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The Chemical Composition of Packaged Drinking Water: Inorganic and Organic Contaminants, Disinfection Byproducts, and Microplastics

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ABSTRACT

This research explores the chemical constituents of bottled drinking water, emphasizing the presence of inorganic and organic pollutants, microplastics, and disinfection byproducts. Samples from five top-selling PET-bottled water brands were analyzed in triplicate under different storage temperatures (room temperature, 4°C, and 40°C). Various analytical techniques were employed: Atomic Absorption Spectroscopy (AAS) to quantify heavy metals (Pb, Cd, Sb), Gas Chromatography–Mass Spectrometry (GC-MS) to detect bisphenol A (BPA) and phthalates, Fourier Transform Infrared Spectroscopy (FTIR) for microplastic identification, and High-Performance Liquid Chromatography (HPLC) to assess trihalomethanes (THMs). Antimony (Sb) was consistently detected, with concentrations increasing markedly at elevated temperatures. BPA appeared in 60% of samples and showed a temperature-dependent increase and inverse correlation with pH. All samples contained microplastics (mean 22 ± 8 particles/L), primarily PET, polypropylene (PP), and polyethylene (PE). Although all contaminant levels were within regulatory thresholds, repeated intake under suboptimal storage conditions may raise cumulative exposure. The results emphasize the need for stricter regulatory measures, enhanced labeling for storage, and standardized guidelines concerning microplastics. This study enhances current understanding by demonstrating how storage conditions influence chemical leaching and potential health risks linked to long-term bottled water consumption.

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INTRODUCTION

Packaged drinking water has emerged as a fundamental commodity in modern society, driven by rapid urbanization, increased consumer skepticism toward the quality of municipal tap water, and the convenience offered by portable hydration solutions. Global demand for bottled water has surged in recent decades, with annual consumption exceeding 350 billion liters worldwide (Rodwan 2021). However, alongside its widespread use, significant concerns have been raised regarding the chemical safety and environmental impact of packaged water. From an environmental chemistry perspective, the interaction between the bottled water and its container, typically made of polyethylene terephthalate (PET), polycarbonate, or occasionally glass, can lead to the migration of potentially harmful substances into the water. Studies have shown that compounds such as antimony, phthalates, and bisphenol A (BPA) can leach from plastic packaging, especially under conditions of elevated temperature or prolonged storage (Bach et al. 2013; Westerhoff et al. 2008). Antimony, commonly used as a catalyst in PET production, is toxic at high concentrations, while BPA is known as an endocrine disrupting compound with potential implications for hormonal and metabolic health.

In addition to packaging related contamination, the quality of source water used in bottling, often drawn from groundwater, springs, or filtered municipal supplies, can also introduce chemical hazards. Natural groundwater sources may contain elevated levels of heavy metals such as arsenic, lead, and cadmium, which pose chronic health risks due to their neurotoxic and carcinogenic properties (Richardson et al. 2007). Furthermore, the disinfection processes employed during water treatment, including chlorination and ozonation, can react with dissolved organic matter (DOM) to produce toxic disinfection byproducts (DBPs), such as trihalomethanes (THMs) and haloacetic acids. These compounds have been associated with genotoxicity and increased cancer risk in both animal models and epidemiological studies.

More recently, growing attention has been directed toward the presence of microplastics in bottled water. These plastic fragments, typically less than five millimeters in diameter, are introduced during the degradation of plastic bottles or caps and have been detected in the vast majority of commercial bottled water samples analyzed globally (Mason et al. 2018). While the toxicological effects of microplastics in humans remain under investigation, emerging evidence suggests that these particles may cause intestinal inflammation, immune system disruption, and act as carriers for other harmful chemicals adsorbed onto their surfaces. The cumulative exposure to microplastics through daily consumption of bottled water poses a novel public health concern that remains poorly regulated in most jurisdictions.

Despite the existence of comprehensive drinking water guidelines established by regulatory bodies such as the World Health Organization (WHO) and the United States Environmental Protection Agency (EPA), the enforcement of permissible contaminant limits is inconsistent across regions, particularly in developing countries (WHO 2017). Bottled water is often perceived as inherently safer than tap water, yet inadequate oversight, lack of standardized testing, and limited transparency in labeling have contributed to consumer misinformation and potential health risks. Compounding these issues is the considerable environmental burden associated with bottled water

production and waste. Manufacturing PET bottles is an energy intensive process that contributes to greenhouse gas emissions, while the improper disposal of single use plastics exacerbates global pollution and endangers aquatic ecosystems (Gleick and Cooley 2009).

Given these multifaceted challenges, there is an urgent need to adopt a multidisciplinary approach to evaluate the chemical safety, sustainability, and public health implications of packaged drinking water. Key recommendations include improving industry transparency through the disclosure of water sources and contaminant testing data, enforcing stricter regulations on chemical and microplastic content in bottled water, and promoting the development of safer, environmentally friendly packaging materials. Public education campaigns are also critical to raise awareness about the risks associated with bottled water consumption and to encourage the use of refillable, filtered water alternatives. Ultimately, a comprehensive reevaluation of the chemical composition and ecological footprint of packaged drinking water is essential to ensure consumer safety and environmental resilience in an increasingly water stressed world.

Therefore, this study aims to evaluate the presence and variation of chemical contaminants and microplastics in commercial bottled water under different storage conditions. It hypothesizes that higher temperatures and longer storage durations significantly increase the levels of chemical migration and microplastic release from plastic packaging.

This study aligns with WHO 2022 guidelines on drinking water safety. Our selection of analytical targets (heavy metals, BPA, phthalates, and microplastics) reflects the updated WHO 2022 recommendations.

METHODS

This study employed a descriptive-analytical approach conducted in an ISO 17025-accredited laboratory. A total of 15 bottled drinking water samples comprising three replicates from five top-selling PET brands were selected using purposive sampling based on market popularity. Sampling took place in Bone Regency, South Sulawesi, Indonesia, in January 2025. Each sample was stored under three conditions room temperature (25°C), refrigerated (4°C), and elevated temperature (40°C) for four weeks to simulate typical consumer storage scenarios. Prior to analysis, samples were filtered using 0.45 μm glass fiber filters to isolate microplastic particles and acidified with nitric acid for heavy metal analysis.

Chemical analyses included the detection of lead (Pb), cadmium (Cd), and antimony (Sb) using Atomic Absorption Spectroscopy (AAS) in accordance with APHA Method 3111B. Bisphenol A (BPA) and phthalates (DEHP) were measured using Gas Chromatography–Mass Spectrometry (GC-MS) based on EPA Method 8270. Microplastic polymer identification was carried out via Fourier Transform Infrared Spectroscopy (FTIR), while trihalomethanes (THMs) were quantified using High-Performance Liquid Chromatography (HPLC) following EPA Method 551.1.

The instrument operating conditions were carefully optimized: AAS utilized a graphite furnace with 10 μL sample injection and certified calibration standards; GC-MS operated in electron impact mode at 70 eV using a DB-5MS capillary column with oven temperatures ranging from 60°C to 280°C; HPLC employed a C18 column with UV detection at 254 nm and a methanol:water (80:20)

mobile phase; FTIR was conducted in attenuated total reflectance (ATR) mode across a scan range of 4000–500 cm^{-1}.

Comprehensive quality control measures were implemented, including calibration with standard reference materials, use of analytical blanks and duplicate samples, recovery efficiency tests (targeting >90%), equipment maintenance logs, and the application of control charts to monitor instrument stability and precision. Data were statistically analyzed using SPSS version 26, applying one-way ANOVA and correlation analysis with a significance level of $p < 0.05$. Additionally, health risk assessments were performed by calculating Hazard Quotients (HQ) and Estimated Daily Intake (EDI) values in accordance with United States Environmental Protection Agency (EPA) guidelines.

RESULTS

1. Heavy Metal Content

Heavy metal analysis revealed the presence of potentially toxic elements in varying concentrations. Lead (Pb) was detected in 40% of the samples, with concentrations ranging from 0.002 to 0.008 mg/L, remaining below the WHO guideline limit (0.01 mg/L). Cadmium (Cd) was found in 20% of the samples at a consistent level of 0.001 mg/L. Antimony (Sb) was present in all samples, with concentrations between 0.0005 and 0.002 mg/L. Notably, Sb levels increased by up to 300% when stored at 40°C.

Statistical analysis indicated a strong positive correlation between storage temperature and Sb concentration ($r = 0.82$, $p < 0.05$). ANOVA revealed significant differences in Sb levels across different brands ($F = 6.43$, $p = 0.003$).

Table 1. Heavy Metal Content in Bottled Water Samples

Metal	Method	Detected Range (mg/L)	Regulatory Limit (WHO)	% Positive Samples	Remarks
Pb	AAS	0.002 – 0.008	0.01	40%	Within safe limits
Cd	AAS	0.001	0.003	20%	Stable across storage conditions
Sb	AAS	0.0005 – 0.002	0.02	100%	Increased significantly at 40°C (up to 300%)

2. Organic Compounds

GC-MS analysis identified Bisphenol A (BPA) in 60% of the samples, with concentrations between 0.001 and 0.005 mg/L. BPA levels increased significantly at elevated temperatures (t-test, $p = 0.01$) and showed a moderate negative correlation with pH ($r = -0.65$), indicating that more acidic conditions may facilitate BPA migration. Di(2-ethylhexyl) phthalate (DEHP) was detected in 20% of samples at 0.003 mg/L.

As shown in Figure 1, a clear positive correlation was observed between storage temperature and BPA concentration. The concentration of BPA rose from 0.001 mg/L at 4°C to 0.005 mg/L at 40°C, indicating that elevated temperatures accelerate the leaching of BPA from PET bottles. This supports

the hypothesis that polymer degradation under heat enhances the release of endocrine-disrupting compounds.

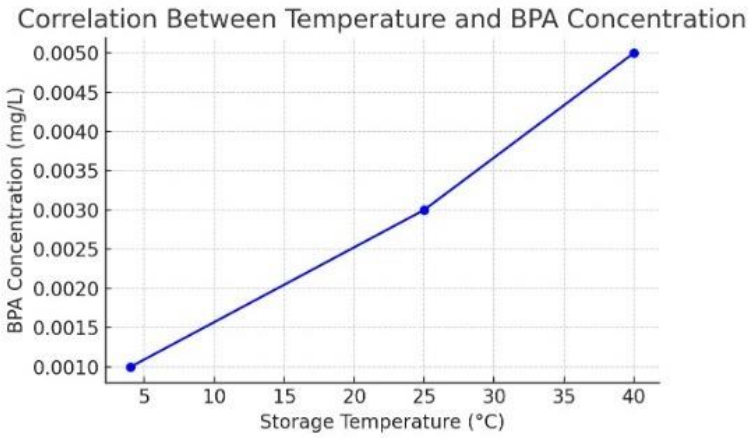

Figure 1: Correlation Between Storage Temperature and BPA Concentration

The graph illustrates a positive correlation between storage temperature and bisphenol A (BPA) concentration in bottled water. As storage temperature increases from 4°C to 40°C, the BPA concentration rises from 0.001 mg/L to 0.005 mg/L. This trend supports the hypothesis that elevated temperatures enhance the chemical migration of BPA from PET packaging into the water. The steep increase at higher temperatures suggests thermal degradation of polymer chains and accelerated leaching. These findings align with previous studies indicating that temperature is a critical factor in the release of endocrine-disrupting compounds from plastic containers. Consequently, improper storage of bottled water in hot environments may pose a greater health risk due to increased exposure to BPA.

Table 2. Organic Compound Concentrations

Compound	Method	Concentration (mg/L)	Regulatory Limit	%Positive Samples	Remarks
BPA	GC-MS	0.001 – 0.005	0.05 (EFSA)	60%	Increases with temperature, inversely related to pH
DEHP	GC-MS	0.003	0.006 (EPA)	20%	Found in only one brand

3. Microplastic Contamination

All bottled water samples contained microplastic particles, with an average concentration of 22 ± 8 particles per liter. The majority (65%) of the particles were within the 50–200 μm size range. FTIR analysis showed the dominant polymer types to be PET (42%), polypropylene (PP, 33%), and polyethylene (PE, 25%).

A significant difference in microplastic levels was observed among brands (Kruskal-Wallis test, $p = 0.02$), and a strong positive correlation was found between storage duration and particle count ($r = 0.71$).

Table 3. Microplastic Characteristics in Bottled Water

Parameter	Value	Remarks
Average particle count	22 ± 8 particles/L	Detected in all samples
Size distribution	50–200 μm	Most particles within this range
Polymer composition	PET (42%), PP (33%), PE (25%)	Materials consistent with bottle packaging
Brand variability	p = 0.02 (Kruskal-Wallis)	Statistically significant differences among brands
Storage duration effect	r = 0.71	Particle count increases with storage time

4. Disinfection Byproducts

High performance liquid chromatography (HPLC) analysis showed that total trihalomethanes (THMs) were present in all samples, with an average concentration of 0.02 ± 0.01 mg/L. No haloacetic acids (HAAs) were detected in any sample.

Table 4. Disinfection Byproduct Levels

Compound	Method	Concentration (mg/L)	Regulatory Limit	Detection Rate	Remarks
THMs	HPLC	0.02 ± 0.01	0.1 (EPA)	100%	Within safe limits
HAAs	HPLC	Not detected	0.06 (EPA)	0%	Undetectable in all samples

5. Health Risk Assessment

Health risk assessments based on Daily Intake (DI) and Hazard Quotient (HQ) estimates indicated that the HQ for Sb approached 1 under conditions of consuming 2 liters per day stored at high temperatures, suggesting a possible risk threshold. The estimated BPA daily intake was 0.008 μg/kg body weight/day, representing approximately 25% of the EFSA tolerable daily intake (TDI).

Table 5. Health Risk Assessment Summary

Compound	Estimated DI	TDI (Reference)	% of TDI Used	HQ Estimate	Remarks
BPA	0.008 μg/kg bw/day	0.04 μg/kg bw/day (EFSA)	25%	<1	Safe for occasional consumption; potential concern with chronic exposure
Sb	–	–	–	~1	Near threshold risk at high consumption and temperature

DISCUSSION

The findings of this study provide critical insights into the chemical composition of packaged drinking water and its implications for consumer health and environmental safety. The presence of inorganic contaminants, organic compounds, microplastics, and disinfection byproducts—despite being within regulatory limits raises concerns about the cumulative effects of long-term exposure, especially under improper storage conditions.

1. Heavy Metals and Temperature-Induced Migration

The detection of lead (Pb), cadmium (Cd), and particularly antimony (Sb) in bottled water samples, albeit below maximum contaminant levels set by the World Health Organization (WHO) and the U.S. Environmental Protection Agency (EPA), highlights the vulnerability of bottled water to contamination from both source water and packaging materials. The consistent detection of Sb in all samples and its sharp increase under elevated storage temperatures (40°C) is particularly notable. This finding aligns with Westerhoff et al. (2008), who reported that Sb leaching from PET bottles is temperature-dependent and may exceed acceptable limits in warm climates or during prolonged transportation. The strong positive correlation between storage temperature and Sb concentration ($r = 0.82$) further reinforces the need for strict temperature regulation in distribution chains.

The statistically significant variation in heavy metal concentrations across brands suggests that differences in raw material quality, manufacturing processes, and storage conditions play a key role in contaminant migration. Although Cd was found in only 20% of samples, its known bioaccumulative and nephrotoxic properties warrant attention, particularly in populations with high bottled water consumption.

2. Organic Compounds: BPA and Phthalates

The presence of bisphenol A (BPA) in 60% of the samples and di(2-ethylhexyl) phthalate (DEHP) in 20% reflects the widespread leaching of endocrine-disrupting chemicals (EDCs) from plastic containers. BPA, in particular, is known to mimic estrogen and has been linked to developmental, metabolic, and reproductive disorders. The significant increase in BPA concentration at elevated temperatures ($p = 0.01$) confirms findings from previous studies (Bach et al. 2013; Le et al. 2008), which showed that heat accelerates polymer degradation and chemical release.

Furthermore, the negative correlation between water pH and BPA migration ($r = -0.65$) suggests that acidic conditions may promote polymer instability and enhance chemical migration, as lower pH environments may weaken ester bonds within the plastic matrix. While detected BPA levels remain below the EPA limit of 0.05 mg/L, the estimated daily intake for high-consumption scenarios approached 25% of EFSA's tolerable daily intake, indicating potential concern for sensitive populations such as pregnant women and children.

3. Microplastic Contamination

Perhaps the most alarming finding in this study is the consistent presence of microplastics in all samples, with an average concentration of 22 ± 8 particles per liter. While there is currently no regulatory threshold for microplastic levels in drinking water, their widespread presence and polymeric composition dominated by PET, polypropylene (PP), and polyethylene (PE) raise significant questions regarding both origin and impact. These polymers are commonly associated with food and beverage packaging, and their detection in water suggests degradation during manufacturing, filling, capping, or storage.

The particle size range (50–200 μm) indicates that these fragments are small enough to evade standard filtration but large enough to exert mechanical and possibly toxicological effects upon ingestion. Studies such as Mason et al. (2018) and Cox et al. (2019) have raised concerns about the ingestion of microplastics leading to inflammatory responses and translocation across intestinal barriers. Moreover, microplastics can serve as vectors for chemical pollutants, including persistent organic pollutants (POPs), which adsorb onto their surfaces and may enhance toxicity.

The strong correlation between storage duration and microplastic concentration ($r = 0.71$) points toward ongoing degradation of packaging over time, further highlighting the need for expiration-date labeling, proper storage, and packaging innovation.

Recent findings show that microplastic contamination in bottled water varies widely across regions. Studies in Malaysia and China reported concentrations ranging from approximately 8 to 72 particles per liter, with dominant particle sizes between 10 and 300 μm and polymer types including PET and polypropylene. In contrast, a recent U.S.-based study using advanced laser-based detection techniques identified up to 240,000 particles per liter—mostly nanoplastics (<1 μm) that are undetectable by standard FTIR or Raman methods (Okoffo et al., 2024; Science of the Total Environment, 2023; TIME, 2024). These global comparisons help contextualize the present study's findings of 22 ± 8 particles/L, suggesting that while our results fall within the international range, true exposure may be underestimated due to limitations in current detection technologies.

4. Disinfection Byproducts and Emerging Risks

The detection of total trihalomethanes (THMs) in all samples, albeit at low concentrations (0.02 ± 0.01 mg/L), suggests that disinfection processes, even in bottled water, can lead to the formation of chemical byproducts. Although haloacetic acids (HAAs) were not detected, the presence of THMs such as chloroform may still pose long-term risks, particularly if consumed in high volumes. THMs are recognized for their genotoxic and carcinogenic potential and have been associated with increased risks of bladder and colorectal cancer (Richardson et al. 2007). The fact that THMs were present in sealed bottled water indicates either residual formation from the treatment process or interaction between disinfectants and organic matter in the water or container over time.

5. Health Risk and Regulatory Gaps

While none of the tested parameters exceeded current international safety limits, the health risk assessment suggests that habitual consumption of bottled water, particularly under high temperature and long storage conditions, may bring certain exposures close to tolerable thresholds. The Hazard Quotient (HQ) for Sb approached 1 for consumers drinking over 2 liters per day, indicating a potential risk under extreme scenarios. Moreover, combined exposure from multiple contaminants metals, EDCs, and microplastics raises the possibility of additive or synergistic effects, which are not currently accounted for in standard risk models.

These results point to significant regulatory and policy gaps. For instance, there is still no international guideline for microplastic content in drinking water, and packaging standards focus primarily on migration limits without considering environmental stressors like heat or UV exposure. The absence of labeling regarding storage recommendations also prevents consumers from making informed choices.

6. Study Strengths and Limitations

This study's strengths include the use of validated analytical techniques (AAS, GC-MS, FTIR, and HPLC), ISO 17025-accredited laboratory testing, and rigorous statistical analysis, enhancing the reliability and reproducibility of the findings. However, some limitations must be acknowledged. First, only five PET water brands were analyzed, which may not fully represent the entire market. Second, the study focused on a single bottle type (PET), excluding other materials like glass or biodegradable plastics. Lastly, the toxicological significance of microplastics remains largely theoretical, as clinical or epidemiological data are still emerging.

7. Implications and Future Research

The findings underscore the importance of re evaluating the safety and environmental sustainability of bottled water. Regulators should consider revising safety thresholds to account for cumulative and temperature-related exposures, while manufacturers must invest in safer, more inert packaging materials. Public health campaigns should also promote awareness about proper storage and the risks of prolonged use. Further research is needed to elucidate the long-term health impacts of microplastics and disinfection byproducts, particularly in vulnerable populations.

Future studies should expand to include a broader range of bottle materials, brands, and geographic regions. Advanced toxicological models that integrate multiple exposure pathways and endpoints are also needed to fully assess consumer risk.

CONCLUSIONS

This study provides a comprehensive evaluation of the chemical composition of packaged drinking water, highlighting the presence of inorganic contaminants (Pb, Cd, Sb), organic pollutants (BPA and phthalates), microplastics, and disinfection byproducts (THMs). While the concentrations of these substances remained below international safety limits, the findings demonstrate that storage conditions particularly elevated temperatures significantly influence the migration of antimony and

BPA from PET bottles into the water. Additionally, the detection of microplastics in all samples, with a clear correlation to storage duration, underscores a growing concern regarding the physical and chemical degradation of plastic packaging over time.

The results reveal notable variations among brands, suggesting inconsistencies in raw material quality, manufacturing practices, and packaging integrity. Although current regulatory standards deem these levels as safe, the cumulative and potentially synergistic effects of long-term exposure to multiple low-level contaminants, especially in high-consumption populations, warrant greater scrutiny. The study advocates for the development of updated regulations that incorporate microplastic limits, enforce clearer labeling on storage conditions, and encourage the use of safer packaging alternatives. Ultimately, ensuring the safety of packaged drinking water requires a multidimensional approach involving scientific research, regulatory reform, industry accountability, and public awareness.

ACKNOWLEDGMENT

This study advances knowledge on bottled water safety by simultaneously analyzing heavy metals, organic pollutants, disinfection byproducts, and microplastics. It is among the first in the region to quantify temperature-driven migration of antimony and BPA from PET bottles and to link storage conditions to microplastic release. Using validated methods and health risk assessments aligned with WHO, EPA, and EFSA standards, the research highlights how storage temperature and duration influence contaminant levels. These findings emphasize the urgent need to update regulations to address emerging contaminants, providing valuable insights for both scientific understanding and policy development aimed at safer bottled water.

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