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Editorial

Editorial for the Special Issue "NMR- and MS-Based Metabolomics Approaches for Local and Traditional Foods' Characterization"

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Metabolomics is a powerful tool in food sciences, widely used in food analysis for authenticity and traceability assessment and regulatory compliance, processing, quality, and safety [1]. The literature on metabolomic research focused on food authenticity and traceability [2] and geographical origin assessment in different matrices, such as olive oils [3], wines [4], honeys [5], and fruit juices [6]. Among foodstuffs, local products are characterized by a specific chemical composition, often exhibiting high nutraceutical and organoleptic values, influenced by several factors (genetics, environment, transportation, and storage conditions). Thus, scientific methods that provide molecular-scale characterizations of traditional food matrices could help valorize these foodstuffs. Moreover, to date, most local landraces do not match the food industry requirements, and the genetic improvement introduces new species with higher commercial values but often impoverished of healthy compounds [7,8]. From this point of view, the characterization of local foodstuffs and their chemical content could relieve the current rate of genetic erosion restoring biodiversity. Moreover, it should be also noted that in recent years, food safety and quality awareness gained significant relevance, as consumers are more interested in authentic foods and drinks with nutraceutical properties [9]. Therefore, analytical methods that detect the presence of bioactive compounds could be successfully used to promote and establish local and traditional product valorization actions, simultaneously meeting consumer requirements. Thus, using foods as ingredients for typical dishes, characterized by chemical fingerprints and nutritional properties (highlighted using metabolomics tools) could be promoted, with possible commercial impacts (e.g., local tourism and territorial development) [10].

Nuclear Magnetic Resonance Spectroscopy (NMR) and Mass Spectrometry (MS) are among the scientific methods and analytical techniques extensively used, combined with chemometrics, in many foodstuff metabolomics studies since both can detect various metabolites with high specificity and reproducibility.

NMR is commonly used to characterize foodstuffs and provides a snapshot of all the molecular components present in a specific complex matrix as a powerful camera. In combination with chemometric methods, NMR allows us to consider the natural variability of the chemical composition of complex matrices and has been widely used for biomarker detection, food quality control, and/or origin discrimination [11]. Together with NMR, Mass Spectrometry (MS) coupled with chemometric techniques is used for foodstuff quality assessment. Using MS in metabolomics is usually coupled to separation techniques, such as liquid chromatography or capillary electrophoresis, providing a detailed metabolomic profile suitable for statistical analyses. MS-based analytical strategies are successfully used in biomarkers discovery, the detection of adulterants, and the analysis of specific classes of secondary metabolites (as phenolic compounds, terpenoids, flavonoids, glucosinolates,

saponins, lignins, and alkaloids) with specific roles in colour, taste, aroma, scents, and, the case of botanicals, including agro-crops, specific defensive responses to biotic and abiotic stresses [12].

Analytical, spectrometric, and statistical techniques used in metabolomic studies allow for the identification of specific characteristics of metabolites, revealing the effects of geographical-specific natural factors (i.e., pedoclimatic conditions) and anthropic factors such as agricultural practices, breeding systems, and production processes. The chemical fingerprinting resulting from these approaches could support the authentication of products with specific characteristics linked to regions' terroir and know-how, with possible contribution also in the consumers' choices [10]. Furthermore, the well-known potential of NMR-MS-based metabolomics methods for authenticity and geographical origin assessment could be used to explain the high added value of specific products and the sustainability of the related supply chain.

This Special Issue aims to publish original research and review articles to increase the knowledge of local and traditional foodstuffs, providing new insights into their chemical characterization and the content of bioactive compounds. Different aspects could be focused on, such as geographical assessment methods, restoring local biodiversity, or even possible commercial applications.

References

1. Cevallos-Cevallos, J.M.; Reyes-De-Corcuera, J.I.; Etxeberria, E.; Danyluk, M.D.; Rodrick, G.E. Metabolomic Analysis in Food Science: A Review. *Trends Food Sci. Technol.* **2009**, *20*, 557–566. [CrossRef]
2. Sobolev, A.P.; Thomas, F.; Donarski, J.; Ingallina, C.; Circi, S.; Cesare Marincola, F.; Capitani, D.; Mannina, L. Use of NMR Applications to Tackle Future Food Fraud Issues. *Trends Food Sci. Technol.* **2019**, *91*, 347–353. [CrossRef]
3. Calò, F.; Girelli, C.R.; Wang, S.C.; Fanizzi, F.P. Geographical Origin Assessment of Extra Virgin Olive Oil via NMR and MS Combined with Chemometrics as Analytical Approaches. *Foods* **2022**, *11*, 113. [CrossRef] [PubMed]
4. Tzachristas, A.; Dasenaki, M.E.; Aalizadeh, R.; Thomaidis, N.S.; Proestos, C. Development of a Wine Metabolomics Approach for the Authenticity Assessment of Selected Greek Red Wines. *Molecules* **2021**, *26*, 2837. [CrossRef] [PubMed]
5. Girelli, C.R.; Schiavone, R.; Vilella, S.; Fanizzi, F.P. Salento Honey (Apulia, South-East Italy): A Preliminary Characterization by 1H-NMR Metabolomic Fingerprinting. *Sustainability* **2020**, *12*, 5009. [CrossRef]
6. Sobolev, A.P.; Mannina, L.; Proietti, N.; Carradori, S.; Daglia, M.; Giusti, A.M.; Antiochia, R.; Capitani, D. Untargeted NMR-Based Methodology in the Study of Fruit Metabolites. *Molecules* **2015**, *20*, 4088–4108. [CrossRef] [PubMed]
7. Renna, M.; Serio, F.; Signore, A.; Santamaria, P. The Yellow–Purple Polignano Carrot (*Daucus Carota* L.): A Multicoloured Landrace from the Puglia Region (Southern Italy) at Risk of Genetic Erosion. *Genet. Resour. Crop. Evol.* **2014**, *61*, 1611–1619. [CrossRef]
8. Girelli, C.R.; Accogli, R.; Del Coco, L.; Angilè, F.; De Bellis, L.; Fanizzi, F.P. 1H-NMR-Based Metabolomic Profiles of Different Sweet Melon (*Cucumis Melo* L.) Salento Varieties: Analysis and Comparison. *Food Res. Int.* **2018**, *114*, 81–89. [CrossRef]
9. Girelli, C.R.; Serio, F.; Accogli, R.; Angilè, F.; De Donno, A.; Fanizzi, F.P. First Insight into Nutraceutical Properties of Local Salento Cichorium Intybus Varieties: NMR-Based Metabolomic Approach. *Int. J. Environ. Res. Public Health* **2021**, *18*, 4057. [CrossRef] [PubMed]
10. Cassago, A.L.L.; Artêncio, M.M.; de Moura Engracia Giraldi, J.; Da Costa, F.B. Metabolomics as a Marketing Tool for Geographical Indication Products: A Literature Review. *Eur. Food Res. Technol.* **2021**, *247*, 2143–2159. [CrossRef] [PubMed]
11. Hatzakis, E. Nuclear Magnetic Resonance (NMR) Spectroscopy in Food Science: A Comprehensive Review. *Compr. Rev. Food Sci. Food Saf.* **2019**, *18*, 189–220. [CrossRef]
12. Liu, Z.; Zhang, M.; Chen, P.; Harnly, J.M.; Sun, J. Mass Spectrometry-Based Nontargeted and Targeted Analytical Approaches in Fingerprinting and Metabolomics of Food and Agricultural Research. *J. Agric. Food Chem.* **2022**, *70*, 11138–11153. [CrossRef] [PubMed]