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Fruit and Vegetable Wastes: Review of Nutritional Composition, Antimicrobial Potential, and Sustainable Applications in Malaysia

Ruma Poddar[1], Jayasree S Kanathasan[2], Idris Adewale Ahmed[3]*

[1-3]School of Applied Science, Lincoln University College, 47301 Petaling Jaya, Selangor, Malaysia
**Corresponding author: idrisahmed@lincoln.edu.my*

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ABSTRACT

Food waste, particularly from fruits and vegetables, represents a major environmental, economic, and social challenge worldwide. Fruit and vegetable peels, seeds, and trimmings are typically discarded, despite being rich in essential nutrients, dietary fibers, bioactive compounds, and minerals. Recent research highlights their potential as renewable resources for nutraceuticals, bioenergy, edible films, and antimicrobial agents. In Malaysia, the rapid expansion of the agro-industrial sector has increased fruit waste generation, especially from highly consumed products such as mango, watermelon, and rambutan. This paper reviews the proximate composition of common fruit and vegetable wastes and their potential applications in addressing food security, antimicrobial resistance, and sustainable waste management. The role of computational bioinformatics, molecular docking, and nanotechnology in enhancing the utilization of bioactive compounds from food waste is also discussed. The study underscores the importance of integrating proximate analysis with innovative biotechnological strategies to reduce municipal solid waste while contributing to public health and sustainable development goals.

INTRODUCTION

Peels from fruits and vegetables are a great source of fiber, proteins, carbs, and phytochemicals, mostly phenolic compounds. Fruit peels are a rich source of antioxidants and certain minerals that can be effectively employed for the production of nutraceuticals and to ensure food security (Hussain et al., 2023; Samsuri et al., 2020). On the other hand, food processing results in a considerable loss of nutritional value, and waste production poses major environmental and economic issues. Fruit and vegetable trimmings include husk, peels, pods, pomace, seeds, and stems; they are often thrown away even though they may contain nutrients, including carotenoids, dietary fibers, enzymes, and polyphenols that may be advantageous (Bhardwaj et al., 2022). Fruit and vegetable waste, particularly peels, is utilized in poor nations to create beneficial goods such as edible films, carbon dots, biochar, and biosorbents. These products are sustainable and environmentally benign, and they may be put to good use. However, since many of these approaches are still in their early stages, further research and advancements in our understanding are needed. Fruit and vegetable peels are becoming more and more popular as a subject for exploration because of their potential applications.

Malaysia is one of the nations that has experienced accelerated economic growth and has a large population. As Malaysia's economy expanded, it also produced a wide range of fruits and vegetables. Not only do Malaysians enjoy this locally farmed food, but it is also exported to other nations. In addition to being farmed for food, Malaysian fruits and vegetables are also industrially processed to make fruit juice, canned fruit, and flavoring.

Fruit wastes such as watermelon rind, mango peel, rambutan skin, and other fruit residues, primarily the peels and seeds, are produced in large quantities, especially in the food industrial area and in large cities like Kuala Lumpur, due to the high consumption and industrial processing of the edible parts of the fruits. Fruit waste is really one of the primary causes of municipal solid waste (MSW), which has become a more serious environmental problem (Ibrahim et al., 2017). The reasons for food waste differ throughout nations; however, it is yet unknown what the characteristics and patterns of food waste are in Malaysia. As a result, changes in consumer behavior might affect the food supply chain and food waste management (Gustavsson et al., 2011; Phooi et al., 2022). The reduction of municipal solid waste is essential, and one method to achieve this is by minimizing fruit and vegetable waste, particularly peels. This paper reviews the proximate composition of common fruit and vegetable wastes and their potential applications in addressing food security, antimicrobial resistance, and sustainable waste management.

OVERVIEW OF HOUSEHOLD KITCHEN WASTE PRODUCTION

According to the definition accepted by the Food and Agriculture Organization, food waste is the waste produced at the end of the consumption chain by consumers and retailers, which constitutes a significant part of municipal solid waste (Mu'azu et al., 2019). Food waste, or food loss, is known to occur mostly during the food cycle in the processing system as well as on-site production, preparation, conveyance, retail, and utilization. The global food loss, or food waste, consists of about 33%, or one-third, of all the delivered food. Thus, food wastage has become a global threat to food security (Ariffin et al., 2023). Household or municipal wastes are usually generated from various sources where different human activities are encountered. Several studies reported that the municipal solid waste that is generated in developing countries is mainly from households (55–80%). This is then followed by commercial or market areas (10–30%). The latter consists of variable quantities generated from industries, streets, institutions and many others (Nabegu, 2010). Industrialized countries are the major contributors to household food waste. Food waste is directly associated with social (e.g., health, equality), economic (e.g., increasing costs, consumption, price volatility, resource efficiency, commodity markets, waste management), and environmental (e.g., water, climate change, energy, depletion of resources, disruption of biogenic cycles due to intensive agricultural activities) impacts (Olle, 2021).

The production of food waste depends on cultural, social, economic, and political factors in society. A variety of factors are identified relevant behind household food waste, including consumer behaviors (e.g., unreasonable purchase plans and cooking skills), consumer perception and attitudes (e.g., attitudes towards food waste, food safety concerns, perceived value of food, and knowledge of food production), consumer socio-demographic characteristics (e.g., age, education, gender, employment status, and marital status), household characteristics (e.g., household size, composition, and income), food-related characteristics (e.g., storage conditions, packaging, and price), and policy and regulation. Regrettably, such an understanding of the characteristics and driving factors behind rural household food waste generation in China is largely missing (Li et al., 2021).

The Malaysian Ministry of Housing and Local Government makes a projection that the quantity of generated daily food waste by households alone may reach about 8745 tons or about 3,192,404 tons per year (Jereme et al., 2018). The comprehensive breakdown illustrates that over 38.32% of total garbage is produced by households, in comparison to restaurants, which are known to produce yearly about 941,608 tons of garbage, or 23.35%. At the moment, only a few studies on waste generation at the national level have focused specifically on food waste (Phooi et al., 2022). However, there is still a paucity of data, especially on food expenditure, choices, as well as the reuse of behavior of food waste. Moreover, a lot of money could be saved by halting food waste.

The Environmental, Economic, and Biological Significance of Food Waste

Resource-intensive food production causes damage to the environment; for instance, water and air pollution, deforestation, soil erosion, and greenhouse gas emissions occur during food production, storage, conveyance, and waste management (Mourad, 2016).

Reports claim that food waste accounts for a share of global carbon emissions equivalent to a medium-sized country (FAO, 2013). Moreover, food loss leads to substantial economic setbacks for farmers, food manufacturers, and retailers, while also posing serious environmental and social challenges. Wasted food contributes to greenhouse gas emissions, depletes land and water resources, and intensifies issues such as food insecurity and hunger in many parts of the world.

The environmental consequences of producing food that is ultimately not consumed are considerable. When food waste ends up in landfills, it decomposes and releases methane a potent greenhouse gas that is 21 times more impactful than carbon dioxide in terms of global warming potential. Worldwide, emissions from food waste account for about 7% of total greenhouse gas emissions. Proper composting of food waste could reduce methane emissions, allowing the release of less harmful carbon dioxide instead.

In addition to landfilling, the environmental burden is further aggravated by the transportation and disposal of food waste over long distances, which requires significant fuel use and contributes to air pollution through vehicle exhaust emissions (Golian & Fasiangova, 2016). In most urban areas, food waste is disposed of in landfills, where the breakdown of organic materials emits carbon dioxide, methane, and hydrogen.

Although carbon dioxide and methane are the main gases produced, there are also smaller amounts of other gases that can be emitted. These gases may include trace amounts of volatile organic compounds, sulfur compounds, and nitrogen oxides. The migration of gas and leachate from landfill sites into the surrounding environment raises serious concerns such as air pollution, groundwater pollution, and climate change (Aljaradin & Persson, 2012). Therefore, to address issues such as water pollution, preserve wildlife, and minimize fossil fuel consumption, food production needs to be sustainable. However, the growing demand for fast production and heavily processed food is creating a major obstacle to preventing environmental damage. One of the major problems with these emissions is the absence of advanced technology to reduce pollution. For example, to reduce the dependence on fossil fuels, renewable energy sources are being introduced, which can significantly lessen carbon dioxide production (Kohli *et al.*, 2024).

Recent developments have led to a significant surge in productivity and marketing within the food and agro-industrial sectors. This progress, however, has also contributed to a substantial increase in agro-industrial food waste. In many developing Asian nations, the continuous rise in food waste is closely tied to ongoing economic expansion and population growth. Food, though invaluable, quickly turns into waste, thereby imposing serious environmental burdens (Badgett & Milbrandt, 2021). Both producers and consumers operate within an interconnected economic framework. Consumer preferences play a key role in shaping producer behavior and, consequently, the generation of food waste. However, the economic system is highly complex and interdependent. Resource consumption is not only dictated by production technology and distribution methods but also heavily influenced by the scale of consumption, which is directly affected by population size. This interconnection makes it impossible to isolate production from consumption; even everyday consumers bear responsibility for the environmental consequences of their consumption choices. Globally, the economic cost of food waste is estimated at around $1 trillion annually. Recognizing the urgency of this issue, food waste has been integrated into the United Nations Sustainable Development Goals (SDGs) under Goal 12: "Responsible Consumption and Production." This goal targets a 50% reduction in per capita global food waste at both the retail and consumer levels and aims to reduce losses along the entire production and supply chain by 2030 (Principato *et al*., 2018).

In less industrialized countries, households are the primary source of food waste, driven by large, diverse populations and widespread poverty. In urban areas, household food waste is often due to overbuying, spoilage, and inadequate storage practices (Liu *et al*., 2023). Farmers may discard produce that does not meet cosmetic standards, while food processing facilities generate waste through by-products such as peels, skins, and seeds. This considerable volume of food waste has significant environmental and economic repercussions—it not only wastes essential resources like water and land but also contributes to greenhouse gas emissions, exacerbating climate change (Chu *et al*., 2023). Efforts are currently underway in various countries to address the food waste crisis. These include programs that promote sustainable consumption patterns and encourage waste reduction at both the household and community levels. Unavoidable food waste may also include items that have spoiled or become contaminated and pose a health risk if consumed. While this type of waste is necessary to ensure food safety, its environmental impact can be mitigated. For instance, inedible food waste can be composted to enrich soil and reduce the reliance on synthetic fertilizers. Furthermore, emerging technologies are enabling the transformation of such waste into valuable resources like biogas for renewable energy. Although it is not possible to eliminate unavoidable food waste, its impact on society and the environment can be significantly reduced through innovative and sustainable practices (Rahman *et al*., 2024).

Kitchen Wastes and Their Composition

Types of Kitchen Wastes

Kitchen waste, often known as food waste, is a substantial component of home waste that includes items abandoned during meal preparation and consumption. It significantly contributes to solid waste globally. Food waste is described as the diversion of food designed for consumption by humans for non-consumption reasons, the usage of food meant for animals, or the disposal of edible food (FAO, 2014). Östergren *et al.* (2014) assert that both edible and non-edible food waste can be recycled or disposed of in an environmentally responsible manner.

Additionally, food waste can be divided into three categories: (a) avoidable waste, which includes food that was once edible but has since gone bad; (b) unavoidable waste, which includes some items that are not edible, such as eggshells; and (c) potentially avoidable food waste, which includes specific wastes that are occasionally consumed but not always, like potato skins (Papargyropoulou *et al*., 2014).

Organic waste in the kitchen includes fruit and vegetable peels, leftover food, meat, fish, and poultry trimmings, eggshells, coffee grounds, and tea bags, as well as carbohydrate residues such as bread, grains, and pasta. These products are frequently wasted during food preparation, resulting in leftovers that deteriorate if not consumed soon. Waste management is critical to keeping a kitchen clean and healthy.

Nutritional and Chemical Composition of Kitchen Waste

Nutritional Composition

The processing of fruits and vegetables yields a diverse array of by-products. Leaves, peels, unwanted pulp, seeds, and discarded fruits exemplify this kind of waste. Despite being discarded, these components are rich in nutrition, including carbohydrates, proteins, fiber, vitamins, and minerals. Typically, they contain a high concentration of carbohydrates, particularly dietary fibers such as pectin, cellulose, and hemicellulose. 10–30% of citrus peels consist of pectin, utilized in the food sector for gelling purposes (Liu *et al.,* 2022). Fruits generally have a low protein content; however, vegetable waste from leguminous plants, such as pea pods, may possess a relatively high protein concentration (Sagar *et al*., 2018). Vegetable waste typically contains around 2–7% protein by dry weight (Müller, 2017). Fruit seeds, such as those from bananas and mangos, contain a considerable amount of oil, with mango seed kernel oil comprising about 7–12% fatty acids, including oleic and stearic acids (Nzikou *et al*., 2010). Vegetable and fruit waste also contains elevated levels of minerals such as calcium, magnesium, and potassium, as well as vitamins including vitamin C and various B-complex vitamins (Ayala-Zavala *et al*., 2011). For example, apple peels are particularly rich in vitamin C (Bhushan *et al*., 2008), whereas banana peels are abundant in potassium (Emaga *et al*., 2007).

Chemical Composition

Fruits and vegetable waste are also a substantial source of bioactive compounds, such as polyphenols, flavonoids, carotenoids, and anthocyanins, which exhibit health-promoting properties. These compounds are recognized for their antioxidant, anti-inflammatory, and antimicrobial activities. Notable phytochemical compounds present in fruit and vegetable waste include phenolic compounds, flavonoids, carotenoids, tannins, and alkaloids (Kumar *et al.*, 2024). Numerous studies have identified that the by-products of fruits and vegetables encompass a diverse array of bioactive compounds. These compounds comprise phytochemical constituents, including flavonoids, anthocyanins, carotenoids, and phenolic acids. A multitude of these compounds has been identified (Aqilah *et al.* 2023).

Natural Products with Antibacterial Activity

Numerous natural compounds derived from plants, animals, and microorganisms exhibit antibacterial properties. However, their effectiveness can differ significantly due to the structural distinctions between Gram-positive and Gram-negative bacteria. Gram-negative bacteria, in particular, pose a major challenge because of their high levels of antibiotic resistance a concern that is especially critical in healthcare settings, where immunocompromised patients are at increased risk (Morris & Cerceo, 2020). Importantly, multidrug-resistant (MDR) bacteria are not confined to hospitals; they are also present in the food supply, largely as a result of the widespread use of antibiotics in livestock for disease treatment, growth enhancement, and preventive measures (Mateescu *et al*., 2014). Consequently, there is an urgent need to discover new antimicrobial agents capable of combating these resistant strains.

Proximate Analysis

Waste valorization, which involves converting waste materials into more useful products, is an important strategy for sustainable resource management. Proximate analysis is a key component of waste valorization and is commonly used to evaluate the nutritional and biochemical composition of organic waste streams such as food waste, agricultural residues, and industrial by-products (Maliki *et al.,* 2023). These parameters are crucial for understanding the bioactive potential of waste-derived materials, particularly in the development of functional ingredients for food, feed, pharmaceuticals, and bioenergy production. The nutritional and functional properties of food materials are significantly influenced by their proximate composition, including moisture, ash, lipids, proteins, and carbohydrates (López-Calabozo *et al.,* 2025). These components play crucial roles in determining various food products' sensory attributes, shelf life, and bioactivity.

Moisture Content

Moisture content is a crucial factor affecting the stability, texture, and sensory properties of food. It influences microbial growth, enzymatic reactions, and the rate of chemical degradation. High moisture content can lead to spoilage and reduce shelf life, while low moisture content can result in undesirable dryness and toughness. Onur *et al.* (2020) demonstrated that drying significantly reduced the total phenolic content and antioxidant activity in hawthorn and wild pear fruits. They also found that lower moisture content was linked to higher antioxidant activity. Additionally, Zhang & Ryu (2023) studied the impact of moisture content on the texture of meat products and observed that maintaining optimal moisture levels was crucial for preserving tenderness and juiciness.

Ash Content

The ash content is the inorganic mineral residue left after the organic matter of food is oxidized. It provides important information about the mineral composition of the food, which is essential for human health. In a previous study, the ash content of various plant-based foods, such as apple pomace, walnut shells, and sunflower husks, was found to vary significantly depending on the species and growing conditions (Adamczyk *et al.*, 2024). Rajurkar & Hand (2011) examined the relationship between ash content and the antioxidant properties of medicinal plants and concluded that higher ash content was correlated with increased antioxidant activity.

Lipid Content

Lipids, also known as fats, are essential nutrients that provide energy, support cell membranes, and act as signaling molecules. The type and amount of lipids in a food can significantly impact its nutritional value, sensory properties, and shelf life. A previous study reported that various nuts and seeds are rich sources of unsaturated fatty acids, which have beneficial health effects (Vecka *et al.*, 2019). Additionally, a recent study investigated the impact of lipid oxidation on the quality and safety of meat products, as well as strategies to prevent lipid rancidity (Pérez-Palacios & Estévez, 2022).

Protein Content

Proteins are vital building blocks of cells and tissues, playing crucial roles in various biological processes such as enzyme catalysis, structural support, and immune function. The protein content of a food is a key factor in determining its nutritional value. Different plant-based protein sources have been found to have excellent protein content, with legumes and grains being particularly good sources of complete proteins (Kumar *et al.*, 2022). Studies on the relationship between protein intake and muscle mass in athletes have concluded that adequate protein intake is essential for optimal muscle growth and recovery (Baranauskas *et al.*, 2023).

Carbohydrate Content

Carbohydrates are the main source of energy for the human body and are divided into simple carbohydrates (sugars) and complex carbohydrates (starches and fiber). The type and amount of carbohydrates in food can affect its glycemic index, energy density, and fiber content. Research on dietary fiber's impact on gut health has shown that a high-fiber diet is linked to better gut microbiota composition and a reduced risk of chronic diseases (Fu *et al.*, 2022). Additionally, Nicholls (2022) studied the glycemic index of various carbohydrate-rich foods and developed strategies for managing blood sugar levels.

Relevance of Proximate Analysis to Bioactivity

The connection between the chemical composition of food and its impact on health is a key focus in the field of food science and nutrition. The essential components of food include moisture, ash, protein, fat, carbohydrates, and fiber, which can influence the health benefits of food, such as its antioxidant, anti-inflammatory, and antimicrobial properties (Rosell *et al.*, 2024). The antioxidant effectiveness of food is affected by the presence of vitamins, minerals, and polyphenols, which are abundant in foods with high levels of phytochemicals (Pruteanu *et al.*, 2023). Additionally, Omega-3 fatty acids like eicosapentaenoic acid (EPA) and docosahexaenoic acid (DHA) found in food have anti-inflammatory properties, reducing the production of inflammatory substances like cytokines and eicosanoids. Dietary fiber, particularly soluble fiber, acts as a prebiotic by providing food for beneficial gut bacteria. These bacteria produce short-chain fatty acids, which support the health of the cells lining the colon. This process is essential for maintaining a healthy gut microbiome, which plays a crucial role in digestion, immunity, and even mental health (Beane *et al.*, 2021). The amino acid profile of a protein can determine its nutritional quality and its ability to support various biological functions. Animal proteins, such as meat, dairy, and eggs, are typically complete proteins. On the other hand, many plant proteins may lack one or more essential amino acids. However, combining different plant proteins, such as rice and beans, can provide a complete amino acid profile, supporting muscle repair, immune function, and other biological processes (Kojima, 2024; Hertzler *et al.*, 2020). The proximate composition of food materials, which includes moisture, ash, lipids, proteins, and carbohydrates, is essential for understanding their nutritional and functional properties. These components play significant roles in determining the sensory attributes, shelf life, and bioactivity of various food products.

Rising Antimicrobial Resistance

The global increase in infections resistant to antibiotics has heightened the hunt for substitute therapeutic approaches. The antibacterial qualities of natural extracts derived from plants, fungi, and other sources are being studied more and more in traditional medicine. Because natural extracts have many target mechanisms, they are less likely to cause pathogen resistance than conventional antibiotics because they frequently contain a variety of active chemicals (Bhat *et al.*, 2022; Osungunna, 2020). Research has demonstrated the potent antibacterial properties of plant extracts, such as those derived from *Ocimum sanctum* (holy basil) and *Curcuma longa* (turmeric), against drug-resistant bacteria and fungi, such as *Staphylococcus aureus* and *Candida albicans* (Abreu *et al.*, 2012; Bhat *et al.*, 2022).

Chemical Diversity and Synergy

The significance of chemical variety and synergy in natural antimicrobial agents has been highlighted by recent studies, especially in the fight against bacteria that are resistant to multiple drugs. Complex combinations of bioactive chemicals, found in natural products like fungi, essential oils, and plant extracts, can work in concert to increase the antimicrobial activity of these products. This multi-pronged strategy breaks down the cell walls of bacteria and fungi, prevents efflux pumps, and obstructs enzyme activity—all of which lessen the chance that resistance will emerge. For instance, it is known that substances like carvacrol, which comes from oregano, and thymol, which comes from thyme, combine to inhibit germs like Escherichia coli and Staphylococcus aureus. Since these chemicals can target many bacterial structures and functions at once, their combined effect is greater than the sum of their separate actions (Bhat *et al.*, 2022; André *et al.*, 2021).

Furthermore, the synergistic effects of secondary metabolites from herbal sources, such as terpenoids, flavonoids, and alkaloids, have been thoroughly researched. These substances can either improve antibiotic penetration or block bacterial resistance pathways when coupled with traditional antibiotics. Because it attacks infections from various angles, this synergy offers a broader approach to antimicrobial therapy, which is crucial in combating the increase of resistant microorganisms. The structural diversity and multi-target mechanisms of natural compounds, especially those derived from East Asian herbs, have been highlighted, which contribute to their strong antibacterial activity. Researchers have been able to increase therapy efficacy against MDR infections, especially in clinical settings, by mixing these natural compounds with conventional antibiotics (Jingru *et al.*, 2022).

Broader Antimicrobial Spectrum

The significance of natural extracts in providing a wider range of antimicrobial protection against Gram-positive and Gram-negative infections, including those that are resistant to several drugs, has been emphasized by recent research. Strong antibacterial properties have been shown by natural items such as fungal metabolites, essential oils (EOs), and chemicals derived from plants. In certain situations, these products have even been shown to outperform conventional antibiotics. *Agastache rugosa* and *Cinnamomum cassia* essential oils, for example, have demonstrated effectiveness against bacteria such as *E. coli* and *S. aureus*, often providing equivalent or superior results to penicillin (Lan *et al.*, 2021). Natural antimicrobial medicines' broad-spectrum efficacy is one of their main advantages. Against a variety of bacteria and fungi, such as Candida, Aspergillus, and antibiotic-resistant strains of *S. aureus* and *E. coli*, allicin from garlic, for instance, demonstrates strong effectiveness (Abouzeed *et al.*, 2013; Santra and Banerjee, 2022). Moreover, bactericidal activity against a variety of diseases has been demonstrated by bioactive compounds from endophytic fungi, such as those from *Curvularia eragrostidis*, which dramatically reduced the microbial load in a matter of hours (Santra & Banerjee, 2022).

One potential way to combat antimicrobial resistance and improve the effectiveness of existing treatments is to explore the diversity of natural chemicals and their potential synergistic effects when combined with antibiotics. In addition to having antibacterial properties, these extracts also have mechanisms that hinder the development of resistance, like regulation of the efflux pump and inhibition of quorum sensing, which help suppress bacterial resilience and communication (Arun & Tabarak, 2024). The wide range of activities exhibited by natural substances highlights the possibility of developing novel antimicrobial treatments and food preservatives, which might effectively address the pressing demand for long-term and efficient substitutes for synthetic antibiotics (Baindara & Mandal, 2022).

In Silico Methods in Antimicrobial Research

Role of Molecular Docking and Bioinformatics in Drug Discovery

Bioinformatics provides a wider context and a set of tools to improve the efficiency of finding new drug candidates in drug development (Dao *et al.*, 2024). It does this by using computational tools and techniques to examine biological data. Target validation and identification, drug target and off-target prediction, route and network analysis, pharmacogenomics, and drug repurposing are some of its functions. Furthermore, through the analysis of genomic, transcriptomic, and proteomic data, bioinformatics aids in the identification and validation of putative therapeutic targets (genes and proteins). It identifies important players and aids in understanding the molecular causes of illnesses. Bioinformatics helps reduce the risk of side effects by predicting possible medication targets and identifying off-target effects by comparing protein sequences and structures (Dao *et al.*, 2024). To determine which genes or proteins are essential in disease pathways and to direct the medication development process, bioinformatics technologies are utilized to examine biological pathways and molecular networks. Drugs that are specifically designed for each patient's genetic profile can be created with the aid of bioinformatics, which aids in the study of how genetic differences affect drug response. Drug development can be sped up by using bioinformatics to help researchers locate novel therapeutic uses for medications based on preexisting data (Chaachouay & Zidane, 2024).

By using molecular docking, scientists may forecast the intensity and mode of an interaction by predicting the preferred orientation of a tiny molecule (ligand) when it binds to a target protein (receptor). A score representing the strength of a drug candidate's binding to its target is produced using docking simulations. Designing more effective inhibitors or activators is guided by the visualization of interactions between the ligand and the protein's active site provided by docking. In addition, docking simulates how molecules fit into the binding site to create and optimize novel medications for targets with known 3D structures (from NMR or X-ray crystallography). Without the need for physical experiments, molecular docking enables the screening of enormous libraries of chemicals against target proteins to find possible leads (Sahu *et al.*, 2024a). In drug discovery, molecular docking and bioinformatics technologies are frequently combined. Bioinformatics can be used to further narrow the selection of possible therapeutic candidates by predicting ADMET (Absorption, Distribution, Metabolism, Excretion, and Toxicity) features and possible side effects, once promising candidates have been identified by molecular docking. Additionally, the combination of molecular docking and bioinformatics can aid in the design of medications that operate on many targets, which is beneficial for complicated diseases such as neurodegenerative disorders or cancer (Sahu *et al.*, 2024b).

Using Computational Methods to Predict the Interaction of Bioactive Compounds with Microbial Targets

A key component of modern drug discovery, especially in the creation of novel antibiotics or antifungal drugs, is the use of computational techniques to forecast how bioactive molecules will interact with microbial targets (Oselusi *et al.*, 2024). Finding promising drug candidates can be done much more quickly and cheaply with the help of these techniques. Finding the microbial target—a protein, enzyme, or nucleic acid—that is essential to the microbe's survival or pathogenicity is the first step in predicting interactions. One can access bioactive compounds from diverse sources such as small-molecule libraries, natural products, or already-identified antimicrobial agents. Subsequently, bioactive chemicals or chemical libraries will be retrieved using resources such as PubChem, ZINC, or ChEMBL databases. These can be filtered according to Lipinski's Rule of Five, molecular weight, solubility, or known antibacterial action. Lastly, the interactions between bioactive chemicals and microbial targets will be anticipated by molecular docking, using tools like AutoDock, PyRx, Schrödinger Glide, or Molecular Operating Environment (MOE) to dock the chemical into the microbial target's active site. Based on energy calculations, the docking software will score the interactions and forecast the optimal binding orientation (Rakshit *et al.*, 2023).

Nanotechnology in Antimicrobial Delivery

Nanotechnology has emerged as a groundbreaking innovation in the field of biomedicine, providing unprecedented opportunities to enhance drug delivery systems, particularly in the treatment of infections. By working at the nanoscale—typically ranging from 1 to 100 nanometers—researchers can manipulate materials at an atomic and molecular level, endowing them with unique properties that traditional bulk materials do not possess. This ability to control the size, shape, surface characteristics, and functionality of materials has opened new frontiers in medicine, especially in the targeted delivery of antimicrobial agents (Mehrabi *et al.*, 2023).

In the context of antimicrobial delivery, nanotechnology offers potential solutions to address critical limitations in current treatment approaches, such as drug resistance, poor bioavailability, rapid degradation of drugs, and the lack of specificity in targeting infected cells or tissues. The controlled design of nanoparticles allows for improved drug stability, reduced toxicity, enhanced delivery to infection sites, and protection of healthy tissues from the adverse effects of potent drugs (Liu *et al.*, 2023). These advances are particularly crucial in an era where microbial resistance is on the rise, making infections harder to treat with conventional therapies. Nanotechnology, therefore, plays a key role in revolutionizing antimicrobial therapies by enhancing drug efficacy, patient compliance, and clinical outcomes.

Benefits of Nanoformulations in Antimicrobial Delivery

The application of nanoparticles in antimicrobial delivery systems confers several important benefits, particularly in terms of improving drug bioavailability, enhancing drug stability, and providing controlled and targeted release. Microorganisms such as bacteria, fungi, viruses, and parasites are responsible for various infectious diseases. According to the report from the World Health Organization, the three leading infectious diseases ranked in the top 10 death causes in 2016 were lower respiratory infection (fourth place), diarrhea disease (ninth place), and tuberculosis (tenth place). Among the infectious microorganisms, bacteria are the leading cause of death in children, the elderly and immunodeficient patients (Aflakian *et al.,* 2023; Yeh *et al.,* 2024).

Enhanced Bioavailability

One of the primary challenges in antimicrobial therapy is the poor bioavailability of certain drugs, which limits their ability to reach therapeutic concentrations in the body. Many antimicrobial agents, especially those that are hydrophobic or poorly soluble in water, face difficulties in crossing biological barriers or are quickly metabolized before they can exert their effects. Nanoparticles significantly improve the bioavailability of these drugs by increasing their solubility, facilitating their transport across cellular membranes, and protecting them from rapid metabolism. For instance, nanoencapsulation can ensure that higher concentrations of the drug reach the infection site, leading to more effective and faster eradication of pathogens (Liu *et al.*, 2023).

Improved Stability

Another major limitation of conventional antimicrobial therapies is the instability of certain drugs, which can degrade quickly in the bloodstream or respond to environmental conditions such as temperature, pH, or enzymes. Nanoparticles act as protective carriers that shield the antimicrobial agents from premature degradation. By encapsulating the drug, nanoparticles preserve its activity and prolong its shelf life. This not only increases the drug's effectiveness but also reduces the risk of therapeutic failure due to the rapid breakdown of the drug before it reaches its target (Nwankwo *et al.*, 2023).

Controlled and Targeted Drug Release

One of the most remarkable advantages of nanotechnology in antimicrobial delivery is the ability to achieve controlled and targeted drug release. Nanoparticles can be engineered to release the encapsulated drug in a slow and sustained manner, ensuring that the drug remains active in the body over a prolonged period. This controlled release reduces the frequency of dosing, improves patient adherence to the treatment regimen, and minimizes the risk of drug resistance development. Furthermore, nanoparticles can be designed to specifically target infected tissues or cells, ensuring that the drug is delivered directly to the site of infection while sparing healthy tissues from unnecessary exposure. This targeted approach reduces the potential for side effects and enhances the overall safety and efficacy of the treatment (Yeh *et al.,* 2024).

CONCLUSIONS

Fruit and vegetable wastes, particularly peels and seeds, are an underutilized resource with significant nutritional, functional, and antimicrobial potential. Proximate analysis reveals that these wastes contain valuable macronutrients and phytochemicals that can be transformed into nutraceuticals, functional food ingredients, and bioproducts. In Malaysia, where agro-industrial waste generation is rising, valorization strategies could play a vital role in reducing municipal solid waste and enhancing food security. Furthermore, bioinformatics and in silico methods offer promising approaches to identify bioactive compounds, while nanotechnology provides innovative solutions for controlled antimicrobial delivery. To maximize these benefits, further research and industrial-scale applications are needed to establish effective valorization pathways. Overall, the sustainable utilization of kitchen and food processing waste aligns with global efforts to reduce food loss, combat antimicrobial resistance, and achieve the United Nations' Sustainable Development Goals on responsible consumption and production.

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AUTHORS' CONTRIBUTIONS

All authors contributed to the research

CONFLICT OF INTERESTS

None.

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