

Centri[®] Applications Compendium



A compilation of the applications of the Centri sample extraction and enrichment platform

Introduction to Centri

A breakthrough in sample extraction and enrichment for GC-MS

Centri is the first platform to offer high-sensitivity unattended extraction and enrichment of volatile and semi-volatile organic compounds (VOCs and SVOCs) in liquid, solid and gaseous samples.

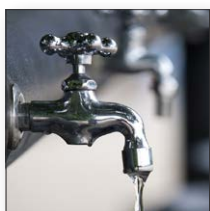
Featuring best-in-class robotic automation and offering multiple sampling modes in a modular design, Centri provides unrivalled application flexibility and sampling robustness. At the same time, the cryogen-free focusing trap optimises analytical sensitivity, enhancing the quality and quantity of information obtained from a sample.



Whichever major brand of GC-MS you're using, Centri lets you **discover more** and **deliver more** from your samples.

The versatility of Centri

Centri can be used for a wide range of applications, including:



Environmental

Centri offers the outstanding sensitivity and automation capability that are key for high-throughput detection of trace pollutants in water, air, and other environmental matrices.



Food

Centri provides the broad analyte range and high sensitivity that allows efficient trace-level aroma profiling of everything from fruit and vegetables to dairy products and dried goods.



Beverages

With its range of water management options, Centri easily deals with the high water (or alcohol) content of beverages, while also avoiding the tedious sample-preparation steps common with other approaches.



Fragrance

Centri offers the sensitivity needed to detect trace-level compounds with low odour thresholds, as well as the ability to purge interferences such as water.



Health

The high throughput and high sensitivity of Centri makes it the ideal choice for health applications, such as biomarker studies.



Forensic

Centri avoids labour-intensive sample preparation, and uses low-temperature thermal desorption, reliably analysing labile analytes such as explosives.



Find out more

In this compendium, we've brought together the full range of Centri-based applications that have been developed by our specialists and by our customers at locations around the world.



In each case, we describe the workflow and the key benefits, and provide a link to download the full application note from our website.

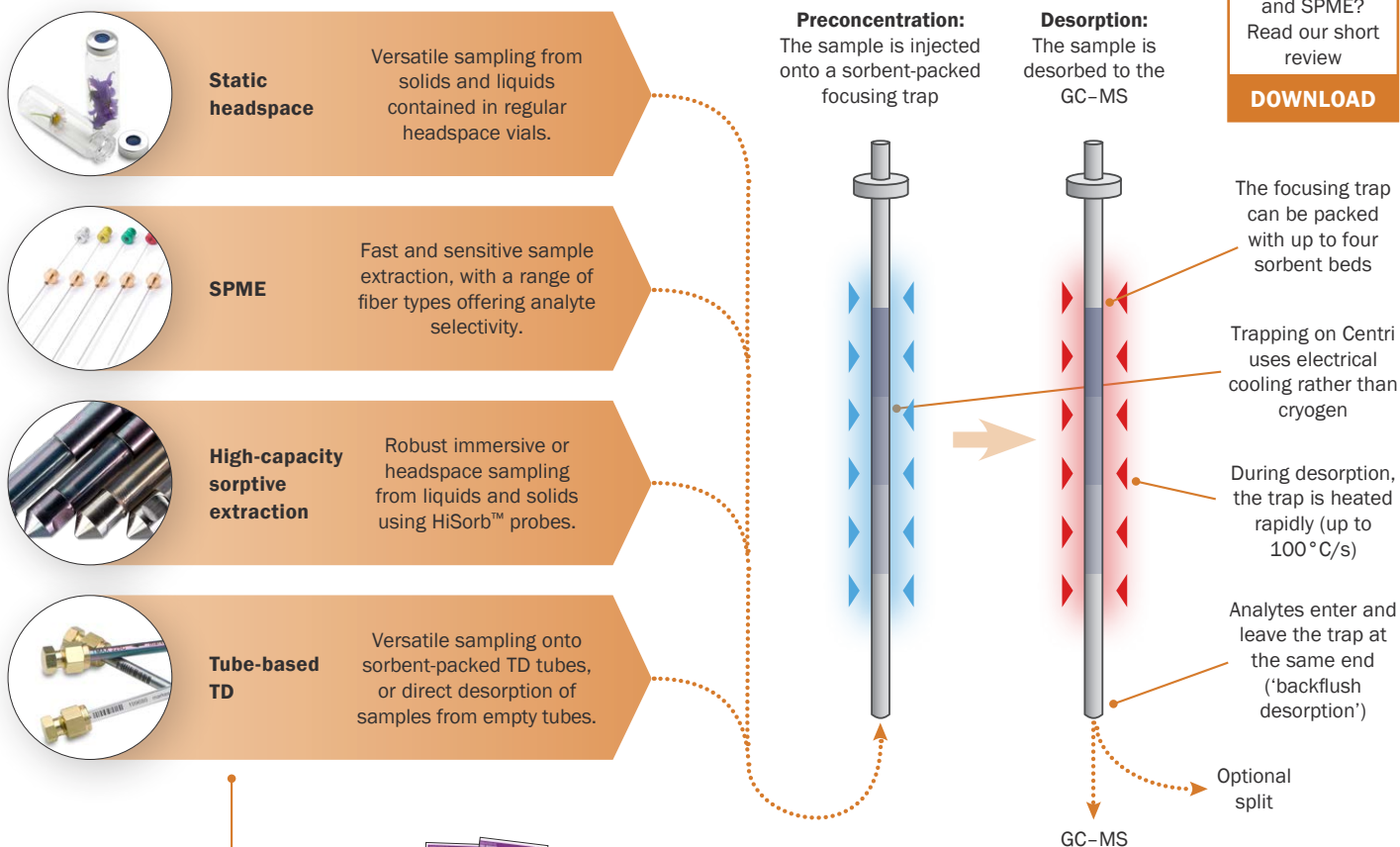
To discuss how Centri could benefit you, please email enquiries@markes.com (see back cover for regional contact details).

How Centri works

Centri offers **four automated sampling modes**. Trap-based preconcentration is an integral part of high-capacity sorptive extraction and tube-based TD, but optional for static headspace and SPME.

Need to know the benefits of adding trapping to headspace and SPME? Read our short review

[DOWNLOAD](#)



New to these techniques? Find out the essentials with our set of infographics

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Benefits of trap-based preconcentration:

- **Improved sensitivity:** Rapidly desorbing the sample to the GC in ~100 µL of vapour produces narrower peaks and so improves sensitivity.
- **Broader analyte range:** The focusing trap contains multiple sorbents placed in order of increasing strength. Combined with 'backflush' operation, this allows a wide volatility range of compounds to be efficiently retained and desorbed in a single analysis.
- **Streamlined operation:** Centri uses electrical cooling, eliminating the cost and inconvenience of cryogen, and avoiding the risk of ice formation in the trap box.
- **More confident identification:** The narrower peaks obtained with trapping result in better spectral matches with compound libraries (such as the NIST database), enabling more confident identification of low-level analytes.

Other methods for enhancing performance:

- **Multi-step enrichment (MSE):** Using Centri, multiple extractions onto the focusing trap can be used to increase both the analyte response and the number of compounds identified. This can be carried out using a single vial, or with replicate samples in multiple vials.
- **Large-volume injection:** The use of trapping allows large volumes of headspace (up to 5 mL) to be preconcentrated, resulting in increased sensitivity without affecting peak shape.
- **Selective purging:** Selective elimination of water (while retaining analytes of interest) is aided by an ambient-temperature purge prior to trap desorption.
- **'Prep-ahead' mode:** The simultaneous extraction of multiple samples while a previous analysis is ongoing offers reductions in overall cycle time and so an improvement in laboratory productivity.
- **Re-collection:** Using Centri, part of the desorbed sample can be transferred to a sorbent tube. This allows sample archiving and reliable data validation, streamlines method development, and opens up the option of obtaining complementary data using different techniques. Such options are particularly useful when samples are unstable or supplies are limited.

Quick application summary

Check the table below to identify the Centri applications and methods you're most interested in, and click on the page numbers to jump straight to the application.

	Focus	Sample type	Extraction methods					Methods for enhancing performance					Page	
			Static headspace SPME	Headspace Immersive	High-capacity sorptive extraction	Tube-based TD	Trap-based pre-concentration	Multi-step enrichment (MSE)	Large-volume injection	Selective purging	'Prep-ahead' mode	Re-collection		
ENVIRONMENTAL	Improving on the performance of purge-and-trap	Water	<input checked="" type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input checked="" type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input checked="" type="checkbox"/>	6
	Detecting low-level contaminants	Water	<input type="checkbox"/>	<input type="checkbox"/>	<input checked="" type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input checked="" type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	<input type="checkbox"/>	7
	Detecting low-level contaminants	Water	<input checked="" type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input checked="" type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	8
	Enhancing extraction for 1,4-dioxane	Water	<input type="checkbox"/>	<input checked="" type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	9
FOOD	Understanding ecosystem health	Soil	<input type="checkbox"/>	<input checked="" type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	<input type="checkbox"/>	<input checked="" type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	10
	Comprehensive aroma profiling	Fruit	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	11
	Comprehensive aroma profiling	Meat	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	12
	Comprehensive aroma profiling	Potato snacks	<input type="checkbox"/>	<input type="checkbox"/>	<input checked="" type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input checked="" type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input checked="" type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	13
	Detecting residual solvents	Food packaging	<input checked="" type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input checked="" type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	14
	Detecting food additives	Dried goods	<input checked="" type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input checked="" type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	15
	Monitoring safety and quality	Dried goods	<input type="checkbox"/>	<input type="checkbox"/>	<input checked="" type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input checked="" type="checkbox"/>	<input type="checkbox"/>	16
	Detecting residual fumigants	Seeds	<input checked="" type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	<input type="checkbox"/>	<input checked="" type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	17
	Discovering authenticity markers	Honey	<input type="checkbox"/>	<input type="checkbox"/>	<input checked="" type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input checked="" type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input checked="" type="checkbox"/>	<input type="checkbox"/>	18
	Evaluating sorptive phase combinations	Honey	<input type="checkbox"/>	<input type="checkbox"/>	<input checked="" type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input checked="" type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input checked="" type="checkbox"/>	<input type="checkbox"/>	19
	Improving the sensitivity of headspace	Food concentrate	<input checked="" type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	20
	Detecting food contaminants	Food concentrate	<input checked="" type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	21
	Enhancing the sensitivity of SPME	Oils	<input type="checkbox"/>	<input checked="" type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	22
BEVERAGES	Detecting additives	Tea	<input checked="" type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input checked="" type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	23
	Comprehensive aroma profiling	Tea	<input type="checkbox"/>	<input checked="" type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	<input type="checkbox"/>	<input checked="" type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	24
	Comprehensive aroma profiling	Tea	<input type="checkbox"/>	<input type="checkbox"/>	<input checked="" type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input checked="" type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	<input type="checkbox"/>	25
	Enhancing the sensitivity of headspace	Fruit juice	<input checked="" type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	26
	Streamlining extraction for low-level 'Brett' odorants	Wine	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input checked="" type="checkbox"/>	<input type="checkbox"/>	<input checked="" type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	27
	Comprehensive aroma profiling	Cider	<input type="checkbox"/>	<input type="checkbox"/>	<input checked="" type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input checked="" type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input checked="" type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	28
	Evaluating sorptive phase combinations	Hard seltzers	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input checked="" type="checkbox"/>	<input type="checkbox"/>	<input checked="" type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	<input type="checkbox"/>	29
	Comprehensive flavour profiling	Hard seltzers	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input checked="" type="checkbox"/>	<input type="checkbox"/>	<input checked="" type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	<input type="checkbox"/>	30
	Avoiding interference from ethanol	Spirits	<input checked="" type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input checked="" type="checkbox"/>	<input type="checkbox"/>	<input checked="" type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	31

Continued on the next page

		Extraction methods					Methods for enhancing performance								
Focus		Sample type		Static headspace SPME	High-capacity sorptive extraction	Headspace	Immersive	Tube-based TD	Trap-based preconcentration	Multi-step enrichment (MSE)	Large-volume injection	Selective purging	'Prep-ahead' mode	Re-collection	Page
FRAGRANCE	Comprehensive fragrance profiling	Personal hygiene products		<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input checked="" type="checkbox"/>	<input type="checkbox"/>	<input checked="" type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	<input type="checkbox"/>	32
HEALTH	Detecting disease biomarkers	Breath		<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	33
FORENSIC	Screening for explosives	Water and fabrics		<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input checked="" type="checkbox"/>	<input type="checkbox"/>	<input checked="" type="checkbox"/>	<input type="checkbox"/>	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	34
GENERAL TOPICS	Improving the sensitivity of SPME by multi-step enrichment			<input type="checkbox"/>	<input checked="" type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	35
	Improving the sensitivity of headspace by large-volume injection			<input checked="" type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input checked="" type="checkbox"/>	<input type="checkbox"/>	<input checked="" type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	36
	Enhancing laboratory throughput by automation			<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input checked="" type="checkbox"/>	<input type="checkbox"/>	<input checked="" type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input checked="" type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	37

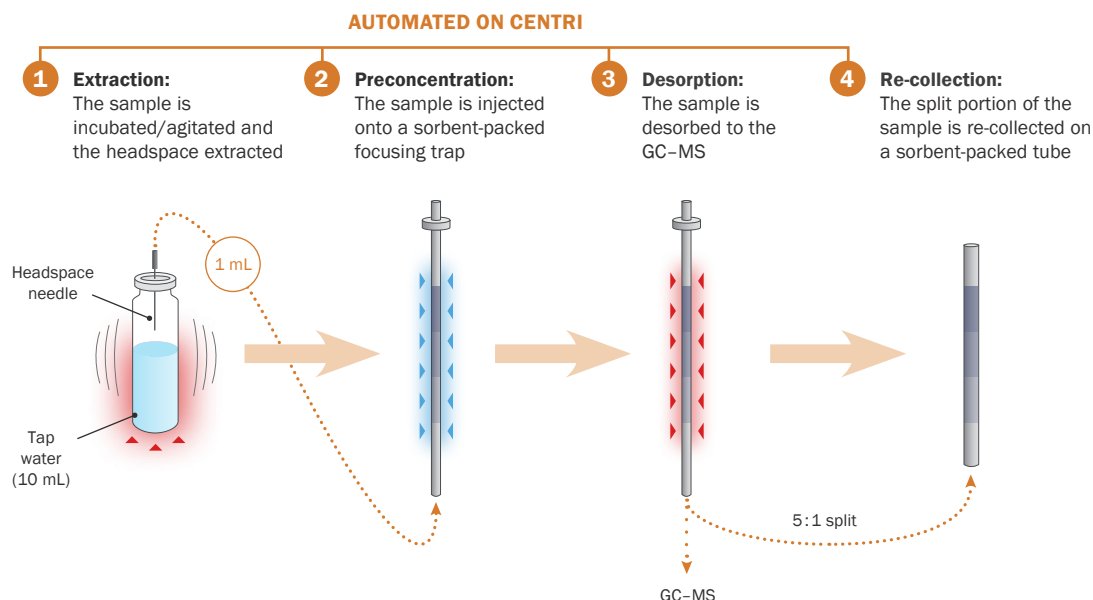
Improving on the performance of purge-and-trap: Water

► CHALLENGE:

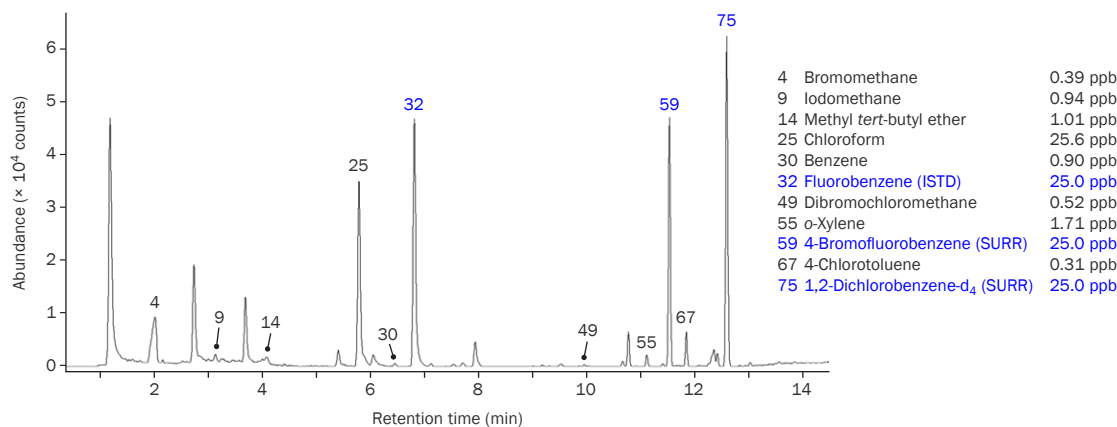
The purge-and-trap process commonly used to identify and quantify volatile pollutants in environmental water (US EPA Method 524.2) can **suffer from foaming and aerosol formation**, leading to poor chromatography.

When strict adherence to the EPA protocol is not required, **headspace-trap** on Centri offers several practical advantages to overcome these issues.

► WORKFLOW:



► EXAMPLE DATASET:



► KEY ADVANTAGES:

- **Lower detection limits:** The mean MDL is 0.13 ppb, which is below the reporting limit stipulated in US EPA Method 524.2.
- **Broad analyte range:** The use of multi-bed focusing traps allows detection of analytes with a wide range of volatilities.
- **Improved peak shapes:** Trapping provides better performance, particularly for early-eluting compounds.
- **Effective water management:** Selective elimination of water (while retaining analytes of interest) is aided by the use of hydrophobic sorbents in the focusing trap, and an ambient-temperature purge of residual water prior to trap desorption.
- **Improved workflow options:** Re-collection of sample split flows for repeat analysis improves method development, sample archiving and method validation.

ENVIRONMENTAL

FOOD

BEVERAGES

FRAGRANCE

HEALTH

FORENSIC

GENERAL TOPICS



Headspace-trap analysis of tap water containing an internal standard and two surrogates (blue) at 25 ppb shows the presence of chloroform at the same level, and a number of other volatile contaminants in the range 0.3–2 ppb.



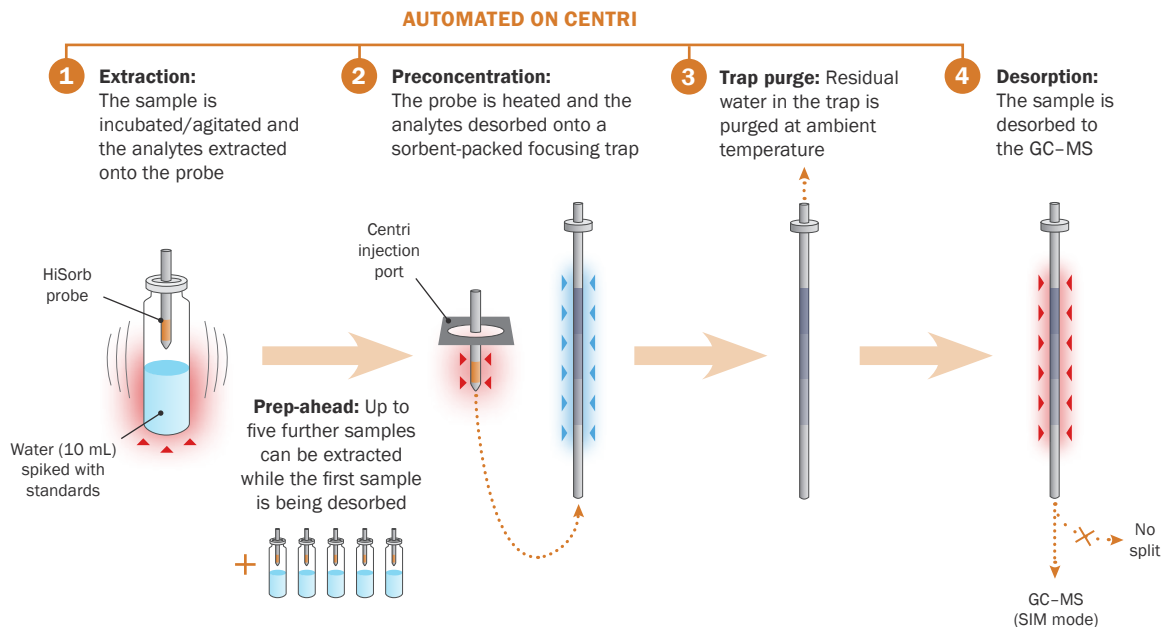
Detecting low-level contaminants: Water

► CHALLENGE:

Some water contaminants have low odour thresholds but are often present at **very low levels**, making them difficult to detect using traditional extraction techniques such as SPME (which also suffers from the **fragility of the fibers**).

High-capacity sorptive extraction on Centri addresses both issues, by providing a larger volume of sorptive phase for greater sensitivity, and by using a robust metal-core probe.

► WORKFLOW:



► KEY ADVANTAGES:

■ Greater sensitivity:

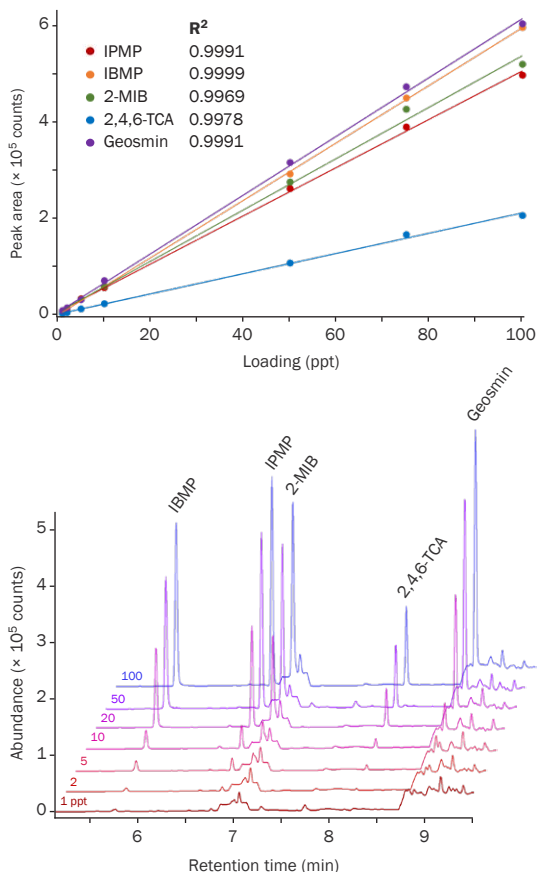
- Probes have more sorptive phase than SPME, resulting in more efficient extraction of low-level and polar compounds.
- The optimised trap design permits low-split (or splitless) operation, allowing a large portion of the sample to be sent to the GC.

■ Improved throughput:

- Full automation of sample extraction, washing/drying of probes, probe desorption and GC injection eliminates time-consuming manual operations.
- Simultaneous extraction of multiple vials is possible with HiSorb probes, unlike SPME (where the tool holds the fiber in the vial for the entire extraction time).

- **Reduced downtime:** HiSorb probes are inherently more robust, easier to handle, and less prone to accidental damage than delicate SPME fibers.

► EXAMPLE DATASET:



Splitless injection and SIM mode enabled calibration of a water standard in the range 1–100 ppt using HiSorb probes in headspace mode, automated on Centri.

For full details
DOWNLOAD
Application Note 255



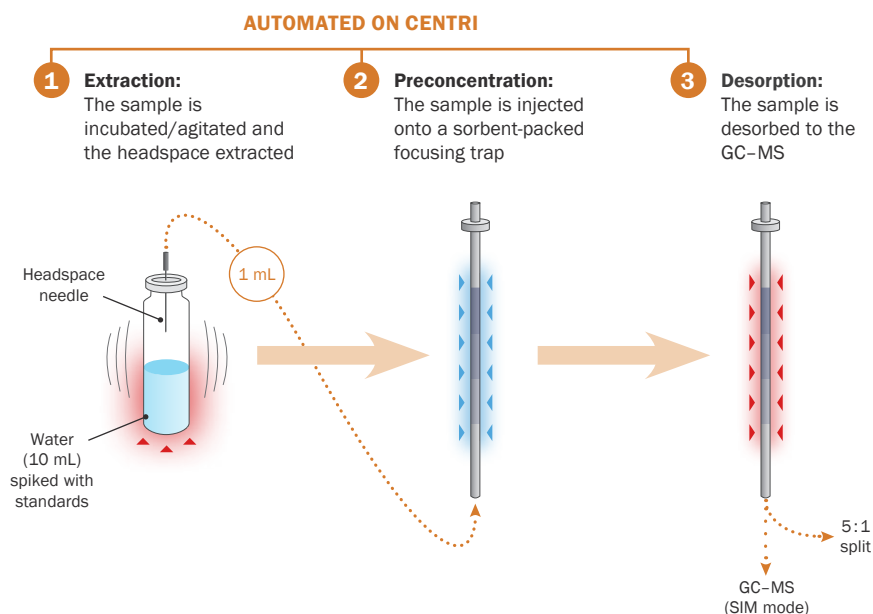
Detecting low-level contaminants: Water

► CHALLENGE:

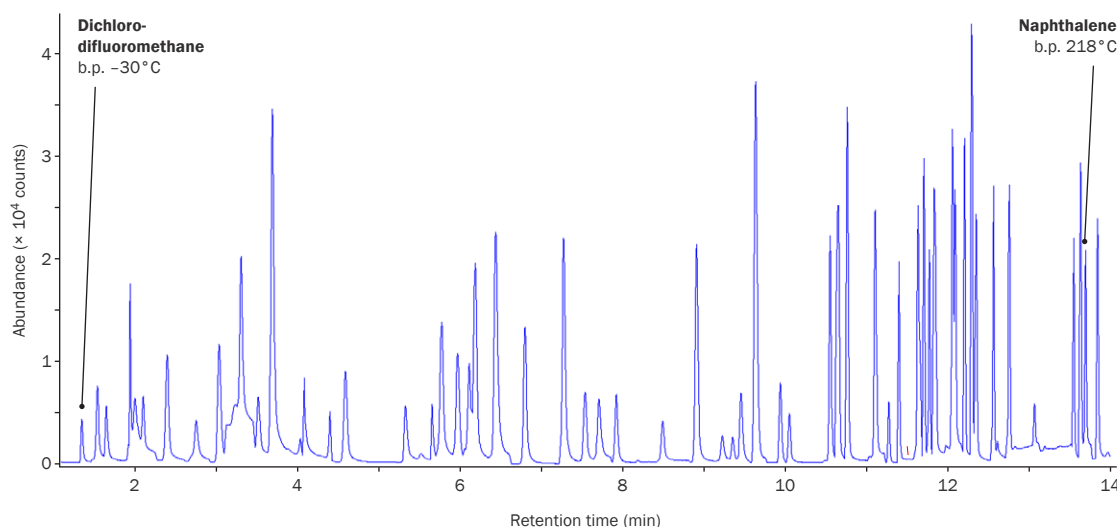
Increasingly stringent water regulations require that contaminants – either environmental pollutants or byproducts of disinfection during water-treatment – must be detected at **very low levels**. However, this can be difficult to achieve using traditional direct headspace methods.

Headspace-trap on Centri overcomes this problem using trap-based preconcentration, allowing low-ppt sensitivity to be achieved within a fully automated workflow.

► WORKFLOW:



► EXAMPLE DATASET:



► KEY ADVANTAGES:

- **Improved sensitivity:** Low-ppt sensitivity is achieved through the optimised trap design, which preconcentrates the 1 mL of headspace into ~ 100 μL of vapour. It also allows low-split (or splitless) operation, allowing a large portion of the sample to be sent to the GC.
- **Generation of comprehensive profiles:** Use of focusing traps containing multiple sorbent beds enables a wide volatility range of compounds to be efficiently retained and desorbed in a single analysis.

ENVIRONMENTAL

FOOD

BEVERAGES

FRAGRANCE

HEALTH

FORENSIC

GENERAL TOPICS



Highly symmetrical peaks are obtained for components of a standard mix across a wide boiling range, using headspace-trap automated on Centri. Acquisition using SIM mode enhances sensitivity further and ensures that performance quantitation limits (PQLs) are well below those required by regulatory bodies.

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Application Note 256



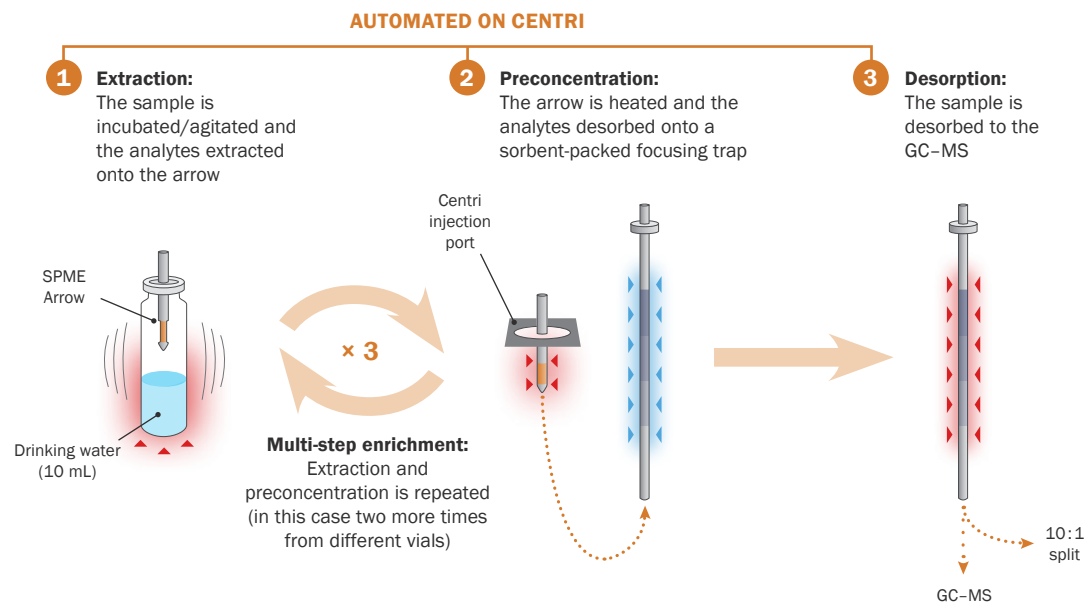
Enhancing extraction for 1,4-dioxane: Water

► CHALLENGE:

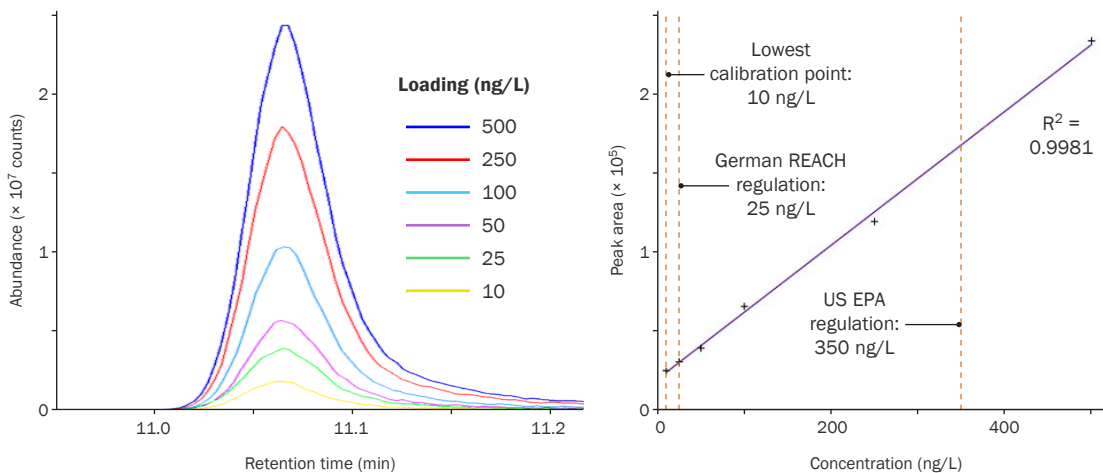
Some water contaminants such as 1,4-dioxane are both volatile and polar, and therefore have a high affinity to the sample matrix, making them **difficult to extract and detect** using traditional automated techniques such as SPME.

SPME Arrow-trap with multi-step enrichment (MSE) on Centri provides a larger volume of sorptive phase. Combined with the ability to take multiple extractions from the same vial to the same trap, this increases the amount of 1,4-dioxane extracted for detection.

► WORKFLOW:



► EXAMPLE DATASET:



► KEY ADVANTAGES:

- **Greater sensitivity:** The optimised trap design not only preconcentrates multiple extractions into $\sim 100 \mu\text{L}$ of vapour, but also allows a low split ratio of 10:1 to be used. The result is that a large portion of the sample is sent to the GC, allowing the detection of low ng/L levels of 1,4-dioxane as required.
- **Improved confidence in results:** The greater sensitivity leads to improved confidence in identification of trace-level compounds.
- **Improved throughput:** Full automation of the MSE workflow eliminates time-consuming manual operations such as those for solid-phase extraction (SPE) methods, and allows automated sample preparation in under an hour.

ENVIRONMENTAL

FOOD

BEVERAGES

FRAGRANCE

HEALTH

FORENSIC

GENERAL TOPICS



SPME Arrow-trap methodology provides excellent detection of 1,4-dioxane, as shown by the set of extracted ion chromatogram overlays for a set of spiked water samples (left). The resulting calibration plots (right) demonstrate very good linearity beyond both the US EPA Method 522 and German REACH regulatory levels.

For full details
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Application Note 282



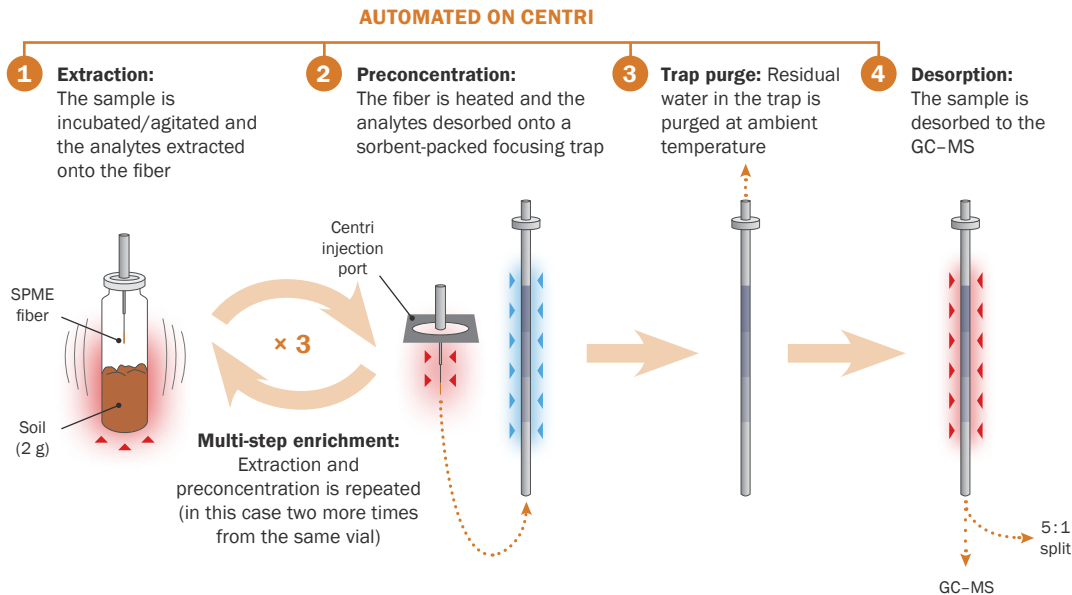
Understanding ecosystem health: Soil

► CHALLENGE:

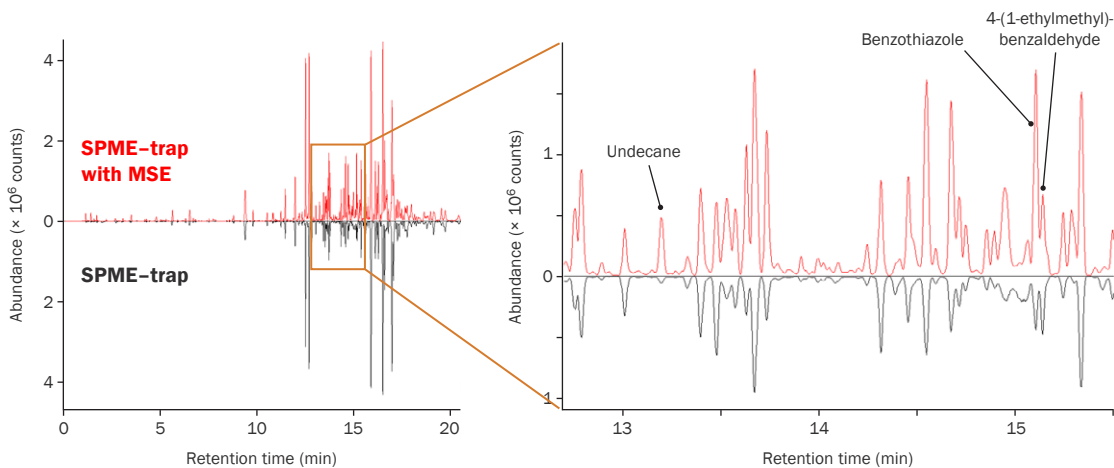
Developing a comprehensive understanding of soil health requires VOC extraction processes that are **efficient, untargeted** and **automated**.

SPME-trap on Centri provides these advantages, allowing compounds at both high and low concentrations to be monitored, with sensitivity boosted further by **multi-step enrichment (MSE)**.

► WORKFLOW:



► EXAMPLE DATASET:



► KEY ADVANTAGES:

- **Greater sensitivity:** The optimised trap design allows a very low split ratio of 5:1 to be used, allowing a large portion of the sample to be sent to the GC, and a consequent improvement in sensitivity.
- **More compounds discovered:** When multi-step enrichment was used, 112 more compounds were discovered.
- **Effective water management:** Selective elimination of water (while retaining analytes of interest) is aided by the use of hydrophobic sorbents in the focusing trap, and an ambient-temperature purge of residual water prior to trap desorption.
- **Greater confidence in identification:** The increased response for low-level compounds enables more confident identification.

In this SPME-trap analysis of soil volatiles, the number of compounds discovered increased from 544 with a single extraction step, to 656 when multi-step enrichment was used.

For full details
DOWNLOAD
Application Note 263



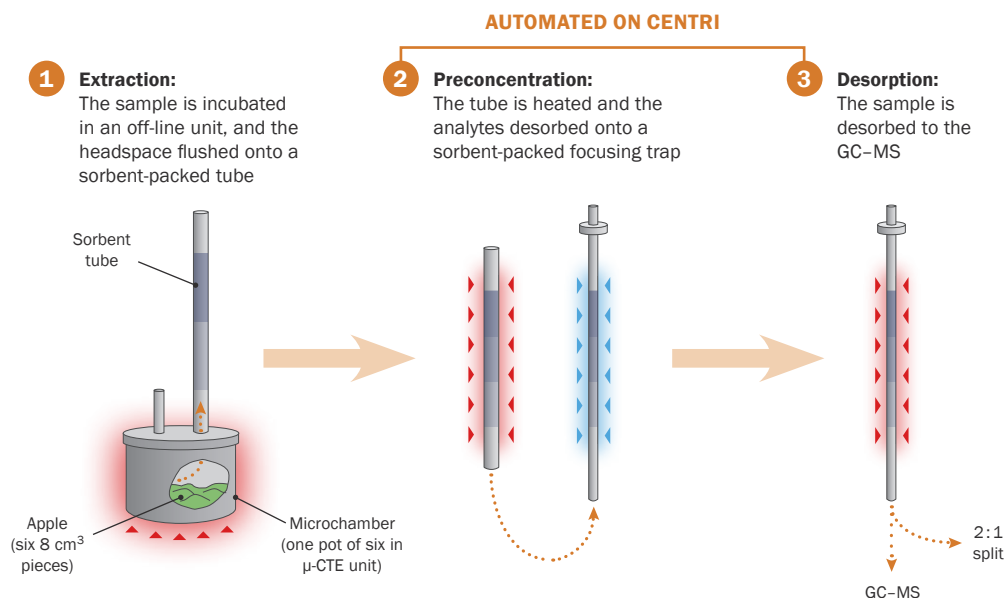
Comprehensive aroma profiling: Fruit

► CHALLENGE:

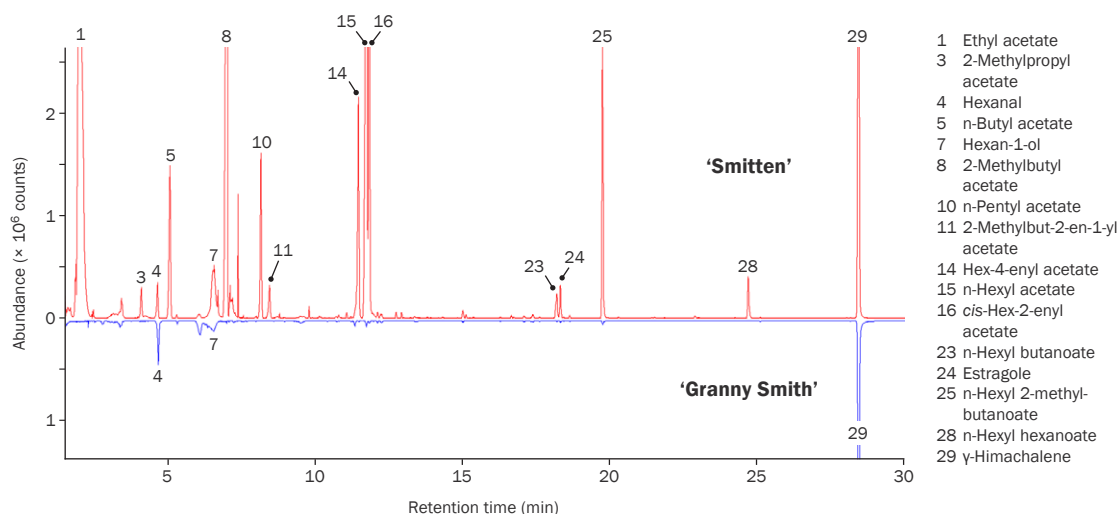
Routine control of food quality, research into extending shelf-life, and the development of new products all require **comprehensive aroma profiles** to be generated, in order that correlations can be made with human sensory analysis (such as olfactometry).

Dynamic headspace sampling onto sorbent tubes, with pre-concentration on Centri, results in the extraction of analytes spanning a broad concentration and volatility range.

► WORKFLOW:



► EXAMPLE DATASET:



► KEY ADVANTAGES:

- **Generation of comprehensive profiles:** Use of focusing traps containing multiple sorbent beds enables a wide volatility range of compounds to be efficiently retained and desorbed in a single analysis.
- **Greater sensitivity:** The optimised trap design allows a very low split ratio of 2:1 to be used, which means that a large portion of the sample can be sent to the GC, consequently improving the sensitivity.
- **Gaining insights into the data:** The comprehensive profiles produced enabled them to be correlated with consumer sensory analysis.

ENVIRONMENTAL

FOOD

BEVERAGES

FRAGRANCE

HEALTH

FORENSIC

GENERAL TOPICS



A wide range of volatiles were captured from fresh samples of two apple cultivars ('Smitten' and 'Granny Smith') using off-line headspace sample extraction, followed by automated analysis on Centri. Sampling at human body temperature (37°C) enhances the release of volatiles experienced by the consumer.



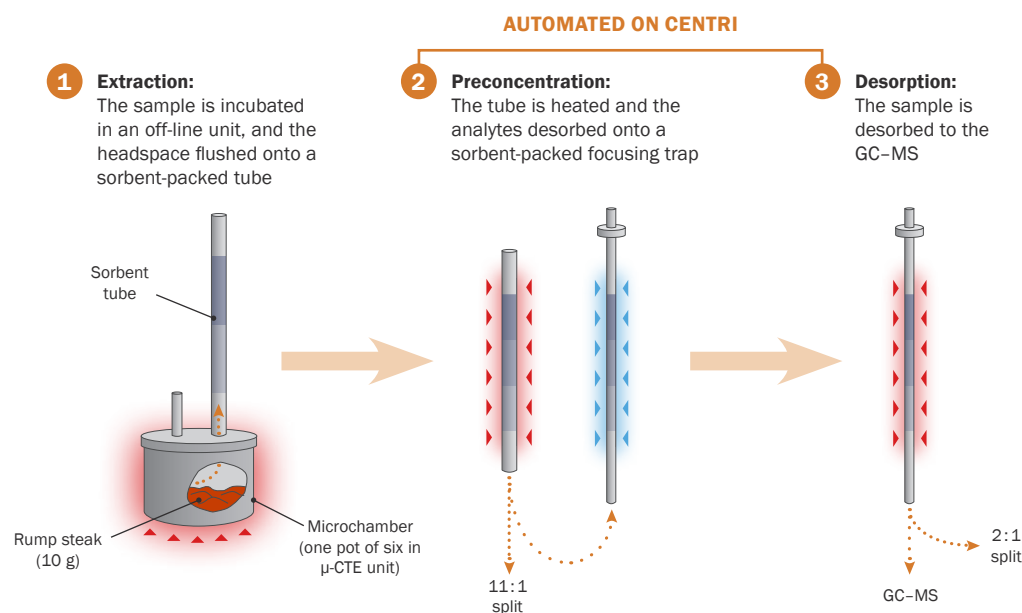
Comprehensive aroma profiling: Meat

► CHALLENGE:

Understanding the factors involved in consumer experience of cooked meat requires the monitoring of a **broad range** of VOCs and SVOCs from a variety of chemical classes.

Dynamic headspace sampling onto sorbent tubes, with trap-based focusing on Centri, results in the extraction of analytes spanning a broad concentration and volatility range.

► WORKFLOW:



ENVIRONMENTAL

FOOD

BEVERAGES

FRAGRANCE

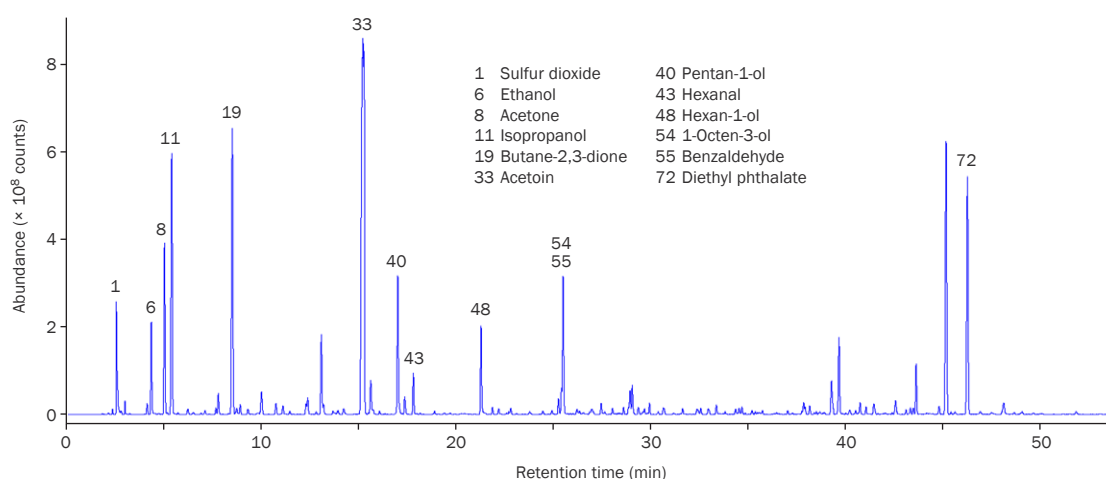
HEALTH

FORENSIC

GENERAL TOPICS



► EXAMPLE DATASET:



Compounds with a broad range of volatilities were found in rump steak, thanks to off-line headspace sample extraction onto tubes containing multiple sorbent beds. Automated analysis on Centri used a focusing trap packed with a similar sorbent mix.

► KEY ADVANTAGES:

- **Analyte range:** The multi-bed sorbent tubes used allow sampling of compounds spanning a wide volatility range (from acetaldehyde up to semi-volatile C_{16} species), to provide useful data that can be correlated to consumer sensory experience.
- **Greater sensitivity:** The optimised trap design allows a low split ratio to be used, allowing a large portion of the sample to be sent to the GC, and a consequent improvement in sensitivity.
- **Easy comparison:** Reproducible sampling and analysis enables meaningful comparison of different samples.



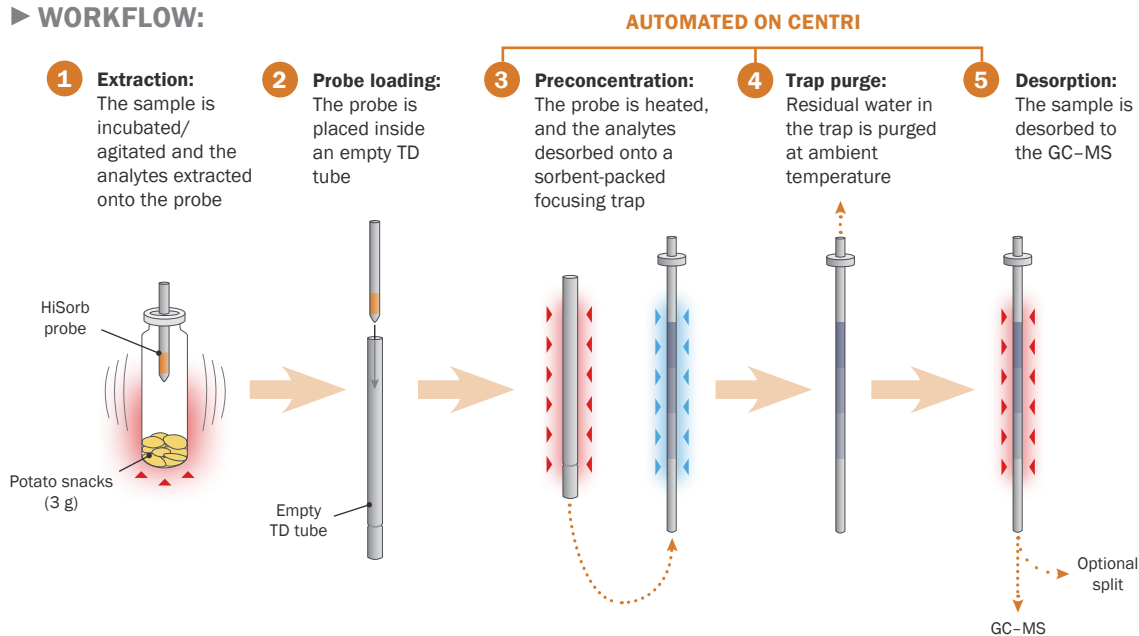
Comprehensive aroma profiling: Potato snacks

► CHALLENGE:

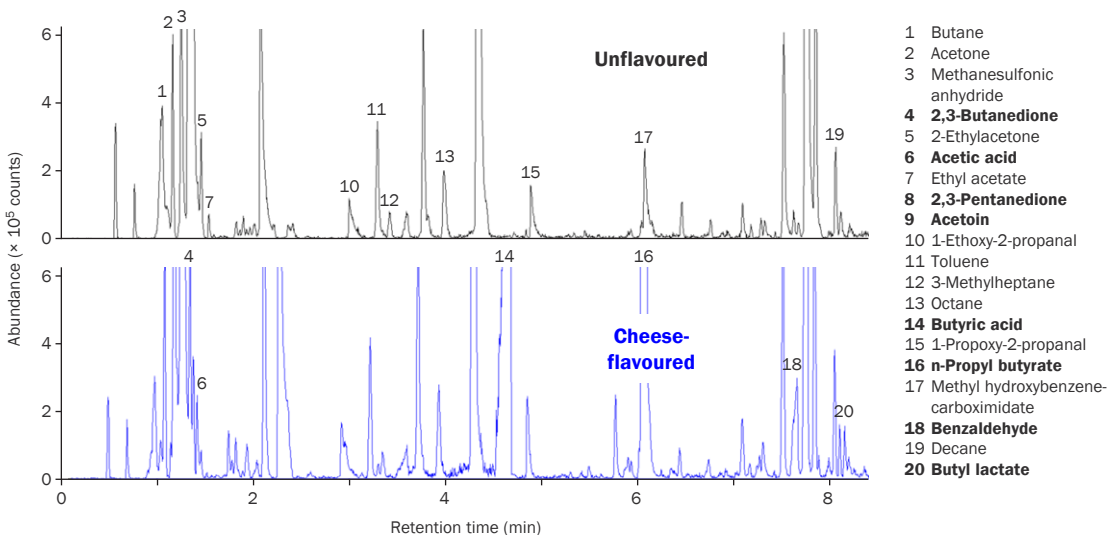
Comprehensive flavour profiling requires that a **wide range of unknown compounds** at varying concentrations is analysed simultaneously. Use of traditional techniques such as SPME risks missing low-abundance but organoleptically important compounds, due to 'competition' with higher-concentration compounds on the small amount of sorptive phase.

High-capacity sorptive extraction probes solve this problem, by providing a larger volume of sorptive phase than SPME fibers, and so greater sensitivity.

► WORKFLOW:



► EXAMPLE DATASET:



Smaller and less abundant peaks are observed during flavour profiling of unflavoured potato snacks (top) compared with those that had cheese flavouring added (bottom). Compounds only present in the flavoured snacks are shown in bold, amongst which is butyric acid (#14), which gives them a cheesy flavour.

► KEY ADVANTAGES:

- **Improved analyte extraction:** The large phase volume on HiSorb probes allows them to extract a wider analyte concentration range than SPME fibers.
- **Comprehensive VOC profiling:** 20 compounds were recovered from flavoured potato snacks, including compounds with key flavour/aroma properties.
- **Simple sample preparation:** Samples are placed into conventional 20 mL vials and crimp-capped, with no liquid extraction step needed, ready for HiSorb extraction.
- **Options for any application:** With a range of phases and phase combinations, HiSorb probes are suitable for targeted and non-targeted analyses from most sample matrices.



Detecting residual solvents: Food packaging

ENVIRONMENTAL

FOOD

BEVERAGES

FRAGRANCE

HEALTH

FORENSIC

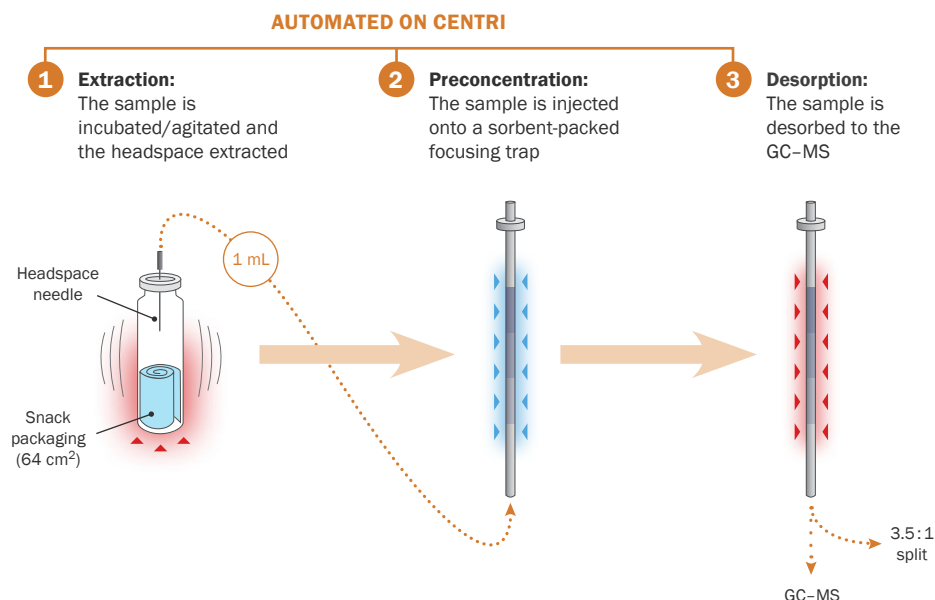
GENERAL TOPICS

► CHALLENGE:

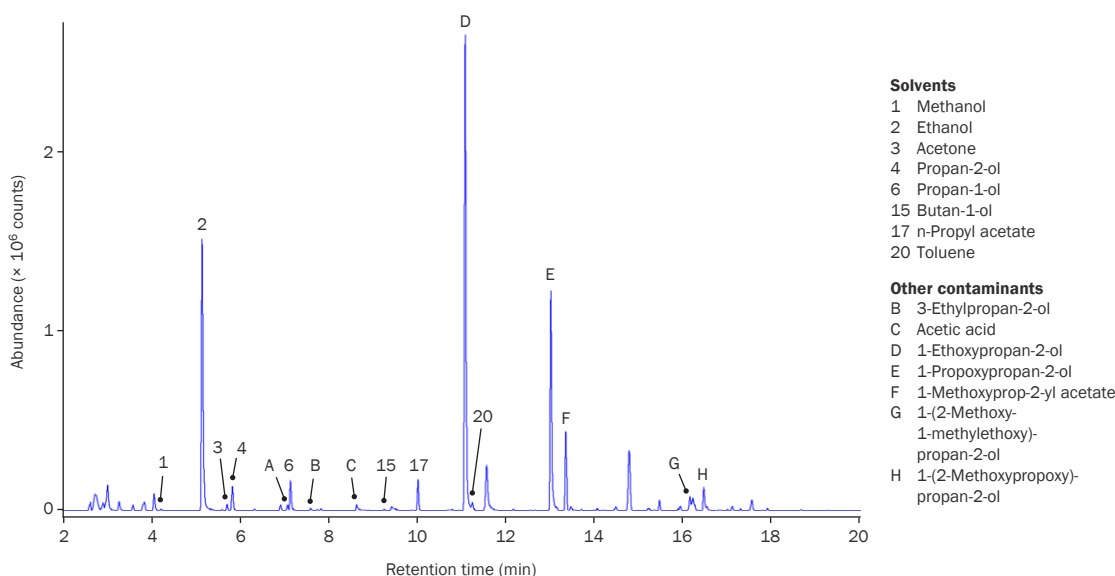
Customer complaints about off-odours and safety-driven regulations demand that residual chemicals in food packaging are monitored using **highly sensitive** analytical techniques.

Headspace-trap on Centri allows sub-ppb sensitivity to be achieved for residual solvents, monomers and additives in food packaging.

► WORKFLOW:



► EXAMPLE DATASET:



Using headspace-trap on Centri, ethanol was found to be the most significant component in a sample of food packaging, with concentrations of 1.92 mg/m², in addition to seven other solvents at trace levels.

► KEY ADVANTAGES:

- **Greater sensitivity:** The optimised trap design not only preconcentrates the 1 mL of headspace into ~100 μ L of vapour, but also allows a very low split ratio of 3.5 : 1 to be used. The result is that a large portion of the sample is sent to the GC, allowing the detection of sub-ppb levels of residual solvents.
- **Better chromatography:** The focusing step results in improved peak shapes (even with these low split ratios), particularly for early-eluting compounds, resulting in more confident identification.

For full details
DOWNLOAD
Application Note 252



Detecting food additives: Dried goods

ENVIRONMENTAL

FOOD

BEVERAGES

FRAGRANCE

HEALTH

FORENSIC

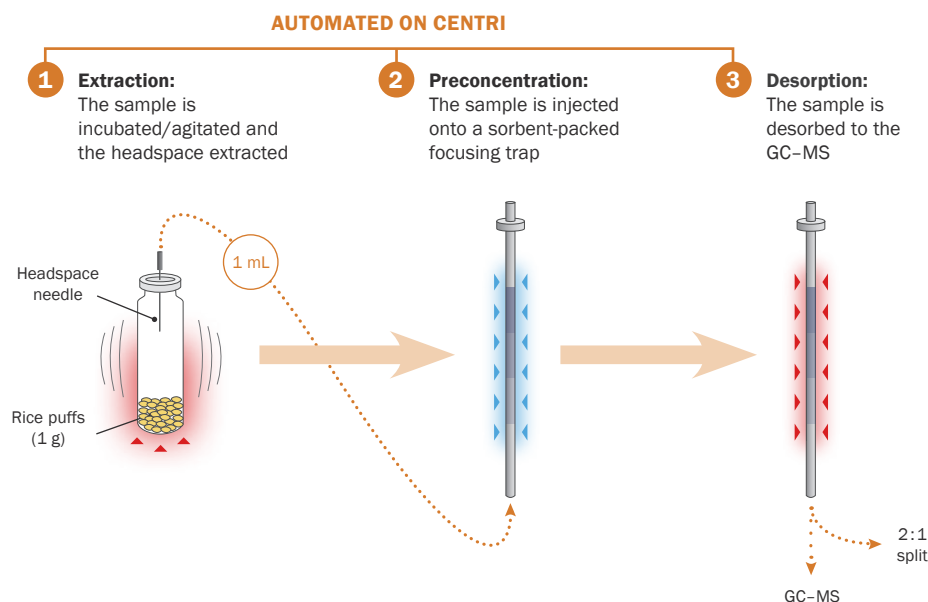
GENERAL TOPICS

► CHALLENGE:

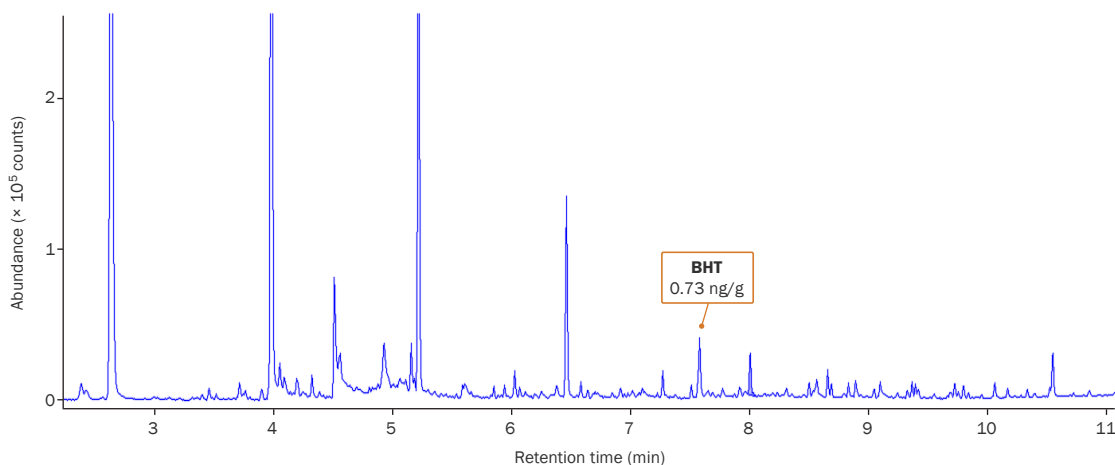
Uncertainties over the safety of the antioxidant butylated hydroxytoluene (BHT) call for analytical methods that can detect this additive at **trace levels**.

Headspace-trap on Centri allows sub-ppb sensitivity to be achieved within a fully automated workflow.

► WORKFLOW:



► EXAMPLE DATASET:



Using headspace-trap on Centri, sub-ppb concentrations of BHT were detected in a sample of rice puffs.

► KEY ADVANTAGES:

- **Greater sensitivity:** The optimised trap design not only preconcentrates the 1 mL of headspace into ~ 100 μL of vapour, but also allows a very low split ratio of 2:1 to be used. The result is that a large portion of the sample is sent to the GC, allowing the detection of sub-ppb levels of BHT.
- **Reduced sample waste:** The use of a low split ratio reduces the amount of sample that is wasted by being sent to the split line.
- **Better chromatography:** The focusing step results in improved peak shapes (even with these low split ratios), particularly for early-eluting compounds, resulting in more confident identification.

For full details
DOWNLOAD
Application Note 251



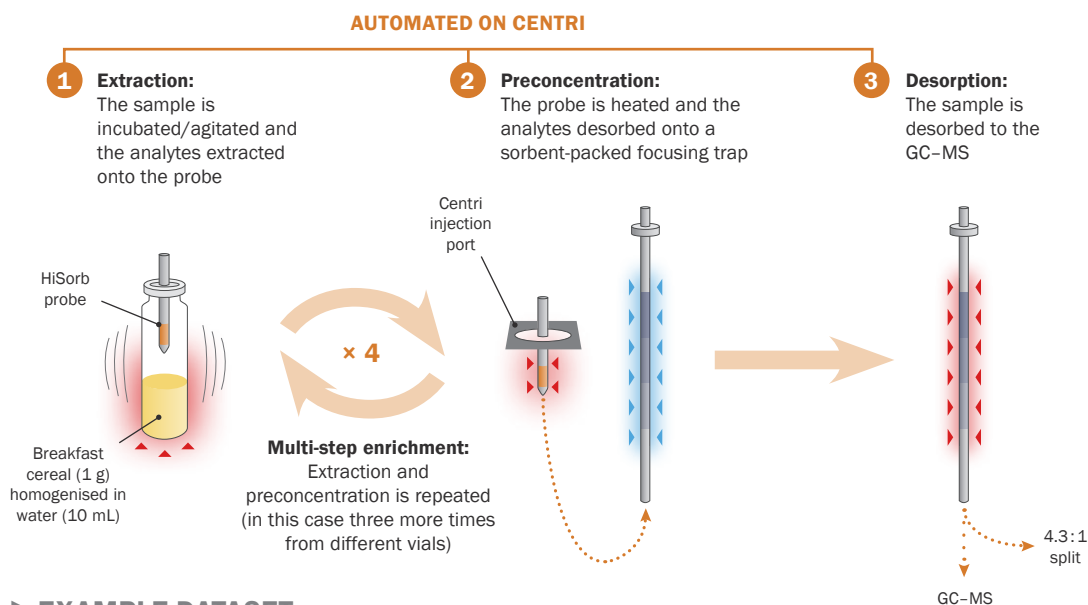
Monitoring safety and quality: Dried goods

► CHALLENGE:

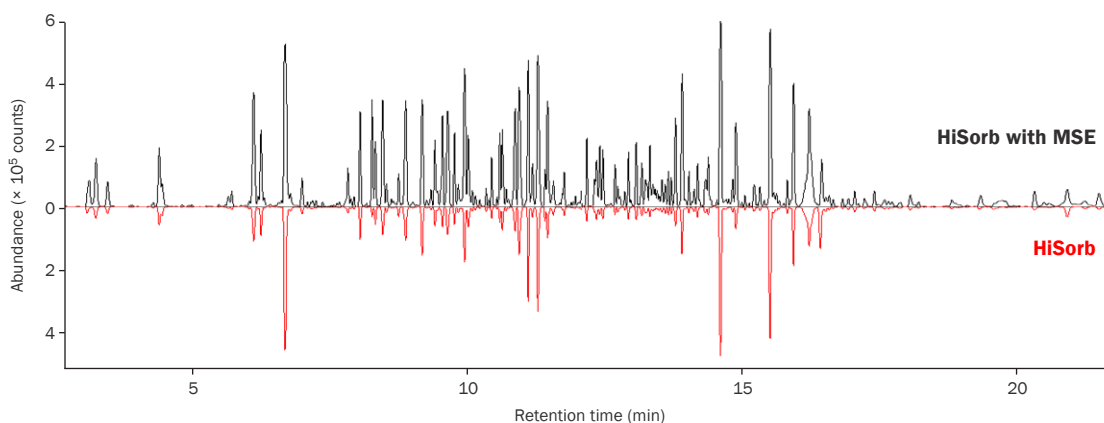
Monitoring food safety and quality requires a detailed understanding of individual components, but the conventional SPME approach is **insufficiently sensitive**, and suffers from the **fragility of the fibers**.

High-capacity sorptive extraction on Centri addresses both issues. A larger volume of sorptive phase, coupled with **multi-step enrichment (MSE)**, improves sensitivity, while a robust metal-core probe avoids the problem of fiber breakage.

► WORKFLOW:



► EXAMPLE DATASET:



► KEY ADVANTAGES:

■ Improved sensitivity:

- A larger volume of sorptive phase compared to a SPME fiber allows more of each analyte to be extracted.
- Multi-step enrichment onto the same focusing trap improves sensitivity further, without sacrificing chromatographic performance, and while maintaining excellent linearity and reproducibility.

■ Generation of comprehensive profiles:

Use of focusing traps containing multiple sorbent beds enables a wide volatility range of compounds to be efficiently retained and desorbed in a single analysis.

■ Improved reliability and productivity:

Operations are streamlined thanks to the robustness of HiSorb probes, and the ease of automation on Centri.

ENVIRONMENTAL

FOOD

BEVERAGES

FRAGRANCE

HEALTH

FORENSIC

GENERAL TOPICS



Multi-step enrichment enhances sensitivity for a wide range of VOCs and SVOCs in a breakfast cereal suspension, using headspace HiSorb probes automated on Centri.



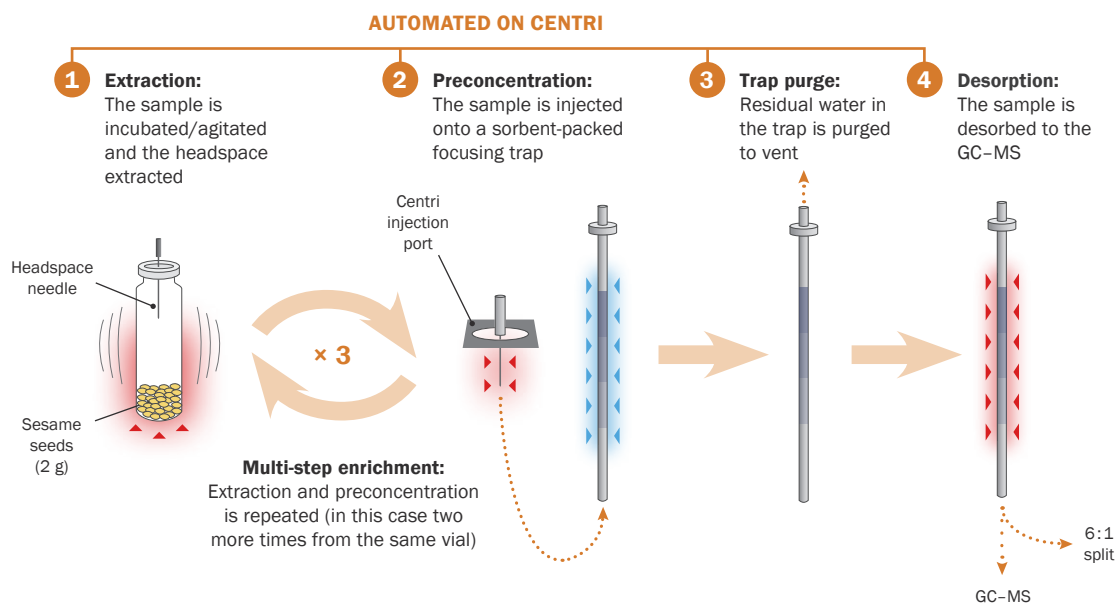
Detecting residual fumigants: Seeds

► CHALLENGE:

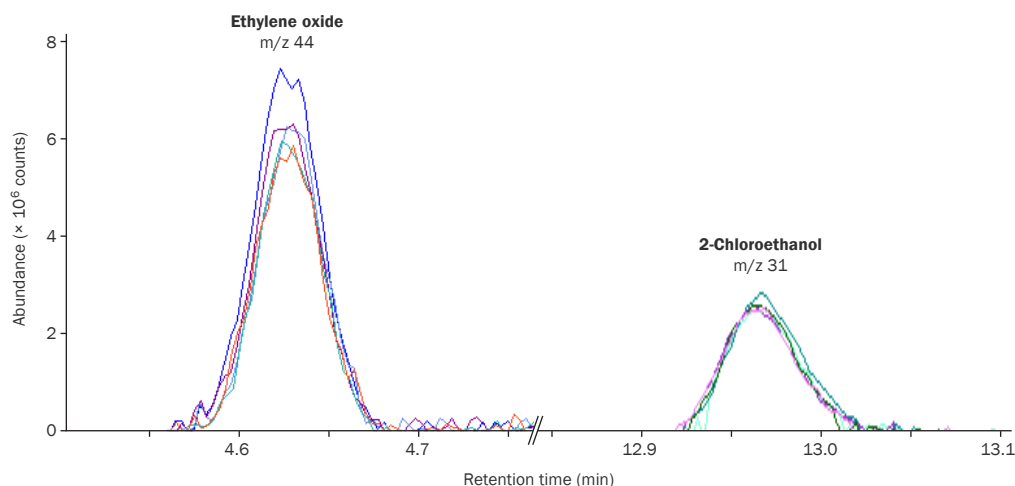
Residual chemicals present in seeds and other agricultural products as a result of fumigation (to eliminate pests) are a concern to human health due to their toxicity, and **safety-driven regulations** demand that they are monitored.

Headspace-trap with multi-step enrichment (MSE) on Centri allows low-ppb sensitivity to be achieved for the simultaneous analysis of residual ethylene oxide and its by-product 2-chloroethanol in sesame seeds.

► WORKFLOW:



► EXAMPLE DATASET:



► KEY ADVANTAGES:

- **Greater sensitivity:** The optimised trap design not only preconcentrates multiple (three) 5 mL headspace extractions into ~ 100 μ L of vapour, but also allows a low split ratio of 6:1 to be used. The result is that a large portion of the sample is sent to the GC, allowing the detection of low-ppb levels of residual fumigants.
- **Better chromatography:** The focusing step results in improved peak shapes (even with low split ratios) particularly for early-eluting volatile compounds like ethylene oxide, resulting in confident identification and improved sensitivity.
- **Wide analyte range:** Use of focusing traps containing multiple sorbent beds enables a wide volatility range of compounds to be efficiently retained and desorbed in a single analysis.

ENVIRONMENTAL

FOOD

BEVERAGES

FRAGRANCE

HEALTH

FORENSIC

GENERAL TOPICS



Excellent reproducibility for the HS-trap methodology is demonstrated by this pair of EIC overlays for five replicate samples, spiked with ethylene oxide and 2-chloroethanol at the maximum residue limit of 0.05 mg/kg, as defined by the EU Reference Laboratories' single residue method.

For full details
DOWNLOAD
Application Note 281



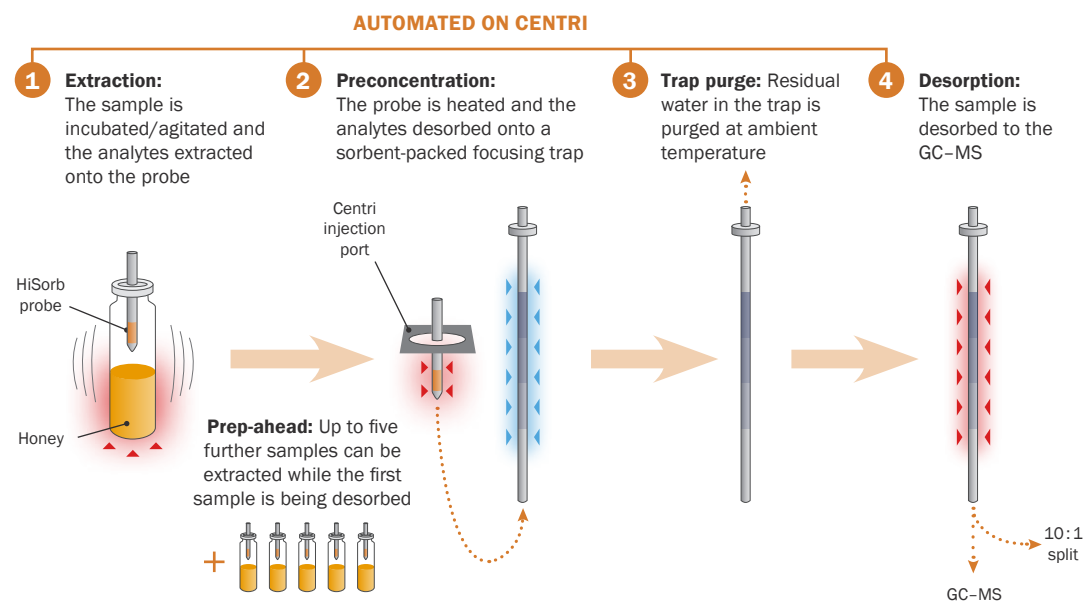
Discovering authenticity markers: Honey

► CHALLENGE:

Honey is prone to food fraud, but current methods, such as pollen analysis, are **time-consuming** and **laborious**. Even methods such as solid-phase microextraction (SPME) can be **insufficiently sensitive** and suffer from the **fragility of the fibers**.

Multi-phase high-capacity sorptive extraction on Centri addresses all these issues, with a larger volume of sorptive phase to extract a wide range of VOCs, and a robust metal-core probe to avoid the problem of fiber breakage. The result is therefore a robust, quick and automated method for discriminating components and prove sample authenticity.

► WORKFLOW:



ENVIRONMENTAL

FOOD

BEVERAGES

FRAGRANCE

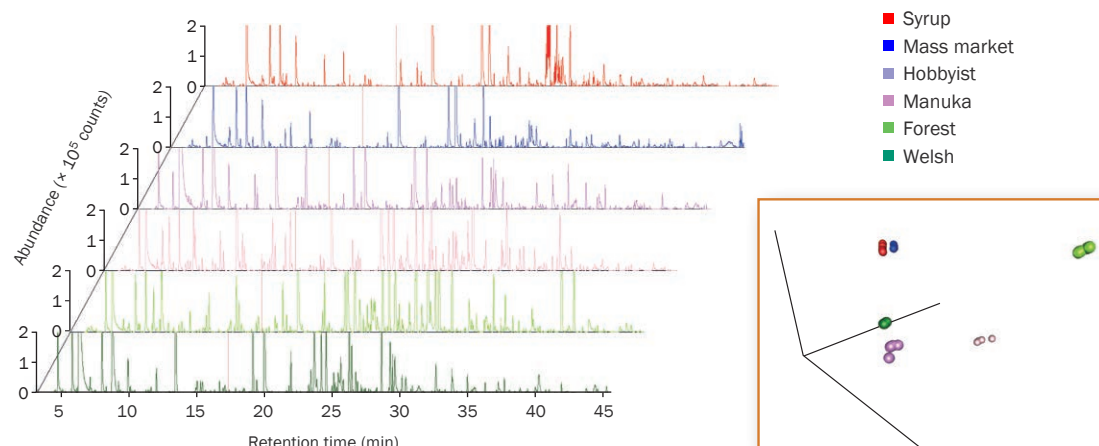
HEALTH

FORENSIC

GENERAL TOPICS



► EXAMPLE DATASET:



► KEY ADVANTAGES:

- **Greater sensitivity:** Probes have more sorptive phase than SPME fibers, resulting in more efficient extraction of low-level and key aroma-active compounds.
- **Comprehensive profiles:** Focusing traps containing multiple sorbent beds enable a wide volatility range of compounds to be efficiently retained and desorbed in a single analysis.
- **Improved reliability and productivity:** Operations are streamlined thanks to the robustness of HiSorb probes, and the ease of automation on Centri.
- **Data insights:** Automated statistical analysis of the data generated using ChromCompare+ (SepSolve Analytical) enables rapid discrimination of honey varieties.

Complex aroma profiles were generated by HiSorb extraction for six honey varieties, and the 79 compounds found overall were screened for automated data-mining using ChromCompare+. This enabled easy separation of the different varieties using a principal components analysis score plot (inset).

For full details
DOWNLOAD
Application Note 275



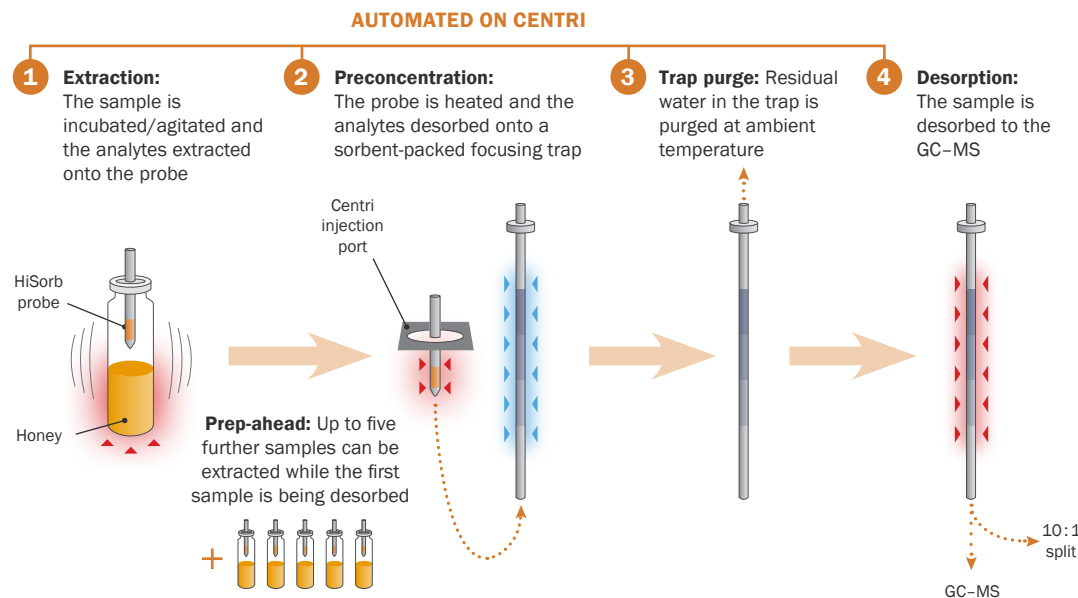
Evaluating sorptive phase combinations: Honey

► CHALLENGE:

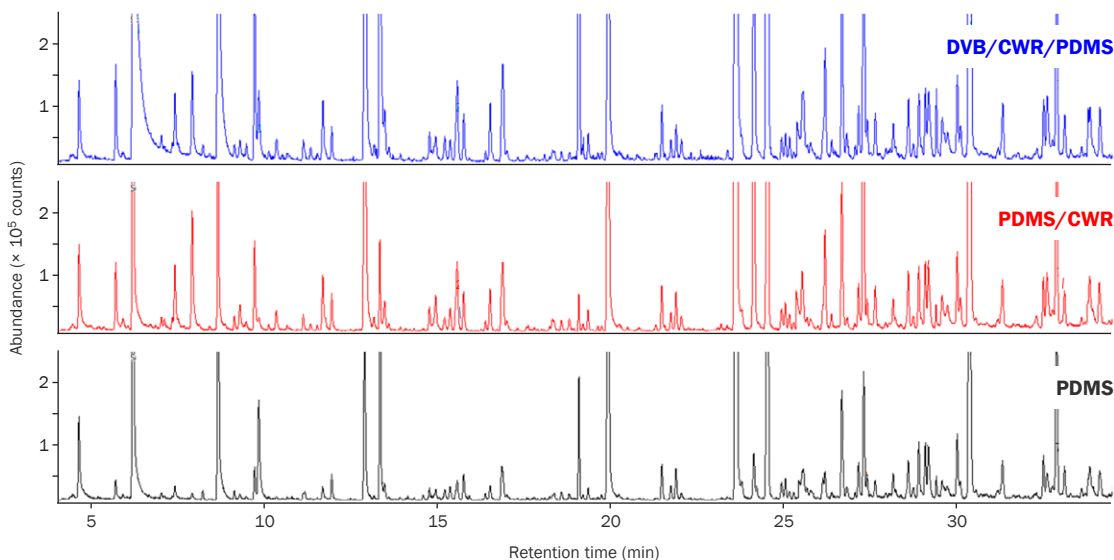
Polydimethylsiloxane (PDMS) is a widely used sorptive phase owing to its broad analyte range. However, it is **less efficient** at extracting more volatile and/or polar compounds.

Including **additional phase types** on **high-capacity sorptive extraction** probes can extend the range of analytes recovered.

► WORKFLOW:



► EXAMPLE DATASET:



► KEY ADVANTAGES:

- **Comprehensive organoleptic profiling:** 92 compounds were recovered from forest honey using DVB/CWR/PDMS, including compounds with key flavour/aroma properties.
- **Wide analyte range:** Use of focusing traps containing multiple sorbent beds enables a wide volatility range of compounds to be efficiently retained and desorbed in a single analysis.
- **Improved sensitivity:** The large phase volume and surface area of the probes (compared to SPME) improved the extraction efficiency of low-level components.
- **Options to suit any application:** With a selection of phase combinations available, HiSorb probes are suitable for targeted and non-targeted analyses from most sample matrices.

Larger and more abundant peaks are observed during flavour profiling of forest honey when carbon wide-range (CWR), or CWR and divinylbenzene (DVB), are used in addition to PDMS for extraction onto HiSorb probes, than with PDMS alone.

For full details
DOWNLOAD
Application Note 279



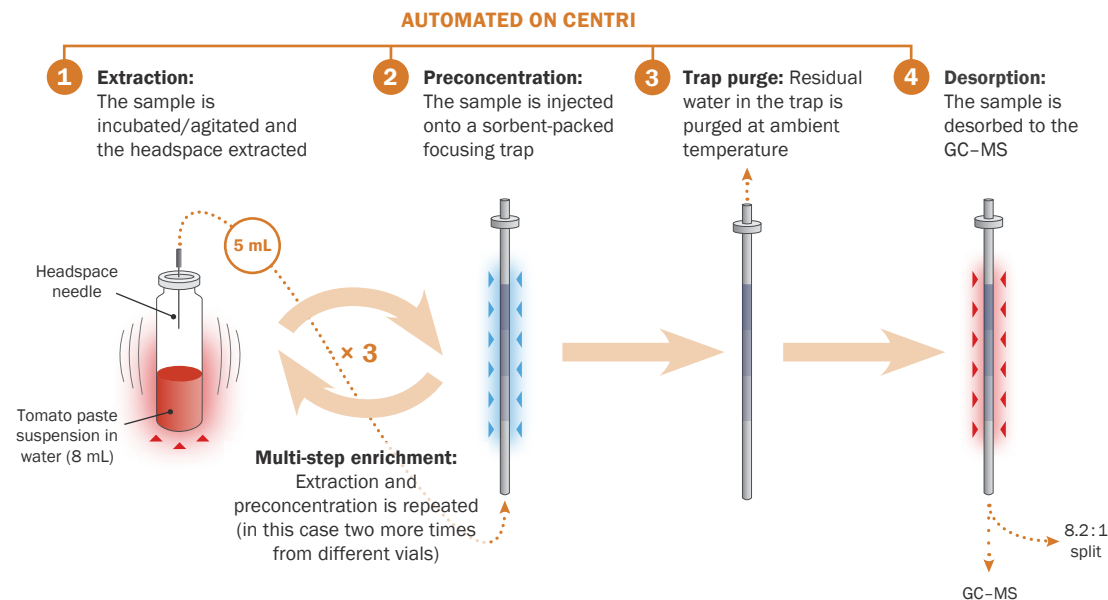
Improving the sensitivity of headspace: Food concentrate

► CHALLENGE:

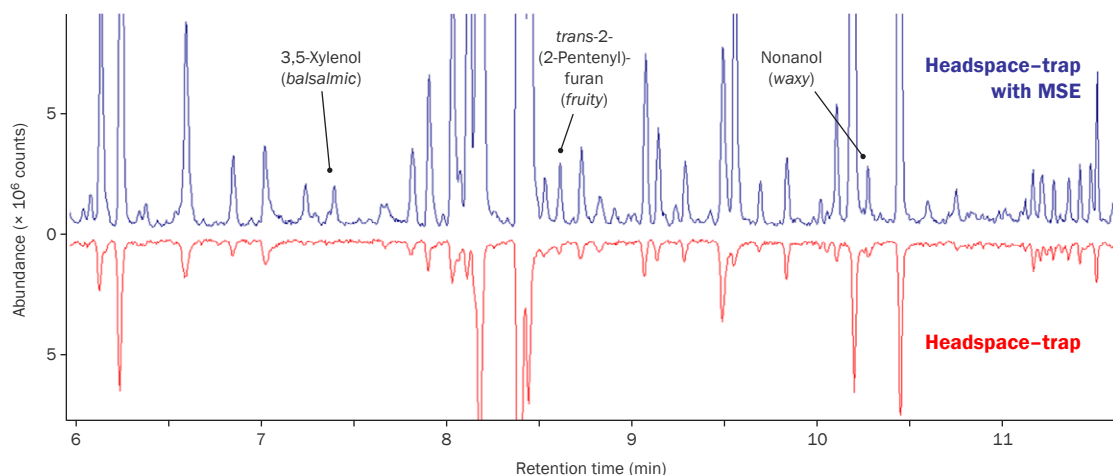
Direct headspace extraction is a popular technique for food analysis, but **extraction volumes** are typically limited to 1 mL, because larger volumes lead to poor chromatography.

Headspace-trap on Centri enhances sensitivity by allowing large volumes of headspace (up to 5 mL) to be preconcentrated, boosted further by **multi-step enrichment (MSE)**.

► WORKFLOW:



► EXAMPLE DATASET:



► KEY ADVANTAGES:

■ Improved sensitivity:

- Large-volume preconcentration on the trap improves sensitivity by allowing larger extraction volumes
- Multi-step enrichment onto the same focusing trap improves sensitivity further, without sacrificing chromatographic performance.

■ Improved confidence in results:

The greater sensitivity leads to the discovery of more compounds, and improved confidence in identification of trace-level compounds.

■ Effective water management:

Selective elimination of water (while retaining analytes of interest) is aided by the use of hydrophobic sorbents in the focusing trap, and an ambient-temperature purge of residual water prior to trap desorption.

ENVIRONMENTAL

FOOD

BEVERAGES

FRAGRANCE

HEALTH

FORENSIC

GENERAL TOPICS



The use of multi-step enrichment results in the detection of three additional flavour compounds in this tomato paste sample, compared to regular headspace-trap on Centri.

For full details
DOWNLOAD
Application Note 270



Detecting food contaminants: Food concentrate

ENVIRONMENTAL

FOOD

BEVERAGES

FRAGRANCE

HEALTH

FORENSIC

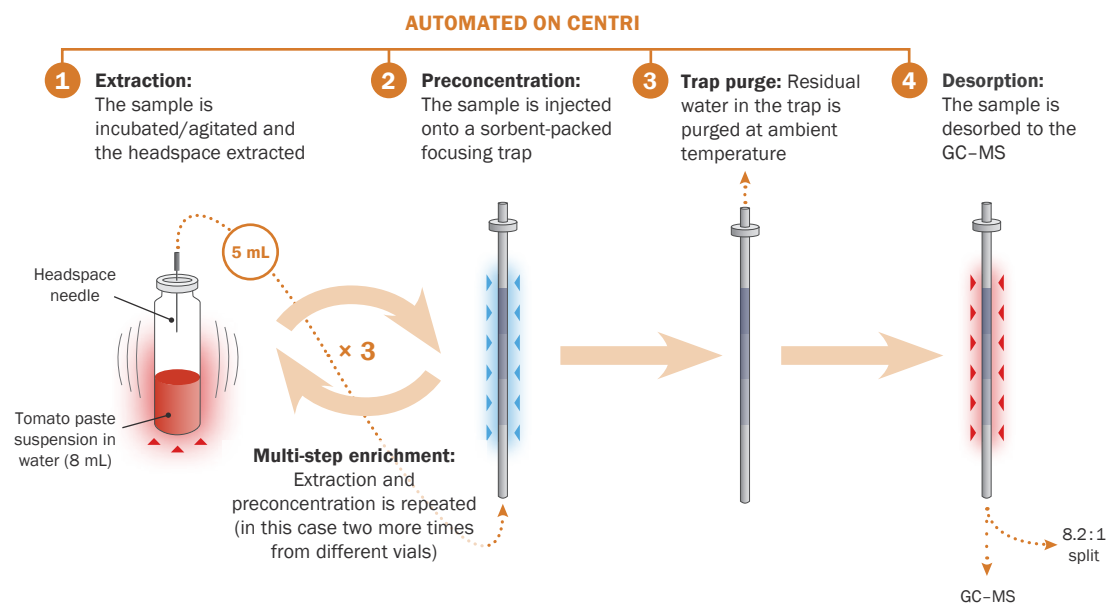
GENERAL TOPICS

► CHALLENGE:

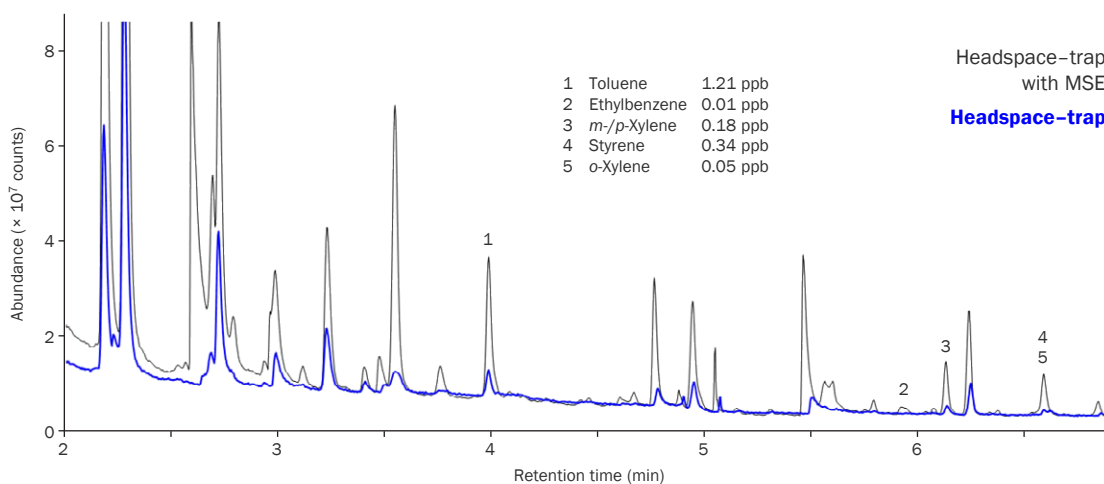
Direct headspace extraction is a popular technique for detecting contamination from residual benzene, toluene, ethylbenzene, xylenes and styrene (BTEXS) in food. But **extraction volumes** are typically limited to 1 mL, because larger volumes lead to water interference and poor chromatography.

Headspace-trap on Centri enhances sensitivity by allowing large volumes of headspace (up to 5 mL) to be preconcentrated, boosted further by **multi-step enrichment (MSE)**.

► WORKFLOW:



► EXAMPLE DATASET:



► KEY ADVANTAGES:

■ Improved sensitivity:

- Large-volume preconcentration on the trap improves sensitivity for BTEXS by allowing larger extraction volumes.
- Multi-step enrichment onto the same focusing trap improves sensitivity further (to sub-ppb levels), without sacrificing chromatographic performance, and while maintaining excellent linearity and reproducibility.

- **Effective water management:** Selective elimination of water (while retaining analytes of interest) is aided by the use of hydrophobic sorbents in the focusing trap, and an ambient-temperature purge of residual water prior to trap desorption.

The sensitivity for food contaminants of headspace-trap on Centri increases four-fold when using multi-step enrichment on this sample of tomato paste.

For full details
DOWNLOAD
Application Note 271



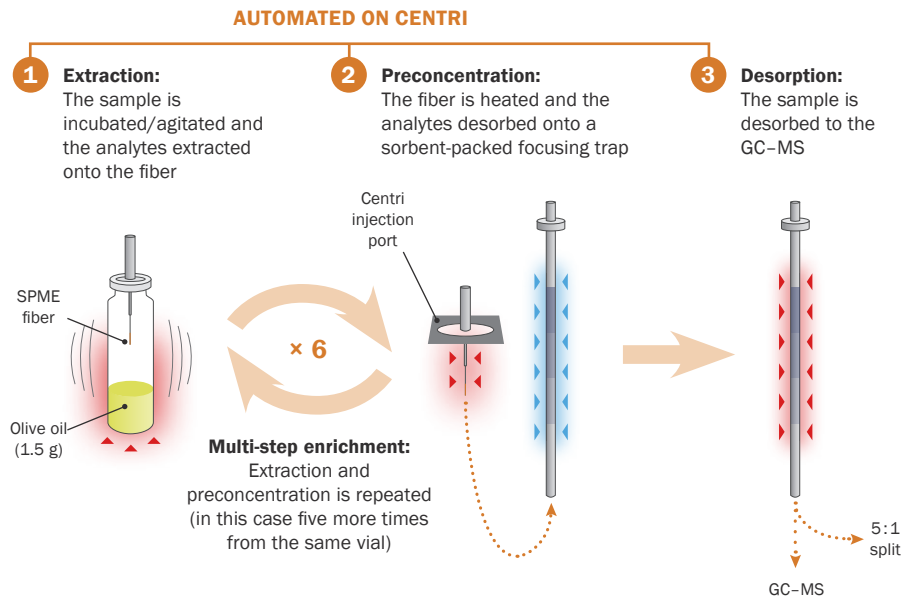
Enhancing the sensitivity of SPME: Oils

► CHALLENGE:

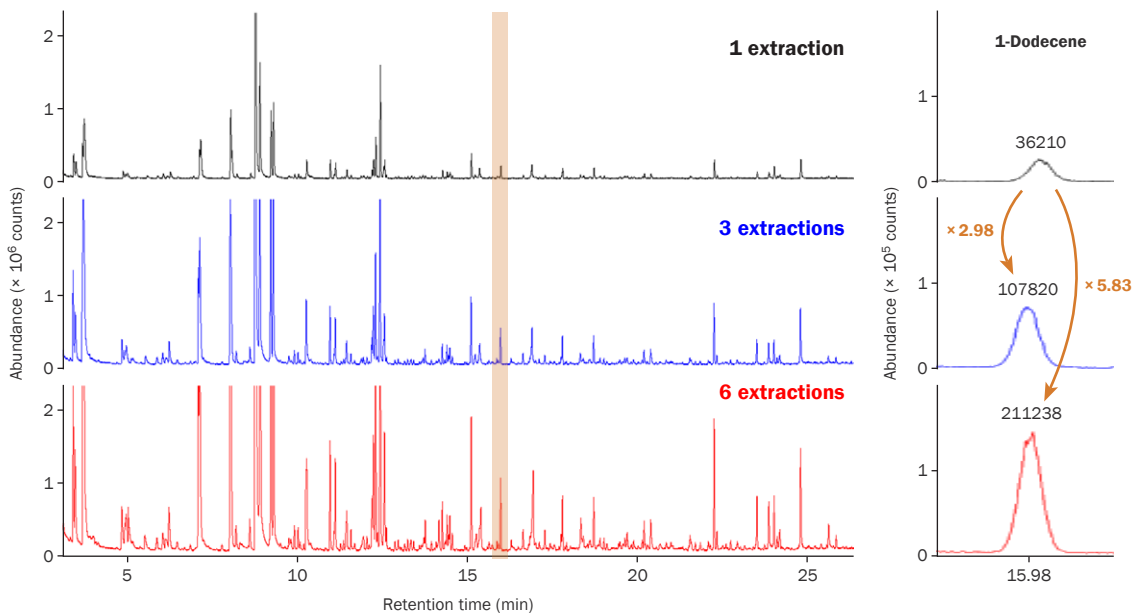
SPME is regularly used for analysis of foods (especially to check authenticity), but conventional ('direct') SPME sometimes suffers from **limited sensitivity**, due to the small volume of sorptive phase and the relatively slow heating rate of GC injection ports.

SPME-trap on Centri overcomes this problem using trap-based pre-concentration, with sensitivity enhanced further by **multi-step enrichment (MSE)**.

► WORKFLOW:



► EXAMPLE DATASET:



► KEY ADVANTAGES:

- **Improved sensitivity:** Multi-step enrichment onto the same focusing trap improves sensitivity, without sacrificing chromatographic performance, and while maintaining excellent linearity and reproducibility.
- **Improved confidence in results:** The greater sensitivity leads to the discovery of more compounds, and thus a more comprehensive profile.

Use of multi-step enrichment increases the sensitivity of this analysis by a factor that is proportional to the number of extractions, as illustrated for an olive oil sample with SPME-trap, automated on Centri.



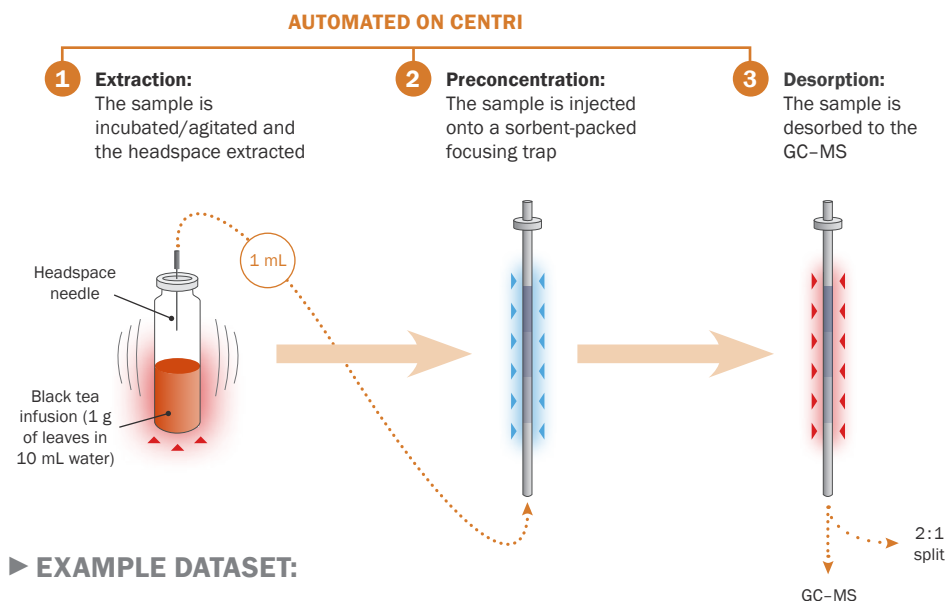
Detecting additives: Tea

► CHALLENGE:

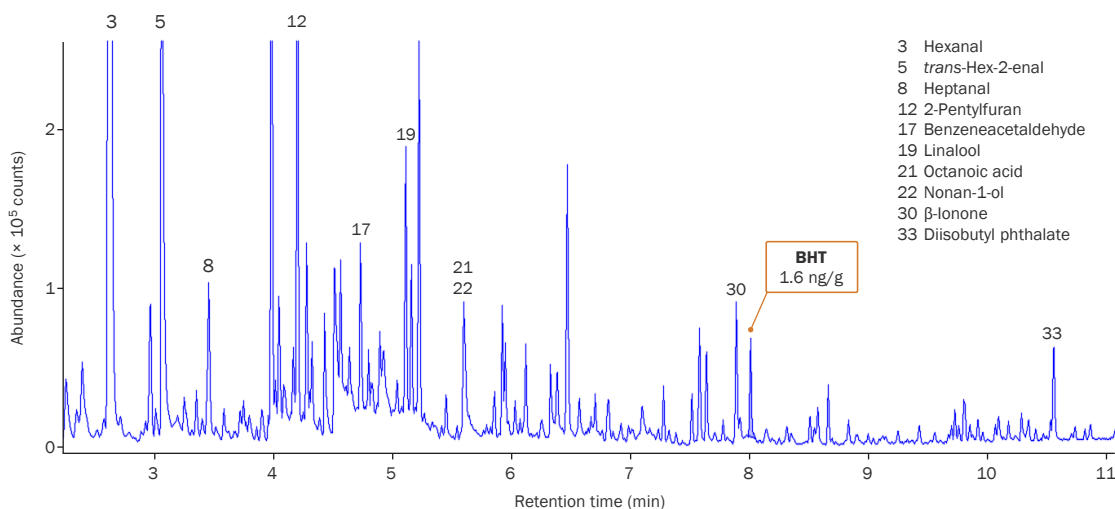
Uncertainties over the safety of the antioxidant butylated hydroxytoluene (BHT) call for analytical methods that can detect this additive at **trace levels**. At the same time, there is a need for more **automated methods** to replace time-consuming manual solid-phase extraction, which is widely used to monitor BHT in aqueous samples.

Headspace-trap on Centri overcomes both these issues, by allowing sub-ppb sensitivity to be achieved within a fully automated workflow.

► WORKFLOW:



► EXAMPLE DATASET:



► KEY ADVANTAGES:

- **Greater sensitivity:** The optimised trap design not only preconcentrates the 1 mL of headspace into ~100 μ L of vapour, but also allows a very low split ratio of 2:1 to be used. The result is that a large portion of the sample is sent to the GC, allowing the detection of sub-ppb levels of BHT.
- **Reduced sample waste:** The use of a low split ratio reduces the amount of sample that is wasted by being sent to the split line.
- **Better chromatography:** The focusing step results in improved peak shapes (even with these low split ratios), particularly for early-eluting compounds, resulting in more confident identification.

ENVIRONMENTAL

FOOD

BEVERAGES

FRAGRANCE

HEALTH

FORENSIC

GENERAL TOPICS



Using headspace-trap on Centri, sub-ppb concentrations of BHT were detected in a sample of black tea.



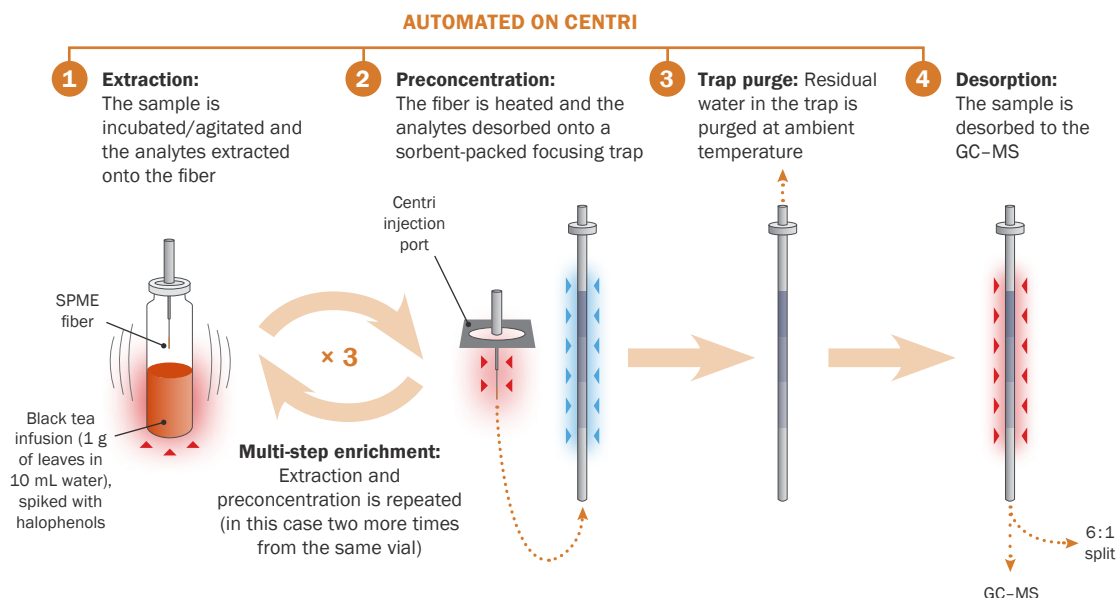
Comprehensive aroma profiling: Tea

► CHALLENGE:

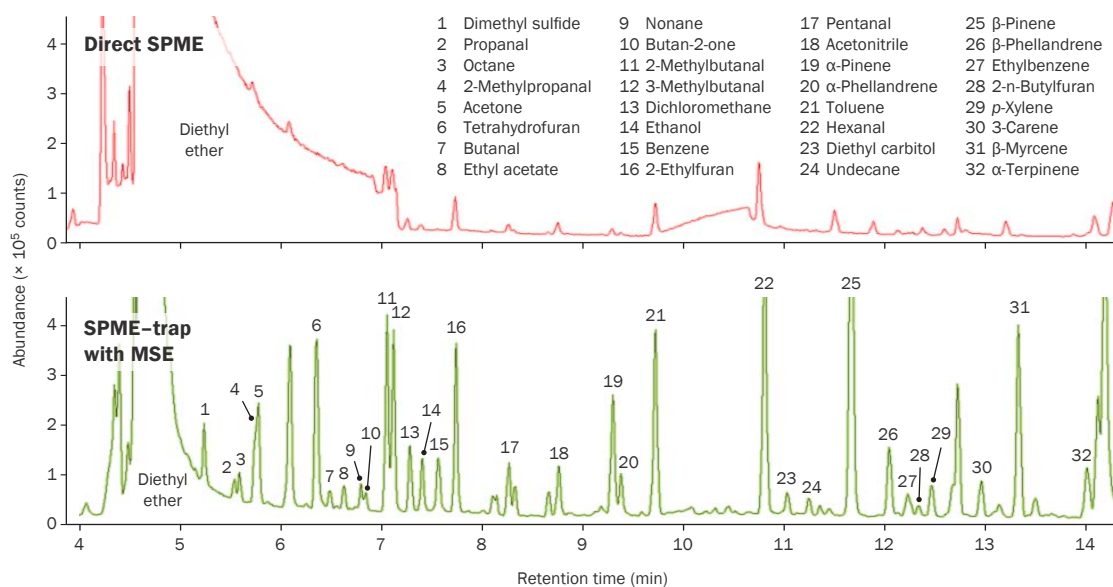
SPME is regularly used for analysis of beverages, but conventional ('direct') SPME sometimes suffers from **limited sensitivity**, due to the small volume of sorptive phase and the relatively slow heating rate of GC injection ports.

SPME-trap on Centri overcomes this problem using trap-based pre-concentration, with sensitivity enhanced further by **multi-step enrichment (MSE)**.

► WORKFLOW:



► EXAMPLE DATASET:



► KEY ADVANTAGES:

- Improved sensitivity:** Multi-step enrichment onto the same focusing trap improves sensitivity further, without sacrificing chromatographic performance, and while maintaining excellent linearity and reproducibility.
- Effective water management:** Selective elimination of water (while retaining analytes of interest) is aided by the use of hydrophobic sorbents in the focusing trap, and an ambient-temperature purge of residual water prior to trap desorption.

ENVIRONMENTAL

FOOD

BEVERAGES

FRAGRANCE

HEALTH

FORENSIC

GENERAL TOPICS

Significantly greater sensitivity is achieved for SPME extraction of tea aroma compounds by using trap-based preconcentration and multi-step enrichment. All operations are automated on Centri.

For full details
DOWNLOAD
 Application Note 268



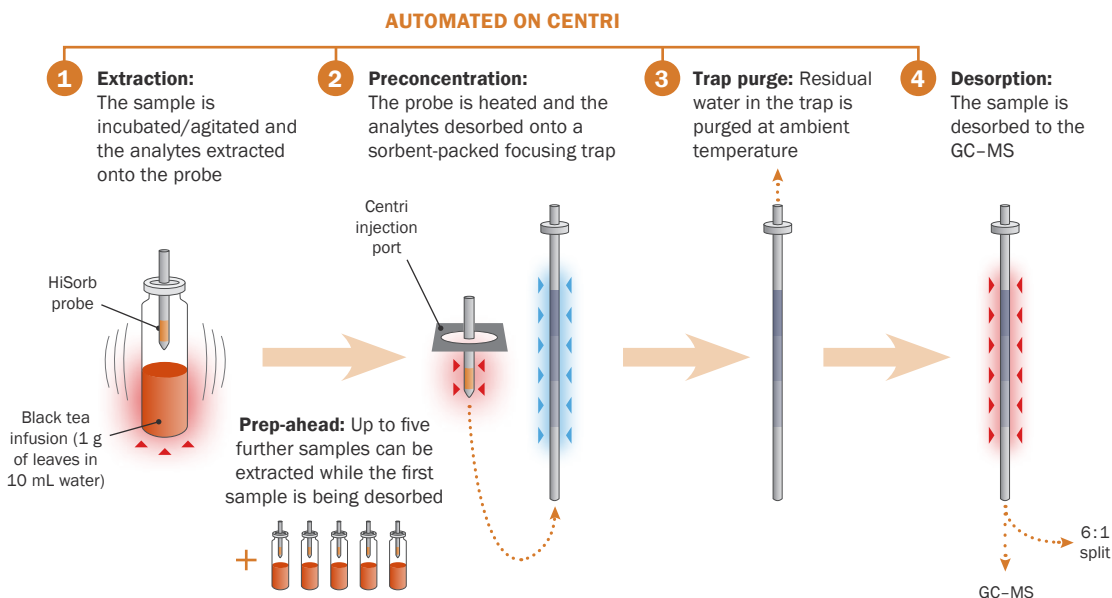
Comprehensive aroma profiling: Tea

► CHALLENGE:

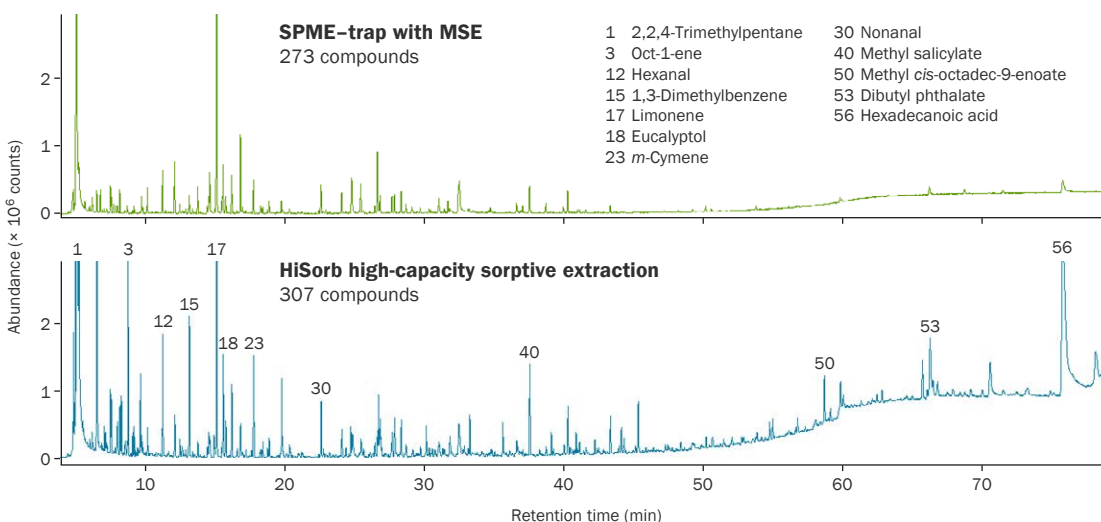
SPME is regularly used for analysis of beverages, but conventional ('direct') SPME sometimes suffers from **limited sensitivity, particularly for high-boiling compounds**.

High-capacity sorptive extraction on Centri addresses this by using a large volume of PDMS sorptive phase, resulting in more efficient extraction of low-level and polar compounds.

► WORKFLOW:



► EXAMPLE DATASET:



► KEY ADVANTAGES:

- **Greater sensitivity:** The high sorptive capacity of the PDMS phase, coupled with the large volume, results in more efficient extraction of low-level and polar analytes, including high-boiling compounds.
- **Improved productivity and reproducibility:** The 'prep-ahead' functionality of Centri allows multiple vials to be simultaneously extracted using multiple HiSorb probes, saving time and improving reproducibility.
- **Effective water management:** Selective elimination of water (while retaining analytes of interest) is aided by the use of hydrophobic sorbents in the focusing trap, and an ambient-temperature purge of residual water prior to trap desorption.

Use of HiSorb high-capacity sorptive extraction, automated on Centri, results in a large increase in the relative abundances of late-eluting compounds, compared to SPME methods.

For full details
DOWNLOAD
Application Note 268



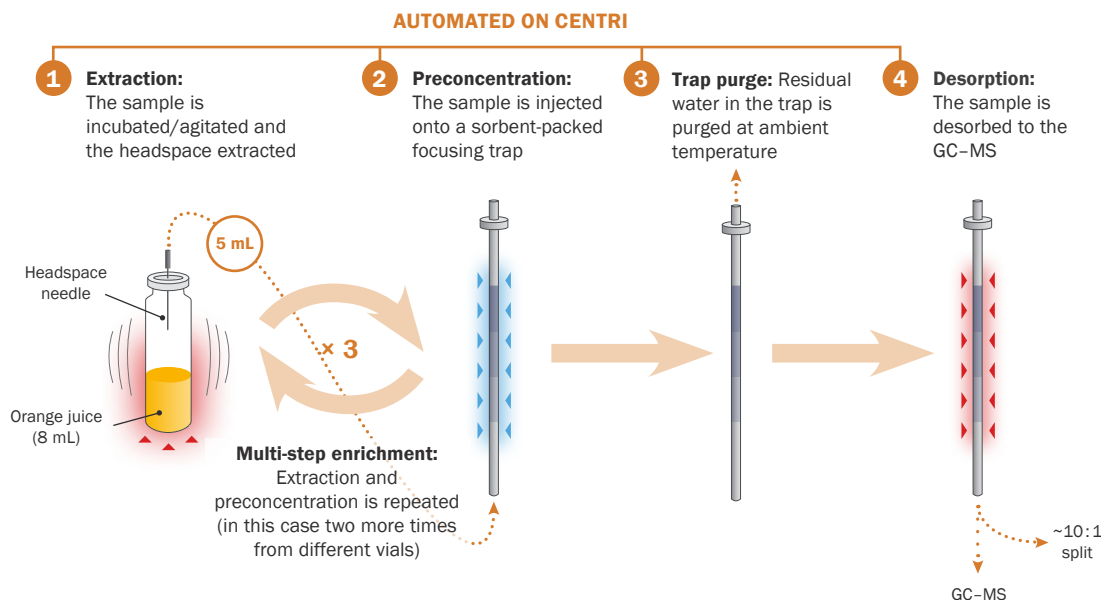
Enhancing the sensitivity of headspace: Fruit juice

► CHALLENGE:

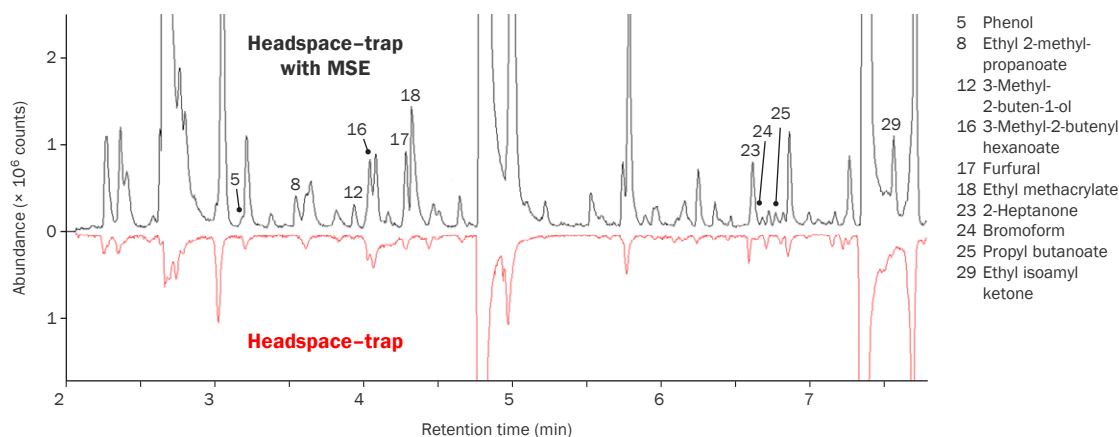
Direct headspace is widely used for aroma profiling of beverages, but the **small sample volumes** typically used mean that trace-level compounds with low odour thresholds may be missed.

Headspace-trap on Centri enhances sensitivity by allowing large volumes of headspace (up to 5 mL) to be pre-concentrated, boosted further by **multi-step enrichment (MSE)**.

► WORKFLOW:



► EXAMPLE DATASET:



Multi-step enrichment of a headspace-trap analysis on Centri results in the identification of more compounds in this sample of orange juice (labelled), compared to a single extraction.

► KEY ADVANTAGES:

- **Effective water management:** Selective elimination of water (while retaining analytes of interest) is aided by the use of hydrophobic sorbents in the focusing trap, and an ambient-temperature purge of residual water prior to trap desorption.
- **Improved sensitivity:**
 - Large-volume preconcentration improves sensitivity by focusing extraction volumes up to 5 mL on the trap, before being sent to the GC in a narrower band of vapour (~100 μ L).
 - Multi-step enrichment onto the same focusing trap improves sensitivity further, for detection of more compounds, without sacrificing chromatographic performance.
- **Increased productivity and reproducibility:** Full automation eliminates time-consuming and error-prone manual operations.

For full details
DOWNLOAD
Application Note 264



Streamlining extraction for low-level 'Brett' odorants: Wine

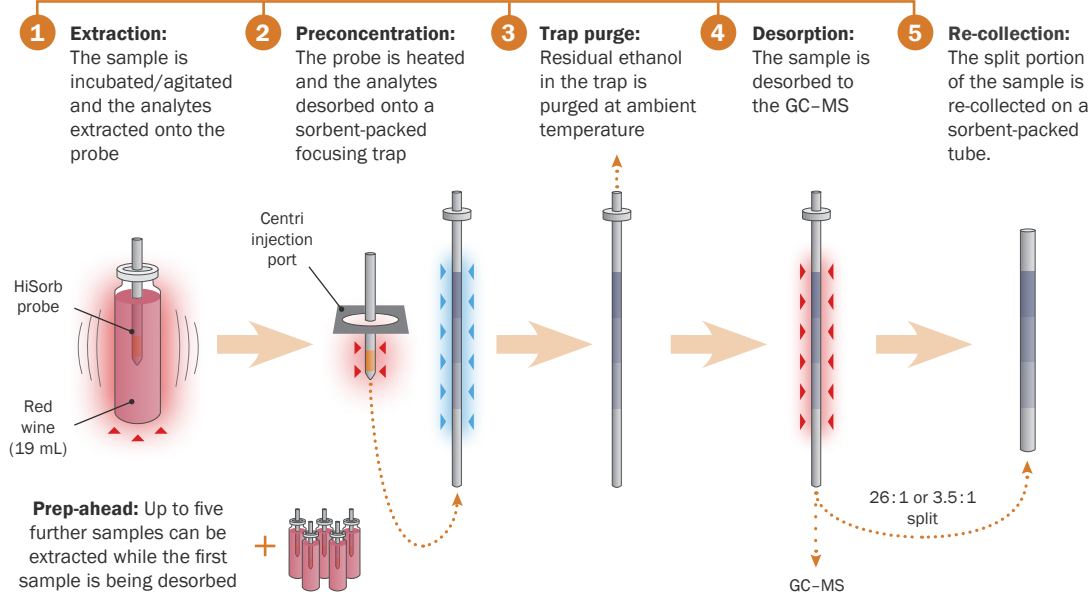
► CHALLENGE:

There is a need to improve upon **inefficient solvent-extraction methods** for identifying the unpleasant 'Brett' odorants 4-ethylphenol (4-EP) and 4-ethylguaiacol (4-EG) in wine.

High-capacity sorptive extraction on Centri greatly simplifies analytical workflows, by allowing fully automated, immersive extraction using a robust metal-core probe.

► WORKFLOW:

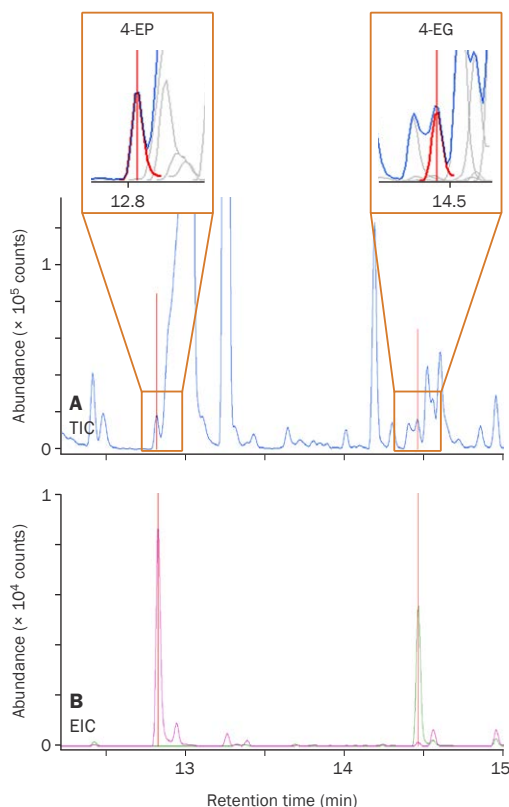
AUTOMATED ON CENTRI



► KEY ADVANTAGES:

- **Improved throughput:** Productivity is enhanced by full automation of sample extraction, washing/drying of probes, probe desorption and GC injection.
- **Elimination of ethanol:** The trap can be held at ambient temperature during probe desorption and trap purging, allowing ethanol to be selectively removed.
- **Generation of comprehensive profiles:** Immersive use of probes enables a wide volatility range of compounds to be extracted.
- **Improved sensitivity:**
 - The large volume of sorptive phase (65 μ L) provides more efficient extraction of low-level and polar compounds
 - Low-split (or splitless) operation allows a large portion of the sample to be sent to the GC.
- **Improved workflow options:** Re-collection of sample split flows for repeat analysis improves method development, sample archiving and method validation.

► EXAMPLE DATASET:



Detection of the 'Brett' odorants 4-EP and 4-EG below sensory threshold values is achieved using a combination of immersive high-capacity sorptive extraction and low split ratios. Re-collection of the sample allows automated re-analysis of the same sample with a different split ratio, allowing quantitation over a wide concentration range.

For full details
DOWNLOAD
Application Note 254



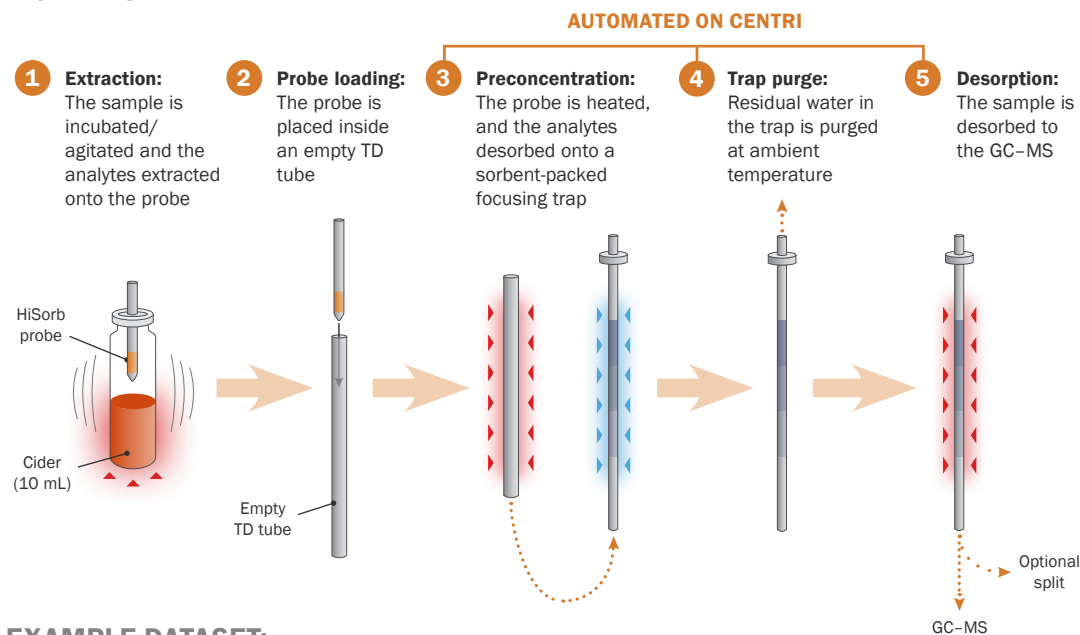
Comprehensive aroma profiling: Cider

► CHALLENGE:

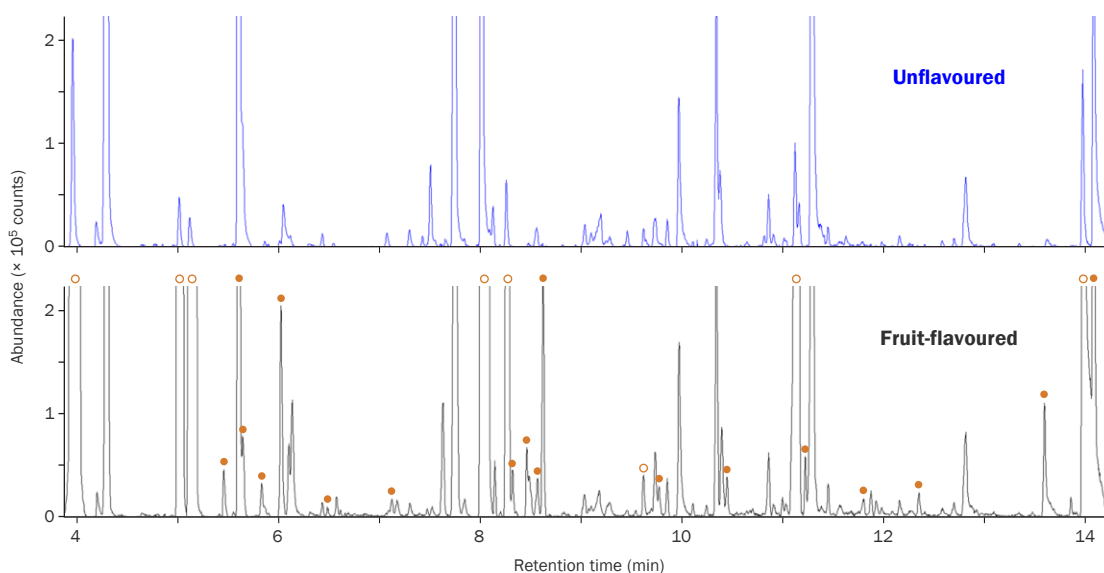
Determining a comprehensive flavour profile of beverages requires extraction processes that are **efficient and untargeted**, and the **simultaneous analysis** of compounds at varying concentrations.

High-capacity sorptive extraction addresses these challenges, by providing a large volume of sorptive phase for greater sensitivity over conventional techniques (such as SPME), and by using robust metal-core probes.

► WORKFLOW:



► EXAMPLE DATASET:



► KEY ADVANTAGES:

- **Large phase volume:** HiSorb probes support a large volume of sorptive phase (~65 μL), increasing sorptive capacity and therefore extraction efficiency relative to SPME.
- **Comprehensive VOC profiling:** 39 compounds were recovered from flavoured cider, including compounds with key flavour/aroma properties.
- **Options to suit any application:** With a selection of phases and phase combinations available, HiSorb probes are suitable for both targeted and non-targeted analyses from most sample matrices.

ENVIRONMENTAL

FOOD

BEVERAGES

FRAGRANCE

HEALTH

FORENSIC

GENERAL TOPICS



Smaller and less abundant peaks are observed during flavour profiling of unflavoured cider (top) compared with fruit-flavoured cider (bottom). Many esters were only identified in the flavoured product (●), or found in much higher abundance (○) compared to the unflavoured product, contributing fruity, sweet and citrus notes.

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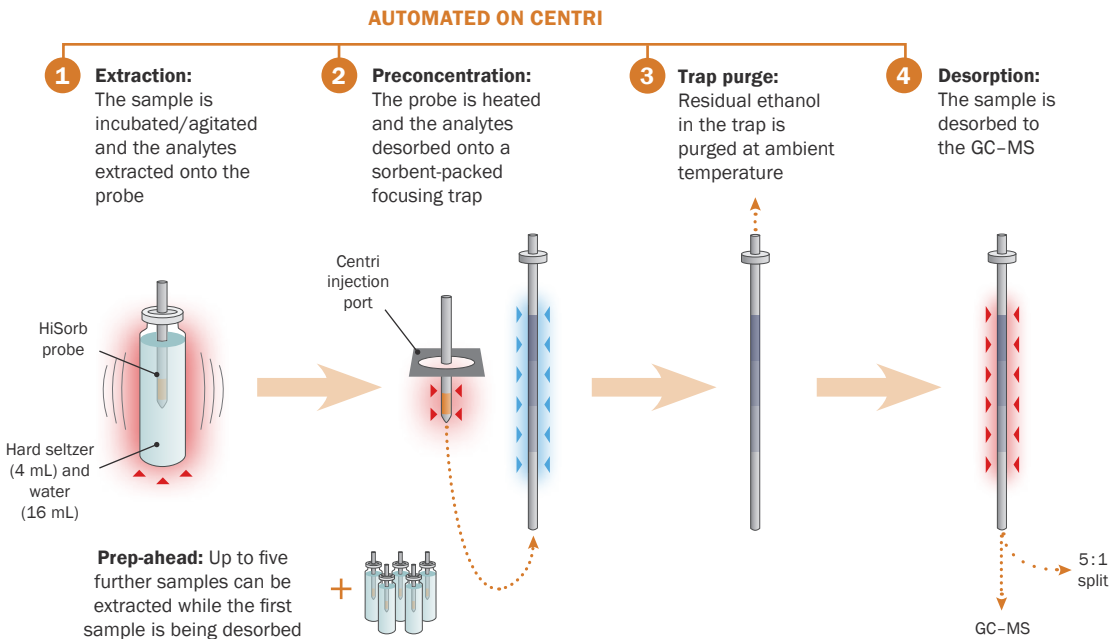
Evaluating sorptive phase combinations: Hard seltzers

► CHALLENGE:

Polydimethylsiloxane (PDMS) is a popular phase for sorptive extraction because of its ability to extract a wide range of compounds. However, PDMS alone has **limited extraction capacity** for certain groups of analytes.

High-capacity sorptive extraction probes with multiple phases show extraction of a wider range of analytes, with workflows fully automated on the Centri platform.

► WORKFLOW:



ENVIRONMENTAL

FOOD

BEVERAGES

FRAGRANCE

HEALTH

FORENSIC

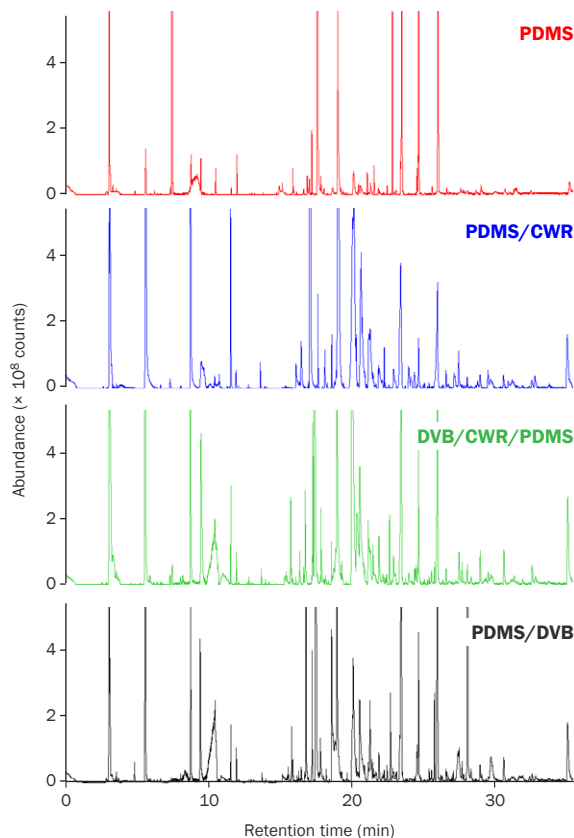
GENERAL TOPICS



► KEY ADVANTAGES:

- **More compounds discovered:** The use of additional phases allows enhanced extraction of more polar and more volatile analytes.
- **Improved sensitivity:** The large phase volume and surface area compared to methods such as SPME improves extraction efficiency of low-level components.
- **Reduced manual handling:** Automation reduces the amount of manual sample preparation required, improving reproducibility and reducing the risk of human error.
- **Generation of comprehensive profiles:** Use of focusing traps with multiple sorbent beds enables a wide range of compounds to be retained and desorbed in a single analysis.
- **Robust analysis and improved reliability:** The stainless-steel probe body provides enhanced robustness compared to SPME, eliminating the risk of breakage.

► EXAMPLE DATASET:



In this comparison of four sorbent combinations for extraction of flavour-active components from hard seltzers, PDMS/DVB (bottom) provided the best performance, and so was selected for further experimental work (see page 30).

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Application Note 277



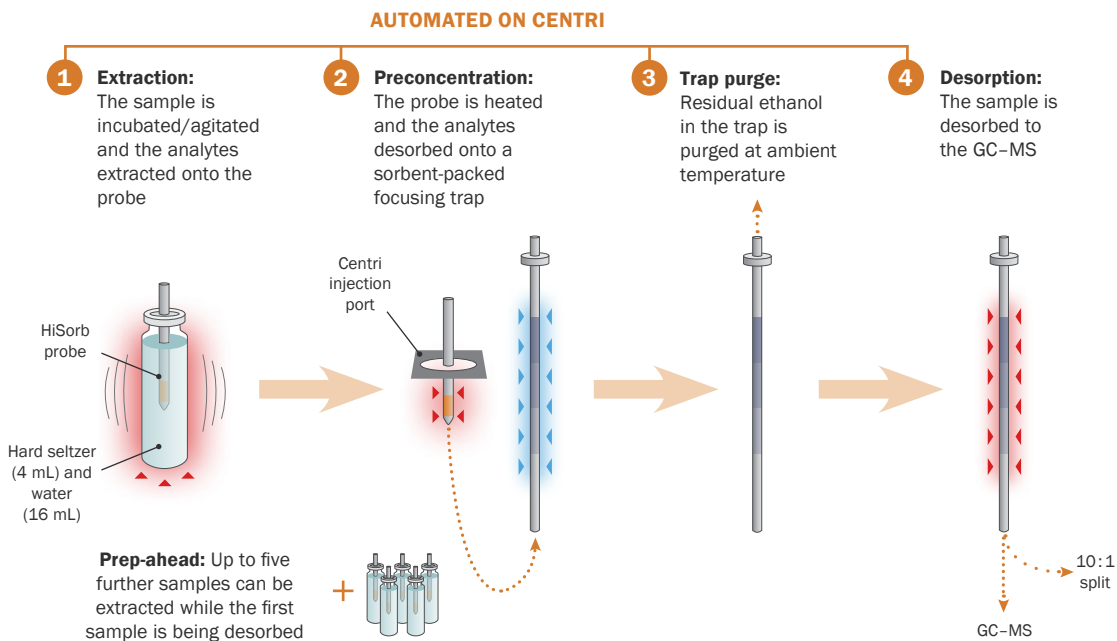
Comprehensive flavour profiling: Hard seltzers

► CHALLENGE:

Flavour profiling is vital for brand quality and authenticity, but flavour-active compounds can remain in the **liquid phase** when using headspace sampling, while immersive SPME sampling suffers from **fiber contamination and breakage**.

High-capacity sorptive extraction with HiSorb probes solves this problem, with a robust design that facilitates immersive sampling.

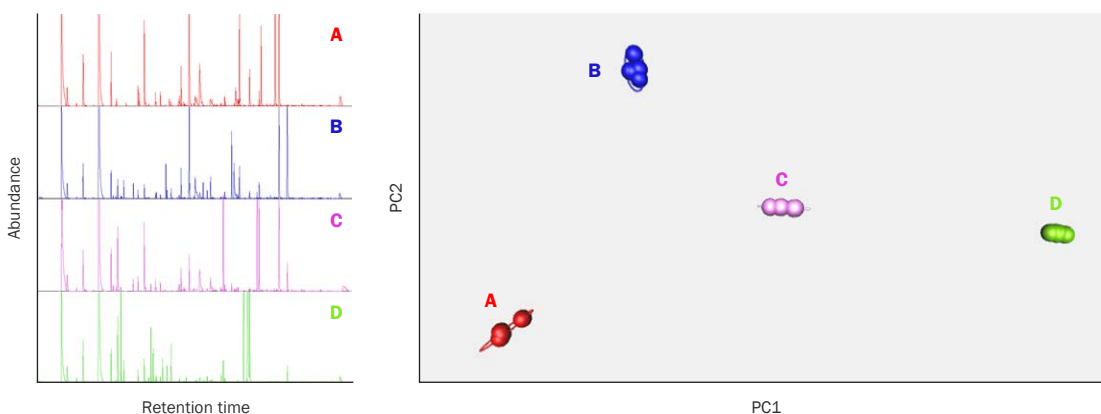
► WORKFLOW:



ENVIRONMENTAL
FOOD
BEVERAGES
FRAGRANCE
HEALTH
FORENSIC
GENERAL TOPICS



► EXAMPLE DATASET:



► KEY ADVANTAGES:

- **Generation of comprehensive profiles:** Immersive use of probes enables a wide volatility range of compounds to be extracted.
- **Improved productivity and reproducibility:** The 'prep-ahead' functionality of Centri allows multiple vials to be simultaneously extracted using multiple HiSorb probes, saving time and improving reproducibility.
- **Improved reliability and throughput:** Operations are streamlined thanks to the robustness of the HiSorb probes, and the ease of automation on Centri.
- **Gaining insights into the data:** Automated statistical analysis of the data generated using ChromCompare+ (SepSolve Analytical) enabled rapid discrimination of products.

In this analysis of four brands of hard seltzer, comprehensive profiles (left) were automatically analysed to reveal 14 key markers for quality and authenticity. Subsequent principal component analysis showed tight clustering of replicate samples.

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Avoiding interference from ethanol: Spirits

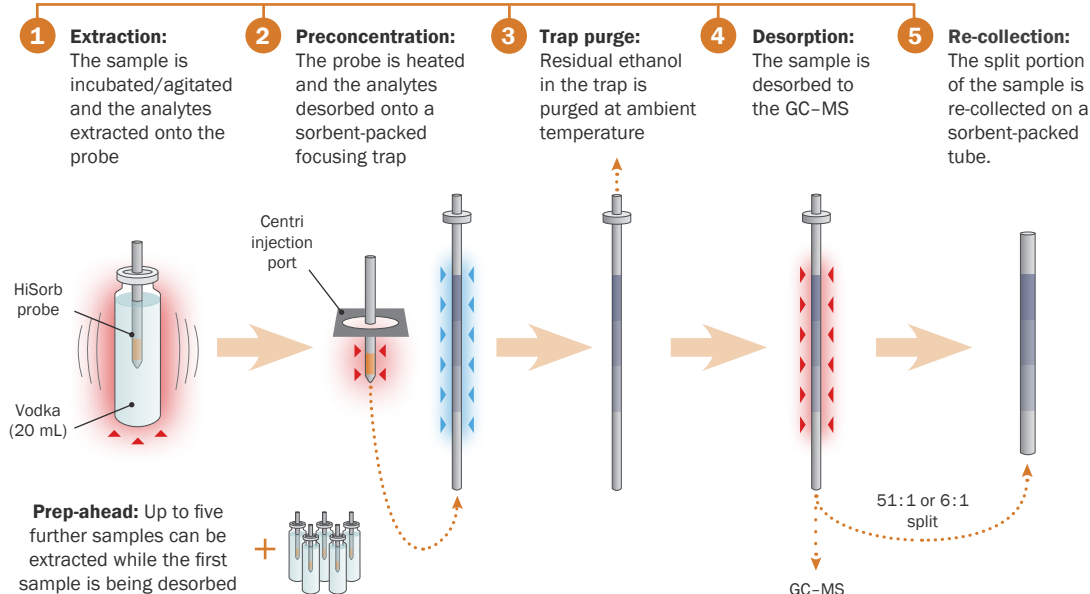
► CHALLENGE:

Existing techniques for analysing VOCs in alcoholic spirits are either **laborious** and **solvent-intensive** (liquid-liquid extraction), result in **chromatographic interference** from excess ethanol (static headspace), or are prone to **sampler breakage** (SPME).

High-capacity sorptive extraction on Centri solves all these problems, by (a) using an easily-automated solvent-free workflow, (b) greatly restricting the amount of ethanol introduced to the GC, and (c) using robust metal-core samplers.

► WORKFLOW:

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ENVIRONMENTAL

FOOD

BEVERAGES

FRAGRANCE

HEALTH

FORENSIC

GENERAL TOPICS

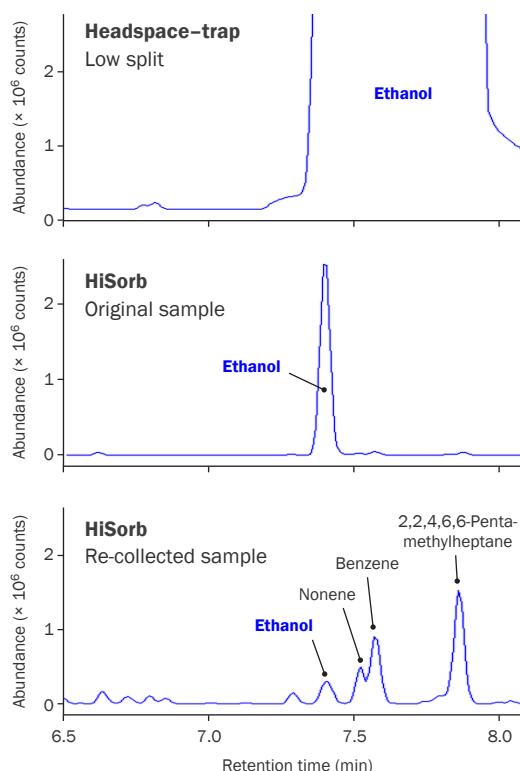


► KEY ADVANTAGES

(SEE ALSO PAGE 3):

- **Elimination of ethanol:** The trap can be held at ambient temperature during probe desorption and trap purging, allowing ethanol to be selectively removed.
- **Improved sensitivity:** Low-split (or splitless) operation allows a large portion of the sample to be sent to the GC.
- **Analyte range:** Immersive sampling allows extraction of compounds spanning a wide volatility range.
- **Improved reliability and productivity:** Operations are streamlined thanks to the robustness of the HiSorb probes, and the ease of automation on Centri.
- **Improved workflow options:** Re-collection of sample split flows for repeat analysis improves method development, sample archiving and method validation.

► EXAMPLE DATASET:



The responses of low-level aroma compounds in vodka are no longer obscured by ethanol, thanks to the use of HiSorb high-capacity sorptive extraction, combined with an ethanol purge. All operations are automated on Centri.

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Comprehensive fragrance profiling: Personal hygiene products

ENVIRONMENTAL

FOOD

BEVERAGES

FRAGRANCE

HEALTH

FORENSIC

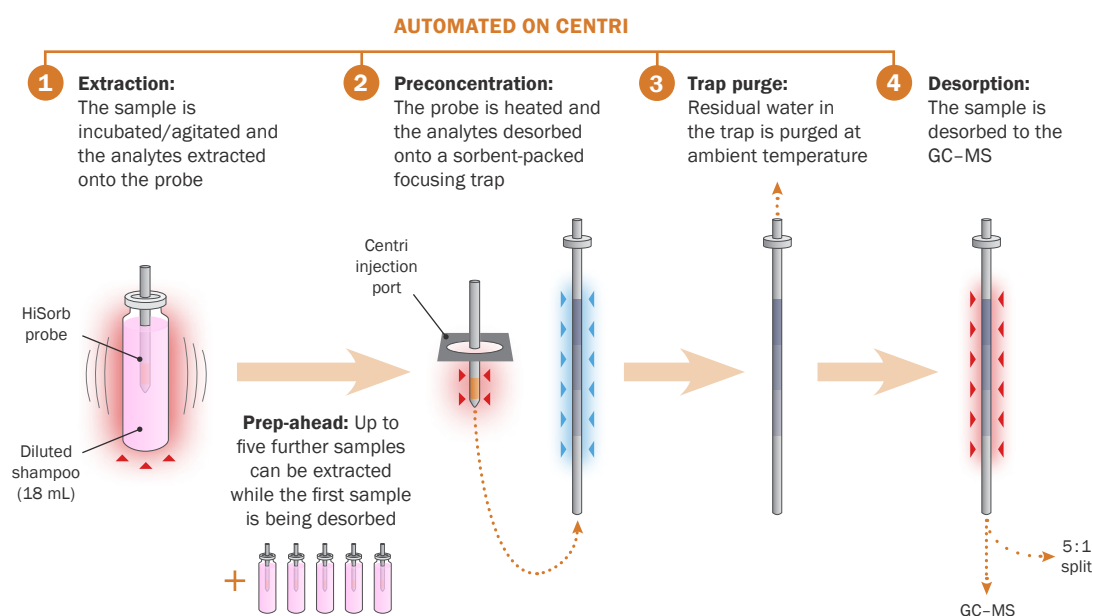
GENERAL TOPICS

► CHALLENGE:

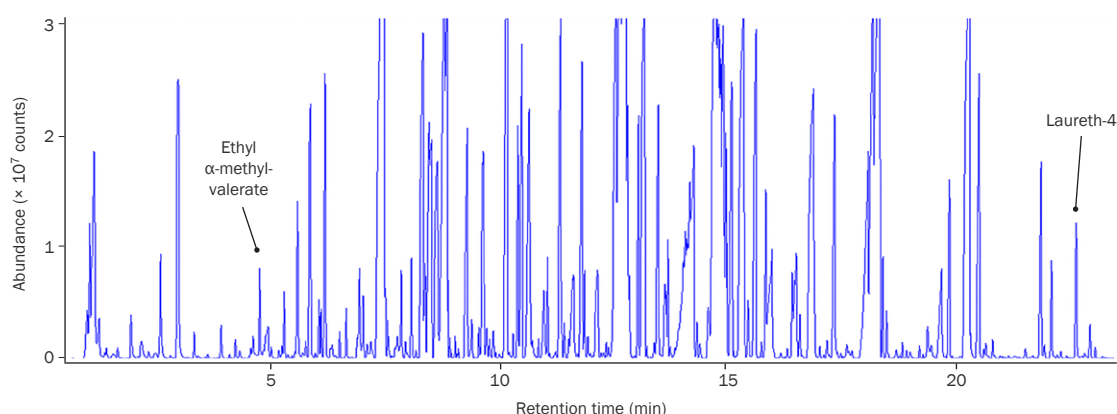
Fragrance profiling of personal care products requires **high sensitivity** for trace-level compounds with low odour thresholds, alongside the ability to **eliminate interferences** such as water, which can affect chromatographic performance.

High-capacity sorptive extraction on Centri addresses both issues, by providing a larger volume of sorptive phase for greater sensitivity, and opening up options for removing water prior to GC injection.

► WORKFLOW:



► EXAMPLE DATASET:



► KEY ADVANTAGES:

- **Analyte range:** Immersive sampling allows extraction of compounds spanning a wide volatility range, so generating comprehensive profiles.
- **Effective water management:** Selective elimination of water (while retaining analytes of interest) is aided by the use of hydrophobic sorbents in the focusing trap, and an ambient-temperature purge of residual water prior to trap desorption.
- **Improved productivity and reproducibility:** The 'prep-ahead' functionality of Centri allows multiple vials to be simultaneously extracted using multiple HiSorb probes, saving time and improving reproducibility.

Immersive high-capacity sorptive extraction of a shampoo sample, automated on Centri, allows compounds over a wide volatility range to be detected.

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Application Note 265



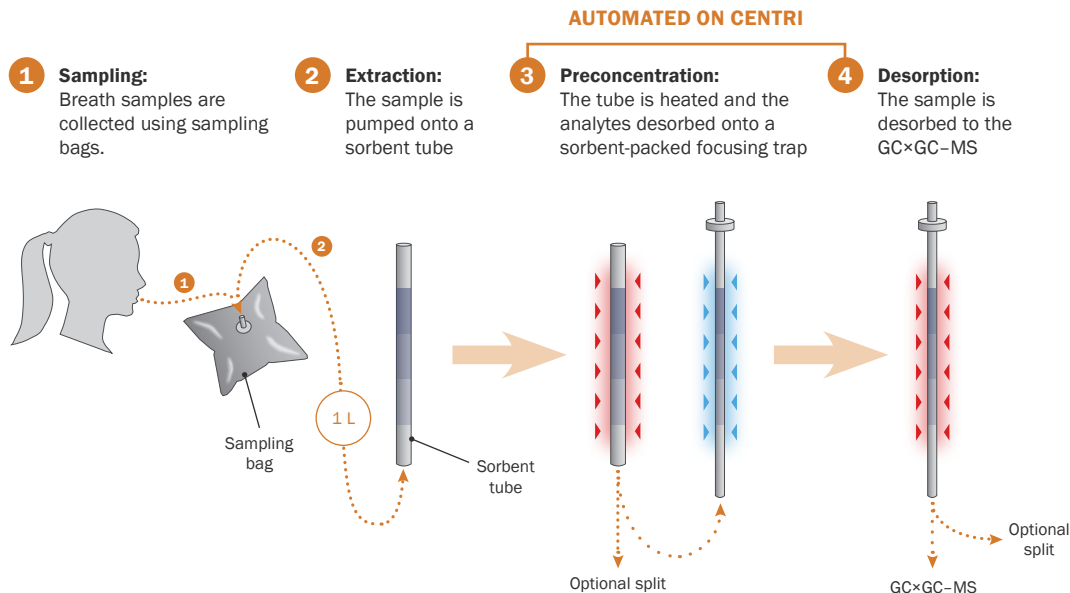
Detecting disease biomarkers: Breath

► CHALLENGE:

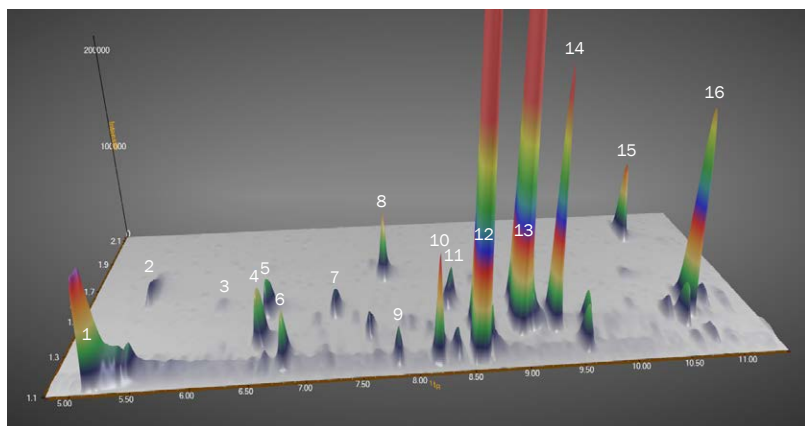
The accurate identification and measurement of biomarkers in samples such as breath, saliva and urine requires **high sensitivity** for the method to realise its full potential for early disease diagnosis.

Pumped sampling of breath onto sorbent tubes, followed by preconcentration on Centri and GC×GC-TOF MS, is a highly sensitive, automated method for screening of breath.

► WORKFLOW:



► EXAMPLE DATASET:



- 1 Carbon dioxide
- 2 Sulfur dioxide
- 3 Ethanol
- 4 Acetone
- 5 Isopropanol
- 6 Isoprene
- 7 Dichloromethane
- 8 Trimethylsilanol
- 9 2-Methylpentane
- 10 3-Methylpentane
- 11 Butane-2,3-dione
- 12 n-Hexane
- 13 Ethyl acetate
- 14 1,3,5-Trifluorobenzene (artefact)
- 15 Butan-1-ol
- 16 Benzene

► KEY ADVANTAGES:

- **High sensitivity:** The use of sorbent tubes and an optimised trap design preconcentrates the 1 L breath sample into ~100 µL of vapour.
- **Sample storage:** The ability to store samples on sorbent tubes for several weeks allows transport to the analytical laboratory without risk of degradation.
- **Improved workflow options:** Re-collection of sample split flows for repeat analysis allows samples to be stored and later re-analysed to confirm compound identity, without having to repeat sample collection.
- **Improved laboratory efficiency:** Automated thermal desorption and sample overlap on Centri speeds up workflows.
- **Range of sampling options:** Centri allows sampling from a wide range of matrices, using HiSorb high-capacity sorptive extraction, SPME and headspace, in addition to TD tubes.

ENVIRONMENTAL

FOOD

BEVERAGES

FRAGRANCE

HEALTH

FORENSIC

GENERAL TOPICS



Sorbent-tube-based workflows, in conjunction with two-dimensional GC, allow highly sensitive detection of low-level breath volatiles, as shown in this expanded region of a GC×GC colour plot.



Screening for explosives: Water and fabrics

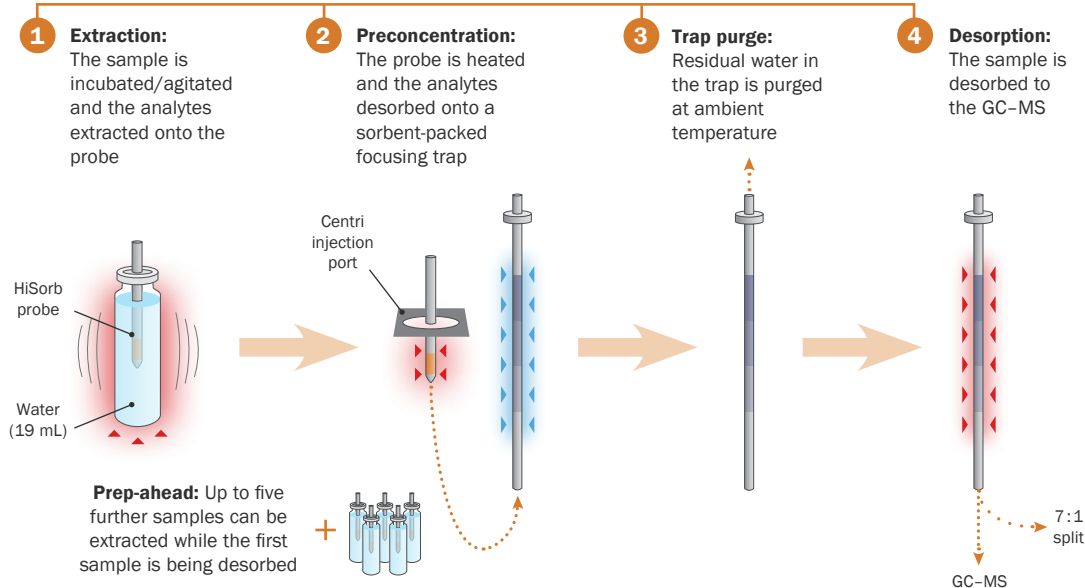
► CHALLENGE:

Identifying trace-level explosive residues in solids and liquids using GC-MS is important for forensic and defence applications, but **some compounds can decompose** before reaching the detector. Another problem is the **labour-intensive** nature of some extraction methods, and their use of large amounts of **hazardous solvents**.

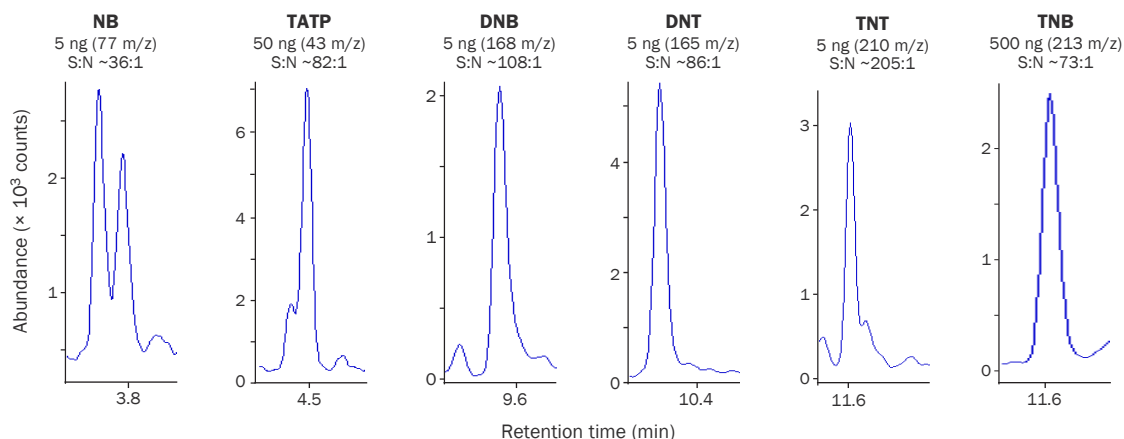
Addressing these issues, **high-capacity sorptive extraction** on Centri is fully automated and solvent-free, and integrates with low-temperature thermal desorption for efficient analysis of explosives.

► WORKFLOW:

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► EXAMPLE DATASET:



► KEY ADVANTAGES:

- **Improved sensitivity:**
 - The greater sampling capacity of HiSorb probes (~100 times more sorptive phase than a SPME fiber) provides more extraction efficiency for trace-level detection
 - Low-split operation allows a larger portion of sample to be sent to the GC.
- **Analyte range:** Immersive sampling combined with backflushed trap operation allows extraction and analysis of a wide volatility range of compounds.
- **Improved reliability:** Operations are streamlined thanks to the robustness of the HiSorb probes, and the ease of automation on Centri.

ENVIRONMENTAL

FOOD

BEVERAGES

FRAGRANCE

HEALTH

FORENSIC

GENERAL TOPICS



The excellent signal-to-noise ratios at low-nanogram loadings of six explosives in water show that HiSorb analysis is relevant to typical contamination scenarios.

NB = Nitrobenzene
TATP = Triacetone triperoxide
DNB = 1,3-Dinitrobenzene
DNT = 2,4-Dinitrotoluene
TNT = Trinitrotoluene
TNB = Trinitrobenzene

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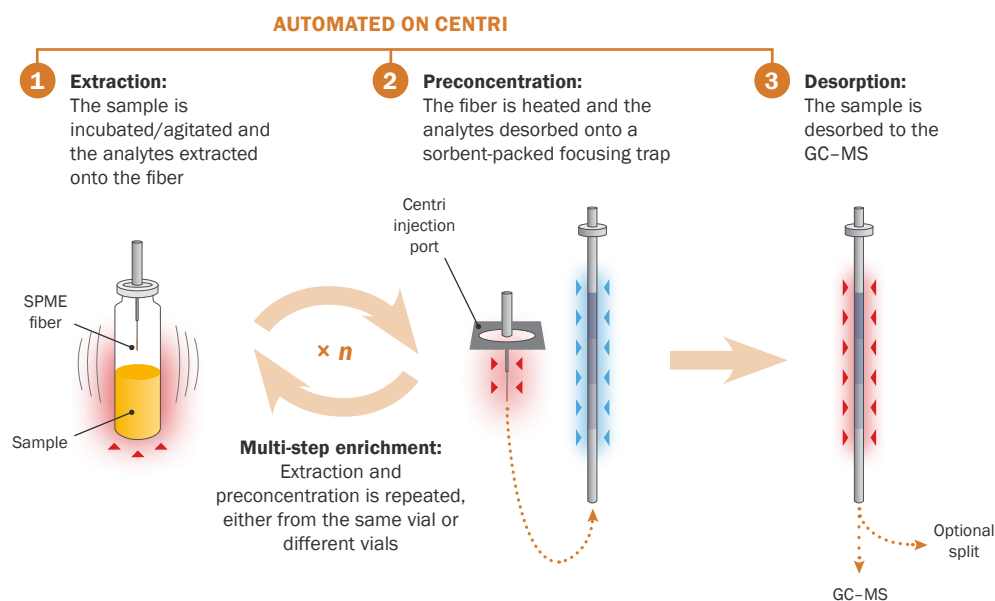
Improving the sensitivity of SPME by multi-step enrichment

► CHALLENGE:

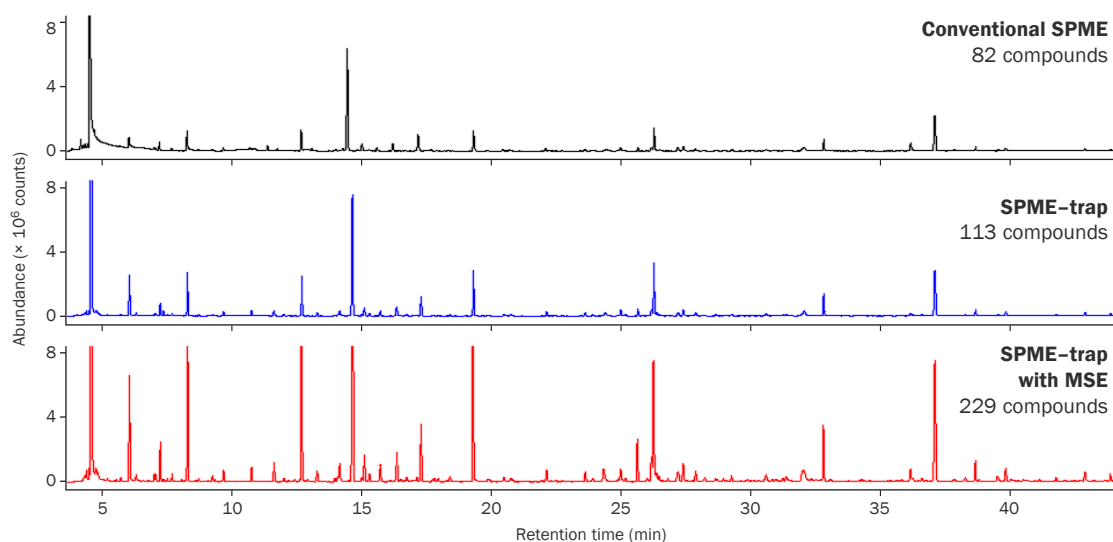
SPME is an easily automated, solventless extraction technique, but **sensitivity is limited**, especially when injector split flows are used to improve the chromatography.

SPME-trap on Centri overcomes this problem using trap-based pre-concentration, with sensitivity enhanced further by **multi-step enrichment (MSE)**.

► WORKFLOW:



► EXAMPLE DATASET:



► KEY ADVANTAGES:

■ Improved sensitivity:

- An optimised trap design pre-concentrates the sample into $\sim 100 \mu\text{L}$ of vapour, providing greater sensitivity than is possible with conventional SPME
- Multi-step enrichment onto the same focusing trap improves sensitivity further, for detection of more compounds
- Low-split (or splitless) operation allows a large portion of the sample to be sent to the GC, without compromising chromatographic performance.

- **More compounds identified:** The greater sensitivity results in the discovery of more compounds in the sample.

ENVIRONMENTAL

FOOD

BEVERAGES

FRAGRANCE

HEALTH

FORENSIC

GENERAL TOPICS



Sample trapping and multi-step enrichment boosts the number of compounds identified using SPME, as exemplified in this analysis of tea headspace on Centri.



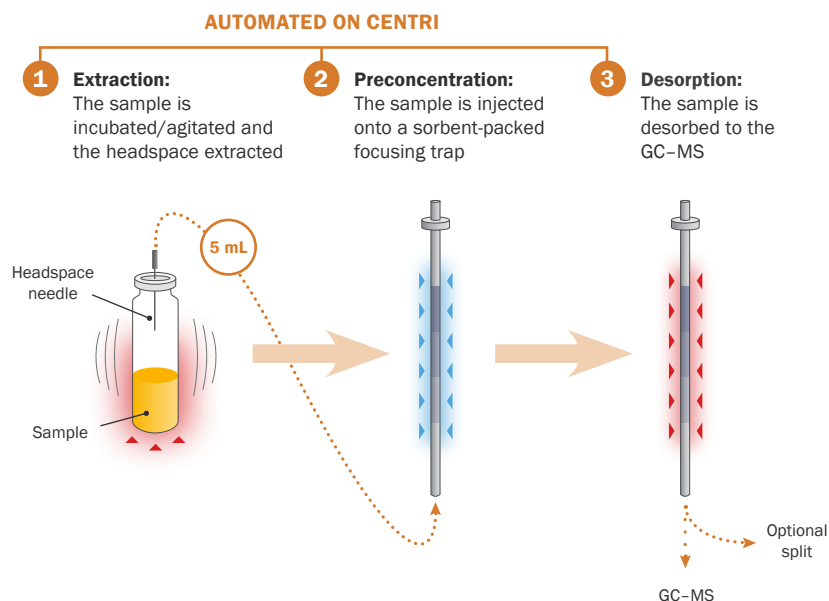
Improving the sensitivity of headspace by large-volume injection

► CHALLENGE:

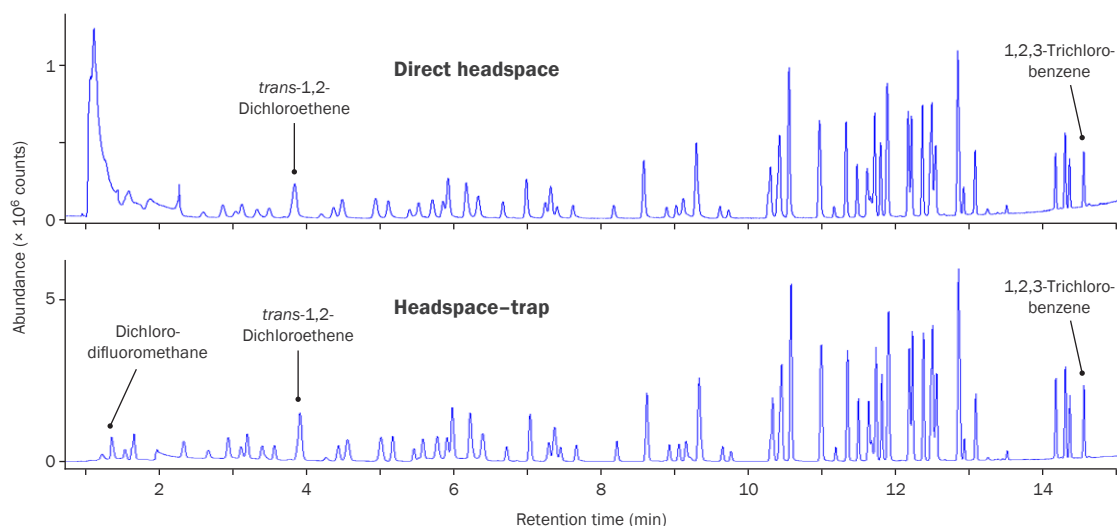
Headspace sample injection is a popular technique for many applications, but it is often difficult to achieve both **high sensitivity** and **good chromatography** within the constraints of injector loop size, injection time, liner capacity and use of split flows. In addition, method development can be **time-consuming**.

Headspace-trap on Centri overcomes these problems because trap-based preconcentration allows larger volumes to be extracted without sacrificing the chromatography. This makes method development much simpler.

► WORKFLOW:



► EXAMPLE DATASET:



► KEY ADVANTAGES:

- **Easy method development:** Trap-based focusing eliminates many of the constraints on method development, allowing sensitivity and chromatography to take priority.
- **Improved sensitivity:** Large-volume injections (>1 mL) and low-split (or splitless) injections allow a large portion of the sample to be sent to the GC.
- **Better chromatography:** The focusing step results in improved peak shapes, particularly for early-eluting compounds, resulting in more confident identification.

ENVIRONMENTAL

FOOD

BEVERAGES

FRAGRANCE

HEALTH

FORENSIC

GENERAL TOPICS



Trapping allows large headspace volumes to be taken, resulting in improved sensitivity and better chromatography, as exemplified in this analysis of a standard, run splitless on Centri.

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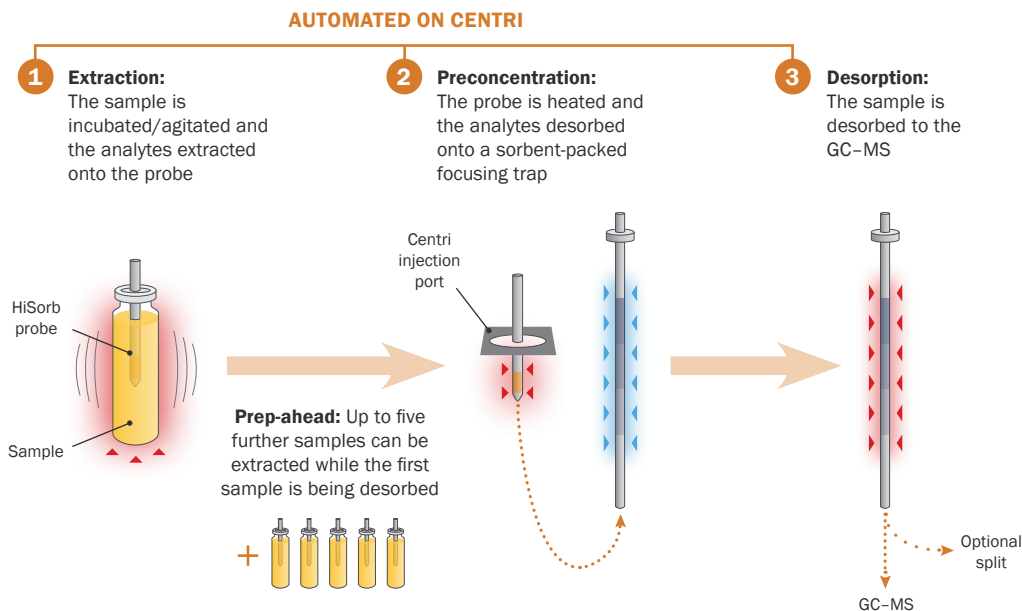
Enhancing laboratory throughput by automation

► CHALLENGE:

Analytical laboratories dealing with large numbers of samples require **fast turnaround**, and also want to reduce time-consuming and costly **manual sample preparation**.

High-capacity sorptive extraction on Centri addresses both issues, by using robust PDMS probes in fully-automated workflows on Centri.

► WORKFLOW:



ENVIRONMENTAL

FOOD

BEVERAGES

FRAGRANCE

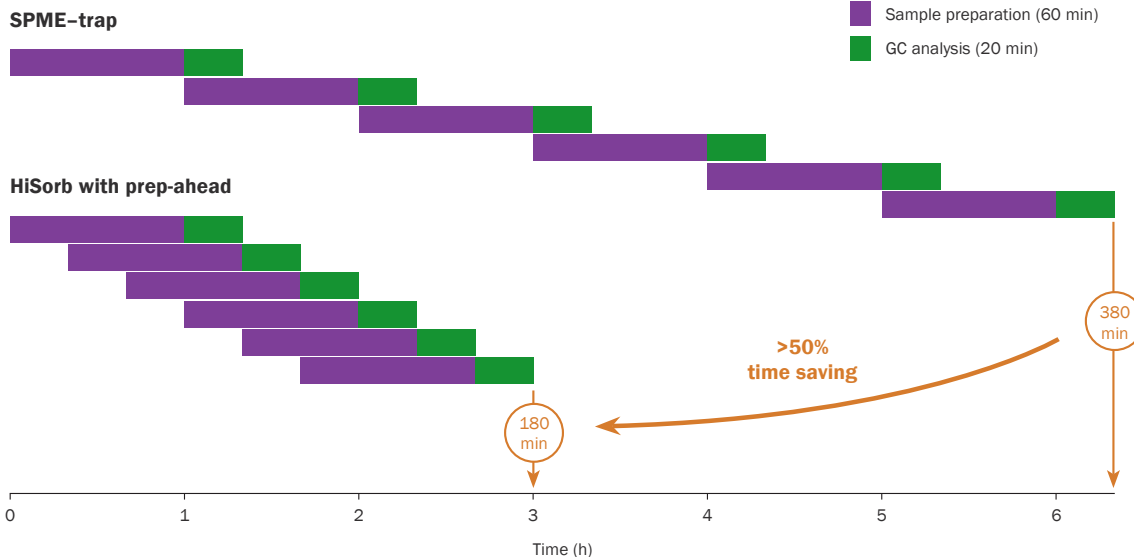
HEALTH

FORENSIC

GENERAL TOPICS



► EXAMPLE DATASET:



The overall time taken to analyse six samples is reduced to less than half by using HiSorb in prep-ahead mode, compared to SPME-trap.

► KEY ADVANTAGES:

- **Increased productivity:** 'Prep-ahead' mode – the simultaneous extraction of multiple samples while a previous analysis is ongoing – offers reductions in overall cycle time and so an improvement in laboratory productivity.
- **Reduced manual handling:** Automation also reduces the amount of manual sample preparation required, improving reproducibility and reducing the risk of human error.

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*Giorgia Purcaro, Analytical Chemistry Professor
University of Liège, Belgium*



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