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Potential of Food By-Products

Valorization of Food By-Products Employing Spectroscopic and Chemical Methods: Characterization and Applications of Functional Biomolecules

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Abstract

Background: Large quantities of by-products and waste materials are inevitably generated throughout food processing and manufacturing operations. Despite being consistently rich in high-value bioactive constituents — including polyphenols, dietary fiber, antioxidant compounds, and bioactive peptides — these by-products are frequently discarded without further utilization, representing a considerable loss of both nutritional and economic potential. Therefore, valorizing such byproducts constitutes a sustainable strategy for reducing food waste while generating added value across food, animal feed, and non-food industrial applications.

Aims: This review aimed to systematically and critically evaluate the current scientific literature pertaining to the characterization and valuation of bioactive compounds extracted from food by-products, with particular emphasis on the spectroscopic and chemical methods employed for their identification and quantification, and on their applications within food systems food systems.

Material and Methods: A structured critical narrative review methodology was adopted for this study. A systematic literature search was conducted across three major academic databases—Scopus, ScienceDirect, and Springer—encompassing publications from 2015 to 2025. The initial search yielded 26,152 documents, from which 17,830 peer-reviewed research articles published in English language were identified. Inclusion criteria were applied to retain publications specifically describing the characterization of bioactive substances employing spectroscopic or chemical analytical methods, and reporting on their primary applications in food-related contexts.

Results: The reviewed literature consistently confirms that food by-products represent potential and underexploited sources of bioactive compounds with biological, technical, and nutritional properties. The integration of spectroscopic techniques — most notably Fourier-transform infrared spectroscopy (FTIR) and near-infrared spectroscopy (NIR) — with conventional chemical analytical methods has demonstrated considerable utility for the rapid and non-destructive characterization of bioactive molecules, quality evaluation, and authenticity verification of food by-product-derived materials. Applications of these compounds in food formulation, preservation, and active packaging have been increasingly documented in the literature; however, persistent challenges remain with respect to analytical standardization, comprehensive safety evaluation, and industrial-scale feasibility.

Conclusions: The valorization of food by-products through the combined application of spectroscopic and chemical analytical approaches presents substantial and scientifically exciting prospects for the development of sustainable, circular food systems. To fully realize the functional and commercial potential of food by-product-derived bioactive compounds, future research should prioritize the standardization of analytical protocols, the rigorous evaluation of safety and toxicological profiles, and enabling their industrial-scale deployment.

Keywords: Food By-Products; Bioactive Compounds; Valorization; Spectroscopic Methods; Chemical Analysis; Functional Biomolecules; Food Applications.

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1 Introduction

One of the most pressing and growing global challenges of the twenty-first century is the generation of food waste and byproducts from agricultural and food industries, attributable to their significant environmental, economic, and public health impacts. Recent estimates indicate that substantial quantities of food are lost or wasted annually across all stages of the food supply chain, including husks, seeds, pulp, bran, and processing residues. Although these byproducts are conventionally considered as waste, accumulating evidence has demonstrated that they constitute valuable sources of bioactive compounds possessing noteworthy nutritional and functional properties, including dietary fiber, natural antioxidants, phenolic compounds, flavonoids, and bioactive peptides (Gómez-García *et al.*, 2021; Sagar *et al.*, 2018).

In response to the growing recognition of the bioactive compounds contained in these materials, the concept of food by-product valorization has emerged in recent years as a cornerstone strategy for advancing circular economy principles and promoting food system sustainability. This paradigm entails the transformation of agricultural and food processing residues into high-value raw materials suitable for diverse applications, including functional foods, active packaging, animal feed, nutraceuticals, and cosmeceutical products (Gómez-García *et al.*, 2021; Mirabella *et al.*, 2014). However, the successful implementation of this strategy largely depends on the ability to accurately characterize bioactive compounds, understand their functional and chemical properties, and ensure their applicability at industrial scale. In this context, chemical and spectroscopic characterization techniques have become essential tools for the identification of active compounds, assessment of their purity, and verification of their biological and functional attributes (Lozada-Ramírez *et al.*, 2021).

Characterization methods have undergone remarkable development in recent decades, with spectroscopic techniques emerging as rapid, non-destructive, and cost-effective tools for the profiling of bioactive compounds. Their capacity to provide accurate molecular fingerprints in a timely manner, coupled with relatively low operational costs, has rendered them particularly attractive for routine analytical applications. Among the most prominent spectroscopic methods are Fourier transform infrared spectroscopy (FTIR), near infrared spectroscopy (NIR), Raman spectroscopy, and Ultraviolet–Visible Spectroscopy (UV–Vis) (Zhang *et al.*, 2025). Conversely, chemical and chromatographic techniques, such as high-performance liquid chromatography (HPLC), gas chromatography-mass spectrometry (GC-MS), and Liquid Chromatography–Mass Spectrometry (LC–MS), despite their elevated cost and operational complexity, remain among the most widely employed techniques owing to their exceptional sensitivity and accuracy in the identification and quantification of individual compounds *(Zhang et al.*, 2025). Despite these advances, considerable heterogeneity persists across studies with regard to the level of analytical validation, industrial applicability, and comparability of results between different studies, that requires a systematic critical evaluation of these analytical tools.

Notwithstanding the substantial and growing body of published scientific reviews addressing the utilization of food waste and the extraction of bioactive compounds, it is noteworthy that the majority of previous investigations have concentrated on descriptive aspects related to the types of waste or extracted compounds and their potential applications. A conspicuous lacuna exists with respect to critical reviews that systematically compare the analytical performance of both spectroscopic and chemical methods across multiple parameters, including sensitivity, accuracy, rapidity, cost, industrial scalability, and experimental validation. Furthermore, the limited methodological consistency observed across studies constrains the derivation of broadly applicable conclusions that may be readily translated to industrial contexts.

Accordingly, the present review aims to provide a comparative critical evaluation of spectroscopic and chemical methodologies employed for the characterization of bioactive compounds derived from food waste, with particular emphasis on analytical performance, advantages and limitations, industrial applicability, and levels of scientific validation. This study further seeks to identify current research gaps and to propose prospective research directions that may facilitate the development of more sustainable and reliable strategies for the valorization of food waste and its conversion into high-value products.

Although prior reviews have addressed the extraction of bioactive compounds from food waste, such as that of Gómez-García *et al.* (2021), which focused on valorization strategies in general, and that of Sagar *et al.* (2018), which specifically examined fruit and vegetable waste, these contributions have not provided a systematic and critical comparison of the analytical performance of spectroscopic and chemical methods in terms of sensitivity, accuracy, rapidity, cost, industrial scalability, and experimental validation. Therefore, the scientific novelty of this review lies in: (1) the provision of a comprehensive comparative and critical evaluation of spectroscopic (FTIR, NIR, Raman, UV-Vis) and chemical (HPLC, GC-MS, LC-MS) methods within the context of food waste valorization; (2) the systematic analysis of the strengths and limitations of each method, with a particular focus on industrial applicability; (3) the proposal of an integrated framework combining the rapidity of spectroscopy with the accuracy of chemical methods; and (4) the identification of research gaps and outlining a roadmap for future investigations in this field.

2 Materials and Methods

2.1 Review Design

The present study adopted a structured critical narrative review methodology, guided by the principles of the Preferred Reporting Items for Systematic Reviews and Meta-Analyses (PRISMA) framework, to ensure transparency methodological rigor, and reproducibility throughout the research process and study selection procedure. The review was specifically designed to evaluate published investigations related to the valorization of food processing waste through the extraction and characterization of bioactive compounds utilizing spectroscopic and chemical analytical methods, with particular emphasis to analytical performance, methodological limitations, and industrial applicability.

2.2 Literature Research Strategy

A comprehensive and systematic literature search was conducted across four major academic databases, including Scopus, ScienceDirect, and Springer, with the objective of identifying relevant studies published between 2015 and 2025. This ten-year time frame was selected to ensure the capture of the most significant and recent developments in the field of spectroscopic and chemical characterization techniques applied to bioactive compounds extracted from food waste and agro-food by-products.

Search queries were systematically adapted to the indexing conventions and syntactic requirements of each individual database in order to maximize search sensitivity and ensure the most comprehensive retrieval of potentially relevant records. The specific search equations employed for each database are presented in Table 1. All searches incorporated Boolean operators (AND, OR) to combine search terms in a structured and reproducible manner. The variation in the number of records retrieved across databases reflects differences in subject coverage, indexing scope, and database-specific search syntax. Scopus yielded the most precise and focused results, whilst ScienceDirect generated the highest absolute number of retrieved publications, and Springer provided intermediate coverage across both parameters.

Table 1. Modified search equations for each database

Database	Modified search equation	Total papers	Research articles	English articles
Scopus	TITLE-ABS-KEY("food waste" OR byproducts) AND TITLE-ABS-KEY("bioactive compounds" OR polyphenols OR antioxidants) AND TITLE-ABS-KEY(spectroscopy OR FTIR OR HPLC OR "GC-MS")	950	915	908
Science Direct	("food waste" OR byproducts) AND ("bioactive compounds" OR polyphenols OR antioxidants) AND (spectroscopy OR FTIR OR HPLC OR "GC-MS")	21,410	14,786	14,786
Springer	("food waste" OR byproducts) AND ("bioactive compounds" OR polyphenols OR antioxidants) AND (spectroscopy OR FTIR OR HPLC OR "GC-MS")	3,792	2,137	2,136

2.3 Eligibility Criteria

Predefined inclusion and exclusion criteria were established prior to the commencement of the study selection process began to ensure methodological consistency and to minimize the risk of selection bias.

Inclusion Criteria

Studies were considered eligible for inclusion if they satisfied all of the following criteria following criteria:

- Published in peer-reviewed scientific journals indexed in the selected databases
- Written in the English language.
- Addressing food waste, agricultural residues, or agro-food processing by-products.
- Incorporating the characterization or analysis of bioactive compounds through spectroscopic or chemical methods.
- Reporting on applications of bioactive compounds or proposing strategies for the valorization of food waste.

Exclusion Criteria:

Studies were excluded from the review if they met any of the following conditions:

- Non-peer-reviewed research publications, including conference abstracts, book chapters, editorial letters, and conference proceedings.
- Publications in languages other than English.
- Studies focusing on non-food waste materials or not incorporating bioactive compound characterization.
- Duplicate records or studies providing insufficient methodological or analytical detail to permit meaningful critical evaluation.

2.4 Study Selection and Screening

The study selection process was conducted in strict accordance with the PRISMA 2020 guidelines. A total of 17,830 research articles were initially identified through the systematic database searches of Scopus, ScienceDirect, and Springer. Following the automated removal of duplicate records, the remaining articles were screened based on their titles and abstracts against the predefined eligibility criteria. Articles meeting the preliminary eligibility requirements were subsequently retrieved in full text and assessed for final inclusion. Only those studies satisfying all established inclusion criteria were retained for qualitative synthesis and critical analysis. The complete study selection and screening process is presented in the PRISMA 2020 flow diagram in Figure 1.

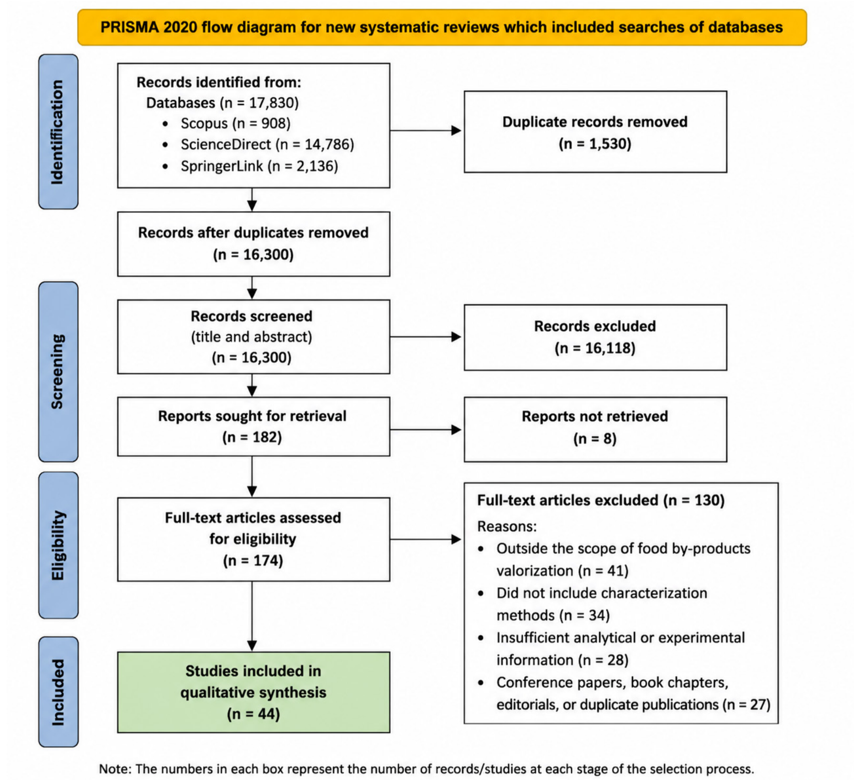

Figure 1. PRISMA 2020 Flow Diagram of the Literature Search and Study Selection Process

To position the present review within the current landscape of systematic reviews addressing food by-product valorization, a selection of recent PRISMA-based systematic reviews were identified and considered as reference studies for methodological comparison (Table 2). These reviews covering a broad range of related topics, including the health effects of foods processed from plant by-products (Pérez-Beltrán *et al.*, 2024), techno-economic aspects of food waste valorization (Tariq *et al.*, 2025), digital transformation for sustainable agri-food waste management (Censi *et al.*, 2025), green extraction of phenolic compounds (López-Salas *et al.*, 2024), marine by-product valorization (Passos *et al.*, 2026), food genomics (Pérez-Beltrán *et al.*, 2022), and mycotoxin occurrence in food by-products (Lopes *et al.*, 2023). As summarized in Table 2, the number of initially identified records and the final number of studies included varied considerably across these reference reviews, reflecting differences in research scope, search strategies, and eligibility criteria. The present review identified 17,830 records and ultimately retained 44 studies for inclusion, placing its scope within the range of recent PRISMA-based systematic reviews in this field.

Table 2. Comparison Between the Present Systematic Review and Selected Recent PRISMA-Based Systematic Reviews in the Field of Food By-Product Valorization

Reference	Topic	Initial records	Final Included
Pérez-Beltrán *et al.* (2024)	Effects of plant by-product consumption on blood lipid levels	15,706	19
Tariq *et al.* (2025)	Economic analysis of food waste valorization across regions	3,964	50
Censi *et al.* (2025)	Digital pathways toward sustainability in agri-food waste	524	373
López-Salas *et al.* (2024)	Phenolic compound extraction using green solvents	282	67
Passos *et al.* (2026)	Characterization of marine by-products and geographical origin tracing	6,443	94–96
Pérez-Beltrán *et al.* (2022)	Gene-diet interactions and effects on lipids	1,110	38
Lopes *et al.* (2023)	Occurrence of mycotoxins in food by-products	Not specified	16
Present review	Spectroscopic and chemical characterization of bioactive compounds from food by-products	4,538	44

The PRISMA 2020 flow diagram presented in Figure 1 provides a transparent and structured overview of all stages of the literature search and study selection process performed, encompassing the identification of records retrieved from the three selected databases, duplicate removal, title and abstract screening, full-text eligibility assessment, and the final inclusion of studies meeting all predefined eligibility criteria. This diagram enhances the methodological transparency and reproducibility of the review.

2.5 Data Extraction and Synthesis

Relevant data were systematically extracted from all included studies employing a standardized data extraction framework. The following information was recorded for each study: the type of food waste or agro-food by-product investigated, the class and identity of bioactive compounds extracted; the spectroscopic and/or chemical analytical methods employed, the principal analytical findings and quantitative results, and the proposed valorization strategies or applications. A comparative critical analysis was subsequently conducted to evaluate and compare the analytical performance of the different characterization methods across the dimensions of accuracy, sensitivity, analytical rapidity, operational cost, and industrial applicability.

2.6 Quality Assessment

To enhance the reliability, scientific rigor, and interpretive robustness of this review, the methodological quality of the selected studies was systematically assessed through predefined methodological quality criteria adapted from established systematic review guidelines (Higgins *et al.*, 2011; Page *et al.*, 2021). The quality assessment focused framework focused on five principal dimensions:

- The clarity and accuracy of the research objectives and study design
- The adequacy and completeness of the description of food by-products and the samples characterization procedure
- The suitability, validity and degree of analytical validation of the spectroscopic or chemical analytical methods employed.
- The reproducibility and methodological transparency of the experimental procedures.
- The scientific significance and practical relevance of the reported results for food by-products valorization and their potential industrial applications.

Each included study underwent rigorous examination according to these criteria to identify methodological strengths and limitations. Studies providing detailed and reproducible experimental protocols, rigorous analytical procedures, and clearly interpretable results were considered to represent higher-quality evidence. Conversely, studies characterized by insufficient methodological reporting or limited analytical validation were interpreted with appropriate caution during the data synthesis process.

The quality assessment was employed primarily as an instrument to support the critical and balanced interpretation of the assembled literature and to minimize the influence of methodological heterogeneity and potential bias on the conclusions of this review. The specific quality assessment criteria applied to the included studies are presented in Table 3, which evaluate study design, sample characterization, analytical validation, experimental reproducibility, and industrial relevance. These criteria were specifically designed for the purposes of the present review to ensure their appropriateness for evaluating the methodological quality and practical relevance of studies addressing the spectroscopic and chemical characterization of bioactive compounds derived from food by-products.

Table 3. Quality Assessment Criteria Employed for the Evaluation of Included Studies

Criterion	Evaluation focus
Study design	Clarity of objectives and
Sample characterization	Adequate description of food by-products
Analytical validation	Validation of spectroscopic or chemical methods
Reproducibility	Availability of sufficient methodological details
Industrial relevance	Potential applicability in real-world valorization processes

3 Results and Critical Review

3.1 Overview of Selected Studies

3.1.1 General Characteristics of Included Studies

The systematic literature research yielded a collection of studies investigating the valorization of food waste through the extraction and characterization of bioactive compounds employing a diverse array of spectroscopic and chemical analytical techniques. The included studies demonstrated considerable heterogeneity with respect to the types of food waste examined, the classes of bioactive compounds targeted, the analytical methods employed, and the proposed end applications of these compounds across various food science, functional food development, and healthcare sectors.

The majority of included studies focused on plant-derived byproducts generated by the food industry — principally fruit peels and pomaces, olive processing residues, cereal bran and milling by-products, and vegetable and legume residues — attributable to their richness in phenolic compounds, flavonoids, dietary fiber, and antioxidants (Gómez-García *et al.*, 2021; Sagar *et al.*, 2018). The results further revealed that phenolic compounds and antioxidants constituted the most extensively studied classes of bioactive compounds, across the included literature, reflecting their established functional significance in enhancing the nutritional and technological properties of food products and in extending shelf life.

A notable divergence was also identified in the analytical approaches adopted across the included studies. A substantial proportion of investigations favored rapid, non-destructive spectroscopic methods such as FTIR and NIR for the preliminary screening and broad characterization of target bioactive compounds, while other investigations relied upon more precise chemical techniques, such as HPLC and GC-MS, for the accurate quantitative and qualitative determination of individual compounds (Kanwal & Musharraf, 2024). This divergence reflects the absence of a clearly established methodological consensus regarding the most appropriate analytical strategy, necessitating a rigorous comparative critical evaluation of the analytical performance, strengths, and limitations of each technique within the context of food by-product valorization.

Table 4 provides a comprehensive summary of the key characteristics of the studies included in this review, including the type of food waste investigated, the targeted bioactive compounds, the analytical methods employed, the principal findings, and the proposed valorization applications.

annual number of publications was recorded in 2025 across all three databases, with ScienceDirect consistently yielding the highest annual publication counts, followed by Springer and Scopus, respectively.

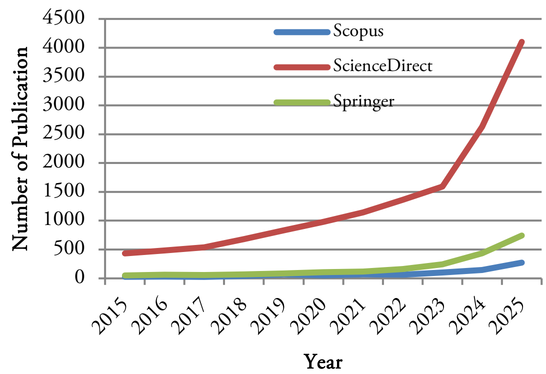

Figure 2. Temporal Distribution of Included Studies Published Between 2015 and 2025

3.1.2 Research Trends and Geographical Distribution of Included Studies

The studies included in this review demonstrate a significant increase in scientific interest in the valorization of food waste in recent years, reflecting the growing shift towards adopting the principles of the circular economy and sustainability in modern food systems. Chronological analysis of the included studies reveals a gradual and progressive increase in the number of publications addressing the extraction and characterization of bioactive compounds from food waste, with a marked acceleration observed further 2020, driven by the growing imperative to develop alternative sources of functional compounds and reduce the environmental and socioeconomic impacts of food waste generation (Gómez-García *et al.*, 2021).

Table 4. Summary of Included Studies on Food By-Product Valorization and Bioactive Compound Characterization

By-product source	Bioactive compounds	Analytical methods	Key findings	Applications
Citrus peels	Flavonoids, dietary fiber	FTIR, HPLC	Rich source of phenolic compounds	Functional foods
Olive pomace	Phenolics, antioxidants	NIR, GC-MS	High antioxidant activity	Natural preservatives
Grape pomace	Anthocyanins, tannins	FTIR, HPLC-DAD	High phenolic content	Nutraceuticals
Cereal bran	Dietary fiber, proteins	FTIR, UV-Vis	Rich in soluble fiber	Food supplements
Vegetable peels	Carotenoids, phenolics	Raman, HPLC	Diverse bioactive compounds	Active packaging
Coffee grounds	Fatty acids, phenolics	GC-MS, HPLC	High volatile compound content	Cosmetic applications
Fruit seeds	Bioactive peptides, oils	LC-MS, FTIR	Rich in unsaturated fatty acids	Health products
Legume husks	Polyphenols, proteins	UV-Vis, HPLC	High antioxidant capacity	Animal feed

Figure 2 illustrates the temporal distribution of publications retrieved from Scopus, ScienceDirect, and Springer between 2015 and 2025. The data demonstrate a progressive and consistent increase in the number of publications across all three databases over the study period, reflecting the growing scientific interest in food waste valorization and bioactive compound characterization. A notable acceleration in publication output is evident following 2020, likely attributable to heightened global attention to circular economy principles and sustainability. The highest

With respect to the nature of the raw materials investigated, the overwhelming majority of included studies focused on plant-derived residues from agricultural and food processing operations — in particular, fruit and vegetable waste, olive residues, and the byproducts of grains and oilseeds — attributable to their high concentrations of phenolic compounds, dietary fiber, and antioxidants. Growing number of studies have additionally examined residues from beverage and dairy production, although to a lesser extent than traditional plant-derived sources (Sagar *et al*., 2018).

Regarding analytical approaches, a discernible trend towards the increased adoption of rapid spectroscopic techniques, particularly FTIR and NIR was observed in more recently published studies due to their lower cost and faster analysis rapidity. Meanwhile, chromatographic chemical techniques, such as HPLC and GC-MS, continue to fulfill a pivotal role in high-resolution quantitative and qualitative analysis. This trend reflects a gradual shift towards the integrated application of rapid, non-destructive techniques in combination with reference chromatographic methods, aimed at simultaneously improving characterization efficiency and ensuring the reliability and scientific validity of analytical results (Tziolas *et al.*, 2021).

A critical review of the included studies further reveals that whilst scientific activity in the domain of food waste valorization has increased substantially since 2020, the majority of studies have concentrated on a relatively limited range of plant-derived waste streams — principally fruit peels, olive pomace, and cereal bran. Gómez-García *et al*., (2021) noted that these categories represent the largest proportion of raw materials studied in the literature, while other food wastes with potentially high value remain comparatively underexplored. Furthermore, Sagar *et al.*, (2018) highlighted that the predominant focus of the existing literature is on the extraction and *in vitro* characterization of bioactive compounds, while only a limited number of studies have addressed aspects related to economic feasibility or practical industrial implementation of the proposed valorization strategies — a critical gap that constrains the translation of research findings into industrial practice.

3.2 Spectroscopic Methods for Food By-Product Characterization

Spectroscopic methods are among the most extensively employed analytical techniques for the characterization of bioactive compounds extracted from food waste, attributable to their ability to deliver rapid and non-destructive analysis with minimal sample preparation requirements. These techniques have gained increasing importance in recent years owing to their ability to improve the efficiency of chemical characterization and reduce operational costs, particularly in industrial applications requiring rapid and scalable analyses. The most widely applied spectroscopic techniques in this domain include FTIR, NIR, Raman spectroscopy, and ultraviolet–visible spectroscopy (UV–Vis) (Hassan *et al*., 2025; Ramachandran *et al*., 2025)

3.2.1 Fourier Transform Infrared Spectroscopy

FTIR constitutes one of the most extensively utilized spectroscopic techniques for the analysis of bioactive compounds extracted from food by-products, owing to its capacity to rapidly identify functional groups and generate a distinctive molecular fingerprint characteristic of the compounds under investigation. The technique operates on the principle of measuring infrared the absorption of infrared radiation by the chemical bonds present within molecular structure, allowing for the determination of the chemical structure , thereby enabling the determination of the chemical and structural characteristics of diverse compound classes, including phenolic compounds, carbohydrates, proteins, and fatty acids (Varas Perez *et al*., 2025).

FTIR has been widely applied to characterize plant-based food processing residues, including citrus waste, fruit peels, olive pomace, and cereal by-products, and has demonstrated efficacy in the rapid detection and preliminary identification of antioxidant compounds and, as well as in monitoring chemical transformations associated with extraction and processing operations (Sun *et al*., 2025). The principal analytical advantages of FTIR include its high rapidity, low operating costs compared to chromatographic techniques, the absence of complex or time-consuming sample preparation requirements, and its non-destructive character, which permits the preservation and subsequent re-analysis of the original sample. These attributes render FTIR a particularly attractive method for industrial applications and quality control within food processing chains (May, 2024; Saji *et al*., 2024).

Notwithstanding these advantages, FTIR is subject to a number of significant analytical limitations. Whilst the technique provides a comprehensive molecular fingerprint of the sample, its sensitivity and selectivity in the identification and quantification of individual compounds remains limited compared to those of chromatographic techniques such as HPLC or GC-MS, especially in the analysis of complex matrices or when target compounds present at low concentrations. Furthermore, the accuracy and reliability of FTIR-based quantification are critically dependent upon the quality of calibration models and reference spectral databases, which can affect the reproducibility of results across different studies (Resende *et al*., 2023).

Therefore, while FTIR may be considered an appropriate technique for rapid preliminary screening and general characterization of bioactive compounds, its independent application is generally insufficient for the accurate identification and quantification of individual target compounds. Consequently, the integrated use of FTIR in conjunction with complementary chromatographic techniques — such as HPLC or GC-MS — is widely recommended in the literature to ensure the accuracy, specificity, and completeness of characterization outcomes, particularly in demanding industrial and regulatory applications.

Several investigations have demonstrated the utility of FTIR spectroscopy for the rapid characterization of phenolic compounds and other bioactive constituents in food by-products. Gómez-García *et al.*, (2021) highlighted the potential of FTIR as a rapid and non-destructive screening tool for valuable bioactive compounds in fruit and olive processing residues. In contract Tziolas *et al.*, (2021) reported that the predictive performance of FTIR-based chemometric models may decline considerably when applied to highly heterogeneous food matrices or when calibration models are transferred across different sample types. This apparent discrepancy suggests that the successful implementation of FTIR depends strongly on sample composition, calibration quality, and the robustness of chemometric modelling approach employed.

3.2.2 Near Infrared Spectroscopy (NIR)

NIR spectroscopy represents a promising and increasingly adopted spectroscopic technique for the characterization of bioactive compounds extracted from food waste, principally by virtue of its capacity to perform rapid, non-destructive analyses with minimal sample preparation. The technique operates through the measurement of electromagnetic radiation absorption in the near-infrared spectral region, enabling the detection of chemical bonds associated with organic compound classes, including phenolic compounds, proteins, lipids, and carbohydrates (Njewa *et al.*, 2025; Yadav *et al.*, 2024).

The application of NIR has undergone substantial expansion within the field of food waste valorization, particularly in assessing the quality of agricultural by-products and the rapid determination of the chemical composition of plant-derived residues. The technique has been applied to the analysis of cereal residues, fruit peels, and oilseed by-products, demonstrating efficacy in the rapid estimation of total phenolic content and antioxidant activity relative to conventional chemical methods (Ayvaz & Doğan, 2025). Among the most significant analytical advantages of NIR is its capacity for high-throughput real-time analysis with minimal consumption of chemical reagents, rendering it an environmentally compatible and friendly technology with promising potential for large-scale industrial applications. Furthermore, the capacity for integration of NIR instrumentation with artificial intelligence (AI) algorithms and advanced chemometric models enhances its predictive capability for the rapid assessment of sample quality and chemical composition (Kanwal & Musharraf, 2024).

Despite these attributes, NIR technology exhibits lower resolution and selectivity for the precise identification and quantification of individual compounds compared with advanced chromatographic techniques such as HPLC and GC-MS. As a consequence, NIR is generally more appropriate for rapid screening and preliminary assessment than for detailed, chemical characterization (Kanwal & Musharraf, 2024).

NIR spectroscopy may therefore be considered an effective and valuable tool for the rapid, non-destructive assessment of bioactive compounds in food waste matrices, particularly in industrial settings that require rapid decision-making and lower analysis costs. However, the enhancement of predictive accuracy and analytical reliability necessitates the development of more robust, reliable calibration models and integrating them with complementary analytical techniques to ensure the accurate characterization of target bioactive constituents.

Published evidence further illustrates the performance characteristics and limitations of NIR in food by-product applications. Cen & He, (2007) demonstrated the capacity of NIR to deliver rapid and non-destructive compositional analysis in relatively homogeneous food matrices. In contrast, Ayvaz & Doğan, (2025) reported a significant reduction in the predictive accuracy of NIR-based models when applied to complex food by-products characterized by highly variable compositions. Collectively, these findings indicate that the transferability of NIR calibration models across diverse categories of food by-products remains limited, and that the development of robust calibration strategies represents a critical requirement for the reliable industrial implementation.

3.2.3 Raman Spectroscopy

Raman spectroscopy constitutes an advanced and increasingly adopted spectroscopic for the characterization of bioactive compounds extracted from food by-products, attributable to its capacity to generate a precise molecular fingerprint. The technique relies on the principle of Raman scattering, where the energy of scattered light changes as a result of its interaction with chemical bonds within molecules, allowing for the determination of the structural and chemical properties of various organic compounds (Vershinina *et al.*, 2025; Yang *et al.*, 2017).

Raman spectroscopy has been applied to the characterization of a broad spectrum of food processing residues, including fruit peels, grain residues, and vegetable oil processing derivatives, with the aim of identifying phenolic compounds, carotenoids, fatty acids, and antioxidants. Published investigations have additionally demonstrated the efficacy of this technique in detecting and monitoring chemical transformations associated with extraction and processing operations, as well as in the verification of the authenticity and quality of food products (Dabić Zagorac *et al.*, 2024; Yang *et al.*, 2017).

Among the most significant advantages of Raman spectroscopy is its capacity to provide accurate molecular information with minimal sample preparation, in addition to its ability to directly analyze hydrated or wet samples, which is a significant advantage compared to some other spectroscopic methods, such as FTIR. Its high accuracy in characterizing organic compounds also makes Its high molecular specificity in the characterization of organic compounds further positions it as a promising instrument for quality control and rapid structural characterization within the food processing industry (Cavdaroglu *et al.*, 2025).

Despite these advantages, Raman spectroscopy is subject to several significant practical challenges that limit its widespread application. The elevated capital cost of Raman instrumentation constitutes a major barrier to large-scale deployment. In addition, the technique exhibits limited sensitivity when applied to compounds present at low concentrations in complex matrices. Signal quality may be substantially compromised by fluorescence interference, particularly in complex plant-derived samples, potentially resulting in reduced spectral resolution and diminished analytical accuracy (Li *et al.*, 2024).

These challenges are further accentuated in the context of the transition from controlled laboratory environments to real-world industrial settings. The majority of published studies have focused on utilizing Raman spectroscopy under controlled laboratory conditions, while research evaluating its performance in actual industrial settings remains exceedingly limited. Consequently, the considerable theoretical analytical potential of this technique has not yet been fully realized in large-scale industrial applications, necessitating further applied studies to assess its economic and technical feasibility in real-world production conditions.

Raman spectroscopy may accordingly be regarded as a powerful technique for advanced molecular characterization of bioactive compounds, particularly in investigations requiring detailed structural elucidation. Nevertheless, its systematic integration with complementary analytical techniques — such as FTIR for broad molecular fingerprinting, or HPLC for quantitative compound-specific analysis — is recommended to achieve a more comprehensive and reliable characterization of complex food by-product matrices.

The divergent findings reported in the literature further illustrate the context-dependent performance of Raman spectroscopy. Vershinina *et al.* (2025) demonstrated the utility of this technique for the structural characterization and quantification of plant-derived bioactive compounds. In contrast, other studies reported that the presence of naturally fluorescent compounds and pigments in plant by-products can generate strong background signals and substantially reduce spectral quality. This apparent discrepancy indicates that, despite its excellent analytical capabilities, the successful application of Raman spectroscopy to heterogeneous food by-products remains highly dependent on sample composition and signal pre-processing strategies.

3.2.4 Ultraviolet –Visible Spectroscopy (UV–Vis)

UV-Vis spectroscopy constitutes one of the most widely employed analytical techniques for the characterization and quantification of bioactive compounds extracted from food by-products. The technique operates on the principle of measuring the absorption of electromagnetic radiation in the ultraviolet and visible spectral ranges, enabling the estimation of the concentration of compounds possessing chromophoric structural groups, such as phenolic compounds, flavonoids, and natural pigments (Njewa *et al.*, 2025).

UV-Vis spectroscopy has been extensively applied to the assessment of antioxidant activity and the estimation of total phenolic, total flavonoid, and carotenoid contents across a broad range of food processing residues, including citrus peels, olive pomace, grain residues, and fruit and vegetable waste. This technique additionally facilitates the rapid evaluation of chemical modifications arising from various extraction processes, making it an effective tool for preliminary screening and quality evaluation in research and industrial settings (Terenzi *et al.*, 2024).

The principal analytical advantages of UV–Vis spectroscopy include its operational simplicity, high analytical rapidity, and lower equipment costs compared to advanced chromatographic reference techniques. Its capacity to deliver rapid quantitative analyses employing relatively simple protocols, renders it particularly appropriate for industrial quality control applications and routine quality control within food processing chains (Tüğen & Taştan Ülkü, 2025).

However, UV–Vis spectroscopy is characterized by several significant and well-recognized methodological limitations. Its capacity to qualitatively differentiate between individual compounds is relatively limited, especially in complex samples containing a mixture of compounds with overlapping absorption spectra. Furthermore, its detection sensitivity is inferior to that of advanced techniques such as HPLC or LC-MS, rendering it more appropriate for macroscopic analysis or rapid screening rather than precise molecular determination (García-Rodríguez *et al.*, 2017; Sanchez *et al.*, 2026).

The limitations of UV–Vis spectroscopy in the context of bioactive compound characterization have been clearly delineated in the published literature. Lozada-Ramírez *et al.* (2021) emphasized that UV–Vis measurements yield only global estimations based on absorbance and do not permit the identification or quantification of individual bioactive compounds. Similarly, Apak *et al.*, (2016) highlighted that spectrophotometric antioxidant assays are highly dependent on reaction conditions and may generate considerable inter-study variability. Collectively, these observations confirm that UV–Vis spectroscopy is most appropriately employed as a rapid and cost-effective preliminary screening tool, and should preferably be combined with chromatographic techniques such as HPLC or LC–MS for comprehensive characterization of food by-products.

UV-Vis spectroscopy may accordingly be regarded as an appropriate technique for the rapid preliminary evaluation of bioactive compounds, particularly in studies aimed at initial comparison or quality control. Its independent application, however, is insufficient for advanced chemical characterization, and its integration with more precise analytical techniques is required to ensure the reliability, specificity, and scientific validity of the characterization outcomes.

Table 5 illustrates a detailed critical comparison of the different spectroscopic methods employed to characterize bioactive compounds extracted from food waste.

Table 5. Critical Comparison of Spectroscopic Methods Employed to Characterize Bioactive Compounds from Food Waste

Method	Principal application	Strengths	Weaknesses	Industrial applicability	Critical interpretation
FTIR	Functional group identification	Rapid, non-destructive	Limited molecular specificity	High	Effective for screening but insufficient for precise compound identification
NIR	Rapid compositional prediction	Real-time analysis	Strong dependence on calibration models	High	Suitable for process monitoring but limited transferability
Raman	Molecular fingerprinting	High chemical specificity	Fluorescence interference	Moderate	Promising but still insufficiently validated industrially
UV–Vis	Total compound estimation	Low cost and simplicity	Low selectivity	High	Useful for preliminary assessment only

3.3 Chemical Methods for Bioactive Compound Analysis

Despite the significant advancements in rapid spectroscopic techniques, advanced chemical and chromatographic analytical methods retain their status as the primary reference methodologies for the characterization of bioactive compounds extracted from food by-products, attributable to their superior accuracy and sensitivity in the quantitative and qualitative determination of individual compounds. These methods include various chromatographic techniques, such as high-performance liquid chromatography (HPLC), gas chromatography-mass spectrometry (GC-MS), and liquid chromatography-mass spectrometry (LC-MS), in addition to conventional chemical assays applied to estimate antioxidant activity and total phenolic content.

3.3.1 High-Performance Liquid Chromatography (HPLC)

High-performance liquid chromatography (HPLC) represents one of the most widely utilized techniques for the characterization of bioactive compounds in food by-products, attributable to its demonstrated capacity for the separation, identification, and quantification of individual constituents within complex multi-component mixtures. This technique relies on the differential interactions of analyte molecules with the stationary and mobile phases, enabling the selective separation and analysis of a wide range of bioactive compound classes (Abderrezag *et al.*, 2025; Njewa *et al.*, 2025).

HPLC has been extensively applied to the analysis of phenolic compounds, flavonoids, carotenoids, and organic acids extracted from fruit, olive, grain, and vegetable waste. The technique has demonstrated particular efficacy in the precise quantitative determination of bioactive compounds, establishing it as one of the most reliable and validated methods for studies aimed at verifying the functional and nutritional properties of plant-derived extracts (Krivošija *et al.*, 2025; Terenzi *et al.*, 2024).

The most significant analytical advantages of HPLC include its high accuracy, its and quantitative precision, its demonstrated capacity to resolve and separate structurally analogous compounds, and its compatibility with various detectors to enhance analytical sensitivity. These attributes collectively render HPLC the method of choice for high-resolution characterization studies requiring unambiguous compound identification and accurate quantification.

Despite its analytical strengths, HPLC is subject to several practical limitations, most notably the high cost of instrumentation and analytical reagents, the requirement for complex and time-consuming sample preparation procedures, and the relatively longer analysis time compared to rapid spectroscopic methods. Furthermore, the advanced operational expertise and maintenance requirements associated with HPLC instrumentation may limit its accessibility and throughput in routine industrial quality control applications (Krivošija *et al.*, 2025; Njewa *et al.*, 2025).

HPLC therefore retains its established status as the reference analytical technique for the detailed characterization of bioactive compounds in food by-products. Nevertheless, combining HPLC with rapid spectroscopic screening methods may improve analytical efficiency while reducing analysis time and overall cost.

Published evidence firmly establishes the analytical precision and selectivity of HPLC for the characterization of complex bioactive extracts from food by-products. Plaza & Turner, (2015) highlighted the high analytical precision and selectivity of HPLC for the characterization of complex bioactive extracts. However, Gómez-García *et al.* (2021) identified substantial inter-study variability in extraction procedures, chromatographic columns, mobile phase composition, and detection conditions, rendering direct comparisons between published datasets difficult. These observations confirm that, despite its status as a reference analytical method, the absence of standardized and universally adopted HPLC methodologies for food by-product characterization remains a significant and persistent limitation in this field.

3.3.2 Gas Chromatography–Mass Spectrometry (GC-MS)

GC–MS constitutes one of the most powerful and analytically sensitive tools available for the identification and structural characterization of volatile and semi-volatile compounds in food by-products. The technique combines the high-resolution chromatographic separation capability of gas chromatography with the structural elucidation and molecular identification power of mass spectrometric detection, enabling the structural characterization of a wide range of volatile metabolites (Abderrezag *et al.*, 2025; Andrade *et al.*, 2022).

GC-MS has been widely applied to analyze essential oils, fatty acids, and volatile aromatic compounds extracted from citrus, olive, and oilseed waste. The technique has additionally played a significant role in identifying compounds of recognized health and technological value within the food and pharmaceutical industries (Andrade *et al.*, 2022; Setiawan *et al.*, 2025). The principal analytical advantages of GC-MS include its high sensitivity, ability to identify compounds with high molecular resolution, and reliability in analyzing complex volatile compounds. These attributes render GC-MS the analytical method of reference in advanced chemical characterization studies focused on volatile bioactive constituents.

Despite these analytical advantages, GC–MS is subject to several practical limitations, including the necessity for derivatization and the relatively high operational cost, both of which may reduce analytical throughput in routine applications.

Several studies have demonstrated the effectiveness of GC–MS for the identification and quantification of volatile compounds, fatty acids, and aroma-related metabolites in food by-products. Plaza & Turner, (2015) highlighted the appropriateness of GC–MS for the comprehensive characterization of volatile bioactive compounds in complex food matrices. However, subsequent investigations have reported that a substantial proportion of phenolic compounds and other non-volatile metabolites require derivatization prior to GC–MS analysis — a requirement that increases sample preparation time and introducing additional sources of variability. These observations indicate that, although GC–MS remains a highly sensitive and selective reference technique, its applicability is largely restricted to volatile or semi-volatile compounds and is therefore generally insufficient as a standalone technique for the comprehensive characterization of the complete bioactive compound profile of food by-products.

GC–MS accordingly remains the analytical method of choice for the characterization of volatile and semi-volatile bioactive compounds. Nevertheless, comprehensive characterization of food by-products generally requires complementary analytical techniques, such as HPLC or LC–MS, to accurately identify and quantify non-volatile constituents. Consequently, integrated analytical strategies combining GC–MS with complementary chromatographic methods provide a more complete understanding of the chemical composition of food by-products.

3.3.3 Liquid Chromatography–Mass Spectrometry (LC-MS)

LC-MS constitutes one of the most advanced analytical platforms for the characterization of bioactive compounds extracted from food waste, owing to its high capacity for precise separation and structural identification of complex compounds present at trace concentrations. This technique integrates the separation efficiency of liquid chromatography with mass spectrometric detection, thereby enabling the simultaneous identification of a substantial number of compounds within complex biological and food matrices (D'Urso *et al.*, 2025; Kharbach *et al.*, 2026).

LC-MS has been increasingly employed for the analysis of phenolic compounds, flavonoids, bioactive peptides, and antioxidants extracted from fruit, vegetable, olive, and cereal by-products. Furthermore, it has demonstrated considerable efficacy in the identification of novel or rare compounds that are difficult to detect by conventional chemical methods (Collado-González *et al.*, 2026; D'Urso *et al.*, 2025; Njewa *et al.*, 2025).

The key advantages of LC-MS reside in its exceptional sensitivity, its capacity to perform both qualitative and quantitative analyses simultaneously, and its aptitude to accurately determine the molecular structure of complex compounds. It additionally constitutes a fundamental tool in advanced metabolomics studies and the characterization of low-concentration bioactive compounds.

However, this technique is subject of several practical limitations, including the requirement for advanced technical expertise, the complexity of data processing, and demanding operational requirements that may restrict its routine industrial application (D'Urso *et al.*, 2025; Kharbach *et al.*, 2026; Njewa *et al.*, 2025).

Therefore, while LC-MS may be regarded as one of the most accurate and comprehensive analytical techniques for the characterization of bioactive compounds, its application is predominantly oriented towards advanced research studies or reference validation applications that demand high levels of sensitivity and accuracy.

Several studies have highlighted the remarkable analytical capabilities of LC–MS for identifying and quantifying bioactive compounds at extremely low concentrations in complex food matrices. Kharbach *et al.* (2026) emphasized that LC–MS/MS has become one of the most powerful techniques for comprehensive food characterization owing to its high sensitivity and molecular specificity. However, other investigations have reported that the high acquisition and maintenance costs of LC–MS instruments, together with the complexity of data processing and interpretation, limit their routine implementation in industrial environments. These observations suggest that, despite its superior analytical performance, the widespread adoption of LC–MS in food by-product valorization continues to face considerable economic and operational challenges.

3.3.4 Conventional Chemical Assays

In addition to advanced chromatographic techniques, traditional chemical assays are widely employed to evaluate the functional properties of bioactive compounds extracted from food by-products, particularly with respect to antioxidant activity and total phenolic content. Among the most commonly applied assays are Folin–Ciocalteu, DPPH, ABTS, and FRAP methods.

The Folin–Ciocalteu assay is primarily employed to estimate total phenolic content. The technique relies on the reaction of phenolic compounds with Folin reagent to form a colored complex that can be measured spectroscopically. While this assay is simple and straightforward to perform, its limited specificity may result in interference from other non-phenolic reducing compounds, potentially compromising the accuracy of the results (Torres *et al.*, 2024).

The DPPH (2,2-diphenyl-1-picrylhydrazyl) assay is widely utilized to evaluate antioxidant activity based on the capacity of bioactive compounds to inhibit free radicals. It is characterized by its rapidity and low cost; however, its sensitivity may vary depending on the solvent employed and the nature of the compounds under investigation (Jia *et al.*, 2024).

Similarly, the ABTS (2,2′-azinobis (3-ethylbenzothiazoline-6-sulfonic acid)) assay is utilized to assess antioxidant capacity and is considered more versatile than DPPH, as it can be applied in both aqueous and organic media. It also permits the evaluation of a broader spectrum of antioxidant compounds (Jia *et al.*, 2024).

In contrast, the FRAP (Ferric Reducing Antioxidant Power) assay measures the reducing capacity of bioactive compounds by converting ferric to ferrous ions. Despite its simplicity and rapidity, it may not reflect all mechanisms of antioxidant activity, thereby limiting its ability to provide a comprehensive assessment when employed in isolation (Apak, 2016).

Several studies have demonstrated that conventional colorimetric assays remain indispensable for the rapid evaluation of antioxidant activity and total phenolic content in food by-products owing to their simplicity and low operational cost. However, Apak, (2016) emphasized that antioxidant assays such as DPPH, ABTS, and FRAP are based on divergent reaction mechanisms and therefore frequently yield non-comparable results. Likewise, Torres *et al.* (2024) reported that the Folin–Ciocalteu assay may overestimate total phenolic content owing to interference from other reducing substances. These findings indicate that conventional chemical assays should be interpreted with caution and preferably combined with chromatographic techniques to obtain a more reliable characterization of bioactive compounds.

Overall, these conventional chemical assays remain valuable tools for the preliminary evaluation of bioactive compounds and antioxidant activity in food by-products. However, their limited specificity and dependence on experimental conditions frequently necessitate their integration with more accurate analytical techniques, such as HPLC or LC-MS, to ensure more reliable interpretation of the results.

3.4 Comparative Critical Analysis of Spectroscopic and Chemical Methods

The studies included in this review demonstrate that the selection of an appropriate analytical technique for characterizing bioactive compounds extracted from food waste depends largely upon the nature of the target compounds, the required level of accuracy, and the ultimate objective of the analysis. Generally, analytical methods can be categorized into two principal groups: rapid spectroscopic methods and chemical reference methods. Each group possesses distinct advantages and limitations that directly influence characterization efficiency and industrial applicability.

Spectroscopic methods, including FTIR, NIR, Raman, and UV–Vis, are particularly appropriate for rapid screening and routine quality control as they enable fast analyses with relatively simple sample preparation, rendering them suitable tools for initial screening, routine quality control, and real-time analysis within food production lines. Furthermore, the limited consumption of chemical reagents renders these methods more closely aligned with the principles of green chemistry and environmental sustainability. In addition, the integration of these methods with chemometric instruments and AI techniques has enhanced their predictive capabilities, particularly in classification and rapid quality detection applications (Li *et al*., 2025; Tziolas *et al*., 2021).

However, the capacity of spectroscopic techniques to accurately and quantitatively identify individual compounds remains relatively limited, especially in complex, multi-component samples. Furthermore, the reliability of their results depends heavily upon the quality of calibration models and reference databases, which may limit the generalizability of results across various types of food waste or varying processing conditions (Njewa *et al*., 2025; Tziolas *et al*., 2021).

In contrast, chemical techniques, such as HPLC, GC-MS, and LC-MS, offer exceptionally high levels of sensitivity and accuracy, rendering them more appropriate for advanced structural characterization and precise quantitative analysis of bioactive compounds. These techniques have proven pivotal in validating results obtained from spectroscopic methods and confirming the molecular identity of target compounds, particularly phenolic compounds, organic acids, and volatile compounds (Njewa *et al*., 2025; Paniagua-García *et al*., 2019).

Nevertheless, chemical techniques face practical challenges, including elevated equipment and maintenance costs, the requirement for more complex sample preparation, and the extended time required for analysis. Furthermore, their routine application in large-scale industrial settings may be constrained by the requirement for specialized technical expertise and high operational requirements (Njewa *et al*., 2025; Tziolas *et al*., 2021).

Although most studies consistently recognize spectroscopy as a rapid and cost-effective analytical approach, considerable disagreement remains regarding its capability to replace conventional chromatographic methods. Gómez-García *et al.* (2021) suggested that spectroscopic techniques may provide sufficiently accurate estimations for routine quality control when supported by robust chemometric models. In contrast, Tziolas *et al.* (2021) reported that prediction accuracy decreases substantially when calibration models are transferred to heterogeneous food matrices. Similarly, Plaza & Turner. (2015) emphasized that chromatographic methods remain indispensable whenever reliable identification and quantification of individual bioactive compounds are required. These contrasting findings indicate that the choice of analytical method should depend upon the intended application rather than upon analytical performance alone.

Based on the available evidence, neither spectroscopic nor chemical methods can be regarded as universally superior. Instead, their analytical performance should be evaluated according to the objectives of the analysis, the complexity of the food matrix, and the intended industrial application. Consequently, integrated analytical workflows that combine rapid spectroscopic screening with confirmatory chromatographic analyses appear to be the most robust strategy for the comprehensive characterization of bioactive compounds in food by-products. Table 6 illustrates a critical comparison between spectroscopic and chemical methods.

3.5 Industrial Applications of Bioactive Compounds Derived from Food By-Products

Recent investigations demonstrate that bioactive compounds extracted from food waste are of significance not only for their nutritional value, but also for their diverse industrial applications, which possess considerable economic and environmental potential. Advances in extraction and characterization technologies have expanded opportunities for utilizing these compounds in the food, pharmaceutical, and smart packaging industries, supporting the principles of the circular economy and reducing food waste (Cinzia Ingallina *et al*., 2025; Shawky *et al*., 2025).

3.5.1 Functional Foods

Bioactive compounds derived from food waste are increasingly employed in the development of functional foods owing to their capacity to enhance the health and nutritional properties of food products. These compounds include phenols, dietary fiber, flavonoids, and antioxidants, which can be incorporated into foods to improve their health value and

Table 6. Critical Comparison Between Spectroscopic and Chemical Methods

Criterion	Spectroscopic methods	Chemical methods	Critical interpretation	Preferred application
Speed	High	Moderate to low	Spectroscopy preferred for rapid screening	Real-time process monitoring and on-line quality control
Accuracy	Moderate	High	Chemical methods remain reference standards	Definitive identification and quantitative analysis
Cost	Low to moderate	High	Industrial implementation favors spectroscopy	Routine industrial quality control
Sample preparation	Minimal	Complex	Major limitation for chemical methods	High-throughput screening and large sample sets
Scalability	High	Moderate	Hybrid approaches appear more realistic	Large-scale industrial monitoring
Sensitivity	Moderate	Very high	Chemical methods detect trace compounds	Trace-level compound detection and metabolite profiling
Operator expertise	Low	High	Chemical methods require specialized training	Routine laboratories (spectroscopy) vs. specialized analytical laboratories (chemical methods)

reduce the risk of chronic diseases (Ahmed *et al.*, 2025; Krishnan & Devarajan, 2025).

3.5.2 Active and Intelligent Packaging

Studies have demonstrated promising potential for the utilization of natural extracts rich in antioxidant and antimicrobial compounds in the development of smart, active food packaging materials. Compounds extracted from fruit peels and plant residues can be incorporated into biofilms to improve food stability and extend shelf life, while reducing reliance on artificial preservatives (Cazón *et al.*, 2025; Dutta *et al.*, 2025; Maddaloni *et al.*, 2025).

3.5.3 Nutraceuticals and Health Products

Food byproducts represent a promising source for the development of nutraceuticals and health supplements, particularly those rich in antioxidants, fatty acids, and anti-inflammatory compounds. Advanced characterization techniques have contributed to a better understanding of the biological activity of these compounds and enhanced their commercial potential (Radha *et al.*, 2024).

3.5.4 Animal Feed Applications

In addition to human food applications, certain food waste has been utilized as functional ingredients in animal feed, owing to their fiber content and biologically active compounds that may contribute to improving animal health and productivity while reducing feed costs (Tedeschini, 2025; Vlasova *et al.*, 2025).

Figure 3 illustrates the principal industrial applications of bioactive compounds derived from food by-products.

Despite the promising industrial applications reported in the literature, the majority of valorization strategies remain at the laboratory or pilot scale. A limited body of research has evaluated long-term economic feasibility, regulatory constraints, or large-scale industrial implementation. Consequently, a significant gap persists between proof-of-concept demonstrations and commercial deployment of bioactive compounds derived from food by-products (Krishnan & Devarajan, 2025).

3.6 Current Challenges and Future Research Directions

Despite significant progress in the field of food waste valorization and bioactive compound extraction, several challenges impede the transition from laboratory findings to large-scale industrial applications. Among the most prominent of these challenges are the absence of standardized protocols for bioactive compound extraction and characterization, and the considerable variability in the physical and chemical properties of food waste, which affects the comparability of results across different studies.

Furthermore, the inconsistency in the selection of analytical techniques and the absence of standardized validation protocols present additional challenges to standardizing results and enhancing their reproducibility. Moreover, certain advanced techniques, such as LC-MS and GC-MS, continue to face limitations related to high cost and operational complexity, restricting their adoption in routine industrial applications.

Conversely, promising opportunities emerge in the future through the integration of spectroscopic techniques with AI tools and chemometric analysis, with the aim of developing more accurate and efficient predictive models for the rapid characterization of bioactive compounds. Developments in smart packaging, functional foods, and the circular economy

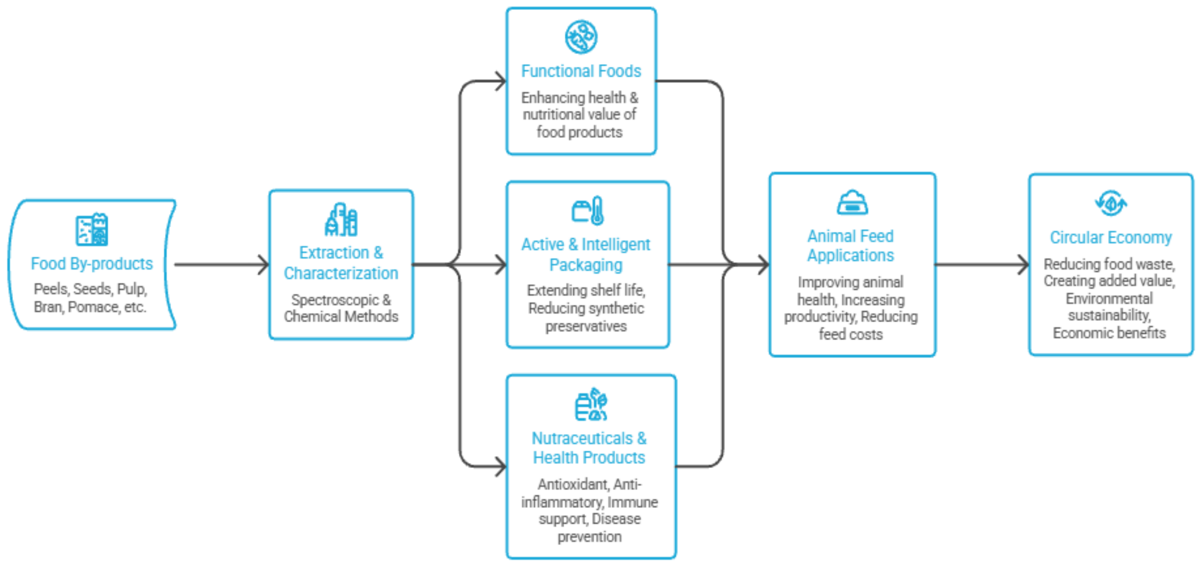

Figure 3. Major Industrial Applications of Bioactive Compounds Derived from Food By-Products

are also expected to contribute to enhancing the economic value of food waste and transforming it into sustainable industrial resources.

Future research should move beyond analytical characterization alone and focus on developing standardized analytical protocols, inter-laboratory validation studies, techno-economic assessments, and real-scale industrial demonstrations. In addition, integrating AI with spectroscopy may substantially improve prediction accuracy and facilitate the industrial adoption of rapid analytical methods (Li *et al.*, 2025; Râpă *et al.*, 2024).

Previous reviews on food by-product valorization have predominantly focused on extraction technologies, the recovery of bioactive compounds, and their nutritional or functional applications (Sagar *et al.*, 2018; Sharma et al., 2017). In contrast, the present review comparatively evaluates both spectroscopic and chemical characterization methods while emphasizing their analytical performance, industrial applicability, and future integration with AI tools. By combining analytical characterization with practical valorization strategies, this review contributes to narrowing the gap between laboratory research and industrial implementation.

Based on the challenges and future opportunities identified in this review, a conceptual framework is proposed to facilitate the integration of rapid spectroscopic techniques, advanced chemical analyses, and AI tools for the sustainable valorization of food by-products. Figure 4 proposes an integrated framework that combines the rapid screening

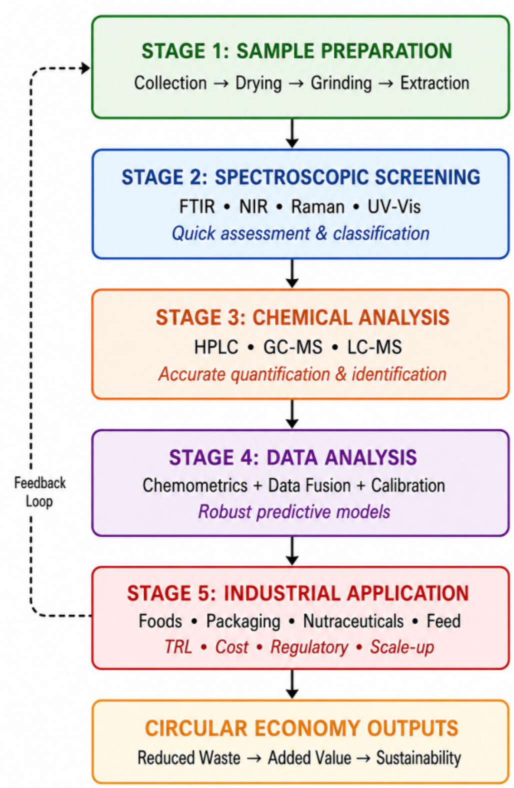

Figure 4. Proposed Integrated Framework for the Valorization of Food By-Products via Combined Spectroscopic and Chemical Characterization Approaches

capabilities of spectroscopic techniques with the high analytical accuracy of chemical methods, thereby bridging the gap between laboratory research and industrial implementation. The proposed framework consists of five interconnected stages: sample preparation, spectroscopic screening, chemical characterization, data analysis and decision-making, and industrial application, supported by a continuous feedback loop to promote method optimization and sustainable valorization strategies.

3.7 Limitations of the Current Review

Despite the rigorous methodology employed in this review, certain limitations must be acknowledged. First, the literature search was limited to major scientific databases and English-language publications, which may have resulted in the exclusion of relevant studies published elsewhere. Second, considerable variation was observed among the included studies regarding extraction protocols, analytical procedures, and reporting practices, making direct comparisons challenging.

Furthermore, several of the reviewed studies were conducted under laboratory conditions, while evidence regarding industrial-scale application remains limited. Consequently, certain conclusions concerning industrial applications should be interpreted with caution. Future reviews would benefit from incorporating more standardized datasets and a greater emphasis on technical and economic evaluations.

4 Discussion

The present review provides a critical evaluation of spectroscopic and chemical methods for the characterization of bioactive compounds derived from food processing waste, with particular emphasis on analytical performance, methodological limitations, and industrial applicability. The collective findings demonstrate that spectroscopic methods, including FTIR, NIR, Raman, and UV-Vis offer significant analytical advantages with respect to rapidity, non-destructiveness, and minimal sample preparation, rendering them well-suited to rapid screening and quality control applications in industrial settings (Li *et al*., 2025; Tziolas *et al*., 2019). However, their limited sensitivity and selectivity for the identification and quantification of individual bioactive compound, combined with their strong dependence upon calibration models remain major challenges (Njewa *et al*., 2025).

In contrast, chemical and chromatographic analytical methods — principally HPLC, GC-MS, and LC-MS — provide superior accuracy, sensitivity, and molecular resolution, enabling precise quantitative and qualitative determination of individual bioactive compounds (Abderrezag *et al*., 2025; D'Urso *et al*., 2025). Nevertheless, their substantially higher instrumentation and reagent costs, considerable operational complexity, and time-consuming sample requirements represent significant practical barriers to their widespread adoption in routine industrial analytical workflows (Krivošija *et al*., 2025).

The considerable divergence in analytical approaches adopted across studies reflects a broader absence of established methodological consensus in this field, as previously highlighted by Gómez-García *et al.* (2021) and Sagar *et al.* (2018). This observation underscores the critical and urgent necessity for the development and adoption of standardized analytical protocols to enhance the comparability, reproducibility, and scientific validity of results across studies. The variability in reported findings for FTIR analysis, as shown by the contrasting results obtained by Gómez-García *et al.* (2021) and Tziolas *et al.* (2021), further illustrates the influence of sample matrix heterogeneity and calibration model quality on the analytical performance.

The systematic reviews consulted as methodological reference benchmarks confirm the rapidly expanding body of literature on food waste valorization, with the number of studies included ranging from 16 to 373 depending on the scope of the research question and stringency of the applied eligibility criteria (Pérez-Beltrán et al., 2024). This considerable variability in review scope and inclusion criteria underscores the importance of rigorous methodological transparency and strict adherence to PRISMA reporting guidelines in systematic review research.

In contradistinction to previous reviews that primarily focused on extraction technologies or specific categories of bioactive compounds in isolation, the present review provides a critical comparative assessment of both spectroscopic and chemical characterization methodologies while emphasizing their industrial applicability and their prospective integration with AI tools and advanced chemometric modelling tools.

The integrated analytical framework proposed in the present review offers a scientifically grounded and practically viable pathway for the systematic combination of spectroscopic screening and chemical methods within food by-product valorization. The implementation of such integrated multi-method approaches, however, requires further validation under real-world industrial conditions prior their broad adoption can be responsibly advocated, as emphasized by Njewa *et al.* (2025) and Tüğen & Taştan Ülkü, (2025).

5 Conclusions

The present review confirms that food processing waste constitutes a valuable and largely underexploited reservoir of bioactive compounds with significant nutritional, technological, and economic potential. Spectroscopic methods — including FTIR, NIR, Raman, and UV-Vis — provide rapid, non-destructive, and cost-effective analytical tools well-suited to preliminary screening and industrial quality control applications. Chemical and chromatographic methods — including HPLC, GC-MS, and LC-MS — remain the established reference standard for the accurate quantification and structural characterization of individual bioactive constituents, by virtue of their superior sensitivity, selectivity, and molecular resolution.

The principal findings of this review may be summarized as follows:

- No single analytical method is universally optimal across all food by-product characterization contexts; an integrated approach combining spectroscopic and chemical methods offers the most comprehensive characterization.
- The analytical performance and reliability of spectroscopic methods are critically dependent upon the quality, robustness, and transferability of calibration models, as well as upon the compositional characteristics and homogeneity of the sample matrix under investigation
- Chemical and chromatographic methods, despite their accuracy, are subject to significant practical challenges related to instrumentation cost, operational complexity, sample preparation requirements, and scalability for routine industrial applications.
- The absence of standardized and universally adopted analytical protocols across the published literature constitutes a major and persistent barrier to the cross-study comparability of results and to the industrial implementation of food by-product characterization strategies.

Future research endeavors should prioritize the development and international validation of standardized analytical protocols for food by-product bioactive compound characterization; the improvement and systematic validation of calibration models for spectroscopic methods across diverse and heterogeneous food matrices; the conduct of rigorous techno-economic feasibility studies evaluating the industrial-scale implementation of integrated analytical frameworks; and the strengthening of collaborative research partnerships between academic institutions and the food processing industry. The integration of AI algorithms and chemometric modeling with spectroscopic instrumentation represents a promising direction for the enhancement of predictive capabilities and real-time quality monitoring.

In conclusion, the sustainable valorization of food processing waste through the application of appropriate analytical characterization strategies constitutes a scientifically sound and practically actionable approach to advancing the principles of the circular bioeconomy. Such valorization contributes to the reduction the environmental burden associated with food waste generation and to the creation of measurable economic value through the recovery and application of high-value bioactive compounds across food, nutraceutical, and pharmaceutical sectors.

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