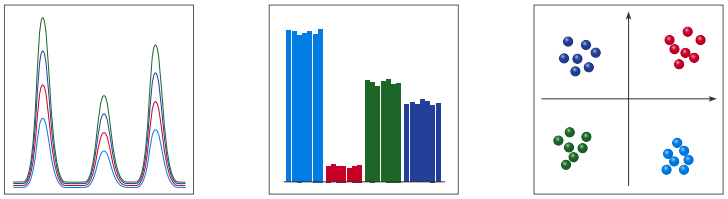
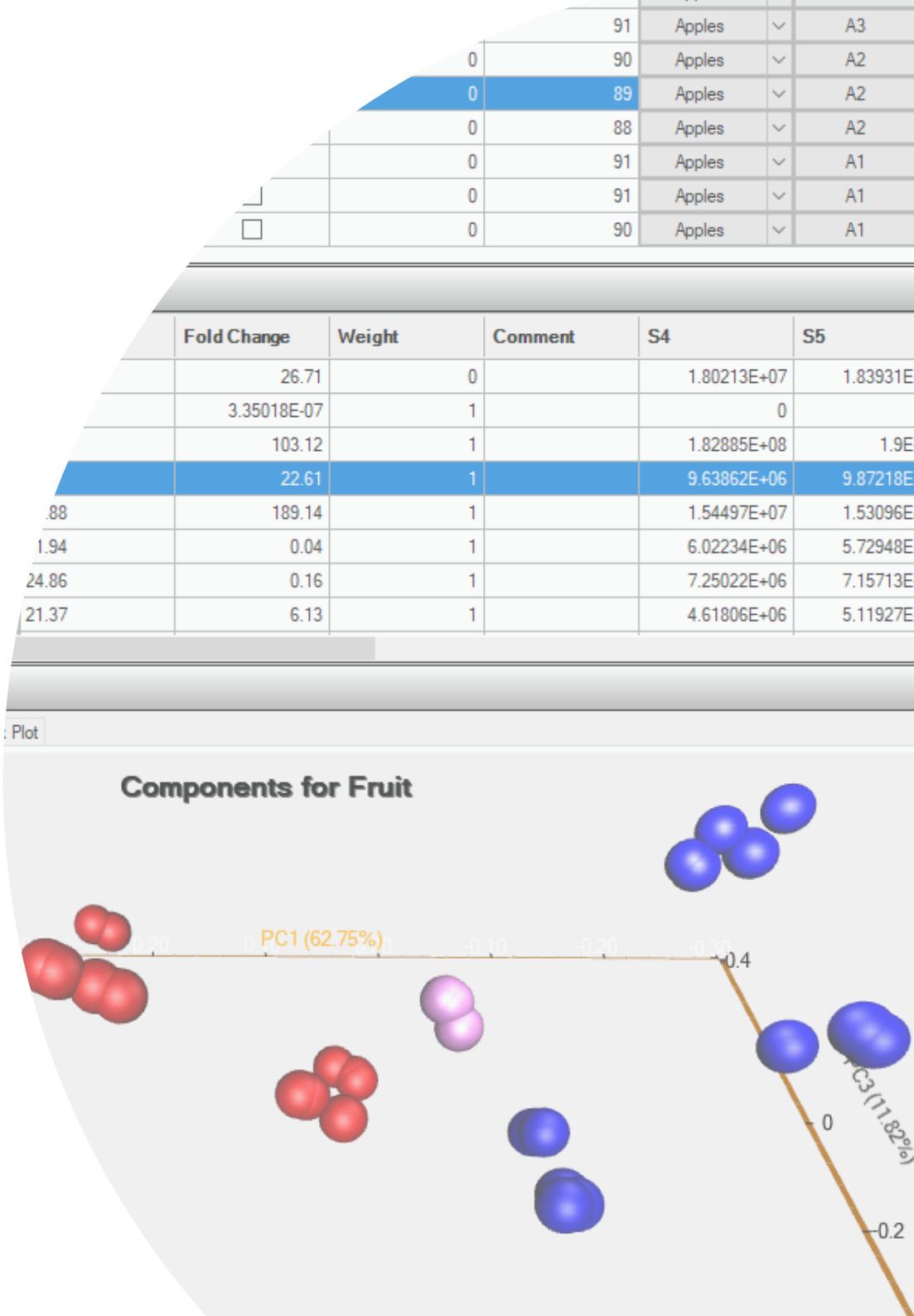
SepSolve Analytical



ChromCompare+™

A powerful chemometrics platform for GC and GC×GC



ChromCompare+™

Transforming complex analytical data into meaningful results

Analytical instrumentation is constantly evolving, allowing us to gain greater insight into sample compositions than ever before.

ChromCompare+ is a powerful, easy-to-use chemometrics platform for comparing multiple chromatograms and extracting useful insights into the constituents present... regardless of your application or GC–MS platform.

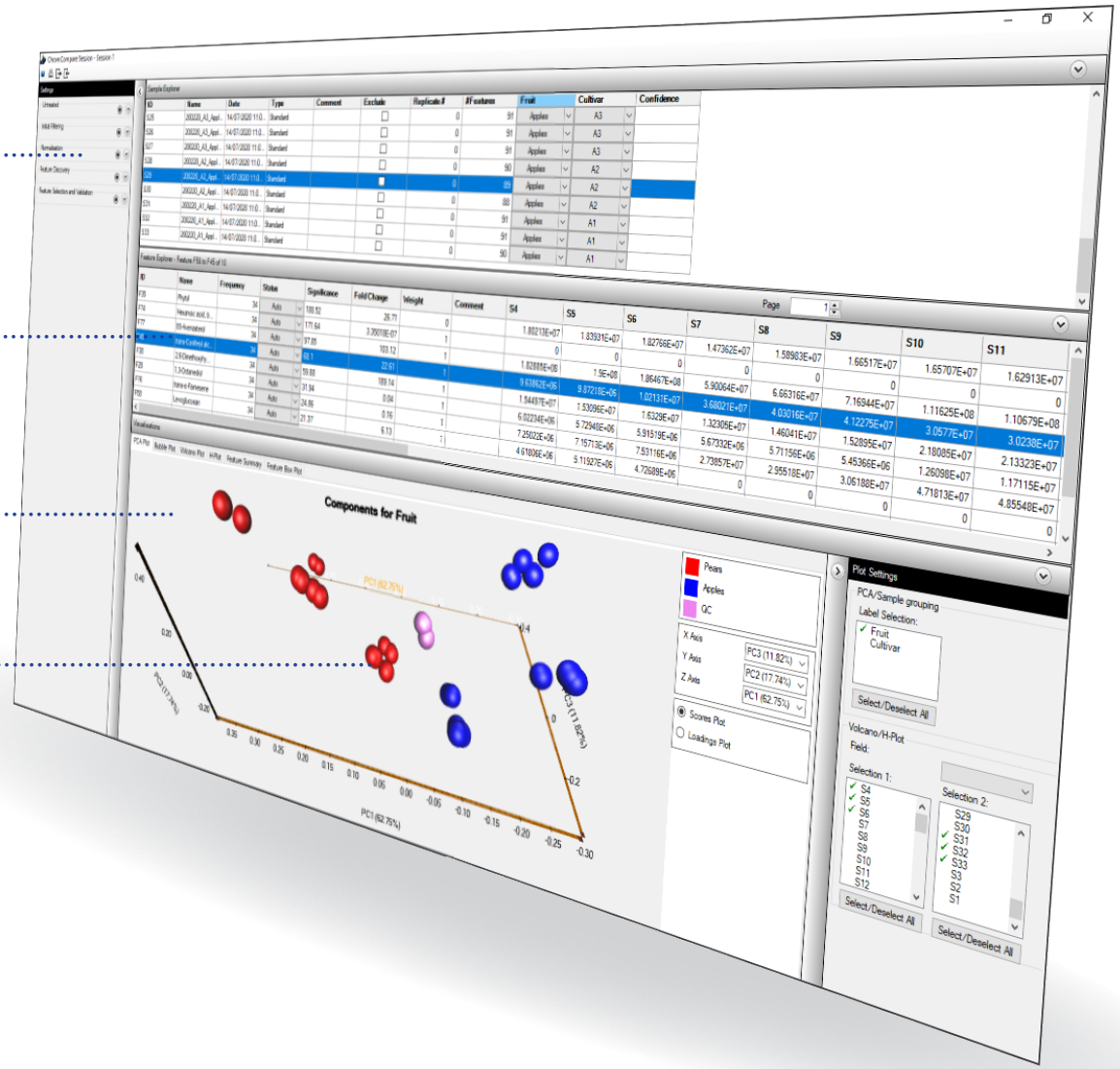
The quality of data-mining software is as critical as the quality of your detector. Get the most out of your datasets with ChromCompare+.

Flexibility to import peak lists or raw data in a range of file formats

Automatic discovery of the most significant differences

Easy visualisation of patterns and trends

Automatic classification of samples using prediction models

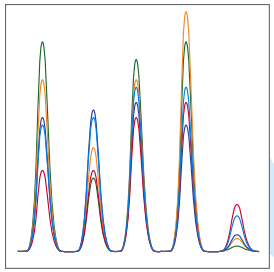


Adapt to different requirements

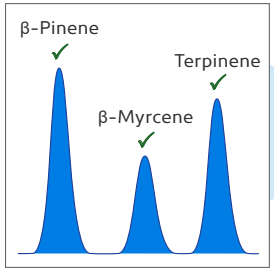
ChromCompare+ offers the flexibility to process 1D and 2D GC–MS data across a range of file formats using various data-mining strategies. The innovative untargeted approach used by ChromCompare+ allows maximum analytical information to be extracted from the raw data when you don't know what you are looking for. This reduces the risk of trace peaks being ignored, and minimises the number of manual steps.

Using ChromCompare+, you can import:

Untargeted datasets:
Align and import raw data to automatically find significant differences in the dataset.

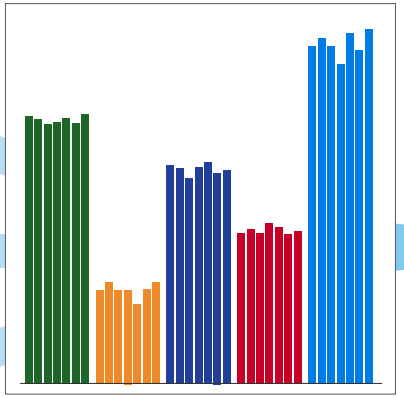


Processed datasets:
Integrate and identify peaks prior to importing for further analysis.

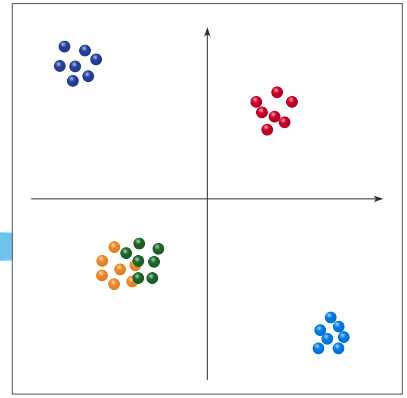


Peak list data:
Import .csv peak lists for additional flexibility in processing historical data.

Peak	Intensity
1	2.04E+06
2	5.85E+05
3	3.12E+07
4	7.34E+05
⋮	⋮
150	6.10E+05



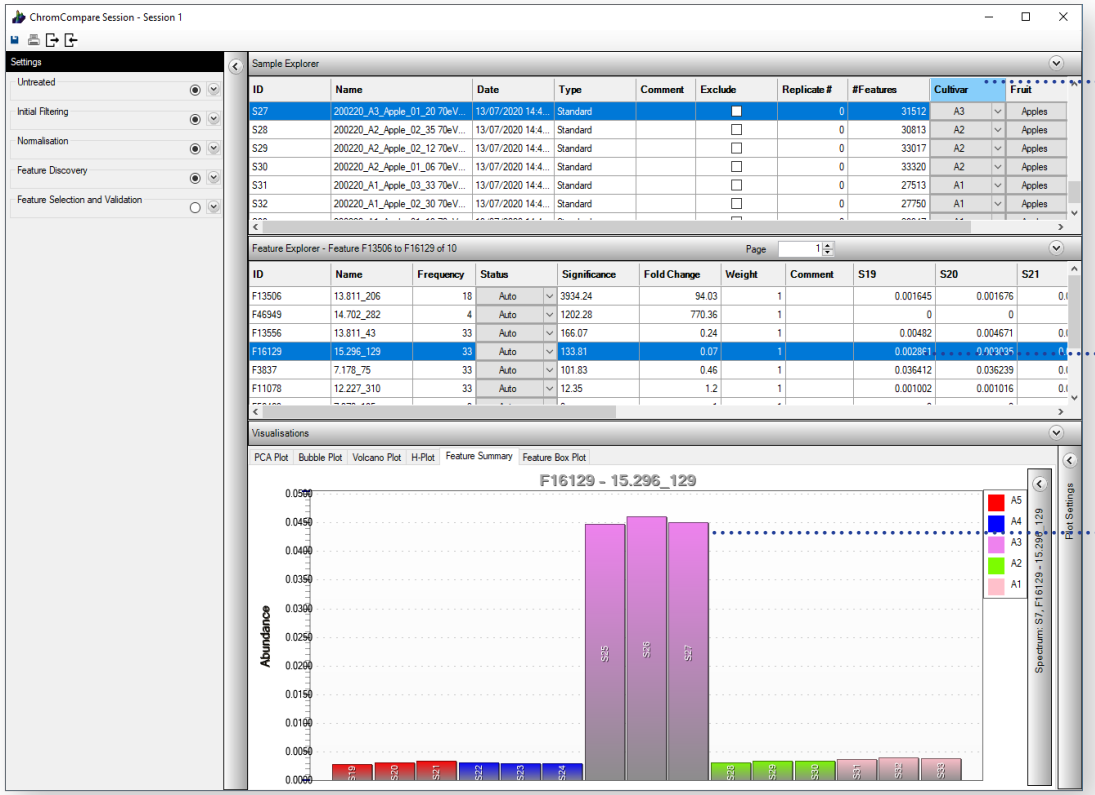
Use chemometrics to automate the discovery of differences among sample types or batches, and so define sample classes on the basis of measurable characteristics rather than prior knowledge.



Create prediction models to easily classify future samples and generate reports.

Minimise manual processing

With ChromCompare+ you don't have to be a statistician to gain greater insight into your complex datasets, and you don't have to know what compounds you are looking for. Raw data can be imported directly in a range of file formats for both 1D and 2D GC–MS, allowing you to quickly and easily discover hidden differences between sample classes.

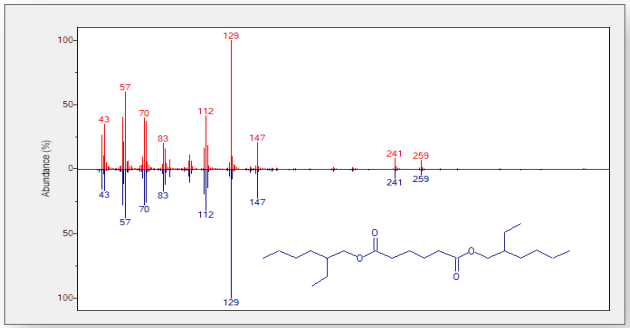


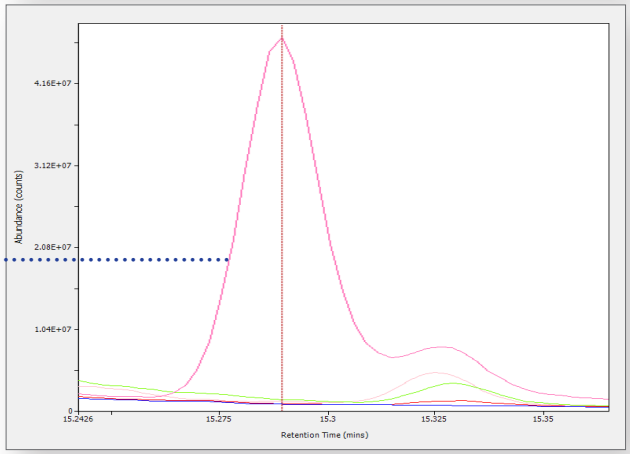
Samples are assigned to known classes

Feature list automatically highlights the most significant differences

Key difference found for m/z 129 in apple cultivar A3

Would you have overlooked this peak using your current workflows?



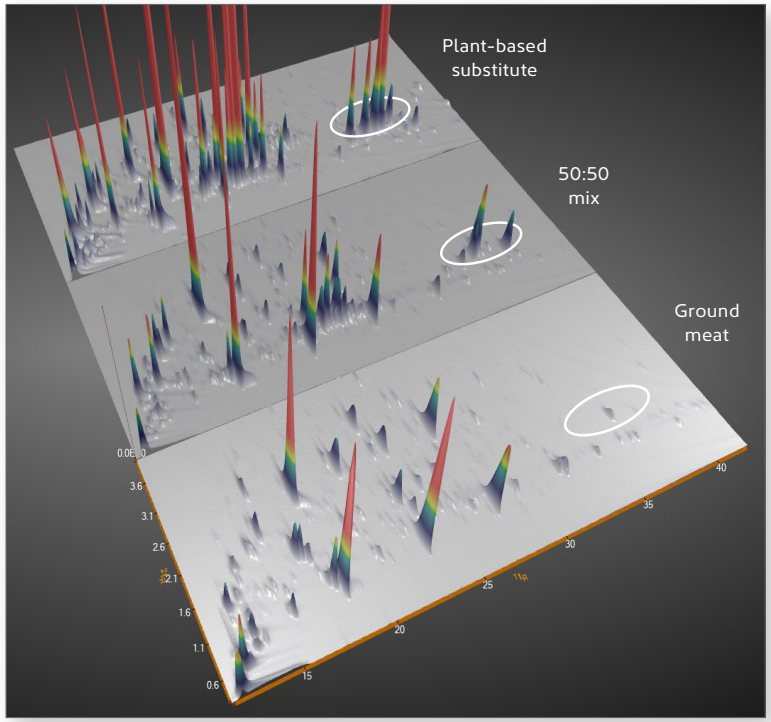


ChromCompare+ quickly highlights key differences between five apple cultivars, with no manual pre-processing steps. Here, the raw GC–MS data for the extracts was imported directly.

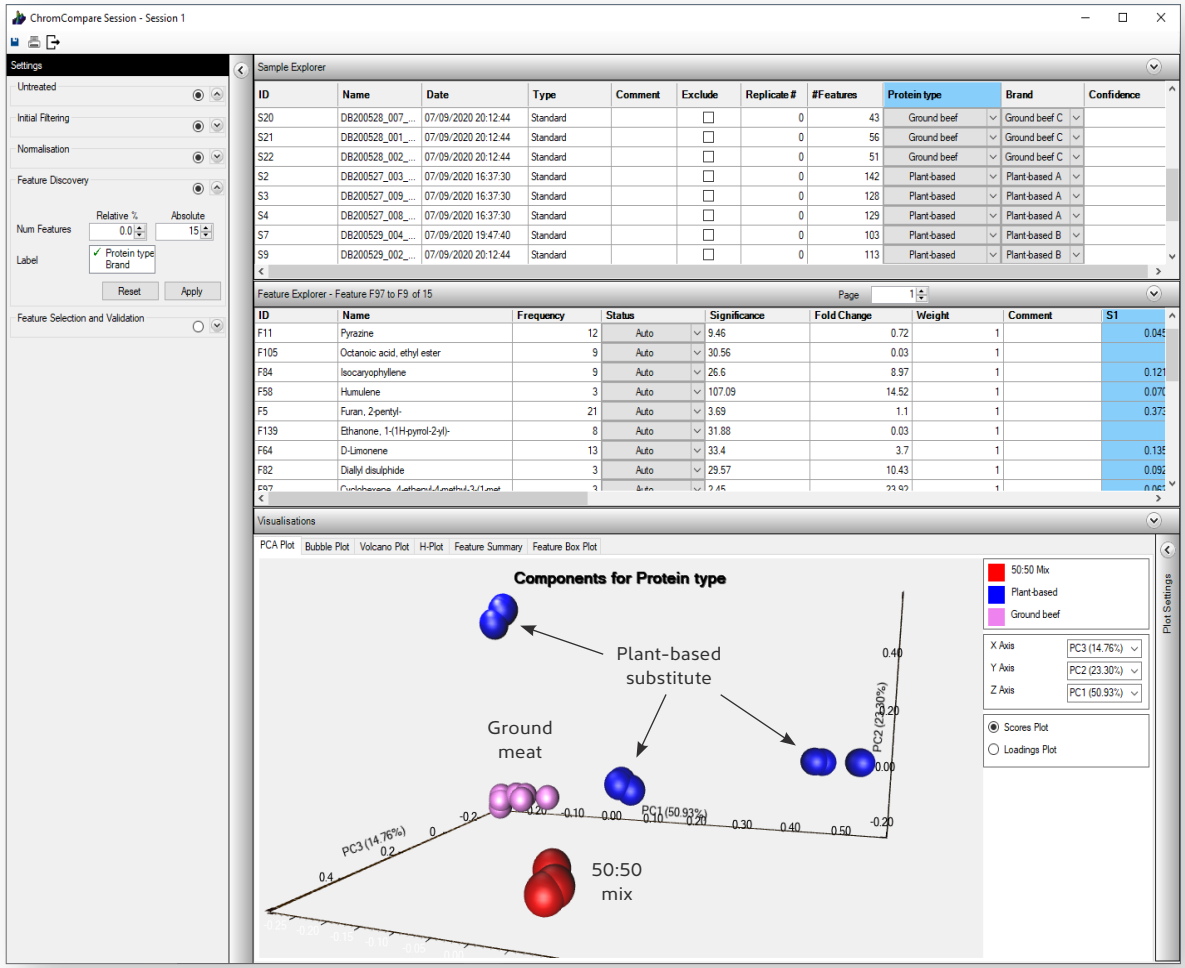
In this case, ChromCompare+ uncovers a plasticiser contaminant in one apple cultivar (A3) that may have migrated from food packaging.

Highlight differences between complex samples

The Feature Discovery function in ChromCompare+ automatically filters datasets to find the most significant differences between samples. This also simplifies any downstream tasks, such as quantitation, by reducing the number of compounds that require further investigation.

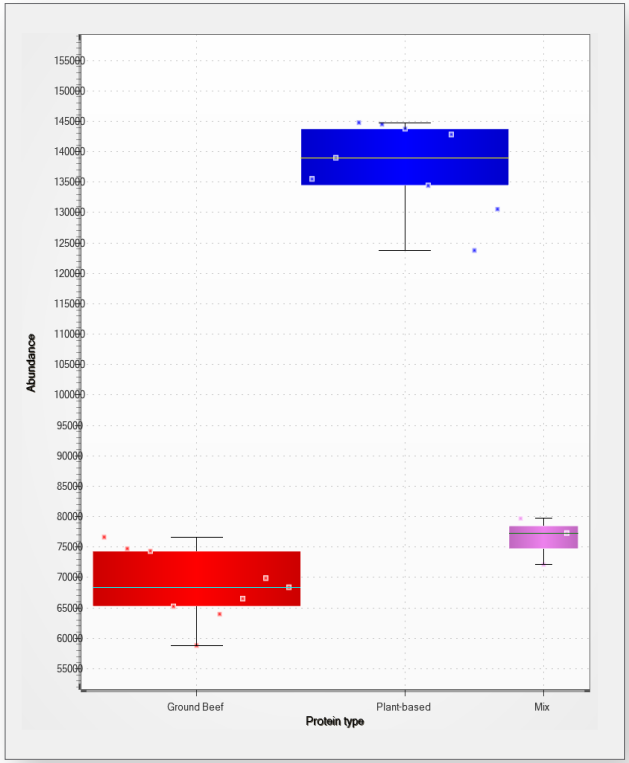


The Feature Discovery option in ChromCompare+ automatically finds the most significant differences between sample classes. Here, the aroma of ground meat is compared to that of two reduced-meat substitutes, with sulfur compounds and terpenes (circled) amongst the key differentiators.

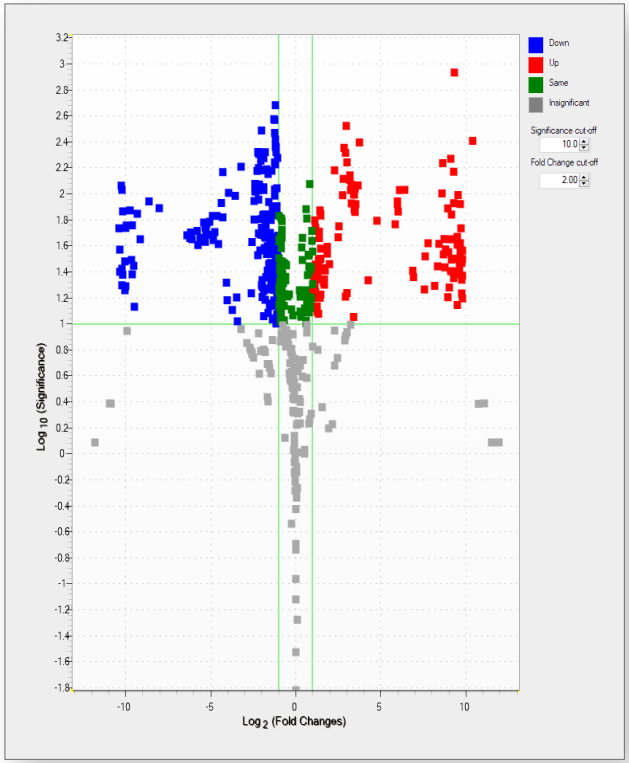


Easily visualise sample relationships

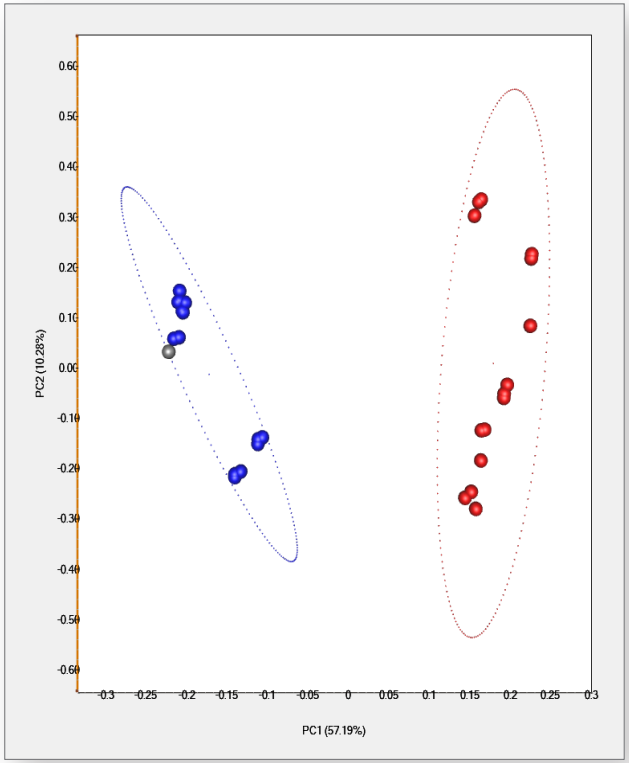
ChromCompare+ provides a suite of advanced visualisation tools to display the key trends and relationships between your samples. These fully interactive charts allow you to see all of the key information at a glance.



Feature box plots are a powerful way of displaying the variability within each class in large datasets, to get a better indication of the distribution of the data and to highlight outliers.



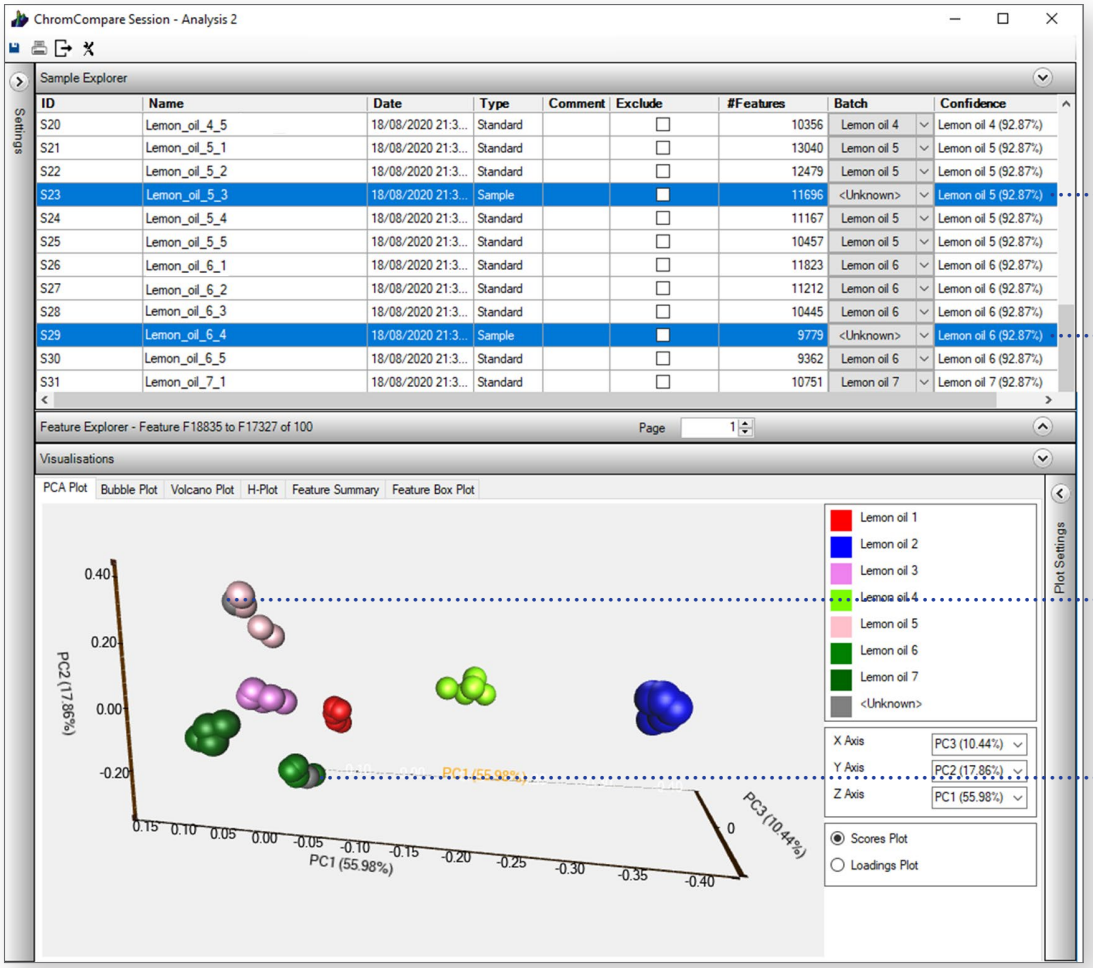
'Volcano plots' display the statistical significance of differences between classes for each feature *versus* the magnitude of this difference. This ensures that small yet significant differences are not missed.



Principal components analysis (PCA) can be used to reduce the dimensionality of the data and emphasise variation. PCA score plots are valuable tools to display key trends and patterns in a dataset.

Predict the class of unknown samples

Class prediction is a useful statistical tool for automatically assigning ‘unknown’ samples to a class.
In ChromCompare+, prediction models can be built, validated and tested to ensure samples are classified correctly regardless of the application. Such models are essential for fast insight into samples of unknown origin in routine quality control as well as authenticity studies.



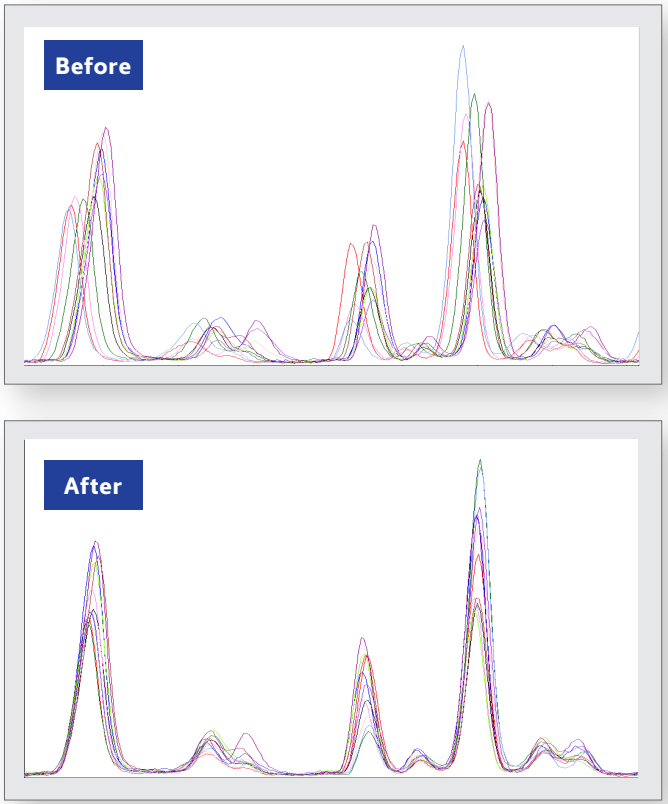
The model (92.87% accuracy) correctly predicts the class for the two samples of unknown origin

A fully-interactive PCA score plot allows the unknown samples to be easily visualised

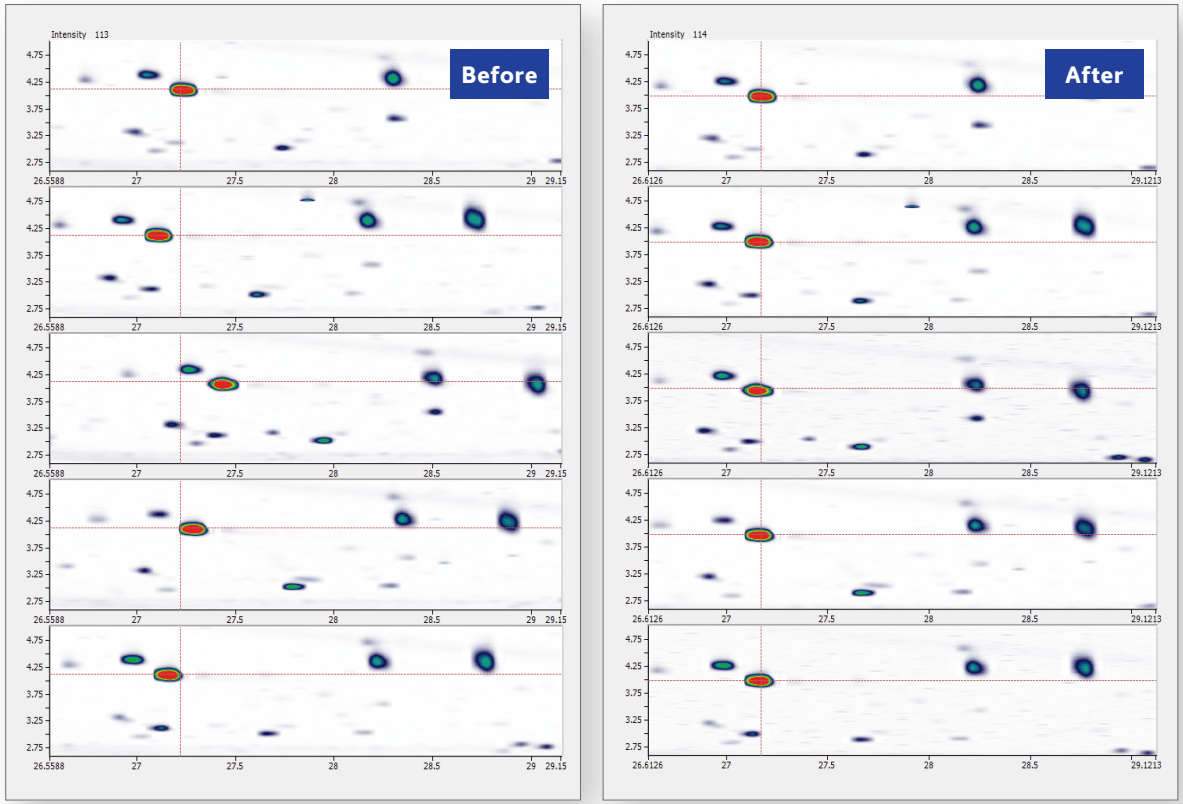
Two lemon oils of unknown origin (grey spheres) are correctly assigned as belonging to batches 5 and 6, respectively, providing fast and simple confirmation of quality and authenticity.

Automatically align chromatograms

ChromCompare+ allows raw data to be imported directly, minimising manual steps and reducing the risk of operator error prior to applying chemometrics. An integral step of this unique workflow is the automated alignment of chromatograms, which accounts for potential retention-time drifts in both 1D and 2D GC–MS.



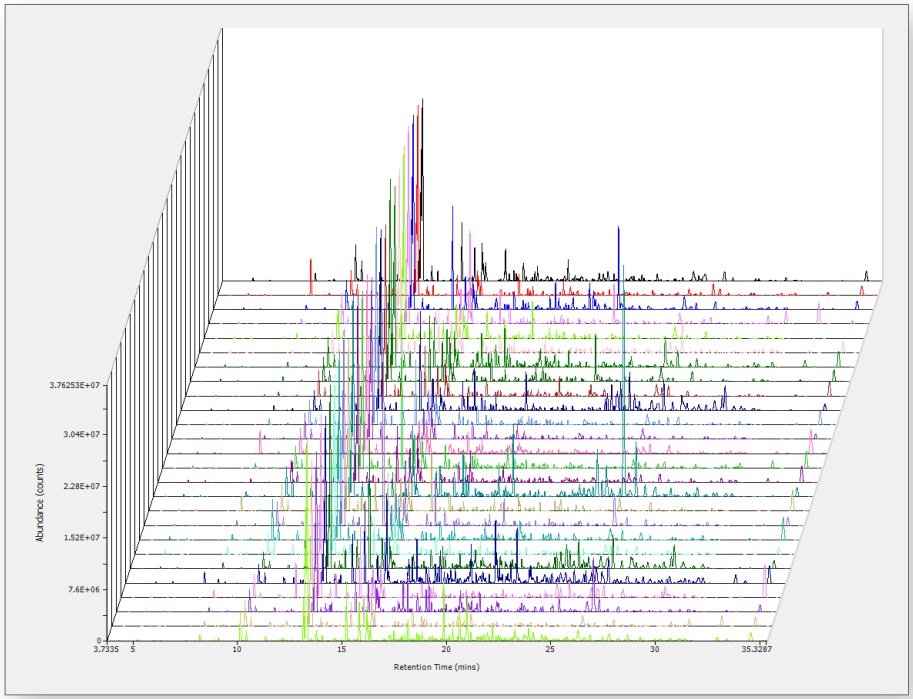
Alignment to a reference file adds confidence in the comparison of large sample batches, where retention time drift may previously have adversely impacted results.



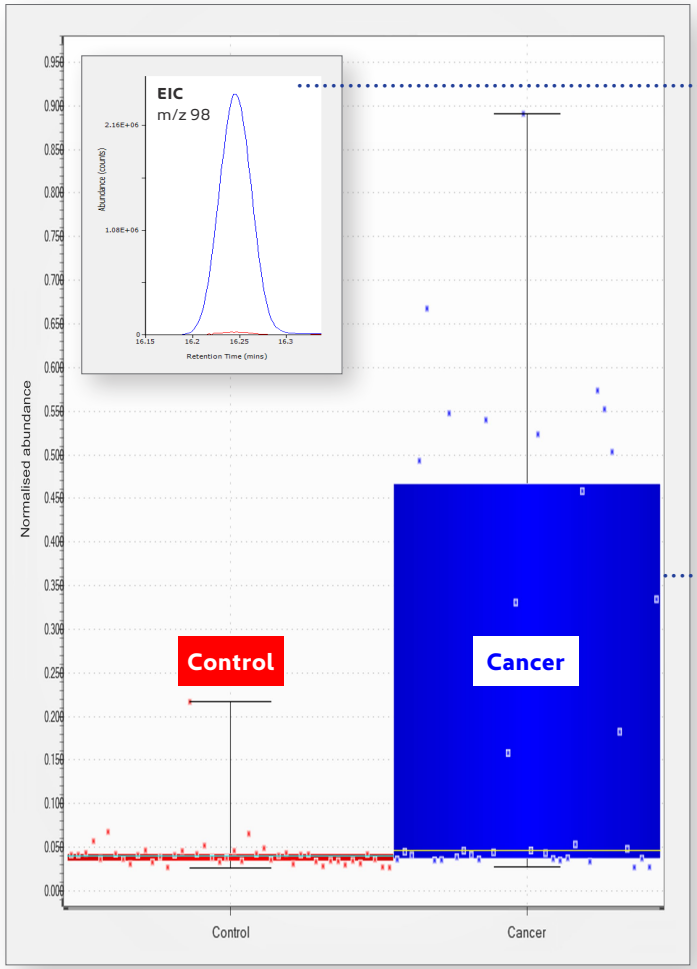
Alignment can also be applied to GC×GC–MS data, in fully automated sequences, for significant time savings.

Accelerate your discovery workflows

In discovery workflows, significant compounds are rarely of high abundance, and can be hidden within complex matrices. As a result, a comprehensive approach is required to identify the maximum number of significant differences. Using an untargeted workflow within ChromCompare+, the entire raw dataset can be automatically aligned and imported, to quickly uncover significant differences, and minimise the risk that compounds of interest are overlooked.



Volatiles from urine were collected from 40 control subjects and 40 cancer patients in a biomarker discovery study. Raw data were first aligned, before significant differences were uncovered as part of an automated, untargeted analysis – reducing normal processing time from days to minutes.

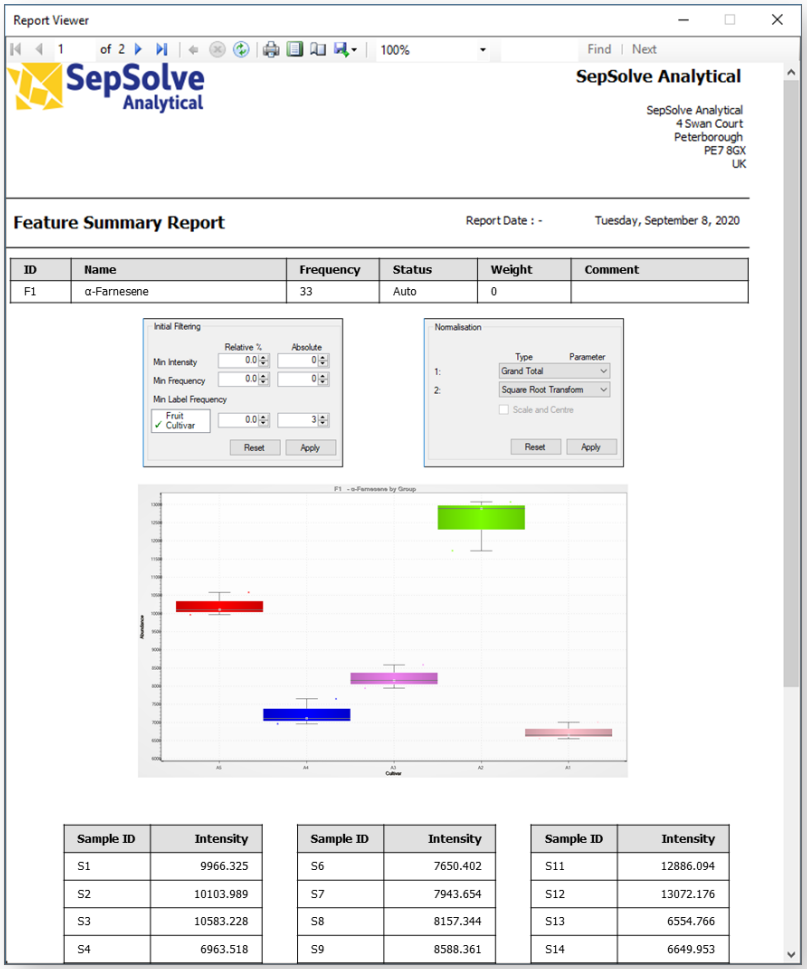


Thousands of individual features are automatically reduced to those of greatest significance – in this case, possible indicators of disease. This response for m/z 98 shows the large difference in response between the sample and control classes.

GC–MS abundances for a potential differentiator between the sample and control classes are displayed as a box plot, for rapid data review

Streamline reporting of results

ChromCompare+ not only delivers greater insight into samples across a wide range of applications, it also makes sharing results easy – with flexible export options, as well as simple report templates.



ID	Name	Frequency	Status	Weight	Comment
F1	α-Farnesene	33	Auto	0	

Sample ID	Intensity	Sample ID	Intensity	Sample ID	Intensity
S1	9966.325	S6	7650.402	S11	12886.094
S2	10103.989	S7	7943.654	S12	13072.176
S3	10583.228	S8	8157.344	S13	6554.766
S4	6963.518	S9	8588.361	S14	6649.953

Share your results with colleagues easily, using simple reporting templates or full export to .csv format.

Request a demo today to see how we can transform your data into usable information, whatever your application.

Biomarker studies for disease diagnosis

Authenticity determination of food and beverages

Quality control of fragrances and other consumer products

Chemical fingerprinting of petroleum products

Source attribution in environmental investigations

Forensic profiling of fire accelerants

Email hello@sepsolve.com to request an online demo of ChromCompare+

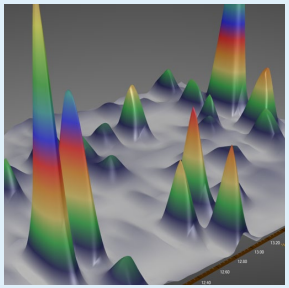
Discover more – Deliver more

ChromCompare+ can be fully integrated into SepSolve's powerful discovery workflows for streamlined analysis, from sample introduction through to data-mining and class prediction.

SAMPLE INTRODUCTION

Flexible sampling, extraction and enrichment to suit your application with Centri®, TD100-xr™ and robotic sample prep systems.

SEPARATION

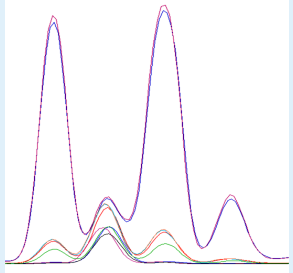


Enhanced separation by GC×GC using INSIGHT® flow modulation, or improved productivity through fast GC.

DETECTION

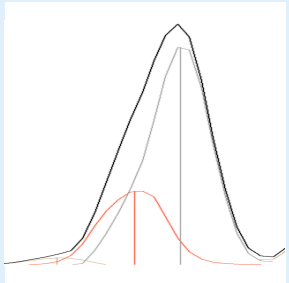
Confident targeted and untargeted screening using BenchTOF™ with unique Tandem Ionisation®.

DATA ALIGNMENT



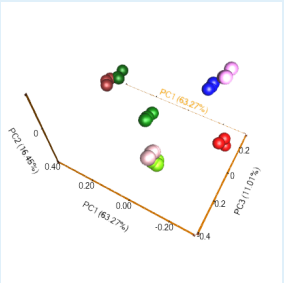
Automated alignment of raw data in GC and GC×GC for seamless comparisons across large data sets.

DATA-MINING



Robust deconvolution, RI matching and much more ensures that important peaks are not overlooked or misidentified.

CHEMOMETRICS



Discovery of important differences between samples using ChromCompare+™.

About SepSolve Analytical

SepSolve Analytical provides analytical platforms for separation scientists, including equipment for automated sample introduction, advanced GC separation, state-of-the-art mass spectrometry and powerful data analysis.

Together, these tools enable you to discover more about your sample, and to deliver higher throughput for both research and routine applications. To ensure you get the best from your investment, our experienced application chemists provide access to the training and support you need, at support centres around the globe.

If you'd like more information on the software shown in this brochure, please get in touch using the contact details below to arrange a free online demonstration.

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