Application Note 122

Flavour profiling of filter coffee using HiSorb sorptive extraction and TD–GC–MS

This study shows that the wide range of volatile and semi-volatile organic compounds (VOCs and SVOCs) giving rise to the flavour of coffee can be identified by high-capacity sorptive extraction using PDMS probes, with analysis by thermal desorption–gas chromatography–mass spectrometry (TD–GC–MS).

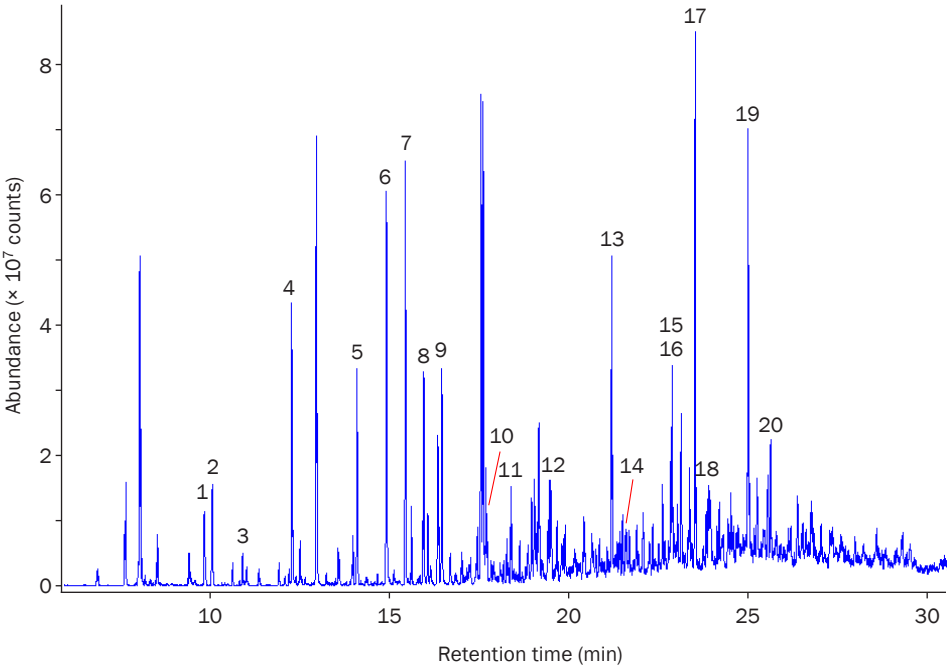
Results and discussion

VOCs and SVOCs in freshly-brewed Colombian filter coffee were sampled by immersing a HiSorb™ PDMS probe in the sample, and agitating it for 1 hour at 40°C using the HiSorb Agitator. This was followed by probe desorption and TD–GC–MS analysis. Figure 1 shows the complex profile obtained, and some of the key components are indicated.

The overall flavour and aroma of coffee results from the combined presence of chemicals from a number of classes, including hydrocarbons, aldehydes, acids, esters as well as sulfur- and nitrogen-containing compounds.

A number of furans are found in this sample, which typically have caramel-like odours, because they result from the pyrolysis of sugars.

Nitrogen-containing compounds are also of particular importance to the aroma of roasted coffee, with pyridine, pyrazines, pyrroles and pyrazoles being found in this sample. However, pyrazines can be common in defective coffee beans, and some of them may contribute undesirable flavours.



1 3-Methylbutanal
2 2-Methylbutanal
3 *N*-Nitrosodimethylamine
4 Pyridine
5 Methylpyrazine
6 Furfural
7 3-Furanmethanol
8 2,5-Dimethylpyrazine
9 2-Acetylfuran
10 Furfuryl hexanoate
11 2-Formyl-1-methylpyrrole
12 *trans*-1,4-Bis(hydroxymethyl) cyclohexane
13 1-(2-Furylmethyl)-1H-pyrrole
14 4-(2-Furyl)but-3-en-2-one
15 4-Ethyl-2-methoxyphenol
16 Difurfuryl ether
17 2-Methoxy-4-vinylphenol
18 5-Amino-1-phenylpyrazole
19 *trans*-1-(2-Furyl)-*N*-(2-furylmethyl) methanimine
20 2-(n-Butyl)furan

Figure 1: Flavour profile of freshly-brewed Colombian coffee, obtained by HiSorb sorptive extraction and TD–GC–MS analysis.

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In conclusion, this study has shown the ability of HiSorb sorptive extraction, combined with analysis by automated TD, to aid the rapid flavour profiling of coffee. The high-capacity PDMS phase results in higher sample loadings than SPME methods, and (combined with Markes' TD pre-concentration technology) offers greater sensitivity across a wider analyte range, in a single run. A further benefit is provided by the unique capability of Markes' instruments to re-collect all split flows, allowing repeat analysis for sample security, method optimisation and characterisation by alternative detection methods.

Experimental

Sample:
Colombian ground coffee was brewed using a coffee machine according to the manufacturer's instructions, and the coffee allowed to cool to 40°C.

Sorptive extraction:

System:	HiSorb probe and Agitator (Markes International)
Sample volume:	15 mL
Probe:	Part no. H1-AXAAC-5 (for 20 mL vials)
Immersion:	1 hour at 40°C
Agitator speed:	300 rpm

TD:

Instrument:	TD100-xr™ (Markes International)
TD tube:	Stainless steel (part no. C0-AXXX-0000)
Tube desorb:	280°C (10 min) with 10:1 outlet split
Cold trap:	General-purpose hydrophobic (part no. U-T2GPH-2S)
Trap low:	25°C
Trap desorb :	280°C (3 min)

GC:

Column:	DB-624™, 60 m × 0.32 mm × 0.5 µm
Oven:	40°C (5 min), then 10°C/min to 240°C (5 min)
Column flow:	Helium, 2 mL/min

Quadrupole MS:

Scan mode:	m/z 35–500
Source:	250°C
Transfer line:	240°C

Background to HiSorb

Markes International's HiSorb system allows high-capacity sorptive extraction from liquids and solids.

Samples are placed inside standard 20 mL or 10 mL vials, sealed with a crimped HiSorb septum cap, and a metal-core PDMS **HiSorb probe** inserted into the vial for either immersive or headspace sampling. The vial and probe are agitated and heated using the **HiSorb Agitator**, and after this the probe is washed, dried, and inserted into a conventional TD tube for desorption and automated TD–GC–MS analysis.

HiSorb has been developed with Welsh Government 'SMART Cymru' funding.

Applications were performed under the stated analytical conditions. Operation under different conditions, or with incompatible sample matrices, may impact the performance shown.

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