White Paper 036
September 2020

Evaluation of fruit quality using GC–TOF MS and innovative chemometrics

This study demonstrates the use of ChromCompare+ software to identify significant differences among fruit cultivars using innovative, automated workflows.

Introduction

Quality management enables the food and beverage industry to meet consumer expectations and maintain brand reputation and product safety.

Analytical instrumentation is constantly evolving, allowing us to gain greater insight into our samples' compositions than ever before, but data processing has remained a challenging prospect. Chromatographic complexity and the vast numbers of samples involved make it difficult to identify trends and differences between sample batches or classes.

ChromCompare+ is a powerful, easy-to-use chemometrics platform to transform your complex 1D or 2D GC–MS data into meaningful and usable results.

Here, we will demonstrate the use of ChromCompare+ software to automatically identify key differentiators across five pear cultivars using all the raw GC–MS data.[1] This innovative approach minimises laborious pre-processing steps and enables automated workflows to be adopted in quality control labs.

Experimental

Samples: Five extracts for different pear cultivars were prepared by QuEChERS extraction and analysed in triplicate.

GC–MS: Instrument: BenchTOF-HD™; Mass range: m/z 40–800; Acquisition rate: 5 Hz.

Software: Instrument control by TOF-DS, data processing in ChromCompare+.

SepSolve Analytical Ltd
T: +44 (0)1733 669222 (UK) +1 888-379-3835 (USA)
E: hello@sepsolve.com
www.sepsolve.com

Results

Untargeted analysis of five pear cultivars was performed using GC–TOF MS (Figure 1) prior to data mining and chemometrics by ChromCompare+.

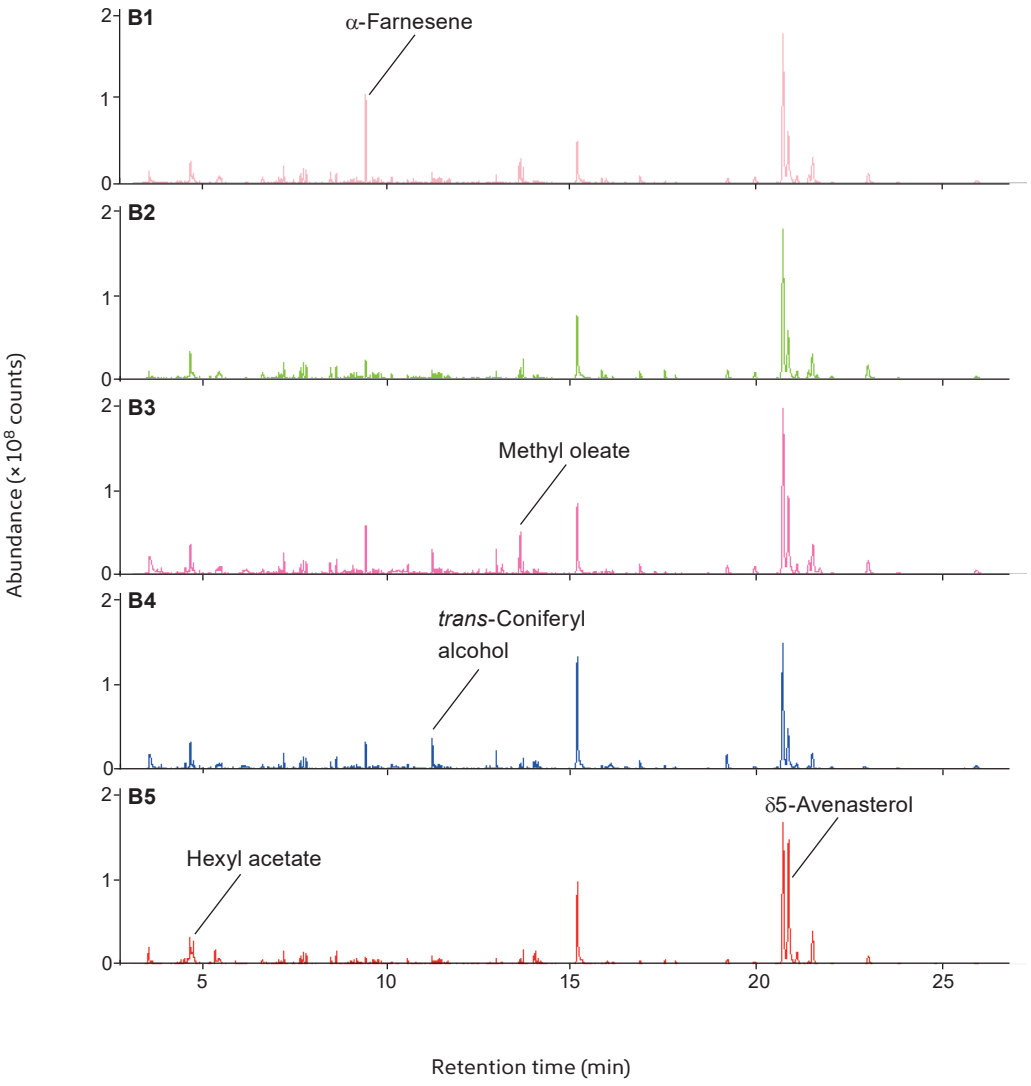

Figure 1

GC–TOF MS chromatograms for extracts from five pear cultivars (B1–B5).

SepSolve Analytical Ltd
T: +44 (0)1733 669222 (UK) +1 888-379-3835 (USA)
E: hello@sepsolve.com

The raw data was imported directly into ChromCompare+ to find differences among the cultivars. 'Feature Discovery' was performed to select the 50 most significant differences from a total of over 30,000 features (Figure 2). The 'Feature Explorer' highlights the retention time and ion that has resulted in a significant difference among the chromatograms, allowing the analyst to quickly review the results and perform identification.

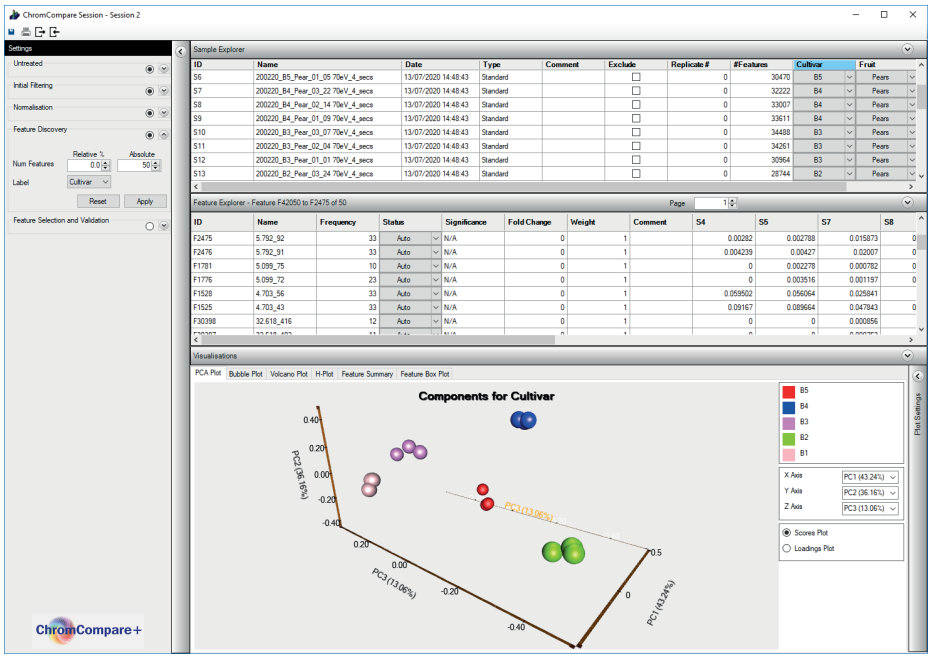

Figure 2

ChromCompare+ results after Feature Discovery using the raw data for the pear cultivars – with all samples showing distinct differences in the PCA score plot.

The principal components analysis (PCA) score plot in Figure 2 shows that cultivars B1 and B3 exhibited the closest similarity, but all cultivars could be differentiated. Some of these differences are easy to see when examining the chromatograms (Figure 1); for example, B5 was found to contain greater abundances of δ5-avenasterol and hexyl acetate, as well as diminished levels of methyl oleate, α-farnesene and *trans*-coniferyl alcohol.

However, a number of trace differences between the cultivars were also listed among the most significant, and these may have escaped notice in manual processing workflows. Interactive feature summary charts can be used in ChromCompare+ to help visualise these differences. Figure 3 provides feature summary charts for some trace differentiators found among the cultivars, as well as the corresponding identification.

For example, cultivar B4 was found to contain a significantly higher level of phenylethyl alcohol than all other samples (Figure 3A) – an important attribute as it can give a characteristic floral, sweet flavour.[2] This untargeted workflow is also useful for identifying potentially harmful compounds; for example, the insecticide etofenprox was only found in cultivar B4 (Figure 3B), while a key differentiator of the B1 cultivar was increased levels of the fungicide cyprodinil (Figure 3C).

These trace peaks had abundances multiple orders of magnitude lower than the highest-loading peaks, and may have been overlooked if peak integration approaches were applied. With ChromCompare+, all of the raw data is utilised for automatic discovery of the important features, regardless of their intensity.

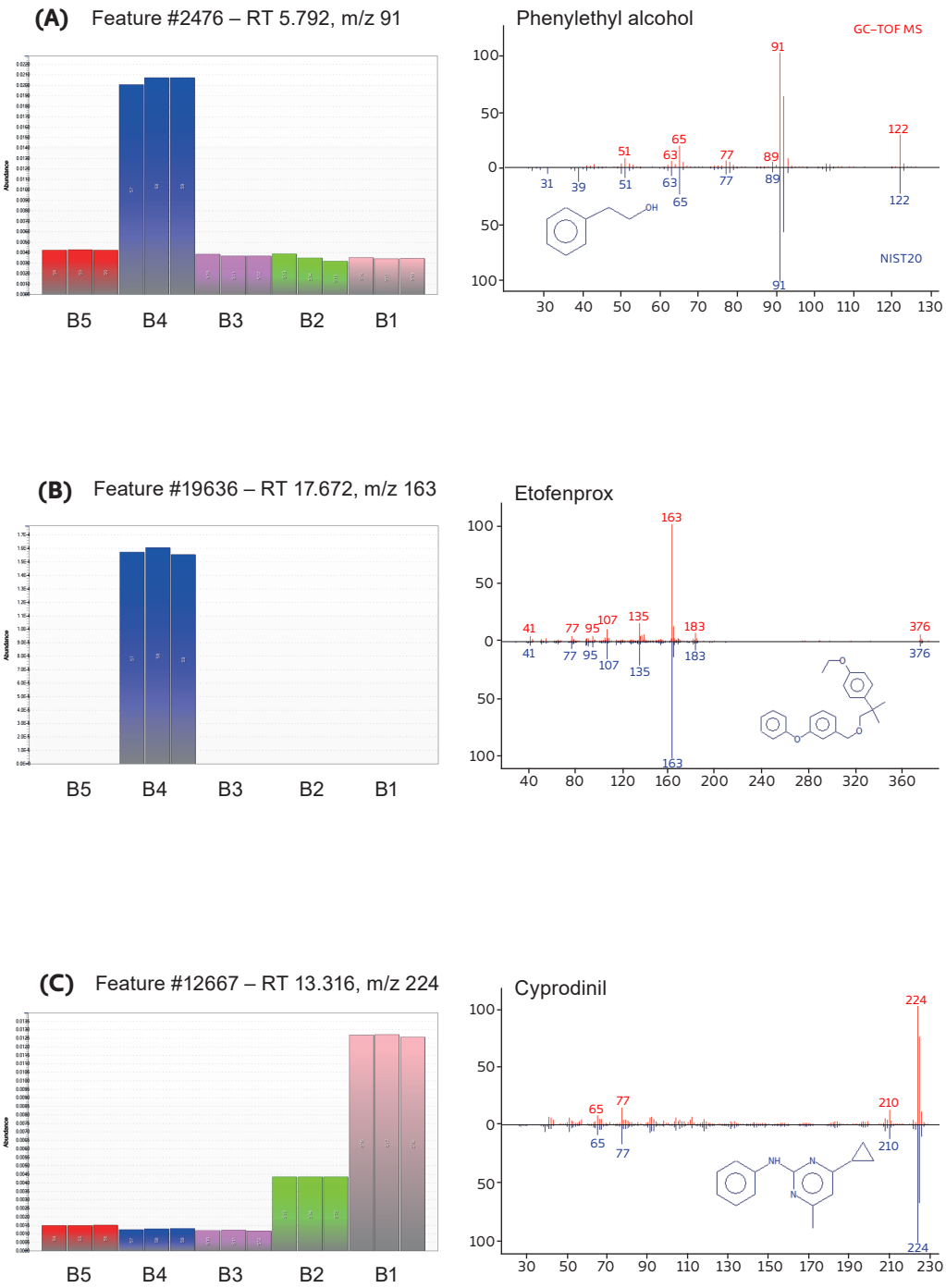

Figure 3

ChromCompare+ feature summary charts highlighting three features that were automatically selected as key differentiators of the pear cultivars. The corresponding identifications based on NIST library searching are also provided.

SepSolve Analytical Ltd
T: +44 (0)1733 669222 (UK) +1 888-379-3835 (USA)
E: hello@sepsolve.com

Conclusions

This white paper has demonstrated that ChromCompare+ is a powerful and easy-to-use tool for chemometrics in the food industry, through the use of:

- Fully automated processes that minimise laborious pre-processing steps and speed up workflows.
- The entire raw dataset to reduce the risk of overlooking trace differences.
- Interactive charts, such as PCA plots and feature summary charts, to easily visualise trends and differences between samples.

For more information on this application, or any of the techniques or products used, please contact SepSolve.

References and notes

[1] C.E. Frye, N.R. Moore and R.E. Synovec, Enhancing the chemical selectivity in discovery-based analysis with tandem ionization time-of-flight mass spectrometry detection for comprehensive two-dimensional gas chromatography, *J. Chromatogr. A.*, 2018, 1537: 99–108.

[2] The Good Scents Company Information System (search facility), www.thegoodscentscompany.com/search2.html (accessed on 13 August 2020).

D0072_1_100920

SepSolve Analytical Ltd
T: +44 (0)1733 669222 (UK) +1 888-379-3835 (USA)
E: hello@sepsolve.com