Environment International 202 (2025) 109650

Contents lists available at ScienceDirect

Environment International

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

Full length article

Screening uncalibrated priority pollutants by improved AHP-CRITIC method at development land

Xinni Wei [a,b], Xiuli Dang [a,*], Peng Liu [a], Ge Gao [b], Hang Zhu [a], Jiayue Shi [a], Qiyuan Zhang [a], Roland Bol [c], Peng Zhang [d], Iseult Lynch [e], Long Zhao [b,*]

[a] College of Land and Environment, National Engineering Research Center for Efficient Utilization of Soil and Fertilizer Resources, Northeast Key Laboratory of Conservation and Improvement of Cultivated Land, Ministry of Agriculture and Rural Affairs, Shenyang Agricultural University, Shenyang 110866, China

[b] Center for Environmental Health Risk Assessment and Research, Chinese Research Academy of Environmental Sciences, Beijing 100012, China

[c] Institute of Bio- and Geosciences, Agrosphere (IBG-3), Forschungszentrum Jülich GmbH, Wilhelm-Johnen-Straße, Jülich 52428, Germany

[d] Department of Environmental Science and Engineering, University of Science and Technology of China, Hefei 230026, China

[e] School of Geography, Earth and Environmental Sciences, University of Birmingham, Edgbaston, Birmingham B15 2TT, United Kingdom

ARTICLE INFO

Handling Editor: Adrian Covaci

Keyword:
Priority pollutants
Uncalibrated pollutants
Screening method
Indicator system
Northeast China

ABSTRACT

Unlisted uncalibrated pollutants in the industrial land of northeast China are continuously accumulating due to insufficient regulatory control, posing a serious threat to the ecological environment and human health. To address this challenge and begin to quantify the currently unlisted uncalibrated pollutants present in the industrial land in northeast China, 170 candidate pollutants were screened based on the literature research method. The Analytical Hierarchy Process (AHP) and the Criteria Importance Through Intercrieria Correlation (CRITIC) were utilized equally to screen for priority control of unlisted uncalibrated pollutants. For the categorical indicators, local modifications were implemented on the toxicity, persistence, and migratory indicators, fully considering the industrial distribution, environmental traits, and pollutant sources in northeast China. The grading standards of these indicators were refined in accordance with the relevant criteria and the availability of monitoring data collected from databases and predicted data by models. 11 types of uncalibrated priority pollutants were screened out using the comprehensive evaluation method and conducting cluster analysis based on total pollutant scores. The order of pollutants identified as candidates for prioritized control measures was as follows: perfluorooctanoic acid (PFOA) > acrolein > perfluorooctane sulfonate (PFOS) > styrene > perfluorobutanoic acid (PFBA) > anthracene (Ant) > methyl isocyanate (MIC) > 2,4-dimethylphenol > hexachlorobutadiene (HCBD) > 2,6-dimethylphenol > perfluorononanoic acid (PFNA). In particular, PFOA has the highest concern with 382 points. It poses long-term and serious potential hazards to the ecological environment and human health of industrial sites in northeast China. Thus, controlling such key pollutants is crucial for northeast China's environmental protection, and the current work supports the prioritization of chemicals for management or remediation.

1. Introduction

Chemical substances that enter the environment are transported through soil, water and air, and are finally enriched in soil. Because of their persistence, easy uptake by living organisms and accumulation, chemical pollutants can adversely affect the soil environment and human health (Burman et al., 2023; Chen et al., 2023; Jiang et al., 2024; Zhao et al., 2023). Priority pollutants, or priority control pollutants, are chemical substances that have been identified as toxic, difficult to degrade, and where they or their residues have high frequency of detection, resulting in their prioritization for control via environmental regulation and management. Uncalibrated pollutants, by contrast, are pollutants that are detected in the environment but for which no clear environmental quality standards or emission limits have been set. There have been many studies on the priority control and screening of pollutants for which there are existing measurement standards and exposure limits such as heavy metals (HMs), polychlorinated biphenyls (PCBs), and organochlorine pesticides (OCPs) (Geng et al., 2025; Melymuk et al., 2022; Mohasin et al., 2023; Peng et al., 2022). However, few studies on priority control and screening of uncalibrated priority

* Corresponding authors.
E-mail addresses: dxl@syau.edu.cn (X. Dang), zhaolong@craes.org.cn (L. Zhao).

https://doi.org/10.1016/j.envint.2025.109650
Received 22 March 2025; Received in revised form 24 June 2025; Accepted 26 June 2025
Available online 28 June 2025

pollutants have been reported. The current state standards of China *Soil environmental quality-Risk control standard for soil contamination of development land* (GB 36600–2018) cover only a limited set of pollutant categories (e.g., benzene, dichloromethane, naphthalene), and many emerging pollutants do not have relevant standards and benchmarks, rendering it challenging to make scientific judgement on the exposure and risks from emerging pollutants. The screening of uncalibrated pollutants and development of effective monitoring and control strategies have thus become a hot research topic. Screening of the breadth of uncalibrated priority pollutants is of great significance for understanding and controlling environmental pollution, prioritizing emerging pollutants for regulatory action, and safeguarding ecological safety and public health.

As an important old industrial base in China, the northeastern region has seen the continued accumulation of a large number of unlisted uncalibrated pollutants with insufficient control during long-term industrial activities, posing a serious threat to the ecological environment and human health. Compared with other regions, the northeast was unique in terms of its industrial structure, climatic conditions and geography, with consequent differences in the distribution, migration and transformation patterns of the pollutants. For example, the long cold winters in the Northeast region may affect the transport and transformation processes of pollutants, making their behaviour in soil and water different from that in other regions. However, there are no recent studies on uncalibrated contaminants, and the existing screening methods do not consider the impacts of regional characteristics on the indicators in the selection, and thus their applicability in this region was limited. Therefore, constructing a priority screening mechanism applicable to uncalibrated pollutants at sites in the Northeast and accurately identifying key pollutants is of great significance for scientifically formulating reasonable management strategies, effectively preventing and controlling environmental pollution, and safeguarding ecological safety and public health.

Screening for priority pollutants has been initiated in various countries with a range of different evaluation indicators. In the United States, the Superfund Act system was established in 1980 to determine priority pollutants by expert review, using exposure and toxicity as evaluation indicators (Agency for Toxic Substances and Disease Registry, 2024). The European Union (EU) uses exposure scores (e.g., toxicity, bioaccumulation, and endocrine disruption) from the Combined Priority Setting Programme (COMMPS) calculation model and monitoring data as pollutant effect indices, and a specific risk ranking methodology (EURAM) as the basis for the development of a list of priority pollutants to be monitored (Publications Office of the European Union, 1999). In China, the blacklist of priority pollutants for the aquatic environment was identified based on the scoring of substances using parameters such as product yield, environmental detection rate, degradability, bioaccumulation, acute and chronic toxicity, carcinogenicity, teratogenicity, mutagenicity and feasibility of monitoring, combined with expert empirical methods (Chou et al., 2023; James et al., 2023). The US method relies on expert review, which may introduce some subjectivity, while the EU method combines exposure scores and monitoring data. The Chinese method also combines multiple factors but with a higher emphasis on empirical methods.

The Analytical hierarchy process (AHP) is a multi-criteria decision-making algorithm for complex decision making, often used in conjunction with a comprehensive evaluation method, which is applicable to the evaluation of optimal solutions under the framework of a multi-level indicator system, and can fully reflect the actual meaning of indicators. Currently, this method has been applied to screening of priority pollutants (Zhao et al., 2024). Liu et al. used AHP, combined with the multi-criteria decision-making (MCDM) methods TOPSIS and VIKOR to screen hazardous substances in groundwater in the Beijing-Tianjin-Hebei region, and a total of 23 priority pollutants with high hazards and potential exposures were screened (Liu et al., 2022). However, AHP relies on expert experience to set different thresholds and ranking weights in the process of quantifying the indicator samples, which has strong subjective factors and easily leads to certain quantification bias. CRITIC is a better objective weighting method than either entropy weighting or the standard deviation method, as it integrates the objective weights of the indicators based on the comparative strengths of the evaluation indicators and the conflict between the indicators, and considers the indicator magnitude of variability and the correlation between indicators, and completely using the objective attributes of the data itself for scientific evaluation (Chang and Zhu, 2021). Chang and Zhu (2020) studied the water security assessment framework of Beijing, Shanghai, Tianjin and Chongqing through CRITIC, and the results showed that Beijing has the best water security situation (Chang and Zhu, 2020), but the method was unable to judge indicators that were difficult to quantify such as mutagenicity, carcinogenicity and so on. Therefore, combining CRITIC with AHP will make up for the subjectivity of expert ratings, consider the importance of the indicators themselves, balance the advantages of subjective and objective assignments, and improve the accuracy and credibility of the weightings, which will help authorities and researchers to screen pollutants better and more accurately.

Therefore, the objective of this study is to determine a screening list covering multiple categories of chemical substances based on literature analysis using uncalibrated contaminants from industrial sites in northeast China. By constructing a hierarchical analysis model, toxicity, persistence and mobility were selected as key indicators based on the actual situation in northeast China. In determining the weights of the indicators, AHP was adopted and the relative importance of the indicators is fully considered by using the expert scoring method. Meanwhile, CRITIC was used to determine the objective weights by combining the data characteristics of the indicators. Subjective and objective weightings were given equal weight, each accounting for 50 % of the weight to ensure the accuracy and credibility of the evaluation. The comprehensive evaluation method was used to calculate the comprehensive score of pollutants, with cluster analysis being used to classify the pollutants and screen for the uncalibrated key pollution sources in the northeast region. This approach provides a scientific basis for environmental pollution management, risk prevention and control in the northeast region, and will assist in the formulation of targeted environmental protection strategies.

2. Research methodology

2.1. Study area

The northeast of China (Fig. 1) has always been the major industrial and agricultural base of China, and is dominated by plains and mountains. It has a continental monsoon climate with distinct seasons. The cold winters and relatively dry climate may affect the mobility and persistence of pollutants. Typical industries include machinery manufacturing, petrochemicals, textiles, rubber and plastic products and the paper industry.

2.2. Obtaining a screening list of uncalibrated pollutants at the site

According to the literature research method for finding uncalibrated pollutants at the site, the keywords used to screen the literature from the China National Knowledge Infrastructure (CNKI, https://www.cnki.net/) database were selected to cover various aspects related to priority pollutants and pollutant characteristics of the industry, such as 'priority pollutants'/'preferred pollutants'/'pollutants at the site'/'pollutants characteristic of the industry'/'toxic and hazardous substances'. For the search of Web literature, the keyword "Priorit* and (pollutant* or contaminate* or pollute* or substance*)" was chosen to capture a broader range of relevant literature. The initial screening list of uncalibrated priority pollutants in the study area was determined by the frequency of detection (detection frequency $>$ 3) (Boris et al., 2023),

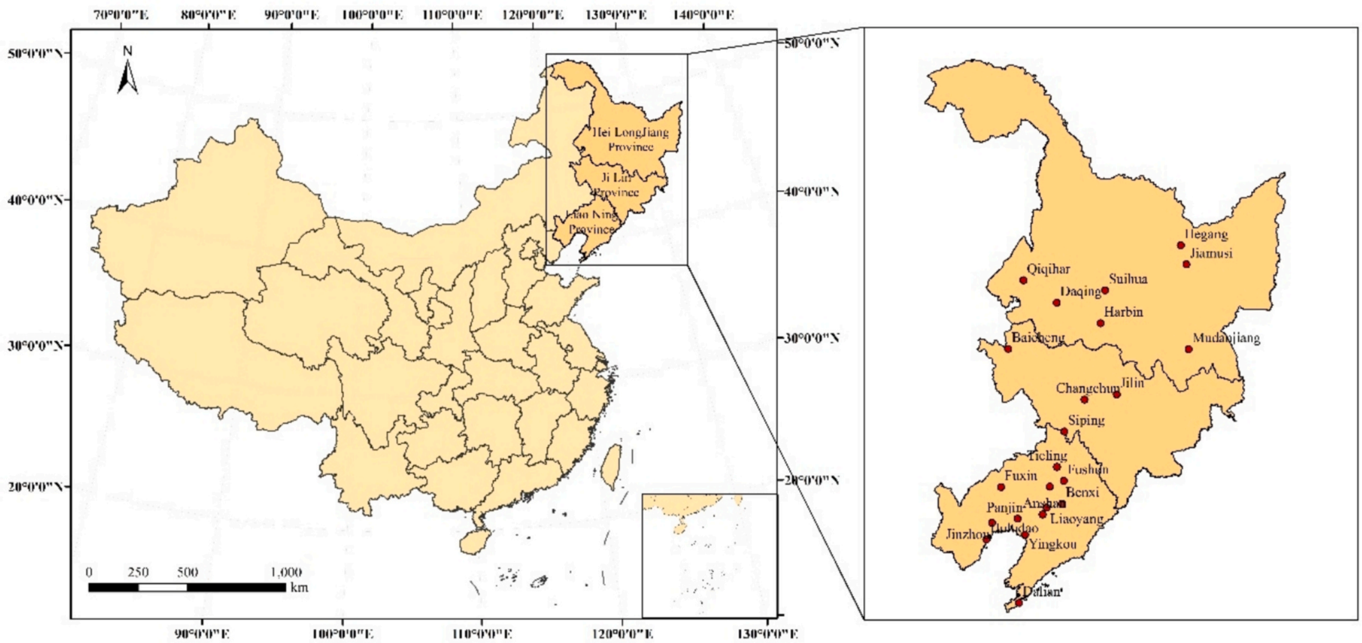

Fig. 1. Study area in the northeast of China, consisting of the Liaoning, Jilin and Heilongjiang provinces.

which means that if one of pollutants at any site was detected more than three times in the literature relating to these sites, then it should be included in the list.

2.3. *Constructing a hierarchical analytical model*

Based on the Technical Guidelines for Assessment of the Environmental and Health Hazards of Chemical Substances, the Catalogue of Hazardous Chemicals, the List of Chemicals for Priority Control and the Action Plan on Controlling New Pollutants of China, a model for

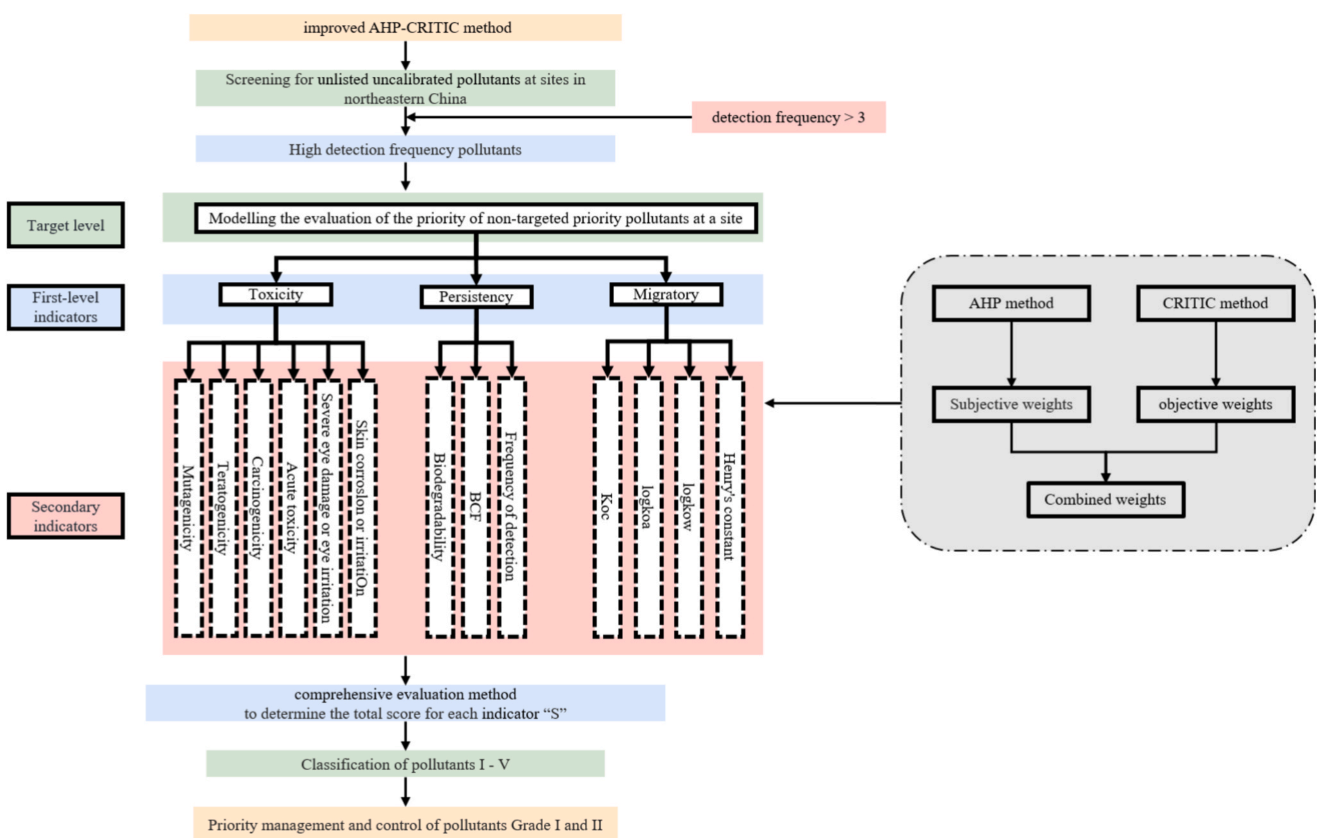

Fig. 2. Evaluation model for the prioritization of uncalibrated priority pollutants at the site of interest (in northeast China).

evaluating the uncalibrated pollutants at the site was constructed (Fig. 2). The selection of toxicity, persistence and migratory as indicators was based on their crucial roles in determining the potential hazards of chemical pollutants. Toxicity indicators include carcinogenicity, teratogenicity, mutagenicity, acute toxicity, severe eye damage or eye irritation, respiratory or skin sensitisation and skin corrosion or irritation. These toxicity indicators were closely related as they all reflect different aspects of the harmful effects of pollutants on living organisms. Persistence includes biodegradability, bioaccumulation, and the frequency of pollutant detection. Bioaccumulation was based on the bioaccumulation coefficient or bioconcentration factor (BCF) of the pollutant; the frequency of the pollutant was based on the number of times the pollutant was found in the literature. The relationship between biodegradability and bioaccumulation was that a more persistent pollutant was likely to have a higher bioaccumulation coefficient. Mobility indicators were the organic chemical absorption constant (Koc), octanol–water partition coefficient ($logK_{ow}$), octanol–air partition coefficient ($logK_{oa}$) and Henry's constant. These mobility indicators are related as they all describe the movement and distribution of pollutants in different environmental media.

2.4. Evaluation criteria and parameters

2.4.1. Parameter acquisition

Measured values were obtained through the European Chemicals Agency (ECHA), the Hazardous Substances Database (HSDB) (National Library of Medicine, 2024), the Toxins and Toxin Targets Database (T3DB), the Chemical Toxicity Database, the Toxicity-Related Databases of Compounds (PubChem) (National Library of Medicine, 2024), the International Agency for Research on Cancer (IARC) (International Agency for Research on Cancer, 2024), and the Organisation for Economic Cooperation and Development (OECD) databases (Organization for Economic Cooperation and Development, 2024). ECHA provides comprehensive data on chemical substances, including their properties and hazards. The HSDB focuses on hazardous substances and offers detailed information on their toxicity and other characteristics. The

Table 1
Indicator hierarchy, classification and values at each level.

Classification of indicators Corresponding score		0 level 0	1 level 1	2 level 2	3 level 3	4 level 4	5 level 5
Toxicity indicators	Carcinogenicity	–	–	IARC Category 3	IARC Category 2B	IARC Category 2A	IARC Category 1
		–	–	IRIS Category D,E	IRIS Category C	IRIS Category B1,B2	IRIS Category A
		–	–	RSLs Category n	–	RSLs Category c	–
	Teratogenicity	–	–	–	Category 2/H362	Category 1B/H361	Category 1A/H360
	Mutagenicity	–	–	–	–	Category 2/H341	Category 1A,1B/ H340
	Acute toxicity (mg/kg)	x ≥ 5000	2000 ≥ x > 5000	300 ≥ x > 2000	50 ≥ x > 300	5 ≥ x > 50	x < 5
	Severe eye damage or eye irritation	–	–	–	Category 2B/H320	Category 2A/H319	Category 1/H318
	Skin corrosion or irritation	–	–	–	Category 3/H316	Category 2/H315	Category 1A ~ 1C/ H314
Persistency indicators	Biodegradability (day)	–	x ≥ 180	90 ≥ x > 180	60 ≥ x > 90	30 ≥ x > 60	x < 30
	BCF	–	0.2 ≤ x ≤ 2.36	2.36 < x ≤ 27.75	27.75 < x ≤ 326.92	326.92 < x ≤ 3851.01	3851.01 < x ≤ 456364
	Frequency of detection	–	3 ≥ x > 8.82	8.82 ≥ x > 25.93	25.93 ≥ x > 76.24	76.24 ≥ x > 224.15	224.15 ≥ x > 659
Migratory indicators	Koc	x ≥ 5000	2000 ≥ x > 5000	500 ≥ x > 2000	150 ≥ x > 500	50 ≥ x > 150	x < 50
	$logK_{ow}$	–	0.05 ≤ x ≤ 0.17	0.17 < x ≤ 0.55	0.55 < x ≤ 1.82	1.82 < x ≤ 6.05	6.05 < x ≤ 20.05
	$logK_{oa}$	–	0.86 ≤ x ≤ 1.64	1.64 < x ≤ 3.12	3.12 < x ≤ 5.95	5.95 < x ≤ 11.35	11.35 < x ≤ 21.63
	Henry's constant (atm-cu m/mole)	–	1.2E-11 ≤ x ≤ 3.13E-08	3.13E-08 < x ≤ 8.19E-05	8.19E-05 < x ≤ 2.14E-01	2.14E-01 < x ≤ 5.59E + 02	5.59E + 02 < x ≤ 1.46E + 06

IARC Category 3: Unclassifiable as to carcinogenicity.
IARC Category 2B: Possibly carcinogenic (limited human/animal evidence).
IARC Category 2A: Probably carcinogenic (strong animal evidence).
IARC Category 1: Carcinogenic to humans.
IRIS Category D,E: Inadequate human evidence (D) or evidence of non-carcinogenicity (E).
IRIS Category C: Possible human carcinogen.
IRIS Category B1,B2: Probable carcinogen (human/animal evidence).
IRIS Category A: Known human carcinogen.
RSLs Category n: No carcinogenic concern.
RSLs Category c: Potential carcinogenic concern.
Teratogenicity Category 2/H362: Suspected of damaging the unborn child (animal evidence).
Teratogenicity Category 1B/H361: Presumed human developmental toxicant (animal evidence).
Teratogenicity Category 1A/H360: Known human developmental toxicant.
Mutagenicity Category 2/H341: Suspected of causing genetic defects.
Mutagenicity Category 1A/H340: Known mutagen (human evidence).
Mutagenicity Category 1B/H340: Presumed mutagen (animal evidence).
Severe eye damage or eye irritation Category 1/H318: Causes irreversible eye damage.
Severe eye damage or eye irritation Category 2A/H319: Causes reversible eye irritation (severe, lasting > 7 days).
Severe eye damage or eye irritation Category 2B/H320: Causes reversible eye irritation (mild, lasting ≤ 7 days).
Skin corrosion or irritation Category 1A-1C/H314: Causes skin corrosion (1A = severe, 1B/1C = moderate).
Skin corrosion or irritation Category 2/H315: Causes skin irritation (reversible damage).
Skin corrosion or irritation Category 3/H316: Causes mild skin irritation (transient effects).

T3DB is dedicated to toxins and their targets, providing valuable data for assessing the toxicity of pollutants. The Chemical Toxicity Database and PubChem offer a wide range of data on chemical compounds, including their toxicity and related properties. IARC is an important source for carcinogenicity data. The OECD databases provide data on various aspects of chemical substances, including their environmental behavior.

If the measured values could not be obtained, the predicted values were obtained, and the Estimation Program Interface (EPI Suite) developed by the U.S. Environmental Protection Agency (EPA) was used to predict the biodegradation half-life, Henry's constant, organic carbon adsorption coefficient (koc), n-octanol–water partitioning coefficient ($logK_{ow}$), n-octanol–air partitioning coefficient ($logK_{oa}$), and bio-concentration coefficient (BCF); and the predicted values were obtained using the OECD and EECD databases. The QSAR toolbox developed by the OECD and ECHA was used to predict skin sensitisation; T.E.S.T. developed by the US EPA was used to predict acute toxicity. The EPI Suite is a useful tool for predicting various parameters when measured values were not available. It uses established algorithms and models to estimate the values. The QSAR toolbox and T.E.S.T. were also important tools for predicting specific properties of pollutants based on their chemical structures and other factors.

2.4.2. Evaluation standardisation

Table 1 shows the indicator hierarchy, classification and values at each level. Carcinogenicity grading was based on international databases (IARC, 2013; US National Library of Medicine, 2017), the US EPA's Integrated Risk Information System (IRIS), and the Risks of Carcinogenicity Classifications (RSLs) (Tabs were as of May 2024). The reason for referring to multiple databases is to ensure a comprehensive and accurate assessment of carcinogenicity. IARC is a leading international authority on carcinogenicity research, providing a global perspective. IRIS offers data on the risk of cancer from exposure to chemical substances in the United States. RSLs provide an additional classification system for carcinogenicity. Teratogenicity, mutagenicity, acute toxicity, severe eye damage or eye irritation and skin corrosion or irritation classification were all based on China's GB30000.24-2013 Specification for Classification and Labelling of Chemicals (National Standardization Administration, 2013a; b, c, d, e). This standard is widely used in China for classifying and labelling chemicals based on their toxicity and other characteristics. It provides a consistent and reliable method for evaluating and comparing these properties of pollutants.

Biodegradability was judged on the basis of the half-life of the substance in water, soil, air and substrate, and the grading is based on the Technical Guidelines for Environmental Safety in the Use of Pesticides; because there is no specific standard for the bioaccumulation coefficient (BCF) and the frequency of the pollutants and the span is large, the equipotential progression method is adopted for its grading. The Technical Guidelines for Environmental Safety in the Use of Pesticures provide a reasonable method for grading biodegradability based on the half-life of the substance.

2.5. Determination of indicator weightings

2.5.1. Subjective weights based on the analytical hierarchy process

AHP was used to calculate the subjective weights of the indicators. Five experts in the environmental field with different academic backgrounds (in China) were selected to score the results. The composition of the experts is as follows: (1) Each expert has an educational background in the field of environmental risk assessment, environmental geochemical behaviour, ecological risk assessment, soil and groundwater remediation, or soil environmental exposures and their health effects, and all of them have PhD degrees. (2) Each expert is familiar with the industrial background of the area and has many years of research experience in this field. Expert scores were obtained by expressing the relative importance of all factors in the current layer compared to a factor (quasi-edge or target) in the previous layer according to a pairwise comparison matrix. The element a_{ij} of the pairwise comparison matrix represents the result of the comparison of the i^{th} factor with respect to the j^{th} factor, and this value is was constructed using Saaty's 1–9 scale (Verma et al., 2022) (Table S1) and combining it with expert scores to construct the judgement matrix A, as shown in Eq. (1).

$$A = \begin{pmatrix} a_{11} & \cdots & a_{1n} \\ \vdots & \ddots & \vdots \\ a_{n1} & \cdots & a_{nn} \end{pmatrix} \tag{1}$$

in which $a_{ij} \neq 0$, i = 1, 2…n, j = 1, 2…n.

The formula for calculating indicator weights was as follows:

The m^{th} power of the product of each row was calculated to obtain an m-dimensional vector, as per Eq. (2):

$$\overline{\omega}_i = \sqrt[n]{\prod_{j=1}^{n} a_{ij}} \tag{2}$$

The subjective weight ω_i is obtained by normalising the $\overline{\omega}_i$ vectors to weight vectors, using Eq. (3):

$$\omega_i = \overline{\omega}_i / \sum_{i=1}^{n} \overline{\omega}_i \tag{3}$$

The largest eigenroot was solved for, and the Consistency Index (CI), Random Index (RI), and Consistency Ratio (CR, calculated by dividing CI by RI) are calculated, and their consistency was assessed (generally CR < 0.1 indicates acceptable consistency).

The maximum characteristic root of the judgement matrix was calculated with Eq. (4):

$$\lambda_{max} = \sum_{i=1}^{n} (A\omega)_i / n\omega_i \tag{4}$$

The CI of the judgement matrix was calculated using Eq. (5):

$$CI = \lambda_{max} - n/n - 1 \tag{5}$$

RI is the average stochastic CI, which is obtained by checking the table of values of stochastic consistency indicator RI obtained by Saaty simulation for 1000 repetitions according to matrix order n. Table S2 shows the values of RI.

The consistency ratio CR of the judgement matrix was calculated using Eq. (6):

$$CR = CI/RI \tag{6}$$

When CR < 0.1 the judgement matrix was considered to satisfy the consistency condition, indicating that the weight allocation was reasonable.

2.5.2. CRITIC based objective weights

The CRITIC method is used to determine the weights of criteria based on the contrast intensity (variability) and conflict (redundancy) between them, leading to a robust and objective weighting. Assuming k pollutants and p evaluation indicators, a raw indicator data matrix was formed, as per Eq. (7):

$$X = \begin{pmatrix} x_{11} & \cdots & x_{1p} \\ \vdots & \ddots & \vdots \\ x_{k1} & \cdots & x_{kp} \end{pmatrix} \tag{7}$$

x_{11} is the original data of the first pollutant and the first indicator. x_{kp} is the original data of the k^{th} pollutant and the p^{th} indicator, In order to eliminate the impact of the different quantitative indicators on the evaluation results, it was necessary to process the indicators. The CRITIC weighting method generally uses forward or reverse processing, the formulas for which are as follows:

Normalisation processing Eq. (8):

$$x_{kp} = x_p - x_{min}/x_{max} - x_{min} \quad (8)$$

where x_p is the original data, x_{min} is the minimum value of all data for that indicator, x_{max} is the maximum value of all data for that indicator, and x'_{kp} is the processed data. Reversal of the treatment, or reverse processing, is used to refine or validate the results obtained from forward processing, and was performed as per Eq. (9):

$$x'_{kp} = x_{max} - x_p/x_{max} - x_{min} \quad (9)$$

Indicator variability was expressed as standard deviation using Eq. (10):

$$\begin{cases} \overline{X}_p = \frac{1}{n}\sum_{k=1}^{n} X_{kp} \\ S_p = \sqrt{\sum_{k=1}^{n} \left(X_{kp} - \overline{X}_p\right)^2 / n - 1} \end{cases} \quad (10)$$

S_p denotes the standard deviation of the p^{th} indicator, which was used in CRITIC to indicate the fluctuation of the difference in the value of each indicator. A higher standard deviation shows that the indicator has a greater variability, meaning it has a stronger influence on distinguishing between alternatives. Thus, indicators with higher standard deviations are considered more important because they provide more information for decision-making.

Indicator conflictability, which measures how much the information provided by one indicator overlaps with or contradicts the information provided by another indicator, is expressed as a coefficient of variation, using Eq. (11):

$$R_p = \sum_{k=1}^{n} (1 - r_{kp}) \quad (11)$$

where r_{kp} denotes the correlation coefficient between evaluation indicators k and p.

Informativeness refers to the ability of an indicator to provide meaningful, relevant, and distinct information that aids in distinguishing between alternatives to make informed decisions, and is determined using Eq. (12):

$$C_p = S_p \times R_p = \sqrt{\sum_{k=1}^{n} \left(X_{kp} - \overline{X}_p\right)^2 / n - 1} \sum_{k=1}^{n} (1 - r_{kp}) \quad (12)$$

Objective weighs are derived from the inherent properties of the data, such as variability or correlation without input from decision-makers or experts, and are calculated using Eq. (13), where ω_j is the objective weight of the j^{th} indicator:

$$\omega_j = C_j / \sum_{j=1}^{p} C_j \quad (13)$$

2.5.3. Combined weights (combining subjective and objective weights)

The choice of 50/50 subjective and objective weighting is based on a consideration of the balance between expert judgement and objective data characteristics. In the field of environmental pollutant screening, experts can make theoretical and practical judgements on the importance of indicators based on their deep professional knowledge and rich experience, and such subjective judgements have a value that cannot be ignored in the assessment process. However, there are some limitations in expert scoring, such as the possibility of being influenced by personal experience, knowledge background and subjective preferences, which leads to a certain degree of subjectivity in the scoring results. Objective data, on the other hand, are derived from a large number of actual monitoring and scientific studies, and accurately reflect the actual performance of pollutant indicators, such as the variability and conflict of the indicators, which provides a solid factual basis for the assessment. However, objective data are not perfect, and some indicators are difficult to quantify or difficult to obtain, which may make the assessment incomplete.

Setting the subjective and objective weightings equal allows the experts' in depth experience in the, analysis of the multi-dimensional characteristics of pollutants to be considered, and ensures the professionalism and accuracy of the assessment. Using the characteristics of the objective data, can reduce the interference of subjective factors and make the results more objective and reliable. Thus, the two complement each other to enhance the scientific robustness and reasonableness of the indicator weightings and provides strong support for the accurate screening of priority pollutants.

The formula for calculating the weighting of composite indicator, ω, is given in Eq. (14):

$$\omega = 50\%\omega_i + 50\%\omega_j \quad (14)$$

ω is the composite weight of the indicators. ω_i is the subjective weight and ω_j is the objective weight. The equal weighting method gives equal importance to both the subjective judgment of the experts and the objective information derived from the data, ensuring a more comprehensive and balanced evaluation of the indicators.

2.6. Combined scoring and determination of priority control pollutants

The list of uncalibrated priority pollutants was prioritised using a comprehensive evaluation method for uncalibrated pollutants.

The composite score for each pollutant was determined from the individual indicator scores and weights using the following formula:

$$S = \sum_{t=1}^{n} S_t \omega_t \quad (15)$$

where S_t is the score of each indicator for the pollutant, ω_t is the weight of each indicator and S means total score.

The comprehensive evaluation method calculates the weighted sum of the scores of all indicators for each pollutant. This weighted sum reflects the overall importance and impact of each indicator on the pollutant priority control grade.

2.7. Data processing and calculations

According to the relative size of the composite score and applying the software SPSS 26.0, the pollutants were classified into five grades (I to V) using the systematic clustering method with the squared Euclidean distance as the measure. The composite scores of the pollutants decreased from I to V, with grades I and II identified as high-priority pollutants, III were listed as medium-priority pollutants, and grades IV and V as low priority pollutants.

3. Results

3.1. Screening results for uncalibrated pollutants at sites in northeast China

The literature research method screened a total of 549 types of uncalibrated pollutants from sites in northeast China, and the initial screening list was formed according to the principle of 'detection frequency > 3', covering a total of 170 types of uncalibrated pollutants. According to their chemical structure, physical and chemical properties and environmental behaviour, the pollutants were classified into eight categories: polycyclic aromatic hydrocarbons (PAHs), perfluorinated and polyfluorinated alkyl compounds (PFAS), organophosphoric esters (OPEs), organochlorine compounds (OCs), phthalates (PAEs), heterocyclic compounds, benzene and benzene derivatives, and other compounds (Table S3). According to the statistics on the frequency of detection of pollutants, PAHs were the main pollutant group (64 % detection frequency), and benzene and benzene derivatives were detected less frequently (11 % detection frequency), as they are involved in a wide range of pollutants (Fig. 3). The thickness of the lines in Fig. 4 indicate the frequency of detection, and the main source of pollutants was the petrochemical industry (76.45 % detection frequency), which is likely related to the raw materials used in the petrochemical industry in northeast China, including the crude oil and coal produced in the Daqing Oilfield and other places. Crude oil contains a large number of organic compounds, some of which can be used as precursor substances for PAHs (Yerulker et al., 2023). During processing, these precursors are converted to PAHs under specific conditions. Coal also contains a certain amount of aromatic hydrocarbons (Xiu et al., 2023), which may increase the generation of PAHs during the petrochemical production process (Howard et al., 2021; Wu et al., 2021).

3.2. Calculation of composite weights for indicators

The five experts compared the indicators one by one, based on the importance of the indicator in screening for unlisted uncalibrated pollutants and the scoring results reflect the degree of importance of the indicators at the previous level. The descriptive statistics are shown in Fig. 4, in which the extreme value was large and the scoring was unevenly distributed, which indicates that the experts have quite different opinions on the degree of importance of the indicators, and there was thus a strong subjectivity. The judgement matrices have passed the consistency test (Table S4).

The CRITIC weighting method was used for objective weight calculation. As can be seen from Table S5, there was no obvious difference between the 13 indicators in terms of indicator conflict; in terms of indicator variability, the indicators of skin corrosion/irritation and severe eye damage/eye irritation have relatively large variability, which means that they fluctuate a lot, and they should thus occupy higher weights. The mammalian acute toxicity, half-life, and organic carbon adsorption coefficient koc indicators are inverted indicators, where lower values are better, while the other indicators are forwarded, meaning that higher values are more desirable. The weights of each indicator were analysed and correlations between the indicators are expressed by the correlation coefficient. The stronger the correlation with other indicators, the less conflict the indicator has with other indicators (Li et al., 2021), reflecting that more information was the same, and thus which weakens the strength of the evaluation of the indicator, and thus the weight assigned to the indicator should be reduced.

The comprehensive weight of the indicator layer relative to the target level (Fig. 2) was calculated according to the formula shown in equation (13). The combined weights after correction using CRITIC were shown in Fig. 5. The weight of the carcinogenicity indicator in the composite weight was 17.69 %, and the weight of the Henry's constant indicator was 3.02 %, which indicates that carcinogenicity was much more important than Henry's constant as an indicator, which was consistent with the expert judgement and environmental science knowledge (Li et al., 2022). In addition, the top three combined weights were carcinogenicity, severe eye damage/eye irritation, and reproductive toxicity, which are all toxicity indicators and should be given sufficient attention in the evaluation process. In the improved method of combining AHP and CRITIC, carcinogenicity was ranked first, followed by severe eye damage/eye irritation.

The weighting results illustrate the significant advantages of the combined AHP-CRITIC approach. This method was able to simultaneously balance the professionalism of the evaluation and the objectivity of the data. In the screening process of priority pollutants, on the one hand, through the analytical hierarchy process (AHP), the knowledge and experience of professionals can be fully utilised to carry out in-depth analysis and assessment of pollutants from multiple perspectives, ensuring that the evaluation process has a high degree of professionalism and accuracy. On the other hand, the CRITIC method, based on the objective characteristics of the data, can effectively explore the information contained in the data itself, avoiding excessive interference from subjective factors and making the screening results more objective and reliable. In summary, the combined AHP-CRITIC method shows strong adaptability and effectiveness in priority pollutants screening, and was very suitable for priority pollutants screening work.

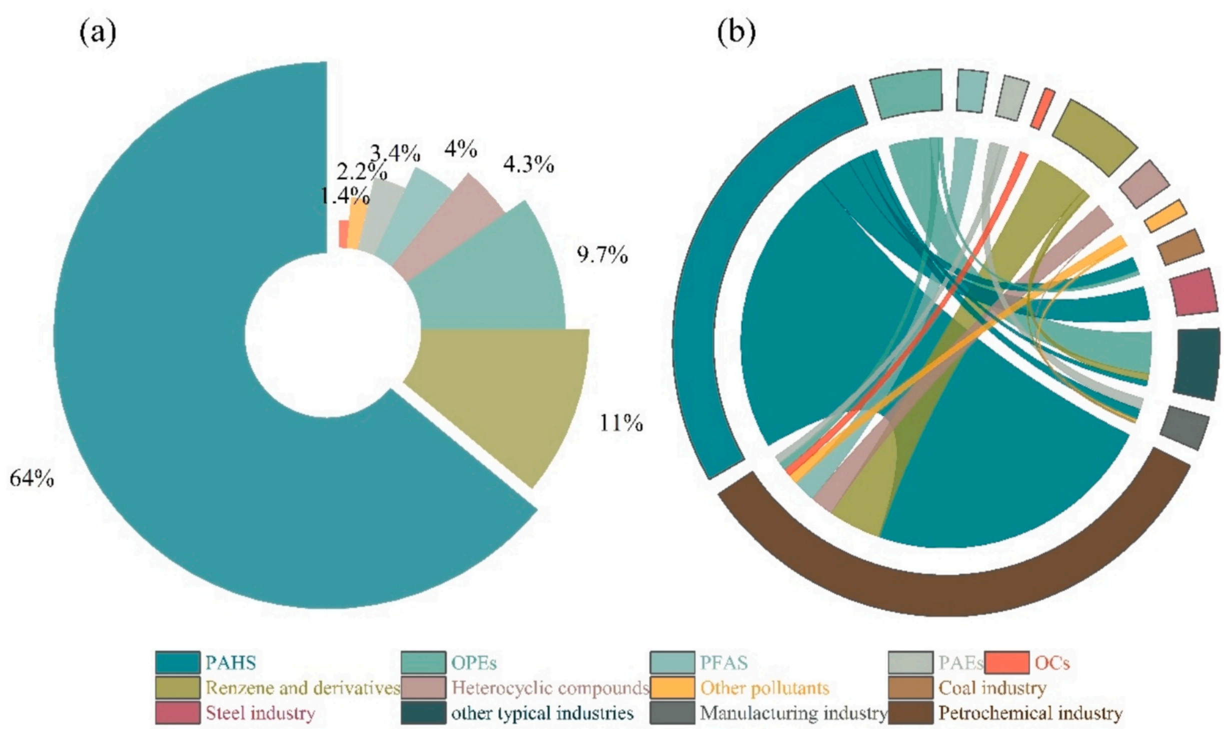

Fig. 3. Proportion of detection frequency for each of the 8 types of pollutants (a); sources of the uncalibrated pollutants by category (b).

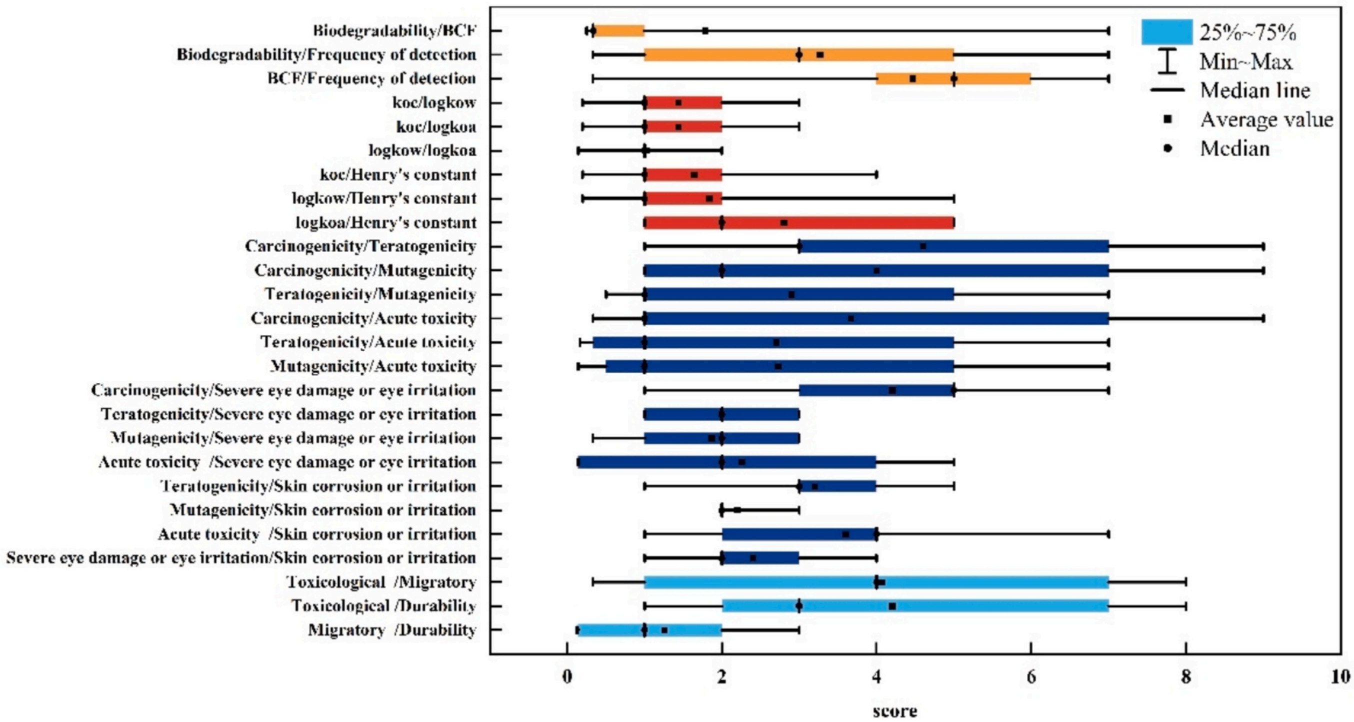

Fig. 4. Distribution of expert scores for the pairwise analysis of indicators.

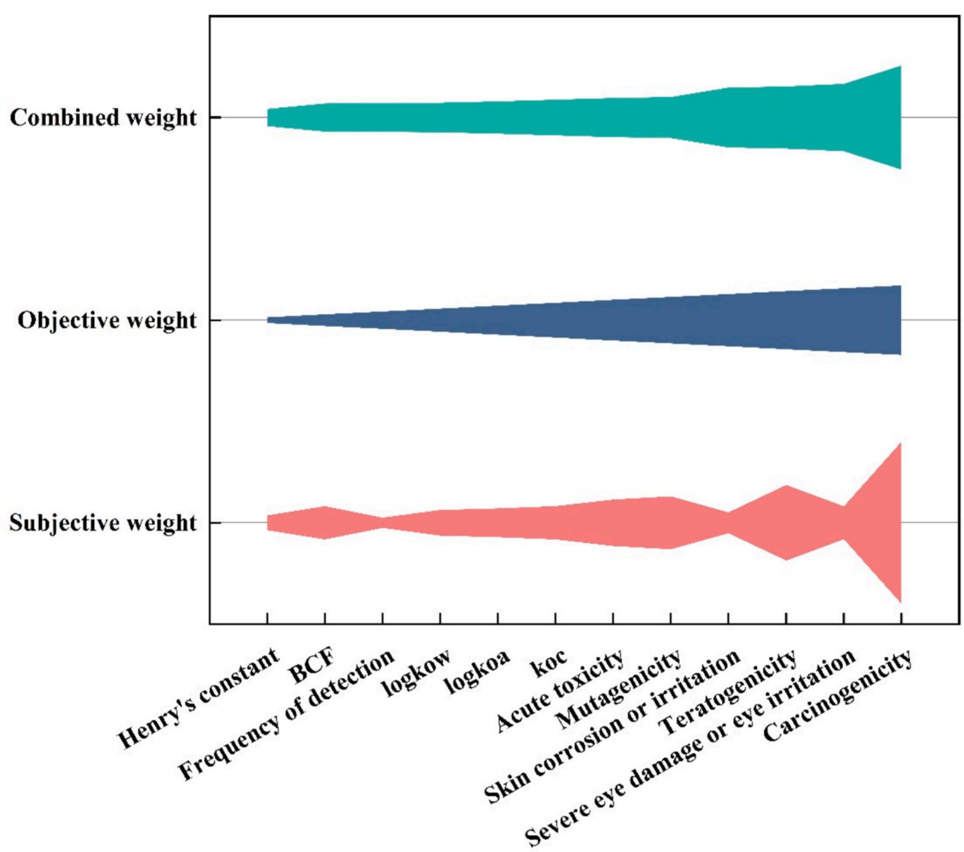

Fig. 5. Combined weights of indicators across the 13 indicators.

3.3. Classification and Inventory Determination of uncalibrated priority pollutants in northeast China

Based on the AHP-CRITIC multi-indicator composite scoring method established in this study, 170 uncalibrated pollutants were screened. The values of pollutant indicators were queried in Table S6 and a cluster analysis was conducted to classify the pollutants based on the total score "S" of the selected uncalibrated pollutants as indicators. The clustering results are shown in Fig. S1. A total of 11 chemicals, including 4 PFAS, 3 benzene and its derivatives, 2 other types of pollutants, 1 PAH, and 1 OCs (Fig. 6), were classified as high-priority pollutants among the uncalibrated pollutants identified from literature as being present at sites in northeast China, based on their total scores (Table 2) with all being either Grade I or Grade II pollutants, with a total score of 265——383; 16 benzene and its derivatives, 7 PAFS, 5 PAHs, 4 heterocyclic compounds, 3 OPEs, 2 OCs, 2 other categories of pollutants, and 1 PAEs with a total score 230——265; were classified as medium-priority pollutants. Another 36 benzene and its derivatives, 24 other categories of pollutants, 21 heterocyclic compounds, 19 PAHs, 11 OPEs, 4 PFAS, 3 PAEs, and 1 OCs, with a total score 138——230, were classified as low priority pollutants. The full list of pollutants and their score are given in Table S7 in the Supplementary Information.

As further evidenced by the contribution of each indicator to the total score of the individual pollutants (Fig. 7), PFOA and PFOS were among the emerging persistent toxic pollutants (per and polyfluoroalkyl substances, PFAS) that were highly prioritized, mainly because of their high carcinogenicity, followed by a sensitive response from a human health perspective, whereas the underlying environmental fate profiles, e.g., persistence and transport, were not dominant factors. Benzene and its derivatives styrene and acrolein were listed as high-priority pollutants mainly because of their carcinogenicity, but other indicators contributed equally, and all had relatively low impacts. Among the PAHs group of pollutants, anthracene was detected very frequently, and carcinogenicity was very strong, and they were also listed as high-priority uncalibrated pollutants.

3.4. Industry sources and cause profiling of uncalibrated priority pollutants

The high priority uncalibrated pollutants at sites in northeast China were mainly composed of chemicals currently produced or used at high grades, as well as PFAS substances that have been used extensively throughout history. The carbon–fluorine bond is the strongest bond known to nature, and is extremely resistant to degradation in the natural environment and in the human body, resulting in bioaccumulation (Liu et al., 2019). For example, PFAS has excellent repellency for water, oil, and dirt, explaining why this class of compounds was widely used in many sectors, including industrial and manufacturing. Among the PFAS family, PFOA was one of the most widely used perfluorosurfactants, being used as a fire (flame) retardant, water repellent, and antifouling agent in the production and processing of consumer goods (textiles, carpets, and leather, etc.) and industrial goods (graphite, semiconductors, and fire-fighting foams, etc.). Similarly, PFOS was used in surface antifouling treatments such as stain, oil and water repellents for personal clothing, home decor, and automotive interiors. PFOA was described as a 'probable carcinogen' or 'suggested carcinogen' in the report of the Science Advisory Board of the U.S. National Environmental Protection Agency (NEPA), and PFOA, PFOS, etc., have now become the second most important carcinogens after organochlorine pesticides (OCPs) and dioxins. PFOA and PFOS are a new type of persistent organic pollutant (POP) alongside OCPs and dioxins, and have been detected in the water bodies of the study area even though they have long been listed as prohibited or restricted organic pollutants under the POPs Convention.

PAHs in sites in northeast China mainly originate from incomplete combustion of fossil fuels such as coal in the petrochemical, coal, and iron and steel industries. PAHs are volatilised at low temperatures to be released from the environment to the atmosphere, and due to their semi-volatility and long-range atmospheric transport capacity, and the natural climatic influences in northeast China, PAHs are ubiquitous in the environment and have become an important source of pollutants in the atmosphere, posing ecological and human health risks to the site.

Organochlorine compounds (OCs) were often made into disinfectants, fungicides, insecticides, etc. Since the outbreak of the global novel coronavirus pneumonia (COVID-19) epidemic in December 2019, chlorine-containing disinfectants have been used in public places such as factories in large quantities, and although their concentration in soil was generally low, they pose a threat to soil biosafety due to their high stability. Unintentional emissions from industrial production, for example, were a major source of HCBD in the environment and were commonly used in the petrochemical industry in the production of trichloroethylene (TCE) and perchloroethylene (PCE) and in the smelting of magnesium, in addition to being solvents for rubber and other polymers, pesticides, herbicides, fungicides, heat-transfer fluids, and hydraulic fluids, etc. The Conference of the Parties to the Stockholm Convention on POPs, at its eighth meeting, in 2017, listed HCBD in Annex C, meaning that governments must "control its unintentional emissions". In China, control standards on HCBD only include surface water, exhibition sites, domestic drinking water, and pollutant discharges from the petrochemical industry, and there is currently a lack of standards in the area of site management and methods for monitoring its emissions (hence it is considered unlisted uncalibrated).

Benzene and its derivatives have a stable cyclic structure, which makes it difficult for them to be degraded naturally in the environment, and their solubility in water and organic solvents allows them to migrate and diffuse through water, soil and other environmental media, expanding the scope of pollution. Petrochemical, pharmaceutical, dye and rubber industries use benzene and its derivatives as raw materials or solvents in their production processes, and these substances may leak, volatilise or be discharged into the environment during production processes. Styrene was an important product in the petrochemical industry chain, and the northeast China has rich oil resources and a related industrial base, so the petrochemical industry was one of the main sources of styrene production in northeast China. In the production of rubber and plastic products, styrene was an important raw material for synthetic rubber and plastic, and there were many rubber and plastic

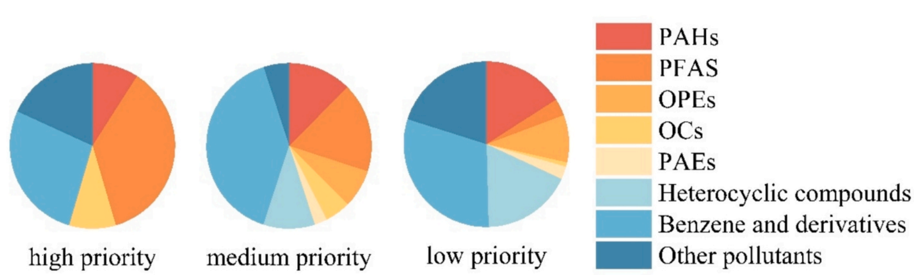

Fig. 6. Priority distribution of pollutants identified in northeast China by category.

Table 2
Clustering results for uncalibrated pollutants identified at sites in northeast China.

Grade	Pollutant
Grade I	perfluorooctanoic acid (PFOA)
Grade II	Acrolein, Perfluorooctane Sulfonate (PFOS), Styrene, Perfluorobutanoic Acid (PFBA), Anthracene (Ant), Methyl Isocyanate (MIC), 2,4-Dimethylphenol, Hexachlorobutadiene (HCBD), 2,6-Dimethylphenol, Perfluorononanoic Acid (PFNA)
Grade III	Perfluorodecanoic Acid (PFDA), 2-Nitrotoluene, Quinoline, Acenaphthylene (Acy), 1-Adamantanamine, N-Hexane, Perfluorododecanoic Acid (PFDoA), Pyrene (Pyr), 3,4-Dimethylphenol, Perfluorohexanesulfonic Acid (PFHxS), P-Methylphenol, Phenol, Trioctyl Phosphate (TEHP), 2,4-Di-Tert-Butylphenol, Perfluoroundecanoic Acid (PFUdA), 1,2,3-Trichlorobenzene, Acenaphthene(Ace), 1,3,5-Trimethylbenzene, Trimethyl Phosphate (TMP), 2,3-Dimethylphenol, 2,5- Dimethylphenol, Perfluorohexanoic Acid (PFHxA), 3,5-Dimethylphenol, Triphenylphosphonic Acid (TPPO), 2-Methylpyridine,1,4-Diethylbenzene, Bis(Trimethylphenyl)Benzene, Perfluorotetradecanoic Acid (PFTeDA), 5-Methyl-1H-Benzotriazole, 3-Ethylphenol, Benzophenanthrene, Fluorene, 2-Ethylphenol, Perfluoroheptanoic Acid (PFHpA), Dimethyl Phthalate (DMP), 1,2,4-Trichlorobenzene, O-Cresol, 3,5-Dimethylpyridine, Tributyl Phosphate (TnBP), 1,2,4-Trimethylbenzene A
Grade IV	1-Bromoadamantane, 1,3-Dichlorobenzene, M−Methylphenol, Carbazole, 2-Vinylnaphthalene, 2-Methylquinoline, 1,3-Diethylbenzene, 2,3,6-Trimethylphenol, 2,3-Benzofuran (Ben), P-Methylstyrene, 4-Ethylphenol, 1-Methylphenanthrene, Perfluorooctadecanoic Acid (PFODA), 2-Ethyltoluene, 1-Naphthol, 2,6-Dimethylpyridine, Perfluoropentanoic Acid (PFPeA), 1,2-Diethylbenzene, Tris (2-Chloroethyl) Phosphate (TCEP), Perfluorohexadecanoic Acid (PFHxDA), 1-Methylisoquinoline, Phenanthrene (Phe), 3-Cyanopyridine, 2,4,6-Trimethylphenol, Guaiacol, 4-Methylquinoline, 4-Methylindole, 1,2,3,4-Tetramethylbenzene, 2,3,5-Trimethylphenol, 1,2,3,4-Tetramethylbenzene, 1,2,3,4-Tetramethylbenzene, 1,2,3,4-Tetramethylphenol, 1,2,3,4-Tetramethylphenol, 2-Ethylbenzene, 2-Ethylbenzene, 1-Ethylbenzene, 1,2,3,5-Trimethylphenol, 2-Ethylbenzene, 2-Ethylbenzene, 2-Ethylbenzene, 2-Ethylbenzene, 1-Ethylbenzene, 1,2,3,4-Tetramethylbenzene, Tripropyl Phosphate (TPrP), Trimethylphenol, 2-Ethyl-6-Methylphenol, 7,8-Benzoquinoline, Phenanthridine, Pentamethylbenzene,2-Methylnaphthalene, N-Octane, 2,6-Di-Tert-Butyl-4-Ethylphenol, 4-Methyl-2-Nitrophenol, 5-Methyl-2-Nitrophenol, 2,6-Diphenylpyridine, Diisobutyl Phthalate (DIBP), Benzo[G,H,I]Perylene, 2-Methylindole, Fluoranthene, 2-Methylphenanthrene, Acetone, O-Aminoacetophenone, Dibenzylidene, Dibenzo[G,H,I]Perylene, 2-Methylindole, Fluorescent Anthracene, 2-Methylphenanthrene, Acetone, O-Aminoacetophenone, O-Aminoacetophenone, Dibenzylidene, Dibenzopyrone, O-Aminoacetophenone. Acetone, O-Aminoacetophenone, Dibenzofuran, 2-Methyl-3-Nitrophenol, 1-Methylnaphthalene, 4-Methoxyphenol, Dibenzopyridine, 2,6-Di-Tert-Butyl-P-Cresol, Indole, 2-Methylthiobenzothiazole, Tris (2-Butoxyethyl) Phosphate (TBEP), Dibutyl Phthalate (DBP), 1-Adamantanemethyl Ketone, Isopropanol, 1-Methylpyrene, 3,4,5-Trimethylphenol, 3-Nitrotoluene, Triethyl Phosphate (TEP), Isobutyl Formate, N-Ethylaniline, Benzotriazole, N-Ethyltriazole. Aniline, Benzotriazole, 3-Chloroaniline, 4-Nitrotoluene, Propylbenzene
Grade V	2-Isopropylnaphthalene, 2-Methoxythiophene, Piperylene Ring, Dodecane, Diethyl Phthalate (DEP), Tris(Nonylphenyl) Phosphite (TNPP Isomers), Tris (1,3-Dichloro-2-Propyl)Phosphate (TDCP), Benzothiazole, 1,3-Dimethylnaphthalene, Oleamide, 1,2-Dimethoxybenzene, Propylene, Perfluorinated 13 Acid (PFTrDA), Phytocarbane, 2,7-Methylnaphthalene, 2,3,5-Trimethylnaphthalene, Decane, Isopentane, Tri (2-Chloropropyl) Phosphate (TCPP), M−Ethyltoluene, N-Butane, 2,4-Dimethylpyridine, Tridecane, Triphenyl Phosphate (TPhP), Propane, 2-Ethylhexyl Diphenyl Phosphate (EHDPP), 1-Methylanthracene, Cis-2-Butene, 6-Methylquinoline, Tetradecane, Pentadecane, 1,2,4,5-Tetramethylbenzene, Patchouli, 3-Acetylpyridine, Triisobutyl Phosphate (TiBP), Tris(Nonylphenyl) Phosphite (TNPP), Hexamethylbenzene, 2-Methylglutaronitrile, Benzyl Benzoate, M−Xylenonitrile, Hexadecanamide

Grade I and Grade II=high priority; Grade III=medium priority; Grade IV and Grade V=low priority.

product enterprises in northeast China, which use styrene from petrochemical enterprises. The machinery manufacturing industry may use rubber or plastic products made from styrene as parts or accessories in the production process, such as for seals, gaskets, rubber hoses, etc.

3.5. Comparative study with major foreign lists

The results of the screening of unlisted priority pollutants in northeast China are compared with nine lists (Table 3). Among the unlisted priority pollutants screened in this study, eight substances are included in the REACH, accounting for 72.73 %. Seven substances are listed in the TSCA, accounting for 63.64 %. The screened pollutants generally cover the major international control lists. PFOA and PFOS are listed as priority control substances in seven international lists (including the REACH, TSCA, and CEPA). Although these substances are included in China's 'List of Key Controlled New Pollutants (2023 Edition),' they still lack site-specific standards. HCBD is listed as a priority control substance in seven international lists and is a new type of persistent organic pollutant.

4. Discussion

The indicator system was fine-tuned to make it highly suitable for the northeast of China and for the specific sites, as well as adapted to the screening of uncalibrated pollutants. The most important primary indicator was toxicity and the most important secondary indicator was carcinogenicity, which was consistent with the results of previous studies. The previous evaluation indicators were mainly centred on exposure and hazard assessment (Zhao et al., 2024) and focused on detection concentration and detection frequency (Liu et al., 2024) whereas the present study focused on indicators of toxicity, persistence and transport. The improved AHP-CRITIC method's global applicability is demonstrated through comparisons with international pollutant lists. The effectiveness of the improved AHP-CRITIC method is reflected in its consistent identification of key pollutants (such as PFOA), which is consistent with the priorities established by major international frameworks. The method's output results are consistent with the European Union's Water Framework Directive's emphasis on PFAS substances and the US EPA's screening levels for industrial site pollutants, and are of significant value in situations where monitoring data is limited.

Most previous studies focused on calibrated pollutants (Ding et al., 2024; Huang et al., 2024; Szabo et al., 2024), while this study screens for uncalibrated pollutants, whose potential hazards were difficult to accurately predict due to the relatively few studies on uncalibrated pollutants, the paucity of relevant data, the difficulty of detection, and the lack of clear measurement standards and criteria. While such predictions provide critical screening insights, they carry inherent uncertainties from model assumptions and limited structural-activity validation for emerging contaminants. Based on conservatism and aligned with the precautionary principle, the selection of more conservative indicators such as toxicity, persistence and mobility can help to ensure an effective assessment of the potential risks of uncalibrated pollutants. By focusing on these key characteristics, the possible impacts of uncalibrated pollutants on the environment and human health can be inferred, providing an important reference for subsequent research and management, and laying the foundation for further exploration of the characteristics of uncalibrated pollutants and their risk assessment.

The northeast China was subject to its own natural climate with relatively low temperatures, which can lead to a slowing down of molecular movement, reducing their diffusion rate in environmental media (Ghosh and Mukherji, 2023; Zhu et al., 2022), and may also lead to a reduction in the solubility of pollutants in soils and water bodies (Neumann et al., 2017), resulting in weaker mobility. At lower temperatures, the degradation of pollutants was slowed down and both chemical and biological degradation processes were significantly inhibited (Tao et al., 2024). Since persistent pollutants may accumulate

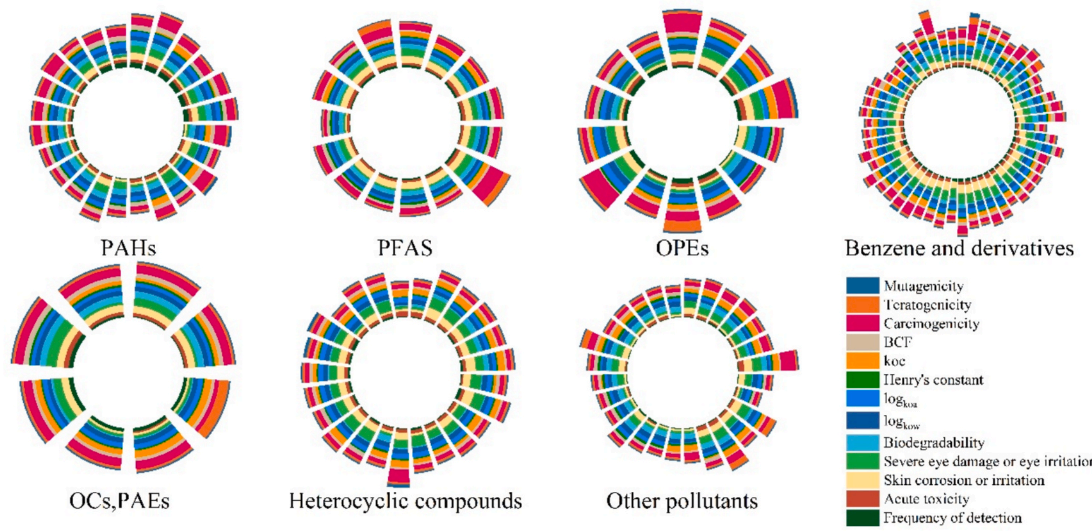

Fig. 7. Combined scores for each type of uncalibrated pollutants for sites in northeast China.

Table 3
Overlap of pollutants screened in this study with the international control list of major pollutants.

Source of list	Total number of controlled substances	Substances overlapping with pollutants screened in this study	Proportion of the same substance (%)
Registration, Evaluation, Authorisation and Restriction of Chemicals (REACH)	Over 2,000	PFOA, PFOS, PFBA, PFNA, HCBD, Ant, Styrene, 2,4-Dimethylphenol	72.73
Toxic Substances Control Act (TSCA)	Over 86,000	PFOA, PFOS, PFBA, PFNA, MIC, Acrolein, Styrene	63.64
Canadian Environmental Protection Act (CEPA)	Approximately 400	PFOA, PFOS, PFBA, HCBD, Ant, MIC	54.55
German Chemical Substance List	Over 1,500	PFOA, PFOS, Ant, Styrene, 2,4-Dimethylphenol	45.45
Safe Drinking Water Act (EPA)	Approximately 100	PFOA, PFOS, HCBD, Styrene, Acrolein	45.45
Chemical Substances Control Law (CSCL)	Existing Chemicals	PFOA, PFOS, HCBD, Styrene, Acrolein	45.45
HAPs (EPA)	187	Styrene, Acrolein, MIC, HCBD	36.36
CERCLA Hazardous Substances Defined	Approximately 375	HCBD, Ant, Styrene, Acrolein	36.36
Stockholm Convention on Persistent Organic Pollutants	Approximately 102	PFOA, PFOS, HCBD, Ant	36.36

in the environment for tens or even hundreds of years, their potential hazards may gradually become apparent over the long term. Therefore, we must pay more attention to the assessment of the persistence and mobility of pollutants in the indicator system to accurately grasp the environmental behaviour and risk of uncalibrated pollutants in northeast China.

The indicator system needs to be tailored to the specificities of the site. Soil plays a crucial role in the environmental system as an enrichment source for water and atmospheric pollution. Pollutants in water and the atmosphere are constantly migrating and accumulating to soil under the influence of natural processes or anthropogenic activities (Chen et al., 2024). Pollutants in soil may cause long-term harm to ecosystems and human health over time through food chain transfer, groundwater contamination, and other pathways (Chen et al., 2024; Wang et al., 2023). In view of the key position of soil in environmental pollution, the accumulation, transformation and potential risk of uncalibrated pollutants in soil must be fully considered in the adjustment of our indicator system. The monitoring and assessment of uncalibrated pollutants in industrial sites can provide a better understanding of the pollution status of the entire environmental system and provide a strong basis for the development of integrated pollution prevention and control strategies.

Among the screened uncalibrated priority pollutants, PFOA (internationally regulated under Stockholm Convention) demands special attention. Our research findings align with those of the US EPA, confirming its persistence in industrial environments. While ECHA focuses more on drug residues, our results underscore the need for continued vigilance regarding PFOA in cold regions. The combination of its global regulatory status, empirical detection patterns, and climate-specific behaviour highlights the importance of PFOA as a priority pollutant across different environmental contexts. PFOA is a prominent member of the PFAS family and has been widely used in various industrial and consumer applications (Wu et al., 2024). PFAS in the study area primarily originate from local petrochemical industries. Its strong carbon–fluorine bond endows (Wallace et al., 2024) it with exceptional resistance to degradation in both the natural environment and the human body, leading to bioaccumulation. The detection of PFOA in the study area, despite being listed as a prohibited or restricted organic pollutant under the POPs Convention, highlights its persistence and potential for long-range transport. The high carcinogenicity of PFOA, as identified in this study, underscores its significant threat to human health. Moreover, its presence in consumer goods such as furniture and industrial products implies that it can enter the human body through multiple pathways, such as ingestion, inhalation, and dermal contact. The current understanding of PFOA's environmental behavior and toxicological effects is still evolving, and further research is needed to fully elucidate its potential impacts on ecosystems and human health. This includes investigations into its transformation products, potential synergistic effects with other pollutants, and the development of more effective remediation strategies.

The uncalibrated priority pollutants screened in this study have certain connections and differences compared to existing environmental standards. On the one hand, some of the uncalibrated pollutants have similar chemical properties and environmental behaviours as pollutants already included in the standards, and they may have the same potential hazards and therefore should be included in the existing standards, but there was a lack of screening and control values for them in practical management in China. For example, the mechanism of toxicity of anthracene (EPA priority pollutant) is similar to that of the calibrated pollutant benzo[a]pyrene, but its environmental threshold has not yet been determined, leading to difficulties in accurately tackling it for pollution assessment and management. On the other hand, some uncalibrated pollutants have unique environmental behaviours and ecological effects that cannot be effectively covered by existing standards. For example, PAHs show strong mobility and bioaccumulation under specific soil and climatic conditions in northeast China, and the existing environmental standards fail to fully consider these characteristics. Therefore, it is necessary to further study the relationship between these uncalibrated pollutants and the existing standards, in order to provide a scientific basis for improving and revising environmental standards.

This study provides the first systematic screening of unlisted uncalibrated pollutants in northeastern China, identifying PFOA and other high-priority pollutants that require urgent attention. However, some limitations should be noted. First, the subjective weights of different indicators, although based on expert judgement, are subjective. Second, for uncalibrated pollutants for which measurement data are not available, we rely on model predictions (e.g., QSAR for toxicity parameters), which introduces additional uncertainty. Thirdly, we were unable to carry out source analysis due to the lack of standardised emission inventories for uncalibrated pollutants and fine-scale social sensitivity data (e.g., information around schools/hospitals). These uncertainties suggest that our prioritised control list should be regarded as tentative and requires further validation through targeted monitoring and testing.

5. Conclusion

A modified AHP-CRITIC method, that combined expert judgment and objective numerical criteria, was used to identify unlisted uncalibrated pollutants that lack regulatory management criteria in industrial sites in northeast China. 170 pollutants were screened and 11 priority pollutants were identified and ranked by constructing a comprehensive evaluation system including toxicity, persistence and migratory indicators. Among the identified pollutants, PFOA scored significantly higher than other pollutants. The research results provide a basis for the control of uncalibrated priority pollutants, such as PFAS and PAHs, at industrial sites across Northeast China, and will help to improve the ecology. Globally, it will provide a basis for the development of control strategies for pollutants in similarly cold and industrially polluted areas and will promote research on the prevention and control of uncalibrated pollutants.

CRediT authorship contribution statement

Xinni Wei: Writing – review & editing, Writing – original draft, Visualization, Investigation, Formal analysis, Data curation, Conceptualization. **Xiuli Dang:** Writing – review & editing, Writing – original draft, Supervision, Methodology, Funding acquisition, Conceptualization. **Peng Liu:** Validation, Formal analysis, Data curation. **Ge Gao:** Formal analysis, Conceptualization. **Hang Zhu:** Visualization. **Jiayue Shi:** Formal analysis, Data curation. **Qiyuan Zhang:** Data curation, Conceptualization. **Roland Bol:** Writing – review & editing, Visualization. **Peng Zhang:** Writing – review & editing, Methodology, Formal analysis, Conceptualization. **Iseult Lynch:** Writing – review & editing, Supervision, Funding acquisition. **Long Zhao:** Supervision, Project administration, Funding acquisition, Conceptualization.

Declaration of competing interest

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

Acknowledgements

We acknowledge National Key Research and Development Program of China (2022YFC3703200), National Natural Science Foundation of China (No. 41301530). IL acknowledges the Horizon 2020 funded SCENARIOS project (Grant agreement No. 101037509).

Appendix A. Supplementary data

Supplementary data to this article can be found online at https://doi.org/10.1016/j.envint.2025.109650.

Data availability

Data will be made available on request.

References

Agency for Toxic Substances and Disease Registry, 2024. Substance Priority List. https://www.atsdr.cdc.gov/programs/substance-priority-list.html (accessed 11 October 2024).
Boris, B., Jonathan, Z., Christian, Z., 2023. Nontarget screening strategies for PFAS prioritization and identification by high resolution mass spectrometry: a review. Trends Environ. Anal. Chem. 40.
Burman, E., Mulvaney, K., Merrill, N., Bradley, M., Wigand, C., 2023. Hazardous and contaminated sites within salt marsh migration corridors in Rhode Island, USA. J. Environ. Manage. 331, 117218. https://doi.org/10.1016/j.jenvman.2023.117218.
Chang, Y.-J., Zhu, D., 2020. Urban water security of China's municipalities: comparison, features and challenges. J. Hydrol. 587, 125023. https://doi.org/10.1016/j.jhydrol.2020.125023.
Chang, Y.-J., Zhu, D., 2021. Water security of the megacities in the Yangtze River basin: comparative assessment and policy implications. J Clean. Prod. 290, 125812. https://doi.org/10.1016/j.jclepro.2021.125812.
Chen, X., Song, Y., Ling, C., Shen, Y., Zhan, X., Xing, B., 2024. Fate of emerging antibiotics in soil-plant systems: a case on fluoroquinolones. Sci. Total Environ. 951, 175487. https://doi.org/10.1016/j.scitotenv.2024.175487.
Chen, Y., Dong, M., Lyu, P., Wang, A., Wang, H., Li, J., 2023. Analysis of metal(loid) pollution and possibilities of electrokinetic phytoremediation of abandoned coking plant soil. Sci. Total Environ. 870, 161982. https://doi.org/10.1016/j.scitotenv.2023.161982.
Chou, L., Zhou, C., Luo, W., Guo, J., Shen, Y., Lin, D., Wang, C., Yu, H., Zhang, X., Wei, S., Shi, W., 2023. Identification of high-concern organic pollutants in tap waters from the Yangtze River in China based on combined screening strategies. Sci. Total Environ. 857, 159416. https://doi.org/10.1016/j.scitotenv.2022.159416.
Ding, S., Li, X., Qiao, X., Liu, Y., Wang, H., Ma, C., 2024. Identification and screening of priority pollutants in printing and dyeing industry wastewater and the importance of these pollutants in environmental management in China. Environ. Pollut. 362, 124938. https://doi.org/10.1016/j.envpol.2024.124938.
Geng, J., Zhao, L., Wang, W., Hou, H., Zhang, Q., Zhang, P., Irshad, S., Bol, R., Dang, X., 2025. Influence of soil properties and residence time on the toxicity of exogenous arsenic to soil-dwelling Caenorhabditis elegans. J. Soils Sedim. 25, 897–911. https://doi.org/10.1007/s11368-025-03974-3.
Ghosh, P., Mukherji, S., 2023. Fate, detection technologies and toxicity of heterocyclic PAHs in the aquatic and soil environments. Sci. Total Environ. 892, 164499. https://doi.org/10.1016/j.scitotenv.2023.164499.
Howard, I.C., Okpara, K.E., Techato, K., 2021. Toxicity and risks assessment of polycyclic aromatic hydrocarbons in river bed sediments of an artisanal crude oil refining area in the Niger Delta, Nigeria. Water 13, 3295. https://doi.org/10.3390/w13223295.
Huang, J., Cheng, F., He, L., Lou, X., Li, H., You, J., 2024. Effect driven prioritization of contaminants in wastewater treatment plants across China: a data mining-based toxicity screening approach. Water Res. 264, 122223. https://doi.org/10.1016/j.watres.2024.122223.
International Agency for Research on Cancer, 2024. List of Classifications. https://monographs.iarc.who.int/list-of-classifications (accessed 12 October 2024).
James, C.A., Sofield, R., Faber, M., Wark, D., Simmons, A., Harding, L., O'Neill, S., 2023. The screening and prioritization of contaminants of emerging concern in the marine environment based on multiple biological response measures. Sci. Total Environ. 886, 163712. https://doi.org/10.1016/j.scitotenv.2023.163712.
Jiang, Y.-Y., Zeng, Y., Long, L., Guo, J., Lu, R.-F., Chen, P.-P., Pan, Z.-J., Zhang, Y.-T., Luo, X.-J., Mai, B.-X., 2024. First report on the trophic transfer and priority list of liquid crystal monomers in the Pearl River Estuary. Environ. Sci. Technol. 58, 16131–16141. https://doi.org/10.1021/acs.est.4c04962.

Li, F., Fan, T., Sun, G., Zhao, L., Zhong, R., Peng, Y., 2022. Systematic QSAR and iQCCR modelling of fused/non-fused aromatic hydrocarbons (FNFAHs) carcinogenicity to rodents: reducing unnecessary chemical synthesis and animal testing. Green Chem. 24, 5304–5319. https://doi.org/10.1039/d2gc00986b.

Li, L., Li, G., Cui, L., He, L., Chen, Y., 2021. Method for modelling ecological competition based on Pareto optimality: a case study of coastal wetlands in Jiangsu Province, China. Ecol. Indic. 129, 107946. https://doi.org/10.1016/j.ecolind.2021.107946.

Liu, J., Ouyang, T., Lu, G., Li, M., Li, Y., Hou, J., He, C., Gao, P., 2024. Ecosystem risk-based prioritization of micropollutants in wastewater treatment plant effluents across China. Water Res. 263, 122168. https://doi.org/10.1016/j.watres.2024.122168.

Liu, J., Yuan, Q., Toste, F.D., Sigman, M.S., 2019. Enantioselective construction of remote tertiary carbon-fluorine bonds. Nat. Chem. 11, 710–715. https://doi.org/10.1038/s41557-019-0289-7.

Liu, Y., Yu, J., Sun, H., Li, T., He, X., Lin, Z., 2022. Screening and prioritizing substances in groundwater in the Beijing-Tianjin-Hebei region of the North China Plain based on exposure and hazard assessments. J. Hazard. Mater. 423, 127142. https://doi.org/10.1016/j.jhazmat.2021.127142.

Melymuk, L., Blumenthal, J., Sanka, O., Shu-Yin, A., Singla, V., Sebkova, K., Fedinick, K. P., Diamond, M.L., 2022. Persistent problem: global challenges to managing PCBs. Environ. Sci. Technol. 56, 9029–9040. https://doi.org/10.1021/acs.est.2c01204.

Mohasin, P., Chakraborty, P., Anand, N., Ray, S., 2023. Risk assessment of persistent pesticide pollution: development of an indicator integrating site-specific characteristics. Sci. Total Environ. 861, 160555. https://doi.org/10.1016/j.scitotenv.2022.160555.

National Library of Medicine, 2024. Explore Chemistry. https://pubchem.ncbi.nlm.nih.gov/ (accessed 11 October 2024).

National Standardization Administration, 2013a. Rules for classification and labelling of chemicals - Part 18: Acute toxicity. https://openstd.samr.gov.cn/bzgk/gb/newGbInfo?hcno=6FAA3711A9BF1B3E706C30AABB8A28F6 (accessed 12 October 2024).

National Standardization Administration, 2013b. Rules for classification and labelling of chemicals - Part 19:Skin corrosion/irritation. https://openstd.samr.gov.cn/bzgk/gb/newGbInfo?hcno=C5B87B85478148F2AD9FBC80991F2D92 (accessed 12 October 2024).

National Standardization Administration, 2013c. Rules for classification and labelling of chemicals - Part 20: Serious eye damage/eye irritation. https://openstd.samr.gov.cn/bzgk/gb/newGbInfo?hcno=406689A7D0C4443BEE5DB91B2BF23C91 (accessed 12 October 2024).

National Standardization Administration, 2013d. Rules for classification and labelling of chemicals - Part 22: Germ cell mutagenicity. https://openstd.samr.gov.cn/bzgk/gb/newGbInfo?hcno=3EE69B7B76FB3E0445F90651EDD4A5EA (accessed 12 October 2024).

National Standardization Administration, 2013e. Rules for classification and labelling of chemicals - Part 24: Reproductive toxicity. https://openstd.samr.gov.cn/bzgk/gb/newGbInfo?hcno=71308BF717E07CF1FD39875FA52F1BBB (accessed 12 October 2024).

Neumann, P., Gonzalez, Z., Vidal, G., 2017. Sequential ultrasound and low-temperature thermal pretreatment: Process optimization and influence on sewage sludge solubilization, enzyme activity and anaerobic digestion. Bioresour Technol. 234, 178–187. https://doi.org/10.1016/j.biortech.2017.03.029.

Organization for Economic Cooperation and Development, 2024. Quick Search. https://www.echemportal.org/echemportal/ (accessed 15 October 2024).

Peng, J.-Y., Zhang, S., Han, Y., Bate, B., Ke, H., Chen, Y., 2022. Soil heavy metal pollution of industrial legacies in China and health risk assessment. Sci. Total Environ. 816, 151632. https://doi.org/10.1016/j.scitotenv.2021.151632.

Publications Office of the European Union, 1999. Study on the prioritisation of substances dangerous to the aquatic environment, first ed. English, Europe.

Szabo, D., Fischer, S., Mathew, A.P., Kruve, A., 2024. Prioritization, identification, and quantification of emerging contaminants in recycled textiles using non-targeted and suspect screening workflows by LC-ESI-HRMS. Anal. Chem. 96, 14150–14159. https://doi.org/10.1021/acs.analchem.4c02041.

Tao, J., Wu, W., Lin, D., Yang, K., 2024. Role of biochar pyrolysis temperature on intracellular and extracellular biodegradation of biochar-adsorbed organic compounds. Environ. Pollut. 346, 123583. https://doi.org/10.1016/j.envpol.2024.123583.

Verma, M., Loganathan, V.A., Bhatt, V.K., 2022. Development of entropy and deviation-based water quality index: Case of river Ganga, India. Ecol. Indic. 143, 109319. https://doi.org/10.1016/j.ecolind.2022.109319.

Wallace, M.A.G., Smeltz, M.G., Mattila, J.M., Liberatore, H.K., Jackson, S.R., Shields, E. P., Xhani, X., Li, E.Y., Johansson, J.H., 2024. A review of sample collection and analytical methods for detecting per- and polyfluoroalkyl substances in indoor and outdoor air. Chemosphere 358, 142129. https://doi.org/10.1016/j.chemosphere.2024.142129.

Wang, J., Deng, P., Wei, X., Zhang, X., Liu, J., Huang, Y., She, J., Liu, Y., Wan, Y., Hu, H., Zhong, W., Chen, D., 2023. Hidden risks from potentially toxic metal(loid)s in paddy soils-rice and source apportionment using lead isotopes: a case study from China. Sci. Total Environ. 856, 158883. https://doi.org/10.1016/j.scitotenv.2022.158883.

Wu, B., Guo, S., Wang, J., 2021. Assessment of the human health risk of polycyclic aromatic hydrocarbons in soils from areas of crude oil exploitation. Environ. Res. 193, 110617. https://doi.org/10.1016/j.envres.2020.110617.

Wu, S., Xie, J., Zhao, H., Zhao, X., Sanchez, O.F., Rochet, J.-C., Freeman, J.L., Yuan, C., 2024. Developmental neurotoxicity of PFOA exposure on hiPSC-derived cortical neurons. Environ. Int. 190, 108914. https://doi.org/10.1016/j.envint.2024.108914.

Xiu, F.-R., Wang, J., Song, Z., Qi, Y., Bai, Q., Wang, S., Lei, X., Yang, R., Gao, Z., 2023. Synergistic Co-liquefaction of waste plastic express bags and low-rank coal based on supercritical water-ethanol system: Waste treatment and resource upgrading. J. Clean. Prod. 425, 138957. https://doi.org/10.1016/j.jclepro.2023.138957.

Yerulker, G., Patel, P., Chafale, A., Rathod, V., Das, S., Pandey, P., Khan, N.A., Devi, A., Munshi, N.S., Dhodapkar, R., Kapley, A., 2023. Comparative assessment of soil microbial community in crude oil contaminated sites. Environ. Pollut. 328, 121578. https://doi.org/10.1016/j.envpol.2023.121578.

Zhao, J., Hu, L., Xiao, S., Zhao, J., Liu, Y., Yang, B., Zhang, Q., Ying, G., 2023. Screening and prioritization of organic chemicals in a large river basin by suspect and non-target analysis. Environ. Pollut. 333, 122098. https://doi.org/10.1016/j.envpol.2023.122098.

Zhao, Y., Wang, C., Cao, X., Song, S., Wei, P., Zhu, G., 2024. Integrated environmental assessment of a diversion-project-type urban water source considering the risks of novel and legacy contaminants. Sci. Total Environ. 951, 175380. https://doi.org/10.1016/j.scitotenv.2024.175380.

Zhu, F.-J., Ma, W.-L., Zhang, Z.-F., Yang, P.-F., Hu, P.-T., Liu, L.-Y., Song, W.-W., 2022. Prediction of the gas/particle partitioning quotient of PAHs based on ambient temperature. Sci. Total Environ. 811, 151411. https://doi.org/10.1016/j.scitotenv.2021.151411.