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Advanced Chromatographic and Spectroscopic Techniques for the Analysis of Emerging Contaminants and Non-Nutritive Sweeteners in Ready-to-Drink Beverages

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Abstract: The global market for ready-to-drink (RTD) beverages made with non-nutritive sweeteners (NNS) has significantly increased due to rising consumer demand for low-calorie and sugar-free options. However, the discovery of emerging contaminants (ECs) such as Bisphenol A (BPA), Bisphenol S (BPS), Furan, and acrylamide in these drinks has highlighted the pressing need for very sensitive and reliable analytical methods for safety evaluation and regulatory compliance. This review provides a comprehensive overview of recent advancements in chromatographic and spectroscopic techniques used for the analysis of NNS and emerging contaminants in RTD beverage matrices. The choice of analytical techniques primarily relies on high-performance liquid chromatography (HPLC), ultra-high-performance liquid chromatography (UHPLC), and tandem mass spectrometry (MS/MS) due to their exceptional sensitivity, selectivity, and multi-residue detection capability. Spectroscopic methods, such as Raman, Fourier-transform infrared (FTIR), near-infrared (NIR), and nuclear magnetic resonance (NMR), offer a rapid and non-destructive alternative for qualitative screening. Recent studies in high-resolution mass spectrometry (HRMS) have enabled non-targeted screening and metabolite profiling, while the integration of chemometric tools such as principal component analysis (PCA) and partial least squares (PLS) has improved data interpretation and classification. The continuous improvement in quantitative NMR (qNMR) and hybrid chromatographic-spectroscopic systems has greatly refined analytical reliability and precision. However, there remain challenges of matrix interferences, detection of trace-level contaminants, and comprehensive evaluation of sweetener mixtures in complex beverage matrices despite the progress made. Future research should target integrated chromatographic-spectroscopic platforms, real-time monitoring, and greener analytical procedures to protect environmental and consumer health. This overview provides vital insights and directions to advance analytical chemistry in food safety monitoring.

Keywords: Chromatography, Spectroscopy, Non-nutritive sweeteners, Emerging contaminants, Ready-to-drink beverages, Mass spectrometry, NMR spectroscopy.

INTRODUCTION

Ready-to-drink (RTD) beverages represent one of the fastest-growing segments in the global food and beverage market, fuelled by consumer demand for satisfaction and taste (Tireki, 2021). To satisfy the preference for low-calorie and sugar-free alternatives, manufacturers increasingly use non-nutritive sweeteners (NNSs) as sugar substitutes. Health-conscious consumers have accelerated this demand towards beverages that provide sweetness with few calories. NNSs, also known as artificial sweeteners, are compounds hundreds to thousands of times sweeter than sucrose but contribute a negligible caloric value (Mathur & Bakshi, 2024). Emerging contaminants and NNSs have raised potential health and environmental concerns due to their chemical persistence and wide use. NNS such as sucralose, aspartame, acesulfame potassium (acesulfame-K), saccharin, and steviol glycosides are dominant in RTD formulations (Garba, Unar, & Kelechi, 2024). Their high stability and resistance to biodegradation enable them to persist in water systems even after treatment, leading to their classification as ECs (X. Yu *et al.*, 2023; Goveas, 2025).

RTD beverages are prone to a variety of contaminants beyond the use of NNSs. (Tireki, 2021; Rot, Gavran, Babić, & Lončarić, 2025). Bisphenol A (BPA), phthalates, per- and polyfluoroalkyl substances (PFAS), and microplastics are the most common ECs reportedly found in beverages (Y. Yu *et al.*, 2024). These compounds, at trace concentrations, have been associated with endocrine disruption, carcinogenicity, and bioaccumulation (Santhanam *et al.*, 2024; Li, 2025). One of the challenges of RTD beverage analysis is its chemical complexity at ultra-trace levels (Idowu-Adebayo, 2022; PS, Thadathil, George, & Varghese, 2024). The detection accuracy and quantification of these analytes often fall short due to matrix interferences and the limited selectivity of existing conventional methods (Raposo & Barceló, 2021). Modern chromatographic and spectroscopic techniques, however, offer high precision and molecular-level insight. Chromatographic methods such as high-performance liquid chromatography (HPLC), Ultra-high-performance liquid chromatography (UHPLC), and Gas chromatography (GC) are

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indispensable for separating analytes based on polarity, volatility, and molecular weight (Hymete, Ahmed, Ashenef, & Abebe, 2024). When coupled with mass spectrometry (MS), they attain detection limits below the micrograms per liter range and enable simultaneous multi-analyte quantification. Recent progress in tandem Mass Spectrometry (MS/MS), high-resolution Mass Spectrometry (HRMS), and time-of-flight Mass Spectrometry (TOF-MS) has enhanced non-targeted screening and structural elucidation in complex beverage matrices (Núñez, 2025; Shang, Wei, Li, Zhao, & Wang, 2025). Complementary spectroscopic methods, including Fourier-transform infrared (FTIR), Raman, and nuclear magnetic resonance (NMR) spectroscopy, provide rapid, non-destructive molecular fingerprinting. FTIR and Raman detect vibrational modes of functional groups such as C=O, C–N, and S=O bonds, while NMR elucidates structural configurations and degradation pathways (Zhu *et al.*, 2025). The combination of these techniques with chemometric techniques has enabled high-throughput screening and quantification in beverage quality control.

Despite these advancements, challenges remain. Sample matrix effects, low detection limits, and the absence of standardized protocols for ECs and NNSs monitoring limit data comparability. Recent studies indicate that some NNSs can alter gut microbiota composition and metabolic processes, while ECs like BPA and PFAS act as endocrine disruptors linked to reproductive and developmental effects (Zhao *et al.*, 2024). These findings highlight the urgent need for comprehensive analytical methods to ensure food safety and environmental protection. Regulatory bodies such as the U.S. Food and Drug Administration (FDA), the European Food Safety Authority (EFSA), and the World Health Organization (WHO) have defined acceptable daily intake (ADI) levels for NNSs based on toxicological assessments (Fitch *et al.*, 2021). For example, the ADI for aspartame is 40 mg/kg body weight/day and 50 mg/kg body weight/day, while the ADI for sucralose is limited to 15 mg/kg body weight/day (Solmaz, Dıraman, & Sezgin, 2021). However, the differences in jurisdictions in assessment approaches create inconsistencies in allowable limits. Although the European Union's Water Framework Directive and the U.S. Environmental Protection Agency (EPA) highlight the need for monitoring emerging pollutants, specific regulatory standards regarding NNSs are still lacking.

The implementation of Green Analytical Chemistry (GAC) principles in beverage analysis provides sustainable, low-solvent, and energy-efficient workflows (Karageorgou, Kalogiouri, & Samanidou, 2025). A comprehensive strategy that integrates the high-resolution separation power of chromatography with the structural elucidation capability of spectroscopic techniques such as Liquid Chromatography-Tandem Mass Spectrometry (LC-MS/MS), Ultra-High Performance Liquid Chromatography- Quadrupole Time-of-Flight Mass Spectrometry (UHPLC-QTOF-MS), and Gas Chromatography-Tandem Mass Spectrometry (GC-MS/MS) offers effective and efficient ways for the simultaneous identification and quantification of analytes (Michal *et al.*, 2025). FTIR and NMR provide molecular confirmation and degradation analysis (Schmidt, Haave, & Wang, 2025). The combination of these methods represents an effective approach for the sensitive, selective, and sustainable analysis of NNSs and ECs in RTD beverages. This review highlights recent advancements in advanced chromatographic and spectroscopic techniques applied for the analysis of emerging contaminants and non-nutritive sweeteners in ready-to-drink beverages. It provides an overview of current trends, methodological challenges, regulatory monitoring, and consumer safety.

ANALYTICAL TARGETS: NNS AND EMERGING CONTAMINANTS IN RTD BEVERAGES

Non-nutritive sweeteners (NNS)

NNS are comprised of a chemically varied group of intense sweeteners, including aspartame, acesulfame-K, sucralose, saccharin, cyclamate, steviol glycosides, neotame, advantame, and newer natural substitutes such as monk fruit and certain oligosaccharide preparations (Patel *et al.*, 2025). These compounds differ in their properties, including polarity, thermal stability, and ionization (Benucci, Lombardelli, & Esti, 2025). All these features directly impact the choice of the analytical method. The wide use of several NNS in beverages and table-top products, mostly in mixtures, makes multi-residue methods relevant. Regulatory bodies such as the U.S. FDA, EFSA, and WHO have defined acceptable daily intake (ADI) limits for NNSs based on toxicological evidence (Fitch *et al.*, 2021). The ADI for aspartame is 40 mg/kg body weight/day and 50 mg/kg body weight/day, while the ADI for sucralose is limited to 15 mg/kg body weight/day (Solmaz *et al.*, 2021). However,

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the newer natural sweeteners, such as monk fruit extract and allulose, remain less regulated, with limited safety and exposure data. This difference in regulation explains the focus on the well-characterized NNSs in RTD while emphasizing the need for continued evaluation of new alternatives.

Emerging contaminants (ECs)

Emerging contaminants (ECs) that concern the beverage industry mainly come from packaging materials, processing equipment, and ingredient residues. The compounds of major concern in ready-to-drink (RTD) beverages are bisphenols (bisphenol A and S), plasticizers (phthalates), per- and polyfluoroalkyl substances (PFAS), and microplastics resulting from the degradation of packaging and the bottling processes (Tumu, Vorst, & Curtzwiler, 2023; Yashwanth *et al.*, 2025). Processing impurities and trace pesticide residues may be introduced through raw ingredients. Environmentally focused ECs, such as pharmaceuticals, personal care products, and steroid hormones, are generally associated with broader aquatic pollution studies and are less commonly found in finished beverages (Arman *et al.*, 2021; Oriji, Isaac, & Ojo, 2024). ECs are quite complex and are often present in very low concentrations, making it necessary to use highly sensitive, reproducible, and multi-residue analytical methods that include both targeted and non-targeted techniques.

Chromatographic Techniques

Chromatography remains the principal method for the separation and quantification of non-nutritive sweeteners and other contaminants. Modern methods are based on ultra-high-performance liquid chromatography (UHPLC) for fast and high-quality separation and tandem/high-resolution mass spectrometry for detection.

HPLC and UHPLC (UV/PDA, fluorescence, Refractive Index)

The traditional HPLC with UV/PDA detection remains applicable for several sweeteners (those with UV-active chromophore) and for sugar profiling if it is coupled with the refractive index (RI) or the evaporative light scattering (ELSD) detectors. The UHPLC technique significantly lessens the total run time and increases the peak capacity, which is a very advantageous feature for screening multiple NNS in beverage matrices on a high-throughput basis. Method development often focuses on mobile phase composition, column chemistry (C18, HILIC for polar analytes), and temperature to find a balance between retention and peak shape (Simon, Kovács, & Szabó, 2025).

LC–MS and LC–MS/MS: targeted multi-residue quantification

The use of liquid chromatography coupled with tandem mass spectrometry (LC–MS/MS) has emerged as the standard method for the quantification of targeted non-nutritive sweeteners (NNS) and various ECs due to its high sensitivity and selectivity. The application of multiple reaction monitoring (MRM) enables the detection of numerous analytes in a low nanogram per liter ($ng \cdot L^{-1}$) range, while isotope-labelled internal standards enhance accuracy in complex matrices (Mirmont, Bœuf, Charmel, Lalère, & Lardy-Fontan, 2023). The simultaneous determination of multiple high-intensity sweeteners during a single run has been proven to be very successful and validated for both tabletop sweeteners and ready-to-drink (RTD) beverages (Nurhayati *et al.*, 2023).

High-resolution mass spectrometry (HRMS) for suspect and non-targeted screening

HRMS platforms (Orbitrap, time-of-flight) facilitate suspect screening and non-targeted workflows, allowing the discovery of unexpected contaminants and transformation products without the need for pre-selection. HRMS's role in environmental and food monitoring and its potential to advocate regulatory surveillance through expanded chemical space coverage have been highlighted in recent reviews (Lai *et al.*, 2024). HRMS datasets, when combined with the techniques of retrospective data mining and spectral library development, greatly enhance the ability of a laboratory to detect emerging threats.

Spectroscopic techniques

Spectroscopic methods are of interest due to their capability to deliver a fast, non-destructive screening and can be utilized in applications that require minimal sample preparation. When combined with chemometrics, they can support classification, authentication, and approximate quantification.

Raman spectroscopy

Raman spectroscopy provides vibrational fingerprints that are directly associated with the molecular structure and has been successfully used to identify and differentiate between sweeteners (sucralose, saccharin, aspartame) and other contaminants. Raman spectroscopy coupled with machine-learning classifications (random forest, SVM) enhances discrimination and allows

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immediate on-site screening. However, without surface enhancement (SERS), Raman's sensitivity can be limited for ultra-trace analytes (Tian *et al.*, 2025).

Fourier-transform infrared (FTIR) and NIR spectroscopy

FTIR and NIR yield rapid spectral acquisition, often with little sample preparation. Coupled with chemometric methods (PCA, PLS-R), they have been applied for authentication, sweetener quantification, and adulteration detection (Dhaulaniya *et al.*, 2020). FTIR combined with machine learning has shown encouraging results for screening artificial sweeteners in beverages. Limitations include spectral overlap for complex mixtures and reduced sensitivity compared to MS (Teklemariam, Chou, Kumaravel, & Van Buskrik, 2024).

Nuclear magnetic resonance (NMR) and quantitative NMR (qNMR)

NMR provides abundant structural details and, when applied for quantification (qNMR), can determine the amounts of sugars and other substances without the need for chromatographic separation. qNMR has proven to be reliable in the quantization of mixtures and can be especially advantageous when certified reference materials are not available (Y. Liu, 2024). There are limitations, which include the cost of the instrument and moderate sensitivity relative to MS, but high sample throughput and minimal preparation advantages for some applications. Recent benchtop NMR spectroscopy developments have improved instrument portability, cost efficiency, and made operations easy (H.-Y. Yu, Myoung, & Ahn, 2021), making it a potential tool for on-site beverage analysis and fast quality control assessments. Benchtop NMR systems typically operate at lower magnetic fields (40–80 MHz) compared to high-field instruments (Riegel & Leskowitz, 2016; H.-Y. Yu *et al.*, 2021). However, technological advances in magnet design and data processing have improved spectral resolution and quantitative reliability, enabling the monitoring of real-time beverage composition in production settings.

Sample preparation strategies and matrix effects

Effective sample preparation is of utmost importance in beverage analysis due to complex matrices (sugars, flavours, preservatives, colorants). The most frequently used methods are:

- Dilution and simple filtration for spectroscopic screening.
- Solid-phase extraction (SPE) or QuEChERS for enrichment of trace ECs before LC–MS analysis.
- Protein precipitation and liquid–liquid extraction (in case it is suitable).
- On-line SPE coupled with LC–MS to minimize manual handling and speed up the process.

Matrix effects remain the leading cause of ion suppression/enhancement in LC–MS; isotope-labelled internal standards, matrix-matched calibration, and matrix removal strategies are standard mitigations.

Chemometrics and data analysis

Spectroscopic methods with chemometric tools (such as PCA, PLS-R, OPLS-DA, random forest, SVM) are central when applying spectroscopic methods to solve overlaps and to extract information quantitatively and qualitatively. With chemometrics, large HRMS datasets in non-targeted workflows are interpreted (feature reduction, suspect prioritization). Reviews highlight the best practices in model validation, the necessity of avoiding overfitting, and the use of independent test sets (Yates, Aandahl, Richards, & Brook, 2023). The combination of machine learning and spectroscopy continues to be an active and productive area in the analysis of beverages.

Hyphenated and integrated platforms

The development of hyphenated systems (e.g., LC–HRMS, LC–NMR, GC–MS/MS, online SPE–LC–MS) clearly indicates the need for both separation techniques and orthogonal structural information. Combining chromatographic separation with NMR or HRMS provides complementary confirmation: LC separates and quantifies, HRMS offers high-accuracy mass data for formula assignment, and NMR delivers detailed structural information for unknown compounds. Recent studies have explored LC–MS combined with vibrational spectroscopy and chemometric overlays to enable quick screening followed by confirmatory analysis (Chen, Shu, Zhao, & Wan, 2023). These workflows optimize throughput while maintaining confidence in identification.

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Non-targeted screening, suspect lists, and retrospective analysis

HRMS non-targeted screening is an effective method of revealing the existence of previously unmonitored contaminants. However, compiling and maintaining suspect lists with in-house and public spectral libraries is very important (Szabo *et al.*, 2024). Improvements in data processing software, feature annotation algorithms, and spectral repositories have progressively enhanced retrospective screening to the extent that archived HRMS datasets can be re-interrogated when new suspects emerge. This helps in proactively monitoring RTD beverages for novel contaminants.

Green Analytical Chemistry and Sustainability

Green chemistry principles, such as solvent minimization, energy consumption reduction, and the use of solvent-free techniques, are now widely accepted and adopted. Solvent consumption per sample is significantly reduced with UHPLC compared to the old HPLC procedures (Nassef, Ahmed, El-Atawy, Alanazi, & Mohamed, 2024). Online Solid Phase Extraction (SPE) and sample dilution techniques aid in the reduction of consumables and solvents (Rani, Nanda, Narang, & Bhatia, 2024). The idea of using spectroscopy as a green first-tier method for sample triaging before resource-intensive confirmatory analyses is becoming increasingly accepted.

Performance Metrics, Validation, and Regulatory Considerations

The international criteria for selectivity, accuracy, precision, linearity, LOD/LOQ, and robustness must be followed for the validation of methods for NNS and ECs. LC–MS/MS methods mostly achieve low-ng·L^{-1} LOQs for many analytes; however, RTD beverages matrix complexity can complicate quantitation. HRMS allows identification but needs thorough validation for quantitative applications. The standardization of methodologies and the need for interlaboratory comparisons are essential to ensure data quality for regulatory enforcement. Regulatory validation frameworks such as the European Commission's SANTE/12682/2019 and the AOAC International Guidelines for Single Laboratory Validation (AOAC, 2016) specify that acceptable performance thresholds for quantitative methods typically demand recoveries in the range of 70–120%, relative standard deviations (RSD) below 20% and a determination coefficient (R^2) above 0.99 (Barbieri, 2021; Simón & Ritieni, 2022). ISO/IEC 17025 accreditation further highlights method traceability, measurement uncertainty, and interlaboratory proficiency testing to ensure analytical reliability (Panagiotidou, Chountalas, Magoutas, & Kitsios, 2025). The standardization of analytical methodologies and interlaboratory comparisons are vital in achieving data comparability and ensuring compliance with global food safety and environmental monitoring regulations (EFSA, EPA).

Case Studies and Notable Applications

Recent advances in analytical techniques have greatly improved the detection, quantification, and classification of non-nutritive sweeteners (NNSs) and emerging contaminants (ECs) in RTD beverages. These innovations combine advanced chromatographic, spectroscopic, and chemometric methods, enabling concurrent multi-analyte analysis, rapid screening, and the discovery of unrecognized compounds. Below are examples of the most significant developments currently influencing analytical processes for RTD drink monitoring:

- Simultaneous Multi-sweetener Quantification: Validated UHPLC–MS/MS workflows capable of quantifying nine high-intensity sweeteners in a single run have been reported, revealing the possibility of high-throughput surveillance for mixtures.
- Spectroscopy coupled with Chemometrics Screening: FTIR or Raman combined with PCA/PLS has quickly categorized and partially quantified sweeteners in beverage matrices, presenting a rapid triage step ahead of confirmatory LC–MS.
- Non-targeted HRMS Discovery: Non-targeted HRMS screening has discovered unexpected packaging and environmental contaminants in food matrices, demonstrating the use of suspect/non-target workflows for RTD beverage safety.

Challenges and current limitations

Analyzing ready-to-drink beverages still remains a challenge due to matrix complexity, the need for detection of contaminants at trace levels, and the issue of sweetener stability during analysis. The continuous use and possible bioaccumulation of non-nutritive sweeteners such as sucralose in the food chain, together with their conversion into very harmful by-products during treatment, are becoming environmental and health concerns. The absence of standardized analytical methods and validation procedures that are uniformly applied in different laboratories continues to limit the comparability and reproducibility of data

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(Chowdhury, Medhi, Bhattacharyya, & Hussain, 2025). While Chromatography methods such as UHPLC–MS/MS and HRMS are very accurate and precise in quantifications, rapid and non-destructive spectroscopic methods such as Raman, FTIR, and NIR are gaining attention for routine screening due to their simplicity and sustainability. Combining spectroscopic techniques (Raman/FTIR/NIR) with chemometrics prior to selected LC–MS/MS or HRMS verification boosts the total throughput and efficiency. Research in the coming years should prioritize expanded HRMS spectral libraries, AI-assisted annotation, and the establishment of inter-laboratory harmonization as the means to strengthen regulatory confidence. In addition, the use of green analytical workflows, which employ solvent-minimized or solvent-free techniques such as SPME and μSPE, is consistent with sustainability goals. Quantitative NMR (qNMR) also provides complementary potential for sugar and sweetener profiling in situations where standards are limited. The future of monitoring and controlling the presence of contaminants and sweeteners in ready-to-drink beverages lies in the integration of multi-technique, eco-efficient, and standardized analytical platforms.

Future directions and recommendations

The existing literature indicates the need for concentrated research and the presence of big gaps. A single technique is not enough to cope with the analytical requirements that emerging contaminants and complicated sweeteners in RTD beverages bring. The combination of chromatographic and spectroscopic methods, possibly through hyphenated systems, could use their strengths in a complementary way (C. Liu, Zuo, Xu, & Wang, 2023). The development of portable, robust, and green analytical technologies enabling real-time monitoring at the consumption or production sites is still considered a necessity. There is a potential for further research to improve the sensitivity and specificity through the integration of chemometric and machine learning algorithms into analytical workflows (Houhou & Bocklitz, 2021). Contemplation of ethical and regulatory matters about the monitoring of sweeteners and their transformation products in the environment leads to the conclusion that an interdisciplinary approach is needed. The standardization of analytical protocols and inter-laboratory validations is an urgent requirement to support the enforcement of regulations and public health protection.

Existing studies point out the presence of significant analytical and regulatory gaps in the detection of both emerging pollutants and non-nutritive sweeteners in ready-to-drink beverages (Drewnowski *et al.*, 2019). The complexity of these multi-component matrices creates the need for complex requirements that no analytical method can handle. The combination of chromatographic and spectroscopic methods, such as LC-MS/MS and LC-NMR, paves the way for obtaining high sensitivity and selectivity and more insight into the molecules (Gathungu, Kautz, Kristal, Bird, & Vouros, 2020). The development of portable and environmentally friendly analytical technologies, such as Raman and FTIR spectrometers, has opened up further prospects for real-time, on-site screening of these substances (Fakayode *et al.*, 2020). The application of chemometric techniques and machine learning algorithms in conducting the analyses has also led to improved data interpretation, non-target screening, and prediction accuracy (Fatholahi *et al.*, 2023). The consideration of the ethical and environmental aspects connected with the presence of sweetener residues and transformation products is a task that requires interdisciplinary collaboration (Varzakas & Antoniadou, 2024). The establishment of common analytical procedures and global regulatory cooperation (ISO, AOAC, EFSA) in inter-laboratory validations will continue to be essential for providing reliable data, regulatory enforcement, and consumer safety.

CONCLUSION

Over the years, the application of advanced analytical techniques in ready-to-drink (RTD) beverages has undergone a significant transformation, and the detection and characterization of complex mixtures of non-nutritive sweeteners (NNSs) and emerging contaminants (ECs) has involved high-performance chromatographic separations, mass spectrometric detection, rapid spectroscopic screening, and advanced chemometric interpretation. Liquid chromatography combined with mass spectrometry (LC–MS/MS) remains the most accepted method for quantitative analysis, while high-resolution mass spectrometry (HRMS) and spectroscopic–chemometric methods present a more exploratory and less invasive approach. The recent progress of machine learning and chemometrics incorporation into analytical workflows has led to an increase in non-targeted screening, peak resolution, and predictive analysis. The issues of matrix interferences, trace-level

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quantification, and a lack of toxicological data continue to be barriers to risk assessment.

The expansion of spectral and mass spectral libraries, the use of joint validation protocols, and the adoption of green analytical practices, such as solvent minimization, microextraction, and the use of portable instruments all contribute to the development of sustainable high-throughput monitoring. The combination of chromatographic and spectroscopic platforms will enhance sensitivity and selectivity in real-time analyses. The collaboration of various disciplines, including analytical chemists, toxicologists, regulators, and industry experts, will be a key factor in translating these technological advancements into standardized, environmentally responsible, and consumer-safe monitoring frameworks for the rapidly growing RTD beverage market.

REFERENCES

1. Arman, N. Z., Salmiati, S., Aris, A., Salim, M. R., Nazifa, T. H., Muhamad, M. S., & Marpongahtun, M. "A review on emerging pollutants in the water environment: Existences, health effects and treatment processes." *Water* 13.22 (2021): 3258.
2. Barbieri, M. V. "Pesticides in the environment: analysis, occurrence, impact and recommendations for their attenuation." (2021).
3. Benucci, I., Lombardelli, C., & Esti, M. "A comprehensive review on natural sweeteners: impact on sensory properties, food structure, and new frontiers for their application." *Critical Reviews in Food Science and Nutrition* 65.24 (2025): 4615–4633.
4. Chen, X., Shu, W., Zhao, L., & Wan, J. "Advanced mass spectrometric and spectroscopic methods coupled with machine learning for in vitro diagnosis." *View* 4.1 (2023): 20220038.
5. Chen, X., Shu, W., Zhao, L., & Wan, J. "Advanced mass spectrometric and spectroscopic methods coupled with machine learning for in vitro diagnosis." *View* 4.1 (2023): 20220038.
6. Chowdhury, P. R., Medhi, H., Bhattacharyya, K. G., & Hussain, C. M. "Guidelines to establish the quality assurance, analytical parameters, and inter-laboratory studies." *Sample Handling and Trace Analysis of Pollutants*. Elsevier, 2025. 435–455.
7. Dhaulaniya, A. S., et al. "Development of an FTIR based chemometric model for the qualitative and quantitative evaluation of cane sugar as an added sugar adulterant in apple fruit juices." *Food Additives & Contaminants: Part A* 37.4 (2020): 539–551.
8. Drewnowski, A., et al. "Sugars and sweeteners: science, innovations, and consumer guidance for Asia." *Asia Pacific Journal of Clinical Nutrition* 28.3 (2019): 645–663.
9. Fakayode, S. O., et al. "Molecular (Raman, NIR, and FTIR) spectroscopy and multivariate analysis in consumable products analysis." *Applied Spectroscopy Reviews* 55.8 (2020): 647–723.
10. Fitch, S. E., et al. "Use of acceptable daily intake (ADI) as a health-based benchmark in nutrition research studies that consider the safety of low-calorie sweeteners (LCS): A systematic map." *BMC Public Health* 21.1 (2021): 956.
11. Garba, A. I., Unar, N. B., & Kelechi, A. J. "Chemistry of Food Sweeteners." *Food Additives—From Chemistry to Safety*. IntechOpen, 2024.
12. Gathungu, R. M., et al. "The integration of LC-MS and NMR for the analysis of low molecular weight trace analytes in complex matrices." *Mass Spectrometry Reviews* 39.1–2 (2020): 35–54.
13. Goveas, L. C. "Artificial Sweeteners and the One Health crisis: Toxicity effects and Ecological consequences." *Discover Applied Sciences* 7.6 (2025): 535.
14. Houhou, R., & Bocklitz, T. "Trends in artificial intelligence, machine learning, and chemometrics applied to chemical data." *Analytical Science Advances* 2.3–4 (2021): 128–141.
15. Hymete, A., et al. "Optimizing Ultra-High-Performance Liquid Chromatography (UHPLC) Methods for Rapid Analysis of Complex Biological Samples." *Relevant Applications of High-Performance Liquid Chromatography in Food, Environmental, Clinical and Biological Fields*. IntechOpen, 2024.
16. Idowu-Adebayo, F. *Adoption of turmeric in street-vended beverages: a case to improve nutritional status and livelihoods in Nigeria*. Wageningen University and Research, 2022.
17. Karageorgou, E. G., Kalogiouri, N. P., & Samanidou, V. F. "Green Approaches in High-Performance Liquid Chromatography for Sustainable Food Analysis: Advances,

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Challenges, and Regulatory Perspectives." *Molecules* 30.17 (2025): 3573.
18. Lai, Y., et al. "High-resolution mass spectrometry for human exposomics: expanding chemical space coverage." *Environmental Science & Technology* 58.29 (2024): 12784–12822.
19. Li, H. "Per- and polyfluoroalkyl substances in agriculture: environmental fate, bioaccumulation and management." *New Contaminants* 1.1 (2025).
20. Liu, C., et al. "Authentication of herbal medicines based on modern analytical technology combined with chemometrics approach: A review." *Critical Reviews in Analytical Chemistry* 53.7 (2023): 1393–1418.
21. Liu, Y. "Quantitative NMR in Quality Control." *Quality Control of Chinese Medicines: Strategies and Methods*. Springer, 2024. 691–757.
22. Mathur, P., & Bakshi, A. "Effect of non-nutritive sweeteners on insulin regulation, glycemic response, appetite and weight management: A systematic review." *Nutrition & Food Science* 54.1 (2024): 100–119.
23. Michal, O., Daria, T., Izabela, J., Gorecka, W., Tadeusz, N., Elzbieta, M., & Magdanena, B.-Z. "Mephedrone and Its Metabolites: A Narrative Review." *International Journal of Molecular Sciences* 26.15 (2025): 7656.
24. Mirmont, E., Bœuf, A., Charmel, M., Lalère, B., & Lardy-Fontan, S. "Validation of an isotope dilution mass spectrometry (IDMS) measurement procedure for the reliable quantification of steroid hormones in waters." *Analytical and Bioanalytical Chemistry* 415.16 (2023): 3215–3229.
25. Nassef, H. M., Ahmed, H. A., El-Atawy, M. A., Alanazi, T. Y., & Mohamed, M. A. "Greens assessment of RP-UPLC method for estimating Triamcinolone Acetonide and its degraded products compared to Box-Behnken and Six Sigma designs." *Green Chemistry Letters and Reviews* 17.1 (2024): 2301315.
26. Núñez, N. "Liquid Chromatography-Mass Spectrometry in Food Analysis." *Mass Spectrometry in Food Analysis: Principles and Applications*. World Scientific, 2025. 1–35.
27. Nurhayati, R., et al. "The developing of reduced-sugar ready-to-drink cocoa beverages: Optimization of stabilizers and sugar replacers concentration." *Food Science and Technology* 43 (2023): e107322.
28. Oriji, A., Isaac, G. O., & Ojo, R. F. "Emerging Contaminants in Drinking Water: Global Perspective." *Emerging Contaminants in Food and Food Products*. CRC Press, 2024. 44–60.
29. Panagiotidou, E., Chountalas, P. T., Magoutas, A. I., & Kitsios, F. C. "The multifaceted impact of ISO/IEC 17025 accreditation: A sector-specific analysis in civil engineering testing and calibration laboratories." *The TQM Journal* 37.4 (2025): 998–1035.
30. Patel, Y., et al. "Rediscovering Sweetness: The Evolution and Impact of Non-Nutritive and Natural Sweeteners." *Current Nutrition Reports* 14.1 (2025): 54.
31. PS, A., Thadathil, D. A., George, L., & Varghese, A. "Food Additives and Evolved Methods of Detection: A Review." *Critical Reviews in Analytical Chemistry* (2024): 1–20.
32. Rani, P., et al. "Advancements in solvent microextraction: Recent developments and diverse applications in the modern era." *Separation Science Plus* 7.6 (2024): 2300243.
33. Raposo, F., & Barceló, D. "Challenges and strategies of matrix effects using chromatography–mass spectrometry: An overview from research versus regulatory viewpoints." *TrAC Trends in Analytical Chemistry* 134 (2021): 116068.
34. Riegel, S. D., & Leskowitz, G. M. "Benchtop NMR spectrometers in academic teaching." *TrAC Trends in Analytical Chemistry* 83 (2016): 27–38.
35. Rot, T., et al. "Occurrence of pesticides, mycotoxins, and heavy metals in distilled alcoholic beverages: A review of contaminants and health risks." *Foods* 14.8 (2025): 1303.
36. Santhanam, S. D., et al. "A combinational threat of micro- and nano-plastics (MNPs) as potential emerging vectors for per- and polyfluoroalkyl substances (PFAS) to human health." *Environmental Monitoring and Assessment* 196.12 (2024): 1182.
37. Schmidt, J., Haave, M., & Wang, W. "Overcoming the challenge of quantifying aged microplastic by qNMR spectroscopy." *Environmental Science: Processes & Impacts* (2025).
38. Shang, W., et al. "Advances in High-Resolution Mass Spectrometry-Based Metabolomics: Applications in Food Analysis and Biomarker Discovery." *Journal of Agricultural and Food Chemistry* 73.6 (2025): 3305–3325.
39. Simón, A. N., & Ritieni, A. *Exposure assessment of mycotoxins in food and biological samples through high-resolution*

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mass spectrometry-based strategies. Universitat de València, 2022.
40. Simon, J., Kovács, M., & Szabó, P. T. "Finding the best column for polar basic analytes across reversed-phase and hydrophilic interaction liquid chromatography." *Heliyon* 11.4 (2025).
41. Solmaz, F. G., Dırman, E., & Sezgin, B. "Current approaches to the use of artificial sweetener aspartame." *GSC Bio Pharm Sci* 14.03 (2021): 36–41.
42. Szabo, D., et al. "Online and Offline Prioritization of Chemicals of Interest in Suspect Screening and Non-Targeted Screening with High-Resolution Mass Spectrometry." *Analytical Chemistry* 96.9 (2024): 3707–3716.
43. Teklemariam, T. A., et al. "ATR-FTIR spectroscopy and machine/deep learning models for detecting adulteration in coconut water with sugars, sugar alcohols, and artificial sweeteners." *Spectrochimica Acta Part A* 322 (2024): 124771.
44. Tian, J., et al. "Exploring the role of surface-enhanced Raman spectroscopy (SERS) in ensuring dairy quality and safety: Recent progress and future prospects." *Critical Reviews in Food Science and Nutrition* (2025): 1–26.
45. Tireki, S. "A review on packed non-alcoholic beverages: Ingredients, production, trends and future opportunities for functional product development." *Trends in Food Science & Technology* 112 (2021): 442–454.
46. Tumu, K., Vorst, K., & Curtzwiler, G. "Endocrine modulating chemicals in food packaging: A review of phthalates and bisphenols." *Comprehensive Reviews in Food Science and Food Safety* 22.2 (2023): 1337–1359.
47. Varzakas, T., & Antoniadou, M. "A holistic approach for ethics and sustainability in the food chain: The gateway to oral and systemic health." *Foods* 13.8 (2024): 1224.
48. Yashwanth, A., et al. "Food packaging solutions in the post-PFAS and microplastics era: A review of functions, materials, and bio-based alternatives." *Comprehensive Reviews in Food Science and Food Safety* 24.1 (2025): e70079.
49. Yates, L. A., et al. "Cross validation for model selection: A review with examples from ecology." *Ecological Monographs* 93.1 (2023): e1557.
50. Yu, H.-Y., Myoung, S., & Ahn, S. "Recent applications of benchtop nuclear magnetic resonance spectroscopy." *Magnetochemistry* 7.9 (2021): 121.
51. Yu, X., et al. "Occurrence, distribution, and ecological risk assessment of artificial sweeteners in surface and ground waters of the Yellow River." *Environmental Science and Pollution Research* 30.18 (2023): 52609–52623.
52. Yu, Y., et al. "A bibliometric analysis of emerging contaminants (ECs) (2001–2021): Evolution of hotspots and research trends." *Science of The Total Environment* 907 (2024): 168116.
53. Zhao, F., et al. "Interactions between gut microbiota and emerging contaminants exposure: New and profound implications for human health." *Environmental Research Communications* 6.7 (2024): 072001.
54. Zhu, Z., et al. "Thermodynamic Properties, Excess Properties, Structural Studies, and Hydrogen Bonding Interaction of Methyldiethanolamine + 1,2-Propylenediamine Mixtures." *Journal of Chemical & Engineering Data* 70.8 (2025): 3200–3215.

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