



REVIEW ARTICLE

Metabolomics and Mass Spectrometry in Postharvest Science: Tools for Quality and Shelf-Life Management

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ABSTRACT

Metabolomics, driven by mass spectrometry and complementary analytical tools, offers powerful insights into the biochemical changes occurring in fruits and vegetables after harvest. This review explores the application of metabolomics in postharvest science, focusing on its capacity to monitor ripening, assess quality, and detect spoilage at the molecular level. Analytical platforms such as GC-MS, LC-MS, and MALDI-TOF provide comprehensive metabolic fingerprints, while data-driven models enhance shelf-life prediction and support non-destructive technologies. Applications range from identifying freshness biomarkers to integrating smart packaging and precision sorting systems. However, commercial adoption is challenged by high costs, technical complexity, and the need for standardization. The review also highlights emerging opportunities in portable MS, AI integration, and the development of real-time decision support tools. With strategic investment and interdisciplinary collaboration, metabolomics is poised to revolutionize postharvest management and contribute to global food quality and sustainability.

Key words: Metabolomics; Postharvest; Mass spectrometry; GC-MS; LC-MS; Food sustainability.

INTRODUCTION

Postharvest losses remain one of the most significant challenges in global food systems, with up to 30–40% of fruits and vegetables being lost between harvest and consumption due to spoilage, senescence, and suboptimal handling conditions (Kader, 2005; FAO, 2022). Traditional postharvest assessment techniques, often based on visual inspection, weight loss, or firmness, fail to capture the complex biochemical processes that underpin fruit ripening, stress responses, and spoilage onset. As supply chains become longer and more complex, and as consumer expectations for freshness and nutritional quality increase, there is a growing need for more precise, real-time, and molecular-level tools to monitor and manage postharvest quality.

Metabolomics—the comprehensive study of small molecules (metabolites) in biological systems—has emerged as a powerful approach for understanding the biochemical shifts that occur in harvested produce. Unlike genomics or proteomics, which focus on potential or intermediate responses, metabolomics

provides a snapshot of the actual physiological state of the organism at a specific moment, making it uniquely suited for postharvest science. By tracking dynamic changes in sugars, organic acids, volatiles, amino acids, lipids, and secondary metabolites, researchers can gain insights into the metabolic pathways involved in ripening, stress tolerance, pathogen resistance, and degradation (Obata & Fernie, 2012; Allwood et al., 2008). This level of molecular detail not only improves our understanding of fruit and vegetable physiology but also offers the potential to develop biomarkers for shelf-life prediction, early spoilage detection, and freshness grading.

At the heart of metabolomics lies a suite of analytical technologies, among which mass spectrometry (MS) stands out due to its sensitivity, specificity, and broad metabolite coverage. Mass spectrometry-based platforms, including gas chromatography-mass spectrometry (GC-MS), liquid chromatography-mass spectrometry (LC-MS), and matrix-assisted laser desorption/ionization time-of-flight (MALDI-TOF), enable the identification and quantification of hundreds to thousands of metabolites

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in a single run. These tools can be applied in both targeted and untargeted metabolomics workflows, offering flexibility in either hypothesis-driven analysis or exploratory profiling. When coupled with robust data processing and bioinformatics pipelines, MS-based metabolomics allows researchers to distinguish subtle biochemical signatures that correlate with postharvest changes such as ethylene production, oxidative browning, and microbial colonization (Rohloff, 2015; Xu et al., 2021).

The relevance of metabolomics in postharvest science is not limited to laboratory studies. Increasingly, this approach is being integrated with precision agriculture technologies, non-destructive sensors, and supply chain monitoring systems to develop real-time quality control tools. For instance, metabolomics can be used to calibrate near-infrared spectroscopy or hyperspectral imaging models, enabling the rapid classification of ripeness stages or detection of latent spoilage without destroying the sample. These advances align with the goals of smart packaging and digital agriculture, in which dynamic quality monitoring can reduce waste, optimize logistics, and ensure consumer satisfaction (Mahajan et al., 2022). Moreover, by identifying specific metabolic pathways involved in chilling injury, pathogen response, or senescence, metabolomics informs breeding programs aimed at improving postharvest resilience in horticultural crops.

This review provides a comprehensive synthesis of how metabolomics and mass spectrometry are revolutionizing postharvest science. It begins with an overview of the conceptual framework and biological relevance of metabolite profiling in harvested crops. It then explores the technical underpinnings of MS-based analysis and complementary tools, followed by a critical examination of their applications in shelf-life prediction, quality control, and spoilage detection. The challenges and opportunities for translating these methods into commercial practice are also discussed, including cost, standardization, and regulatory considerations. Finally, the review identifies future directions in postharvest metabolomics, including the integration of AI-driven analytics, portable MS devices, and real-time monitoring platforms for enhanced food system sustainability (Fig. 1).

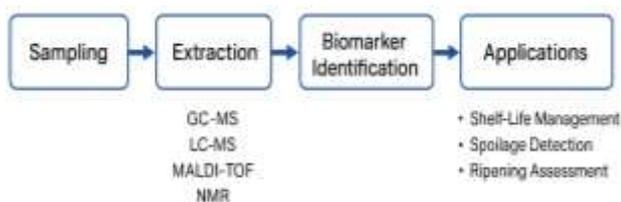


Fig. 1: Integrated workflow of metabolomics in postharvest science, illustrating the sequential process from sampling and extraction to biomarker identification and practical applications such as shelf-life prediction, spoilage detection, and ripening assessment.

1. Fundamentals of Metabolomics and Its Relevance to Postharvest Science

Metabolomics refers to the comprehensive analysis of small molecular weight compounds—metabolites—within a biological system. These metabolites represent the final downstream products of gene expression and enzymatic activity, providing a highly responsive and integrative view of the organism's physiological state. In the context of postharvest science, this responsiveness is particularly valuable because harvested plant tissues undergo rapid biochemical changes that are not always detectable through traditional physical or visual assessments. These include shifts in respiration rate, ethylene production, cell wall degradation, membrane integrity, and oxidative stress responses, all of which directly influence product quality and shelf-life (Fernie & Schauer, 2009; De Vos et al., 2007).

Metabolites are broadly classified into primary and secondary categories. Primary metabolites include compounds essential for basic cellular function, such as sugars, amino acids, organic acids, and lipids. These molecules play direct roles in energy metabolism, respiration, and structural integrity and are thus closely linked to processes such as fruit ripening, starch degradation, and senescence. For example, the conversion of starch to glucose and fructose in bananas or the accumulation of malic and citric acids in citrus fruits during storage are primary metabolic events that determine sweetness, acidity, and consumer acceptability (González-Agüero et al., 2009). Secondary metabolites, by contrast, include a wide range of phenolics, flavonoids, alkaloids, terpenes, and volatile organic compounds that serve roles in defense, pigmentation, aroma, and stress signaling. These compounds often act as key indicators of postharvest stress, pathogen attack, or exposure to chilling injury and are therefore central to metabolomics studies in quality control and spoilage detection (Wang et al., 2019).

One of the primary advantages of metabolomics in postharvest science is its capacity to reveal early biochemical changes that precede visible symptoms of deterioration. As fruit and vegetables progress through postharvest phases, metabolite profiles evolve dynamically in response to both internal metabolic programming and external environmental conditions such as temperature, humidity, gas composition, and microbial load. For instance, the decline of specific antioxidants or the rise of lipid peroxidation products may signal oxidative stress before any physical softening or discoloration becomes apparent (Zhang et al., 2020). These early markers provide a window of opportunity for intervention, whether by adjusting storage conditions, applying protective coatings, or initiating processing to prevent economic loss.

Furthermore, metabolomics enables the differentiation of closely related physiological states that may be indistinguishable by conventional

methods. Fruits at different stages of ripening or exposed to different postharvest treatments can exhibit overlapping visual characteristics but possess distinct metabolic fingerprints. This has been demonstrated in climacteric fruits such as tomatoes and mangoes, where metabolic profiling can distinguish between ethylene-induced and chilling-induced ripening pathways based on specific amino acids, volatiles, or phenolic signatures (Tzafrir et al., 2021). Similarly, in non-climacteric crops like grapes and strawberries, metabolomics can track subtle biochemical responses to cold storage, modified atmosphere packaging, or UV-C treatments, providing insights into stress adaptation and quality retention strategies.

In addition to quality assessment, metabolomics is increasingly applied to understand postharvest disease resistance mechanisms. Pathogen infection induces significant shifts in host metabolism, often resulting in the accumulation of defense-related metabolites such as phytoalexins, salicylic acid, and reactive oxygen species. Monitoring these shifts can help identify resistant cultivars or evaluate the efficacy of biocontrol agents and storage treatments. For instance, metabolomic studies have revealed that fruits treated with antagonistic yeasts or essential oils show distinct metabolic responses that correlate with enhanced resistance to fungal pathogens (Zhou et al., 2022). Such insights support the development of residue-free, sustainable postharvest technologies.

Another growing application is the use of metabolomics to guide breeding programs for postharvest traits. While traditional breeding has focused on yield, size, and appearance, metabolomics provides a tool to evaluate flavour, nutritional content, and shelf stability at the biochemical level. By identifying metabolite markers linked to desirable traits such as aroma, firmness retention, or low chilling sensitivity, researchers can accelerate the selection of superior genotypes. This approach also facilitates the screening of landraces or wild relatives for novel metabolites that confer improved storability or stress tolerance, thereby broadening the genetic base for crop improvement.

2. Analytical Platforms — The Role of Mass Spectrometry and Complementary Techniques

The effectiveness of metabolomics in postharvest research is largely determined by the sensitivity, accuracy, and versatility of the analytical platforms used to profile small molecules. Among these, mass spectrometry (MS) stands as the cornerstone of metabolite analysis, offering unparalleled capabilities for both targeted and untargeted detection across a broad range of compound classes. Its ability to identify metabolites based on mass-to-charge ratios, fragmentation patterns, and retention times makes MS particularly suitable for deciphering the complex metabolic alterations that occur in fruit and vegetable

tissues during storage, transport, and shelf-life (Dettmer et al., 2007). Mass spectrometry's high throughput, precision, and dynamic range allow researchers to detect subtle changes in metabolite concentrations associated with quality loss, spoilage, or stress adaptation—factors critical for postharvest management.

Gas chromatography–mass spectrometry (GC-MS) is one of the most widely used MS techniques in postharvest metabolomics. It is particularly well-suited for analyzing volatile compounds and small polar metabolites, including organic acids, sugars, and amino acids. GC-MS has been extensively used to profile aroma volatiles in fruits such as apples, bananas, and melons, providing insights into ripening, fermentation, and senescence pathways (Gómez-Cortés et al., 2020). Sample preparation often involves derivatization to increase compound volatility, followed by separation on a GC column and ionization in the mass spectrometer. The resulting spectra are compared with reference libraries for compound identification, enabling both qualitative and quantitative assessments. GC-MS excels in reproducibility and resolution but is limited in its ability to analyze non-volatile or thermally labile compounds.

Liquid chromatography–mass spectrometry (LC-MS), in contrast, is more versatile for analyzing a broader range of non-volatile, thermolabile, and higher molecular weight metabolites. It is commonly used to detect phenolics, flavonoids, alkaloids, and lipid derivatives—many of which serve as biomarkers for stress, decay, or senescence in postharvest tissues. LC-MS requires minimal derivatization, allowing for faster and more flexible workflows compared to GC-MS. Moreover, the use of electrospray ionization (ESI) facilitates the detection of fragile molecules with minimal fragmentation, enhancing analytical sensitivity (Dunn et al., 2011). Recent applications of LC-MS in postharvest research include the monitoring of chilling injury in tomatoes, antifungal responses in citrus fruit, and antioxidant depletion in cut vegetables.

Matrix-assisted laser desorption/ionization time-of-flight (MALDI-TOF) mass spectrometry is another technique gaining traction in the postharvest metabolomics domain, especially for spatially resolved metabolite profiling. MALDI-TOF allows the direct analysis of tissue surfaces, producing molecular images that reveal spatial distributions of key metabolites without extensive sample processing. This is particularly useful for mapping metabolite gradients across fruit peels, wounds, or fungal infection sites, providing insights into localized metabolic responses to stress or damage (Boughton et al., 2015). However, the technique is more qualitative than quantitative and is best used in combination with other platforms for comprehensive analysis.

Complementary techniques such as nuclear magnetic resonance (NMR) spectroscopy and Fourier-transform infrared (FTIR) spectroscopy are often

employed alongside MS to enhance metabolite coverage and data reliability. NMR is highly reproducible and non-destructive, making it ideal for quantifying high-abundance compounds such as sugars and organic acids in intact fruit extracts. Its structural elucidation capabilities are valuable for identifying unknown metabolites and verifying MS-based findings. While NMR lacks the sensitivity of MS, it provides quantitative data without the need for calibration curves or derivatization (Emwas et al., 2019). FTIR, on the other hand, provides rapid fingerprinting of biochemical compositions based on vibrational spectra, enabling non-targeted assessments of water content, carbohydrate profiles, and cell wall modifications.

The integration of multiple platforms—referred to as multiplatform metabolomics—is increasingly used to overcome the limitations of any single technique and provide a more comprehensive view of the postharvest metabolome. For instance, GC-MS may be used to capture volatile profiles, LC-MS to target phenolic or lipid fractions, and NMR to quantify organic acids—all from the same sample batch. Such integrative approaches enhance data richness and enable more robust interpretations of physiological status and quality dynamics during postharvest storage.

To handle the large and complex datasets generated from these techniques, advanced data processing and statistical tools are essential. Software packages for spectral deconvolution, peak alignment, normalization, and multivariate analysis—such as principal component analysis (PCA) and orthogonal partial least squares-discriminant analysis (OPLS-DA)—are commonly used to extract biologically meaningful patterns from raw MS data. These computational workflows are critical for biomarker discovery, classification of storage treatments, and building predictive models for shelf-life estimation (Schrimpe-Rutledge et al., 2016).

3. Applications in Shelf-Life Prediction, Ripeness Assessment, and Spoilage Detection

The most impactful contributions of metabolomics and mass spectrometry in postharvest science lie in their ability to detect biochemical changes associated with ripening, senescence, and spoilage long before they manifest visually (Figure 2). By capturing the dynamic metabolic fingerprint of a fruit or vegetable during storage, these technologies enable the prediction of shelf-life, assessment of ripeness, and early detection of deterioration with unprecedented precision. These applications hold significant promise for optimizing harvest timing, reducing postharvest waste, and improving supply chain logistics.

Shelf-life prediction is a key focus in metabolomics-based postharvest studies. Traditional models rely on temperature, humidity, or CO₂ levels as proxies for quality loss, but these parameters lack specificity. In contrast, metabolite profiling allows for the identification of biochemical markers directly linked to

degradation pathways. For instance, rising levels of lipid peroxidation products and declining antioxidant metabolites such as ascorbate or glutathione can indicate oxidative stress and impending quality loss in fresh-cut produce (Zhang et al., 2020). Studies in bananas and papayas have demonstrated that accumulation of specific amino acids and organic acids correlates strongly with tissue senescence and flavor decline, offering metabolite panels that can serve as predictive indicators of remaining shelf-life (Singh et al., 2022). By integrating these markers into logistic models or sensor-driven alert systems, distributors can make real-time decisions about cold storage adjustments, market redirection, or processing options.

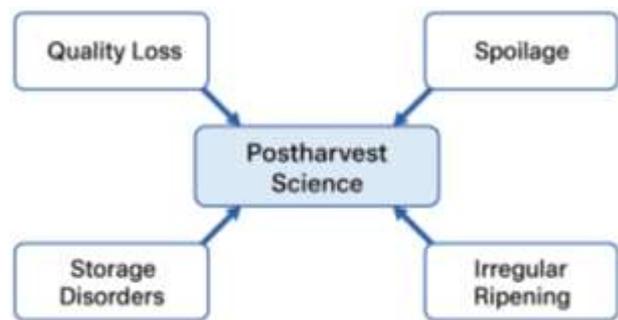


Fig. 2: Key postharvest challenges—quality loss, spoilage, storage disorders, and irregular ripening—that can be addressed through metabolomics-based interventions and diagnostics.

In ripeness assessment, metabolomics offers a molecular lens that complements and surpasses external indicators such as firmness or color. Ripening is accompanied by shifts in sugars, volatiles, pigments, and cell wall-degrading enzymes, many of which can be tracked through targeted or untargeted MS-based analyses. In climacteric fruits like mango, tomato, and avocado, ethylene-triggered increases in compounds such as β -ionone, hexenal, and linolenic acid derivatives provide precise biochemical staging of ripening (Tzafrir et al., 2021). In non-climacteric fruits such as citrus, strawberry, or grape, secondary metabolites like flavonoids and anthocyanins play a greater role and are easily quantified using LC-MS. These markers not only support consumer-oriented quality grading but also aid in determining optimal harvest windows to synchronize ripeness at the retail level. The ability to match internal ripening stages with external market demands adds strategic value for exporters and large-scale retailers seeking to minimize losses due to over- or under-ripe shipments.

Spoilage detection is perhaps the most critical application of metabolomics in food safety and quality assurance. Spoilage often begins at the molecular level, long before microbial growth or textural breakdown becomes observable. Mass spectrometry enables the detection of microbial metabolites, stress-related volatiles, and tissue degradation products that signify the onset of spoilage. In apples and pears, for example,

early production of methanol and ethanol—associated with fermentative metabolism—is detectable through GC-MS before the fruits exhibit off-odors or softening (Obando-Ulloa et al., 2008). Similarly, changes in sulfur-containing compounds can indicate microbial invasion or anaerobic respiration under modified atmosphere storage. These early biochemical shifts provide a valuable opportunity for quality control interventions such as removal from circulation, modified atmosphere adjustments, or microbial testing.

One promising avenue is the use of metabolomics to calibrate or validate non-destructive techniques such as near-infrared (NIR) spectroscopy, hyperspectral imaging, and electronic noses. These tools are increasingly used in commercial settings due to their speed and portability, but their accuracy often depends on robust biochemical calibration datasets. Metabolite-based fingerprints derived from mass spectrometry provide ground-truth datasets that improve the predictive power of these rapid tools (Wu et al., 2021). In this way, metabolomics serves not only as a diagnostic platform but also as an enabler of high-throughput quality monitoring technologies.

Furthermore, spoilage detection using metabolomics has expanded into the realm of smart packaging. Volatile organic compound (VOC) sensors embedded in packaging can be tuned to detect biomarkers identified through GC-MS, enabling real-time monitoring of product freshness during storage and transit. This has been explored for leafy greens, berries, and meat analogues, where the buildup of spoilage-associated volatiles triggers color changes or digital alerts (Jafari et al., 2021). The integration of metabolite-specific sensors with QR codes, blockchain, and cloud platforms also facilitates traceability, enhancing consumer trust and regulatory compliance in the postharvest sector.

4. Opportunities and Challenges for Commercial Implementation

While metabolomics and mass spectrometry have demonstrated significant potential in postharvest science, their application at the commercial level remains limited due to various logistical, technical, and economic constraints. Bridging the gap between laboratory-based insights and real-world implementation requires innovations not only in analytical platforms but also in data interpretation, regulatory compliance, and cost-effective integration with existing postharvest infrastructure. Nevertheless, the growing interest in smart agriculture, food safety, and traceability offers a conducive environment for the gradual adoption of metabolomics-based tools in the agri-food industry.

One of the key opportunities lies in the translation of biomarker discovery into actionable, real-time decision-making systems. Metabolomic studies have already identified numerous compounds that correlate with freshness, ripening, and spoilage. The next step

involves embedding this knowledge into portable devices or software systems that can assist producers, distributors, and retailers in assessing produce quality on-site. Recent advancements in portable mass spectrometry and miniaturized sample preparation systems have made it feasible to bring lab-grade analytics closer to the field or packinghouse floor (Cosio et al., 2020). Although still in developmental stages, these instruments have the potential to revolutionize quality control, especially when paired with user-friendly interfaces and cloud-based reporting tools.

Additionally, metabolomics plays a pivotal role in precision sorting and grading. Conventional methods typically rely on visual cues or destructive sampling, which may not reflect the internal quality or biochemical status of produce. By integrating metabolite data into machine vision algorithms, non-destructive quality sorting systems can be trained to detect internal defects, predict shelf-life, or group products by ripening stage more accurately than current commercial systems. These innovations are particularly valuable for export markets, where uniformity and extended shelf-life are critical quality attributes. Moreover, incorporating metabolomics into postharvest treatment evaluation—for instance, assessing the biochemical impact of coatings, irradiation, or controlled atmosphere storage—can optimize interventions to preserve nutritional and sensory quality without compromising safety or regulatory thresholds.

However, several challenges hinder the full-scale deployment of metabolomics in commercial settings. Chief among these is the high cost of instrumentation and maintenance. High-resolution mass spectrometers, NMR machines, and complementary platforms require significant capital investment, as well as skilled personnel for operation, data processing, and interpretation. While centralized testing laboratories may support large-scale exporters or vertically integrated supply chains, smallholder farmers and decentralized markets often lack access to such facilities. Developing lower-cost platforms and remote diagnostic services—where samples can be shipped and results returned rapidly via digital platforms—could help democratize access to metabolomics-based insights (Nicodemo et al., 2020).

Reproducibility and standardization also pose major hurdles. Postharvest metabolomic profiles are highly sensitive to pre-analytical variables such as sample handling, extraction protocols, and environmental conditions. Without standard operating procedures, data from different facilities or studies may be difficult to compare or integrate into predictive models. Regulatory acceptance of metabolomics-derived markers for shelf-life or spoilage certification will require validated protocols, certified reference materials, and inter-laboratory reproducibility studies (Allwood et al., 2008). Moreover, interpreting complex

metabolic datasets often demands advanced bioinformatics expertise and access to curated databases, which are not always readily available in commercial environments.

Data management and security are additional considerations. As metabolomics platforms are increasingly integrated with cloud-based tools and Internet of Things (IoT) systems, the volume and sensitivity of stored data grow significantly. Ensuring data privacy, secure transmission, and compliance with regional data protection regulations is essential, especially for multinational companies operating across jurisdictions. Additionally, intellectual property issues may arise regarding biomarker patents, proprietary metabolite libraries, or algorithm-based predictive models. Transparent data governance frameworks are needed to facilitate collaboration while protecting commercial interests and promoting open innovation.

Despite these limitations, the increasing convergence of metabolomics with AI, sensor technologies, and supply chain informatics suggests a promising trajectory. The use of machine learning algorithms to automate pattern recognition, anomaly detection, and predictive analytics can reduce dependence on human expertise and enhance the usability of metabolomics systems across diverse stakeholders. High-throughput metabolomics platforms capable of processing hundreds of samples per day are also being developed, which would drastically reduce analysis time and cost, making routine screening more feasible for exporters and retailers.

5. Conclusion and Future Directions

Metabolomics, underpinned by advanced mass spectrometry and complementary analytical techniques, has emerged as a transformative tool in postharvest science. By enabling high-resolution insights into the biochemical shifts associated with ripening, senescence, and spoilage, metabolomics allows for a more nuanced and predictive understanding of quality dynamics in horticultural commodities. From discovering biomarkers for shelf-life prediction to identifying early signals of pathogen attack, metabolomic profiling bridges a long-standing gap between subjective postharvest assessments and molecular-level diagnostics. Its integration with non-destructive sensing technologies, smart packaging systems, and machine learning platforms further expands its utility across research, breeding, logistics, and quality assurance.

Despite these advancements, translating metabolomics from laboratory research to routine commercial practice remains a complex challenge. Issues of cost, accessibility, data complexity, and regulatory validation continue to limit its widespread adoption, especially among smallholder producers and in low-resource settings. Additionally, standardization of workflows and metabolite databases remains an

urgent priority for ensuring reproducibility and comparability across studies and operational contexts. The development of portable MS instruments, cloud-based analytics, and open-access bioinformatics tools offers promising pathways to democratize metabolomics and embed it more deeply into postharvest decision-making systems.

Future research should focus on identifying universal and crop-specific metabolic markers that can serve as standards for freshness, safety, and sensory quality across the supply chain. Greater collaboration between plant physiologists, chemometricians, engineers, and industry stakeholders will be essential to develop interoperable platforms that support both real-time monitoring and strategic interventions. Furthermore, coupling metabolomics with transcriptomic and proteomic datasets can deepen our systems-level understanding of postharvest biology, facilitating the design of crops with enhanced shelf stability and resilience to storage conditions.

Ultimately, metabolomics has the potential to become a foundational pillar of precision postharvest management. Its continued advancement, guided by the principles of scalability, affordability, and sustainability, will play a vital role in reducing food loss, enhancing nutritional quality, and securing global food systems for the future.

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