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PFAS in bottled water from China: High prevalence of ultrashort-chain compounds, health risks, and global insights

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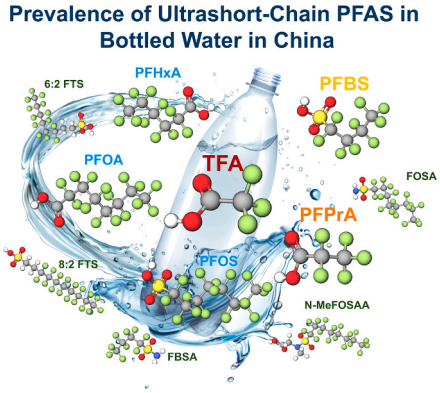
HIGHLIGHTS

- First national-scale survey revealed dominance of ultrashort-chain PFAA in China.
- TFA and PFPrA reached 46.2 and 64.0 ng/L, respectively, in bottled water.
- Significant correlations suggest precursor-to-terminal PFAA transformation pathways.
- Most PFAA posed low health risks, except for PFOA and PFOS.
- A global analysis revealed rising ultrashort-chain PFAA and precursors in bottled water.

GRAPHICAL ABSTRACT



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ABSTRACT

Per- and polyfluoroalkyl substances (PFAS) are persistent environmental contaminants, with drinking water serving as a major human exposure pathway. This study analyzed 52 bottled water products across China for 50 PFAS analytes, covering ultrashort-chain, short-chain, long-chain compounds, and precursors. A total of 21 PFAS were detected, with Σ_{21}PFAS concentrations ranging from 2.69 to 97.0 ng/L. Ultrashort-chain PFAS, trifluoroacetic acid (TFA) and perfluoropropanoic acid (PFPrA), were the most abundant with median concentrations of 7.40 and 3.98 ng/L. PFAS levels varied notably across product types, water sources and treatment. Spring water showed the highest average Σ_{21}PFAS concentration (37.5 ng/L), likely due to shallow, surface-impacted sources and minimal treatment. In contrast, lower levels were observed in mineral and purified waters, especially those from deeper aquifers or with reverse osmosis (RO) treatment. Risk quotient analysis indicated that, apart from PFOA and PFOS, most PFAS posed low to very low health risks under existing guidelines. Additionally, a global synthesis further revealed rising levels of ultrashort-chain PFAA and precursors, suggesting a shifting PFAS exposure profile. These findings underscore the need for expanded monitoring, toxicity evaluation, and regulatory frameworks that account for overlooked PFAS classes in drinking water supplies.

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1. Introduction

Per- and polyfluoroalkyl substances (PFAS) are a diverse group of synthetic chemicals widely used in industrial applications and consumer products for their unique physicochemical properties and desired performance [1,2]. However, their strong carbon-fluorine bonds render them highly resistant to environmental degradation [3,4], leading to persistent and widespread occurrence. Consequently, PFAS have been detected in various environmental matrices [5,6], food [7], consumer products [8], drinking water [9], and even human blood [10], raising increasing concern over associated health risks, including cancer, immune system suppression, and endocrine disruption [11].

Among various exposure pathways, drinking water is a major contributor to human PFAS exposure. Despite the phase-out of legacy long-chain perfluoroalkyl acids (PFAAs), including perfluorooctanoic acid (PFOA) and perfluorooctanesulfonic acid (PFOS) over the past two decades [12], they remain the most frequently detected in global drinking water [9,13,14]. In response, several countries have updated drinking water guidelines: the U.S. Environmental Protection Agency (U.S. EPA) set maximum contaminant levels (MCLs) at 4 ng/L for both PFOA and PFOS in 2024, while China's Drinking Water Quality Standards (GB 5749–2022) established MCLs of 80 ng/L for PFOA and 40 ng/L for PFOS, respectively.

Bottled water, widely perceived as a safer alternative to tap water, is increasingly consumed worldwide [15]. In 2024, the global bottled water market was valued at USD 351.9 billion and is projected to grow to USD 674.8 billion by 2033 [16]. China, the largest consumer of bottled water, accounts for 15 % of global consumption [17]. In 2021, the market value of China's bottled water industry reached USD 49.174 billion, with an average annual compound growth rate of approximately 10.8 % in recent years. By 2023, national bottled water consumption exceeded 50 billion liters, with Guangdong, Zhejiang, and Jiangsu provinces together accounting for about 45 % of the total volume (data from China Puhua Industry Research Institute). Bottled water typically undergoes additional treatments, as represented by distillation, filtration, and reverse osmosis (RO), to improve taste and remove conventional contaminants [18,19]. However, despite these additional treatments, the safety of bottled water remains uncertain, as the levels of contaminants, especially PFAS, are not yet well characterized. Studies have revealed PFAS contamination in bottled water, with median concentrations of 0.98 ng/L in the USA [20], 0.48 ng/L in Turkey [21], 15.0 ng/L in Brazil, 14.9 ng/L in France and 11.3 ng/L in Spain [22]. Despite growing global concern, research on PFAS contamination in bottled water in China remains limited.

Notably, increasing regulatory restrictions on long-chain PFAAs ($C \geq 8$) have prompted the widespread use and detection of ultrashort-chain (C2-C3), short-chain (C4-C7) [23], and PFAA precursors (e.g., 6:2 fluorotelomer sulfonic acid (6:2 FTS)) [24], many of which exhibit greater environmental mobility and persistence. For example, a recent study found that ultrashort-chain PFAS constituted up to 97 % of ΣPFAS in tap water from Shanghai, China—highlighting the environmental dominance and monitoring importance of these compounds [25]. Nevertheless, most existing studies on bottled water have focused primarily on long-chain PFAAs [22,26,27], while comprehensive profiling of ultrashort-chain, short-chain, and other PFAA precursors remains limited.

To fill this knowledge gap, this study conducted a comprehensive investigation of PFAS contamination in 52 bottled water products sold in China. A broad spectrum of PFAS was analyzed, including ultrashort-chain, short-chain, long-chain, and precursor compounds. The study further examined differences in PFAS concentrations across product types, water sources, treatment processes, as well as correlations with water quality parameters and product price. In addition, potential human health risks associated with PFAS in bottled water products were evaluated. An analysis of published data on PFAS occurrence in bottled water worldwide was also conducted to examine spatial and temporal variations across countries and regions. This large-scale, multi-class PFAS survey provides critical data to support regulatory development, raise public awareness, and inform international efforts to ensure drinking water safety and environmental health protection.

2. Materials and methods

2.1. Chemicals and standards

Standard solutions of 50 PFAS and 19 isotope-labeled internal standards were purchased from Wellington Laboratories (Canada). The target PFAS included perfluorocarboxylic acids (PFCAs), perfluorosulfonic acids (PFSAs), fluorotelomer sulfonic acids (FTSs), perfluoroalkyl sulfonamide derivatives (PFASDs) and other PFAS subclasses (Table S1 in the Supplementary Information (SI)). The solvents methanol, ammonium hydroxide (25 %), and acetonitrile were obtained from Merck (Germany) and Sigma-Aldrich (USA). Ultrapure water was supplied by a Milli-Q system (Millipore, USA).

2.2. Bottled water sample selection and characterization

A total of 52 bottled water products from 40 brands were collected in Guangzhou, China, from five retail food stores and 35 online stores. These products represented those readily accessible to consumers. The selection included the top six national brands, together accounting for 80.5 % of the bottled water market share, and encompassed water sources from 18 provinces across the country (Figure S1), thereby ensuring broad market representation and geographic coverage. All samples were non-flavored and non-nutritive, and were classified into four types: purified water (PW, n = 12), natural mineral water (NMW, n = 25), spring water (SW, n = 11), and natural soda water (NSW, n = 4). Only four NSW samples were included, as this category represents a minor share of the bottled water market and was not a major focus of this study. Definitions of these four water types are detailed in Text S1. Information on water classification and sources was obtained from product labels and packaging (Table S2).

Conductivity and pH were measured within 24 h of the opening of the bottled water using calibrated meters (Hach HQ2200). Total organic carbon (TOC) and total inorganic carbon (TIC) were analyzed using a TOC analyzer (Shimadzu, TOC-VCPH). Total carbon (TC) was calculated as the sum of TOC and TIC. Detailed physicochemical characteristics of the bottled water samples are provided in Table S3.

2.3. PFAS extraction and analysis

All bottled water products were extracted on the day of receipt. Before analysis, unopened bottles were stored at room temperature (~25 ℃) in the dark. After homogenization, 500 mL of each sample was transferred to a pre-cleaned polypropylene bottle for solid-phase extraction (SPE). Prior to extraction, the SPE lines were rinsed three times with methanol. Each sample was then spiked with 10 ng of internal standard mixture (listed in Table S1), followed by extraction using a weak anion exchange column (Oasis WAX, 6 mL, 150 mg, 30 μm; Waters). The analytes were eluted with 4 mL methanol and 4 mL 1 % ammonium hydroxide in methanol, and the eluates were subsequently evaporated to near dryness under a gentle nitrogen stream at 40 °C. The residues were reconstituted to a final volume of 1 mL with methanol for instrumental analysis [28].

PFAS concentrations were quantified using ultra-performance liquid chromatography (UPLC; Agilent Technologies) coupled with a triple quadrupole mass spectrometer (API 5500; AB SCIEX) operating in negative electrospray ionization mode. Separation of long-chain and short-chain PFAS was conducted using a ZORBAX SB-C18 column (3.5 μm, 2.1 mm × 100 mm; Agilent), while ultrashort-chain PFAS (C2-C3) were separated using an ion-exchange column (RSpak JJ-50 2D; Shodex). Quantification was performed using isotope dilution with ^{13}C-

labeled internal standards spiked into each sample prior to extraction. Internal standards were selected to match representative chain lengths and chemical structures of target PFAS. Calibration curves were constructed using inverse concentration-weighted linear regression with coefficients of determination (R^2) > 0.99.

Instrumental limits of quantification (LOQs) were defined as the lowest calibration concentrations corresponding to a signal-to-noise (S/N) ratio of 10 [29]. Method LOQs were calculated by dividing the instrumental LOQ by the SPE concentration factor (e.g., 500 mL concentrated to 1 mL) (EURACHEM, 2014). Except for low levels of PFOA, all procedural blanks were below the corresponding LOQs; therefore, blank correction was applied only for PFOA. Detailed extraction methods, analytical procedures, and MS/MS parameters are provided in Text S2 and Tables S4-S6.

2.4. Quality assurance and quality control (QA/QC)

All solvents used, including methanol and ammonia, were LC–MS grade. Polypropylene bottles, SPE cartridges, and other labware were pre-screened to ensure negligible PFAS background contamination. Sample containers were covered with aluminum foil during storage and handling to prevent photodegradation or volatilization of target compounds.

Procedural blanks (Milli-Q water processed through the same extraction and analysis steps) were included in each batch to evaluate background levels and potential cross-contamination. No target PFAS (except for PFOA) were detected above the LOQ in any blank samples. Spiked recovery tests were conducted by fortifying selected samples at known concentrations. Method recoveries ranged from 78 % to 118 %, with relative standard deviations (RSDs) below 20 %, indicating acceptable analytical accuracy and precision. Instrumental calibration was verified using multi-point calibration curves, and all measurements met internal QA criteria. Information on QA/QC, procedure blank, and spike recoveries can be found in Text S3 and Table S7.

2.5. Risk assessment

To assess the potential health risks associated with PFAS exposure through bottled water, we compared the concentration of target PFAS in the samples with the health guidelines for PFAS in drinking water issued by different authorities or scholars [30]. We then calculated the risk quotient (RQ) as shown below:

$$RQ = \frac{C_{PFAS}}{HBV_s}$$

Where C_{PFAS} is the concentration of PFAS, ng/L; HBV_S is the health guidance value of PFAS in drinking water proposed by different institutions (e.g., U.S. EPA) or scholars, ng/L. In selecting HBV_S, we prioritized the most recent values issued by the U.S. EPA when available; for PFAS without EPA guidelines, the lowest available limits from other international or national authoritative agencies were adopted to ensure a conservative assessment. Due to the lack of established health guidelines for certain PFAS, RQs were only calculated for compounds with available reference values.

In addition, we calculated the estimated daily intake (EDI) of PFAS across different population groups, including kids (6–11 years), teenagers (12–19 years), adults (20–60 years), and seniors (> 60 years). The detailed methodology is provided in Text S4 of the SI.

2.6. Statistical analysis

Statistical analyses were conducted using SPSS Statistics software (version 18.0; IBM, New York, USA). Non-parametric comparisons between groups were performed using the Mann–Whitney *U* test, and correlations among variables were assessed using Spearman's rank correlation. Pearson's correlation coefficient was applied to evaluate the relationships between PFAS concentrations and water quality parameters. A p-values less than 0.05 was considered statistically significant. For descriptive statistics (e.g., average, median and total PFAS concentrations), only values above the LOQ were included to avoid bias from non-detects. The average/mean concentration was calculated as the arithmetic mean of all quantified values, whereas the median concentration represented the middle value of the ordered dataset. For correlation analyses, values below the LOQ were replaced with one-half of the LOQ, a commonly applied approach in environmental studies for handling non-detects.

3. Results and discussion

3.1. The presence and levels of PFAS in bottled water

Among 50 targeted PFAS analytes, 21 compounds were detected (≥ LOQ) across 52 bottled water products (Table 1 and Fig. 1). The total concentrations of these 21 PFAS (Σ_{21}PFAS) ranged from 2.69 to 97.0 ng/L (Table S8). The detected PFAS included PFCAs (C2-C10), PFSAs (C3-C5 and C7-C8), FTSs (6:2 FTS and 8:2 FTS), and PFASDs (e.g., perfluorooctane sulfonamide (FOSA), perfluoro-1-butanesulfonamide (FBSA), N-methylperfluoro-1-octanesulfonamidoacetic acid (N-MeFOSAA), N-ethylperfluoro-1-octanesulfonamidoacetic acid (N-EtFOSAA)). On average, the detection frequencies followed the order: PFCAs > FTSs > PFSAs > PFASDs. Grouped by chain length, ultrashort-chain PFAS (C2-C3) showed the highest detection rates, followed by short-chain (C4-C7) and long-chain (C ≥ 8) PFAS.

3.1.1. Long-chain PFAAs

Legacy PFAS, PFOA and PFOS, remained dominant in most bottled water samples with detection frequencies of 100 % and 71 %, and median concentrations of 2.14 and 1.14 ng/L, respectively. These findings are consistent with a previous nationwide survey involving 526 drinking water samples from 66 cities across China, which also identified PFOA and PFOS as the most prevalent PFAS, except in remote areas, including Urumqi, Lhasa, and parts of northeastern China [31]. The relatively high concentrations of these two PFAAs are likely attributed to historical extensive use in fluoropolymer manufacturing, textiles, and surface treatment [32]. Their inefficient removal by current treatment technologies further promotes their persistence in aquatic environments [33]. Notably, both the detection frequency and concentration of PFOA were higher than those of PFOS, likely reflecting the earlier and more stringent regulatory restrictions on PFOS, especially following its listing under the Stockholm Convention in 2009 [34]. Previous studies have also indicated that PFOA occurrence in Chinese drinking water is significantly associated with polytetrafluoroethylene (PTFE) production, with extremely high concentrations observed in provinces with PTFE manufacturing facilities (e.g., Sichuan and Zhejiang) [31,35]. Other long-chain PFCAs and PFSAs—perfluorononanoic acid (PFNA), perfluorodecanoic acid (PFDA), perfluorododecanoic acid (PFDoDA), and perfluorononane sulfonic acid (PFNS)—were detected at relatively lower concentrations. This pattern may be explained by ongoing global phase-out efforts and increasingly strict regulations on their production and use [36]. In addition, the physicochemical properties of long-chain PFAAs, especially their high hydrophobicity and strong affinity for organic matter, promote sorption onto soils, sediments, and suspended particles, thereby reducing their abundance in aqueous phase [37].

3.1.2. Short-chain PFAAs

With the phase-out of long-chain PFAAs, short-chain analogues were introduced as alternatives due to their smaller molecular size and lower bioaccumulation potential [38]. However, this substitution has led to elevated environmental concentrations of short-chain PFAAs [39]. In this study, perfluorohexanoic acid (PFHxA) and perfluorobutane sulfonic acid (PFBS) were frequently detected, with detection rates of 83 %

Table 1
Overview of PFAS detections in bottled water samples (n = 52). Twenty-one PFAS were detected and 29 other PFAS were below LOQ. A complete list of PFAS analytes can be found in Tables S1 and S8.

Analyte		Detection frequencies (%)	Detected concentrations (ng/L)[a]			Relative mass abundance[b]
			Median	Minimum	Maximum	
PFCAs	TFA	87	7.40	0.010	46.2	35.9
	PFPrA	83	3.98	0.210	64.0	19.2
	PFBA	15	0.468	0.079	2.81	0.449
	PFPeA	46	0.534	0.006	3.46	1.22
	PFHxA	83	0.200	0.003	2.20	0.862
	PFHpA	54	0.170	0.016	1.42	0.506
	PFOA	100	2.14	0.265	62.8	15.0
	PFNA	52	0.038	0.005	0.725	0.174
	PFDA	40	0.131	0.019	1.39	0.296
	PFDoDA	8	0.351	0.165	0.430	0.084
PFSAs	PFPrS	23	0.282	0.018	1.57	0.349
	PFBS	96	1.22	0.018	36.9	14.1
	PFHxS	23	0.121	0.007	0.991	0.296
	PFOS	71	1.14	0.120	2.85	2.74
	PFNS	12	0.155	0.055	0.290	0.063
FTSs	6:2 FTS	65	0.614	0.044	54.6	5.56
	8:2 FTS	52	0.121	0.033	1.75	0.562
PFASDs	FBSA	29	0.018	0.014	13.6	0.895
	FOSA	44	0.227	0.006	11.1	1.61
	N-MeFOSAA	10	0.122	0.028	0.726	0.096
	N-EtFOSAA	13	0.095	0.025	0.724	0.119

[a] Concentrations calculated based only on positive detections above LOQ.

[b] Fraction of total PFAS mass detected in across all samples $= \sum_{n=1}^{52} \frac{[\text{Analyte} \geq \text{LOQ}]}{\Sigma\text{PFAS}}$

and 96 % and median concentrations of 0.200 and 1.22 ng/L, respectively. These compounds have also been reported as the most prevalent short-chain PFAAs in tap water across several European countries. For example, both PFHxA and PFBS were detected in over 80 % of samples in a national survey of Czech drinking water [40], and similarly widespread occurrence was observed in both raw and treated water in the Netherlands [9]. The frequent detection of PFHxA and PFBS is largely attributed to their extensive production and application, especially the use of PFBS as a substitute for PFOS due to its lower toxicity and favorable regulatory profile [41]. In addition, several studies have demonstrated that precursor compounds can degrade into short-chain PFAAs in the environment, further contributing to their environmental prevalence [42–44]. Short-chain PFAAs also exhibit low organic carbon–water partition coefficients (K_{oc}), resulting in weak sorption onto soils and sediments and high mobility in aquatic environments [45,46]. These physicochemical traits make them more difficult to be removed through conventional drinking water treatment processes (e.g., activated carbon adsorption), compared to long-chain PFAAs [9]. Moreover, their high mobility facilitates long-range transport via seawater, enabling them to reach remote regions [39]. Consequently, these compounds are now commonly found across various water matrices, including drinking water [27,47], surface water [48], and groundwater worldwide [49], raising growing concerns about long-range transport and chronic exposure risks.

3.1.3. Ultrashort-chain PFAAs

Ultrashort-chain PFAAs, trifluoroacetic acid (TFA) and perfluoropropanoic acid (PFPrA), exhibited high detection frequencies of 87 % and 83 %, respectively. The median concentrations of TFA and PFPrA were 7.40 and 3.98 ng/L, with maximum values reaching 46.2 and 64.0 ng/L, respectively—substantially higher than those of most other PFAS detected in this study. Similar detections of these compounds have been reported in drinking water from the Netherlands and Germany [9,50], however, the concentrations observed in our samples were notably higher. In China, a previous study reported an average TFA concentration of 6.61 ng/L in six bottled water products [29], which is significantly lower than the 12.4 ng/L observed (45/52) in this study. These findings suggest that ultrashort-chain PFAA are increasingly prevalent in aquatic environments. TFA and PFPrA originate not only from direct industrial uses and synthesis byproducts but also from secondary pathways, including atmospheric oxidation of precursors, refrigerant degradation, fluoropolymer breakdown, and biotransformation of pesticides or pharmaceuticals [39]. The diversity of these sources, combined with their high water solubility, minimal adsorption onto conventional sorbents, and strong resistance to degradation, contributes to their widespread presence and persistence [51]. This is further supported by a recent study, which found no significant differences in the concentrations of ultrashort-chain PFAS between raw and treated drinking water, nor between surface water and groundwater [9].

Taken together, these results underscore the emerging environmental and human health concerns associated with ultrashort-chain PFAS (e.g., TFA and PFPrA), and highlight the urgent need for more comprehensive monitoring, source identification, and toxicological risk assessment in future research.

3.1.4. PFAA precursors

Several PFAA precursors were detected, including 6:2 FTS (detection frequency of 65 %), 8:2 FTS (52 %), FOSA (44 %), FBSA (29 %), N-MeFOSAA (10 %), and N-EtFOSAA (13 %), with corresponding median concentrations of 0.614, 0.121, 0.227, 0.018, 0.122, and 0.095 ng/L, respectively. Many of these compounds, including 6:2 FTS, FOSA, and N-EtFOSAA, are known to undergo environmental or biological transformation into persistent PFAAs, including PFOA and PFOS [24,52,53]. However, the occurrence of these precursors in bottled or drinking water has been rarely reported in previous studies or has typically observed at relatively low rates and levels (often < LOQ) [9,13,20]. Notably, Chen et al. reported elevated levels of 6:2 FTS, FOSA and N-EtFOSAA in surface waters near wastewater treatment plants in China, with significant correlations among these compounds suggesting common emission sources and potentially shared degradation pathways [48]. These findings suggest the ongoing environmental input and transformation of PFAA precursors, which may contribute to the formation of terminal PFOS and PFOA.

Overall, this study underscores the growing complexity of PFAS contamination, highlighting the importance of monitoring not only terminal PFAA but also their precursors to better understand their

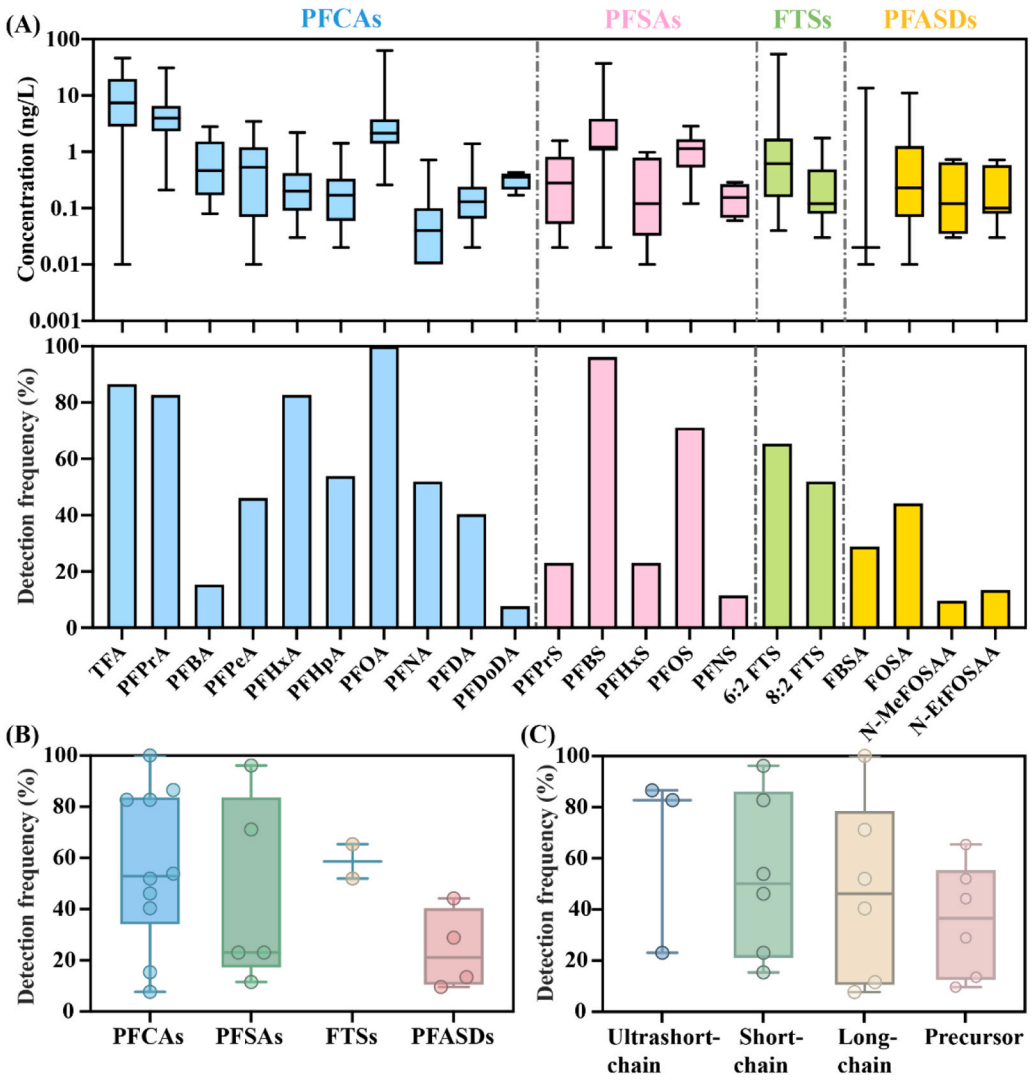

Fig. 1. (A) Concentration and detection frequency of 21 detected PFAS (29 other PFAS were not detected) in bottled water products (n = 52). (B) Detection frequency of different PFAS classes: PFCAs (n = 10), PFSAs (n = 5), FTSs (n = 2), PFASDs (n = 4). (C) Detection frequency of different PFAS classes: ultrashort-chain (n = 3), short-chain (n = 6), long-chain (n = 6) PFAA and precursors (n = 6).

environmental fate, persistence, and associated human health risks.

3.2. Correlation analysis among individual PFAS

To explore potential relationships among PFAS compounds in bottled water, Spearman correlation analysis was performed based on the concentrations of 21 detected PFAS (Fig. 2). Significant positive correlations were observed among both short-chain and long-chain PFCAs, suggesting common sources or similar environmental behaviors [54,55]. For example, perfluorobutanoic acid (PFBA) showed strong correlations with PFHpA, PFNA, and PFDA ($\rho > 0.45$, $p < 0.001$), while PFHxA was highly correlated with PFNA ($\rho = 0.50$, $p < 0.001$), and PFNA with PFDA ($\rho = 0.62$, $p < 0.001$). In contrast, correlations among PFSAs were generally weaker. No significant associations were found between short-chain and long-chain PFSAs, except for a notable correlation between PFBS and perfluoropropanesulfonic acid (PFPrS) ($\rho = 0.49$, $p < 0.001$), suggesting more diverse sources or transformation pathways for sulfonated compounds. Interestingly, cross-class correlations between PFCAs and PFSAs were also evident, including PFBA with PFHxS ($\rho = 0.63$, $p < 0.001$), PFHxA with PFPrS ($\rho = 0.70$, $p < 0.001$), and PFDoDA with PFNS ($\rho = 0.72$, $p < 0.001$), indicating potential co-occurrence or shared release mechanisms.

Several PFAA precursor, including 6:2 FTS, 8:2 FTS, N-MeFOSAA, and N-EtFOSAA, also exhibited positive correlations with both PFCAs and PFSAs. In particular, 6:2 FTS was strongly correlated with PFHxA, PFNA, and PFNS ($\rho > 0.45$, $p < 0.001$), while 8:2 FTS showed strong correlations with PFPeA, PFHpA, and PFDA ($\rho > 0.45$, $p < 0.001$), and moderate correlations with PFBA, PFNA, and PFOS ($\rho > 0.34$, $p < 0.05$). Such correlations are consistent with previous studies showing that PFAA precursors can be transformed into terminal PFAAs via diverse abiotic and biotic processes. For example, Maldonado et al. reported that sulfonamide- and fluorotelomer-based precursors were electrochemically transformed into PFCAs during leachate treatment [43]. Yang et al. demonstrated that 6:2 FTS was biodegraded into PFPeA, PFHxA, and PFHpA in soil, while Dasu et al. showed that aerobic biodegradation of 8:2 FTS produced PFHxA, PFHpA, and PFOA [42]. Therefore, the observed positive correlations between 6:2 FTS/8:2 FTS and several PFAAs may indicate potential transformation pathways or common sources [24,52,53]. In addition, a significant correlation was observed between N-MeFOSAA and N-EtFOSAA ($\rho = 0.96$, $p < 0.001$), reflecting their structural similarity and likely co-occurrence. Both compounds were also highly correlated with PFDoDA ($\rho > 0.82$, $p < 0.001$) and moderately with PFNS ($\rho > 0.44$, $p < 0.01$), further supporting their potential role as transformation intermediates contributing to the

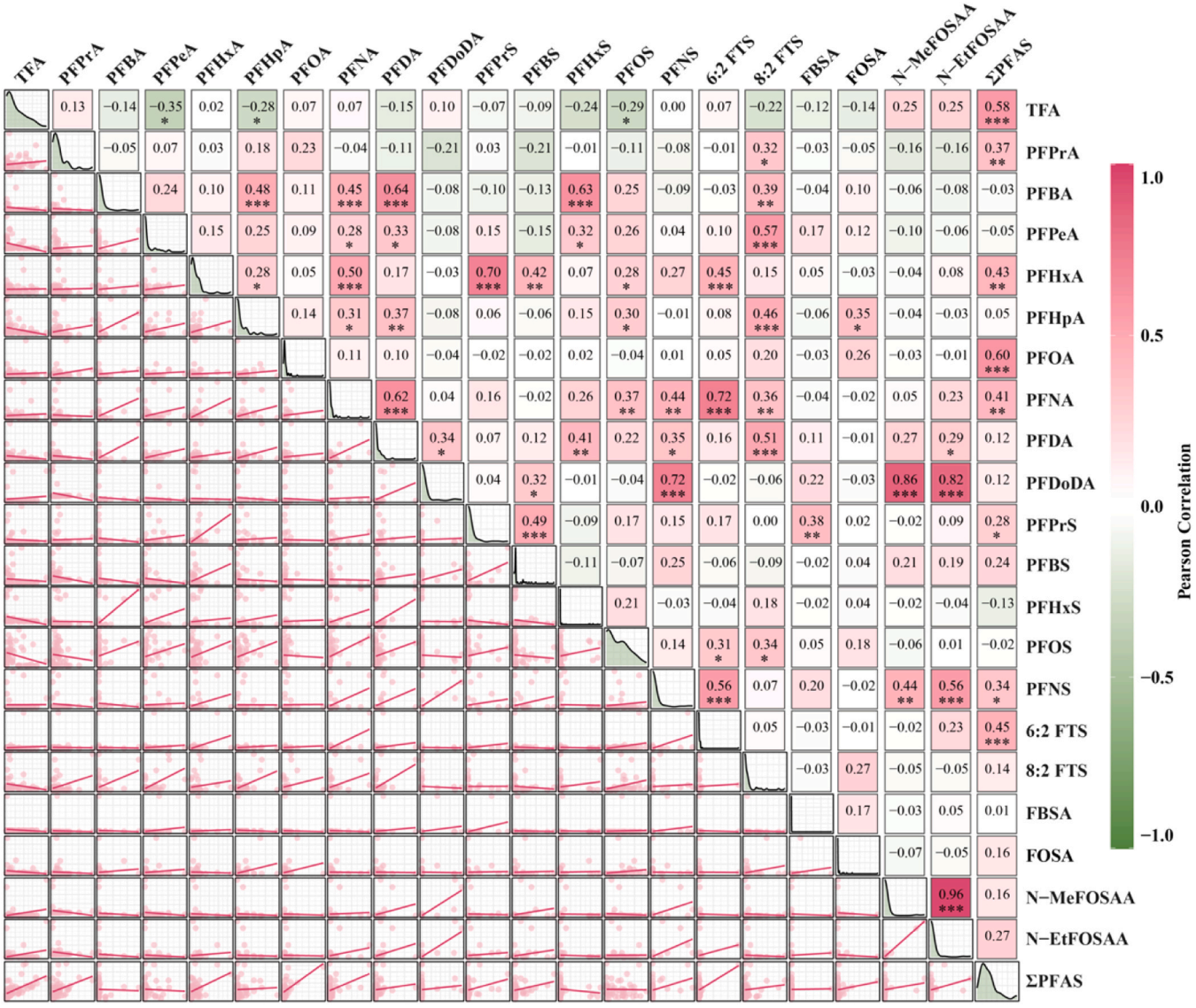

Fig. 2. Spearman correlation matrix of individual PFAS concentrations detected in bottled water samples (n = 52). Each cell represents the pairwise Spearman correlation coefficient (ρ) between two PFAS compounds. Color intensity indicates the strength and direction of the correlation (red: positive; green: negative). Statistically significant correlations are denoted by asterisks (* $p < 0.05$; ** $p < 0.01$; *** $p < 0.001$).

presence of terminal PFAS. These correlation patterns collectively highlight the interconnectedness between precursor and terminal PFAS, emphasizing the necessity of including precursor compounds in environmental monitoring and risk assessment frameworks.

3.3. Comparison of product type, source and treatment

Comparative analyses were conducted to reveal differences in PFAS levels among bottled water samples based on product type, water source, and the use of RO treatment (Fig. 3). It should be noted that the sample size for natural soda water (n = 4) was limited by product availability, which may constrain statistical power; further studies with larger datasets are warranted to validate the conclusions. PFAS concentrations ranged from 10.8 to 51.6 ng/L in PW, 2.69–97.0 ng/L in NMW, 4.84–94.0 ng/L in SW, and 9.12–41.3 ng/L in NSW (Fig. 3 A). Among these, SW exhibited the highest average Σ_{21}PFAS concentration (37.5 ng/L), followed by NMW (26.8 ng/L), PW (26.6 ng/L), and NSW (23.4 ng/L). The higher levels in SW may be due to its susceptibility to environmental contamination from shallow source waters [14,56] and the limited treatment typically applied to maintain its "natural" characteristics. NMW, although also minimally treated, is generally sourced from deeper aquifers less exposed to surface pollution. In contrast, PFAS levels in PW were slightly lower, potentially due to additional purification processes, including RO or advanced filtration. Notably, the PFAS concentrations obtained in this study were higher than those reported in previous studies, as evidenced by bottled water samples from the U.S. showing Σ_{32}PFAS levels ranging from 0.170 to 18.9 ng/L [20], and samples from Japan and New Zealand exhibiting Σ_{10}PFAS levels of 14.1 ng/L and 16.1 ng/L, respectively [27]. These discrepancies underscore regional variations in source water quality and environmental PFAS prevalence, as well as the broader analytical scope of this study, which included ultrashort-chain PFAS (e.g., TFA).

To gain more detailed insights, the distribution patterns of individual PFAS were further examined across different product types (Fig. 3B). TFA was the predominant PFAS in all categories, with notably high mean concentrations observed in SW (16.8 ng/L) and NSW (16.6 ng/L). These findings are consistent with the widespread occurrence of TFA in surface-impacted waters [57,58]. In contrast, PW and NMW showed comparatively lower TFA levels (11.8 and 10.2 ng/L), likely due to deeper water sources or partial treatment. These patterns were further

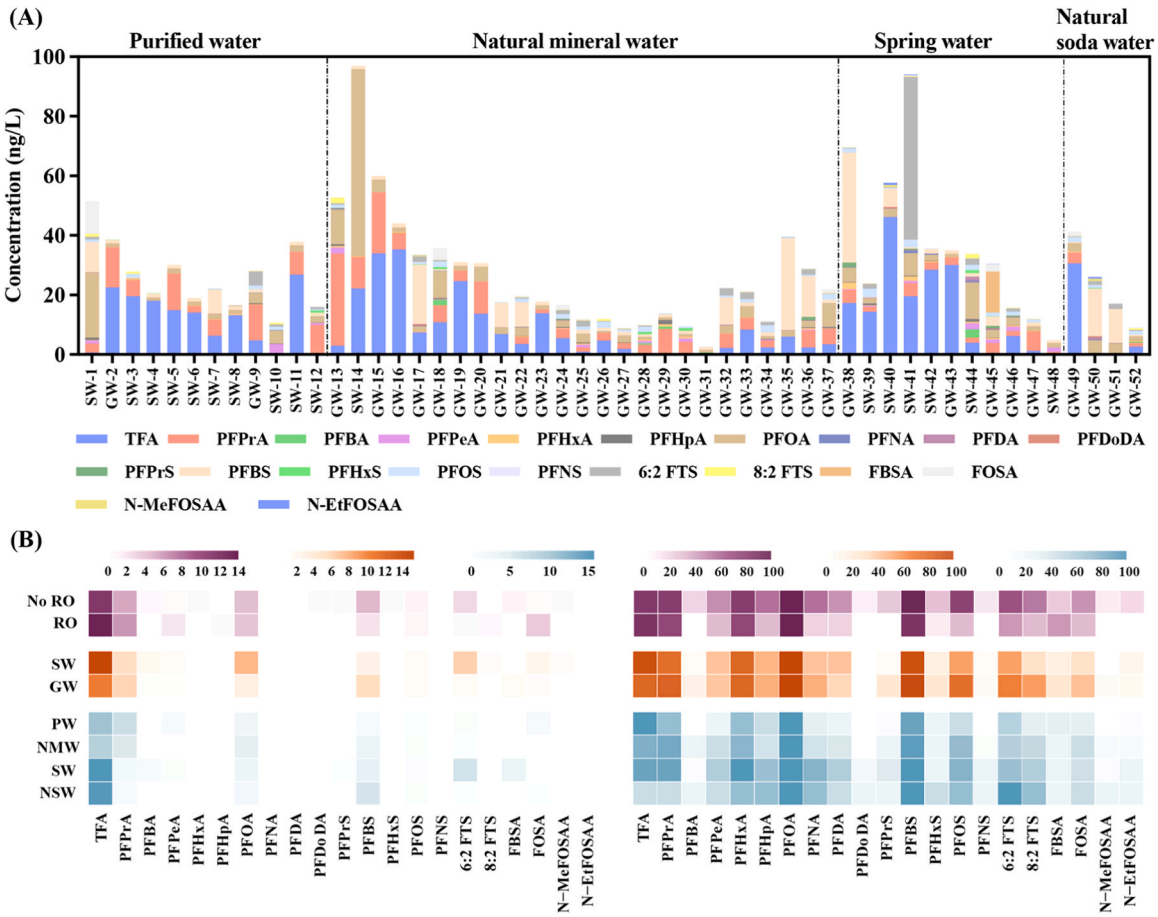

Fig. 3. (A) The distribution of PFAS was examined across 52 bottled water products, classified into four different categories: PW (n = 12), NMW (n = 25), SW (n = 11), and NSW (n = 4). (B) Comparative analysis of PFAS occurrence by reverse osmosis treatment, source (SW and GW mean surface water and groundwater), and product type. The data represent the mean concentrations (ng/L, left) and detected frequencies (%, right) of each PFAS in the different categories.

supported by our source-based comparison (Fig. 3B). PFOA and PFBS were also consistently detected across all product types, with average detection frequencies of 100 % and over 92 %, respectively, and showed no significant concentration differences among PW, NMW, SW, and NSW. Their widespread occurrence is consistent with previous reports in various aquatic environments [31,48,59]. Notably, PFOA levels were generally higher in surface water-sourced products, whereas PFBS was more prominent in groundwater-based products, likely due to its greater mobility and weaker adsorption to environmental media [60]. In addition, 6:2 FTS was significantly elevated in SW and surface water–sourced products, consistent with previous studies reporting higher concentrations of 6:2 FTS in surface waters than in groundwater [61].

These findings underscore the widespread presence of PFAS in both surface water and groundwater sources across China and highlight the limitations of current bottled water treatment processes in effectively removing PFAS. Previous studies have reported ΣPFAS concentrations as high as 2500 ng/L in surface water in Tianjin and up to 26,700 ng/L in groundwater in eastern China [48,59]. In addition, drinking water in many cities and regions across China, especially in East, South and Southwest China, has been found to be contaminated with PFAS, with average concentrations ranging from 59.9 to 503 ng/L [31]. These patterns are consistent with the geographical distribution of PFAS contamination observed in our bottled water samples (Figure S1). As one of the world's largest producers and consumers of fluorinated chemicals, China accounts for over 55 % of global production of basic and general-purpose fluorine compounds, which significantly contributes to environmental PFAS pollution.

Water treatment process is another contributing factor to the variation in PFAS levels among bottled water products. However, among the available product information, RO was the only treatment process explicitly indicated. Based on this, the products were categorized as either RO-treated (n = 9) or non-RO-treated (n = 43). Most PFAS exhibited lower detection frequencies in RO-treated products, except for TFA, PFPrA, PFHxA, PFOA, PFBS, and FBSA (Fig. 3B). The mean concentrations of PFOA, PFBS and FBSA were also lower in RO-treated products compared to those without RO. Additionally, several PFAS, including PFBA, PFPrS, PFHxS, 6:2 FTS, N-MeFOSAA, and N-EtFOSAA, were significantly reduced in RO-treated products, indicating that RO is generally effective in removing a wide range of PFAS. However, TFA and PFPrA concentrations remained largely unaffected by RO treatment, which is consistent with previous studies [9,62,63]. This is likely due to their low molecular weights and high solubility, the limited size exclusion and selectivity of RO membranes, and the influence of water conductivity [64].

Finally, no significant correlations were found between PFAS concentrations and water quality parameters (e.g., conductivity, pH, TC, TIC, TOC) or product price (Figure S2). This indicates that higher-priced bottled water does not necessarily offer greater safety in terms of PFAS contamination.

3.4. Risk assessment, regulations, and health guidance

This study assessed the potential health risks of PFAS in 52 bottled water samples using RQ values (Fig. 4), calculated as the ratio of PFAS concentrations to health-based guidance values from authoritative agencies (e.g., U.S. EPA) (Table S9). Based on these values, PFAS were

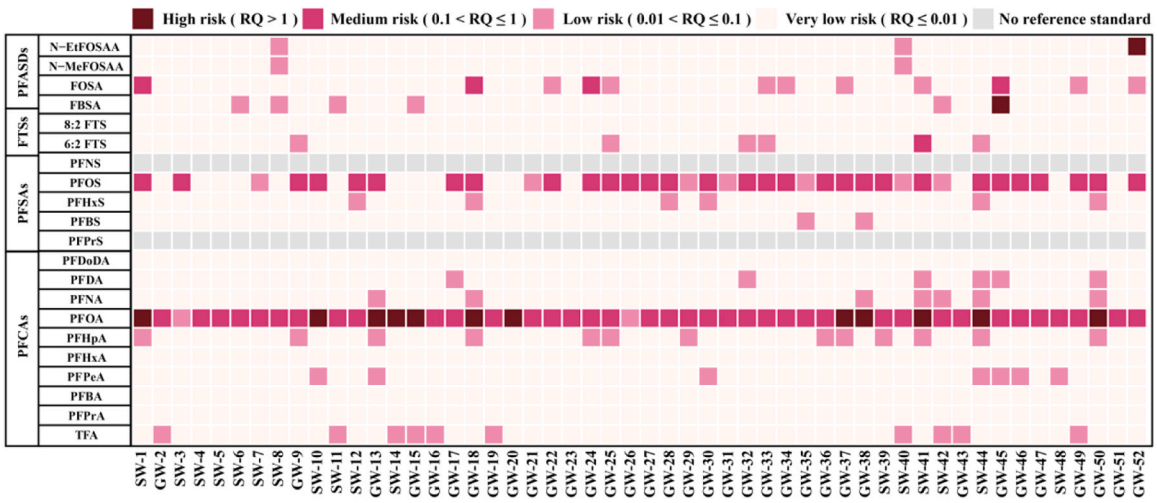

Fig. 4. Potential health risk distribution of each detected PFAS across 52 bottled water products. RQ values were calculated based on current health guidelines listed in Table S9.

categorized into four risk levels: high (RQ > 1), medium (0.1 < RQ ≤ 1), low (0.01 < RQ ≤ 0.1), and very low (RQ ≤ 0.01) [65]. Among all analytes, legacy PFOA and PFOS exhibited relatively higher risks. Notably, 23 % of the samples exceeded the high-risk threshold for PFOA, and 73 % fell into the medium-risk range, while PFOS was classified as medium-risk in 58 % of samples. This aligns with recent global regulatory updates, underscoring the increasing recognition and prioritization of the health risks posed by these compounds.

Other PFAS, including FBSA and N-EtFOSAA, reached high-risk levels in specific samples (e.g., GW-45 and GW-52), while FOSA was classified as medium risk in four samples, indicating moderate health concerns. In contrast, PFAS like PFPrA, PFBA, PFHxA, and 8:2 FTS exhibited RQ values below 0.01 in all samples, suggesting minimal direct health risks. Overall, except for PFOA and PFOS, most detected PFAS posed low to very low risks, likely attributable to the relatively high health-based guidance values, which in turn stem from limited toxicological data for these compounds [66–68].

A notable example is ultrashort-chain TFA, the predominant PFAS in the bottled water samples, with median and maximum concentration of 7.4 and 46.2 ng/L, respectively. The associated risks were very low in most samples, based on RQ values calculated using a health-based guidance value of 2200 ng/L. Although current drinking water regulations in most countries lack specific limits for TFA, it is classified under the EU's Classification, Labelling and Packaging (CLP) Regulation as harmful to aquatic life with long-lasting effects (Aquatic Chronic 3) [69]. Additionally, the proposed revision of the EU's Drinking Water Directive incorporates TFA within its "total PFAS" limit of 500 ng/L [70]. This highlights that the long-term health and environmental effects of TFA and other PFAA precursors warrant further research, along with the establishment of comprehensive policies and health guidelines.

Furthermore, we calculated the EDI to assess PFAS exposure through bottled water across different population groups (Table S10). Consistent with previous studies [71,72], children exhibited the highest EDIs on a body-weight basis, followed by teenagers, adults, and seniors. Among the detected compounds, TFA showed the highest contribution, with EDI values ranging from 0.161 to 0.289 ng/kg bw/day across different population groups. PFPrA, PFOA, and PFBS also represented major contributors, with comparable EDIs of 0.071–0.127, 0.067–0.121, and 0.063–0.113 ng/kg bw/day, respectively. These findings highlight that, although legacy PFOA remain of concern, ultrashort-chain and short compounds now represent major contributors to human exposure and therefore warrant greater regulatory attention.

3.5. Occurrence of PFAS in bottled water globally

The global distribution of PFAS in bottled water—categorized into ultrashort-chain, short-chain, long-chain PFAA and precursors—was systematically summarized to reveal spatial and temporal variations across countries and regions (Fig. 5). Data were compiled from peer-reviewed studies published between 2008 and 2025 (provided in Table S11), encompassing 25 countries with diverse geographic and economic backgrounds. The background map is color-coded based on GDP per capita in 2022, providing a comparative perspective on the relationship between national income levels and PFAS contamination in bottled water.

Over the past two decades, most studies investigating PFAS in bottled water have primarily focused on short-chain and long-chain PFAAs. The earliest such investigation was conducted by Ericson et al. in Spain, targeting PFCAs (C6–C14), PFSAs (C4, C6, C8, C10), and two precursors—1 H,1 H,2 H,2H-perfluorooctanesulfonic acid (THPFOS) and FOSA [26]. The total concentrations of short-chain, long-chain PFAAs, and precursors were reported as 1.42, 4.64, and 1.19 ng/L, respectively. Around the same period, similar studies were conducted in Thailand and Australia, reporting short-chain and long-chain PFAAs concentrations of 0.87 and 10.72 ng/L, and 3.66 and 1.95 ng/L, respectively [73,74]. In Germany, Gellrich et al. analyzed 14 PFAAs (C4-C14) and four precursors in 119 bottled water products, reporting concentrations of 5.70 ng/L (short-chain) and 6.10 ng/L (long-chain), with no precursors detected above the LOQ [47].

In the past decade, the concentrations of short-chain and long-chain PFAAs in bottled water have increased significantly in several countries. For example, in Spain, the levels of short-chain and long-chain PFAAs reached 18.3 and 19.5 ng/L in 2016, approximately 13-fold and 4-fold higher than those reported in 2008 [22]. The same study also documented PFAS levels in bottled water from Brazil and France, with respective concentrations of 10.2 and 53.1 ng/L in Brazil, and 20.9 and 123 ng/L in France [22]. This upward trend may be attributed to the widespread production and use of PFAS, coupled with rising background levels in source waters. In contrast, much lower concentrations were observed in Korea in 2014 (0.12 and 0.36 ng/L) [75], Canada in 2018 (0.76 and 0.14 ng/L) [76], and Turkey in 2019 (0.84 and 0.25 ng/L) [21], suggesting notable regional differences in PFAS usage, source water quality, and regulatory frameworks. Notably, PFAA precursors were largely undetected in most countries during this period, which may reflect low environmental occurrence or limited analytical coverage in earlier studies.

More recently, the detection of ultrashort-chain PFAAs and certain

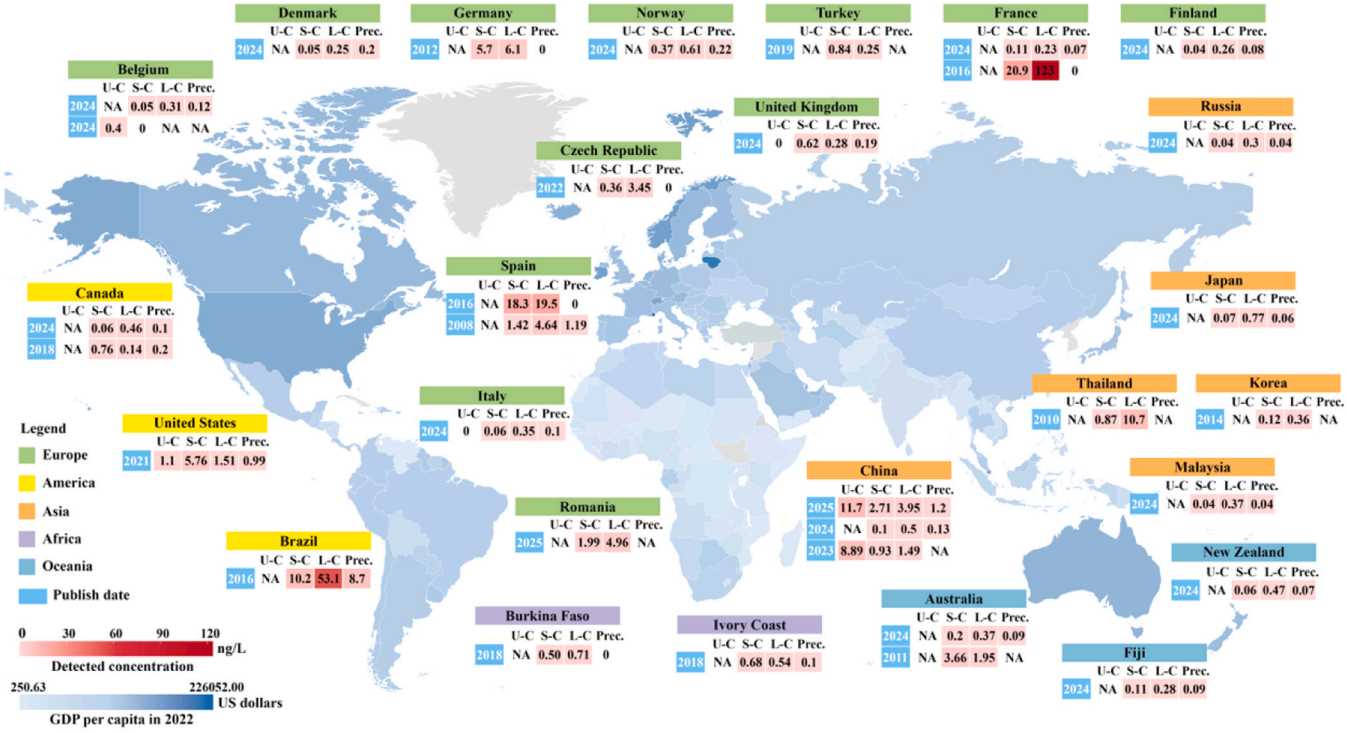

Fig. 5. GDP and the detected concentrations of ultrashort-chain (U-C), short-chain (S-C), long-chain (L-C) PFAAs, and precursor (Prec.) PFAS in global bottled water products over the past decades. The concentrations are presented as either mean or median values, depending on what was reported in the original studies. GDP data originated from the World Bank database; base map created with MapChart (http://www.mapchart.net/). NA: not available; 0: below the LOQ.

precursors has increased, partly due to regulatory restrictions on long-chain PFAAs. In 2021, PFPrA and PFPrS were first reported in bottled water from the United States, with concentrations of ultrashort-chain, short-chain, long-chain PFAAs, and precursors reported at 1.10, 5.76, 1.51, and 0.99 ng/L, respectively [20]. Subsequently, Dong et al. documented the presence of TFA in six bottled water products in China, with ultrashort-chain PFAAs concentrations reaching up to 8.89 ng/L [29]. Our study further demonstrated that ultrashort-chain PFAAs (e.g., TFA and PFPrA) predominated in most bottled water products in China, with concentrations reaching 11.7 ng/L—noticeably higher than previously reported values. The concentrations of short-chain, long-chain PFAAs, and precursors were 2.71, 3.95, and 1.20 ng/L, respectively. In addition, Gao et al. analyzed 10 PFAS, including PFCAs (C8 and C10), PFSAs (C4, C6, and C8), and five precursors in bottled water from 15 countries [27]. The results showed that precursor compounds were widely detected across all sampled countries, with concentrations ranging from 0.04 to 0.22 ng/L. These findings reflect a growing shift in PFAS exposure patterns, with increasing relevance of ultrashort-chain and precursor compounds in global bottled water supplies.

4. Conclusion

This study conducted a nationwide survey of bottled water products across China, encompassing a broad spectrum of PFAS classes, including ultrashort-, short-, and long-chain compounds, as well as precursors. A total of 21 PFAS were quantified above the LOQ, with Σ_{21}PFAS concentrations ranging from 2.69 to 97.0 ng/L. Overall, the detection frequencies followed the order: PFCAs > FTSs > PFSAs > PFASDs, with ultrashort-chain PFAAs being the most prevalent, followed by short- and long-chain compounds. Among ultrashort-chain PFAAs, TFA and PFPrA exhibited the highest detection rates (87 % and 83 %, respectively), with median concentrations of 7.40 ng/L and 3.98 ng/L. For short-chain PFAAs, PFHxA and PFBS were frequently detected (83 % and 96 %), while long-chain PFOA and PFOS were predominant (100 % and 71 %, respectively) in most samples. Several precursors, including 6:2 FTS, 8:2 FTS, and FOSA, were also commonly observed.

Correlation analysis of individual PFAS revealed positive associations among short- and long-chain PFCAs and PFSAs, as well as between several precursors and terminal PFAS, suggesting potential transformation pathways or shared sources. Substantial differences in PFAS concentrations were observed across product types, water sources and the use of RO treatment. Spring water showed the highest PFAS levels (average Σ_{21}PFAS: 37.5 ng/L), likely due to its shallow source and minimal treatment. In contrast, natural mineral and purified waters generally exhibited lower PFAS levels, especially in products sourced from deeper aquifers or subjected to more advanced treatment processes. Additionally, both surface water and groundwater across China have been contaminated by different PFAS to varying degrees. Although RO treatment was generally effective in reducing a broad spectrum of PFAS, it proved insufficient for ultrashort-chain compounds, likely due to their low molecular weight, high solubility, and weak retention by membrane filtration. Overall, deeper source waters combined with RO treatment may offer relatively lower PFAS exposure risks and thus be considered a safer option.

Furthermore, RQ analysis showed, aside from PFOA and PFOS, most detected PFAS posed low to very low risks. This may be attributable to relatively high health-based guidance values, which in many cases reflect the lack of toxicological data for most PFAS. The occurrence of ultrashort-chain PFAA and precursors in both Chinese and global bottled water highlights a shifting exposure profile that warrants greater regulatory attention. Given their mobility, persistence, and resistance to conventional treatment, there is an urgent need to strengthen PFAS monitoring frameworks, establish health-based thresholds for overlooked compounds, and promote source-control strategies to reduce PFAS contamination in drinking water supplies. Future research incorporating multi-season and longitudinal investigations will be essential to capture temporal variability and improve understanding of PFAS contamination dynamics in bottled water.

Environmental implication

This study establishes the first nationwide profile of PFAS contamination in bottled water across China, highlighting the high prevalence of ultrashort-chain compounds (TFA and PFPrA). Systematic analysis of concentration differences across product types, water sources, and treatment technologies revealed distinct contamination patterns and the limited removal of ultrashort-chain PFAS by reverse osmosis. A global analysis further identified rising levels of ultrashort-chain PFAA and precursors, indicating a shifting exposure profile. These findings underscore the need for strengthened regulatory oversight, improved treatment technologies, and expanded global monitoring to mitigate human exposure through bottled water consumption.

CRediT authorship contribution statement

Rui Li: Writing – review & editing, Supervision, Project administration, Funding acquisition, Conceptualization. **Zhen Zhong:** Investigation. **Fahui Ji:** Writing – original draft, Visualization, Formal analysis, Data curation. **Haoting Quan:** Writing – original draft, Visualization, Investigation. **Lu Hui:** Writing – review & editing, Supervision, Project administration, Conceptualization.

Declaration of Competing Interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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Disclaimer

The findings and conclusions presented in this study are based solely on scientific analysis and interpretation of the collected bottled water samples. No specific brand names were mentioned, and all samples were anonymized using coded identifiers to ensure objectivity and neutrality. This study does not aim to target, criticize, or promote any company, brand, or product. The research was conducted independently and is intended solely to contribute to the scientific understanding of PFAS contamination in bottled water.

Appendix A. Supporting information

Supplementary data associated with this article can be found in the online version at doi:10.1016/j.jhazmat.2025.140184.

Data availability

Data will be made available on request.

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