SHIMADZU
Excellence in Science

Identifying And Quantifying Aroma Compounds

Flavor & Fragrance Analysis Solutions

Introduction

Aroma analysis plays a crucial role in food, beverages, and consumer products, including essential oils, perfumes, cosmetics, and more. The aroma of a product not only influences consumer perception but also impacts its overall quality and marketability. Whether it's the enticing scent of a perfume, the flavor profile of food, or the fragrance of skincare products, aroma analysis is crucial for quality control, product development, and innovation, enabling the creation of sensory-driven, high-quality products.

What Is Aroma Analysis?

Aroma analysis involves identifying and quantifying the volatile compounds responsible for the scent and flavor of food. Typically, these aroma components can be classified into top note, middle note and base note, based on their volatility. Since all types of components influence flavor composition, it is crucial to choose the most suitable sampling method, tailored to specific requirements such as trace-level analysis or automation.

Generally, these volatile compounds can be detected using analytical instruments, allowing scientists to map aroma profiles and pinpoint specific components that cause desirable or undesirable flavors. These advanced techniques complement the human sense of smell in sensory testing by providing an objective evaluation of aromas, thereby supporting efforts to maintain product quality, predict shelf-life, and drive innovations in food science.




Workflow Solutions

The analytical workflow often relies on methods such as gas chromatography mass spectrometry (GC-MS), but sample complexity can pose challenges in analysis. Shimadzu simplifies this process with well-established end-to-end workflows, robust instruments, and comprehensive databases, enabling accurate results and a boost in productivity.

Routine Analysis Confirmation Of Known Components

- GC-MS(/MS) can analyze high-concentration samples and known components
- HS Trap can be used to concentrate the sample for high-sensitivity in trace-level analysis

Aroma Component Analysis With Aroma Database

- Aroma Database contains >500 aroma compounds
- Identification of aroma compounds is now simplified using characteristic ions, retention times, and mass spectra in the database

GC-MS Off-Flavor Analysis System

- GC-MS Off-Flavor Analyzer is a turnkey solution to identify disinfectant odour, paint odour, resin odour, mouldy odour, and more
- MRM and SIM analysis can detect odour threshold concentration levels

Research Development Search For Causal Agents

- SPME-GCMS(/MS) can be used for highly selective and sensitive measurement of target components
- Used with Aroma Database, aroma components are easily identified, enhancing R&D efforts

Application Insights

Aroma Analysis of Essential Oils

Applications Insights

In this section, we will explore how Shimadzu's advanced solutions support aroma analysis, particularly in essential oils. From effective identification of aroma components and off-flavors to leveraging the comprehensive FFNSC library and streamlining multivariate analysis with eMSTAT, Shimadzu's solutions are designed to deliver accuracy and reliability.

Analysis Of Fragrant Components In Aroma Oils Using GC-MS Off-Flavor Analyzer

A given compound's scent can be considered as pleasant or unpleasant depending on its concentration and the surrounding aroma profile characterized by co-existing compounds.

This workflow highlights the use of Shimadzu GC-MS Off-Flavor Analyzer as a turnkey solution for analyzing the fragrant characteristics of four commercially available aroma oils—Jasmine, Lavender, Rose, and Citrus. With minimal sample preparation, this system ensures accurate identification even in the presence of nature-derived contaminants.

Workflow Solution

Analysis Of Essential Oil Using GC-MS/FID Detector Splitting System

Hinoki contains diverse aromatic components that may evoke a sense of comfort and relaxation, which reminds of cedar wood aromas.

In this application, five types of Hinoki oils, including Shimadzu's award-winning Hinoki oil, which earned recognition in the Brands & Communication Design category of the prestigious Red Dot Design Award 2021, were analyzed using a detector splitting system between MS and FID. The MS results were further evaluated using the eMSTAT Solution to analyze the composition of the components.

Workflow Solution

Characterization Of The Volatile Fraction Of Brazilian Essential Oil, Namely Cordia Verbenaceae

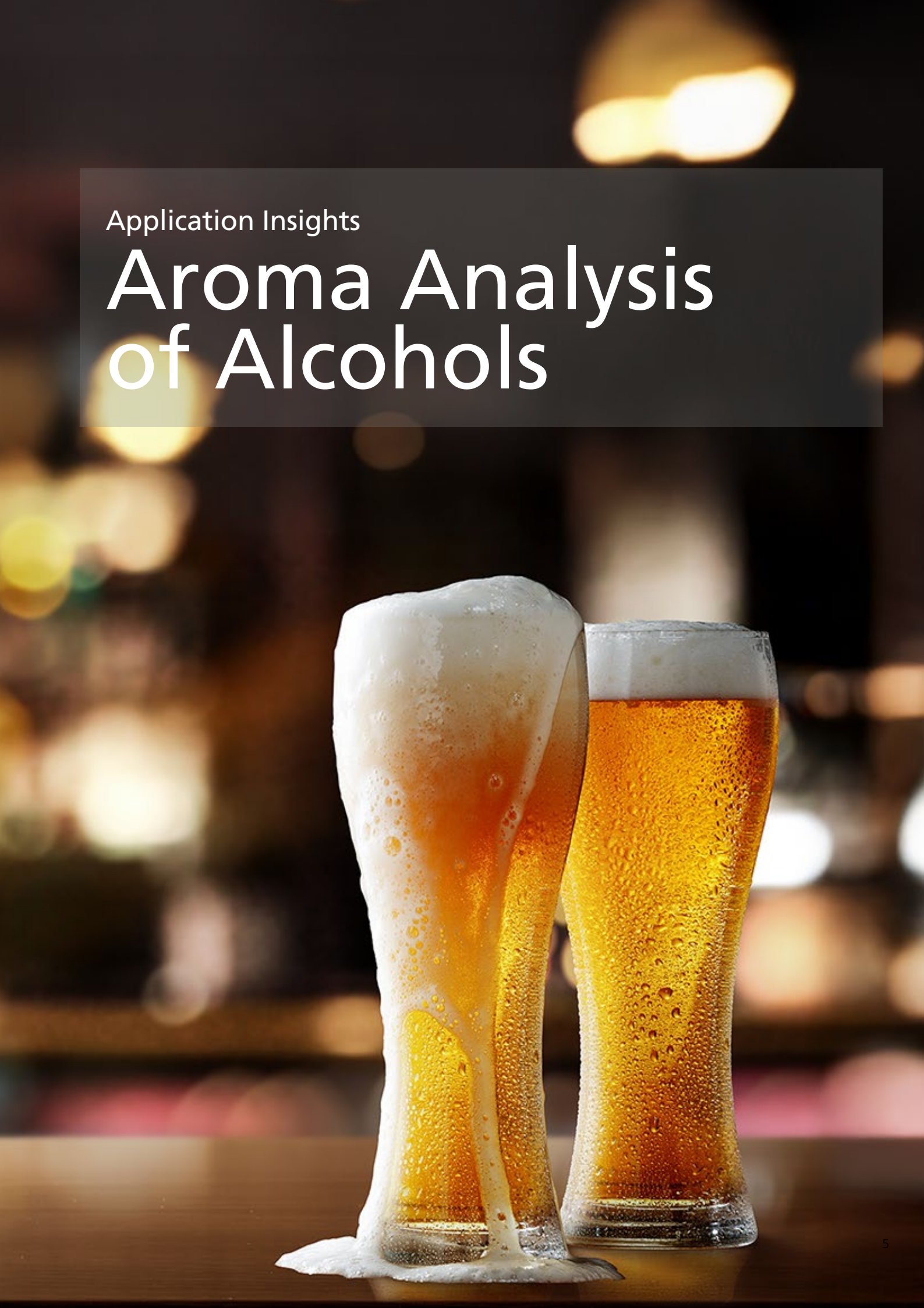
The flavors and Fragrances of Natural and Synthetic Compounds (FFNSC) MS spectral library contains Linear Retention Index (LRI) data, which can be crucial for reliable peak assignment in the identification process.

Although major components of the essential oil are usually identified through MS spectral comparison and reference literature, this may be difficult for compounds such as sesquiterpenes due to their highly similar mass fragmentation patterns. The FFNSC library, with its LRI data, can hence be used together with MS similarity data to improve identification accuracy.

Workflow Solution

Application Insights

Aroma Analysis of Alcohols



Applications Insights

Herein, we will demonstrate the benefits of Shimadzu's Aroma Database in supporting wide-scope targeted analysis and high-sensitivity target analysis using selected ion monitoring (SIM) and multiple reaction monitoring (MRM). With just a simple adjustment of retention times using a standard n-alkane mixture, analytical method can be easily created. Results can then be used to automatically identify target aroma compounds based on retention times, similarity scores and ion ratios.

Science-Based Evaluation And Visualization Of Sake Flavors And Providing This Information To Consumers

One of the appeals of Japanese sake is the wide variety of tastes and aromas (flavors) offered by sake brands and individual products.

Using GC-MS to analyze aroma compounds and LC-MS for taste-related components, this workflow integrates statistical analysis to produce a visual distribution of sake flavors. An example of flavor map is presented, providing a practical tool to classify and position sake based on its flavor profile. This evidence-based approach helps consumers identify sake products that align with their personal taste preferences.

Workflow Solution

Aroma And Metabolite Analysis Using GC-MS And LC-MS And Approach To Craft Beer Development

Craft beers are renowned for their distinct flavors, and analytical methods can be used to enhance beer quality and innovation.

Herein, a spicy aroma compound, characteristic of wild yeast, was identified using GC-MS. Targeted metabolomic analysis with GC-MS and LC-MS revealed characteristic metabolite compounds in each beer, which helps in refining brewing processes. Finally, non-targeted metabolomic analysis using LC-QTOF provided precise mass data, enabling the identification of unknown compounds in the analytical workflow.

Workflow Solution

Analysis Of Aroma For Beverage R&D Using Aroma Database And SPME Arrow

Beer aroma and taste can differ significantly depending on the malt type and fermentation method used.

To support R&D efforts, SPME Arrow can be used to extract aroma compounds from beer samples, followed by GC-MS analysis using the Aroma Database, which includes over 500 aroma-related compounds. The identified compounds are then analyzed using Principal Component Analysis (PCA) to effectively compare and characterize aroma differences across various beer types and brewing methods.

Workflow Solution

Application Insights

Aroma Analysis of Consumer Products

Applications Insights

When it comes to consumer products, the objective identification and quantification of off-flavor components can be achieved using advanced analytical tools such as GC-MS. Qualitative analysis determines the components present, which can then be verified against the sensory information. Quantitative analysis calculates the concentration of the detected components, assessing whether the levels surpass off-flavor thresholds, thus ensuring product quality and consistency.

Analysis Of Aroma Compounds In Cosmetics Using The Aroma Database

Cosmetics and personal care products often contain fragrances or active ingredients derived from natural substances.

These components are typically detected alongside interfering peaks, making accurate quantification challenging due to overlapping signals from quantitation ions and contaminants, even for SIM mode analysis of a narrow mass range. MRM mode analysis can minimize contaminant interference due to higher selectivity, although it can be time-consuming. With Aroma Database, MRM methods for selected compounds can be automatically created, which can save time and boost productivity.

Workflow Solution

Highly Sensitive Analysis Of Fragrance Allergens In Cosmetics Using Triple Quadrupole GC-MS

The EU Cosmetics Regulation (EC 1223/2009) currently regulates 24 fragrance compounds in cosmetics as allergens, with potential plans to expand the list to over 80 compounds. Accurate monitoring of these allergens in raw materials and finished products is hence essential.

This end-to-end workflow demonstrates the capabilities of GCMS-TQ8040 NX in analyzing 57 fragrance allergens in hair oil. As MRM analysis offers high sensitivity, it allows for greater sample dilution, thereby reducing the possibility of contamination in the injector and enables more stable quality control.

Workflow Solution

Off-Flavor Analysis In Chemical Material Using A Thermal Desorption Method

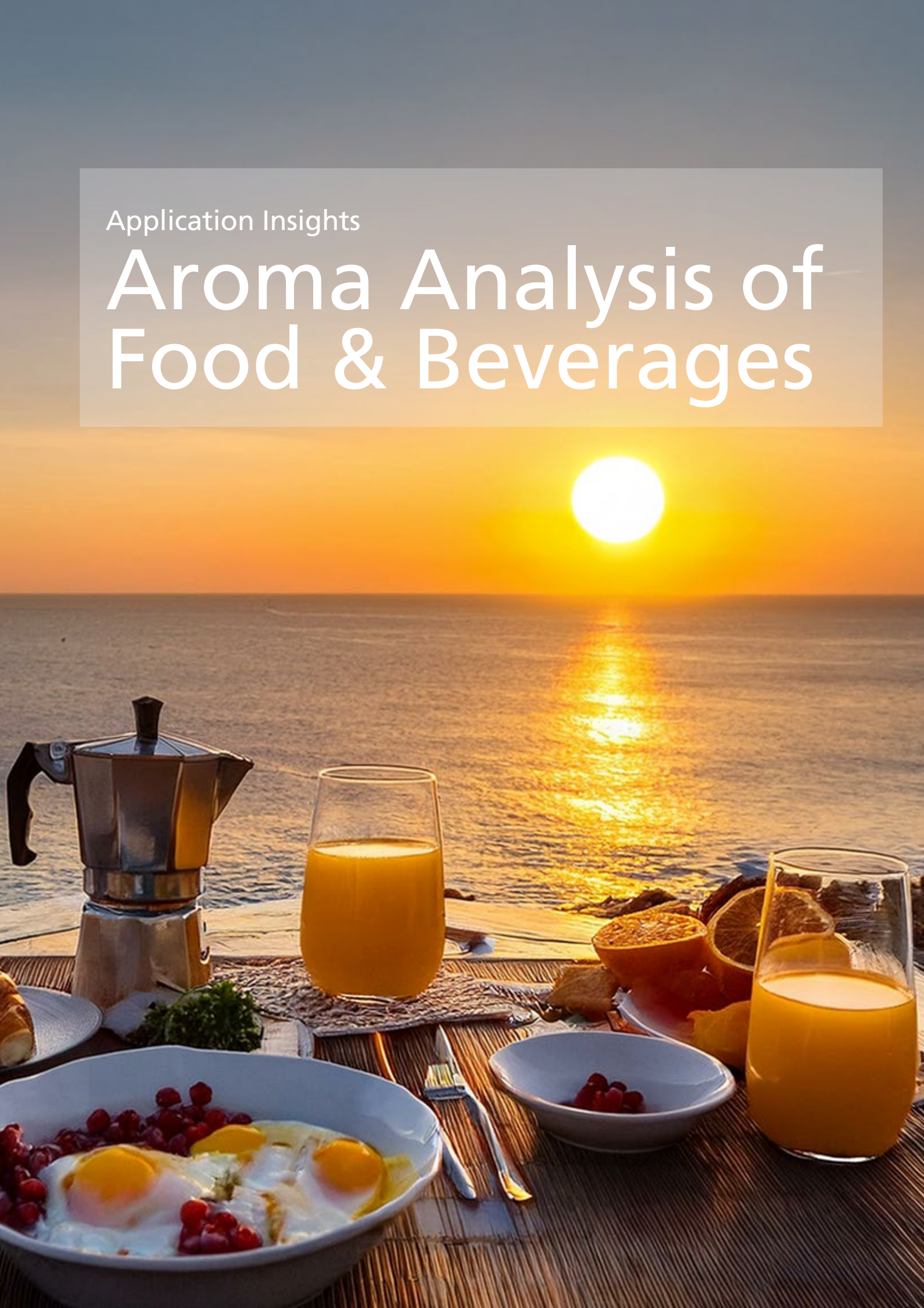
For off-flavor analysis, samples can be pretreated using the thermal desorption method. This process involves heating the sample or adsorbent to a high temperature, producing gases that are then introduced into a GC-MS(/MS) system for analysis.

Shimadzu's GC-MS Off-Flavor Analyzer offers a turnkey solution to aroma analysis. With essential parameters for identifying key off-flavor compounds already in the database, it allows users of all levels to perform accurate and reliable analyses with ease.

Workflow Solution

Application Insights

Aroma Analysis of Food & Beverages



Applications Insights

Aroma transformations during cooking can bring significant changes, such as the shift from the characteristic odors of raw fish to the development of complex and distinctive aroma compounds. The Maillard (aminocarbonyl) reaction plays a crucial role in this process. Advanced tools, such as GC-MS systems, combined with Aroma Database, enable the precise identification and analysis of the key components that contribute to these aromas.

High-Sensitivity Analysis Of Fragrance Components By Trap Mode Of HS-20 Trap Headspace Sampler

Headspace samplers enable high-sensitivity analysis of volatile components by maintaining the sample under controlled time and temperature conditions, introducing the gas phase (headspace gas) into GC.

The Shimadzu HS-20 Trap headspace sampler takes it a step further with its trap mode, which concentrates the headspace gas to detect ultra-trace components previously undetectable with conventional samplers. To showcase its capabilities, the sensitivity of ordinary headspace analysis (loop mode) is compared with trap mode by analyzing fragrance components in a liquid food sample.

Workflow Solution

Evaluation Of Aroma Characteristics Using The Aroma Database – Simple Calculation Of OAV

In aroma analysis, it is essential to determine if compounds are present at concentrations exceeding their sensory thresholds to understand their contribution to the overall aroma.

This workflow highlights the Aroma Database's semi-quantitative function (SQF), which simplifies the traditionally labor-intensive process of calculating the Odor Activity Value (OAV)—a key metric for evaluating an aromatic compound's contribution to overall aroma. By leveraging the SQF, this approach significantly saves time and effort, thereby boosting productivity.

Workflow Solution

Analysis Of Aroma Components In Milk Using Aroma Database

The aroma components of milk greatly influence its deliciousness but can vary based on region, feed, sterilization, and storage. However, their extremely low concentrations make comprehensive analysis challenging.

In this application note, six milk types were analyzed by concentrating their aroma components using the solid-phase microextraction method (SPME Arrow). The samples were then examined using Shimadzu's advanced GC-MS system and Aroma Database, facilitating a detailed and successful comparative study of the aroma components across the different milk samples.

Workflow Solution

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DIGITAL CLASSROOMS

Digital Classrooms

From food and beverages to perfumes, household products, and beyond, aroma analysis is becoming increasingly crucial for enhancing product formulation, ensuring quality control, meeting regulatory requirements, and maintaining sensory consistency.

In this latest session of Shimadzu's Digital Classrooms, explore how Shimadzu's advanced GC-MS systems, Aroma Database, along with other innovative solutions can streamline conventional aroma analysis with accuracy. Together with our experts, gain an in-depth understanding of GC-MS principles, review real-world case studies, and witness how Shimadzu's technologies are enabling industries to drive efficient quality control and accelerate R&D efforts in aroma analysis.

Don't miss this opportunity! Register now and discover the latest insights with us.

LEARNING OBJECTIVES

- Explore advanced GC-MS methodologies for analyzing aroma profiles with precision.
- Discover Shimadzu's solutions designed to enhance identification sensitivity and improve analytical accuracy.
- Examine recent advancements in GC-MS technology and evaluate their transformative potential in aroma analysis workflows.

Register Now

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