Journal of Environmental Sciences 165 (2026) 379–386

Contents lists available at ScienceDirect

Journal of Environmental Sciences

journal homepage: www.elsevier.com/locate/jes

JES JOURNAL OF ENVIRONMENTAL SCIENCES www.jesc.ac.cn

Research Article

Development of nontarget method based on GC-QTOF-HRMS for analyzing organic pollutants in human serum

Congcong Yue[a,b], Chang He[a,b], Hailing Li[a,b], Zhiquan Yuan[c], Guiying Li[a,b], Shengtao Ma[a,b], Xin Zhang[d], Taicheng An[a,b,*]

[a] *Guangdong-Hong Kong-Macao Joint Laboratory for Contaminants Exposure and Health, Guangdong Key Laboratory of Environmental Catalysis and Health Risk Control, Institute of Environmental Health and Pollution Control, Guangdong University of Technology, Guangzhou 510006, China*
[b] *Guangzhou Key Laboratory of Environmental Catalysis and Pollution Control, Guangdong Basic Research Center of Excellence for Ecological Security and Green Development, School of Environmental Science and Engineering, Guangdong University of Technology, Guangzhou 510006, China*
[c] *Agilent Technologies (China) Co. Ltd., Guangzhou 510700, China*
[d] *Institute of Environmental Science, Shanxi University, Taiyuan 030006, China*

ARTICLE INFO

Keywords:
Nontarget analysis
Biomonitoring method
Human serum sample
Organic pollutants
GC-QTOF-HRMS

ABSTRACT

Traditional targeted analyses often overlook unknown or emerging contaminants, highlighting the significance of nontarget and suspect screening approaches. A novel and high-sensitivity methodology for nontarget analysis of organic pollutants in human serum was newly-developed based on gas chromatography coupled with quadrupole time-of-flight high-resolution mass spectrometry. The extraction protocol employing an acetonitrile-ethyl acetate (9:1, *V*:*V*) mixture significantly improved the extraction efficiency while minimizing matrix effect. A hybridized analytical strategy integrating nontarget and suspect screening was developed to achieve comprehensive identification and classification of pollutants, employing the National Institute of Standards and Technology (NIST) 20 library and Agilent Technologies Personal Compound Database and Library (PCDL). This approach successfully characterized 273 organic contaminants spanning 12 categories, including polycyclic aromatic hydrocarbons (PAHs) and their derivatives, esters, and phenolic compounds in human serum, with a significant increase in detection specificity compared to conventional workflows. The methodology used serum samples of the workers from coking industry, revealing widespread contamination dominated by PAHs and PAH derivatives. Among the target analytes, three were identified solely by NIST and six solely by PCDL, indicating the complementary benefits of combining these different databases. Notably, this work reported the first confirmed detection of 2-naphthalenamine in human serum. This optimized approach demonstrates enhanced sensitivity and reliability in serum analysis, advancing biomonitoring capabilities and providing a deep understanding of human exposure to environmental pollutants.

1. Introduction

In the contemporary era, the ubiquity of environmental contaminants has escalated due to industrialization, urbanization, and anthropogenic activities (He et al., 2025; McDonough et al., 2020; Xiang et al., 2024), leading to widespread exposure to complex mixtures of pollutants, including polycyclic aromatic hydrocarbons (PAHs) (Deng et al., 2023; Jia et al., 2023; Zhang et al., 2022), pesticides (Mali et al., 2023; Mu et al., 2022), and other toxic chemicals (Khan et al., 2022). Growing evidence have linked cumulative exposure to these substances with adverse health outcomes, driving demand for analytical methods capable of detecting both known and unknown contaminants (Wang et al., 2021b). Although traditional targeted analysis method remains valuable for quantifying predefined compounds, its reliance on prior knowledge limits its ability to identify unknown pollutants (Baduel et al., 2015; Díaz et al., 2012). This gap underscores the critical role of nontarget screening in environmental and human exposure studies, enabling comprehensive detection of contaminants without requiring a priori information about their identities (Li et al., 2022, 2023; Phillips et al., 2024; Xu et al., 2021).

Recent advances in high-resolution mass spectrometry (HRMS) coupled with gas chromatography (GC) have revolutionized nontarget analysis, allowing identification of diverse contaminants in environmental matrices including air, soil, and water. Unlike suspect screening, which examines a predetermined list of potential analytes (Mohammed Taha et al., 2022), the nontarget analysis can detect unknown contaminants without prior knowledge of their identity (Tang et al., 2023; Wang et al., 2022). This is particularly relevant to human biomonitor-

* Corresponding author.
E-mail address: antc99@gdut.edu.cn (T. An).

https://doi.org/10.1016/j.jes.2025.11.032
Received 10 June 2025; Received in revised form 10 November 2025; Accepted 11 November 2025
Available online 13 November 2025

ing, where understanding full spectrum of internal exposure requires methods that transcend limitations of targeted analyses (Hallberg et al., 2021; Zhu et al., 2024). However, despite its success in environmental matrices, the application of nontarget screening in human biological samples, particularly blood or serum samples remains underdeveloped due to technical and methodological challenges (Plassmann et al., 2018; Wang et al., 2021a).

The complexity of serum matrices poses significant difficulties on the nontarget analysis (Guo et al., 2020). Blood contains abundant proteins, lipids, and endogenous metabolites that can interfere with detection of trace environmental pollutants in blood or serum samples (Wu et al., 2024), compromising analytical sensitivity and accuracy. Furthermore, the absence of standardized protocols for serum sample preparation worsens these challenges, with limited studies successfully applying nontarget analysis to human serum samples (Greco et al., 2023; Renner and Reuschenbach, 2023). The scarcity of studies on the nontarget screening in serum highlights need for optimized methodologies to suite such complex matrices, facilitating accurate detection and identification of contaminants at very trace levels. However, HRMS, like quadrupole time-of-flight (QTOF), offers unparalleled mass accuracy and high resolution for differentiating compounds (Lin et al., 2015; Partington et al., 2024). Gas chromatography quadrupole time-of-flight high-resolution mass spectrometry (GC-QTOF-HRMS), particularly, is well-suited for detecting various organics, many of which are biomarkers of human exposure (Zhao et al., 2023). By integrating the nontarget and suspect screening, this approach enables the identification of unknown chemical and cross-reference screening of suspected compounds against established databases (Pan et al., 2020; Tang and Tan, 2018). Despite these advancements, critical knowledge gaps still persist, and few studies have systematically optimized serum-specific protocols, particularly for effective extraction method of these contaminants in serum with very low concentration. Given high lipid and protein content in serum samples, an efficient cleanup procedure is also very essential to reduce matrix effects and enhance analytical sensitivity (Hajeb et al., 2022; Musatadi et al., 2023).

Therefore, this work mainly aims to (1) develop a robust serum pretreatment method for comprehensive screening of trace organic contaminants, and (2) implement a hybrid nontarget/suspect screening strategy to characterize the organic pollutant profiles in human serum using GC-QTOF-HRMS. By overcoming limitations of current monitoring methods and advancing human exposome, this work seeks to enhance understanding of human exposure to organic pollutants based on our newly-developed nontarget method.

2. Materials and methods

2.1. Chemicals and materials

Chemical standards, including 16 PAHs, 7 methyl-PAHs (MPAHs), 4 oxygenated-PAHs (OPAHs), and 18 heterocyclic PAHs (HPAHs) were purchased from AccuStandard (New Haven, USA). All solvents were of high-performance liquid chromatography (HPLC) grade and were obtained from CNW Technologies GmbH (Germany). The detailed information on all chemicals and materials used in this study are provided in the **Appendix A Text S1**.

2.2. Serum sampling

A total of 240 serum samples were collected from workers at a coking industry for this work to verify the method. The information of all participants is given in **Appendix A Text S2**. All samples were collected by medical professionals at a local hospital and were centrifuged within three hours of collection, transferred to lyophilized tubes, and stored at −80 °C until analysis. Each participant completed a brief questionnaire and was fully informed about the purpose of the study. Ethical approval for the project was granted by the Ethics Committee of Guangdong University of Technology. Pooled samples were obtained by combining individual samples from all coking plant workers for nontarget and suspect screening and 47 individual serum samples were selected for target analysis.

2.3. Sample pre-treatment

For each sample, 1 mL of serum was spiked with 2.5 ng internal standards. Protein precipitation was conducted by adding different solvent, including pure acetonitrile (ACN) and ethyl acetate (EtAc). Following vortexing for 30 s, the samples were centrifuged at 4000 r/min for 10 min at 4 °C. The resulting supernatant was subjected to further cleanup using either Enhanced Matrix Removal (EMR)-lipid (6 mL, 600 mg) or Florisil (1 g, 6 mL; 60–100 mesh) solid phase extraction (SPE) cartridges. The purified extract was concentrated under a nitrogen stream, and then reconstituted in 50 μL isooctane. Procedural blanks (fetal bovine serum) were prepared in the same batch as described for the pooled serum samples.

2.4. Sample analysis

For the nontarget analysis and suspect screening, an 8890 GC equipped with two HP-5MS (15 m × 250 μm, 0.25 μm) columns was coupled to a 7250 Q-TOF (Agilent Technologies, USA) operated in the electron ionization (EI) mode. Linear temperature gradients of 50–300 °C and 60–310 °C were chosen for separating all major peaks in the analysis of the serum extract for the nontarget and suspect screening, respectively. Full scan mass spectrometry (MS) (Agilent Technologies, USA) were acquired using the exact masses with the mass ranged from 45 to 650 *m/z*. The temperature of the transfer line, source, and quad was 280 °C, 280 °C, and 150 °C, respectively, and the electron energy was 70 eV. Detailed information on the instrumental analyses is available in **Appendix A Table S1**.

Target analysis was also applied for method validation using a GC tandem mass spectrometry system (GC–MS/MS-TQ8040, Shimadzu, Japan) in the EI mode, and a DB-5MS capillary column (30 m × 0.25 mm, 0.25 μm) was used for chromatographic separation. The oven temperature was programmed as follows: the initial temperature was set at 80 °C (held for 0.5 min), then raised to 280 °C at 5 °C/min, to 300 °C at 15 °C/min, to 315 °C at 20 °C/min (held for 0.5 min) and finally held for 0.5 min at 315 °C. The ion source and interface temperatures were set at 230 °C and 300 °C, respectively. The detailed parameters of GC–MS/MS are described in **Appendix A Table S2**.

2.5. Chemical screening

For the chemical screening, a dual identification process was applied. First, the nontarget analysis was conducted by Agilent Unknown MassHunter (B.10.0), using SureMass Deconvolution for feature matching. Each feature's deconvoluted spectra were compared against the National Institute of Standards and Technology (NIST) library, with criteria of signal-to-noise ratio (S/N) ≥ 3, retention time index (RI) deviation < 5 %, matching factor > 70 %, and *m/z* deviation < 10 ppm. A mixture of n-alkanes was also injected to calculate RI of each feature identified in serum samples, and the deviation of ± 5 % between library RI and test RI was considered acceptable. Manual blank subtraction was applied, where compounds were excluded if their intensities were less than three times that observed in the procedural blanks.

Second, the suspect screening was carried out by using Agilent MassHunter Qualitative Analysis (B.10.0), and compounds were screened using Agilent Personal Compound Database and Library (PCDL), with tools for spectral matching, retention time (RT) alignment, and semi-quantitation. Suspect screening combined with the retention time locked (RTL) method makes it easier to compare RT of compounds in real samples with their library RTs, which allows for high cer-

tainty of identified compounds. The criteria for the screening included S/N ≥ 3, retention time < 0.2 min, matching factor > 75 %, qualified fragments > 2, and *m/z* deviation < 5 ppm. In addition, the reference standards (listed in **Appendix A Table S3**) were purchased for some of these provisionally identified compounds (with a confidence level of 1) (Schymanski et al., 2014a) for definitive confirmation.

3. Results and discussion

3.1. Development of the nontarget analytic method

To address the challenges of analyzing trace organic pollutants in human serum, a novel sample preparation protocol combining polarity optimized protein precipitation and broad spectrum solid-phase extraction was developed. The quality control (QC) samples were prepared by pooling serum from 240 workers from coking industry, with six aliquots analyzed to ensure methodological reproducibility (Fig. 1). To optimize the sample preparation procedure, methods for protein precipitation, extraction, and cleanup methods were systematically evaluated. Initial protein precipitation trials compared pure ACN and ACN/EtAc mixtures. While 100 % ACN yielded detection of 381–493 compounds via GC-QTOF-HRMS, a 9:1 (*V*:*V*) ACN/EtAc mixture increased detectable compounds by 13 % (497–517 compounds), demonstrating superior recovery of semi-volatile and non-polar species including phthalate esters and halogenated hydrocarbons. This enhancement of detection was likely caused by the capacity of EtAc to disrupt hydrophobic protein-lipid-contaminant complexes that typically entrap low-polarity analytes during conventional ACN precipitation. A previous study also suggested that adding EtAc could improve extraction efficiency of polybrominated diphenyl ethers, polychlorinated biphenyls, and PAHs in fish (Kalachova et al., 2011). The possible reason for this is that the optimized solvent mixture reduced the nonspecific binding by weakening van der Waals interactions between serum proteins and hydrophobic pollutants, thereby minimizing co-precipitation artifacts that compromise traditional methods.

For the cleanup procedure, both Captiva EMR-lipid and Florisil PR cartridges were systematically evaluated to compare the polarity-dependent recovery challenges in the nontarget analysis. Firstly, by using Captiva EMR-lipid cartridges, eluted with ACN/water (4:1, *V*:*V*), 381 compounds were identified but exhibited limited recovery efficiency (64 % ± 16 %) for spiked standards. Secondly, by using Florisil pr cartridges, which were eluted with dichloromethane (DCM)/Hex (1:1, *V*:*V*), EtAc/Hex (1:1, *V*:*V*), and EtAc/DCM (1:1, *V*:*V*), the numbers of identified compounds were 439, 480, and 493, respectively. Therefore, a 9:1 (*V*:*V*) ACN/EtAc mixture as the protein precipitation solvent and EtAc/DCM (1:1, *V*:*V*) as the elution solvent were combined to comprehensively screen organic contaminants in serum. In contrast, precipitating proteins with a 9:1 (*V*:*V*) ACN/EtAc mixture and eluting Florisil PR cartridges with EtAc/DCM (1:1, *V*:*V*) demonstrated a superior performance, recovering 517 compounds with significantly high recovery efficiency (88 % ± 12 %). This enhancement directly correlates with tunable surface chemistry of Florisil, which balances hydrophilic-lipophilic interactions to minimize irreversible adsorption of ultra-trace analytes (Andrade-Eiroa et al., 2016). However, the selectivity of EMR-lipid toward aromatic species (16 identified heterocycles) limited its applicability for broad-spectrum analysis, while the moderate polarity of Florisil enabled efficient elution of both polar and non-polar chemicals. The optimized Florisil/EtAc-DCM protocol achieved a 13 % improvement in compound detection over conventional ACN-based methods, establishing its robustness for trace-level pollutant analysis. This workflow (Fig. 1) was ultimately selected for its ability to harmonize matrix cleanup with analyte preservation across a 5-order-of-magnitude polarity range.

3.2. Optimization of chemical screening

To investigate the presence of both known and previously unidentified contaminants, an initial nontargeted screening was conducted on serum samples using the optimized workflow (Fig. 1). Total 11,621 chromatographic features were produced by SureMass deconvolution in QC samples, with 6316 candidates retained after blank correction. Nontarget screening using the NIST 20 database identified 463 compounds that fulfill the screening criteria, leveraging its extensive coverage of > 200,000 chemicals (Schymanski et al., 2015; Weiss et al., 2011). How-

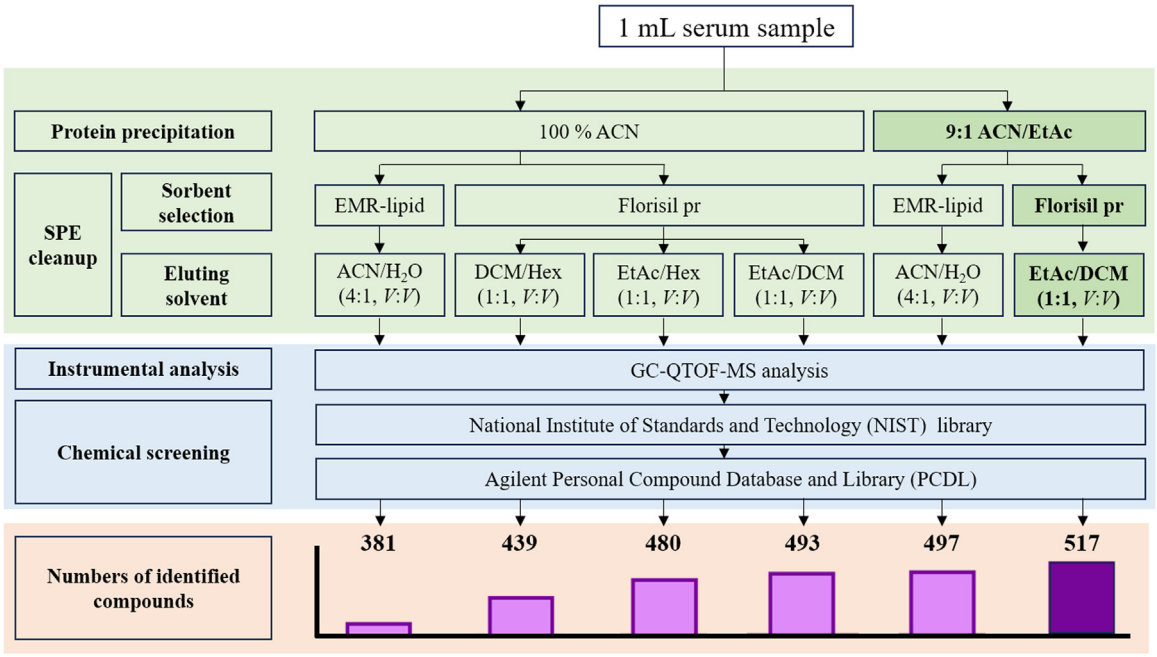

Fig. 1 – Optimization of the extraction and cleanup procedurals for the nontarget and suspect screening of serum samples, where the optimized protocol was highlighted. (ACN: acetonitrile; EtAc: ethyl acetate; EMR: Enhanced Matrix Removal; DCM: dichloromethane; GC-QTOF-HRMS: Gas chromatography quadrupole time-of-flight high-resolution mass spectrometry).

ever, the analysis based on NIST 20 database could only provide level 2 confidence with probable structure identification (Schymanski et al., 2014b), resulting in potential false positive in chemical identification. To address this limitation, the suspect screening using Agilent PCDL database was implemented by combining retention time locking (deviation < 0.2 min) and exact mass fragment matching ($\Delta m/z$ < 5 ppm and qualified fragments > 2) to enhance identification certainty. Iterative filtering was applied to 120 PCDL candidates tentatively identified through retention time alignment, spectral matching scores, qualifying fragments, and m/z deviation, refining the candidate list to 94, 75, 59 and 54, respectively. Notably, among 54 high confidence identifications, 46 compounds were overlapped between the nontarget and suspect screenings, while 8 unique PAHs (i.e., benzo[a]pyrene, 9-fluorenone) were exclusively detected through suspect screening. This screening technique combining both the nontarget and suspect screenings addresses critical gaps in complex matrix analysis, where the extensive coverage of nontarget screening minimizes library bias (Dürig et al., 2019; Mardal et al., 2019), while the validation of suspect screening reduces false positives inherent to probabilistic matching (Moschet et al., 2018; Zedda and Zwiener, 2012). The introduction of RT alignment in the suspect screening increased the confidence of identification, while 23 PAHs and PAH derivatives were further confirmed by reference standards (listed in **Appendix A Table S3**), increased the confidence level from Level 2 to Level 1 (Charbonnet et al., 2022). Combining nontarget screening with suspect screening can enable the extensive identification of pollutants while improving the accuracy of identification.

An example of the identified compounds using two different methods is shown in Fig. 2, where the nontarget screening achieved near-perfect deconvolution (component shape quality: 96.8) for a representative compound (Naphthalene), with spectral matching (match factor: 96.8) and RI alignment confirming structural assignment. A component shape quality of 96.8 indicates a perfect deconvolution process, which can be revealed from the coelution diagrams of the five primary deconvoluted fragments. An exceptionally high match factor of 96.8 was observed between the deconvoluted spectrum and NIST 20 library spectrum, with the measured RI well matched with that in NIST library values. Such a high matching result allowed for identification of this compound with high confidence. The suspect screening further enhanced specificity through RTL method (deviation < 0.05 min) and superior deconvolution (component shape quality: 98.9), enabling trace-level identification of chemicals (Fig. 2c and d). However, the nontarget screening showed advantages in detecting diverse contaminants, and the suspect screening provided high confidence identification of chemicals at trace levels, with frequently evade detection due to matrix suppression. Together, this dual methodology overcomes limitations inherent to single approaches, establishing a synergistic framework for both exploratory discovery and hypothesis-driven analysis.

3.3. Method performance evaluation and validation

The optimized workflow enabled comprehensive profiling of serum pollutants, with 517 compounds initially matched through the combined nontarget and suspect screening. Following exclusion of endogenous long-chain alkanes, alkenes, acids, and esters (limited relevance to exogenous exposure or health risks) (Hollender et al., 2023; Kunzelmann et al., 2018), the detected 273 contaminants were classified into 12 priority categories (Fig. 3). PAHs and their derivatives dominated the profile (20.1 %), heterocyclic compounds (12.8 %), phosphates/aromatic esters (11.7 %), and phenols (10.9 %) also constituted other major classes, reflecting diverse exposure sources from coking industrial processes to consumer products. Generally, the coking industries are known as an important source of PAHs and worker exposure

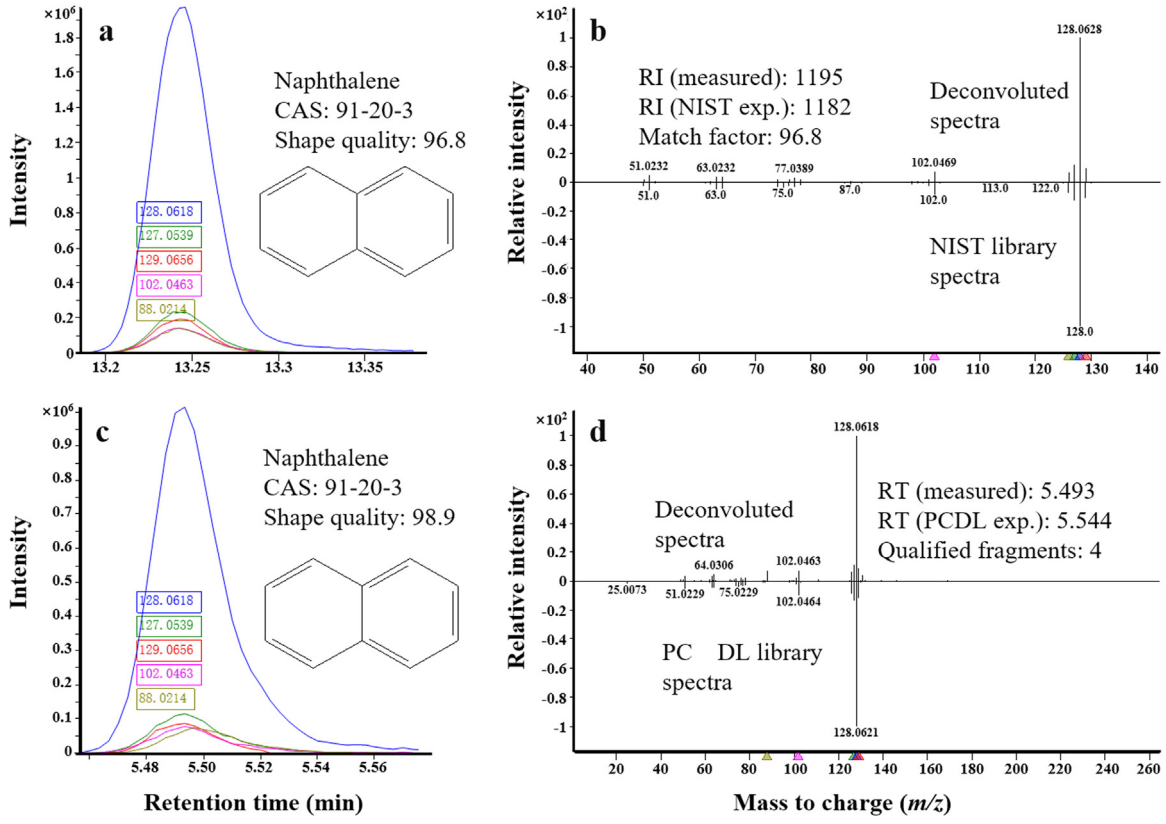

Fig. 2 – Example of Naphthalene (CAS 91–20–3) detected by nontarget and suspect screening. (a) Co-elution plot of five main deconvoluted fragments in a real serum sample by nontarget screening. (b) Differential plot between deconvoluted spectrum and NIST 20 library spectrum. (c) Co-elution plot of five main deconvoluted fragments in a real serum sample by suspect screening. (d) Differential plot between deconvoluted spectrum and PCDL library spectrum. RI: retention time index; exp.: experimental; RT: retention time.

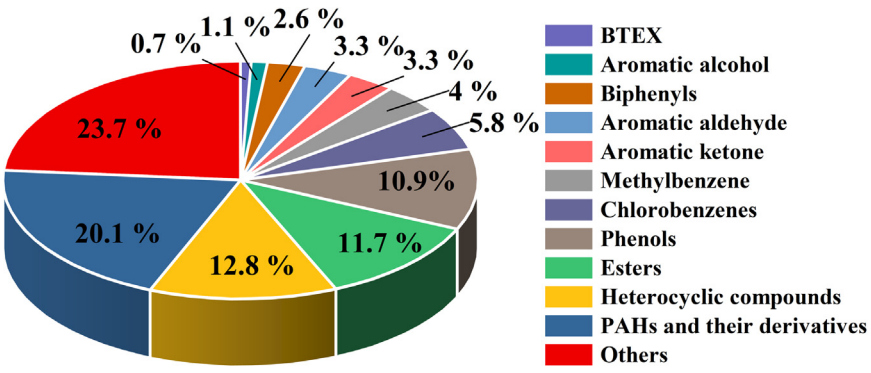

Fig. 3 – Profile of compounds detected the serum quality control (QC) samples using nontarget and suspect screening.

to PAHs are well-documented (Du et al., 2020; Fu et al., 2022), but traditional target analyses focusing on 16 prioritized PAHs may underestimate the exposure risk to humans. In this study, alongside the 16 prioritized PAHs, PAH derivatives, such as quinoline, carbazole, and dibenzothiophene, which have been classified as carcinogens by International Agency for Research on Cancer (IARC) (IARC, 2013) but not captured by conventional methods, were also identified. The findings demonstrated the advantage of the nontarget and suspect screening over traditional target analyses in comprehensive assessment of human exposure to chemicals.

Furthermore, our results indicate that the established protocol was sensitive. For example, indole was consistently identified in all QC samples (n = 6) by both nontarget and suspect screening, yet the suspect screening achieved higher confidence than nontarget screening (matching score 99.9 vs. 86.5 for nontarget) due to RTL method and fragment pattern validation (**Appendix A Table S4**). In contrast, diphenylamine was detected exclusively via suspect screening, highlighting additional suspect screening enhanced sensitivity for low concentration chemicals in serum. Moreover, the matching scores of all contaminants identified by both nontarget and suspect screening are summarized in **Appendix A Table S5**. Notably, the matching scores of contaminants identified by suspect screening are consistently higher than those identified by nontarget screening, further validating the high certainty of suspect screening. Additionally, the nontarget screening uniquely identified 2-naphthalenamine (2-ANaP) (CAS 91–59–8), and a high matching result was obtained for it (Shape quality: 91 and match factor: 88.5) (**Appendix A Fig. S1**). To our knowledge, this was the first detection of 2-ANaP in human serums. It is worth noting that the IARC has identified 2-ANaP as Group 1, suggesting its potential carcinogenicity to humans. Despite its prohibited status in many countries (IARC, 2012), the identification of 2-ANaP indicates a higher capability of the established protocol in detecting the unlisted or emerging contaminants. In addition, among the 273 identified contaminants, 121 are regularly monitored in human biomonitoring programs, including prioritized PAHs, PAH derivatives, phenols, chlorobenzenes, and esters, etc. Besides, 13 contaminants were detected for the first time in human serum through literature retrieval based on the key words of “Human serum” and “Contaminant name”, including 2-ANaP, 2-dibenzofuranol and 4,4′-dimethylbiphenyl, though few studies have identified them in human urine or environmental samples (**Appendix A Table S6**).

To validate the accuracy and repeatability of the analyses, a procedural blank and a spiked matrix were included for every batch of 10 serum samples, the recoveries of PAHs and their derivatives in spiked matrices were 48.2 %–108 %, with relative standard deviations of 2.9 %–13.6 % (**Appendix A Table S7**), indicating that this method has good accuracy and reproducibility. After nontarget analysis and suspect screening validation of the pooled QC samples, the target analysis was further applied to all individual serum samples (n = 47) from coking industry to analyze PAHs and their derivatives (i.e. MPAHs, OPAHs, and HPAHs). In total, 34 out of 49 analytes were detected in the target analysis, while 23 of them were identified in the nontarget and suspect screening (Table 1). Among those identified analytes, fourteen were identified by both the nontarget analysis using NIST Library and the suspect screening using PCDL, three were identified by NIST only, and six were identified by PCDL only. These results indicate the complementary benefits of combination of those different databases. Moreover, the estimated identification limits from the nontarget or suspect screening for each compound, defined as the lowest concentration capable of producing a peak with an intensity three times that of noise, are shown in Table 1. The identification limits of compounds were consistently higher (1.03–11.4 times) than the quantification limits for target analysis. Interestingly, the identification limits were still lower than those reported previously, even from target analysis (Baduel et al., 2015; Zhang et al., 2017). All these demonstrate the developed method has high sensitivity for nontarget analysis of organic pollutants in human serum.

3.4. Semi-quantitative and quantitative analyses of PAHs and their derivatives

The semi-quantification (mixed samples) of PAHs and their derivatives was performed to assess their prevalence in the serum of coking plant workers. Total of 10 PAHs, 6 MPAHs, 6 HPAHs, and 1 OPAH were identified in serum samples by nontarget and suspect screening (**Appendix A Fig. S2 and Table 1**). The detection frequencies of PAHs and their derivatives were all > 50 %, except for benzo[a]pyrene (BaP) (33.3 %), indicating wide exposure of coking plant workers to PAHs and their derivatives. Total concentrations of PAHs (Σ_{10}PAHs) in serum samples ranged from 359 to 3446 ng/g lipid with a mean concentration of 1859 ng/g lipid, which were higher than those of Σ_6MPAHs (range: 148–996 ng/g lipid; mean: 524 ng/g lipid), Σ_6HPAHs (range: 198–1768 ng/g lipid; mean: 742 ng/g lipid), and Σ_1OPAHs (range: not detected-41.0 ng/g lipid; mean: 23.9 ng/g lipid). Despite lower concentrations than those of unsubstituted PAHs, PAH derivatives are also non-negligible pollutants in coking sites due to high toxicity (Krzyszczak and Czech, 2021; Peng et al., 2023). For individual PAHs, Nap exhibited the highest mean concentration (901 ng/g lipid), flowed by phenanthrene (Phe) (366 ng/g lipid) and fluorene (Flu) (296 ng/g lipid). This is different from PAH levels in atmospheric samples gathered from the same coking plant (Deng et al., 2023), which may be attributed to the fact that Nap is primarily distributed in the gaseous phase and thus more easily absorbed by human body. For PAH derivatives, the mean concentrations of 1-methylfluorene (1-Mflu) (151 ng/g lipid) and indole (516 ng/g lipid) were the highest among MPAHs and HPAHs, respectively.

In addition, the results of nontarget and suspect screening were compared with those of targeted analysis (**Appendix A Fig. S2**). The mean concentrations of Σ_{10}PAHs (2593 ng/g lipid, range: 472–7588 ng/g lipid), Σ_6MPAHs (799 ng/g lipid, range: 117–2547 ng/g lipid), Σ_6HPAHs (1164 ng/g lipid, range: 374–3955 ng/g lipid), and Σ_1OPAHs (23.0 ng/g lipid, range: n.d.–71.1 ng/g lipid) determined by target analysis were 0.96–1.57 times those determined by nontarget and suspect screening. Consistent with nontarget and suspect screening, the mean concentration of NaP (1236 ng/g lipid) was the highest among

Table 1 – Comparison between target analysis and nontarget analysis, using concentrations of PAHs and their derivatives (ng/g lipid, n = 47) and their identification by nontarget and suspect screening*.

Category	Chemical	Target analysis				Nontarget and suspect screening					The rate of identification limits (T/N + S)
		Average (ng/g lipid)	Range (ng/g lipid)	Detection rate (%)	Identification limit (ng/g lipid)	Average (ng/g lipid)	Range (ng/g lipid)	Detection rate (%)	Identification limit (ng/g lipid)	Workflow	
PAHs	Nap	1236	n.d.–4750	95.7	2.17	901	n.d.–1638	83.3	11.6	N + S	5.35
	Acy	131	n.d.–959	97.9	2.67	107	n.d.–161	83.3	14.1	N + S	5.28
	Ace	68.2	n.d.–286	93.6	2.67	32.8	n.d.–69.8	66.7	30.4	N + S	11.4
	Flu	407	n.d.–1610	97.9	2.17	296	n.d.–644	83.3	16.1	N + S	7.42
	Phe	550	9.26–1490	100	3.00	366	211–594	100	10.3	N + S	3.43
	Ant	88.7	n.d.–329	97.9	3.67	48.1	n.d.–103	83.3	15.7	N + S	4.28
	FluA	34.9	n.d.–162	87.2	4.33	24.3	n.d.–43.1	83.3	19.2	N + S	4.43
	Pyr	62.2	n.d.–434	76.6	1.83	65.1	n.d.–173	66.7	14.5	N + S	7.92
	Chr	10.5	n.d.–93.0	36.2	2.67	14.1	n.d.–37.1	66.7	7.88	N	2.95
	BaP	3.95	n.d.–31.5	27.7	3.67	4.06	n.d.–18.7	33.3	3.77	S	1.03
MPAHs	1,3-DMNap	134	7.90–576	100	4.50	104	18.4 – 172	100	21.9	N + S	4.87
	1,4-DMNap	64.2	n.d.–475	83.0	3.83	49.2	n.d.–121	83.3	17.5	N + S	4.57
	2,7-DMNap	238	n.d.–1400	93.6	2.67	123	9.03–273	100	22.2	N + S	8.31
	1,6,7-TMNap	114	n.d.–493	95.7	4.50	66.4	n.d.–107	83.3	15.9	N + S	3.53
	1,4,6,7-TMNap	38.2	n.d.–115	89.4	4.00	29.8	n.d.–60.3	83.3	16.8	N + S	4.20
	1-Mflu	210	25.7 – 978	100	3.00	151	n.d.–450	66.7	13.1	S	4.37
	3-Mcholant	23.1	n.d.–117	97.9	4.67	-	-	-	n.a.	n.a.	-
OPAHs	9-Fluorenone	23.0	n.d.–71.1	85.1	2.17	23.9	n.d.–41.0	66.7	14.7	S	6.77
HPAHs	QL	26.1	n.d.–153	85.1	2.67	29.7	n.d.–60.3	66.7	10.6	S	3.97
	IQL	9.63	n.d.–40.7	68.1	6.33	-	-	-	n.a.	n.a.	-
	Indole	768	56.0 – 2810	100	2.00	516	201–1391	100	19.1	N + S	9.55
	DBF	142	n.d.–488	93.6	4.17	69.4	n.d.–122	66.7	12.4	N	2.97
	4-MDBF	157	7.03–635	100	5.50	95.3	17.9 – 236	100	8.77	S	1.59
	DBT	30.7	n.d.–96.7	93.6	4.83	-	-	-	n.a.	n.a.	-
	Acridine	33.5	n.d.–127	66.0	4.67	-	-	-	n.a.	n.a.	-
	4-MDBT	64.7	2.89–261	100	3.17	27.6	n.d.–78.6	66.7	12.5	S	3.94
	5,6-BQL	29.3	n.d.–152	85.1	5.83	-	-	-	n.a.	n.a.	-
	3-MDBT	2.58	n.d.–64.8	21.3	3.50	-	-	-	n.a.	n.a.	-
	CBZ	5.05	n.d.–66.2	38.3	4.00	3.47	n.d.–8.75	50	4.85	N	1.21
	4,6-DBT	2.05	n.d.–39.0	23.4	5.17	-	-	-	n.a.	n.a.	-
	1,8-DMCBZ	5.55	n.d.–44.6	59.6	4.00	-	-	-	n.a.	n.a.	-
	3M-CBZ	47.4	n.d.–145	87.2	3.67	-	-	-	n.a.	n.a.	-
	2,8-DMDBT	3.91	n.d.–44.4	29.8	3.17	-	-	-	n.a.	n.a.	-
	1,4-DMCBZ	1.58	n.d.–24.8	21.3	3.33	-	-	-	n.a.	n.a.	-
	7-MB[b]nap[2,3-d]T	4.53	n.d.–74.0	19.1	4.83	-	-	-	n.a.	n.a.	-

T: target analysis; N: confirmed by nontarget screening; S: confirmed by suspect screening; N + S: by both nontarget and suspect screening; n.d.: not detected; n.a.: not available.

* Results are not shown when chemicals are not detected in the nontarget and suspect analysis.

the 10 PAH isomers in target analysis, followed by Phe (550 ng/g lipid) and Flu (407 ng/g lipid), while indole was the most abundant (516 ng/g lipid) in HPAHs. In contrast, 1-Mflu was the most abundant in MPAHs in nontarget and suspect screening, whereas 2,7-dimethylnaphthalene (2,7-DMNap) (238 ng/g lipid) showed the highest mean concentration in target analysis, which may be attributed to the certain uncertainties of semi-quantification (Wang et al., 2022). Despite that, both 1-Mflu and 2,7-DMNap were the major MPAHs in both nontarget/suspect screening and target analysis.

As evidenced by the above results, although the semi-quantitative concentrations calculated based on the ratio of the peak areas of the identified contaminants to their corresponding surrogate standards have discrepancy compared with target analysis, they can basically reflect the exposure levels and distribution characteristics of PAHs and their derivatives in the serum of coking plant workers. This also further validates the accuracy of the nontarget and suspect screening method.

3.5. Strengths and limitations

In this study, by innovatively integrating the nontarget and suspect screening strategies with complementary NIST and PCDL databases, a multidimensional compound identification system was first established, offering superior detection specificity to conventional methods. This established system not only successfully resolved critical challenge identifying low-concentration analytes in complex biological matrices, but also provided major advancements for assessing human exposome to chemicals, particularly in advancing nontarget analysis of chemicals in human serums through methodological innovation and empirical breakthroughs. By optimizing solvent mixtures and SPE protocols, this newdeveloped method improved the recovery efficiency compared to conventional approaches, meanwhile, minimizing matrix effects. Furthermore, the integration of nontarget and suspect screening leveraged complementary databases (NIST and PCDL) to mitigate false positives while identifying emerging contaminants like 2-ANaP, a compound previously undetected in serum despite its regulatory significance. Such high capabilities are important for uncovering unknown exposure pathways, particularly in high-risk populations such as industrial workers exposed to complex chemical mixtures.

Furthermore, the dominance of PAH derivatives in serum samples from coking industry workers clearly showed exposure from industrial emissions, highlighting an urgent need for enhanced accurate analytical method for assessing their exposure to PAH derivatives. With the improved identification limits compared to conventional target analyses, this established method also enhanced the detection of trace organic pollutants, thereby supporting early warning systems and management. Its application in serums from coking workers not only validated its robustness but also established a framework for global human biomonitoring efforts.

Despite those strengths, there are also some limitations. For example, the absence of a dependable and precise mass spectrometry library

may lead to inaccurate matching of features such as isomers in the NIST library. Furthermore, the suspect screening library is narrow, which makes it more difficult to identify compounds without EI spectra in the database. Therefore, accurate and reliable large-scale mass libraries are needed to precisely identify unknown pollutants.

Overall, this methodology filled the gap between environmental contamination exposure and human health impacts, empowering policymakers to prioritize contaminants based on real-world exposure data and advancing paradigm of evidence-based environmental governance.

4. Conclusions

Overall, in this study, a sensitive method was established for nontarget analysis and suspect screening of organics in serum. This developed method included a rapid sample pre-treatment, liquid-liquid extraction steps and SPE cleanup procedures, together with chemical screening using both NIST library and PCDL. Total 517 compounds were tentatively identified by using the optimized workflow, including PAHs and their derivatives, heterocyclic compounds, phosphates/aromatic esters, phenols, and others. The combination of two libraries enhanced the sensitivity of the compounds screening of traditional nontarget analysis. This approach was then successfully applied to analyze PAHs and their derivatives in the 47 serum samples collected from coking plant workers, and the identification limits of some compounds were consistently higher than quantification limits for target analysis. This study not only offers valuable references for identifying chemicals in human serum samples but also brings brand-new perspectives for comprehensively analyzing the toxic contaminants in various industries practically in the coking industry.

Statement

This work has received approval for research ethics from Guangdong University of Technology and a proof/certificate of approval is available upon request.

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.

CRediT authorship contribution statement

Congcong Yue: Writing – original draft, Validation, Methodology, Investigation, Formal analysis, Data curation. **Chang He:** Writing – review & editing, Visualization, Validation, Data curation. **Hailing Li:** Writing – review & editing, Visualization, Data curation. **Zhiquan Yuan:** Resources, Methodology. **Guiying Li:** Writing – review & editing, Visualization, Funding acquisition. **Shengtao Ma:** Visualization, Methodology. **Xin Zhang:** Visualization, Resources. **Taicheng An:** Writing – review & editing, Supervision, Funding acquisition, Conceptualization.

Acknowledgments

This work was supported by the National Key Research and Development Project (Nos. 2023YFC3905102 and 2024YFC3713201), and the National Natural Science Foundation of China (Nos. 42207485 and 42407567).

Appendix A Supplementary data

Supplementary material associated with this article can be found in the online version at doi:10.1016/j.jes.2025.11.032.

References

Andrade-Eiroa, A., Canle, M., Leroy-Cancellieri, V., Cerdà, V., 2016. Solid-phase extraction of organic compounds: a critical review. Part ii. Trends Analyt. Chem. 80, 655–667.

Baduel, C., Mueller, J.F., Tsai, H., Ramos, M.J.G., 2015. Development of sample extraction and clean-up strategies for target and non-target analysis of environmental contaminants in biological matrices. J. Chromatogr. A 1426, 33–47.

Charbonnet, J.A., McDonough, C.A., Xiao, F., Schwichtenberg, T., Cao, D., Kaserzon, S., et al., 2022. Communicating confidence of per- and polyfluoroalkyl substance identification via high-resolution mass spectrometry. Environ. Sci. Technol. Lett. 9, 473–481.

Deng, W., Wen, M., Wang, C., Huang, J., Zhang, S., Ma, S., et al., 2023. Atmospheric occurrences and health risk assessment of polycyclic aromatic hydrocarbons and their derivatives in a typical coking facility and surrounding areas. Chemosphere 341, 139994.

Díaz, R., Ibáñez, M., Sancho, J.V., Hernández, F., 2012. Target and non-target screening strategies for organic contaminants, residues and illicit substances in food, environmental and human biological samples by UHPLC-QTOF-MS. Anal. Methods 4, 196–209.

Du, J., Pan, B., Cao, X., Li, J., Yang, J., Nie, J., 2020. Urinary polycyclic aromatic hydrocarbon metabolites, peripheral blood mitochondrial DNA copy number, and neurobehavioral function in coke oven workers. Chemosphere 261, 127628.

Dürig, W., Tröger, R., Andersson, P.L., Rybacka, A., Fischer, S., Wiberg, K., et al., 2019. Development of a suspect screening prioritization tool for organic compounds in water and biota. Chemosphere 222, 904–912.

Fu, M., Wang, H., Bai, Q., Du, J., Niu, Q., Nie, J., 2022. Urinary polycyclic aromatic hydrocarbon metabolites, plasma p-tau231 and mild cognitive impairment in coke oven workers. Chemosphere 307, 135911.

Greco, V., Locatelli, M., Savini, F., Grazia, U.d., Montanaro, O., Rosato, E., et al., 2023. New challenges in (bio)analytical sample treatment procedures for clinical applications. Separations 10, 62.

Guo, Z., Huang, S., Wang, J., Feng, Y., 2020. Recent advances in non-targeted screening analysis using liquid chromatography-high resolution mass spectrometry to explore new biomarkers for human exposure. Talanta 219, 121339.

Hajeb, P., Zhu, L., Bossi, R., Vorkamp, K., 2022. Sample preparation techniques for suspect and non-target screening of emerging contaminants. Chemosphere 287, 132306.

Hallberg, I., Plassmann, M., Olovsson, M., Holte, J., Damdimopoulou, P., Sjunnesson, Y.C., et al., 2021. Suspect and non-target screening of ovarian follicular fluid and serum–identification of anthropogenic chemicals and investigation of their association to fertility. Environ. Sci. Process. Impacts 23, 1578–1588.

He, R., Zhong, H., He, C., Li, H., Wang, Z., Zheng, J., et al., 2025. Individual and mixture effects of BTEX occupational exposure with hematologic and hepatic profiles in petrochemical workers and the metabolic mechanism. J. Environ. Sci. 154, 163–173.

Hollender, J., Schymanski, E.L., Ahrens, L., Alygizakis, N., Béen, F., Bijlsma, L., et al., 2023. NORMAN guidance on suspect and non-target screening in environmental monitoring. Environ. Sci. Eur. 35, 75.

IARC (International Agency for Research on Cancer), 2012. 2-Naphthylamine. Lyon, France. World Health Organization. Available at: https://www.ncbi.nlm.nih.gov/books/NBK304406/. Accessed November 6, 2025.

Jia, Y., Li, W., Li, Y., Zhao, L., Li, C., Wang, L., et al., 2023. The levels of polycyclic aromatic hydrocarbons and their derivatives in plasma and their effect on mitochondrial DNA methylation in the oilfield workers. Toxics 11, 466.

Kalachova, K., Pulkrabova, J., Drabova, L., Cajka, T., Kocourek, V., Hajslova, J., 2011. Simplified and rapid determination of polychlorinated biphenyls, polybrominated diphenyl ethers, and polycyclic aromatic hydrocarbons in fish and shrimps integrated into a single method. Anal. Chim. Acta 707, 84–91.

Khan, S., Naushad, M., Govarthanan, M., Iqbal, J., Alfadul, S.M., 2022. Emerging contaminants of high concern for the environment: current trends and future research. Environ. Res. 207, 112609.

Krzyszczak, A., Czech, B., 2021. Occurrence and toxicity of polycyclic aromatic hydrocarbons derivatives in environmental matrices. Sci. Total Environ. 788, 147738.

Kunzelmann, M., Winter, M., Åberg, M., Hellenäs, K.-E., Rosén, J., 2018. Non-targeted analysis of unexpected food contaminants using LC-HRMS. Anal. Bioanal. Chem. 410, 5593–5602.

Li, H., Zhang, S., Yao, C., He, R., Lu, P., Li, G., et al., 2023. Nontarget screening of novel urinary biomarkers for occupational exposure to toxic chemicals from coking industry using HPLC-QTOF-MS. Environ. Sci. Technol. 57, 13004–13014.

Li, J., Zhang, H., Wang, J., Yu, Z., Li, H., Yang, M., 2022. Identification of unknown disinfection byproducts in drinking water produced from Taihu Lake source water. J. Environ. Sci. 113, 1–11.

Lin, L., Lin, H., Zhang, M., Dong, X., Yin, X., Qu, C., et al., 2015. Types, principle, and characteristics of tandem high-resolution mass spectrometry and its applications. RSC Adv. 5, 107623–107636.

Mali, H., Shah, C., Raghunandan, B.H., Prajapati, A.S., Patel, D.H., Trivedi, U., et al., 2023. Organophosphate pesticides an emerging environmental contaminant: pollution, toxicity, bioremediation progress, and remaining challenges. J. Environ. Sci. 127, 234–250.

Mardal, M., Andreasen, M.F., Mollerup, C.B., Stockham, P., Telving, R., Thomaidis, N.S., et al., 2019. HighResNPS. Com: an online crowd-sourced HR-MS database for suspect and non-targeted screening of new psychoactive substances. J. Anal. Toxicol. 43, 520–527.

McDonough, L.K., Santos, I.R., Andersen, M.S., O'Carroll, D.M., Rutlidge, H., Meredith, K., et al., 2020. Changes in global groundwater organic carbon driven by climate change and urbanization. Nat. Commun. 11, 1279.

Mohammed Taha, H., Aalizadeh, R., Alygizakis, N., Antignac, J.-P., Arp, H.P.H., Bade, R., et al., 2022. The norman suspect list exchange (NORMAN-SLE): facilitating European and worldwide collaboration on suspect screening in high resolution mass spectrometry. Environ. Sci. Eur. 34, 104.

Moschet, C., Anumol, T., Lew, B.M., Bennett, D.H., Young, T.M., 2018. Household dust as a repository of chemical accumulation: new insights from a comprehensive high-resolution mass spectrometric study. Environ. Sci. Technol. 52, 2878–2887.

Mu, H., Zhang, J., Yang, X., Wang, K., Xu, W., Zhang, H., et al., 2022. Pesticide screening and health risk assessment of residential dust in a rural region of the North China Plain. Chemosphere 303, 135115.

Musatadi, M., Andrés-Maguregi, A., De Angelis, F., Prieto, A., Anakabe, E., Olivares, M., et al., 2023. The role of sample preparation in suspect and non-target screening for exposome analysis using human urine. Chemosphere 339, 139690.

Pan, Y., Wang, J., Yeung, L.W., Wei, S., Dai, J., 2020. Analysis of emerging per-and polyfluoroalkyl substances: progress and current issues. Trends Analyt. Chem. 124, 115481.

Partington, J.M., Rana, S., Szabo, D., Anumol, T., Clarke, B.O., 2024. Comparison of high--resolution mass spectrometry acquisition methods for the simultaneous quantification and identification of per- and polyfluoroalkyl substances (PFAS). Anal. Bioanal. Chem. 416, 895–912.

Peng, B., Dong, Q., Li, F., Wang, T., Qiu, X., Zhu, T., 2023. A systematic review of polycyclic aromatic hydrocarbon derivatives: occurrences, levels, biotransformation, exposure biomarkers, and toxicity. Environ. Sci. Technol. 57, 15314–15355.

Phillips, K.A., Chao, A., Church, R.L., Favela, K., Garantziotis, S., Isaacs, K.K., et al., 2024. Suspect screening analysis of pooled human serum samples using GC × GC/TOF-MS. Environ. Sci. Technol. 58, 1802–1812.

Plassmann, M.M., Fischer, S., Benskin, J.P., 2018. Nontarget time trend screening in human blood. Environ. Sci. Technol. Lett. 5, 335–340.

Renner, G., Reuschenbach, M., 2023. Critical review on data processing algorithms in non-target screening: challenges and opportunities to improve result comparability. Anal. Bioanal. Chem. 415, 4111–4123.

Schymanski, E.L., Jeon, J., Gulde, R., Fenner, K., Ruff, M., Singer, H.P., et al., 2014a. Identifying small molecules via high resolution mass spectrometry: communicating confidence. Environ. Sci. Technol. 48, 2097–2098.

Schymanski, E.L., Jeon, J., Gulde, R., Fenner, K., Ruff, M., Singer, H.P., et al., 2014b. Identifying small molecules via high resolution mass spectrometry: communicating confidence. Environ. Sci. Technol. 48, 2097–2098.

Schymanski, E.L., Singer, H.P., Slobodnik, J., Ipolyi, I.M., Oswald, P., Krauss, M., et al., 2015. Non-target screening with high-resolution mass spectrometry: critical review using a collaborative trial on water analysis. Anal. Bioanal. Chem. 407, 6237–6255.

Tang, C., Tan, J., 2018. Quasi-targeted analysis of halogenated organic pollutants in fly ash, soil, ambient air and flue gas using gas chromatography-high resolution mass spectrometry with isotopologue distribution comparison and predicted retention time alignment. J. Chromatogr. A 1555, 74–88.

Tang, C., Zhu, Y., Liang, Y., Zeng, Y.H., Peng, X., Mai, B.X., et al., 2023. First discovery of iodinated polyfluoroalkyl acids by nontarget mass-spectrometric analysis and iodine-specific screening algorithm. Environ. Sci. Technol. 57, 1378–1390.

Wang, A., Abrahamsson, D.P., Jiang, T., Wang, M., Morello-Frosch, R., Park, J.-S., et al., 2021a. Suspect screening, prioritization, and confirmation of environmental chemicals in maternal-newborn pairs from San Francisco. Environ. Sci. Technol. 55, 5037–5049.

Wang, L., Xiao, Q., Yuan, M., Lu, S., 2022. Discovery of 18 organophosphate esters and 3 organophosphite antioxidants in food contact materials using suspect and nontarget screening: implications for human exposure. Environ. Sci. Technol. 56, 17870–17879.

Wang, X., Huang, K., Zeng, L., Zhang, X., Cheng, D., Li, R., et al., 2021b. Integration of 103 semivolatile organic compounds into one multianalyte method for human serum analysis: an innovative approach within exposure assessment. Environ. Sci. Technol. Lett. 8, 419–424.

Weiss, J.M., Simon, E., Stroomberg, G.J., De Boer, R., De Boer, J., Van der Linden, S.C., et al., 2011. Identification strategy for unknown pollutants using high-resolution mass spectrometry: androgen-disrupting compounds identified through effect-directed analysis. Anal. Bioanal. Chem. 400, 3141–3149.

Wu, J., Yao, S., Wang, Y., Fan, S., Cui, X., Chen, D., et al., 2024. Fast determination of organophosphate esters and their metabolites in human matrices by a straightforward cold-induced strategy coupled with HPLC–MS/MS. Anal. Bioanal. Chem. 416, 6663–6677.

Xiang, Y., Liu, G., Yin, Y., Li, Y., Wang, D., Cai, Y., et al., 2024. Human activities shape important geographic differences in fish mercury concentration levels. Nat. Food 5, 836–845.

Xu, C., Gao, L., Zheng, M., Qiao, L., Wang, K., Huang, D., et al., 2021. Nontarget screening of polycyclic aromatic compounds in atmospheric particulate matter using ultrahigh resolution mass spectrometry and comprehensive two-dimensional gas chromatography. Environ. Sci. Technol. 55, 109–119.

Zedda, M., Zwiener, C., 2012. Is nontarget screening of emerging contaminants by LC-HRMS successful? A plea for compound libraries and computer tools. Anal. Bioanal. Chem. 403, 2493–2502.

Zhang, X., Li, X., Jing, Y., Fang, X., Zhang, X., Lei, B., et al., 2017. Transplacental transfer of polycyclic aromatic hydrocarbons in paired samples of maternal serum, umbilical cord serum, and placenta in Shanghai, China. Environ. Pollut. 222, 267–275.

Zhang, Z.F., Chen, J.C., Zhao, Y.X., Wang, L., Teng, Y.Q., Cai, M.H., et al., 2022. Determination of 123 polycyclic aromatic hydrocarbons and their derivatives in atmospheric samples. Chemosphere 296, 134025.

Zhao, Y., Chen, D., Duan, H., Li, P., Wu, W., Wang, X., et al., 2023. Sample preparation and mass spectrometry for determining mycotoxins, hazardous fungi, and their metabolites in the environment, food, and healthcare. Trends Analyt. Chem. 160, 116962.

Zhu, L., Bossi, R., Carvalho, P.N., Rigét, F.F., Christensen, J.H., Weihe, P., et al., 2024. Suspect and non-target screening of chemicals of emerging Arctic concern in biota, air and human serum. Environ. Pollut. 360, 124605.