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GC-MS GCMS-TQ™ 8040 NX
Energy Dispersive X-ray Fluorescence Spectrometer EDX-7200

Application News

Quantifying the Similarity of Two Coffee Bean Products by GC/MS and EDXRF

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User Benefits

- By using the Smart Aroma Database™, trace aroma components that are difficult to detect in the Scan mode can be detected by the MRM mode.
- EDX can be used to analyze minerals in foods either as is or by simple sample preparation.

■ Introduction

Coffee plays an important role as a drink. Coffee beans are produced mainly in South American countries such as Brazil and Colombia. These countries grow high-quality coffee beans in warm climates and rich precipitation. On the other hand, the countries that consume coffee are different from the countries that produce it. In Western countries, coffee culture is rich, and various coffee products (such as dark roast and latte art) are enjoyed. It is important for consumers to ensure the quality of coffee beans in both producing and consuming countries across geographical and cultural differences.

To improve the quality and safety of coffee beans, elemental analysis should be conducted in addition to that of the texture, taste, and flavor. Coffee beans contain trace amounts of elements, but their effects are not small. For example, if there is a lot of iron in coffee beans, they may oxidize easily and deteriorate their flavor. Also, too much zinc and copper can have a negative effect on the body when consumed. In addition, toxic cadmium is easily absorbed from soil and water by plants, such as coffee trees, and can cause health risks if it accumulates in the body when ingested. In terms of taste and flavor, when metal containers and utensils come into contact with coffee beans, metal ions can leach out and change the flavor and quality of the coffee. For this reason, it is important to regularly inspect the elements contained in coffee beans to ensure that they meet safety standards.

This application news presents two types of commercially available coffee beans measured using an energy-dispersive X-ray fluorescence spectrometer EDX-7200 and a gas chromatograph mass spectrometer GCMS-TQ8040 NX equipped with an AOC-6000Plus (Fig. 1).

Fig. 1 EDX-7200 (left) and GCMS-TQ™8040 NX (right)

■ Experimental

Two types of commercial coffee beans were prepared, and 476 components were measured by SPME by the Smart Aroma Database for flavor measurement, and 502 components, including amino acids, fatty acids, organic acids, and sugars, were measured by GC/MS by the Smart Metabolites Database Ver.2 and the pretreatment handbook for taste measurement. EDXRF performed elemental analysis under the conditions described in Table 1, and quantitative values were calculated by the FP method.

Because each measurement was performed with n=1, a similarity score was calculated instead of performing multivariate analyses such as principal component analysis and volcano plot.

Table 1 EDX analytical conditions

Element	: $_{11}$Na-$_{92}$U
Analysis Type	: Qualitative and quantitative
Detector	: SDD
X-ray tube bulb	: Rh Target
Tube voltage	: 15 [kV] (Na-S), (Cl-V) 50 [kV] (Cr-Fe), (Ni-Nb, As, Pb), (Mo-Xe)
Tube current	: Auto [µA]
Collimator	: 10 [mmφ]
Primary Filter	: Nothing (Na-S) , #2 (Cl-V) , #3 (Cr-Fe) , #4 (Ni-Nb, As, Pb) , #1 (Mo-Xe)
Atmosphere	: Helium
Integration time	: 100 [sec] × 5 (Na-S), (Cl-V) (Cr-Fe), (Ni-Nb, As, Pb), (Mo-Xe)
Dead time	: Maximum 30 [%]

■ Results

Comparable compounds and elements were detected in coffee beans A and B in all taste, flavor, and elemental analyses (Table 2). On the other hand, coffee bean B was found to be rich in both taste and flavor.

Table 2 Measurement results

	Taste (502 targets)	Flavor (476 targets)	Element (82 targets)
Found in A	235	194	14
Found in B	230	188	14
Found in only A	15	35	0
Found in only B	20	24	0
X10 abundant in A	4	9	1
X10 abundant in B	21	28	0

Table 3 EDXRF results (ppm)

	K	Mg	S	Ca	P	Cl	Fe
Coffee Bean A	21996.3	1786.4	1384.9	1528.7	1085.6	141.2	38.8
Coffee Bean B	21270.1	1669.4	1219.4	1174.6	1069.9	164.3	37.5
	Mn	**Rb**	**Br**	**Cu**	**Zn**	**Sr**	**Ni**
Coffee Bean A	37.8	16.9	0.2	17.6	6.6	4.1	1.2
Coffee Bean B	31.4	16.4	16.1	16.0	5.5	3.0	1.4

* Quantitation calculation was performed assuming CH_2O balance.

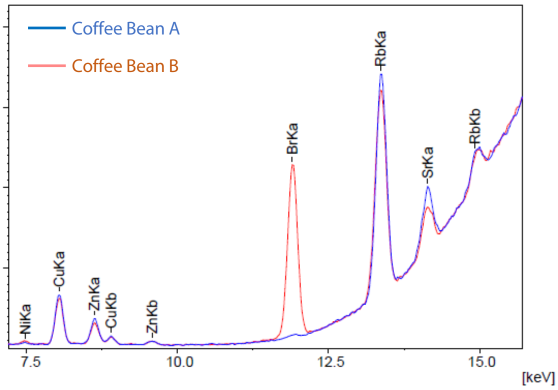

Fig. 2 Profile Superposition near Bromine

The elements detected included minerals such as K, Mg, and Zn but not harmful heavy metals such as As, Pb, and Cd, which are related to food safety. Bromine (Coffee beans A at 0.2 ppm, B at 16.1 ppm), specifically detected at high levels in coffee bean B, is known to affect taste and flavor (Table 3, Fig. 2). As an element, bromine produces a pungent odor, and as an organic bromine compound, each compound structure has a different flavor (For example, bromopropane has a sweet smell, dibromobenzene has a chemical smell, etc.).

$$\text{Similarity Score} = \left[1 - \frac{\Sigma \left| Area_A - Area_B \right|}{\Sigma \left(Area_A + Area_B \right)} \right] \times 100$$

	Taste (502 targets)	Flavor (476 targets)	Element (82 targets)
Similarity Score	89 %	**47 %**	97 %

	Sweet	Bitter	Spice	Apple
Similarity Score	74 %	86 %	74 %	48 %

Fig. 3 Similarity calculation of coffee beans A and B

When the similarity between coffee beans A and B was calculated using the formula shown in Fig. 3, it was found that the taste and the elements contained in the two types of beans were highly similar. In contrast, the similarity in flavor was low. Based on the functional information in the Smart Aroma Database, the classes were classified (Sweetly or bitterly), and the similarity was calculated for each class. There was a difference between A and B in the smell of apples. Among them, methyl -2 methylbutyrate and methyl isovalerate were detected explicitly at high levels in coffee bean A (Fig. 4). In addition to the odors shown in Fig. 3, there are various sensory information, such as forest-like and cinnamon-like scents, so we calculated the similarity of only representative odors.

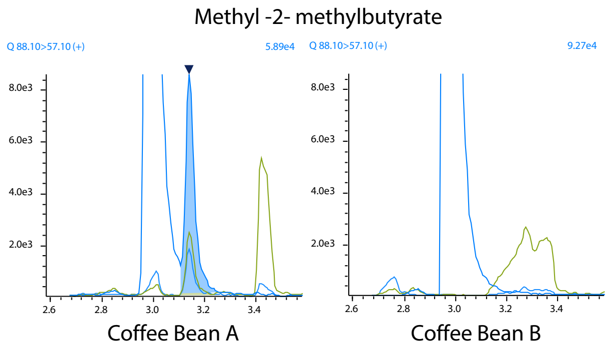

Fig. 4 Example of a chromatogram for flavor

■ Summary

In a multifaceted evaluation of 2 types of commercial coffee beans using GCMS and EDXRF, less than 250 flavor components, less than 200 flavor components, and 14 elements were detected in each sample.

As in this report, it is challenging to perform multivariate analysis such as principal component analysis or volcano plot, which analyzes the relationship between multiple variables to understand patterns and trends when n number or sample size is small (n =1 for two types). However, even when data is sparse, qualitative analysis, such as similarity calculations and sensory information in the Smart Aroma Database, can provide helpful information.

<Related Applications>

1. Vegetable Juice Evaluation by Particle Analyzer and GC/MS, Application News No. 01-00691-EN

01-00748-EN First Edition: Jun. 2024