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Unravelling the chemistry of PFAS transfer from packaging to food

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ABSTRACT

Background: Per- and polyfluoroalkyl substances (PFAS) pose significant risks to both human health and the environment. One of their common applications is in food packaging, which serves as a direct source of human exposure. The migration of PFAS from food packaging into food is a chemically complex and context-dependent process that has significant implications for public health and environmental safety.

Scope and approach: This review explores PFAS chemistry, migration from food packaging and factors involved in the migration of PFAS from food contact materials (FCM) into food.

Conclusion: The migration of PFAS from food packaging into food is a chemically complex that has significant health implications. Currently, highly sensitive and specific methods like LC-MS/MS have been approved by FDA for food and feed and EPA for water. With PFAS levels varying globally, emerging tools, including ML algorithms and advanced analytical techniques, are increasingly applied for detection, monitoring, and toxicity assessment, underscoring the need for harmonized regulations and coordinated international efforts to safeguard public health.

1. Introduction

Global research highlights PFAS as pervasive anthropogenic environmental contaminants, due to their exceptional chemical stability, which has led to their designation as “forever chemicals” (Manojkumar et al., 2023). The presence of C_nF_{2n+1} (perfluoroalkyl moieties) within their molecular structure imparts high polarity, amphiphilic characteristics, elevated surface activity, and thermal resistance, rendering PFAS uniquely persistent and highly mobile in environmental systems (Bonato et al., 2025). Since their introduction in the mid-twentieth century (1950s), recent findings revealed that the total number of PFAS structures may be far greater than previously estimated, with current projections suggesting approximately seven million distinct compounds in a wide range of industrial and consumer applications (Bonato et al., 2025).

This group comprises of both long chains ($C \geq 8$) identified as “legacy PFAS” (e.g., perfluoro octane sulfonate (PFOS) and perfluoro octanoic acid (PFOA)) and short chain PFAS ($C < 8$) as “emerging PFAS” including

GenX (chemicals ammonium perfluoro-2-propoxypropionate) (Pasecnaja et al., 2022). Tragically, various PFAAs with long chains ($C \geq 8$), such as PFOA and PFOS, are identified as bio-accumulative, persistent, and hazardous (Cheng & Ng, 2019; Pasecnaja et al., 2022). Increasing evidence indicate that even at low concentrations, these chemicals exhibit significant toxicological potential across various environmental compartments. Their widespread distribution has led to contamination of food sources, groundwater, and both aquatic and terrestrial ecosystems—even extending to remote regions such as the Arctic and Antarctic. This pervasive presence raises serious concerns regarding their implications for both human health and ecological integrity (Eze et al., 2024). Moreover, toxicological studies have linked these specific PFAS compounds to adverse effects on liver function, reproductive and developmental health, immune response, and other physiological outcomes (Fenton et al., 2021). Recognizing the complexity of PFAS mixtures and the adverse effects already observed in biota and humans, as well as the potential risks that may arise without timely interventions, the present review aims to critically examine the

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transfer of PFAS compounds from environmental sources into the food chain, with a focus on leaching mechanisms from food matrices to humans. It also highlights recent advances in analytical detection, explores the emerging role of artificial intelligence (AI) in PFAS monitoring for risk assessment analysis, and reviews current regulatory frameworks to support enhanced environmental safety and public health protection.

2. Study design

This review aims to provide a structured analysis of the literature on PFAS and food. A systematic search using the keywords “PFAS migration in the food chain”, “PFAS detection tools”, “Risk assessment analysis of PFAS using AI”, “PFAS health implications”, and “PFAS related regulations” was conducted in Scopus. The analysis indicated that, as of May 2025, <342 relevant publications were indexed in Scopus. The present review primarily incorporates recent publications; however, in certain instances, older references have been cited to substantiate specific facts.

3. Tracing the silent PFAS from industry to dietary intake

PFAS accumulate in living organisms through the food web, resulting in higher contamination among higher trophic species and potentially posing risks to wildlife survival and population stability (Ohoro et al., 2024). The environmental distribution and accumulation of PFAS, however, occur via multiple dispersion routes and exposure pathways, ultimately impacting final receptors, particularly humans. Human exposure to PFAS originates from both direct and diffuse sources. Direct sources are mainly associated with response sites, industrial activities and fire training camps, while diffuse sources include potable water, food and corresponding packaging material. The transport and environmental fate of PFAS are governed by their chemical properties, resulting in migration into groundwater, runoff to surface water, or long-range atmospheric deposition processes that can contaminate agricultural products and increase human exposure. Among the various exposure routes, ingestion of contaminated water and food is recognized as the most prominent pathway (Wee & Aris, 2023). Collectively, these mechanisms contribute to both short and long-term PFAS exposure in aquatic, terrestrial ecosystems, as well as in human populations. According to the most recent dataset (mid-2024 to mid-2025) reported by Ohoro and Ngole-Jeme (2025), the highest PFAS concentrations were reported in sediment from China (19,300 pg/g), and in both surface water (12,293 ng/L) and fish (9620 ng/kg) from the United States. In comparison, earlier findings Ohoro et al. (2024) identified China, Finland, and Sweden as hotspots in surface water, sediment, and biota, respectively. This shift highlights changing contamination patterns and suggests a potential increase in PFAS usage. In recent years, numerous studies have examined the PFAS across different food groups, identifying fish, eggs, meat, fruits, and vegetables as the major sources of dietary exposure (Pasecnaja et al., 2022). Among the detected compounds, PFOA and PFOS were the most prevalent (Bonato et al., 2025). Transfer of PFAS from water and feed to livestock is considered the primary driver of their accumulation, with dietary intake of animal-derived foods regarded as a major exposure pathway for humans. The extent of PFAS bioaccumulation appears to vary among species; for instance, carnivorous fish generally accumulate higher levels than omnivorous fish, whereas poultry seems to metabolize PFAS more rapidly than mammals (Ohoro et al., 2024). Eggs have been reported as the most contaminated among animal-derived products, with PFOA concentrations exceeding 100 ng/g (Bonato et al., 2025). Fish and seafood, meanwhile, remain the most extensively studied food categories for PFAS contamination in aquatic environments. Additionally, a recent study in Poland highlighted that regular consumption of wild boar meat could represent a significant PFAS exposure source for children (Mikolajczyk et al., 2024).

Crops can bioaccumulate PFAS primarily through uptake from

contaminated soil and irrigation water, with aerial deposition contributing in areas near fluorochemical industries (Lesmeister et al., 2021). Long-chain PFAS (C10–C11) tend to remain on root surfaces, whereas short-chain PFAS are more readily translocated to shoots via the transpiration stream due to higher solubility, mobility, and weaker soil sorption (Bolan et al., 2021; Li et al., 2021). This root-to-shoot movement can affect crop yield and nutritional quality and may increase human exposure through consumption of contaminated plants or animal products from livestock fed on such crops (Ohoro & Ngole-Jeme, 2025). Recent studies indicated that vegetables accumulate higher PFAS levels compared to fruits, grains or animal-derived foods such as fish, with accumulation occurring mainly in vegetative tissues rather than roots or storage organs (Ohoro & Ngole-Jeme, 2025).

PFAS are widely incorporated into food contact materials (FCM) owing to their strong oil- and water-repellent properties (Schwartz-Narbonne et al., 2023), which has led to their common use in fast-food wrappers, bakery papers, and non-stick cookware. Across studies, the most commonly detected PFAS in such materials include perfluoroalkyl carboxylic acids (PFCA), perfluoroalkanesulfonic acids (PFBS), fluorotelomer sulfonates (6:2 FTS), fluorotelomer alcohols (FTOH), and polyfluoroalkyl phosphate ester (PAP/diPAP) precursors (Yashwanth et al., 2025). Migration can occur either as individual molecules or through the release of PFAS-containing particles or fragments, and is strongly influenced by the type and composition of the food packaging material (Yashwanth et al., 2025). According to Gupta et al. (2024), PFAS migration from FCM into food is governed by complex physico-chemical processes, including diffusion-adsorption-desorption dynamics as discussed below:

- Diffusion:** Chemicals within the packaging migrate through the spaces between polymer molecules to the packaging surface, from where they can enter the food. Diffusion, governed by Fick's law, is often the rate-limiting step in migration and depends on factors such as the diffusion coefficient, which varies with the molecular size of the migrant, polymer matrix properties, temperature, and packaging thickness. Higher temperatures and thinner packaging accelerate diffusion, whereas crystalline or cross-linked polymers limit it by restricting molecular mobility (Gupta et al., 2024).
- Desorption:** Chemicals attached to the packaging surface can detach and transfer to the food upon contact. In polymer-based packaging, this process is influenced by monomers, plasticizers, stabilizers, processing aids, chemical composition, and time of contact, all of which can leach into the food matrix (Gupta et al., 2024). Diffusion through the packaging matrix often drives this desorption from the inner surface into the food.
- Adsorption:** Food components can attach to the packaging surface through chemical or physical interactions, such as electrostatic or hydrophobic forces. This adsorption can induce a reverse migration of substances from the packaging into the food (Zhang et al., 2025).

Recent studies demonstrate that PFAS migration varies substantially across polymer matrices due to differences in material structure, surface chemistry, and the manner in which PFAS are incorporated ((Ramírez Carnero et al., 2021). Elevated temperatures, prolonged contact, and the nature and composition of the food further amplify diffusion-driven transfer (Begley et al., 2008). Evidence consistently shows that paper and fibre-based packaging display the highest migration potential, as PFAS are often applied as surface coatings and the porous, hydrophilic structure of these materials facilitates rapid transfer into food. In contrast, polyethylene generally exhibits much lower migration because PFAS, when present, are typically residual additives or processing by-products embedded within a hydrophobic, low-permeability matrix. Migration from polyethylene remains limited unless the films are extremely thin, chemically degraded, or intentionally surface-treated with PFAS-based coatings (Phelps et al., 2024). One such complementary evidence from Vera et al. (2024) illustrates how packaging type and

regional manufacturing differences influence PFAS behaviour. Their comparative evaluation of cardboard, recycled cardboard, paper, biopolymer, and Teflon-coated trays showed minimal PFAS migration in Spanish products, while several Chinese trays exhibited detectable PFCA and PFSA migration ranging from 1.55 to 22.3 $\mu\text{g}/\text{kg}$, with the highest PFOA concentration (22.3 $\mu\text{g}/\text{kg}$) detected in a recycled cardboard sushi tray. Fluorotelomer sulfonates were not detected above LOD in any sample, and only PFOA migrated above LOD from Teflon-coated trays. Notably, the migration levels increased markedly with temperature, reinforcing the temperature-diffusion relationship, showing that higher temperatures increase molecular kinetic energy, thereby enhancing mobility within the material matrix even when the contact time is relatively short. This explains the counterintuitive observation that short, high-temperature exposures can still yield higher PFAS transfer than longer exposures at lower temperatures. Another explorative assessment of PFAS occurrence in twenty-five paper and board-based FCM was conducted by Zabaleta et al. (2020) and examined their migration into various food simulants (50 % ethanol, 95 % ethanol, and Tenax®) under controlled contact time (15, 30, and 60 min) and temperature conditions (room temperature and 60 °C). Among all tested materials, pet food bags showed the highest PFAS contamination, particularly in the multi-layer structure composed of an outer printed paper and an inner brown paper. Migration tests further showed clear influence of both simulant composition and experimental conditions, with the strongest effects observed for 95 % ethanol. A chain-length-dependent pattern was evident: short-chain PFCA (PFPeA, PFHxA) migrated more readily into 50 % ethanol, whereas long-chain PFCA (PFOA, PFNA, PFDA) exhibited greater migration into 95 % ethanol, reflecting the role of hydrophobicity in partitioning. Regarding the assays performed at different temperature conditions, when temperature was raised to 60 °C, migration into 95 % ethanol reached a near-constant level for all PFCA, regardless of chain length, indicating a plateau in diffusion-driven release under high-energy conditions. In contrast, migration to Tenax® was minimal, with PFCA migration ranging only from 0.1 to 0.4 % at both 60 °C (10 days) and 150 °C (15 min), preventing differentiation among compounds. To evaluate real-world relevance, Zabaleta et al. (2020) further examined PFAS transfer to real food products (cereals, rice, and infant milk powder) stored for six months. Their findings demonstrated a clear dependence of migration on food type, with the trend cereals < rice < milk powder, reflecting increasing fat content and the strong affinity of PFAS, particularly long-chain compounds and precursor species, for lipid-rich matrices. Similarly, (Wang et al., 2024a) investigated PFAS release from takeaway food packaging waste in China and showed that it contributes substantially to environmental PFAS loads, with 87 % of emissions originating from paper packaging and only 13 % from plastic. To elucidate these differences, six representative FCM types—burger wrappers, burger paperboard, disposable plastic meal boxes, and various food-contact papers were examined based on their intended use. PFAS concentrations varied widely across samples, with 21 PFAS detected at levels ranging from 3.2 to 377 ng/g, and PFCA represented the dominant class in five of the six materials. This PFCA prevalence was largely attributed to the presence and oxidative degradation of precursor compounds such as FTOH and PAP. Notably, for the compostable plastic meal box, oxidative processes resulted in a marked increase in PFBA (C4) and the formation of PFPeA (C5), indicating the presence of C4-C5-based precursors and aligning with the high proportion of short-chain PFCAs (52.1 %) identified in this material. Importantly, the study underscores that although paper packaging is increasingly promoted as an alternative to plastics, it often contains higher PFAS levels and therefore contributes disproportionately to PFAS release during waste disposal. Furthermore, many biodegradable or plant-fibre products, such as polylactic acid items and bagasse-based tableware, achieve water- or oil-resistance through PFAS surface treatments and therefore exhibit migration behaviour comparable to paper. For example, Simionetti et al. (2024) assessed PFAS migration from seven bio-based

disposable FCM made from sugarcane bagasse or cellulose pulp using 95 % ethanol (fatty food simulant) and 3 % acetic acid (acidic food simulant) under standardized time-temperature conditions. Their results showed consistently higher migration into acidic aqueous simulants, reflecting the greater polarity and solubility of many PFAS. The effect was most pronounced at 100 °C for 1 h, where elevated temperatures accelerated diffusion and significantly increased migration from baking papers and food boxes. These findings demonstrate that even biodegradable or bio-based packaging, despite being marketed as environmentally friendly, can act as notable sources of PFAS either through intentional coatings or contamination during processing, indicating that “green” materials do not inherently guarantee chemical safety, particularly when used with acidic foods or under heating conditions. Thus, complementary comparative analysis, including data from the Food Contact Chemicals – Migrates and Extracts database, further show that PFAS detections are most common in paper and board (72.5 %), followed by plastics (8.9 %) and coated metals (4.5 %), confirming that paper-based matrices are the predominant contributors to PFAS migration (Phelps et al., 2024). The documented sources of PFAS contamination along with their associated impacts on the food chain is presented in (Table 1).

4. Determinants of PFAS migration from FCM to food

The increasing PFAS usage in food packaging has been associated with their elevated occurrence in food, as direct contact with FCM allows migration into food matrices, which occurs in two steps: (i) release from the packaging surface, which depends on whether PFAS are surface-bound or absorbed into the material, and (ii) dissolution of the compounds into food (Ramírez Carnero et al., 2021) as shown in (Fig. 1). Moreover, this extent of migration is influenced by several factors, including food contact conditions (temperature, time), material properties, and compound-material interactions, expressed as the distribution coefficient, concentration, mass fractions, type, and length of the PFAS chain, as well as physico-chemical properties of the food (Ramírez Carnero et al., 2021), as discussed in detail below:

4.1. Influence of PFAS chain length and structure

The migration and toxicity of PFAS are strongly influenced by structure-activity relationships, especially carbon-chain length, polarity, and functional groups. For instance, chain lengths of PFCA and FTOH were studied for PFAS migration from paper and cardboard to the simulants of ethanol:water solutions (10:90, 30:70, and 50:50). The migration of 6:2 FTOH to 10 % ethanol, for instance, was 0.00024 $\mu\text{g}/\text{cm}^2$, and at 50 % ethanol, it was 0.013 $\mu\text{g}/\text{cm}^2$, it was increasing as the ethanol proportion increased. It was also noticed that the migration was higher from paper and cardboard towards water and different ethanol solutions when the length of fluorinated chain is small as compared to a longer fluorinated chain (Yuan et al., 2016). Gomis et al. (2018) highlighted that short-chain PFAS, such as PFBA and PFHxA, possess higher polarity and water solubility, enabling easier diffusion and greater migration into aqueous foods due to their smaller molecular size and weaker interactions with polymer matrices, resulting in low bio-accumulation potential owing to rapid renal clearance and weak protein binding. In contrast, long-chain PFAS ($\geq\text{C8}$), including PFOA and PFOS, show limited migration but persist longer because of strong hydrophobic interactions and high affinity for serum proteins (Sunderland et al., 2019). Moreover, functional groups also play a crucial role in influencing PFAS migration, persistence, and toxicity. For instance, sulfonate PFAS (e.g., PFOS, PFHxS) exhibit greater environmental persistence, stronger protein binding, and slower renal clearance than their carboxylate (e.g., PFOA, PFHxA) counterparts, but can still accumulate with repeated exposure (Fischer et al., 2024).

Table 1

Reported sources of PFAS compounds and their effects in the food chain from published studies.

Sources	PFAS components and concentration	Key findings	References
Agriculture produce			
Wheat grains	(in µg/kg) PFOA; 0.46–1.45 PFHxS; 0–1.23 PFHpS; 0.04–0.44 PFPeS; 0.06–0.52 PFBA; 0.54–2.58 HFPO-DA; 0.14–0.34	Low pH favoured PFAS bioaccumulation in wheat.	Yang et al. (2024)
Rice	(in ng/kg) PFBA; 5–30 PFPeS; 0–5 PFHxS; 0–10	LOQ ranged between 2 ng/kg and 32 ng/kg.	Consolato et al. (2024)
Maize	(in ng/g) PFBA; ~0.09 PFOA; ~0.1 Cumulative PFAS; 0.25	Transpiration aids PFAS uptake in maize, making it a potential source of human PFAS exposure through animal-derived foods.	Li et al. (2024)
Soyabean	(in µg/kg) PFHxA; 55.66 PFBA; 12.20 PFBS; 3.24	Progeny plants showed increased uptake and accumulation of PFCA.	Zhang et al. (2022)
Lettuce	(in ng/g) PFBA; 2148 PFCA; 4758 PFOA; 182 HFPO-DA; 121	HFPO-DA translocated more to edible parts than PFOA, while 8:2 Cl-PFESA accumulated mainly in roots with minimal movement to aerial parts compared to PFOS in lettuce and Chinese cabbage.	Gu et al. (2023)
Chinese cabbage	(in ng/g) PFBA; 4335 PFCA; 120,41 PFOA; 323 HFPO-DA; 308		
Seafood, meat and eggs			
Brown trout and Mottled Sculpin Fish	(in ng/g) PFDA; 0.62–9.76 PFDS; 0.22–0.38 PFHxA; 1.05–3.44 PFUDa; 0.55–2.63 PFDoA; 0.46–4.93 FOSA; 0.09–3.20	Fish contained multiple PFAS, with frequent PFDA detection, and many samples exceeded European safety limits, indicating dietary risk.	Sapozhnikova et al. (2025)
Chicken Liver	(in µg/kg) PFOA; 0.48–0.66 PFOS; 0.17–0.58 PFNA; 0.04–0.12 PFHxS; 0.03–0.32	PFAS levels were higher in livers of rural free-range chickens than indoor ones, suggesting outdoor exposure increases contamination.	Depau et al. (2025)
Whole eggs	(in ng/g) PFBA; 0.4–0.91 PFOA; 0.13–0.26 PFNA; 0–0.73 PFDA; 0–1.6 PFUnDA; 0.33–0.91	Younger laying hens had higher egg PFOA levels.	Lasters et al. (2022)
FCM			
Donut bags	(in ng/g) PFBA; 11.3 PFHxA; 0.65 Long-chain PFCA; 372 to 624	Side-chain fluorinated polymers in fast food packaging, breaks down with time and release short-chain PFAS and their precursors, leading to the formation of toxic compounds gradually.	Schwartz-Narbonne et al. (2023)
Printed FCM	PFBS and N-methylperfluorobutane sulfonamidoethanol	Out of 68 PFAS detected in FCM extracts, only 7 are listed in global regulations or industry inventories; almost 90 % are by-products, impurities that are unlisted and toxicology data for these PFAS is unknown.	Phelps et al. (2024)
Frying pans, bakeware, baking paper	(in µg/L) PFODA; 3.05 PFNA; 2.12 (in oatmeal porridge) PFPeA; 0.24–0.4 PFHxA; 1.49–1.96 PFHpA; 0.03–0.06 6:2 FTOH; 2.83–4.26 (in tomato soup) PFPeA; 0.71–0.81 PFHxA; 1.89–2.63 PFHpA; 0.04–0.26 6:2 FTOH; 11.3	PFAS migrate from packaging into food, migration depends on conditions of use, such as temperature, food type, and contact time. PFODA migrated in n-heptane. PFNA migrated in 50 % ethanol.	Ramírez Carnero et al. (2021)

PFBA: Perfluorobutanoic acid, PFOA: Perfluorooctanoic acid, PFNA: Perfluorononanoic acid, PFHxS: Perfluorohexanesulfonic acid. PFOS: Perfluorooctane sulfonic acid, PFODA, Perfluorooctadecanoic acid, PFNA: Perfluorononanoic acid, PFPeA: Perfluoropentanoic acid, PFHxA: Perfluorohexanoic acid, PFHpA: Perfluoroheptanoic acid, PFHpS: Perfluoroheptane sulfonic acid, HFPO-DA: Hexafluoropropylene oxide dimer acid, FTOH: Fluorotelomer alcohol; LOQ: Limit of Quantification, PFBS: Perfluorobutane sulfonic acid, PFUnDA: Perfluoroundecanoic acid, PFHxDA: Perfluorohexadecanoic acid, PAP: Polyfluoroalkyl phosphate ester, diPAP: Polyfluoroalkyl diphosphate ester, PFCA: Perfluoroalkyl carboxylic acids.

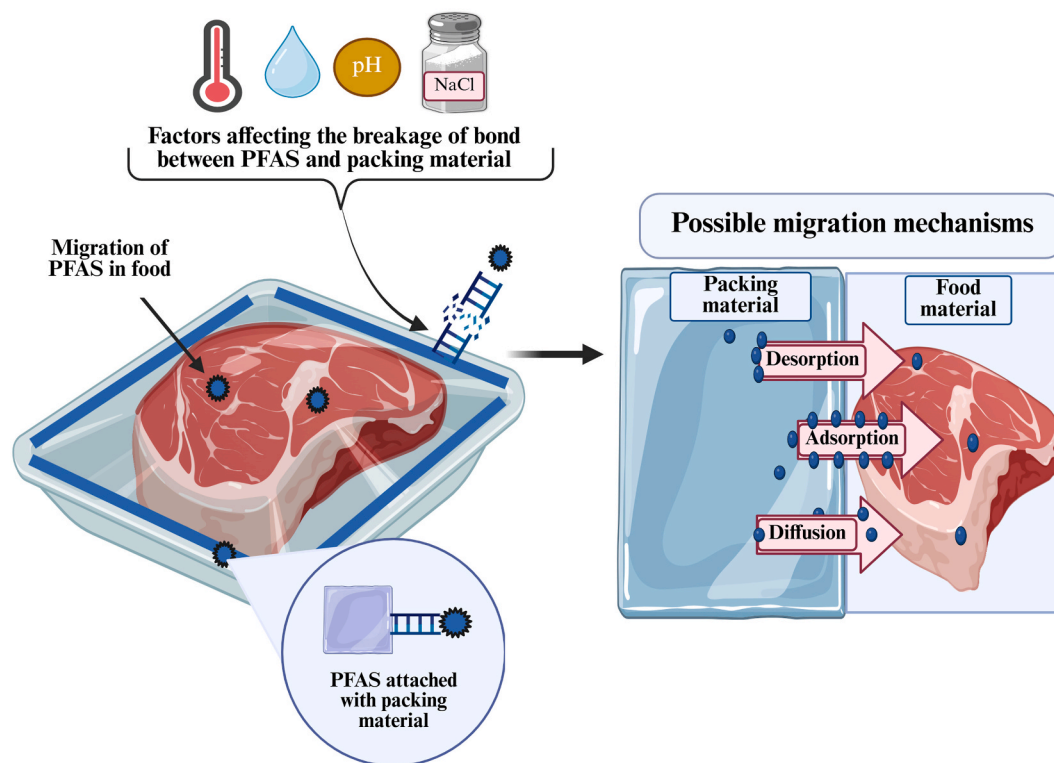


Fig. 1. Factors affecting PFAS migration and the possible mechanism of migration from food packaging material to food.

4.2. Physico-chemical properties of food on PFAS migration

4.2.1. Influence of pH

pH is a key determinant of PFAS migration in food matrices, affecting their stability and transfer. PFAS are more stable in acidic conditions, facilitating greater migration into acidic foods, whereas migration is reduced in more basic environments, for example, vegetables (Eze et al., 2024). Mohamed et al. (2019) elevated concentrations of PFAS in acidic tomato sauce, 18.30 µg/kg for PFOS and 16.55 µg/kg for PFOA, compared to those found in more basic white dry beans, which showed slightly lower levels of 18.08 µg/kg and 16.03 µg/kg, respectively.

4.2.2. Influence of fat content

PFAS are commonly found in protein-rich foods, such as meat, liver and fish, due to their affinity for proteins. However, in migration studies, fat content exerts a stronger influence than protein, as packaging materials often interact with lipids in fast foods and ultra-processed food items (Eze et al., 2024). A comprehensive assessment conducted by Choi et al. (2018), involving 312 consumer product samples including cooking pans, baking equipment, electric rice cookers, grills, and baking papers, provided valuable insights into the differential migration behaviour of perfluoroalkyl compounds (PFCs) across a range of simulant environments. The studies revealed that migration is highly matrix-dependent, for instance, highly polar short-chain, PFAS preferentially migrate into aqueous-based foods, owing to higher solubility and low sorption, whereas less polar long-chain PFAS have greater affinity for lipid-rich matrices and thus tend to accumulate in dairy, meat, and oils due to strong lipophilic interactions that enhance their mobility (Choi et al., 2018; Sunderland et al., 2019).

4.2.3. Influence of salt content

Ionic strength, particularly from dietary salt in the form of sodium chloride, is an important factor influencing PFAS migration into food (Eze et al., 2024). The WHO estimates that between 10 and 12 g of salt are ingested daily (Eze et al., 2024). This salt is present in both

pre-cooked meals and added during the cooking process. For instance, previous research conducted by Mohamed et al. (2019) demonstrated that sodium chloride accelerates PFAS migration; when comparing salted and unsalted matrices, PFOS and PFOA transfers from Tefal cookware increased from 13.11 ng/kg to 18.08 ng/kg and from 9.28 ng/kg to 16.03 ng/kg, respectively.

4.2.4. Influence of moisture content on PFAS migration

Due to their hydrophobic nature, PFAS preferentially associate with fats and oils (Eze et al., 2024). For instance, Fengler et al. (2011) reported that in muffin samples, higher moisture content corresponded to lower FTOH levels, likely due to increased evaporation reducing PFAS concentration in the food.

4.3. Influence of food contact conditions on PFAS migration

4.3.1. Contact time and temperature

The contact time and thermal conditions play a pivotal role in modulating the migration kinetics of PFAS from polymeric matrices into food (Ramírez Carnero et al., 2021). For instance, contact time is short in fast-food or takeaway packaging but longer when materials are used for cooking or processing. Similarly, at room temperature, water's high surface tension limits wetting of paper or cardboard and thus PFAS release; however, at higher temperatures, reduced surface tension promotes migration. Elizalde et al. (2018) reported that migration to Tenax® simulant at 160 °C doubled, reaching up to 25 % of the initial amount present in paper.

4.3.2. Repeated use of FCM

Food packaging is typically discarded after single use, whereas non-stick cookware such as pots, oven racks and pans, is used repeatedly. One such study was investigated by Mohamed et al. (2019) observed that repeated use of non-stick cookware leads to increasing migration of PFOA and PFOS into food with the increasing number of exposures.

5. Mechanism of PFAS transfer from food to humans

PFAS distribution within biological systems plays a vital role in assessing their potential health impacts (Fenton et al., 2021). In humans, the toxicokinetics of PFAS are primarily determined by their absorption, distribution, metabolism, and elimination. Reported investigations have studied several exposure pathways, with oral ingestion being the most common route of exposure, accounting for more than 90 % of total

intake, whereas data on inhalation and dermal absorption remain limited (Bharal et al., 2024). The persistent nature of PFAS makes them highly resistant to degradation, and upon entering the body, they tend to accumulate in various tissues (Cao & Ng, 2021). Accumulation of PFAS in blood, liver, kidneys, heart, muscles, and brain of the population has been reported in many studies, causing neurotoxic effects through direct mechanism, and disruption of neuronal signalling, oxidative stress, impaired cognitive function and developmental neurotoxicity through

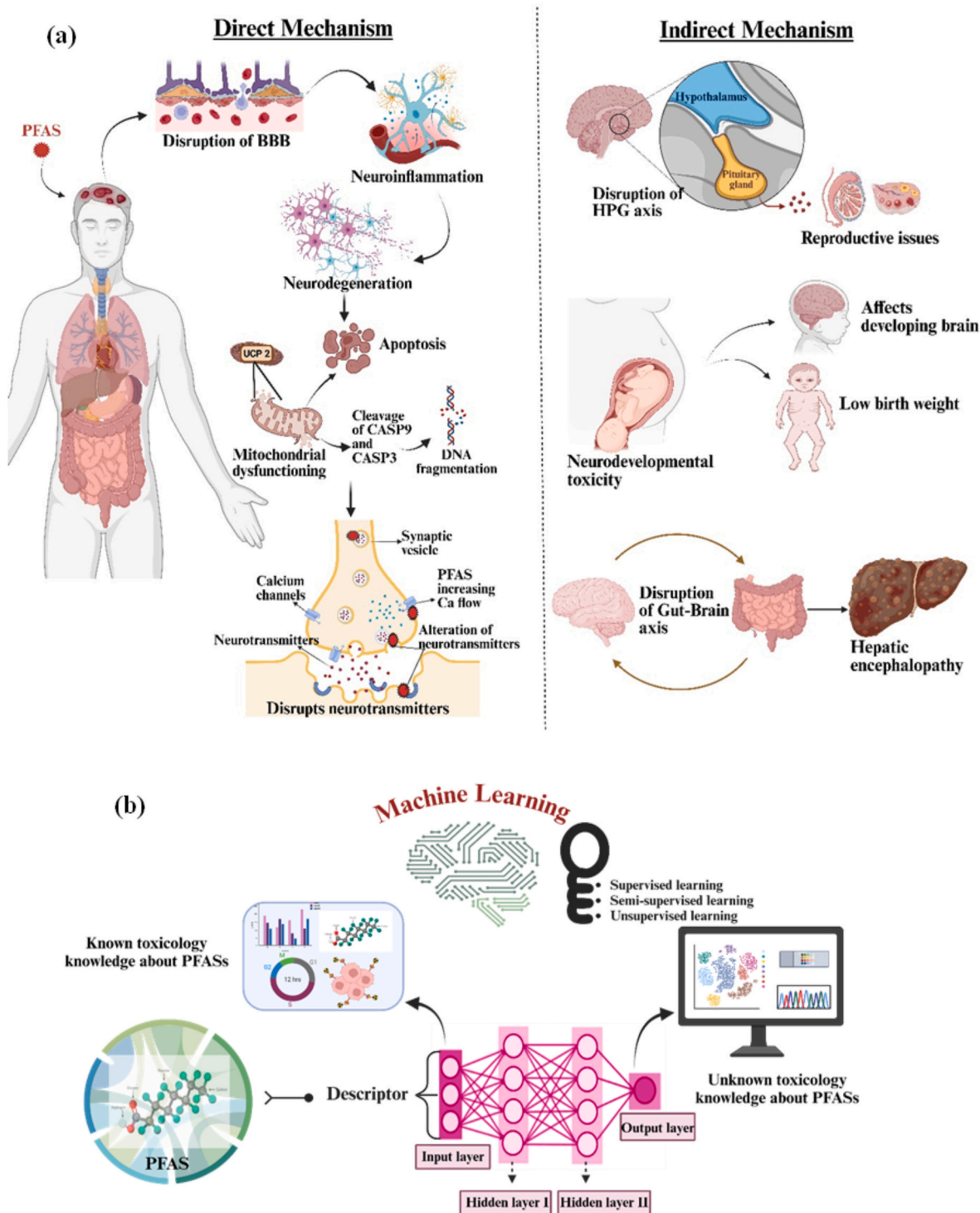


Fig. 2. (a) Underlying mechanisms and consequences of PFAS bioaccumulation in humans affecting the brain through direct mechanisms and indirectly arising through systemic pathways linked to organs such as the liver, kidney, endocrine system, and immune system; (b) Schematic diagram of Deep Learning (a sub-set of Machine Learning) to predict PFAS toxicity using Neural Networks.

indirect mechanism (Bharal et al., 2024) as shown (Fig. 2a). The normal functioning of the brain is ensured by the uptake of oxygen, nutrients and other substances via blood, and this cerebral transfer of compounds aids in the entry of PFAS in the brain (Bharal et al., 2024). However, the movement of xenobiotics is restricted in the brain by the protective cerebral barriers like blood-brain barrier (BBB) and the blood–cerebrospinal fluid barrier (BCSFB), which are meant to safeguard the central nervous system (CNS), by restricting the entry of any toxins and pathogen and allowing the entry of only essential chemicals (Covarrubias et al., 2014).

5.1. Direct mechanism of PFAS bioaccumulation

- a. **Disruption of cerebral barriers:** Epidemiological, animal, and wildlife studies indicate that PFAS can bypass the BBB and blood–cerebrospinal fluid barrier (BCSFB), leading to their accumulation in brain tissue (Bell & O'Shaughnessy, 2022). Proposed mechanisms include disruption of tight junctions, passive diffusion, and active transport via proteins such as serum albumin and brain-type FABP. Accumulation varies with PFAS structure, with long-chain compounds crossing brain barriers more efficiently than short-chain analogs (Pedersen et al., 2015). Despite consistent detection of PFAS in brain tissue, the exact mechanisms of penetration and retention remain unclear (Dassuncao et al., 2019).
- b. **Modulation in neuro-transmitters:** PFAS exposure has been shown to alter neurotransmitter levels, including dopamine, serotonin, and glutamate (Grønnestad et al., 2021). Since these neurotransmitters regulate key functions such as mood, motor activity, appetite, and excitotoxicity, their modulation by PFAS may contribute to neurological disorders (Cao & Ng, 2021).
- c. **Malfunction in mitochondria:** PFAS-induced mitochondrial dysfunction is primarily driven by disrupted calcium homeostasis, leading to neurotoxicity (Chen et al., 2014). Excessive glutamate release and overactivation of NMDA receptors, Na^+/K^+ channels, and L-type voltage-gated calcium channels elevate intracellular calcium, causing mitochondrial overload. This imbalance impairs mitochondrial stability and promotes oxidative stress through increased ROS and RNS generation (Bharal et al., 2024).
- d. **Impact on cerebral cells:** According to Zhuchen et al. (2023), PFOS exposure leads to apoptosis in cerebellar cells by impairing calcium ion homeostasis, disturbing redox balance, and activating protein kinase C signalling by ROS. These disruptions affect neurodevelopmental proteins, including CaMKII (Ca^{2+} /calmodulin-dependent protein kinase II), CREB (cAMP response element-binding protein), and GAP-43 (Growth-associated protein 43), resulting in neurodevelopmental effects.

5.2. Indirect mechanism of PFAS bioaccumulation

- a. **Hepatic issues:** PFAS exposure has been shown to significantly impair liver function and contribute to the development of hepatic encephalopathy (HE) through multiple mechanisms. Studies in both humans and rodents indicate that PFAS can induce liver damage (Roth et al., 2021). In rodents, PFAS exposure has been associated with elevated markers of liver injury, while a meta-analysis in humans reported increased levels of liver enzyme, reflecting hepatic damage linked to PFAS exposure (Choi et al., 2022).
- b. **Alteration in Hypothalamic–pituitary–gonadal (HPG) axis:** The endocrine-disrupting nature of PFAS mediates the activation of the gonadal system, resulting in elevation of hormonal levels in the bloodstream (Davidsen et al., 2022; Rodriguez-Carrillo et al., 2023). This dysregulation can further disturb hypothalamic homeostasis, a central regulator of the hypothalamic–pituitary–gonadal (HPG) axis (Davidsen et al., 2022). Disruptions in HPG axis function may consequently affect brain activity, potentially impairing

reproductive behaviour, hormone regulation, and neurodevelopment (Zeng et al., 2019).

- c. **Developmental neurotoxicity:** Zhuchen et al. (2023) reported that the developing brain is particularly vulnerable to toxic exposures during critical growth periods, such as pregnancy and early childhood. PFAS compounds can cross biological barriers, including the placenta, enabling them to reach the foetal brain and potentially disrupt essential neurodevelopmental processes.

Moreover, the rate and degree of PFAS absorption differ according to their physico-chemical qualities (Nielsen et al., 2024) and individual biological parameters such as age, gender, and health state. Over the past several decades, epidemiological studies have consistently linked PFAS exposure to a range of chronic health conditions, including hyperlipidaemia, non-alcoholic fatty liver disease (Roth et al., 2020), various cancers (Steenland & Winquist, 2021), thyroid dysfunction (Preston et al., 2020), testicular and renal disorders, and developmental toxicity (Gaballah et al., 2020). Moreover, the long-term toxicity of PFAS exposure has raised significant concerns to neurodegenerative diseases such as Alzheimer's, Parkinson's, multiple sclerosis, amyotrophic lateral sclerosis (Lou Gehrig's disease), Huntington's disease, and other conditions associated with neuroinflammation (Delcourt et al., 2024).

6. Data-driven risk assessment of PFAS using AI

The vast diversity and structural complexity of PFAS, shaped by both environmental and anthropogenic factors, pose significant challenges, as their interactions with physical, chemical, and biological systems are intricate, especially in light of limited information, making detection and prediction in environmental systems challenging (Currie et al., 2025). Conventional mechanistic models rely on extensive experimental data, including toxicological studies on animals, making the process time-consuming, costly, labour-intensive, lengthy, and prone to uncertainties when extrapolating results (Meng et al., 2024). As a result, AI-driven approaches serve as a valuable tool for processing massive datasets, accelerating hazard identification, improving consistency, and assisting regulatory decision-making and risk assessment in less time via pattern recognition and data-driven learning (Bacon et al., 2024; Currie et al., 2025). Using advanced and robust algorithms, AI systems process vast data, spot trends, and adapt to new information. ML, an indispensable AI tool, eliminates reliance on prior knowledge by finding patterns, comprehending complicated relationships, anticipating trends, and discovering hidden insights by learning PFAS characteristics directly from available datasets, reducing reliance on complex experimental procedures (Park et al., 2025). ML consist of three components: (a) Algorithm structure; (b) Learning goals, and (c) Training techniques. Based on whether labelled data is used during model development, ML algorithm structures are classified into Supervised Learning, Unsupervised Learning, or Semi-supervised Learning based on the learning logic (Meng et al., 2024).

- a. **Supervised learning ML models:** These models are trained on labelled data, enabling them to learn patterns from inputs and make predictions. In this approach, the input dataset is divided into training and test data, while the target or output values are already assigned to the training data to enable model learning (Pandey et al., 2019). They are generally classified into regression and classification models, depending on whether the target variable is continuous or categorical (Park et al., 2025). Common algorithms include Support Vector Machines (SVM), Discriminant Analysis, Naïve Bayes, k-Nearest Neighbors, regression methods, ensemble techniques, decision trees, and neural networks (Pandey et al., 2019).
- b. **Unsupervised learning ML models:** These are trained on unlabelled data, allowing them to uncover hidden structures and patterns within the dataset to explore the underlying data distribution rather

than predicting predefined outcomes (Park et al., 2025). This model approach includes principal component analysis (PCA), K-means clustering, Neural networks (Pandey et al., 2019).

- c. **Semi-supervised learning ML models:** These models use a combination of labelled and unlabelled data for training. These models attempt to exploit when only a small portion of the data is labelled, but a large amount of unlabelled data is available for optimizing machine learning models. Common semi-supervised model approaches include generative models, semi-supervised SVM, graph-based methods, and disagreement-based methods.

Various ML models have been applied in PFAS management for tasks such as classification, detection, and prediction. These include artificial neural networks (ANNs), including deep neural networks (DNNs); ensemble methods like random forests (RF) and gradient boosting decision trees (GBDT); and individual algorithms such as support vector machines (SVMs). Among these, ANNs are particularly prevalent, with applications ranging from early-stage ML implementations to advanced deep learning techniques. Moreover, as illustrated (Fig. 2b) Deep Learning (DL) is currently trending in the AI field, which can imitate the learning procedure in the human mind and capture more hidden layers non-linear correlations in input data using ANN. Although many studies have been undertaken to investigate techniques for PFAS removal, very few have employed ML approaches for PFAS investigations (Table 2). For instance, PFAS bioactivity is an aspect investigated by Cheng and Ng (2019) that employed ML-based quantitative structure-activity relationship models like RF, Logistic Regression (LR), Multimodal Attentional Neural Networks (MANN), and Graph-based methods to estimate the biological activity range of PFAS. ML models have also been employed to optimize PFAS removal processes involving photocatalysis and adsorption. To identify the source of PFAS contamination using a comprehensive global dataset containing 1197 water samples, 4 Supervised ML algorithms, including Support Vector Machines, Extra Trees, and K-Neighbors (as traditional ML classifiers), as well as a Multi-Layer Perceptron Feed-Forward Deep Neural Network was reported by Kibbey et al. (2020). The results indicated that Deep Neural Networks and Extra Trees outperformed the other methodologies tested when it came to categorizing data from diverse sources. Another study by Navidpour et al. (2024) demonstrated that algorithms, including AdaBoost, Gradient Boosting Machine (GBM), RF can accurately predict PFOA degradation through photocatalysis. Similarly, Wang et al. (2024b) introduced an automated PFAS identification platform (APP-ID) that integrates an enhanced molecular-networking algorithm with ML to screen environmental samples and uncover previously unrecognized PFAS structures. The platform outperformed existing algorithms by achieving a substantially lower false-positive rate, and the incorporated SVM model successfully identified unknown PFAS in the test set with an accuracy of 58.3 %. Currie et al. (2025) applied an additional machine learning approach, integrating artificial-intelligence-based image analysis through the DeepImageJ framework with the HPA cell segmentation model into a high-throughput, high-content screening platform using *Caenorhabditis elegans* dopaminergic neurons. This strategy effectively identified PFAS-induced neurodevelopmental toxicity, showing pronounced effects from individual compounds, particularly PFOS and even stronger impacts from mixtures. The study provides a valuable tool for prioritizing PFAS in risk assessment.

7. Analytical approaches for PFAS detection in food and water

Evidence of the environmental and health risks of PFAS, including their high toxicity even at low concentrations, continues to grow. This emphasizes the need for highly sensitive analytical methods capable of rapid, trace-level detection in the field (Pasecnaja et al., 2022; Rehman et al., 2023). Although nearly 5000 PFAS are in use globally, fewer than 30 are routinely quantified (Pasecnaja et al., 2022). While many studies

report both standardized and non-standardized extraction and analytical methods, comprehensive reviews focusing specifically on standardized detection approaches approved by regulatory bodies, illustrated in (Fig. 3), particularly for complex food matrices and water, remain scarce.

7.1. Conventional analytical approaches for PFAS detection

Among the conventional methods, liquid chromatography coupled with quadrupole tandem mass spectrometry (LC-MS/MS) has become the most widely adopted approach for targeted analysis with available standards. Currently, standards exist for <100 of the thousands of potentially significant PFAS (Rehman et al., 2023). LC-MS/MS analysis is FDA (2025, Method C-010.03) for detecting 30 PFAS in food and feed, and EPA-approved (2018, Method 537.1) for drinking water, offering high sensitivity, specificity, and simultaneous multi-compound analysis, LC-MS/MS remains a robust and reliable tool for regulatory monitoring and safety assessments. This method includes sample preparation such as SPE and QuEChERS that are commonly used to isolate and concentrate PFAS from food and water samples prior to analysis. In this technique, chromatography separates individual components before MS detection, providing retention time data that reflects physico-chemical properties such as vapor pressure and octanol-water partition coefficients (Kow). For homologous PFAS classes, retention time, log Kow relationships support compound classification (Baygi et al., 2016). This chromatographic behaviour complements MS data in determining molecular formulas of unknown features, while newly identified PFAS can be catalogued in spectral libraries to aid future analysis. This is a selective and quantitative approach that determines compound occurrence and concentrations using multiple lines of evidence, such as retention time and precursor/product ion pairs, referenced against standards, with detection limits reaching the low ppt range (Cui et al., 2024; Rehman et al., 2023). Targeted MS methods are limited by the absence of standards for many novel PFAS (Cui et al., 2024).

While LC-MS/MS remains the standard for consistent performance, advances in non-targeted approaches such as LC high-resolution mass spectrometry (LC-HRMS) have made the technology more accessible. LC-HRMS offers high accuracy, sensitivity, and speed, enabling both quantitative analysis and screening of unknown PFAS, particularly valuable for trace analysis in complex matrices (Cui et al., 2024; Pasecnaja et al., 2022; Rehman et al., 2023). Modern HRMS instruments, such as quadrupole-TOF and quadrupole-Orbitrap, can operate in full-scan mode and allow retrospective data evaluation, offering far greater flexibility than MS/MS (Pasecnaja et al., 2022). This progress is primarily attributed to the combination of high resolving power, which minimizes spectral interferences and helps detect low-abundance features, and accurate mass measurements, which enable reliable molecular formula prediction. Additional improvements, such as rapid full-scan acquisition rates (>1 Hz) that facilitate seamless coupling with chromatography, and exceptional sensitivity capable of detecting contaminants at femtogram levels under full-scan conditions, further expand HRMS applications in PFAS research (Liu et al., 2019) (Fig 3). The data processing in the all the non-targeted studies generally follow similar working pattern, even if the approaches of performing are different: (1) generating high-resolution full-scan chromatograms and/or spectra; (2) selecting peak features to capture all detectable ions in the sample by mass filtering, often assuming homologous series); (3) assigning molecular formula with PFAS-specific features according to the profiling data; (4) applying MSⁿ ($n \geq 2$) generic fragmentation to confirm molecular formula and obtain structural details; and (5) proposing and validating structures through database searches (Cui et al., 2024; Liu et al., 2019). Prior study by Van Leeuw et al. (2024) analysed 268 food samples in his study using LC-HRMS and found at least one type of PFAS in 43 % samples with PFOS being the most detected compound and present in 19 % samples. Moreover, advances in HRMS and non-targeted screening have enhanced the detection of emerging

Table 2

Applications of specialized ML algorithms for PFAS in various target directions for risk assessment.

PFAS application type	ML algorithm	Target direction	Target system	Sample size/ Dataset	Prediction strength	Relevance to risk assessment	Key highlights	Reference
Toxicity studies	LR, MMN, RF, GC model, Weave model	Bioreactivity	Binary classification for 26 different bioassays/ML-based QSAR models	1012 PFAS across 26 bioassays	0.916	High	Biologically active PFAS mostly <12 carbons, classified into fluorotelomer-related compounds and perfluoroalkyl acids/precursors.	Cheng and Ng (2019)
	RR	Reproductive toxicity	PFAS adsorbed on microplastics in drinking water to evaluate joint toxicity in female reproductive system	45	–	High	PFAS + microplastics in drinking water increase reproductive toxicity, guiding safer PFAS alternatives with lower female reproductive toxicity.	Du et al. (2023)
Exposure risk parameters	RF, SVM, XGB, LGB, CB, and MLP, DNN, and GNN algorithms, such as GCN, GAT, and AFP	Plasma-binding fraction	Human plasma: prediction of unbound fraction of compounds in plasma	2274	0.92	High	Predicted PFAS bioaccumulation and plasma-binding fraction, enabling safer PFAS design with lower accumulation potential	Cao et al. (2022)
	RF	Toxicokinetic half-life to prioritize PFAS for exposure assessment	4 model species (human, monkey, rat, mouse)	11 PFAS	0.861	High	Enables large-scale PFAS screening and prioritization for exposure assessment, reverse dosimetry, cross-species extrapolation, and identifying candidates for higher-tier testing.	Dawson et al. (2023)
Complex toxicity characterization	RF	Combined toxicity	Zebrafish	Combinations of 2 TMDC × 7 PFAS	1.72 and 0.63	High	PFAS-TMDC interactions can increase bioaccumulation and toxicity in aquatic environments	Liu et al. (2023)
Computational toxicology/ Hazard screening of emerging PFAS	Stacking deep-learning architecture called GXDNet	Endocrine-disrupting toxicity from PFAS	Screening estrogen receptor α activity (ER α) and identification of potential ER α binders. In vivo: zebrafish experimental validation	10,067	–	High	Deep-learning model predicted ER α binding with high accuracy. Docking and MD simulations reveal molecular mechanisms. Many PFAS show high endocrine-disrupting potential similar to PFOS	Pang et al. (2025)
PFAS classification	RF classifier	Predict the most compositionally similar known site/data-source for an unknown water sample; also compute probability that sample is AFFF (aqueous film-forming foam) vs non-AFFF origin	Environmental water samples from different sources	>13,000	Extremely strong performance	High	ML rapidly classified PFAS-contaminated water samples, differentiated AFFF from non-AFFF sources and is useful for source tracking and site remediation	Kibbey et al. (2024)
Process modelling for PFAS degradation by photocatalytic treatment	Adaptive Boosting (AdaBoost), GBM, and RF	Predict the photocatalytic degradation of PFOA	Contaminated water	1343	GMB: 0.878 RF: 0.867 AdaBoost: 0.574	High	GBM model performed best for predicting PFOA photocatalytic degradation by identifying process parameters and catalysts for higher efficiency.	Navidpour et al. (2024)

(continued on next page)

Table 2 (continued)

PFAS application type	ML algorithm	Target direction	Target system	Sample size/Dataset	Prediction strength	Relevance to risk assessment	Key highlights	Reference
Analytical method development to discriminate between distinct PFAS compounds detection and characterization	PCA and t-SNE, PCA and t-SNE	Screening of PFAS species and and diagnostic Raman marker bands that indicate PFAS contamination	Raman spectral signatures (DFT-computed and noise-augmented spectral library) representing 40 PFAS of interest	40	–	Medium–high	It supports decision-making for PFAS mitigation t-SNE and PCA classified PFAS. It identified diagnostic marker bands for detection and improves PFAS characterization for environmental and health monitoring	Chen et al. (2024)
Sensor development	Autoencoder neural network	ML-assisted liquid crystal array platform to capture critical features of LC droplet arrays treated with water samples containing different concentrations	Water samples (ultrapure water, municipal tap water, and simulated river water containing dissolved organic matter	3	0.802	High	ML-assisted LC droplet array detected PFAS at low ppt levels. It transfers learning distinguished PFOS, PFOA, and mixtures. Outperformed EPA detection limits (4 ppt). It provides basis for low-cost PFAS monitoring sensors	Wang et al. (2025)

Artificial Neural Network (ANN), Attentive FP (AFP), Categorical Boosting (CB), Deep Neural Network (DNN), Extreme Gradient Boosting (XGB), Gradient Boosting Machine (GBM), Graph Attention Networks (GAT), Graph Convolutional (GC), Graph Convolutional Networks (GCN), Graph Neural Network (GNN), Light Gradient Boosting (LGB), Logistic Regression (LR), Multi-layer Perceptron (MLP), Multi-task Neural Network (MMN), Principal Component Analysis (PCA), Quantitative Structure-Activity Relationship (QSAR), Random Forest (RF), Ridge Regression (RR), Support Vector Machine (SVM), t-distributed Stochastic Neighbor Embedding (t-SNE); Least Absolute Shrinkage (LAS), Selection Operator (SO), Feed- Forward Neural Network (FFNN).

and previously unidentified PFAS compounds, which is essential in ensuring food safety. However, non-targeted MS detection of PFAS remains challenging because fluorine lacks stable isotopes. As a result, current approaches rely on fluorine-related mass defects, with tools such as Kendrick mass defect plots used to identify homologous PFAS series. An overview of conventional methods used to detect PFAS in food is summarized in (Table 3).

7.2. Emerging analytical approaches for PFAS detection

Although conventional detection techniques offer the necessary sensitivity and selectivity, their reliance on specialized instrumentation and expertise makes analysis costly (>\$200 per sample), time-consuming, and complex, with some PFAS precursors remaining undetected (Rehman et al., 2023). These limitations significantly constrain current testing capabilities. In response, the EPA PFAS Action Plan (EPA, 2019) emphasized the need for emerging analytical methods and tools to more comprehensively monitor PFAS distribution, impact, and concentrations. These emerging techniques include colorimetric, spectrofluorometric, and electrochemical methods, as depicted in (Table 4), along with field-deployable sensors offer low-cost and portable alternatives for detection of PFAS in drinking water and wastewater streams, while supporting remediation efforts in areas heavily impacted by PFAS contamination. These tools improve spatial and temporal resolution in PFAS screening but still require refinement to reach regulatory-level sensitivity. While they may not replace conventional or semi-quantitative methods, they can serve as complementary screening tools, enabling analysis of larger sample sets (Rehman et al., 2023).

8. Insights of global and regulatory frameworks for PFAS management

The environmental persistence of PFAS and their links to adverse health effects have raised considerable concern, underscoring the urgent need for comprehensive policies and regulatory strategies to control

their production, use, discharge, and remediation, as well as to limit their spread. PFAS concentrations vary across industries, regions, and countries; for instance, studies indicate relatively high levels in the United States and Austria, but lower levels in Uganda and Italy. Moreover, a country's gross domestic product (GDP) per capita may correlate with PFAS presence in wastewater, as higher-income countries often produce and use more PFAS, resulting in elevated concentrations (Park et al., 2025). These disparities highlight the importance of tailored regulatory strategies and coordinated global efforts to mitigate PFAS pollution. In response, recent regulations have been introduced to restrict PFAS concentrations across various media, reflecting growing recognition of their potential risks (Park et al., 2025). Collectively, such measures reflect an increasing worldwide awareness of PFAS-related risks and encourage proactive actions by governments and industries to protect public health.

8.1. European regulations guidelines

Building on the European Food Safety Authority (EFSA) 2020 scientific opinion, which established a group tolerable weekly intake (TWI) of 4.4 ng/kg body weight for the combined exposure to PFOA, PFOS, PFNA and PFHxS (Corsini et al., 2024), the European Union (EU) introduced regulatory controls for PFAS in food. Commission Regulation (EU) 2023/915 sets maximum levels for PFAS in several food categories (eggs, fish, meat, bivalve molluscs, crustaceans, game and certain offal), with the provision on the sum of PFAS substances effective from January 1, 2023; foods exceeding those levels may not be placed on the EU market. To support consistent monitoring and enforcement, Commission Implementing Regulation 2022/1428 (August 24, 2022) established harmonized methods for sampling and analysis of PFAS in designated foodstuffs. The EU's Drinking Water Directive sets limit values for PFAS in drinking water and mandates continuous monitoring, while separate regulations specify maximum concentrations in foods, such as 1–2 ng/g in eggs, 1.3 ng/g in bovine meat, and up to 45 ng/g for some fish species (Commission Regulation 2023/915, 2023).

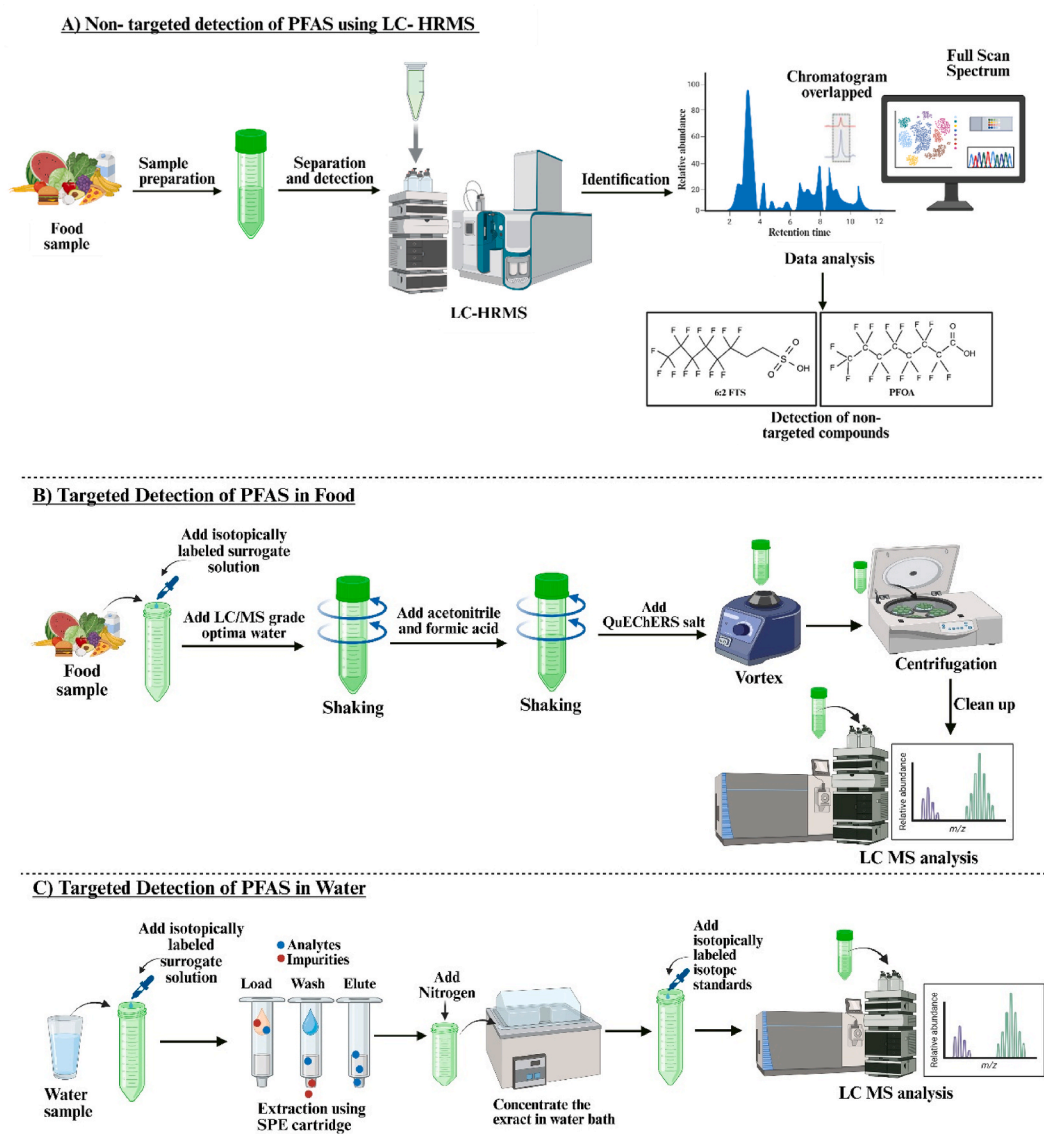


Fig. 3. (A) Non-targeted approach LC-HRMS for the identification of unknown or emerging PFAS; (B) and (C) LC-MS/MS based quantitative determination of specific PFAS in food and water samples, respectively.

8.2. U.S regulatory guidelines

Since 2019, the U.S. Food and Drug Administration (FDA) has been monitoring dietary exposure to PFAS by developing analytical methods to detect 30 PFAS compounds and testing nearly 1300 fresh and processed food samples. In 2020, the FDA's post-market review raised concerns about the safety of short-chain PFAS containing 6:2 fluorotelomer alcohol (6:2 FTOH), leading three manufacturers to commit to a voluntary three-year phase-out, completed by December 31, 2023. Following this, the FDA announced in February 2024 that grease-proofing substances containing PFAS were no longer sold by manufacturers for food contact use, effectively eliminating the primary source of dietary PFAS exposure from authorized food packaging applications. In January 2025, the agency revoked the effectiveness of 35 Food Contact Notifications (FCNs) involving PFAS. By mid-2025, the sale of intentionally added PFAS in paper- and fibre-based food packaging was prohibited nationwide, alongside additional state-level restrictions. While some PFAS remain authorized for specific uses such as cookware, food packaging, and food processing, the FDA continues to conduct rigorous pre-market reviews and post-market reassessments to ensure these applications remain safe (<https://www.fda.gov/food/enviro>

[mental-contaminants-food/and-polyfluoroalkyl-substances-pfas](#)).

On the other hand, the U.S. Environmental Protection Agency (EPA) has progressively tightened regulations on PFAS in response to growing evidence of health and environmental risks. The EPA has finalized maximum contaminant levels for drinking water as 4 ppt for PFOA and PFOS individually, and 10 ppt for a group of other PFAS (PHHxS, PFNA and HFDO-DA), with the health-based goal set at zero due to potential risks even at trace levels (U.S. EPA, 2024). Under waste management statutes, the EPA has strengthened PFAS oversight through both the Comprehensive Environmental Response, Compensation, and Liability Act (CERCLA) and the Resource Conservation and Recovery Act (RCRA). In April 2024, the agency finalized a rule designating PFOA and PFOS, including their salts and structural isomers, as hazardous substances under CERCLA, thereby enhancing enforcement mechanisms for cleanup and liability. Earlier, in February 2024, the EPA proposed two rules under RCRA: (i) to list nine additional PFAS, along with their salts and isomers, as hazardous constituents, ensuring they are considered in facility assessments and corrective actions; and (ii) to clarify the definition of hazardous waste, reinforcing federal and state authority to require cleanup at permitted hazardous waste facilities. These proposed rules are still under review following public comment, underscoring the

Table 3

Overview of food applications of conventional techniques in PFAS compounds detection.

Technique used	Sample	Compound detected	Spiked concentration	LOD	Reference
FULSE	FCM (popcorn bags)	several PFAS compounds	20 µL from 0.3 ng/µL solution of surrogate standards.	0.6–2.2 ng/g	Zabaleta et al. (2017)
MA/MMF-SPME-HPLC	Milk and water	PFCA	10.0 µg/kg	0.9–12.1 ng/L (milk) 0.40–4.40 ng/L (water)	Huang et al. (2018)
µSPE-LCMS/MS	Water	13 PFAS compounds	Up to 898 ng/L	less than 10 ng/L	Lockwood et al. (2019)
SPME-LCMS	Tap water and river water	PFOA, PFOS	upto 35 ng/L	1.5 ng/L (PFOA) 3.2 ng/L (PFOS)	Rodriguez et al. (2020)
ICECLES and HPLC-MS	Potable water	14 PFAS	–	0.05–0.3 ng/L	Skaggs and Logue (2021)
HR-CS-GFMAS	Water samples	PFCA, PFBS, PFOA	0, 1 and 2 ng fluorine	0.1 mg/L (SPE not used) 300 ng/L (SPE used)	Simon et al. (2022) Akhthar et al. (2020)
HPLC-MS/MS	Food and FCM	22 PFAS compounds	–	0.33 ng/kg (plant-based foods) 1.6 ng/kg (animal-based foods)	Aßhoff et al. (2024)

LOD: Limit of Detection, HPLC: High-performance liquid chromatography-Mass Spectrometry, MMF-SPME: Multiple Monolithic Fiber Solid-Phase Microextraction, MIP: molecularly imprinted polymer, HR-CS-GFMAS: High resolution-continuum source-graphite furnace molecular absorption spectrometry, FULSE: Focused Ultrasonic solid-liquid extraction, LC-Q-ToF-MS: Liquid Chromatography-quadrupole time-of-flight mass spectrometry, ICECLES: Ice Concentration Linked with Extractive Stirrer, d-SPE: Dispersive solid phase extraction, SPME-LCMS: Solid-Phase Microextraction - Liquid Chromatography-Mass Spectrometry, µSPE: Micro-SPE; NMR: Nuclear magnetic resonance spectroscopy, SPE: Solid phase extraction.

urgency of addressing PFAS contamination (Park et al., 2025).

8.3. International agreements and global standards

In May 2025, the European Parliament and stakeholders urged broader PFAS restrictions as part of the EU Water Resilience Strategy, calling for updated limits and stronger pollution controls. Internationally, key PFAS, including PFOS, PFOA and PFHxS are listed under the Stockholm Convention on Persistent Organic Pollutants, which requires Parties to restrict or eliminate their production and use (Figuière et al., 2025). To address practical compliance and detection challenges for legacy uses, certain limited exemptions for PFOA-containing firefighting foams were extended through December 3, 2025, although pressure is mounting to phase out even these essential uses. While food-specific PFAS rules remain relatively limited, signalling a global shift toward phasing out PFAS and promoting safer alternatives.

8.4. Alignment of PFAS regulatory standards with analytical detection in food and water monitoring

To enforce these regulations, analytical detection techniques must reliably quantify PFAS at levels at or below these thresholds. The standard methods, largely based on LC-MS/MS and EPA Method 537.1, can achieve limits of detection in the range of 0.71–2.8 ppt in water and as low as 0.2 ng/g in food matrices, which are sufficiently sensitive for compliance monitoring (Menger et al., 2021). Emerging methods, such as SPME-MS, have demonstrated detection limits as low as 0.1–13 ng/L for environmental water samples, offering the potential for rapid and field-deployable applications (Jalili et al., 2023). The alternative detection methods, such as fluorescence, colorimetry, and impedance-based measurements, are increasingly being developed to supplement PFAS detection. Fluorescence techniques have demonstrated LOD typically between 0.24 and 7.5 ppb for common PFAS such as PFOA and PFOS, with further improvements yielding sensor arrays capable of differentiation down to 5 nM (Menger et al., 2021). Colorimetric approaches, leveraging small molecule or dye-based reactions, are generally suited for rapid, onsite threshold detection; however, their LOD are higher, usually in the range of 1–10 ppm for practical field applications, making them useful for gross contamination screening but insufficient for regulatory compliance in drinking water. In contrast, impedance measurement (such as electrochemical impedance spectroscopy with molecularly imprinted polymer-modified electrodes) has yielded highly sensitive results, with LODs reported as low as 3.4 pM for

PFOS, easily surpassing the most stringent regulatory limits (Thompson et al., 2024).

9. Challenges and future outlook

9.1. Addressing research gaps in PFAS transformation, degradation, and bioaccumulation modelling

Despite significant advancements in understanding PFAS behaviour, most of the experimental studies and scientific data still predominantly focus on a few well-known compounds, such as PFOA and PFOS, even though more than 4700 PFAS substances have been identified to date (Panieri et al., 2022). This vast chemical diversity makes it nearly impossible to assess the specific ecological and human health impacts of each compound over short- and long-term scales. Furthermore, many experimental studies are conducted under controlled laboratory conditions that do not accurately reflect natural environmental complexities, such as variable salinity, pH, ionic strength, or the diverse physico-chemical interactions among PFAS sub-classes (e.g., polarity, functional groups, chain length). While long-chain PFAS have traditionally received the most attention, emerging evidence indicates that short-chain analogs may pose comparable risks due to their high mobility and bioaccumulative potential. Therefore, further research is needed to elucidate the bioaccumulation patterns of short-chain PFAS in different food matrices. Additionally, long-term investigations into the chronic health effects of dietary PFAS exposure are essential to fully understand their risks and to inform more robust predictive and regulatory models (Barhoumi et al., 2022).

9.2. Integration of AI and advanced sensor technologies for real-time monitoring

Traditionally, assessing a diverse range of PFAS compounds, each exhibiting unique characteristics across sub-classes, has distinct impacts on human health and thus requires extensive biological and chemical experimentation, which is both time- and resource-intensive.

AI-driven ML models offer a powerful alternative by leveraging existing data to predict toxicity, monitor environmental behaviour, and enhance remediation strategies in real time. For instance, ML models have been used to predict oral median lethal doses (LD₅₀) in rats based on chemical structure data, classifying toxicity levels according to U.S. EPA standards (Feinstein et al., 2021). Similarly, a semi-supervised ML model was developed to predict the bioactivities of PFAS listed in the

Table 4
Overview of emerging techniques for identification and quantification of PFAS compounds.

Primary Detection Technique	Secondary Detection Technique	Working Principle	Limit of Detection (LOD)	Advantages	Disadvantages	Target Compounds	Key features of relevant studies	References
Colorimetric	Aggregation using nanoparticles	The detection relies on target compound-induced changes in the surface charge and aggregation of colloidal nanoparticles, causing spectral shifts and visible color changes.	10 ppb	Fast, sensitive, low-cost detection, Selective PFAS binding	Costly, complex, laborious, optimization required	PFOS	Sample: Water Colormetric material: Citrate-coated gold nanoparticles functionalized with perfluoroalkyl receptors Target compound: PFAS LOD: 4.96 µM (best sensitivity to PFOA)	Rehman et al. (2023); Jung et al. (2024); Kumar and Narayan (2025)
	Using redox dyes	The dyes like MB and MG detect target compounds via ion-pair binding, producing concentration-dependent changes in UV-Vis absorbance intensity.	0.5 ppb	On-site, rapid detection, Stable, sensitive reading, Interference removal	Low visual sensitivity, needs stable lighting	PFOS, PFOA	Sample: Spiked in tap/groundwater Colormetric material: Detecting anionic surfactants like PFOA and PFOS by forming a hydrophobic ion-pair with ethyl violet, extracting it into an organic phase, and measuring RGB values Target compound: PFOA and PFOS LOD: For PFOA, 10 ppb (LPE) and 0.5 ppb (SPE)	
	Paper-based analytical device	The target compounds form colored ion pairs with cationic dyes producing a purple spot whose diameter—controlled by wax-printed hydrophobic barriers—can be measured as a simple, concentration-dependent optical readout.	10 ppm	Fast, inexpensive, portable, Simple visual Avoids complex instruments, Stable, consistent results	Sensitive to ionic strength, Partial surfactant interference, lack of selectivity and high LOD	PFOS	Employed a paper-based platform functionalized with a colorimetric indicator that undergoes a visible color change upon interaction with high concentrations of PFOS (>50 ppm)	
Electrochemical	Voltammetry	It detects target compounds by signal suppression from blocked electron transfer at molecularly imprinted polymer (MIP) modified electrodes.	30 µg/L	High selectivity, Rapid response, Cost-effective, Versatile analyte detection	Interference from gases, Dependent on bubble dynamics	PFOA, PFOS	Sample: Water Electrode material: Ion-selective electrodes with fluorine anion-exchanger membranes Target compound: PFOA, PFOS LOD: 1.08 ppb	Kazemi et al. (2020); Cheng et al. (2020); Park et al. (2022)
	Potentiometry	It detects target compounds by measuring potential changes caused by	0.05 nM	Ultra-sensitive detection, Interferent-tolerant	Limited PFAS species selectivity,	PFOS	Sample: Water Electrode material: Screen-printed	

(continued on next page)

Table 4 (continued)

Primary Detection Technique	Secondary Detection Technique	Working Principle	Limit of Detection (LOD)	Advantages	Disadvantages	Target Compounds	Key features of relevant studies	References
Fluorescence		their binding to MIP modified electrodes.			Requires careful calibration		carbon electrode Target compound: PFOA LOD: 0.07 ng/L (PFOA) and 0.43 ng/L (PFOS) Sample: Water Electrode material: MOF capture probes sandwiched between interdigitated microelectrodes Target compound: PFOS LOD: 0.5 ng/L Sample: Water Electrode material: MIP functionalized utg-C3N4 nanosheets Target compound: PFOA LOD: 10 ng/L Sample: Water Fluorescence material: Fluorescent dye ethidium bromide and nitrogen doped carbon dots Target compound: PFOS LOD: 1.4×10^4 ng/L Sample: Aqueous solutions/ laboratory-spiked water samples Fluorescence material: water-soluble CdTe quantum dots Target compound: PFOS and PFOA LOD: 13.26 ng/L (PFOA) and 21.99 ng/L (PFOS) Sample: Water Fluorescence material: bacterial biosensor engineered with a regulatory gene to express green fluorescent protein Target	
	Impedance Measurement	It detects target compounds measuring impedance changes at nanomaterial- or MIP-modified electrodes.	0.5 ng/L	Label-free, real-time detection, Ultra-low detection limit, Molecular-level selectivity	Scaling challenges, Limited PFAS range	PFOS		
	Electrochemiluminescence	It detects target compounds by converting electrochemical reactions at molecularly imprinted or nanomaterial-modified electrodes into measurable light signals.	0.01 ppb	Rapid, stable signal, Low-cost, simple, Minimal interferences	Limited to PFOA, ECL signal quenching, Specialized instrumentation	PFOA		
	Fluorescent dyes	commonly used as fluorescent markers in fluorescence sensing. They are typically composed of benzene or heterocyclic rings with conjugated double bonds and can be either natural or synthetic	6.2 μ M	selective and sensitive detection	Most dyes lack stability and are easily bleached or quenched, many fluorescent probes also face issues of low water solubility and high cost.	PFOA, PFOS		Rehman et al. (2023); Cui et al. (2024); Cui et al. (2024)
	Quantum dots	Nanoscale semiconductor quantum dots (2–20 nm) are employed as fluorescent probes due to broad excitation, narrow tunable emission, and strong fluorescence	124 ppb	Sensitive, excellent selectivity, cost-effective, effectively reduces matrix interference and eliminate background interferences	Heavy metals like cadmium or selenium cause toxicity, along with light flicker, low solubility, and poor biocompatibility.	PFOS and PFOA		
	Other fluorescent sensing	Genetically engineered bacteria used as biosensors	NM	convenient and affordable solutions for the fast determination of PFAS in real samples	due to the complexity surrounding PFAS determination, further research is required	PFOA, PFOS		

(continued on next page)

Table 4 (continued)

Primary Detection Technique	Secondary Detection Technique	Working Principle	Limit of Detection (LOD)	Advantages	Disadvantages	Target Compounds	Key features of relevant studies	References
compound: PFOS and PFOA LOD: 70 ng/L								

MB: Methylene Blue, MG: Methylene Green, MIP: Molecularly Imprinted Polymer; ECL: Electrochemiluminescence; LPE: Liquid Phase Extraction; SPE: Solid Phase Extraction; NM: Not mentioned, PFOA: Perfluorooctanoic acid, PFOS: Perfluorooctane sulfonic a.

Organisation of Economic Cooperation and Development (OECD) database across multiple human biological targets, including enzymes, genes, proteins, and cell lines. However, realizing the potential of AI-assisted approaches requires continued model development and validation, and solutions to challenges related to data availability, model selection, large-scale implementation, and integration with existing detection technologies. With increasing regulatory pressure and interest in PFAS management, sensor-based technologies such as electrochemical and biosensors for water quality monitoring are gaining prominence for their simplicity and real-time capability. Recent studies further demonstrate the promise of integrating AI with analytical tools, such as combining ML with MS for improved compound identification or enhancing sensor performance for real-time PFAS detection (Park et al., 2025).

9.3. Harmonized international regulatory frameworks for PFAS management

Despite variations in regulatory frameworks, ensuring food safety continues to be a global priority, with nations striving toward the shared objective of safeguarding public health through stringent regulatory measures and harmonized international standards. For instance, the European Chemicals Agency has actively implemented restrictions on the use of PFAS. In contrast, WHO highlights that establishing health-based guidance values remains challenging due to reliance on animal studies and limited epidemiological data. These disparities represent a major obstacle, alongside the high cost and technical complexity of PFAS remediation (Ohoro & Ngole-Jeme, 2025), thereby emphasizing the urgent need for tailored regulatory approaches and coordinated global efforts in effective PFAS management and mitigation.

9.4. PFAS-free packaging and sustainable alternatives

The growing regulations on PFAS in food-contact materials has accelerated the development of PFAS-free packaging coatings and biodegradable barriers. More recent advancements in food-contact coatings involve fluorine-free hydrophobic and oleophobic coatings that comprise polysaccharides, lignin, chitosan, and polyvinyl alcohol. These coatings achieve grease resistance through crosslinking and nanostructuring, rather than relying on fluorination. Biodegradable coatings based on polylactic acid, starch and protein matrices achieve moisture and oil resistance as per useful state standards for short-term food-contact applications while also staying compostable (Jerić et al., 2025). Several adsorptive removal technologies being researched and developed for PFAS from waste or coating residues include biochar, cyclodextrin composites and plasma-based surface treatments. Biochar with engineered porosity can selectively trap perfluoroalkyl acids (PFAA) for reuse (Song et al., 2024). Cyclodextrin polymer networks can entrap PFAS using hydrophobic cavities, adding cost-effective PFAS remediation methods for treatment (Wang et al., 2022). Aligning with these processes and material-level developments will not only create circular economy opportunities, but also exemplify a movement towards safer, fluorine-free food packaging systems that meet future regulatory demands.

10. Conclusion

This systematic review highlights the pervasive presence of PFAS (a large class of synthetic pollutants) found across nearly all aspects of life, often at trace concentrations that are estimated to impact 98 % of the global population. Food packaging material treated with PFAS improves its physicochemical capabilities, like water repellence, oil and grease resistivity, thereby making it significantly more appropriate for use in packaging purposes. The migration of PFAS from food packaging into food is a chemically complex and context-dependent process that has significant implications for public health and environmental safety. Owing to their chemical stability, PFAS persist in the environment, food, and bioaccumulate in the human body, and contribute to various organ-specific toxicities. Currently, highly sensitive and specific methods like LC-MS/MS have been approved by the FDA for food and feed and the EPA for water. While “MS-based methods are reliable and robust, but constrained by high costs and operational complexity. Emerging techniques driven by advances in nanotechnology and materials science, though unlikely to replace conventional methods, can serve as complementary tools that expand screening capacity. Given the global variation in PFAS levels across industries and regions, harmonized regulations and coordinated international efforts are essential to protect public health. As food safety is a global priority and PFAS levels vary widely across industries and regions, harmonized regulations and coordinated international action are crucial to safeguard public health.

Author contributions

Bhawna Bisht: Conceptualization; Investigation; Data curation; Writing – original draft; Shivani Dimri: Data curation; Writing – review & editing; Mikhail S. Vlaskin: Writing – review & editing; Alexey A. Dmitriev: Writing – review & editing; Monu Verma: Writing – review & editing; Arun Kumar: Writing – review & editing; Krishna Aayush: Writing – review & editing; Hyunook Kim: Supervision; Proof-reading; Vinod Kumar: Conceptualization; Supervision; Proof-reading.

Ethics statement

The authors have nothing to report.

Declaration of competing interest

The authors declare no conflicts.

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Data availability

No data was used for the research described in the article.

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