

Review Article

From Sea to Table: The Power of Metabolomics in Marine Food Science and Facing Challenges

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ABSTRACT

Marine food science has gained increasing attention owing to its potential to offer valuable bioactive compounds beneficial for human health aside from nutritive value. Metabolomics, a cutting-edge analytical technology aims to provide a comprehensive insight into the chemical composition of marine food systems, ensuring quality and safety. This review explores the integration of metabolomics in marine food science, emphasising its ability to profile metabolites for quality control, authentication, and safety assessment in seafood products. Metabolomics can aid in identifying geographical origin, detecting contaminants, and monitoring freshness levels in seafood. Additionally, it plays a critical role in advancing aquaculture by monitoring the health and nutritional quality of farmed fish species. The use of advanced spectroscopy, exemplified by nuclear magnetic resonance (NMR) and mass spectrometry (MS), enables the discovery of novel bioactive compounds with therapeutic potential, thereby enhancing the nutritional value of seafood. Despite the challenges in data interpretation due to the complexity of marine metabolites and their origin, the combination of metabolomics with other "omics" technologies holds promise to revolutionise our understanding of marine ecosystems. Further research is needed to overcome current analytical challenges and translate these findings into practical applications for the food industry.

Keywords: Aquaculture, Authentication, Marine food, Metabolomics

1. INTRODUCTION TO MARINE FOOD SCIENCE AND ITS ECONOMIC VALUE

Recently, the marine bioprocess industry has shown great interest converting and using most marine food products as valuable functional ingredients. Novel bioprocessing technologies are being developed for the isolation of bioactive substances from marine sources, which can be used as functional foods and nutraceuticals.^[1] Such development and optimisation of novel technologies, such as enzymatic hydrolysis, membrane filtration, supercritical fluid extraction, and fermentation, have revolutionised bioactive molecule discovery from marine organisms. These techniques facilitate the efficient extraction of compounds such as peptides, polysaccharides, polyunsaturated fatty acids (PUFAs), sterols, carotenoids, and phenolic compounds, which exhibit potential health benefits.^[2] Studies have provided evidence that marine-derived functional ingredients play a vital role in human health and nutrition. The wide range of biological activities including antioxidant, anti-inflammatory, antihypertensive, antimicrobial, antidiabetic, and anticancer activities, associated with the bioactive ingredients derived from marine food sources have the potential to expand its health-beneficial value.^[3] Hence, marine bioactive compounds hold a significant potential to be a promising candidate in the value-added nutraceutical, functional food ingredient,

and natural health product sector that can be used for health promotion and food preservation.^[4-7] Their unique structural characteristics, often shaped by the harsh and dynamic marine environment, make them attractive candidates for drug discovery and the development of skin care products with anti-ageing, photoprotective, or skin-repairing properties.^[7] Consequently, the economic value of marine food science continues to grow, driven by increasing consumer demand for natural, sustainable, and health-promoting products. Owing to the expansion of consumer market demand for marine products, quality assurance approaches are important, including standardisation of analytical methods for assessing sensory properties to ensure consumer acceptance.^[4] In this review, the impact of implementing metabolomics in marine food science using modern technological platforms is presented, ensuring seafood quality and safety, authenticity and traceability, fingerprinting and chemical profiling to highlight its nutritional and beneficial health effects, as well as overcoming challenges observed in aquacultures.

2. GLOBAL USE AND IMPORTANCE OF MARINE-DERIVED FOODS

Marine-derived foods are essential contributors to global nutrition and food security, supplying more than 3.3 billion people with at least 20% of their average intake of animal protein.^[5] The total global seafood consumption has more than doubled from 9.0 kg per capita in 1961 to 20.5 kg in 2020. According to the Food and Agriculture Organisation (FAO), over 179 million tonnes of fish and other aquatic animals were produced in 2020, of which 88% were used for direct human consumption. Aquaculture now contributes more than 50% of fish destined for consumption, marking a significant shift from traditional wild capture to farming systems. Moreover, marine-derived foods, such as seaweeds are increasingly valued not only as food but also as sources of nutraceuticals and functional ingredients, with the global seaweed market expected to reach USD 30 billion by the end of 2025.^[6]

3. METABOLOMICS AND ITS POTENTIAL IN FOOD SCIENCE

Due to the continuous growth in the food consumption, ensuring food safety, traceability, authenticity, and nutritional quality has become a top priority for both regulatory authorities and the food industry.^[8] To meet these demands, advanced analytical techniques have been developed to support quality assurance in food production systems, particularly in marine food products where authenticity and freshness are critical.^[9] Among these tools, metabolomics emerged

as a powerful and versatile technology for comprehensive food analysis.^[10] Metabolomics is the systematic study of the complete set of small-molecule metabolites, often referred to as the metabolome, present within a biological system under specific physiological or environmental conditions.^[11] In the context of food science, metabolomics offers insight into the biochemical composition of food products, enabling researchers and industry professionals to assess quality, detect adulteration, monitor processing effects, and verify geographical or botanical origin.^[8,12] However, the complete set of small molecule metabolites present in foods that make up the human diet, alongside the role of food production in altering the food metabolome, are still largely unknown. Such comprehensive analyses can be achieved through metabolomics, an “omics” technology defined as the study of all the metabolites or small molecules present in an organism, cell, or tissue under certain conditions.^[13] Metabolomics represents a transformative approach capable of capturing the dynamic nature of food matrices influenced by environmental, genetic, and technological factors. Modern metabolomic platforms, typically based on high-resolution nuclear magnetic resonance (NMR) spectroscopy and mass spectrometry (MS) coupled with liquid or gas chromatographic techniques (GC or LC), are capable of detecting hundreds to thousands of metabolites in a single analytical run.^[14] In foodomics, metabolomic applications are broadly categorised into untargeted and targeted approaches. Untargeted metabolomics, often described as metabolic fingerprinting, aims to capture a holistic profile of metabolites without prior bias.^[13] This method emphasises pattern recognition and is commonly used for sample classification, authentication, and comparative studies using multivariate chemometric analysis.^[13] It is particularly effective in distinguishing food products based on origin, species, processing stage, or storage duration. In contrast, targeted metabolomics or metabolite profiling involves the precise quantification of a predefined set of metabolites related to specific biochemical pathways or nutritional components. This approach is essential for understanding the functional relationships between bioactive compounds and their health effects, especially in nutraceutical and functional food development.^[15] Overall, metabolomics holds vast potential in modern food science as it bridges the gap between molecular composition and functional properties of foods. In combination with other “omics” technologies, such as genomics and proteomics, food traceability systems and personalised dietary strategies can be further advanced, thereby reshaping the future of food safety and health-oriented food design.

4. HOW METABOLOMICS CAN REVOLUTIONISE OUR UNDERSTANDING OF MARINE FOOD?

Marine ecosystems are hosts to a vast array of organisms, being among the most abundantly biodiverse locations on the planet. The study of these ecosystems is warranted, as they are not only a significant source of food but also have become an enriched source of bioactive compounds with therapeutic potential.^[11] Metabolomics has been used to deepen the understanding of interactions between marine organisms and their environment at a metabolic level and to discover new metabolites biosynthesised by these organisms.^[16] The exposure of marine organisms to environmental conditions, which can be intrinsic to their ecosystems or induced by anthropogenic activities, results in metabolic changes.^[16] Such metabolomic profiling studies are well documented for terrestrial-derived food from plants, but far less understood in the case of marine resources. In this context, a comprehensive analysis of metabolites produced by marine organisms is crucial in understanding the dynamics of marine ecosystems.^[16] Such untargeted analysis is a powerful tool in the study of marine organisms because it provides a comprehensive overview of the metabolites inside (metabolic fingerprinting) and outside (metabolic footprinting) to study the metabolic changes caused by genetic, environmental, or biological factors.^[11] For this reason, metabolomics approaches could provide a holistic viewpoint of metabolism, which would be impossible in classical targeted metabolic studies. Through unbiased metabolomic analysis, biomarkers for toxicity, diseases, or putative novel molecules with biological activity can be identified without previous knowledge of specific metabolites or metabolic pathways involved in the studied phenomena.

5. UNDERSTANDING THE METABOLOME OF MARINE ORGANISMS

The marine environment is a rich source of diverse structurally unique metabolites. So far, more than 40,000 marine metabolites have been reported from various marine organisms like sponges, algae, cnidarians, mollusks, tunicates, echinoderms, bryozoans, and microorganisms.^[17] These metabolites exhibit immense chemical diversity, including terpenes, steroids, polyketides, peptides, alkaloids, macrocyclic lactones, and porphyrins, many of which are unique to marine environments,^[18] and exhibit numerous biological activities, including antitumor, antiviral, and antimicrobial properties.^[18,19] Such chemical diversity is attributed to the unique environmental pressures (*i.e.*, salinity, temperature, and pressure), the symbiotic relationship, and the niche specialisation.

Marine metabolites play crucial roles in various biological processes such as metabolism, reproduction, and development, in response to biotic and abiotic factors, and in defense against competitors, predators, and other environmental stressors.^[20] Most of the reported metabolites are believed to originate from the symbiotic microorganisms living in coherence with marine creatures, which is much more complex in the scenario than in terrestrial plants. Such metabolites are primarily produced to protect the sessile marine organisms from potential parasitic and microbial infections.^[17] Such interactive symbiotic relationships have been the research focus for the discovery of many new bioactive scaffolds, and to better understand the regulation mechanisms covering production. The major detected classes of metabolites in marine organisms and the analytical techniques used for their detection are presented in Table 1.

Table 1: Major classes detected in marine organisms and the analytical techniques used for their detection

Class of metabolites	Examples	Analytical techniques	Marine resources
Amino acids/Peptides	Carnitine, glycine, taurine, bioactive peptides	NMR, GC/MS	Fish, crustaceans, mollusks
Fatty acids/Lipids	Omega-3-fatty acids, phospholipids, sterols	NMR, GC/MS, LC/MS/MS	Fish, algae, sea cucumbers
Organic acids	Lactic acid, succinic acid, malic acid	LC/MS/MS,	Crustaceans, shellfish
Carbohydrates	Glucose, trehalose, mannose...etc	GC/MS, NMR	Sea cucumbers, mollusks
Alkaloids/Amines	Trimethylamine (TMA), cadaverine	GC/MS, LC/MS/MS	Spoiled fish, squids
Phenolic compounds	Bromophenols, polyphenols,...etc	LC/MS/MS	Algae, sponges, mollusks
Terpenes and polyketides	Carotenoids, triterpenes	LC/MS/MS	Algae, sea cucumber
Vitamins	Vitamin B, tocopherols...etc	LC	Seaweeds, algae, crustaceans
Toxins	Okadaic acid, saxitoxins, domoic acid	LC/MS/MS, GC/MS	Bivalves, algae, sponges, shellfish
Saponins	Holotoxin A, lessonioside D	LC/MS/MS	Sea cucumbers
Sulfated metabolites	Holothurin D, holothurin B	LC/MS/MS	Sea cucumbers

NMR: Nuclear magnetic resonance, GC/MS: Gas chromatography mass spectrometry, LC/MS/MS: Liquid chromatography coupled to tandem mass spectrometry, LC: Liquid chromatography

6. POTENTIAL APPLICATIONS OF METABOLOMICS IN MARINE FOOD SCIENCE

Marine metabolomics, a powerful approach for profiling small-molecule metabolites in biological systems, plays a vital role in advancing seafood research and safeguarding its supply chains using integrated and advanced analytical techniques such as NMR, liquid or gas chromatography coupled to mass spectrometry (LC/MS, GC/MS) aided by multivariate data analyses i.e. principal component analysis (PCA) and unsupervised multivariate data analysis (MVA) (i.e., orthogonal partial least squares (OPLS) and molecular networking. Over the last decade, it has proven to be a golden mine for providing deep insight into the biochemical processes within marine organisms enabling it to expand its applications significantly as mentioned below in the next subsections for different applications [Figure 1].

6.1. Seafood quality and safety

Marine metabolomics aids in monitoring and ensuring the quality, freshness, and safety of seafood. By analysing profile fingerprints, it becomes possible to detect indicators for geographical origins, changes in metabolite profile associated with adulteration, spoilage, microbial contamination, chemical residues, or the impact of processing techniques such as storage, drying, freezing, and/or cooking.^[9,21-24] For instance, metabolomics can identify heavy metals

contamination or pollutants in seafood^[9,25] and can offer rapid detection of volatile and non-volatile compounds that are associated with microbial spoilage in fish such as trimethylamine oxide (TMAO) and its breakdown product trimethylamine (TMA), thus enabling timely interventions and ensuring food safety. Additionally, it aids in detecting paralytic shellfish biotoxins in bivalves and other seafood.^[9,23,26-29] On the other hand, metabolomics can reveal changes that occur in key metabolites that influence flavour, texture, and taste; thus aiding in optimising the processing methods for the overall quality of seafood products.^[30-33] This approach not only ensures compliance with consumers' preferences but also minimises risks to public health by preventing foodborne illness following the regulatory standards as hazard analysis critical control point guidelines by the Food & Drug Administration (HACCP, FDA).

6.3. Marine sources nutritional value and bioactive compounds

Seafood offers a valuable nutritional resource due to its highly enriched content of protein, vitamins (B12, D), minerals (selenium, iodine), fatty acids (particularly omega-3 eicosapentaenoic acid and docosahexaenoic acid), and essential amino acids. Moreover, it is recognised by the diverse content of unique secondary metabolites that belong to polyphenols, terpenes, sterols, and carotenoids among others,

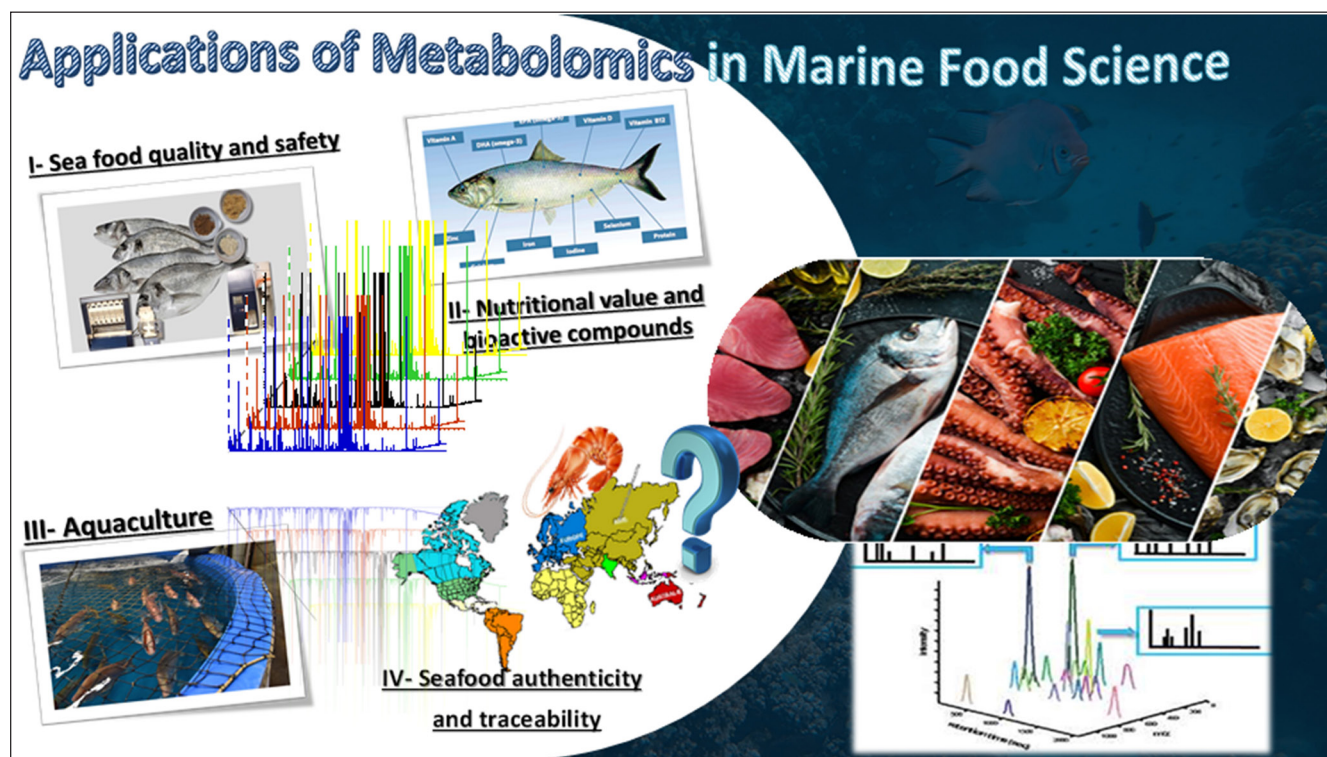


Figure 1: Applications of metabolomics in marine food science.

that exhibit pharmacological and therapeutic activities which, consequently, contribute to health-promoting purposes. This includes reducing the risk of cardiovascular diseases, enhancing brain function, and managing osteoporosis as well as anticancer, anti-inflammatory, antimicrobial, and antioxidant activities.^[34-39]

Metabolomics provides a significant advancement in the profiling of seafood primary and secondary metabolites. By analysing marine metabolome, researchers can determine, qualitatively and quantitatively, the impact of species and environmental variations (water quality, diet, temperature, geographical impact, climate changes, pollution, acidification, etc.) on seafood nutritional profile and bioactive components, as well as tracking the effect of stress factors on their metabolomes.^[37,40-43] This, in turn, can aid in the development of functional food and nutraceuticals from marine resources of potential in the healthcare field as well as optimising dietary recommendations.

6.4. Aquaculture

Aquaculture contributes significantly to seafood production to meet global demands as it can provide sustainable production of marine organisms, decrease the pressure on wild fisheries, and maintain a controlled environment for quality and safety management. Metabolomics is implemented in aquaculture to monitor the health and growth of the cultured species. Since metabolome profiling of fish, shellfish and crustaceans aids in assessing the impact of diet, environmental stressors, and water quality, it thus, improves the quality of farmed seafood.^[44] Furthermore, it aids in disease management by detecting metabolites' changes or assigning biomarkers associated with infections, enabling timely interventions that, subsequently, reduce economic loss of seafood. For instance, metabolomics was used to evaluate the effect of probiotics on fish metabolism to optimise their feed formulations and sensory attributes. On the other hand, it allows timely interventions for disease management in shrimps through the early detection of *Vibrio* infection among them, thus preventing massive losses in the farmed shrimps.^[44-47]

6.5. Seafood authenticity and traceability

Metabolomics offers a robust tool for tracking seafood authenticity by distinguishing between species, geographical origins, and different production methods, thus avoiding concerns about fraud, mislabelling of low-valued species as premium ones, and potential adulteration of seafood products. Metabolome profiling allows for generating unique fingerprints for different species and/or sources of seafood, assigning species-specific biomarkers, and detecting adulterants or substitutes.^[9,48] For example, metabolome

analysis was used to differentiate between the wild-caught fish and the aquaculture-farmed fish.^[9,44,49] Other metabolomic studies authenticated the species identity, geographical origin, and production methods of commercially important shrimps and prawns.^[50] This approach allows the consumers to make an informed choice and protects them from fraud, as well as ensuring compliance with regulatory laws.

7. ANALYTICAL CHALLENGES AND FUTURE DIRECTIONS IN MARINE FOOD OMICS

Regardless of the broad applications of metabolomics in studying marine organisms, its implementation is limited by practical obstacles, such as the broad chemical diversity of the metabolome delineating a challenge in the use of a single approach for extraction and analysis, in addition to the high salt and lipid content which necessitates sample pretreatment to obtain compatible extracts for metabolomic analysis.^[51] Additionally, the lack of standardised protocols for sample preparation from different marine matrices limits reproducibility.

7.1. Complexity of marine metabolomes

The main objective of metabolomics studies is to acquire a snapshot of the existing metabolome of an organism, yet none of the existing protocols allow the detection of the whole metabolome. Yet for marine organisms, the challenge is more crucial owing to the vast diversity and complexity of the existing chemistry being derived typically from several symbiotic relationships^[11]. Marine metabolites are distinguished by unique chemical features such as macrocyclic rings, nitrogenated and halogenated structures, and immense stereochemistry, all contributing to the challenge of their analysis.^[52] Aside from the lack of comprehensive databases for marine foods to aid in identification, especially using MS and NMR techniques.

7.2. Sensitivity and specificity of analytical techniques

NMR metabolomics is a widely used analytical platform and is especially useful in profiling highly abundant metabolites, yet its application is limited in the detection of less abundant metabolites owing to its low sensitivity and signal overlap in the spectra.^[11]

In contrast to NMR metabolomics, LC-MS enables the profiling of the less abundant metabolites and provides more information as reflected by the chromatographic and fragmentation behaviour of the metabolites. Yet the annotation step remains a huge bottleneck in the analysis workflow. The complementation of both techniques in food omics has been reported extensively recently,^[53] but is yet to be examined in the case of marine food analysis.

Compared to LC-MS, which is better suited for secondary metabolites, GC-MS can provide a definitive overview of the primary metabolites (i.e., amino acids, lipids, and carbohydrates), along with the volatiles, especially when integrated with *in situ* sampling tools (i.e., headspace and solid phase microextraction).^[54] Nevertheless, it is much less used in the study of the marine metabolome when compared to the widely used LC-MS technique.

Conclusively, the incorporation of various metabolomics tools can provide a more comprehensive overview of the particular organism under study, especially when combined with other analytical platforms such as capillary electrophoresis-mass spectrometry (CE-MS), supercritical fluid chromatography-mass spectrometry (SFC-MS), high-performance thin layer chromatography (HPTLC), and IR-based metabolomics.^[11] Nevertheless, the incorporation of new analytical tools does not ultimately assure more valuable findings.

7.3. Data analysis and interpretation

A major challenge in marine metabolomics studies lies in data mining and dereplication owing to the scarcity of marine chemical standards, limitations of the existing spectral libraries, and the difficulty of the isolation which is hampered by the limited availability of the sample. These obstacles could be overcome by the *in silico* dereplication tools (such as Sirius),^[55] which speed up the annotation step and allow the discovery of novel scaffolds.

Yet, sometimes metabolite detection fails within the complex mixture and requires isolation for their identification, which is often hindered by the scarcity of the samples which could be overcome by microscale isolation protocols.

Recently, the GNPS platform (Global Natural Products Social Network) has facilitated the grouping of structurally similar metabolites, aiding in the data mining of the acquired complex datasets.^[56] Incorporation of the *in silico* dereplication tools with the molecular networking (via the GNPS platform), such as NAP (network annotation propagator), MS2LDA, and MolNetEnhancer is a potential approach for metabolite identification or compound families. Additionally, the application of networking tools in correlation with bioactivity in regression models or food attributes could aid in identifying specific moieties for a targeted effect or use.

Another significant approach in mining complex metabolomics datasets lies in the integration of multivariate analysis (MVA). Given the massive number of variables generated from metabolomics analysis (ranging from hundreds to tens of thousands), the reduction of data dimensionality is crucial for deriving hidden and significant information from the complex data matrix. Both supervised

(i.e., principal component analysis (PCA)) and unsupervised MVA (i.e., orthogonal partial least squares (OPLS)) can be applied to reduce the data dimensionality, regardless of the employed metabolomics protocol.^[11] For the unsupervised MVA, (PCA) is the most commonly adopted to gather most of the existing variance using principal components (new orthogonal variables).

The produced predictive models can be used for food authentication, detection of adulteration, and the formed hazardous substances during processing or storage.^[57,58]

7.4. Standardisation and data sharing of marine-derived datasets

The ultimate goal of metabolomics research is to identify the significant metabolites highlighted from the MVA, however this process is yet limited by the huge chemical diversity of the marine metabolome and the availability of reliable databases. Most of the available databases provide information about the chemical structure and the physicochemical properties of the compounds regardless of their biological origin, with databases devoted to plants, animals, or microbial metabolites, such as Super Natural II, Dictionary of Natural Products, NP Atlas, and AntiBase, and a few are for the marine metabolites.^[11] Recently, marine specialised databases were developed, such as Marinlit (<https://marinlit.rsc.org/>), seaweed metabolite database (SWMD),^[59] CMNPD: a comprehensive marine natural products database,^[60] and MarinChem3D, which could aid in the identification of marine secondary metabolites, besides the generic databases for exploring the primary metabolome. The continuous contribution of the natural products community to the growth of mass spectrometry databases is crucial and could be extremely helpful in the dereplication step, even though the instruments and experimental parameters may differ which could greatly affect the acquired mass spectra.

Likewise, the incorporation of more NMR spectroscopic data on marine metabolites is critical to boost the annotation in NMR metabolomics, which could be of benefit to *in-silico* prediction tools such as ACD/Labs.^[11] Another challenge in marine metabolomics studies is the data assimilation across different laboratories, with distinct instruments and independent protocols,^[61] necessitating the development of standardised protocols to improve data comparability and reproducibility across studies and laboratories.

7.5. Combining metabolomics with other omics for a more comprehensive understanding of marine organisms

Other-omics tools could be integrated with metabolomics according to the analytical objectives or targeted question in mind [Figure 2]. For instance, lipidomics can be used in

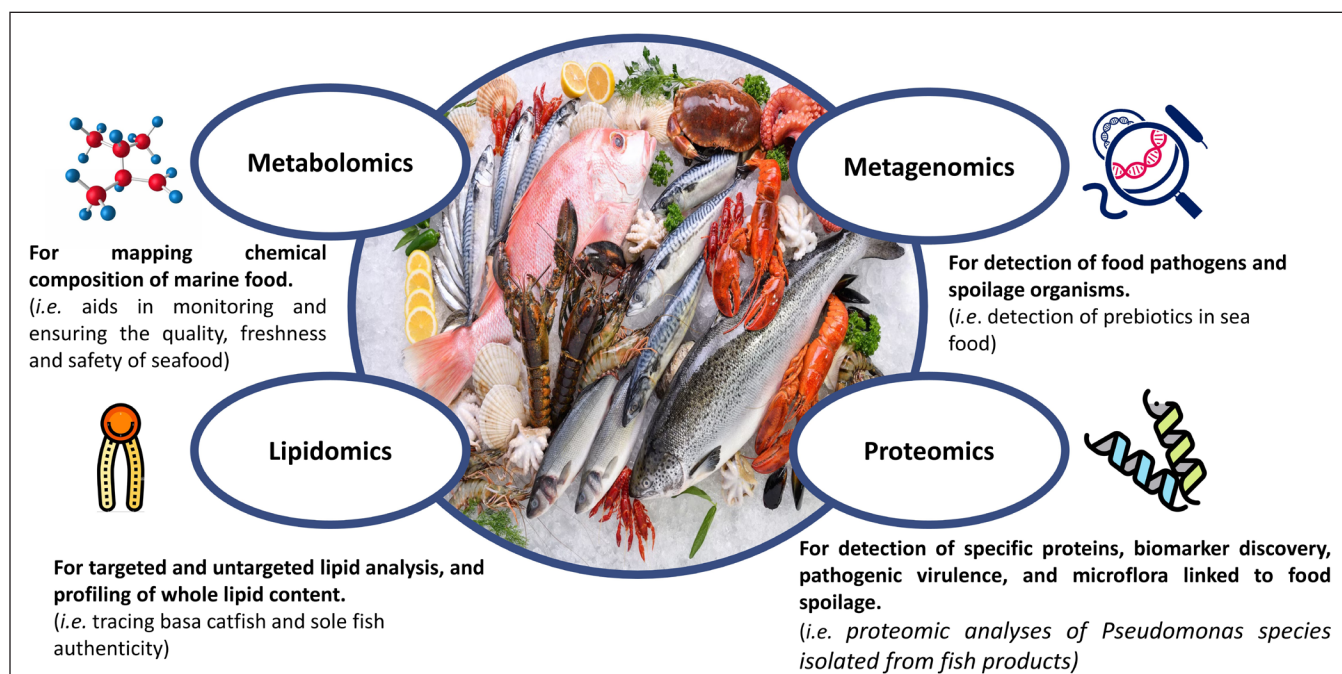


Figure 2: Integration of metabolomics with other omics techniques for a better understanding of marine organisms.

both targeted and untargeted manners to analyse specific lipids or profile the entire lipid content in samples.^[58] Similarly, targeted or untargeted proteomics analysis could be integrated for the detection of specific proteins and biomarker discovery respectively, thus providing further information about the safety and quality of marine foods.^[62] Additionally, proteomics has recently been popular for the prediction of pathogenic virulence during the processing and storage of seafood, and for the detection of microflora linked to seafood spoilage and foodborne diseases through next-generation sequencing.^[63,64] Compared to extensive reports on prebiotics of plant origin and how they interact with gut microbiota,^[14] less is known about marine-derived prebiotics and should be considered using metagenomics and metabolomics technologies.

Furthermore, the detection of food pathogens and spoilage microorganisms could be accomplished by incorporating metagenomics, which also enables the identification of other unknown microbes through observing the modifications in the entire microbial communities, thus improving the quality and safety of marine food.^[65]

Nevertheless, the integration of other omics techniques could provide a more comprehensive understanding of marine life, but it also requires sophisticated analytical tools and bioinformatics resources to handle and interpret the large datasets generated.

8. CONCLUSION

Owing to the increasing popularity of marine-derived food, tracing its quality and safety is a major concern for producers, traders, and consumers. The integration of different -omics tools could pave the way for molecular labelling to reflect the safety and quality of marine-derived food. Combining metabolomics, proteomics, lipidomics, and metagenomics data with MVA can undoubtedly establish and contribute to improved quality control analysis of marine-derived food in the context of their origin, freshness, lipid oxidation, processing, storage, and detection of contaminants and microbial pathogens. Emphasising the importance of translating research findings derived from metabolomics reports into practical applications to benefit the food industry is crucial in capitalising more on seafood and its applications.

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