30 minutes Recap : Food Ingredient Analysis by LC-MS

An Advanced Analytical Technique for Food Safety and Quality

PRESENTED BY

Pongsagon Pothavorn, Sci Spec Co., Ltd.

Primary Ingredients : The Foundation of Food

Grains & Staples

Rice, flour, and sugar form food bases in many cultures.

Proteins

Meat, fish, and eggs provide essential amino acids.

Produce

Vegetables and fruits deliver vitamins and flavor diversity.

Dairy & Legumes

Milk products, legumes, seeds, and nuts support nutrition and texture.

Food Additive : Enhancing & Preserving

Type	Examples	Common Codes
Preservatives	Sodium benzoate, Sorbic acid	E211, E200
Coloring Agents	Synthetic dyes, Beta-carotene	E102, E160a
Flavourings	Vanillin, Fruit extracts	Often not coded
Sweeteners	Aspartame, Sucralose	E951, E955
Stabilizers & Thickeners	Gelatin, Gum arabic, Modified starch	E441, E414, E1400–1450
Gelling Agents	Agar, Carrageenan	E406, E407
Acidity Regulators	Citric acid	E330

Processing Aids

Enzymes

Amylase and protease aid in food processing but do not remain in products.

Solvents

Ethanol and others help extract components during manufacturing.

Filtering Agents

Used to clarify liquids; mostly removed before final food packaging.

Seasonings and Flavorings

Sauces

Soy, oyster, and fish sauces boost umami.

Flavourings

Natural or artificial agents enhance taste.

Basic Seasonings

Salt and sugar balance flavor profiles.

Herbs and Spices

Garlic, pepper, and others add aroma and zest.

Food Allergens

- Gluten from wheat, barley, rye
- Milk and dairy
- Eggs
- Peanuts and tree nuts (almonds, walnuts)
- Soybeans
- Fish and shellfish like shrimp, crab

Functional Ingredients

Functional Ingredients

- Dietary fiber boosts digestion
- Probiotics support gut health
- Fortified vitamins and proteins enhance nutrition

Why it matter

Safety & Quality Assurance

Ensures ingredients meet safety standards and quality expectations.

Product Innovation

Adjust taste, texture, shelf-life. Use of novel or substitute ingredients

Label Accuracy

Verifies nutritional content, allergens, additives claims on packaging and labels.

Understanding LC-MS

Wide Compound Range

Identifies and measures diverse chemical compounds in food.

Trace Detection

Finds contaminants and residues at extremely low levels.

Minimal Preparation

Efficient analysis with less elaborate sample processing.

Case Studies: Real-World Applications

Adulterant Detection

Melamine in milk detectable at parts-per-billion levels.

Vitamin Quantification

Accurate measurement of vitamin D in fortified foods.

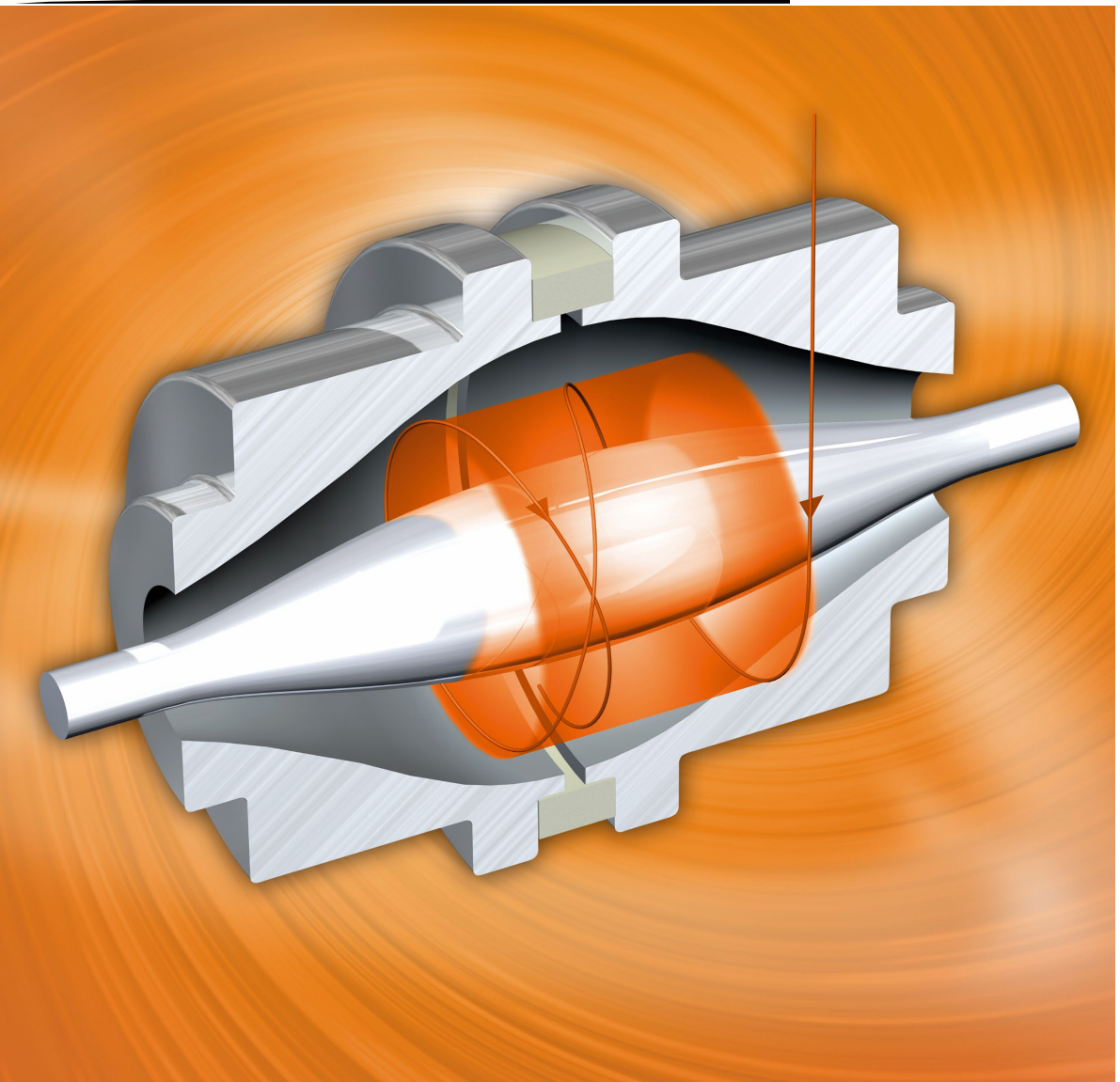
Food Allergens

Detection of allergens such as proteins in tree nuts, eggs, milk, soy, gluten, etc

Fatty Acid Analysis

Profiling omega-3 and omega-6 contents in oils.

Orbitrap : High-Resolution Accurate Mass



Orbitrap Analysis: Targeted & Untargeted Food Ingredient Screening

Explore how Orbitrap revolutionizes food safety and quality control. This presentation covers HRAM spectrometry principles, challenges in food matrices, and advanced screening methods.

Discovery Components

Comprehensive Profiling

Detects all compounds without prior knowledge.

Advanced Software Tools

Data analysis with XCMS and MZmine for peak detection.

I.D. & Applications

Detect adulterants, authenticate products, and assure quality.

Nutritional Analysis

Nutrient Quantification

Measures vitamins, amino acids, and essential nutrients accurately.

Label Verification

Ensures nutritional claims on packaging are truthful and reliable.

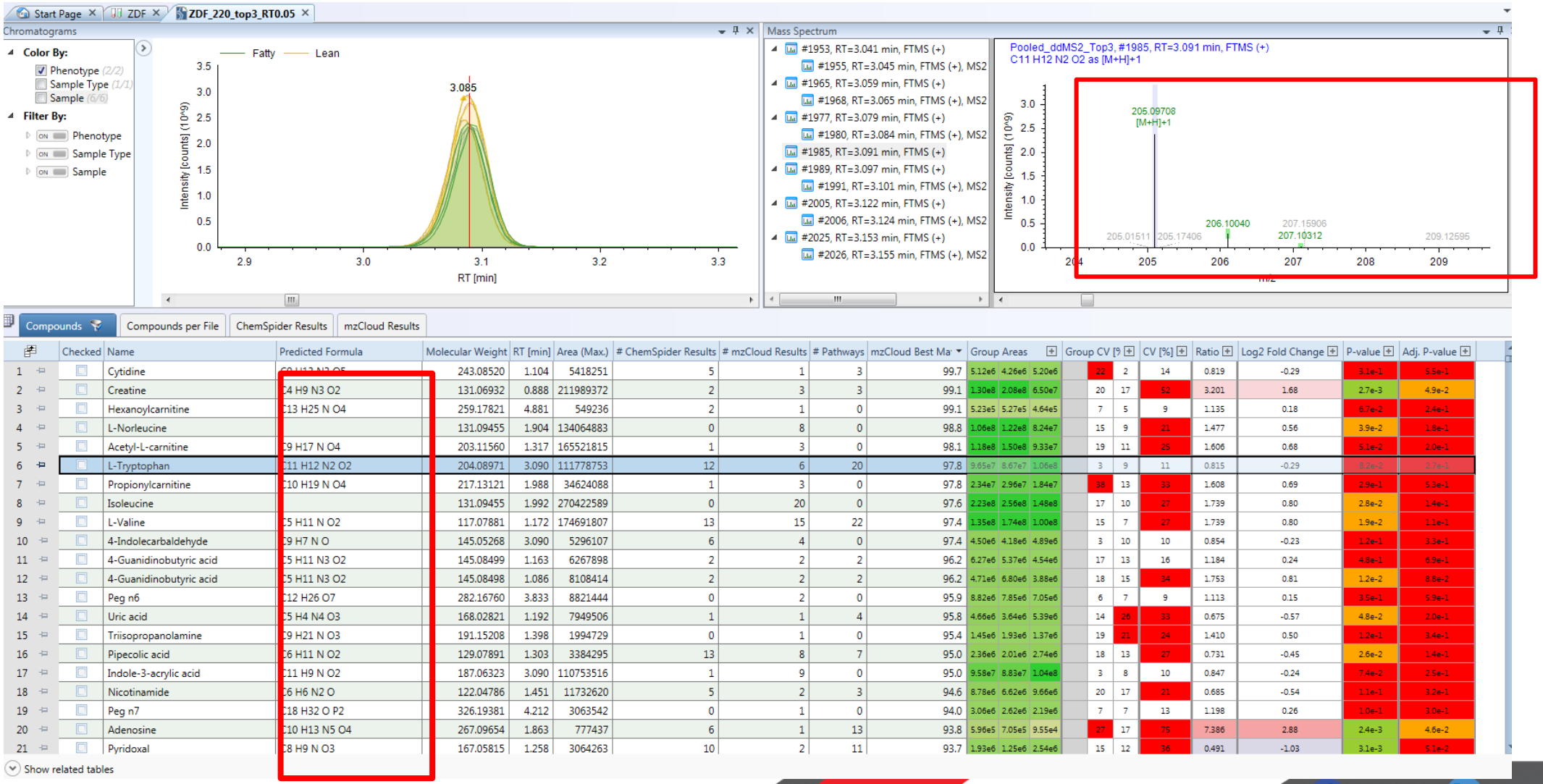
Precision

LC-MS delivers reproducible and sensitive results for nutrition.

Example

Vitamin D levels in fortified milk precisely analyzed by LC-MS.

Predicted Elemental Composition



	Checked	Name	Predicted Formula	Molecular Weight	RT [min]	Area (Max.)	# ChemSpider Results	# mzCloud Results	# Pathways	mzCloud Best Ma	Group Areas	Group CV [%	CV [%]	Ratio	Log2 Fold Change	P-value	Adj. P-value
1		Cytidine	C9 H13 N3 O5	243.08520	1.104	5418251	5	1	3	99.7	5.12e6 4.26e6 5.20e6	22 2	14	0.819	-0.29	3.1e-1	5.5e-1
2		Creatine	C4 H9 N3 O2	131.06932	0.888	211989372	2	3	3	99.1	1.30e8 2.08e8 6.50e7	20 17	52	3.201	1.68	2.7e-3	4.9e-2
3		Hexanoylcarnitine	C13 H25 N O4	259.17821	4.881	549236	2	1	0	99.1	5.23e5 5.27e5 4.64e5	7 5	9	1.135	0.18	6.7e-2	2.4e-1
4		L-Norleucine		131.09455	1.904	134064883	0	8	0	98.8	1.06e8 1.22e8 8.24e7	15 9	21	1.477	0.56	3.9e-2	1.8e-1
5		Acetyl-L-carnitine	C9 H17 N O4	203.11560	1.317	165521815	1	3	0	98.1	1.18e8 1.50e8 9.33e7	19 11	25	1.606	0.68	5.1e-2	2.0e-1
6		L-Tryptophan	C11 H12 N2 O2	204.08971	3.090	111778753	12	6	20	97.8	9.65e7 8.67e7 1.06e8	3 9	11	0.815	-0.29	8.2e-2	2.7e-1
7		Propionylcarnitine	C10 H19 N O4	217.13121	1.988	34624088	1	3	0	97.8	2.34e7 2.96e7 1.84e7	38 13	33	1.608	0.69	2.9e-1	5.3e-1
8		Isoleucine		131.09455	1.992	270422589	0	20	0	97.6	2.23e8 2.56e8 1.48e8	17 10	27	1.739	0.80	2.8e-2	1.4e-1
9		L-Valine	C5 H11 N O2	117.07881	1.172	174691807	13	15	22	97.4	1.35e8 1.74e8 1.00e8	15 7	27	1.739	0.80	1.9e-2	1.1e-1
10		4-Indolecarbaldehyde	C9 H7 N O	145.05268	3.090	5296107	6	4	0	97.4	4.50e6 4.18e6 4.89e6	3 10	10	0.854	-0.23	1.2e-1	3.3e-1
11		4-Guanidinobutyric acid	C5 H11 N3 O2	145.08499	1.163	6267898	2	2	2	96.2	6.27e6 5.37e6 4.54e6	17 13	16	1.184	0.24	4.8e-1	6.9e-1
12		4-Guanidinobutyric acid	C5 H11 N3 O2	145.08498	1.086	8108414	2	2	2	96.2	4.71e6 6.80e6 3.88e6	18 15	34	1.753	0.81	1.2e-2	8.8e-2
13		Peg n6	C12 H26 O7	282.16760	3.833	8821444	0	2	0	95.9	8.82e6 7.85e6 7.05e6	6 7	9	1.113	0.15	3.5e-1	5.9e-1
14		Uric acid	C5 H4 N4 O3	168.02821	1.192	7949506	1	1	4	95.8	4.66e6 3.64e6 5.39e6	14 26	33	0.675	-0.57	4.8e-2	2.0e-1
15		Triisopropanolamine	C9 H21 N O3	191.15208	1.398	1994729	0	1	0	95.4	1.45e6 1.93e6 1.37e6	19 21	24	1.410	0.50	1.2e-1	3.4e-1
16		Pipecolic acid	C6 H11 N O2	129.07891	1.303	3384295	13	8	7	95.0	2.36e6 2.01e6 2.74e6	18 13	27	0.731	-0.45	2.6e-2	1.4e-1
17		Indole-3-acrylic acid	C11 H9 N O2	187.06323	3.090	110753516	1	9	0	95.0	9.58e7 8.83e7 1.04e8	3 8	10	0.847	-0.24	7.4e-2	2.5e-1
18		Nicotinamide	C6 H6 N2 O	122.04786	1.451	11732620	5	2	3	94.6	8.78e6 6.62e6 9.66e6	20 17	21	0.685	-0.54	1.1e-1	3.2e-1
19		Peg n7	C18 H32 O P2	326.19381	4.212	3063542	0	1	0	94.0	3.06e6 2.62e6 2.19e6	7 7	13	1.198	0.26	1.0e-1	3.0e-1
20		Adenosine	C10 H13 N5 O4	267.09654	1.863	777437	6	1	13	93.8	5.96e5 7.05e5 9.55e4	27 17	75	7.386	2.88	2.4e-3	4.6e-2
21		Pyridoxal	C8 H9 N O3	167.05815	1.258	3064263	10	2	11	93.7	1.93e6 1.25e6 2.54e6	15 12	36	0.491	-1.03	3.1e-3	5.1e-2

Food Bioactive Compounds

foods

MDPI

Review

Food Bioactive Compounds and Emerging Techniques for Their Extraction: Polyphenols as a Case Study

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Abstract: Experimental studies have provided convincing evidence that food bioactive compounds (FBCs) have a positive biological impact on human health, exerting protective effects against non-communicable diseases (NCD) including cancer and cardiovascular (CVDs), metabolic, and neurodegenerative disorders (NDDs). These benefits have been associated with the presence of secondary metabolites, namely polyphenols, glucosinolates, carotenoids, terpenoids, alkaloids, saponins, vitamins, and fibres, among others, derived from their antioxidant, antiatherogenic, anti-inflammatory, antimicrobial, antithrombotic, cardioprotective, and vasodilator properties. Polyphenols as one of the most abundant classes of bioactive compounds present in plant-based foods emerge as a promising approach for the development of efficacious preventive agents against NCDs with reduced side effects. The aim of this review is to present comprehensive and deep insights into the potential of polyphenols, from their chemical structure classification and biosynthesis to preventive effects on NCDs, namely cancer, CVDs, and NDDS. The challenge of polyphenols bioavailability and bioaccessibility will be explored in addition to useful industrial and environmental applications. Advanced and emerging extraction techniques will be highlighted and the high-resolution analytical techniques used for FBCs characterization, identification, and quantification will be considered.

Keywords: food bioactive compounds (FBCs); polyphenols; disease protection; cancer; cardiovascular diseases (CVDs); neurodegenerative diseases (NDs); bioavailability and bioaccessibility

check for updates

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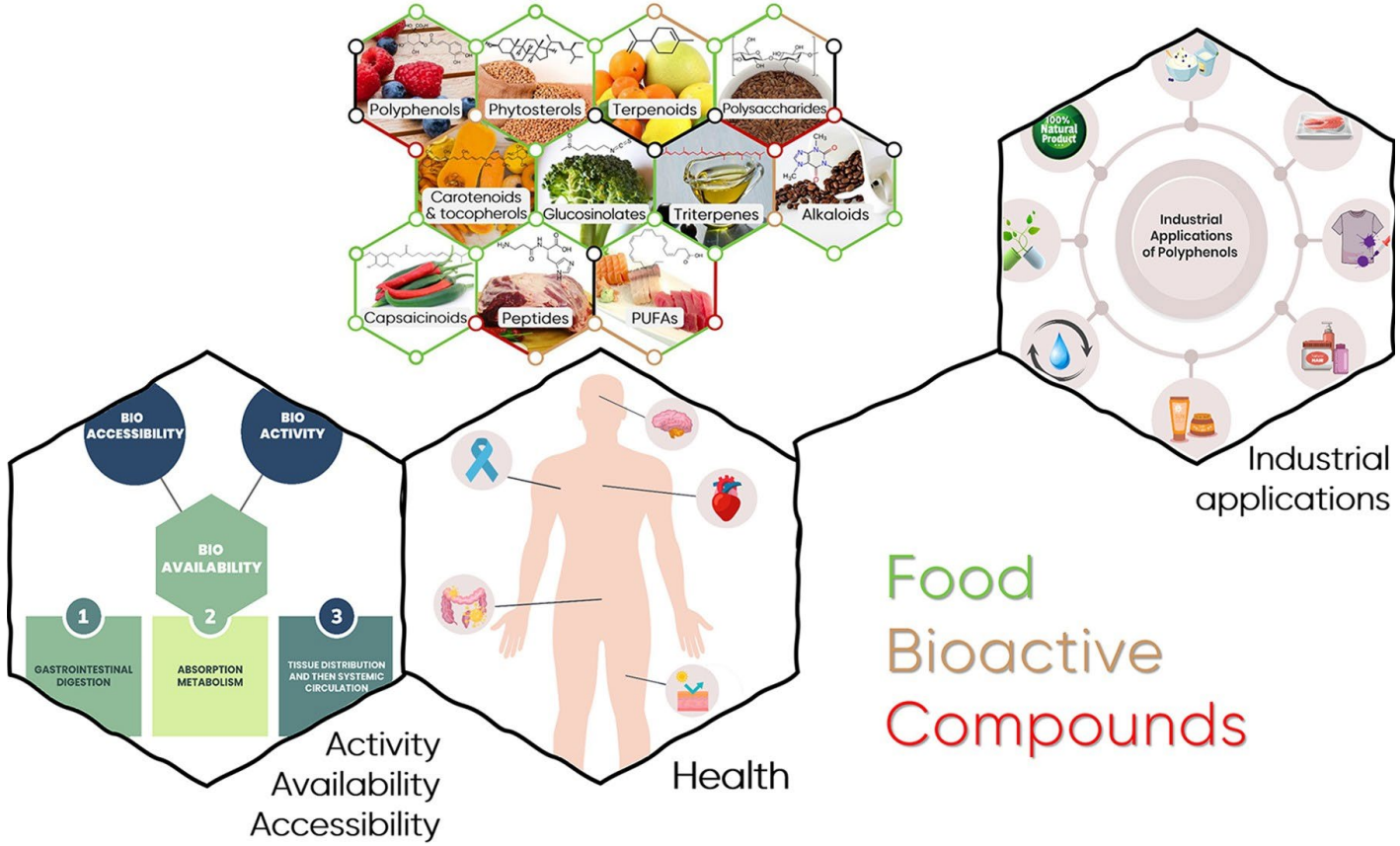
1. Introduction

Non-communicable diseases (NCDs), mainly cardiovascular diseases (CVDs), cancer, chronic respiratory diseases, neurodegenerative diseases (NDs), and diabetes, represent a severe burden worldwide. According to the most recent data, NCDs caused over 70% of the 57 million deaths worldwide in 2016 [1]. The major risk factors contributing to this scenario have been identified as the combination of an unhealthy diet, poor physical activity, and alcohol and smoking abuse. Diet, in particular, is considered a leading risk factor for illness, death, and disability and it is estimated that one in five deaths are associated with a



Orbitrap HRMS in Food Analysis

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Taylor & Francis

Future perspectives in Orbitrap™-high-resolution mass spectrometry in food analysis: a review

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A literature search from 2007 to 2014 was conducted to identify publications where principally LC-Orbitrap™-high-resolution mass spectrometry (HRMS) has been employed in food analysis. Of a total of 212 relevant references, only 22 papers were from 2007–10, but in subsequent years there has been a steady growth in publications with 38–55 relevant papers being published each year from 2011 to 2014. In the food safety area, over 50% of the published papers were equally divided between pesticides, veterinary drug residues and natural toxins (including mycotoxins) focused primarily on multi-analyte target analysis. LC-Orbitrap-HRMS was also found to be increasingly important for the analysis of bioactive substances, principally phenolic compounds in foods. A number of studies reported for the first time the identification of new fungal metabolites, predominantly various conjugated forms of known mycotoxins. Novel process contaminants were also identified by LC-Orbitrap-HRMS, as were various substances used for food adulteration and bioactive substances in herbal products and dietary supplements. Untargeted analysis is seen as a major future trend where HRMS plays a significant role. Retrospective analysis of scanned high-resolution mass spectra in conjunction with relevant databases can provide new insights. Metabolomics is also being increasingly used where foods are being profiled through fingerprinting using HRMS. All evidence points towards future growth in the number of applications of HRMS in food safety and quality, as the power of this technique gains wider recognition.

Keywords: review; Orbitrap; high resolution mass spectrometry; pesticides, veterinary drugs, natural toxins; process contaminants; adulteration; bioactive substances; non-target analysis; metabolomics

Introduction

Over the past 20 years there have been a number of key developments in mass spectrometry (MS) which have led to step-changes in the way food analysis has been conducted. In LC-MS the development of electrospray (ESI) and atmospheric pressure chemical ionisation (APCI) interfaces together with progressive improvements in MS designs opened up LC-MS to the wider analytical community. Improvements in the ease of use of LC-MS through better software, improved reliability and lower purchase costs have led to significantly wider accessibility, which had been initially restricted to specialists. Latterly, further improvements have seen movement from LC-MS to LC-MS/MS, which has now become the standard approach, whether it be with bench-top instruments or more sophisticated MS configurations. Another step change has been the development of high-resolution LC-MS through Orbitrap technology enabling resolutions of 10 000–200 000 to be achieved (Zubarev & Makarov 2013) together with development of time-of-flight (TOF) instruments in the form of LC-TOF-MS in various configurations (Holčapek et al. 2012). The same trend with HRMS, as was the case with LC-MS, has been apparent in the last few years in terms of software being progressively improved and lower capital investment required with the introduction of LC-HRMS bench-top instruments such as the Exactive™ (a single-stage Orbitrap-MS). There are, what can appear to be, a confusing array of different LC-MS configurations, and a useful overview of commercial systems has been provided comparing the technical specifications of individual manufacturers instruments (Holčapek et al. 2012). Applications of different types of mass detector including Orbitrap™ configurations have been reviewed (Wang, Wang, et al. 2013) highlighting newly developed MS methods, including MALDI TOF-MS (MALDI = matrix-assisted laser desorption ionisation) imaging and ambient ionisation MS for direct analysis in real time (DART). The advantages and the limitations of different MS techniques in their application to food safety and quality have been assessed (Wang, Wang, et al. 2013).

In the food safety area, the use of HPLC was limited to fluorescence or diode array detection which provided the only viable options offering the sensitivity needed in residue and contaminant analysis. However, with MS available as a detection option, methods quickly migrated onto LC-MS platforms and this transformation was particularly apparent in the pesticide and veterinary drug residue areas, where multi-residue and multi-class methods were developed (Kaufmann et al. 2011a; Mol et al. 2012). A review of LC-MS in food safety

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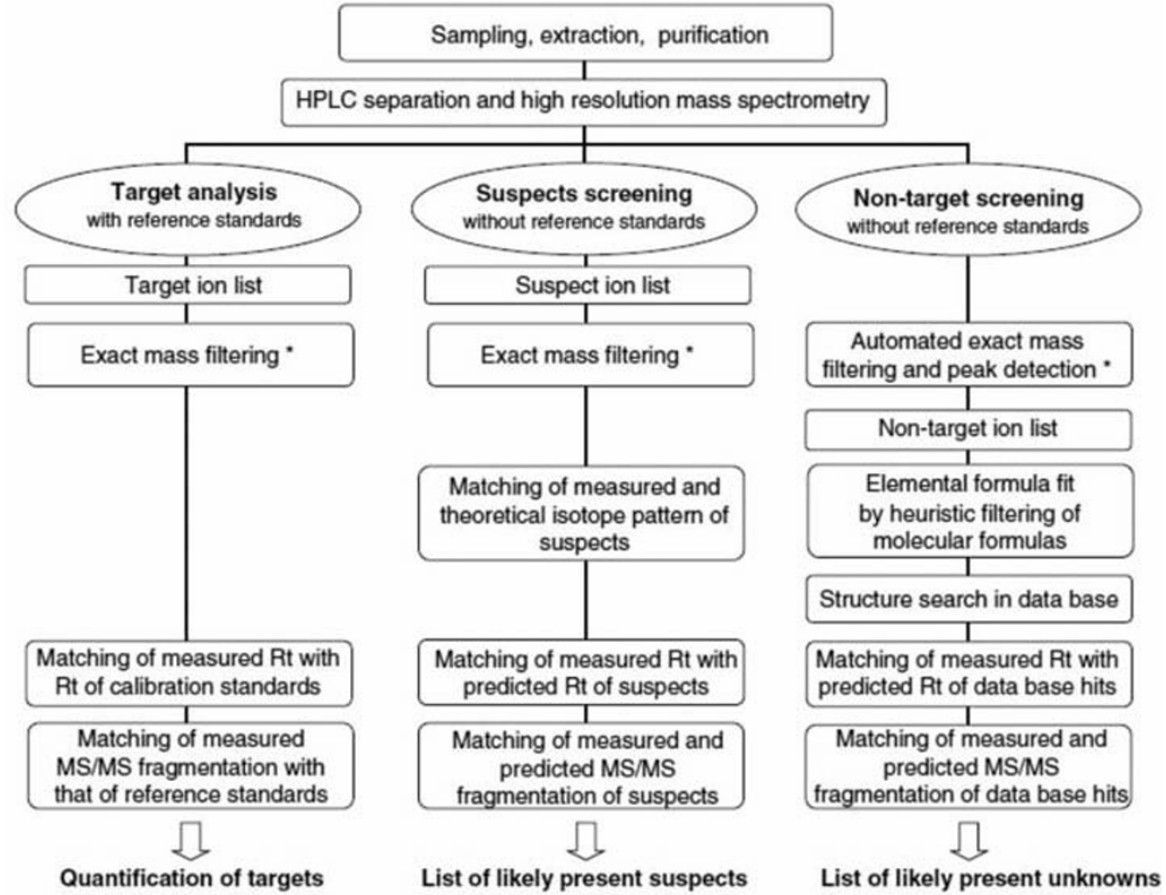

Compound Identification

Know more unknowns

Database	Molecular Ion (Precursor Ion)	MS^2 Spectrum	Metabolic Pathway
Online	• ChemSpider	• mzCloud	• Metabolika Pathways • KEGG • BioCyc
Offline In-house Database	• Mass Lists Optional Import from ChemSpider	• mzVault	• Metabolika Pathways

Automatically identify components

- Spectral library searching
  - Online mzCloud™ spectral library
  - In-house Thermo Scientific™ mzVault™ spectral libraries
- mzCloud can provide similarity search results, giving you even more information to use for unknown identification
- Determine elemental composition, including fine isotopes, using HRAM MS and MS/MS data. Then, use this information to search multiple chemical databases for further annotation information
- Structure proposals automatically annotated on an experimental spectrum

Orbitrap HRMS in Food Analysis

Group	Specific compounds (number identified)	Matrix	Basis for identification	Reference
Mycotoxins	Fusarins (10)	Culture medium	LC-HRMS and ^{13}C-NMR	Kleigrewe et al. (2012)
	DON conjugates (8)	Wheat	LC-HRMS, SIL	Kluger et al. (2013)
	DON oligoglycosides (3)	Malt, beer, bread	IAC, LC-HRMS	Zachariasova et al. (2012)
	Fusarenon X-glucoside	Wheat	LC-HRMS	Nakagawa et al. (2011)
	A. flavus anthraquinone metabolites	Culture medium	LC-HRMS, LC-ITMS	Malysheva et al. (2014)
Marine biotoxins	Pinnatoxins (6)	Mussels	LC-HRMS and synthesis	McCarron et al. (2012)
Plant toxins	Acetogenins (80)	Tropical fruit	HPLC-UV-LTQ-Orbitrap	Le Ven et al. (2014)
	Quinoline, carboline and glycinamide compounds	Cow's milk	HPLC/DAD/HRMS and 1D and 2D NMR	Rouge et al. (2013)
Veterinary drugs	Enrofloxacin metabolites	Chicken	LC-LTQ-Orbitrap and LC-QqToF	Morales-Gutiérrez et al. (2014)
	Mequindox metabolites (24)	Chicken bile, plasma, faeces, tissues	LC-HRMS	Shan et al. (2012)
	Estradiol-dipeptide biomarker	Urine	LC-LTQ-Orbitrap	Regal et al. (2013)
Process contaminants	MCPD derivatives	Palm oil	LC-LTQ-Orbitrap – mass defect filtering	Nagy et al. (2011)
	Mepiquat	Coffee	LC-Q-Exactive MS	Hammel et al. (2014)
Adulteration	Sildenafil analogue	Dietary supplement	LC-LTQ-Orbitrap-MS	Kee et al. (2013)
	Basic red 46 dye	Spices	LC-Exactive	Ruf et al. (2012)
Bioactive substances	Flavonoids, phenolic acids, phenylpropanoid glycosides (56)	TCM	UHPLC-ESI/LTQ-Orbitrap-MS	Chen et al. (2014)
	Caffeoyl derivatives, flavonoids, coumarins and sesquiterpenoids (50)	TCM	LC-HRMS and ^{1}H-NMR, ^{13}C-NMR	Li et al. (2011)
	Flavanol, flavanone, dihydrochalcone derivatives (38 compounds)	Tomatoes	LC-LTQ-Orbitrap-MS and LC-MS/MS	Vallverdu-Queralt et al. (2010)
	Quercotriterpenoside (2 compounds)	Wine	LC-HRMS, LC-MS/MS 2D ^{1}H-NMR, ^{13}C-NMR	Marchal et al. (2011)

Food Allergens

Analytical and Bioanalytical Chemistry
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RESEARCH PAPER

In-house validation of an LC–MS method for the multiplexed quantitative determination of total allergenic food in chocolate

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Abstract
Mass spectrometry has been widely accepted as a confirmatory tool for the sensitive detection of undeclared presence of allergenic ingredients. Multiple methods have been developed so far, achieving different levels of sensitivity and robustness, still lacking harmonization of the analytical validation and impairing comparability of results. In this investigation, a quantitative method has been validated in-house for the determination of six allergenic ingredients (cow's milk, hen's egg, peanut, soybean, hazelnut, and almond) in a chocolate-based matrix. The latter has been produced in a food pilot plant to provide a real and well-characterized matrix for proper assessment of method performance characteristics according to official guidelines. In particular, recent considerations issued by the European Committee for Standardization have been followed to guide a rigorous single-laboratory validation and to feature the main method performance, such as selectivity, linearity, and sensitivity. Synthetic surrogates of the peptide markers have been used both in native and labelled forms in matrix-matched calibration curves as external calibrants and internal standards, respectively. A two-order of magnitude range was investigated, focusing on the low concentration range for proper assessment of the detection and quantification limits (LOD and LOQ) by rigorous calibration approach. Conversion factors for all six allergenic ingredients have been determined for the first time to report the final quantitative information as fraction of total allergenic food protein (TAFP) per mass of food ($\mu g_{TAFP}/g_{food}$), since such a reporting unit is exploitable in allergenic risk assessment plans. The method achieved good sensitivity with LOD values ranging between 0.08 and 0.2 $\mu g_{TAFP}/g_{food}$, for all ingredients besides egg and soybean, whose quantitative markers reported a slightly higher limit (1.1 and 1.2 $\mu g_{TAFP}/g_{food}$, respectively). Different samples of chocolate bar incurred at four defined concentration levels close to the currently available threshold doses have been analyzed to test the quantitative performance of the analytical method, with a proper estimate of the measurement uncertainty from different sources of variability. The sensitivity achieved resulted in compliance with the various threshold doses issued or recommended worldwide.

Keywords Food allergen · Mass spectrometry · Quantitative method · In-house validation · Uncertainty · Conversion factors

🔍 Highlights of Orbitrap Mass Spectrometry in Allergen Detection

- 🧪 Simultaneous detection of multiple allergens

⟶ Covers 5 types: low-fat milk, whole egg, soy flour, hazelnut, and peanut.

- 🔊 Protein extraction via ultrasonic treatment

⟶ Simple 30-minute protocol + cleanup using exclusion cartridge.

- ⏱️ Full MS/DIA acquisition mode

⟶ Ensures high sensitivity and precision in measurement.

- 🧬 17 allergen-specific peptides detected

⟶ All identified in a single run from processed cookie samples.

- 📉 Detection limits: 60–100 µg/g

⟶ Capable of detecting trace levels in complex food matrices.

- 🧪✅ Validated with in-lab precision testing

⟶ Demonstrates reliability and consistency for real-world use.

- 🆚 Superior to traditional methods (ELISA / PCR)

⟶ No need for allergen-specific kits

⟶ Saves time, expands coverage

⟶ Detects processed allergens with altered protein structures

Protein & Peptide Biomarkers

Available online at www.sciencedirect.com
ScienceDirect
Current Opinion in Food Science

Proteins and peptides: proteomics approaches for food authentication and allergen profiling

Mónica Carrera[1], Ana G Abril[1], Manuel Pazos[1], Pilar Calo-Mata[2], Tomás G Villa[3] and Jorge Barros-Velázquez[2]

Food authentication and food allergy profiling are relevant topics that must be carefully considered by authorities, food production and manufacturing industries, and customers. Precise, sensitive, and efficient detection procedures are crucial for authenticating food and identifying allergens. In this paper, we present a current review of advanced proteomic approaches for food authentication and allergen profiling. We discuss three proteomics strategies, namely, discovery proteomics, targeted proteomics, and proteomics-based systems biology, used to authenticate food and profile allergens. This review includes a selection of the most representative papers published in this field in the last few years. Furthermore, we discuss future directions and potential opportunities in this field.

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Introduction

Food authentication and allergy profiling are important measures to ensure food quality and safety. Confirming the authenticity of food products is essential for preventing the consumption of harmful substances and protecting consumer health. Regulatory bodies are increasingly focused on accurately verifying products and preventing the substitution of species, addressing the concerns of customers and the food industry. These regulations comprise the U.S. Food and Drug Administration's Food Safety Modernization Act 2011, the European Regulation (EC) No 178/2002 identified as the General Food Law Regulation, and the Food Information to Consumers Regulation (Regulation [EU] No 1169/2011). The guidelines require food labels to clearly state the species or commercial name of the product.

Accurate labels with information about potential allergens also help people with food allergies obtain safe food. Approximately 6–8% of kids and 2–4% of adults are diagnosed with food allergies [1]. The European Food Safety Authority has recognized 14 food items as allergens, including fish, mollusks, shellfish, milk, eggs, soybeans, nuts, celery, peanuts, mustard, wheat, lupin, sesame, and sulfur dioxide/sulfites. Numerous countries have implemented stringent regulations for the labeling of allergens to safeguard consumers, as outlined in Directive 2007/68/EC.

Authorities, the food industry, and customers play a role in guaranteeing food quality/safety, as food authentication and allergy profiling have become topics of interest. To meet these guidelines, accurate and efficient detection methods are needed for identifying food species and controlling allergies. Various analytical methodologies have been applied to authenticate food and profile allergens. There are several commonly utilized methods, including high-performance liquid chromatography, near-infrared spectroscopy, nuclear magnetic resonance spectroscopy, immunoassays, and stable isotope ratio; in addition, genomics, metabolomics, and proteomics approaches have been recently applied [2–4]. In this sense, omics methodologies have profoundly impacted the research community and are increasingly being utilized in modern food science.

Research in the proteomics field examines proteins within a biological system on a large scale [5]. The objective of this field is to clarify the assembly, function, modifications, interactions, and regulation of proteins, thereby offering valuable knowledge on the dynamic