Application Note

Coffee Aroma Profiling - Direct SICRIT® HR-MS Analysis

Introduction

Coffee is one of the most popular beverages and known for its manifold aroma profiles. Aroma is one of the first senses experienced when preparing or consuming a coffee beverage and arises from different volatile compounds produced during the roasting of coffee beans.

Figure 1 - Representative photograph of coffee olfactoric testing.

However, the chemical composition of the coffee aroma is very complex. More than 1000 volatile compounds have been identified that are associated with flavour in coffee. The main volatile compounds in coffee include carbonyl, sulfur alicyclic, aromatic benzenoid, and heterocyclic compounds.

...SICRIT MS allows for real-time MS based aroma profiling either direct from a coffee bean or during the coffee roasting process

The aroma of roasted coffee beans allows conclusions about the bean origin, the roasting conditions, and the storage of the roasted beans. Therefore, a high-resolving analysis of volatile compounds would be helpful to optimize the roasting and blending process regarding the resulting aroma profile. Furthermore, a comprehensive screening of VOCs in the beans would supply the manufacturer's quality control and their search for better aroma-conserving packaging materials.
The manufacturer's quality control is mainly based on sensory analysis of roasted beans by professional tasters and physical properties as roasting temperature, color, and weight of the beans after roasting.
In lab analysis, coffee aroma compounds are commonly identified by GC-MS of brewed coffee extracts. However, this method requires tedious sample pretreatment by solid phase microextraction before headspace-GC analysis (HS-SPME/GC-MS).
Therefore, analytical methods which allow for direct online-monitoring of a broad range of VOCs would open new possibilities in the coffee bean processing.

Setup

The SICRIT® technology is particularly suitable for direct screening of complex samples without sample pre-treatment. The special design of the SICRIT ion source allows for easy interfacing the direct sampling of VOCs out of the whole bean with untargeted and high-resolved detection by mass spectrometry.
For fast and direct online-screening purposes, the beans just have to be placed in front of the SICRIT® ion source. Even semivolatile compounds can be measured by application of a heated gas stream (100°C). The desorbed VOCs are drawn in the MS by the applied permanent vacuum and detected instantaneously.
Of course, the SICRIT® solution is also applicable for SPME-sampling of coffee extracts and combinable with GC by using our GC/SPME-module.

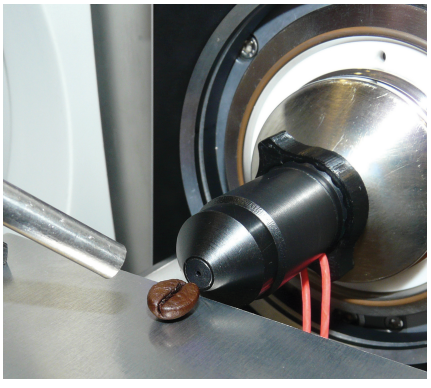

Figure 2 -Coffee aroma profiling by direct VOC desorption in front of the SICRIT® ion source

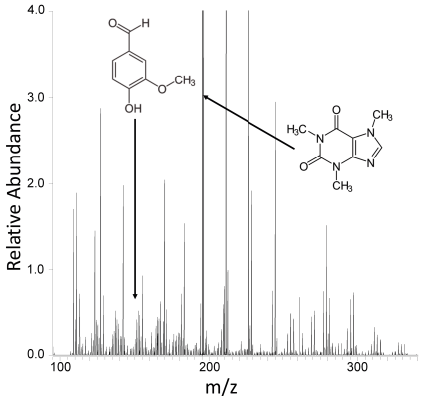

Figure 3 - Aroma profile of a single coffee bean acquired using a SICRIT® ion source attached to a Thermo LTQ Orbitrap MS; vanilline (m/z 153) and caffeine (m/z 195).

Results

The singularity of the SICRIT® technology is the possibility to easily interface it with any mass spectrometer. Thus, there's no given limitation in the mass resolution by using the SICRIT®

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Table 1 - Matching of coffee aroma compounds by exact mass. HR-MS resolution 100,000.

Flavour compound (excerpt)	Sum formula	M+H (calc)	M+H (meas)	Dev (mmu)
2-ethyl-3.5-dimethylpyrazine	$C_8H_{12}N_2$	137.1073	137.1077	0.37
2.3-diethyl-5-methylpyrazine	$C_9H_{14}N_2$	151.1230	151.1235	0.53
(E)-beta-damascenone	$C_{13}H_{18}O$	191.1430	191.1437	0.66
Guaiacol	$C_7H_8O_2$	125.0597	125.0603	0.59
4-vinylguaiacol	$C_9H_{10}O_2$	151.0754	151.0760	0.64
4-ethylguaiacol	$C_9H_{12}O_2$	153.0910	153.0915	0.49
vanilin	$C_8H_8O_3$	153.0546	153.0551	0.48
5-ethyl-3-hydroxy-4-methyl-2(5H)-furanone	$C_7H_{10}O_3$	143.0703	143.0707	0.43
2-isobutyl-3-methoxypyrazine	$C_9H_{14}N_2O$	167.1179	167.1184	0.51
propionic acid	$C_3H_6O_2$	75.0441	75.0456	1.51
cresol	C_7H_8O	109.0648	109.0652	0.41
trigonelline	$C_7H_7NO_2$	138.0550	138.0554	0.42
caffeine	$C_8H_{10}N_4O_2$	195.0877	195.0882	0.56
6-methyl-3-pyridinol	C_6H_7NO	110.0600	110.0604	0.35
3-hydroxypyridine	C_5H_5NO	96.0444	96.0446	0.20
2-methylpyrazine	$C_5H_6N_2$	95.0604	95.0606	0.27
1-methylpyrrole	C_5H_7N	82.0651	82.0651	0.00
2.5-dimethyl-4-hydroxy-3(2H)-furanone	$C_6H_8O_3$	129.0546	129.0550	0.40
furfural	$C_5H_4O_2$	97.0284	97.0286	0.21
2-acetylfuran	$C_6H_6O_2$	111.0441	111.0444	0.35
5-hydroxymethylfurfural	$C_6H_6O_3$	127.0390	127.0394	0.41
4.4-dimethyl-2-cyclopenten-1-one	$C_7H_{10}O$	111.0804	111.0808	0.34
2.3-dimethyl-2-cyclopenten-1-one	$C_7H_{10}O$	111.0804	111.0808	0.34
2-hydroxy-3-methyl-2-cyclopenten-1-one	$C_6H_8O_2$	113.0597	113.0601	0.35
3-ethyl-2-hydroxy-2-cyclopenten-1-one	$C_7H_{10}O_2$	127.0754	127.0758	0.39
phenol	C_6H_6O	95.0492	95.0494	0.22

ion source. Combined with the soft ionization process (positive and negative), hundreds of volatile compounds can be identified in less than one second without any sample pretreatment. Furthermore, the smart design of the SICRIT® ion source enables a loss-free transfer of the ionized analyte molecules and hence increases the sensitivity. The high potential of the SICRIT®-MS for online-coffee aroma profiling is demonstrated by direct screening of single coffee beans using a SICRIT®-Thermo LTQ Orbitrap XL system. With a resolution setting of 100.000 the results depicted in Figure 3, 4 and Table 1 were aquired. Figure 4 shows the resolving power on example of the nominal mass 143, where multiple isobaric peaks can be discriminated and precisely assigned. The shown separation

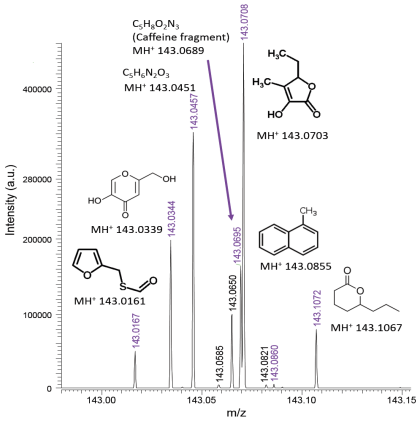

Figure 4 - Illustration of high-resolving power using SICRIT®-MS at m/z 143. Data acquired on a Thermo LTQ Orbitrap MS.

of 143.069 and 143.071 mass traces emphazise the need for a high resolution or MS/MS method, when dealing with direct trace VOC measurement and especially for direct quantitation.

Conclusions

SICRIT® enables the direct real time detection and identification of way more than 300 aroma compounds emitted from one single coffee bean. Thus, SICRIT® enables ultrasensitive real time coffee profiling or roasting monitoring with any conventional API MS. Especially the combination with high resolution MS instruments enables in-dephts analysis never seen before. Thus, the only limit to face is the enormous information gained by such a powerful combination. Moreover, SICRIT® enables isomer separation and precise quantita- by direct interfacing of any GC- or HPLC system, maintaining its soft and broad ionization benefits.

SICRIT® Coffee Analysis Benefits

- Direct identification of coffee aroma compounds (profiling)
- Enbales real time monitoring of coffee roasting processes
- No limitation in resolution
- Can be easily interfaced with GC, LC and SPME
- Broad ionization range (e.g. acids, PAH and alkanes)

References

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Fujioka K., Shibamoto T., J. Agric. *Food Chem.* 2006, 54, 6054−6058.

Rocha, S. et al., J. Sc. *Food and Agric.*, London, 2003, 84, 43-51

Further reading

Technical Note

TN_01 SICRIT®: Soft Ionization by Chemical Reaction in Transfer

Product Notes

PN_02 SICRIT® SC-20X Ionization Set

PN_03 SICRIT® GC/SPME Module

KW AN_02_03/18

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