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Application News

GC-MS, GCMS-TQ™ Series, Smart Metabolites Database™

Efficient Data Analysis for Food Samples by Using Smart Metabolites Database

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User Benefits

- The Smart Metabolites Database Ver. 2 enables highly sensitive and widely targeted MRM-based analysis.
- It is possible to narrow down the components being targeted for analysis based on the sample type to reduce data analysis times while still obtaining highly reliable results.

■ Introduction

Metabolomics is a technology for comprehensive analysis of components in biological samples using chromatograph-mass spectrometers and other analytical instruments. In the field of food science, metabolomics is used to investigate a wide variety of food materials and products to develop new functional foods and assess food sensory performance. Performing multivariate analysis on component data from multiple samples allows for the identification of characteristic features in the component profile of each sample. However, this approach to data analysis increases labor requirements due to the huge amounts of chromatographic data being handled.

This article presents an approach to food analysis that uses the Smart Metabolites Database Ver. 2 to achieve efficient data analysis with ease, even by novices in the field.

■ Widely Targeted Analysis in MRM Mode

Metabolomic analysis normally utilizes non-targeted analysis performed in Scan mode. This approach produces huge amounts of chromatographic data from numerous samples and requires high levels of skill and experience and a significant investment of time to analyze the resulting data. Such an approach can identify unknown compounds but also increases labor requirements and may not guarantee component identification or the generation of useful information.

The Smart Metabolites Database Ver. 2 enables a user to easily create methods for the simultaneous analysis of biological samples for 540 hydrophilic low-molecular-weight components that have known important functions (Fig. 1). The Smart Metabolites Database Ver. 2 contains retention indices and mass spectra for a wide range of components that can be used to automatically determine the presence of those components in a sample. This approach provides a wealth of metabolomic information while also taking advantage of the simplicity of targeted data analysis. The Smart Metabolites Database Ver. 2 can be used to analyze food samples for a wide range of taste and functional components. Using MRM mode that only detects ions characteristic to each component also reduces peaks caused by contaminants and noise, and allows detection at higher sensitivities than Scan mode (Fig. 2).

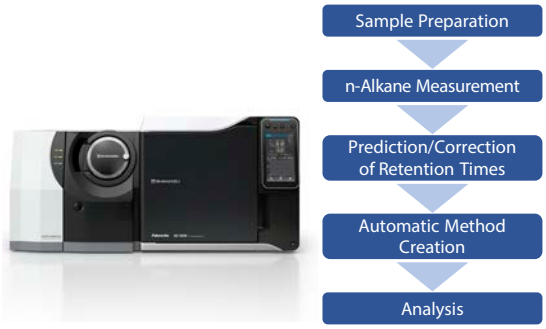


Fig. 1 Smart Metabolites Database Ver. 2 Analysis Workflow

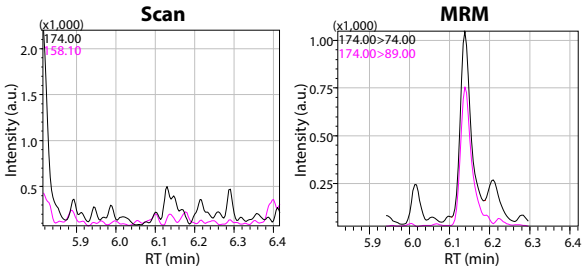


Fig. 2 Chromatogram of Pyruvic Acid (TMS-Derivatized) in Lemon

■ Filter Function that Narrows Down Components Targeted for Analysis

The types of components in a food sample vary depending on its raw materials. The Smart Metabolites Database Ver. 2 contains information on 540 components detected in a wide variety of biological samples, but any one sample may only contain around 20% of these components. Properly judging whether a detected peak represents a given component of interest requires not just time and effort, but also introduces the risk of a false positive result. The Smart Metabolites Database Ver. 2 is equipped with a filter function that enables more efficient data analysis of specific sample materials with a reduced risk of false positives (Fig. 3). The filter function contains 5 filters designed for different sample materials: plant (food), animal (food), urine, blood, and cells. A user can either use the Smart Database™ filter function to narrow down the number of components targeted by analysis, or measure all components and then use the LabSolutions Insight™ flag function to narrow down the number of component targeted for data analysis. The filter function allows the user to limit analysis to only those components detected in similar sample materials based on past reports.

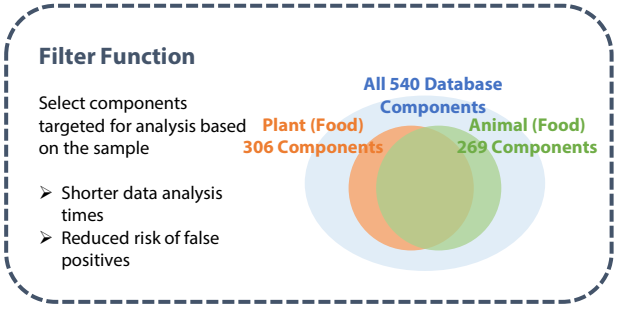


Fig. 3 Overview of Filter Function

■ Applying the Filter Function in Food Analysis

The effectiveness of the filter function included with the Smart Metabolites Database Ver. 2 was evaluated using various food samples that included processed and fermented foods. The filters applied were selected based on the raw materials in the sample. When a sample contained both plant and animal material, such as Plant (Corn) and Animal (Milk) in corn soup, both the Plant (Food) and Animal (Food) filters were used in combination. The number of components detected after applying filters based on the food sample was compared to the number detected when the filter function was not applied (simultaneous analysis for 540 components). Table 1 shows the analytical conditions used and Table 2 compares the numbers of components detected in each analysis.

The detection ratio is the number of components detected applying the filter function as a percentage of the number of components detected without applying the filter function. Detection ratios show that 90 % or more components were detected in all food samples when using the filter function.

Principal component analysis (PCA) was also used to examine component data obtained from crab and 3 imitation crab product samples when applying the filter function. As shown in Fig. 4, differences between the component profiles of each sample are visualized even when applying the filter function, thereby providing clues for the development of imitation foods that better mimic the original food.

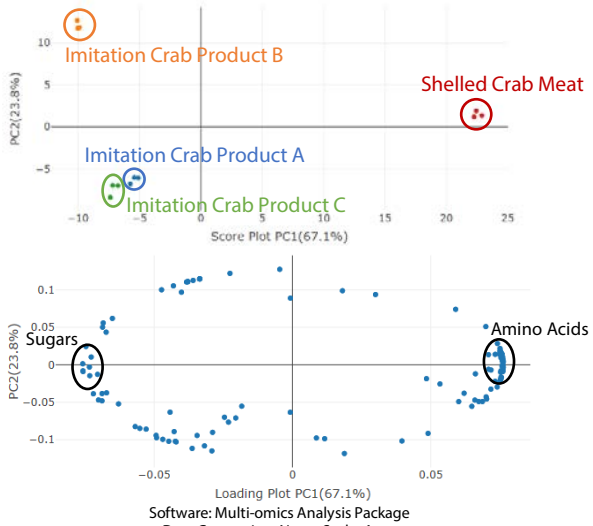
Table 1 Equipment Configuration and Analytical Conditions

GC-MS:	GCMS-TQ8050 NX
Autoinjector:	AOC™-20i/20s
Column:	BPX5 (30 m × 0.25 mm, I.D. 0.25 µm)
[GC Conditions]	
Injection Mode:	Split
Split Ratio:	30
Carrier Gas:	He
Carrier Gas Control:	Constant linear velocity (39.0 cm/sec)
Injection Volume:	1 µL
Injection Temp.:	250 ˚C
Column Oven Temp.:	60 °C (2 min) → 15 °C/min → 330 °C (3 min)
[MS Conditions]	
Ion Source Temp.:	200 °C
Interface Temp.:	280 °C
Data Acquisition Mode:	MRM

Table 2 Component Analysis of Processed and Fermented Foods with and without the Filter Function

Sample	Soy Milk	Beer	Coffee	Cheese	Thai Fish Sauce	Corn Soup	Imitation Crab
Filter Type	Plant (Food)	Plant (Food)	Plant (Food)	Animal (Food)	Animal (Food)	Plant (Food)+ Animal (Food) *2	Plant (Food)+ Animal (Food) *2
No. of Components Detected (No Filter)	87	95	89	100	132	104	102
Detected Components (With Filter)	85	93	84	92	119	101	99
Detection Ratio (%) *1	98	98	94	92	90	97	97

*1 Detection ratio = No. of Components Detected (With Filter) / No. of Components Detected (No Filter) × 100 (%)
*2 Components targeted for analysis constitute the union of the orange and green sets in the Venn diagram in Fig. 3.



Software: Multi-omics Analysis Package
Data Conversion: None, Scale: Auto

Fig. 4 Primary Component Analysis of Crab and Imitation Crab (3 Products)

■ Conclusion

The Smart Metabolites Database Ver. 2 allows simultaneous analysis of 540 components known to be present in biological samples. The filter function included with Smart Metabolites Database Ver. 2 can also be used to select which components to target based on sample type, reducing the labor involved in data analysis.

Until now, metabolomic data analysis has required a high level of skill from the user. The Smart Metabolites Database Ver. 2 removes existing barriers to metabolomics and supports the easy acquisition of highly valid metabolomic data.

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