

Analytical Solutions for Food Development



List of Products by Purpose of Analysis





Analyzing Deliciousness Scientifically

At Shimadzu, we use our technologies to support the realization of everyone's wish: to eat safe and delicious food.

Shimadzu offers a variety of analytical instruments for objectively evaluating food texture, aroma, flavor, and various other subjective factors that determine whether something tastes good. Such evaluation methods have been developed to obtain objective, quantitative results for supplementing conventional sensory tests in organizations involved in product development or quality control.

Factors Evaluated	Type of Analysis	Instrument	Page	
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	Particle Size Distribution	Particle Size Analyzer	6-7	
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	Mouth Melt Evaluation	Differential Scanning Calorimeter (DSC)	10	
1	Aroma Component Analysis			
Fragrance/ Aroma	Off-flavor Analysis	Gas Chromatograph Mass Spectrometer (GC-MS)	11-13	
	Components with Functional Benefits and Taste Components (bitterness, astringency,	High-Performance Liquid Chromatograph (HPLC) Liquid Chromatograph Mass Spectrometer (LC-MS)	14-17	
	Food Metabolomics	Liquid Chromatograph Mass Spectrometer (LC-MS) Gas Chromatograph Mass Spectrometer (GC-MS)	18-19	
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Flavor	Nutrient Components Vitamins, Amino Acids, Organic Acids, Sugars, Fats/Oils (fatty acids and triglycerides), and	Fourier Transform Infrared Spectrophotometer (FTIR)	_ 24	
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Texture

Food texture characteristics, such as crispiness, chewiness, tooth feel, and tongue feel, are closely related to mechanical properties. Texture analyzers evaluate the physical properties and texture of food materials by applying compression, shear, penetration, or other forces to cause deformation. Because texture analyzers provide measurement results that correlate closely with sensory tests, Shimadzu offers an extensive line of jigs designed for different food characteristics and shapes. By changing jigs or measurement parameters, a variety of food materials can be measured.

■ Examples of Texture Jigs









































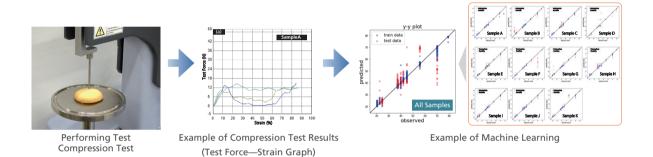


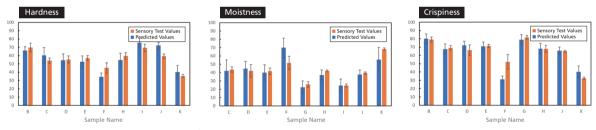


- The EZ Test texture analyzer can be used to test food texture.
- The jig platform enables a wide variety of jigs to be replaced easily.

■ Using Machine Learning to Predict Sensory Test Values for Confectionery (Cookies)

Texture is considered an important factor for determining how food tastes. Though texture is mainly evaluated based on sensory tests, instrument measurements are also used to ensure objectivity and reproducibility. Measuring the complex texture characteristics of food with instruments had been considered very difficult, but approximate predictions can be obtained by using machine learning to predict sensory test values.





Comparison of Sensory Test Results and Machine Learning Predicted Values

Texture Analyzers EZ Test Series

This compact single-column design is available in three capacities: 5 kN, 2 kN, and 500 N. This stylish compact testing machine is packed with extensive functionality that enables convenient and efficient testing operations. EZ Test series offers an ample selection of specialized jigs and applications to support a wide variety of customer needs, such as testing the strength of foods, vegetables, and other food materials, processed foods, and various packaging materials.





Particle Size Distribution

With food products, the particle size distribution is said to have an impact on food texture, including the feeling on the tongue and crunchiness. The human tongue is very sensitive, and is said to be able to recognize the touch of particles several dozen micrometers or larger. As a result, the particle size distribution is an important factor in food product development because the particles can be tiny and uniform, creating a smooth impression, or conversely, large and non-uniform, producing a subtle food texture.

Numerical Quantification of Food Textures

Foods that Contain Solid Particles

- $\bullet \ \, \text{Coarse or non-uniform/irregularly shaped particles}.$
 - → Grainy texture
- · Tiny, uniformly shaped particles
 - → Smooth texture

Food Quality Evaluation

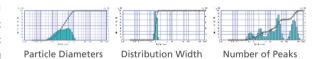
Evaluation of the stability of emulsions, etc. (checking for aggregates/foreign matter)
Stabilizing quality through numerical control

Liquid Foods

- High concentration → Rich or smooth
- Low concentration \rightarrow Refreshing or light

Laser Diffraction/Scattering Method

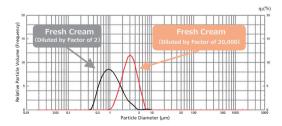
This method irradiates particle groups with laser light and calculates the particle size distribution based on the light intensity distribution pattern of the diffracted or scattered light emitted from the particle groups. In addition to evaluating primary particles, it can also determine the dispersion or cohesion status based on the particle size distribution.



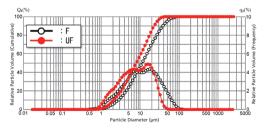


- Reliably captures the particle size distribution as it varies depending on particle concentration.
- The SALD series can measure a wide range of particle concentrations from 0.1 ppm to 20%, which minimizes variations in the dispersion status due to dilution. Therefore, it can evaluate particle distributions in a state as close to the actual product as possible.

Example of Evaluating High Concentrations in a Liquid Product



■ Example of Evaluating Chocolate



Laser Diffraction Particle Size Analyzer SALD-2300

Measurement Range: 17 nm to 2500 µm

Suitable for a variety of measurement samples and objectives, including wet measurement, dry measurement, and high-concentration sample measurement.



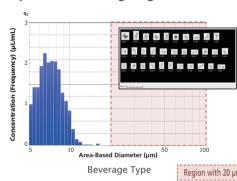
Dynamic Image Analysis

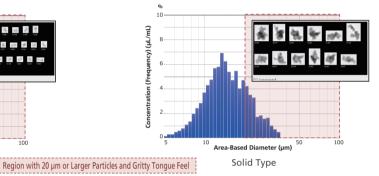
This method can provide a wide variety of information, such as the size concentration and shape of particles, by converting captured images to particle diameter values.



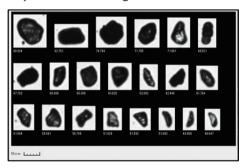
- Texture-related parameters can be evaluated quantitatively by obtaining information about the concentration and shape of 20 µm or larger particles.
- The iSpect DIA-10 is ideal for quantitative evaluations of food texture because it can analyze tens
 of thousands of particles within a few minutes, determining not only their sizes but also their
 concentrations, shapes, and images.

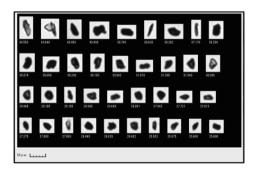
■ Example of Evaluating Yogurt





Example of Evaluating Chocolate





Concentration and Quantity of Particles Larger than a Specified Diameter in Chocolate

	Sample		Max. Length	
	Jample	20 μm or Longer	40 μm or Longer	50 μm or Longer
Count Concentration	F	308	36	19
(Count/mL)	UF	128	5	0
Solid Particle Content	F	308×10 ⁴	36×10 ⁴	19×10 ⁴
(Count/g)	UF	128×10 ⁴	5×10 ⁴	0

Dynamic Particle Image Analysis System iSpect DIA-10

This single system can be used to analyze particle images, particle shapes, particle size distributions, contaminants, and particle count concentrations, which were previously analyzed using multiple specialized instruments, such as particle size analyzers and microscopes.



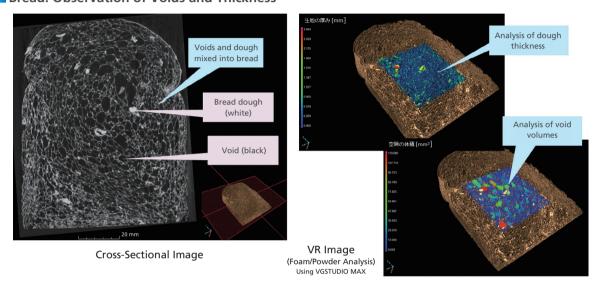
Non-Destructive Observation of Interior Objects



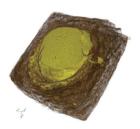


- X-ray CT systems enable the non-destructive visualization of internal structures in objects.
- Enables observing the internal state of bread and other foods with complex porous structures or foods containing mixtures of different substances.
- Voids and thickness distributions within foods can be visualized three-dimensionally and their respective sizes can be calculated.

■ Bread: Observation of Voids and Thickness



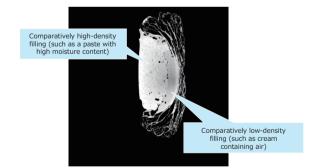
Danish Pastry: Observation of Filling



Enables color-coding 3D images



Enables 3D image clipping for checking filling mixture status



Bench-Top X-Ray CT System XSeeker 8000

The compact XSeeker 8000 bench-top X-ray CT system enables threedimensional observation and imaging inside objects. It offers easy operation, high throughput, and dedicated software that enables acquiring data, reconstructing images, and displaying cross-section images with ease. It assists with detailed observations for product development and quality evaluation.



Product



Measuring Moisture Content

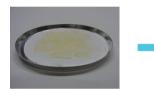
Moisture is one of a food product's constituent substances. In addition to having a major impact on food texture, including firmness and smoothness, it acts as a solvent for the gustatory components sensed as flavor and fragrance. A moisture analyzer determines the moisture content by heating the sample to vaporize the moisture and then calculating the change in mass before and after heating.



- The MOC63u electronic moisture analyzer can accurately measure moisture content quickly and easily.
- Measurements are started by simply placing the sample on the sample pan and closing the cover.
- It can measure a wide variety of samples and contributes to higher productivity.

■ Measurement of Mayonnaise Using a Fiberglass Sheet

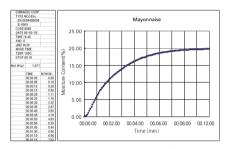
Mayonnaise is highly viscous. Placing the sample on a fiberglass sheet (optionally available), and then spreading it out to a uniform thickness using a spatula before measurement, can shorten the drying time and provide highly reproducible data.



(Before measurement)
The sample is placed on a fiberglass sheet and is then spread out uniformly using a spatula.



(After measurement)
The drying surface of the mayonnaise is increased by the fiberglass sheet so it dries uniformly.



Using the computer connection function, the data can be imported into Excel.

■ Measurement of Moisture Content in Various Foods

The table below summarizes the moisture content measurements for various food product samples using a moisture analyzer. For more details, refer to the Shimadzu website.

	Sample	Measurement Mode		Heating Temp.	Measurement	Moisture	
Sample Name	Amount	Ending Mode	Ending Criterion (% or Minutes)	(°C)	Time (Minutes)	Content (%)	CV Value (%)
Mayonnaise	1g	TIME	10Minutes	160°C	10:00	20.61%	0.46%
Instant coffee	1g	TIME	10Minutes	120°C	10:00	7.43%	1.18%
Chocolate	3g	AUTO	0.01%	140°C	6:18	2.36%	1.49%
Corn starch	5g	AUTO	0.05%	200°C	7:54	12.94%	0.16%
White rice	5g	AUTO	0.05%	200°C	12:30	15.12%	0.53%
Tea	5g	AUTO	0.05%	120°C	9:05	3.76%	0.41%
Milk	1g	AUTO	0.05%	140°C	7:30	87.36%	0.04%

Moisture Analyzer MOC63u

Simply place the sample in the sample pan, and close the cover to begin the measurement. The sample pan has a large diameter of 95 mm and the sample can be uniformly heated, enabling high-precision measurements.

With a variety of measurement modes, the instrument can measure samples in a range of forms, including powders (e.g., wheat flour), granules (e.g., grains), solids (e.g., dried noodles and processed foods), liquids (e.g., beverages), and pastes (e.g., flavorings).





Analysis of Food Melting in the Mouth and Changes over Time

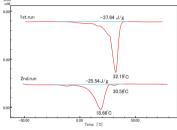




- Differential scanning calorimeters (DSC) can measure phase transitions, such as melting, crystallization, and glass transitions, as well as curing reactions, thermal denaturation, and other thermal processes.
- They can evaluate food melting in the mouth using sample quantities as small as a few tens of milligrams.

Evaluation of Chocolate Melting Behavior in the Mouth

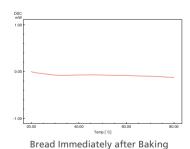
Six forms of crystals are present in cocoa butter contained in chocolate. Of these form V is considered to have good thermal stability. Given that form V crystals melt at about 33 °C, the state of form V crystal formation in chocolate can be determined by measuring the chocolate with a DSC. The DSC graph shown below labeled "1st run" was obtained when the chocolate was heated at a rate of 3 °C/min. The DSC graph labeled "2nd run" was obtained when melted chocolate was hardened by cooling to -50 °C and then reheated. Note that the peak that appears at 32.19 °C in the 1st run graph has disappeared in the 2nd run graph. That indicates that the crystal form in the cocoa butter changed.



DSC Graphs of Chocolate

■ Measurement of Time-Course Changes in Bread

The relationship between the degradation of bread and the number of days after baking was investigated by measuring bread degradation. The graphs show that the transition heat increases with the increasing number of days elapsed but remains unchanged after nine days. These results indicate that the bread in this example begins degrading immediately after baking, but stops degrading after nine days. Note, however, that the degradation speed varies depending on the type of starch used, the sugar content, whether it contains oil or fat, and other factors.



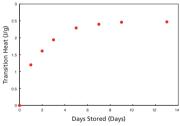
After 1 Day Heat: -1.09 J/g

After 5 Days Heat: -2.29 J/g

After 9 Days Heat: -2.46 J/g

-1.00

After 9 Days Heat: -2.46 J/g



Bread 1, 5, and 9 Days after Baking

Transition Heat vs. Days of Bread Storage

Differential Scanning Calorimeter DSC-60 Plus

Used to determine changes in the temperature and heat content of samples due to glass transitions, melting, crystallization, or other transitions/reactions by measuring the temperature difference between the sample and reference substance.



- Ensures a wide ±150 mW dynamic range
- Compact space-saving design (W320 × D500 × H290 mm)





Aroma Component Analysis

Flavor compounds, which comprise fragrance/aroma and flavor components, are the main factors that affect consumer recognition. Gas chromatograph mass spectrometer (GC-MS) systems are used to analyze the aroma components of foods and beverages due to their superior qualitative analysis capabilities. Multiple methods are used to sample aroma components, which are classified as top-note, middle-note, or base-note components depending on their volatility, any of which can affect the composition of flavors. Various sampling methods, such as trace analysis or automation, are available for configuring the best method for given needs. The following example describes using headspace GC/MS and SPME GC/MS methods.

Headspace (Trap) Method

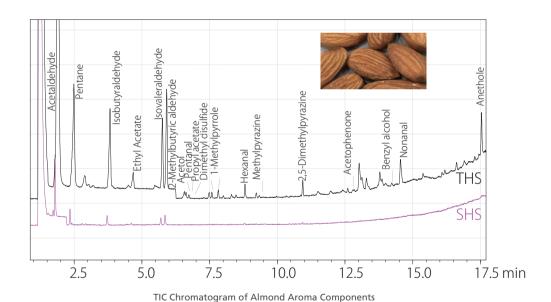


- Components with boiling points ranging from low to high can be quickly analyzed at the same time.
- Achieves about 5 to 20 times higher sensitivity than static headspace (SHS) analysis.
- Both trap and loop modes can be used by switching back and forth based on the concentration level

■ Analysis of Aroma Components Emitted from Almonds



Samples were sealed in headspace vials and heated in an autosampler (HS-20 NX TRAP). Then, the evolved gases were injected by the standard mode (SHS) and trap mode (THS) for analysis. A measurement example is shown.



Headspace Sampler HS-20 NX Gas Chromatograph Mass Spectrometer GCMS-QP2050

This system uses a gas chromatograph (GC) to separate the compounds contained in a sample based on their components and then ionizes the components to analyze their masses. It enables more accurate qualitative analysis than gas chromatography and can separate components even in the presence of contaminant components. It also offers higher sensitivity and can measure lower concentrations.



Aroma Component Analysis

SPME Arrow Method

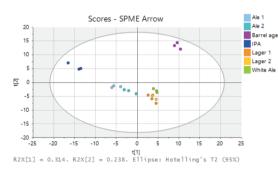


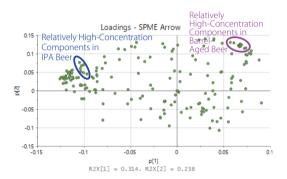
- The Smart Aroma Database enables efficient analysis of aroma components using information about approximately 500 aroma-related components registered in the database.
- Methods can be created easily using the Smart Aroma Database without having to reconsider analytical conditions.
- Concentrating components with an SPME Arrow can achieve high-sensitivity analysis, which is
 especially useful for research and development of aroma components.

■ Analysis of a Wide Range of Target Aroma Components in Beer



Seven types of commercially sold beers were used as samples. Each vial was filled with 8 g of beer and 3 g of NaCl, sealed, and measured. Compounds were identified based on the retention time, ion, and mass spectrum information registered for each compound in the Smart Aroma Database. As a result, 204 aroma components were identified from 7 types of beer. The score plot and loading plot from primary component analysis (PCA) of the detected components are shown below.





Principal Component Analysis of Aroma Components in 7 Types of Beer (Left: Score Plot, Right: Loading Plot)

Components contained in relatively high concentrations in two of the beer types, IPA and barrel-aged, and the characteristics of those components are listed below. The results show that the barrel-aged beer contained higher concentrations of honey, vanilla, coconut, and other components that provide a rich sweet aroma, whereas the IPA contained higher concentrations of components that provide a herbal and grassy aroma.

Components Contained in Relatively High Concentrations in Respective Beers

Barr	el aged	IPA		
Compound	Odor Characteristics	Compound	Odor Characteristics	
Ethyl lactate	fruit	3-Methyl-2-buten-1-ol	herb	
4-Ethyl-2-methoxyphenol	spice, clove	1-Hexanol	resin, flower, green	
3-Ethylphenol	must	trans-Rose Oxide	flower	
Diethyl succinate	wine, fruit	3-Ethoxy-1-propanol	fruit	
Benzyl alcohol	sweet, flower	cis-3-Hexen-1-ol	grass	
Eugenol	clove, honey	Geranyl acetate	rose	
(E)-Whiskey lactone	flower, lactone	Methyl salicylate	peppermint	
(Z)-whiskey lactone	coconut	Ethyl salicylate	wintergreen, mint	
gamma-Decalactone	peach, fat			
Ethyl vanillate	flower, fruit, sweet, vanilla			
Benzaldehyde	almond, burnt sugar			

Database for GC-MS(/MS) Aroma Analysis Smart Aroma Database

This database provides comprehensive support for analyzing aroma components using a GC-MS (or GC-MS/MS) system. The database includes analytical information (MRM and SIM modes) and compound information for over 500 components, which enables reliable and easy detection of components based on retention time, characteristic ion, and mass spectral information.



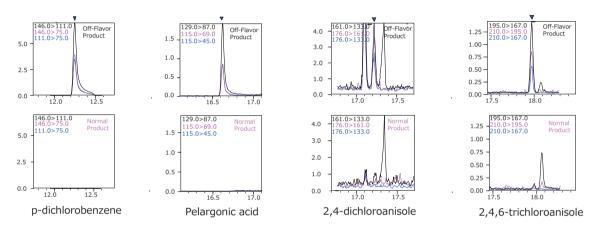


Off-Flavor Analysis



- With expert knowledge about off-flavor analysis consolidated in database form, the database allows even users with minimal experience to start analyzing odors.
- Enables accurate identification and easy quantitation even without standard samples.
- The GC/MS (or GC-MS/MS) high-sensitivity MRM or SIM modes can be used to detect odor threshold values.
- Odor-causing substances can be identified based on the odor characteristics and the odor threshold values.

The GC/MS Off-Flavor Analysis System was used to compare measurements from normal and off-flavor food samples. Results from identifying components contained in higher concentrations in off-flavor samples than in normal samples are shown below.



Results from Measuring 4 Components Contained in Higher Concentrations in Off-Flavor Samples

Estimated concentration values (simplified quantitation results), odor characteristics of respective components, and odor threshold values are listed below for comparing concentration and odor threshold values. Given that the estimated concentration was higher than the odor threshold value for 2,4,6-trichloroanisole but below the odor threshold values for the other 3 components, despite being detected, the odor-causing component could be identified as 2,4,6-trichloroanisole.

Comparison of Concentrations and Odor Threshold Values, and Corresponding Odor Characteristics

Four Components with Higher	Estimated Concentration (pg/mg)		Odor Threshold Value	O de a Chemante de de	
Concentrations in Off-Flavor Samples than in Normal Samples	Normal Product	Off-Flavor Product	(pg/mg)	Odor Characteristics	
p-dichlorobenzene	0.052	66.998	1000.000	Insect repellent	
Pelargonic acid	0	0.851	100.000	Dried fruit	
2,4-dichloroanisole	0	0.003	10.000	Mold	
2,4,6-trichloroanisole	0	0.009	0.001	Mold	

GC/MS Off-Flavor Analysis System

The solid phase microextraction (SPME) method concentrates components, by adsorbing them onto a fiber, before injection into the GC-MS system, which enables high sensitivity analysis.

This system enables all steps, from pretreatment to analysis, to be fully automated

The GC/MS Off-Flavor Analysis System is software specialized for assisting the analysis of off-flavor components.



Analyzing Functional and Taste Components

"Functional components" refer to food components that help regulate biological processes and are considered beneficial for maintaining health when consistently ingested as food. Agricultural products and foods that contain high levels of such functionally beneficial components and foods or supplements with those components actively added have attracted considerable attention. Some functionally beneficial components also provide taste, such as umami, sweetness, bitterness, or acidity, and can significantly affect the flavor of foods depending on their type or concentration. Various types of polyphenols, catechins, and other components have a bitter, astringent, or acidic taste, which are not only important flavor elements but also widely known to offer functional benefits for inhibiting oxidation and promoting metabolism. Such trace quantities of functional components in food are analyzed using a high-performance liquid chromatograph (HPLC) or high-performance liquid chromatograph mass spectrometer (LC-MS).

Examples of Methods Used to Measure Functional Components

Functionality	Component	Measurement Method
Bitterness, Astringency, and Acidity	Catechins, caffeine, chlorogenic acid, caffeic acid, trigonelline, humulinone, iso-α-acid, α-acid, and β-acid	HPLC
	Catechins and theaflavins	LC-MS
Umami, Sweetness, Bitterness, and Acidity	D/L-amino acids	HPLC, LC-MS
Non-Taste Functions	Pyrocatechol, xanthohumol, and isoxanthohumol	HPLC

High-Performance Liquid Chromatograph

i-Series integrated LC systems consistently provide highly reliable analytical results with flexibility for satisfying the needs of increasingly diverse personnel, workplaces, the same outstanding performance as previous HPLC systems.

Nexera series ultra high performance liquid chromatography (UHPLC) systems serve as the industry standard in terms of intelligence, efficiency, and design.

High-Performance Liquid Chromatograph Mass Spectrometer

To satisfy the increasingly diverse needs of analytical workplaces, LCMS-TQ RX series triple quadrupole mass spectrometers are designed to offer reliability, resilience, and responsibility based on a combination of state-of-the-art Shimadzu technologies. Boasting hardware with outstanding reliability and consistency and software that offers outstanding operability and exceptional automation technology, these systems provide new value.





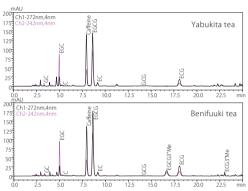
Analysis of Catechins





 This test method is prevalidated for all steps from sample pretreatment, according to the method jointly developed with the National Agriculture and Food Research Organization, to measurements by HPLC.

Chromatograms from analyzing leaf extract solutions are shown below. Two types of tea leaves were quantitated to determine the difference in catechin content depending on the variety.



Chromatograms from Tea Leaf Extract Solutions

Catechin Analysis Kit

Using the test method indicated above, this kit provides support for quickly and easily quantitating the concentrations of catechins contained in tea leaves and a green tea beverage. The kit enables highly reliable catechin measurements to be performed easily, with quantitative results immediately available for checking in a report. Thus, it offers powerful support for acquiring data needed for development of foods with functional claims, application for approval, and quality control.



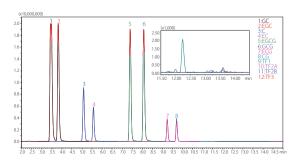
Simultaneous Analysis of Catechins and Theaflavins



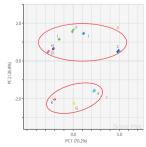


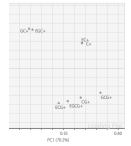
- Enables simultaneous analysis of 8 types of catechins and 4 types of theaflavins contained in tea.
- Traverse MS data analysis software enables easy multivariate analysis by quickly processing MRM data from multiple analytes and components.

Chromatograms from green tea and results from using Traverse MS software for principal component analysis (PCA) of 9 types of green tea are shown below. Multivariate analysis provides easy-to-visualize and understand data analysis results.



Chromatograms of Green Tea





PCA Results

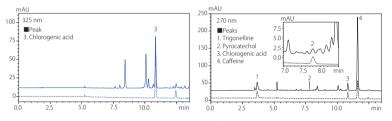
Analysis of Coffee



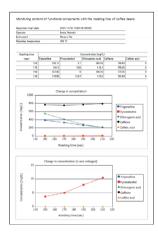


- Highly polar coffee components ranging from acidic to basic can be analyzed simultaneously.
- Retains peaks with good reproducibility for substances that contain basic portions with low retention in a typical reversed-phase column.
- Can quickly and efficiently create reports for multiple analyses by automating the transcription of analytical results and graphing.

Among the functionally beneficial components in coffee, trigonelline levels are known to decrease as coffee beans are roasted, whereas chlorogenic acid is known to be hydrolyzed by the coffee bean roasting process, which converts it to pyrocatechol via caffeic and quinic acids. The content of respective functional components in coffee relative to the roasting time can be monitored by acquiring analytical results from different roasting times and then using a multi-data report to automatically create a spreadsheet file.



Chromatograms of Coffee



Multi-Data Report

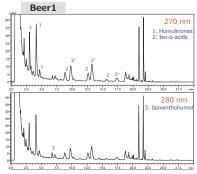
Analysis of Beer

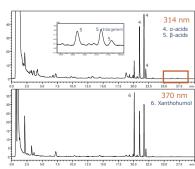




- Enables simultaneous analysis of xanthohumol and isoxanthohumol, which reportedly provide health benefits, and components involved in providing bitterness (humulinones, iso- α -acids, α -acids, and β -acids).
- Analytical conditions that inhibit the effects of contaminant components improve the ability to quantitate components.

Hops contain components that contribute to the bitterness of beer, such as humulinones, iso- α -acids, and β -acids. Chromatograms from analyzing beers are shown below. Improved separation of contaminant components from the xanthohumol, isoxanthohumol, humulinones, iso- α -acids, α -acids, and β -acids contained in beer results in simultaneous analysis that is less affected by contaminant components.





Chromatograms of Beer

Analysis of D/L Amino Acids in Yogurt Drinks

Application -



- Multiple D/L-amino acid components can be analyzed simultaneously using the LC/MS/MS method package.
- Without the need for derivatization, high-speed, high-separation, and high-sensitivity analysis
 can be executed automatically.

L and D-amino acids taste different, with D-amino acids reportedly exerting a broad influence on the flavor of fermented foods and aged foods. Furthermore, D-amino acids have attracted attention for product development and quality control applications, with D-amino acids anticipated for use as a new umami component or sweetener. Results from analyzing D/L-amino acids in yogurt drinks from different manufacturers are indicated in the table on the right. For some amino acids, the D-amino acid ratio is relatively high, and significant differences in the component ratio of D/L amino acids are evident depending on the manufacturer. It is suggested that this may contribute to differences in flavor qualities.

High-Performance Liquid Chromatograph Mass Spectrometer with LC/MS/MS Method Package for D/L Amino Acids

With two types of chiral separation columns, this analysis system uses an LC/MS/MS method package that includes parameter settings for simultaneous analysis of 42 D/L-amino acid components in 10 minutes. Because derivatization is not necessary for pretreatment, D/L-amino acids can be analyzed quickly with high sensitivity, which means analytical operations can be executed efficiently.

Note: The analysis methods in this method package were developed based on the research results of the Fukusaki Laboratory in the Graduate School of Engineering at Osaka University.

References: Y. Nakano, Y. Konya, M. Taniguchi, E. Fukusaki, *Journal* of *Bioscience and Bioengineering*, 123, 134-138 (2016)



D/L Ratio in Yogurt Drinks

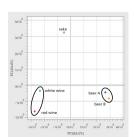
D/L Component Ratio	Yoghurt A	Yoghurt B
Alanine	164.0%	40.2%
Arginine	6.9%	36.5%
Asparagine	43.2%	16.5%
Aspartic acid	38.1%	15.3%
Cysteine	-	-
Glutamine	0.6%	19.8%
Glutamic acid	4091.1%	5069.6%
Histidine	-	5.2%
Isoleucine	0.8%	1.0%
Alloisoleucine	59.4%	39.3%
Leucine	1.0%	-
Lysine	73.5%	3.5%
Methionine	0.9%	-
Phenylalanine	0.5%	1.5%
Serine	14.4%	29.3%
Threonine	1.5%	4.6%
Allothreonine	42.5%	23.7%
Tryptophan	1.9%	13.3%
Tyrosine	2.1%	107.4%
Valine	0.4%	0.9%

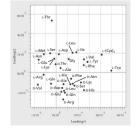
Analysis of D/L-Amino Acids in Alcoholic Beverages



- Using a simple UHPLC system configuration enables simultaneous analysis of D/L-amino acid components without using MS or multidimensional LC systems.
- Simple and high-sensitivity analysis with high quantitative accuracy can be achieved using automatic mobile phase preparation and automatic pre-column derivatization.

Using a general-purpose UHPLC system in combination with automatic mobile phase preparation and automatic pre-column derivatization enables simple quantitation results with high reproducibility. PCA analysis results from analyzing D/L-amino acids in alcoholic beverages are shown below. It suggests that PC1 indicates the differences between the types of alcoholic beverages and PC2 indicates the differences between isomers. This method could presumably be used for profiling D/L-amino acids in alcoholic beverages.





PCA Results (n = 4)

References: N. Iwata, M. Kobayashi, *Chromatography*,45, 63-72 (2024)

Statistical Analysis Software eMSTAT Solution

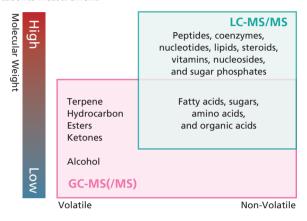
Conventional qualitative and quantitative analysis methods are inadequate for identifying differences between different groups involved in product development or quality control. Multivariate analysis using massive amounts of chromatogram and MS spectral data enables the search for differentiation markers and the visualization of characteristics. Equipped with a wide variety of statistical analysis functionality, eMSTAT Solution provides easy access to multivariate analysis without the need for operating proficiency.



Comprehensive Metabolomic Analysis



Metabolites in biological samples are widely involved in the flavor and aroma of food products. Accordingly, metabolomic methods, which involve a comprehensive analysis of metabolites, are being actively applied to research and development, including for analyzing taste components and the stability of fermented food quality. "Wide target quantitative metabolome analysis" is an approach used in the food development field to efficiently search for taste components by using a triple quadrupole mass spectrometer (GC-MS/MS or LC-MS/MS), which provides excellent resolution, quantitative analysis capability, and consistency, in combination with a database for primary metabolite measurement.







LC-MS/MS

Gas Chromatograph Mass Spectrometer

- Hundreds of components can be analyzed simultaneously in a single measurement.
- Excellent robustness.

Liquid Chromatograph Mass Spectrometer

- Specific metabolites (up to 100 components) can be measured easily.
- Non-volatile metabolites with a high molecular weight can be measured.

GC/MS Database—Smart Metabolites Database Ver. 2

Registered Compounds	Derivatization Method	Measurement Method	Number of Compounds Registered
Organic acids, fatty acids, amino acids,	TMS	SIM	627
sugars, etc.	11013	MRM	540
Fatty acids	Methylation	SIM	50
	Wethylation	MRM	50
Sugars	Acatulation	SIM	24
Sugars	Acetylation	MRM	24

LC/MS Database—LC/MS/MS Method Package Ver. 3

Registered Compounds	Method	Number of Compounds Registered
Metabolites, amino acids, nucleotides, etc. in the major metabolic pathways	Ion pair reagent used	114
Amino acids, organic acids, bases, etc.	PFPP columns used	143

Example of a Food Metabolomics Application

Item	Target	Component	Sample
Deliciousness	Taste Components	Primary metabolites and dipeptides	Liquors, beverages, fermented food products,
Deliciousness	Odor	Volatile components	agricultural crops
Functionality	Functional Components	Secondary metabolites	Agricultural crops, fermented foods, herbal medicines
Functionality	Effects of Components	Primary metabolites	Blood, urine, cells
Quality and	Fermented and Brewed Products	Primary metabolites	Fermented food products
Productivity	Plant Breeding (Agricultural Products)	Primary metabolites, phytohormones	Agricultural crops
Distribution and Storage	Degradation of Components (Mislabeled Food or Quality during Distribution/Storage)	Volatile components, primary metabolites	Agricultural crops, food products

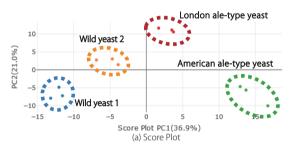
Approach for Using Metabolomics for Beer Development

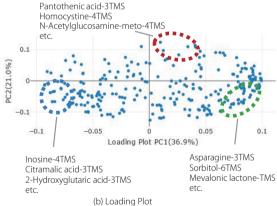




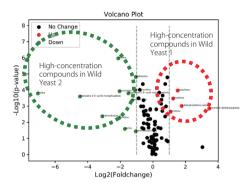
- Enables comprehensive aroma and metabolite analysis using Smart Aroma Database and Smart Metabolites Database ver. 2.
- Metabolomic data obtained by GC-MS or LC-MS can be efficiently analyzed using the Multi-omics Analysis Package.

The metabolite components in beer were analyzed using GC-MS/MS and LC-MS/MS systems. The GC-MS analysis identified 235 components, mainly consisting of amino acids, organic acids, and sugars, whereas the LC-MS analysis identified 104 components, mainly consisting of amino acids, vitamins, and nucleic acid bases. Multivariate analysis results confirmed that the 4 types of beers had characteristic metabolite components.

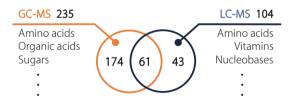




Results from Principal Component Analysis of Metabolite Components Detected by GC-MS



Volcano Plot (LC-MS Analysis of Wild Yeasts 2 vs 1)



Number of Metabolites Detected by GC-MS and LC-MS

Multi-omics Analysis Package

The Multi-omics Analysis Package is metabolic engineering software that can automatically plot metabolic maps and perform a variety of data analysis functions based on the vast amounts of mass spectrometry data generated, such as from metabolomics, proteomics, and flux analysis. In combination with the various method packages and databases offered by Shimadzu for metabolomic analysis, the Multi-omics Analysis Package can increase the efficiency of metabolomic data analysis operations. By presenting data in an easy-to-understand format, it provides powerful support for drug discovery, functional food bioengineering, and other life science research applications.



Nutrient Component Analysis

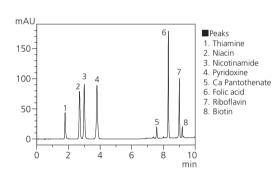
Vitamins serve to maintain proper body functions, but almost none of them can be synthesized within the body, so they must be obtained from foods. Vitamins can be classified as either water-soluble vitamins that dissolve easily in water or fat-soluble vitamins that do not dissolve easily in water. Both types of vitamins can be analyzed with high sensitivity and accuracy using a high-performance liquid chromatograph or high-performance liquid chromatograph mass spectrometer.

Simultaneous Analysis of Water-Soluble Vitamins



• Using a Shim-pack MAqC-ODS I column, even water-soluble vitamins with weak retention in a typical reversed-phase mode column can be analyzed without using an ion-pair reagent.

The following is an example of analyzing water-soluble vitamins in a multivitamin tablet. Typically, an ODS column is used for simultaneous analysis of water-soluble vitamins, with an ion-pair reagent added to the mobile phase. If a Shim-pack MAqC-ODS I column is used, vitamins can be analyzed simultaneously without adding an ion-pair reagent to the mobile phase.



Shim-pack Series Shim-pack MAqC-ODS I

Shim-pack MAqC-ODS I reversed-phase columns are packed with a silica gel containing metal and added octadecylsilyl groups. In addition to hydrophobic characteristics due to the ODS, the metal content also provides cation-exchange effects. That significantly increases the retention of basic compounds and enables the analysis of water-soluble vitamins using regular mobile phase.



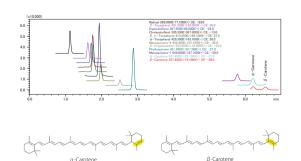
Simultaneous Analysis of Fat-Soluble Vitamins





• Enables simultaneous analysis of 13 fat-soluble vitamins and individual quantitation of α - and β -carotene.

The following is an example of simultaneously analyzing 13 fat-soluble vitamins in vegetable juice. It enables individual quantitation of α -and β -carotene, which are structural isomers.



High-Performance Liquid Chromatograph Mass Spectrometer LCMS-8050RX

This enables simultaneous analysis of multiple components by mass separation. The RX series includes CoreSpray technology that enables significantly more consistent analysis than previous models.





Analysis of Amino Acids in Food





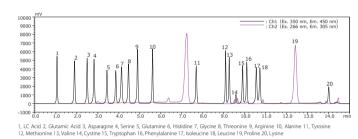
More than any other amino acid, glutamic acid is widely known as a component that provides an umami flavor. Similarly, glycine and alanine provide sweetness, valine and leucine add bitterness, and aspartic and glutamic acids provide acidity. Thus, amino acids can have a major effect on the flavor of foods depending on their type and ratio.



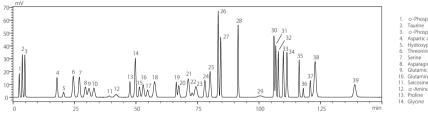
- HPLC provides an excellent way to quantitatively analyze amino acids.
- With a pre-column, amino acids can be analyzed quickly using a general-purpose HPLC system.
- The post-column amino acid analysis system that performs derivatization after separation is less susceptible to the effects of contaminants.

■ Amino Acid Measurement Methods

Either pre-column or post-column methods can be used for HPLC analysis. Though a variety of pre-column methods are available, a typical example using general-purpose HPLC analysis is shown to the right. The derivatization reaction is performed within the autosampler for selective and high-sensitivity measurement by a fluorescence detector. The post-column method involves using a dedicated amino acid analysis system that can analyze 37 free amino acid components.



Example of Pre-Column Amino Acid Analysis



Example of Post-Column Amino Acid Analysis

15. Alanine (28. y -Aminobutyric. (GARA) (GARA) (GARA) (GARA) (SARA) (SA

Pre-Column Amino Acid Analysis: i-Series/Nexera Series + RF-20AXS System

The automatic pretreatment functionality of the autosampler was used for amino acid analysis by the pre-column derivatization method. In addition to automating pre-column derivatization operations to reduce labor requirements, the system enables high-accuracy measurements. Because a general-purpose HPLC system is used, it can also be used for applications other than amino acid analysis.



Product -

Nexera Post-Column Amino Acid Analysis System

Amino acid analysis is not only important for food analysis but also serves an important role in natural substances, pharmaceuticals, and other fields. The system can selectively and sensitively quantitate amino acids in samples containing high quantities of contaminant components by using post-column fluorescent derivatization detection, which uses an o-phthalaldehyde (OPA)/ N-acetylcysteine reaction reagent.





Measurement of Organic Acids in Foods

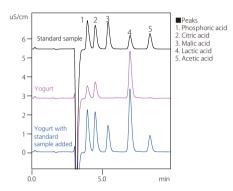




 Organic acids can be quantitated even more selectively by using the post-column pH buffering method for HPLC.

Organic acids are analyzed in a wide variety of fields, not only as flavor and aroma components in foods, but also as potential ingredients in drugs and chemical products. HPLC analysis of organic acids allows selecting from multiple separation modes, such as ion-exclusion, ion-exchange, and reversed-phase, and also choosing between UV, electrical conductivity, and other detection modes.

lon-exclusion column and post-column pH-buffered electrical conductivity detection methods can selectively detect organic acids by inhibiting matrix effects originating from the sample.



Chromatogram of Pretreated Yogurt

Organic Acid Analysis System



- Separation by Ion-Exclusion Chromatography
- → Offers high separation selectivity due to the difference between the acid dissociation constant and the hydrophobicity of organic acids.
- Combination of post-column pH-buffered method and electrical conductivity detection.
 - → Both high sensitivity and high selectivity.
 - \rightarrow Easy to analyze simultaneously due to consistent peak intensity.
- Set of reagents increases productivity.
 - → Simplifies the process up to starting analysis by minimizing wasted time and preparation errors.
 Product







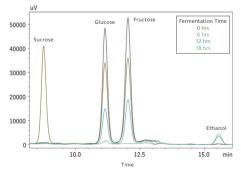
Sugars are often measured by HPLC due to their high water solubility that stabilizes them in aqueous solutions. Different HPLC separation columns, such as ligand exchange, HILIC, size exclusion, and anion exchange columns, are used for different applications. Furthermore, since sugars and sugar alcohols exhibit almost no UV absorption, they are detected using a differential refractive index detector or an evaporative light scattering detector.

Fermentation Monitoring Measurements by Sugar Analysis



- Ligand exchange columns enable analysis using only water as the mobile phase and eliminate the trouble of mobile phase preparation.
- Ability to analyze monosaccharides easily enables monitoring measurements.

A ligand exchange column for sugar analysis can be used to discriminate between glucose, fructose, and other isomers with hydroxyl groups in different positions within chair conformations. Isomers can be separated based on differences in the strength of complexes formed between hydroxyl groups in sugar and the metal ions in the stationary phase.



Chromatogram of Yeast Fermentation Culture Solutions

Nexera Series Differential Refractive Index Detector

The RID-20A differential refractive index detector includes a dual temperature control function of the optical system and lamp performance improvements that ensure stable baselines that are not affected by room temperature changes.



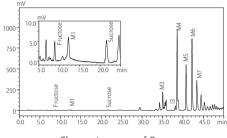
■ Measurement of Monosaccharides to Sugar Alcohols and Oligosaccharides





- In addition to mono- and disaccharides, hydrophilic interaction chromatography (HILIC) can be used to analyze oligosaccharides.
- Using an ELSD-LT III evaporative light scattering detector allows simultaneous analysis of sugars by gradient elution.

An Evaporative Light Scattering Detector (ELSD) enables separation of maltooligosaccharides, isomaltooligosaccharides, and other sugars, enabling the quantitative analysis of those components in beer. Using functionality for extending the dynamic range of the ELSD-LT III, sugar components can be quantitated with optimal sensitivity without reviewing sensitivity settings, even for samples with large differences in component concentrations.



Chromatograms of Beer

HPLC Nexera Series Evaporative Light Scattering Detector ELSD-LT III



Evaporative light scattering detectors (ELSD) are general-purpose (universal) detectors that can even detect components with no UV absorption, such as sugars, lipids, surfactants, and synthetic polymers.* The ELSD-LT III model offers exceptional sensitivity, a wide dynamic range provided by Analytical Intelligence, and easy operation using LabSolutions software. Consequently, it is commonly used in a wide variety of fields.

* Excluding some volatile compounds.

Product -

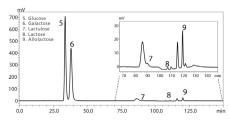
■ High-Sensitivity Measurement of Lactose in Low-Lactose Product





This post-column reducing sugar analysis system can analyze reducing sugars with high sensitivity.

Lactose is a disaccharide formed from galactose and glucose that is contained in large quantities in dairy products. However, over 70 percent of the world's population is known to suffer from lactose intolerance, which is a digestive disorder that occurs if there is insufficient lactase, the enzyme that breaks down lactose by hydrolysis, activity or secretion within the intestines. Therefore, a variety of low-lactose and lactose-free products are being developed for people with lactose intolerance. The reducing sugar analysis system enables simultaneous analysis of lactose, allolactose, lactulose, and other sugars in low-lactose dairy products.



Chromatogram of Low-Lactose Milk (100-Fold Dilution)

Nexera Reducing Sugar Analysis System

The Nexera reducing sugar analysis system is based on Shimadzu's proprietary method of post-column boric acid-arginine fluorescence derivatization. Offering both high sensitivity and a wide dynamic range, the system can simultaneously analyze all sugars in samples even if there are large differences between their respective concentrations.



The taste of meats and fish is determined not only by gustatory components, but is often enhanced by the fat components contained in adipose tissue that provide a smooth mouthfeel.

Fats serve an important role in the physical structure of food, such as by providing a crispy texture or producing a creamy texture by entrapping tiny air bubbles. Therefore, the types and content levels of triacylglycerol and fatty acids, which are the main components in fats, are commonly analyzed to check the chemical characteristics of fats in food.

Analysis of Fatty Acids in Fish Oil

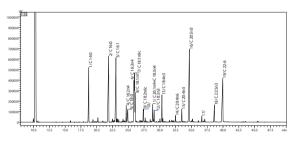


 Enables precisely measuring the number of carbons or the composition of fatty acids with different degrees of unsaturation (double bonds).

This example shows the measurement of fish oil by hydrolysis and methyl esterification.

The fatty acid methyl esters were identified by using a standard sample to determine separation and retention times.

The C18:1n9 label in the chromatogram indicates the component contains 18 carbons and 1 double bond in position 9, which corresponds to oleic acid.



Fatty Acid Methyl Esters in Fish Oil

Gas Chromatograph Brevis GC-2050



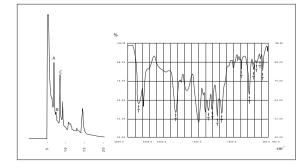


Analysis of Fatty Acids in Red Wine



- A combination of various analytical techniques is used to efficiently analyze foods composed of various compounds.
- Enables structural estimation of compounds based on infrared absorption spectra.

This example describes the use of a liquid chromatograph to separate components in a red wine that was filtered through a membrane filter, followed by measuring the separated components with an infrared spectrophotometer. A peak attributed to tartaric acid (a fatty acid) is clearly detected.



Fourier Transform Infrared Spectrophotometer IRXross

This instrument primarily performs structural estimations of organic compounds. When molecules are irradiated with infrared rays, the absorbance of the infrared rays differs depending on the structure of the molecules. Quantification



and structural estimations of compounds are performed by investigating the absorbance (infrared absorption spectrum) pattern. Measurements can be performed with relatively simple pretreatment. A wide range of samples can be analyzed, making it especially useful in the fields of food product development and quality control.



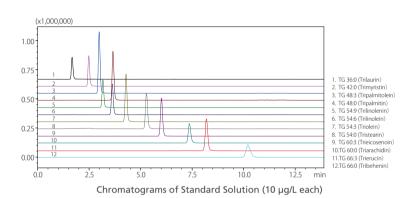
Analysis of Triglycerides in Cooking Oil

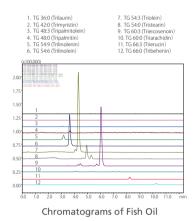




 Supercritical fluid chromatography can be used to measure components that are difficult to separate by HPLC.

Triglycerides are neutral fats stored in adipose and other tissues of animals and decomposed to supply energy whenever cells need energy. Large amounts of triglycerides are also contained in foods and are known to be a principal component of vegetable oils. Triglycerides are highly hydrophobic molecules that consist of 3 fatty acids (acyl groups) bonded to a glycerol (glycerin) and exist in many different forms depending on differences in the acyl group composition or bond positions. The types of acyl groups that form triglycerides in vegetable oil differ depending on the raw material used to produce the oil. The following is an example of using supercritical fluid chromatography (SFC) to analyze triglycerides.





Supercritical Fluid Extraction/Supercritical Fluid Chromatograph Nexera UC

Supercritical fluid chromatography (SFC) is a separation technique that uses supercritical carbon dioxide as the mobile phase. Due to the different retention behavior of SFC compared to HPLC, SFC can provide new separation selectivity. Additionally, the high penetration and diffusivity characteristics of the supercritical fluid can provide better peak shape and separation than HPLC. Furthermore, the broad line of Nexera UC systems offered can help maximize instrument uptime rates and achieve more efficient preparative purification operations. In addition, by using supercritical fluid as an extraction solvent (SFE), it can reduce the labor required for pretreatment processes and can even significantly increase the efficiency of overall analytical operations by connecting SFE and SFC processes online.

- Enables the ultimate in high separation.
- ightarrow Enables shorter analysis times without sacrificing separation, even when using faster flow speeds than HPLC.
- Enables both UHPLC and SFC analysis with a single system.
- \rightarrow Two different separation methods can be used for screening during method development.
- Automates processes from extraction to analysis.
 - \rightarrow Preparative fractions can be dispensed into MTP plates by adding a fraction collector.
- Supports small-quantity preparative separation.
- → Previous pretreatment methods involved adding reagents, centrifugal separation, and many other steps, but Nexera UC systems require no such complicated operations, which can significantly improve the efficiency of analysis operations.
- Supports reducing environmental impact.
- ightarrow Compared to using normal phase HPLC for the same analysis, Nexera UC can reduce solvent consumption by 94 %.





Analysis of Minerals in Food



Minerals are one of the five major sources of nutrients, along with proteins, fats, carbohydrates, and vitamins. Sixteen minerals, including sodium, calcium, and iron, are considered essential nutrients for humans. They perform important functions such as supporting the activities of organs and cells or forming teeth and bones.



- EDX analyzers can analyze minerals in foods directly or with only simple pretreatment.
- Enables the non-destructive analysis of various sample forms, such as solids, liquids, and powders.
- Light elements can be analyzed with higher sensitivity by analyzing samples in a vacuum or in a helium-purged environment.

Samples were prepared by pulverizing cabbage core or leaves in a mixer, drying the material for 6 hours at 85 °C, packing it into 22 mm diameter PVC rings, and press forming the material for 10 seconds at 40 kN. An overview of the pretreatment process is shown in Fig. 1. An overlay of the profiles from the core and leaves is shown in Fig. 2 and FP quantitation results are listed in Table 1. Assuming the presence of cellulose (C6H10O5) as a principal component, the balance (remaining material) was quantified by the Fundamental Parameter (FP) method. The results show that there were no differences between the elements detected in the cabbage core and leaves, but the cores contained more phosphorus (P), potassium (K), and other minerals.



Fig. 1 Pretreatment Overview

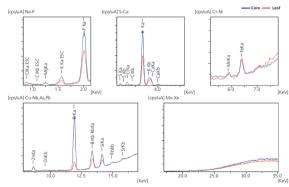


Fig. 2 Overlay of Profiles from Cabbage Core and Leaf

Table 1 FP Quantitative Analysis Results*1

Element	Core (mass%)	Leaf (mass%)	Element	Core (ppm)	Leaf (ppm)
Mg	0.14	0.13	Mn	6.20	11.4
P	0.50	0.32	Fe	27.1	23.2
S	0.93	0.78	Zn	31.4	27.5
а	1.14	0.18	Br	159.9	17.1
K	6.32	2.82	Rb	23.0	13.2
Ca	0.51	0.44	Sr	23.2	8.70
				*1 Quantitated assu	ming the remainder is $C_0H_{10}O_5$.

Energy Dispersive X-ray Fluorescence Spectrometer EDX-8100/ALTRACE

Energy dispersive X-ray fluorescence spectrometers are used to determine the type and concentration of elements in samples by irradiating them with X-rays and then analyzing the energy level (wavelength) or intensity of fluorescent X-rays emitted from the sample.

Shimadzu offers various types of EDX systems, from ALTRACE models designed for high-speed analysis of trace elements to EDX-8100 models that support analyzing light elements.







■ Direct Measurement of Mineral Components (Fe, Zn, Cu, and Mn) in Wine





- Flame atomic absorption spectrometry can directly measure samples even with high matrix levels.
- The system is easy to operate and maintain.

The following is an example of using flame atomic absorption spectrometry to directly measure Fe, Zn, Cu, and Mn in wine. Commercially available red and white wines were directly used as measurement samples. After adding a fixed quantity of standard solution, the wines were measured using spike-and-recovery testing.

1 % Absorption Concentration and Lower Limit of Detection

				Offic. Hig/L
Measured Element	Fe	Zn	Cu	Mn
Analysis Wavelength	248.3 nm	213.9 nm	324.8 nm	279.5 nm
1 % Absorption Concentration	0.04	0.007	0.03	0.02
Lower Limit of Detection (3σ)	0.04	0.007	0.005	0.01

Wine Measurement Results

				Unit: mg/L
	Fe	Zn	Cu	Mn
White Wine	0.68	< 0.007	<0.005	0.54
vvnite vvine	(94 %)	(99 %)	(99 %)	(91 %)
Red Wine	1.7	0.44	0.01*	0.57
Red Wine	(88 %)	(88 %)	(94 %)	(90 %)

^{*} For reference (less than lower limit of quantitation)

Atomic Absorption Spectrophotometer AA-7800 Series

Shimadzu AA-7800 series atomic absorption spectrophotometers are general-purpose models suitable for a wide variety of applications and offer safety measures and easy operation, even for inexperienced users. In combination with an autosampler, they provide a high degree of operational flexibility for various working styles, such as serial analysis or remote data analysis via a network.



Analysis of Minerals and Hazardous Elements in Powdered Milk





- Enables the simultaneous analysis of essential minerals in powdered milk.
- ICPE-9820 systems can simultaneously analyze various components across both low and high concentration ranges.

Powdered infant formula contains a healthy balance of minerals necessary for infant growth.

The Japanese Health Promotion Act specifies that, as a special-application product (prepared specifically for nursing infants), infant formula must contain specified amounts of calcium (Ca), iron (Fe), copper (Cu), and other essential minerals and mandates corresponding labeling.

Results from using an ICPE-9820 system to analyze acid-digested NMIJ-certified standard infant formula powder (trace elemental analysis grade) (NMIJ CRM 7512-a: No. MI-040) are indicated in the table below. Using the ICPE-9820 enabled simultaneous analysis of all targets in the infant formula, ranging from high-concentration minerals to trace amounts of hazardous elements.

Results from Analyzing Certified Standard Infant Formula Powder (NMIJ CRM 7512-a)

	Unit	Analysis Value (in Powder)	NMIJ Certified Value	Expanded Uncertainty	Detection Limit in Powder
Ca	g/kg	8.63	8.65	0.38	0.0000002
Fe		0.100	0.104	0.007	0.000006
K		8.66	8.41	0.33	0.00002
Mg		0.838	0.819	0.024	0.0000002
Na		1.78	1.87	0.09	0.00001
P		5.52	5.62	0.23	0.0002
Cu	mg/kg	4.70	4.66	0.23	0.02
Mn		0.957	0.931	0.032	0.002
Mo		0.229	0.223	0.012	0.02
Sr		5.89	5.88	0.20	0.0008
Zn		40.9	41.3	1.4	0.01
Cd		<dl< td=""><td>-</td><td>-</td><td>10</td></dl<>	-	-	10
Cr	μg/kg	<dl< td=""><td>-</td><td>-</td><td>15</td></dl<>	-	-	15
Pb] ' "	<dl< td=""><td>-</td><td>-</td><td>97</td></dl<>	-	-	97

<DL: Less than detection limit (3 σ) (concentration in measurement solution) Spike Recovery Rate (%) = (Spike-and-Recovery Test Sample Analysis Value - Analysis Value) / Spike Concentration × 100

Simultaneous ICP Atomic Emission Spectrometers ICPE-9800 Series

ICPE-9800 series simultaneous ICP atomic emission spectrometers are next-generation systems that provide the superior accuracy necessary to simultaneously and quickly analyze multiple elements regardless of their concentration levels. They also feature user-friendly software that simplifies analysis.



■ Simultaneous Analysis of Minerals in Powdered Infant Formula





- From trace-concentration Se to high-concentration alkaline elements, all elements can be analyzed simultaneously with high accuracy.
- Because the analysis is based solely on collision parameter settings, analysis times can be shortened.
- Running costs can be reduced by using a mini-torch that consumes about half the argon gas typically used.

The CODEX STAN 72-1981 standard is specified to ensure the quality and safety of infant formula products.

An ICP-MS system was used to simultaneously analyze the 12 elements contained in the certified standard infant formula.

NIST SRM 1849a Analysis Results

		311111 10 134 7 1114	,	
Element	mlz	Certified Value	Analysis Result	Instrument Lower Limit of Quantitation*1
				ILOQ
		mg/kg	mg/kg	mg/kg
Na	23	4265 ±83	4236	4
Mg	24	1648 ±36	1638	0.14
Р	31	3990 ±140	4120	1.2
К	39	9220 ±110	9167	4
Ca	42	5253 ±51	5186	3
Cr	52	1.072 ±0.032	1.056	0.007
Mn	55	49.59 ±0.97	48.17	0.008
Fe	56	175.6 ±2.9	172	0.5
Cu	65	19.78 ± 0.26	19.72	0.01
Zn	66	151.0 ±5.6	145.6	0.04
Se	78	0.812 ±0.029	0.79	0.009
Мо	95	1.707 ±0.04	1.689	0.0014

 $^{^{\}star}1$: ILOQ = 10 \times Standard deviation (n = 10) of calibration curve blank \times Slope of calibration curve

Inductively Coupled Plasma Mass Spectrometer ICPMS-2040/2050

Shimadzu's proprietary advanced mini-torch offers both superior environmental performance and high-level analytical performance, helping to shorten measurement times and improve operational productivity without requiring any special optional products.





Measuring Color

■ Measurement of Vegetable Juice Color



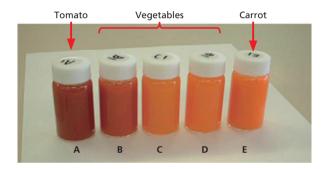
Of all the aspects of the appearance of food products, color has the greatest impact on human emotion. Even a slight difference in color can have an impact on appetite.



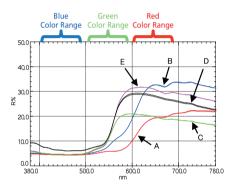
• Color can be expressed in terms of objective numerical values that enable color comparisons between samples by measuring food product samples with a spectrophotometer and then calculating color values based on those results.

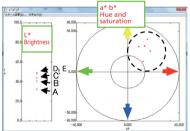
Reflectance data obtained from various vegetable juices in screw-top containers using a spectrophotometer were analyzed with color measurement software.

The results were plotted on a 2D chromaticity chart, enabling differences in color between samples to be represented objectively.









UV-VIS-NIR Spectrophotometer UV-3600i Plus

This spectrophotometer can measure a wide range of wavelengths, from ultraviolet to visible and near-infrared.

In addition to the main unit, the large sample compartment and the integrating sphere attachment of the UV-3600i are designed to support three detectors, enabling high-sensitivity measurements even for solid samples.





Analysis of Food Additives

Preservatives, sweeteners, colorants, flavorings, and other additives are widely used in food manufacturing processes to improve food processing or storage characteristics.

However, they must be used appropriately in accordance with applicable standards and regulations in respective countries.

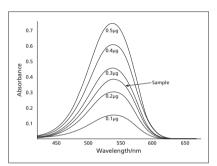
Given our modern dietary lifestyles, food additives have become inextricably linked to the quality of food products, including their taste, flavor, color, and freshness. Shimadzu supports food product development through the high-accuracy analysis of food additives using various analytical instruments.

Analysis of Preservatives



 A wide variety of components can be accurately analyzed using only simple pretreatment and measurement methods.

This example shows the analysis of preservatives in food products, the usage standards for which are prescribed by the Japanese Food Sanitation Act.



Sodium Nitrite in Meats

UV-VIS Spectrophotometer UV-1900i

This instrument is used to confirm the concentrations and molecular structures of organic compounds and inorganic ions primarily in solutions, using the characteristic absorption of light by specific components.

It is also used to quantify preservatives, vitamins, and food colorings in food products.

Powdered and solid samples can also be measured using appropriate accessories.

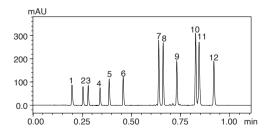


Analysis of Artificial Colorants



- Enables high-speed simultaneous analysis of 12 artificial coloring components.
- A total of 21 components can be analyzed simultaneously by changing gradient elution parameters.

The 12 artificial colorant components were separated within 1 minute. Good retention time and peak area reproducibility results were obtained for all peaks measured from 6 successive injections.



- 1. Y4 (Tartrazine), 2. R2 (Amaranth), 3. B2 (Indigo Carmine),
- 4. R102 (New Coccine), 5. Y5 (Sunset Yellow FCF), 6. R40 (Allura Red AC), 7. G3 (Fast Green FCF),
- 8. B1 (Brilliant Blue FCF), 9. R3 (Erythrosine), 10. R106 (Acid Red),
- 11. R104 (Phloxine), 12. R105 (Rose Bengale)

High-Performance Liquid Chromatograph



In addition to performance improvements that maximize throughput, such as fast injection and low carryover, IoT technologies help ensure stable equipment operation and improve operational efficiency. Systems are designed to be both exceptionally space-saving and energy-efficient while also providing exceptional LC performance, ensuring consistent data acquisition regardless of the installation site.



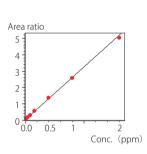
■ Measurement of Sulfites in Foods and Beverages



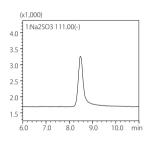


- Enables high-speed analysis of sulfites added as antioxidants to foods and beverages.
- Designed based on the method specified by the FDA (C-004.03), it enables excellent quantitative analysis of sulfites.
- Enables safe pretreatment due to not using dichloromethane as a specified chemical substance during pretreatment.

Sulfite was mixed with a 0.2 % formaldehyde extract solution to convert it to hydroxymethylsulfonatee (HMS) and detected. The calibration curve created for the 0.02 to 2 ppm range had good linearity with $R^2 > 0.999$ (n = 3).



Calibration Curve for HMS



HMS in Mango

Liquid Chromatograph Mass Spectrometer LCMS-2050

fields.



The LCMS-2050 offers both the easy usability as an LC detector and the superior capacity of an MS system, resulting in a compact, easy-to-use system that also offers excellent performance. The LCMS-2050 can measure a wide range of target compounds, from small lower-mass molecules to large polymers and with polarities ranging from low to high, making it suitable for a wide variety of applications and



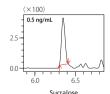
■ Simultaneous Analysis of Sweeteners

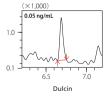


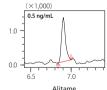


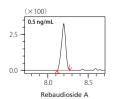
- Enables simultaneous analysis of 16 sweetener components.
- Using the solvent extraction method, samples can be pretreated quickly and easily without any special equipment.

Chromatograms of some compounds near the lower limit of quantitation are shown below. Good linearity with a correlation coefficient of 0.997 or higher was obtained for all the compounds. Spike-and-recovery tests of soy sauce and other actual samples resulted in recovery rates of 80 to 110 %









Liquid Chromatograph Mass Spectrometer LCMS-8050RX

Equipped with the newly developed CoreSpray nebulizer nozzle, it features improved nebulizer flow uniformity. With the addition of "consistency" to existing high-sensitivity and high-speed characteristics, the system offers trusted reliability in an easy-to-use design.





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