The Quest for Quality

Analytical techniques govern our standard of living across all sectors.
From the water we drink to the fuel we consume, proven extraction methods coupled with powerful detection approaches like MS ensure consumer safety and satisfaction.
This book details an array of essential applications across fields.

Food & Drink

Petrochemicals

Enivronment

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Direct Rapid Analysis of Tetrodotoxin Contained in Fugu Using DPiMS™-8060

Fugu (pufferfish) is widely consumed, especially in Japan. Incidents of fugu poisoning occur frequently due to careless control, despite wide acknowledgement that certain parts and species of fugu contain the deadly poison tetrodotoxin (TTX). Establishment of a quick and simple detection method for fugu TTX is desired for both quality control and consumer protection purposes.

We present a quick TTX analysis method using the new Shimadzu DPiMS-8060 (Figure 1), which combines probe electrospray ionization (PESI) with a tandem-type mass spectrometer. We also present an approach free of pretreatment. This method is applicable to the liver, ovaries, skin and muscle of fugu.

As a standard sample, fugu TTX was prepared in a 50 percent ethanol solution and 10 µL of sample solution was injected into the dedicated liquid sample plate of the DPiMS-8060. A product ion scan was conducted, conditions enabling confirmation of the characteristic fragment (ion m/z 162.1) were studied, and the conditions shown in Table 1 were applied. The samples were measured under MRM conditions, a calibration curve was prepared, and values for the detection limit and lower quantitative limit were established (Figure 2).

Samples of approximately 3 mm^2 were taken from the muscle, skin, liver and ovary of the fine-patterned puffer (*Takifugu poecilonotus*). Samples were inserted into the dedicated biological sample plate of the DPiMS-8060, 35 µL of the 50 percent ethanol solution was added as an ionization accelerator, and a product ion scan was conducted. Fragment ions of TTX were detected in all tissues. Differences in detection sensitivity were also observed between tissues, suggesting that the respective magnitudes of TTX concentration can be measured simply and without pretreatment using the DPiMS-8060.

The Shimadzu DPiMS-8060 eliminates the need for pretreatment in TTX analysis, which is often essential when applying LC-MS to study this high-polarity component. Therefore, the DPiMS-8060 may be effective for quick and simple in-field inspections of food safety.

Collision Energy	-30 V
MRM Transition	m/z : 320.2 > 162.1 (Monitoring conducted using proton adduct as precursor ion.)
Survey Event : Product	m/z : 100-370
Ion Scan MS Range	
Scan Speed	5,000 u/sec
Event Time	0.06 sec
Desolvation Line	250 °C
Heat Block	50 °C
Polarity	Positive
Acquisition time	0.5 min

Table 1 TTX Analysis Conditions for DPiMS-8060

Fig. 1 DPiMS™-8060

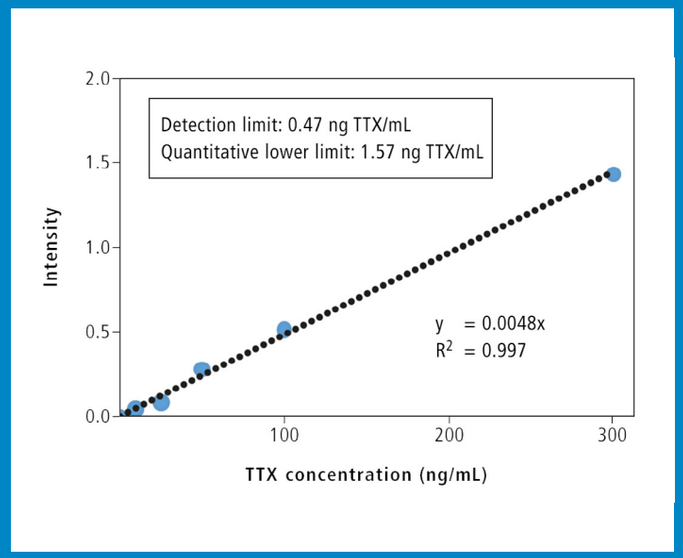
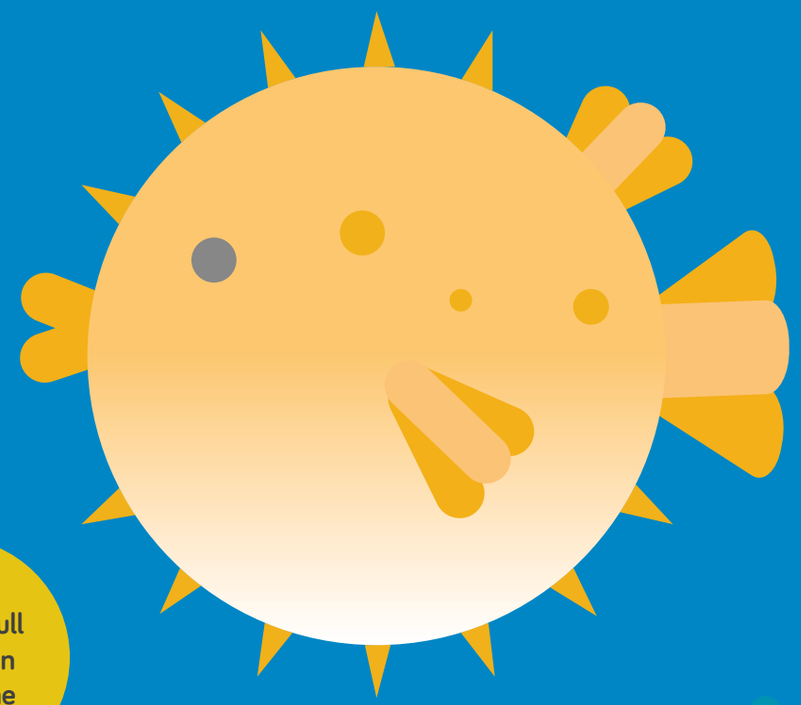


Fig. 2 Calibration Curve of TTX Standard Sample



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Cost-effective Proximate Analysis in Food Products with Robust and Reliable BUCHI Instrumentation

Proximate analysis is used to quantify important components of food items, such as protein, fat, carbohydrates, moisture and ash. Combinations of techniques to quantify these substances are well documented due to legal requirements. In the case of milk, for example, fat content is determined by NIR at several points before distribution to consumers, as are protein and dry matter content. There is thus a clear need for rapid, robust and reliable methods to conduct these analyses.

BUCHI offer state-of-the-art instruments to support analysis across the spectrum of food analysis, from simple macromolecular quantification to QC testing and beyond. For instance, the BUCHI NIRFlex N-500 with BUCHI precalibration for sausage quality parameters is a valuable tool for QC per industry standards. All BUCHI precalibrations are accurate and robust – essential features in a strictly regulated field. NIR carries many obvious advantages for such purposes, namely the lack of chemical waste and resultant cost savings.

Mead Johnson have specific requirements for Vendor Change Control and Raw Material Quality in the USA. By applying the Solids Measurement Cell (suitable for powder, fine powder, and whole and ground seeds) with the BUCHI NIRFlex N-500, analysis of infant formula for QC purposes has been successful in identifying cases of supplier mislabeling, including wrong particle size, incorrect materials and undisclosed manufacturing changes. For at-line applications, the NIRMaster with transflectance cover provides the perfect tool.

When studying fat content by extraction, the Extraction SOX, Extraction HE and Extraction ECE are available for Soxhlet, Hot Extraction, and Economic Continuous Extraction, respectively. Each is ideal for the handling of distinct samples, and each presents with its own advantages, from cost-saving to speed and reproducibility. In short, BUCHI instruments are available to streamline food analysis in all settings.

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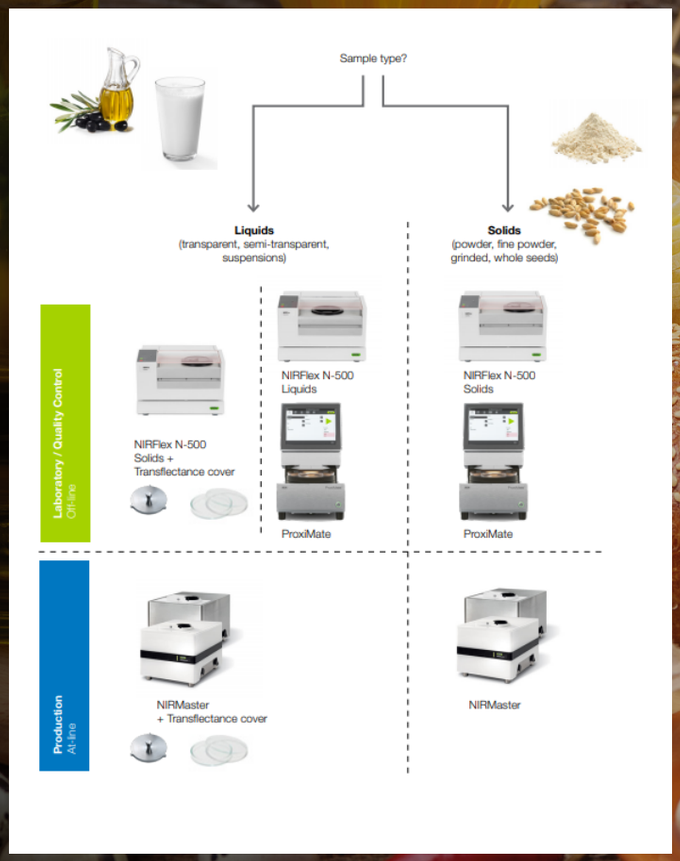

Fig 1. Cost-effective proximate analysis by NIR

Area of application	Fat «Extraction»	Protein «Kjeldahl»	Proximate «NIR»
R&D	+++	+++	+
Production	+	+	+++
Goods inspection	+	+	+++
Quality control / labeling	+++	+++	++
Characterictics			
Range of applications	+	++	+++
Variation in sample types	+++	+++	++
Automated throughput	++	+++	+
Speed of analysis	+	+	+++
Compliance [1]	+++	+++	+
Detection of adulterants	+	++ (NPN)	+++
Unattended operation	++	+++	+
No contact with chemicals	+	+	+++
Ingress protection rating	+ (IP 20)	+ (IP 20)	+++ (IP 65)
Low initial costs	+++	+++ / ++ / + [2]	+
Low running costs	++	+	+++
Eco-friendly	++	+	+++
Technical Data			
Throughput in 9 h [3]	~ 36 samples	120 samples	400+ samples
Analysis time	~ 90 min/6 samples	200 min/20 samples	~ 15 s/sample
Max. sample amount	10 g	> 4 g/400 mL	395 cm
Limit of detection (LOD)	0.1 %	0.02 mg N	0.1 %

[1] With respect to application regulations such as AOAC, ISO, DIN etc.
[2] Initial costs of the Kjeldahl products are very much depending on the level of automation
[3] Depending on sample composition, packaging material. No shift work assumed.
+ applicable ++ more applicable +++ most applicable

Fig. 2 Find your perfect match

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Application Note
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Interference-free TS Determination by UV-Fluorescence in Fuels with N-containing Cetane Improvers

During the production of motor fuels by hydration of coal or vegetable oil, as well as during the production of traditional fuels based on mineral oil with biodiesel addition, end products with altered ignition characteristics can occur. In this case, special additives — generally known as cetane improver — are used to enhance the ignitability (cetane number). Nitrogen compounds have proven to be especially suitable and cost-efficient.

The elevated nitrogen content in these fuels presents a challenge when conducting sulfur analysis, often leading to false positive results when determining the TS content. Given that many fuels classed as sulfur-free have an actual TS content close to the common limit value of 10 ppm, the sulfur content determined can exceed the specified threshold easily if nitrogen cross-sensitivity is not accounted for.

The Micro Plasma Optimization (MPO), a patented technique developed as an enhancement of the classic sulfur detection by UV-fluorescence, guarantees reliable results with a short measurement time by converting the interfering NO molecules to harmless species. Plus, there is no need for additional auxiliary materials (e.g., catalysts), multiple injections, or matrix separation by trap-and-release approaches.

This application note shows how the new compEAct S-MPO facilitates fast and interference-free determination of sulfur contents in the presence of nitrogen-containing additives. Especially designed for fuel applications, it enables reliable analysis of challenging matrices and simplifies routine work.

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Fig. 1 The compEAct S-MPO

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Analysis of Elemental Impurities in Naphtha by ICP-MS According to ASTM D8110-17

The monitoring of trace metal contents in naphtha is important for a number of reasons. In the refinery, certain elements can poison catalysts or promote equipment corrosion, and emissions of toxic elements are an environmental concern. Thus, various elements are analyzed in product quality control to ensure a consistently performing product.

For the analysis of small impurities in naphtha, ICP-MS is the technique of choice as it achieves the lowest limits of detection. However, due to the complex nature of naphtha, the analysis by ICP-MS requires special attention to minimize the formation of carbon deposits on the sampler and skimmer cones, and to avoid the instability or complete extinction of the plasma due to organic vapor overloading. Interferences due to polyatomic species, originating from the carbon matrix and plasma, must also be considered and eliminated.

This application note demonstrates the performance of the PlasmaQuant MS and its unmatched tolerance to organic solvents, which allow routine analysis of highly volatile organic solvent samples according to ASTM D8110-17, with results exceeding the requirements for accuracy and long-term stability.

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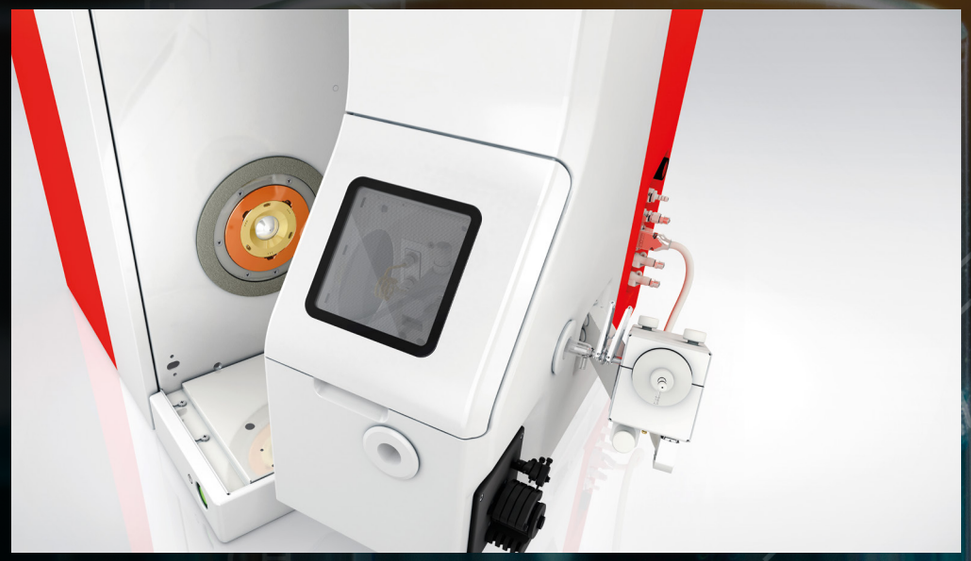

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ICP-MS tailored to your requirements

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Speed Up Your Work: High-Throughput Analysis of Drinking Water with ICP-MS

Drinking water is the world's most essential resource, the quality control of which is regulated by international and national regulations and norms. For example, the U.S. Environmental Protection Agency (EPA) has released the Method 200.8, which specifies criteria for the determination of trace elements in waters and wastes by ICP-MS.

For labs requiring high sample throughput each day, the speed of analysis is an important factor to consider alongside the accuracy, precision and robustness of the method. The more samples that can be analyzed per hour, the lower the cost per sample.

Fast sampling systems were developed for ICP mass spectrometers, dramatically decreasing sample uptake time and total analysis time per sample. The limiting factor is no longer the supply and rinsing time of the sample, but the measuring time, which depends on the number of elements to be analyzed.

However, reducing the data acquisition time will directly affect the precision of the results as less averaging is possible with greater time constraints. Therefore, precision is the key parameter for evaluating high-throughput methods. Since ICP-MS precision is mainly dependent on the counting statistics for the analyte ion and background, higher detection sensitivity is advantageous – it allows reaching the same counting statistics in a shorter time, and thus allows higher sample throughput without sacrificing performance. This application note shows how the industry-leading sensitivity of the PlasmaQuant MS Elite, combined with a fast sampling system, can exceed a throughput of 80 samples per hour, while still fulfilling all requirements of the EPA 200.8 method.

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TOC Determination in Raw and Drinking Water

The traditional method for total organic carbon (TOC) determination is based on a differential measurement of total (TC) and inorganic carbon (IC), where TOC = TC – IC. When analyzing trace TOC contents in water samples with high IC content, this differential method suffers from poor precision because the uncertainty of the IC measurement may already be greater than the actual TOC content, thus producing meaningless results. It is also a time-consuming method due to the need for two separate analyses of a sample.

The NPOC method is a suitable alternative because IC is purged out of the sample, and TOC can be detected directly, which greatly reduces the analysis time per sample. An optional control measurement for residual IC guarantees a complete purge, and therefore accurate results.

The parallel purge-and-analyze function further increases the sample throughput. Here, while one sample is being analyzed, the next sample is already being purged automatically and is immediately ready to be analyzed once the first sample is finished.

The two most common oxidation methods, thermocatalytic combustion and UV-assisted wet-chemical oxidation, are compared with respect to differences in method parameters. Additional instrument features, such as the VITA gas flow management and the EasyCal calibration strategy, and their benefits are explained.

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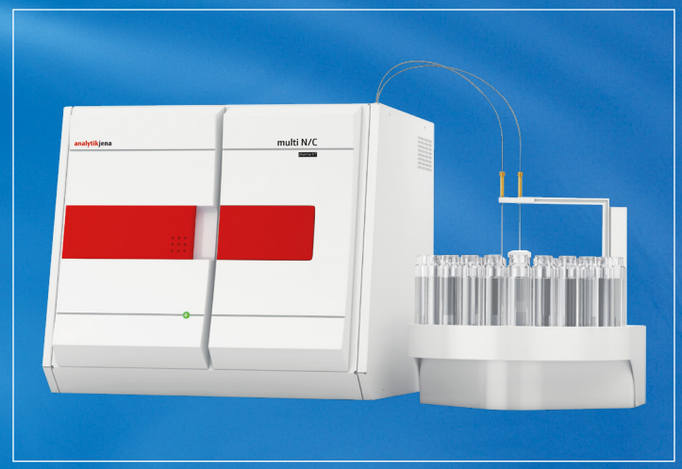

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