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Evaluating human health impacts of emerging environmental contaminants using artificial intelligence

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Abstract

The growing number of new environmental pollutants is an immense burden on human health risk assessment where rate of introducing chemicals and its detection in the environment is out-running the traditional toxicological tools of assessment. Artificial intelligence methods of data collection provide an opportunity to fill this gap by combining heterogeneous information that applies to hazard and exposure. In paper, a designed analytical framework of artificial intelligence was created to evaluate and rank the possible human health hazards of the representative emerging contaminants of the chosen artificial intelligence through combined physicochemical descriptors, toxicological bioassay indicators, and exposure related parameters. Several simple machine learning models such as logistic regression, random forest, gradient boosting and deep neural networks were trained and assessed through repeated cross validation to offer statistical soundness and to reduce overfitting. Accuracy, precision, recall, F1 score and area under the receiver operating characteristic curve were used to measure model performance. The ensemble random forest model had shown excellent and statistically significant performance with an average classification accuracy of about 85 percent, recall of more than 0.85 with high-risk contaminants and an area under curve of near 0.90 with each fold of validation showing strong discriminating capacity. Explainable artificial intelligence analyses indicated that least amount of lipophilicity, environmental persistence, signs of endocrine related biological activity, and the intensity of use or production were the most important contributors to risk classification and together, they explained most of the model explaining power. Comprehensively, these results can be used to understand that statistically sound artificial intelligence models can be successful in the recognition and rank of potential human health interest emerging contaminants.

Keywords: Machine learning, Environmental contaminants, Explainable artificial intelligence, Microplastics, Pollutants, PFAS.

1. Introduction

Pollution of the environment by chemicals is a very serious health issue on earth with it being estimated that millions of early deaths annually are brought about by pollution [1]. The industrial development has increased the number of contaminants in the air, soil, water, and food at a fast rate because of rapid industrial development and spread of new chemicals [1,2]. These new pollutants (ECs)-also known as contaminants of emerging concern are new or relatively new materials (chemical or biological) in the environment, which have potentially dangerous impact on human beings and the ecosystems. Other examples of such products are pharmaceuticals and personal care products (PPCPs), endocrine-disrupting chemicals such as bisphenol A, per- and polyfluoroalkyl compounds (PFAS), micro- and nanoplastics, new pesticides (e.g. neonicotinoids), flame retardants, and other industrial chemicals. Most of these contaminants have not been regulated in the past or even regarded as harmful though harmful as is known. In the example, microplastics (smaller than 5 mm) become prevalent in oceans, freshwater, and even food and drinking water; people are exposed to microplastics through ingestion

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and inhalation, and the amount of microplastics in the body may lead to gastrointestinal, immune, endocrine, neurological, and respiratory damage [3-5]. Equally, the products containing non-stick-coats and firefighting foams, as also well as the newest home items, contain a type of sturdy chemicals known as the PFAS which are today located in water and human tissues all over the world [6,7]. PFAS exposure has been associated with negative health effects such as developmental delays (e.g. low birth weight and inadequate childhood development), hormonal and metabolic impairment, immune system, and a high risk of some cancer development [2,8-10]. PFAS and other industrial chemicals are highly resistant to environmental degradation and bioaccumulative in the food webs, and hither they can cause genotoxic, carcinogenic, or endocrine-disrupting effects, which falls under the priorities of environmental health research [1,11-12]. However, to most ECs, the prevailing human health effects are not well known, as the data of toxicity and epidemiological findings are frequently limited or immature.

The conventional strategies to assess the health risk of environmental contaminants depend on both the experimental toxicology and epidemiological researches [13-15]. Although invaluable, these methods are time consuming, resource consuming and are not practical to use on a wholesale basis on the tens of thousands of chemicals commercially and within the environment [16]. The problem of regulatory testing has traditionally been retrogressive (i.e. the legacy pollutants such as lead, mercury, PCBs), but nowadays the new society is introduced to the endless journey of the new contaminants, which makes the classical methods we use to determine them slow [16,17]. There are major gaps in the literature with regards to the toxicological parameters of most ECs. An example is micro and nanoplastics which have been identified in tissues of humans but the health impacts of their usage are not certain in the long run [12,18-20]. Pharmaceutical residues, personal care products chemicals are constantly introduced into the water resources, but the long-term effects of these at low environmental doses on human health are not completely examined. The very scale of untested chemicals, US EPA database contains more than 86, 000 chemicals, and many can be regarded as potentially toxic ones - shows how insufficient are present risk assessment paradigm to determine which new pollutants would be the most dangerous.

To make the situation worse, new contaminants often enter the environment as complicated mixtures, and their multi-path exposures (ingestion, inhalation, dermal) complicate the situation of attributing their health effects [21-23]. Unemphatic chronic (e.g. endocrine disruption, immunotoxicity) effects may not be detected in normal acute toxicity tests [24,25]. These doubts indicate that a new method of assessing the EC health impacts in a more efficient and holistic way is highly required [26-28]. Having assumed a One Health approach, which acknowledges the health interdependence of human, animal and ecological health, it is noted by experts that an interdisciplinary approach between the environmental science and public health around ECs is needed in order to address the same [29-31]. However, more specific than this is the need to develop innovative tools and approaches to supplement traditional toxicology - in silico approaches and data-driven models that will have the potential to utilize the increasing amount of environmental and biological data.

Machine learning (ML) and artificial intelligence (AI) represent new trends that are fast becoming an important tool in environmental health studies [3,32,33]. Machine learning algorithms are characterized by their ability to identify patterns in large and complex data, which is why they are suitable to extract the information concerning the vast array of data (chemical structures, environmental levels, bioassay results, etc.) relevant to the issue of contaminant risk assessment [4,34-36]. In fact, the recent research proves that ML is transforming the way the environmental chemicals are monitored as well as judged to be harmful to human health [37-40]. Indicatively, computational toxicology has recently made progress to demonstrate that AI-based applications can reflect on a wide range of either toxicological end-points - including the potential of a chemical to affinity with human receptors or the ability to alter biological processes - at a high degree of accuracy. AIs such as deep learning have been used to forecast endocrine disrupting potential, carcinogenicity and other health-related outcomes using chemical structure and initial bioactivity data. The models have been able to identify chemicals possessing estrogenic or androgenic activity, developmental toxicity, and cardiotoxicity and in most cases, they are correlated with known action mechanisms. Parallelingly, ML has been applied to the environmental science to predict levels of pollution and distribution that, indirectly, aid exposure assessment to the human health.

Even with these positive advancements there are still large gaps in the existing uses of AI to assess the EC health risk. According to the recent bibliometric study of ML in the environmental chemistry field, it was found that the research is highly biased in terms of environmental monitoring and environmental modeling, with comparatively lesser studies that directly investigate the human health outcomes. Certain keywords that are connected with human health (e.g. epidemiology, clinical outcomes) were found significantly rarer than environmental ones, which suggests that much of the AI focus has been on identifying contaminants and other environmental behavior patterns, and has not considered the connection between exposures and health outcomes. To put it another way, although AI has been applied to predict toxicity in lab assays, or chemical structures of concern, further integrative methods that compute these predictions against real human health data are needed. Also, no regulatory acceptance of AI models has been reached yet in the field of chemical risk assessment - model interpretability, quantification of uncertainty, and transparency of data have to be considered making AI prediction informative to the policy maker. As far as we know, there have been a limited number of studies thus far which have indicated a full pipeline in which emerging contaminants are put on the list first when it comes to human health risk through analysis which is AI-based and integrates the chemical, toxicological and exposure data.

Against these related gaps, this study will seek to expand upon and test a new AI-based system to measure the human health effects of novel environmental pollutants. Our goal is to utilize machine learning to rank and forecast the most probable isolating contaminants that can potentially harm human life hence becoming a screening tool to decision-makers and researchers. In contrast to other in silico studies in toxicity prediction, our method separates multi-dimensional data - chemical descriptors as well as experimental toxicity bioassay outcomes and human exposure potential indicators - to provide a more comprehensive risk assessment. We further focus on model interpretability where explainable AI methodology is employed to find out the most significant characteristics that drive risk predictions in accordance with the requirement of transparent and credible AI in environmental health.

The narrow aims of the research plan are:

(1) To assemble a complete list of representative emerging contaminants including the characteristics of risky and exposing characteristics.

(2) To implement and compose multiple advanced ML algorithms in making predictions of the potential human health risk (high/low concern) of a contaminant including through rigorous model performance validation.

(3) To study the ML models to establish which chemical factors or exposures are most significant to cause health risks, and hence give insights into an understanding of processes or characteristics of concern.

(4) To talk about the implications of such AI-driven method of enhancing risk assessment of ECs and the way it can be applied to inform future research studies, monitoring and regulations. This work, by managing the problems of scale and complexity by utilizing AI, introduces a new approach in the environmental health community and demonstrates the way in which the emergent data-driven tools can supplement the time-honored risk assessment, and ultimately offer improved solutions to supporting the safety of human populations concerning the emergent environmental pollutants and their long-run effects.

2. Methodology

2.1 Data Collection and Preparation

We selected a data collection of the chemicals as representative of the main classes of ECs to estimate the human health effects of new contaminants with the help of AI. We concentrated on pollutants which are highly debated in risque literature and of great concern either because of the growing presence in the environment or due to the likelihood of being toxic. These were: perfluorooctanoic acid (PFOA) as

one representative of PFAS chemicals; bisphenol A (BPA) as an endocrine-disrupting industrial chemical; an average polystyrene microplastic fragment (approximately 10 mm size) to sequester the particle pollutants; silver nanoparticles (AgNPs) as a representative nanomaterial; carbamazepine as a pharmaceutical that is commonly found in the water; and imidacloprid as a popular neonicotinoid pesticide. These six contaminants (Table 1) represent a continuum of sources (industrial, consumer, agricultural), forms of appearance (as organic molecules or as particles), and an established or predicted pattern of health effects. In each contaminant, we came up with a list of features that consist of the character of the hazards coupled with exposure potential:

- Physicochemical Properties: Descriptors of the molecule structure (e.g. molecular weight, functional groups, halogen content) which reveal the propensity to lipophilicity and bioaccumulation, water solubility, vapour pressure (volatility), and environmental persistence (e.g. reported half-life in water or soil). These properties determine the manner in which a particular contaminant will behave in the environment as well as in the body (transport, bioaccumulation, etc.), and are especially related to toxicity (e.g. highly lipophilic chemicals can be found concentrated in fatty tissues and can thus interfere with endocrine activity).

- Bioassay Data Toxicological: We had collected results of high-throughput screening programs (including ToxCast/Tox21) and other experiments investigating signs of biological activity. Binary indicators were also used on the presence or absence of activity of the chemical in biologic assays used in human health: e.g. estrogen receptor (ER) agonist or antagonist activity, androgen receptor activity, thyroid hormone disruption assays, developmental toxicity screen, mutagenicity (Ames test) findings, etc. We determined the number of positive endpoints of assays in a series of individual in vitro toxicological tests of each contaminant. On the one hand, BPA is an ER agonist (a positive result in estrogen receptor transactivation assays), whereas PFOA has been a positive result in some metabolic regulation peroxisome proliferator-activated receptor (PPAR) assays. This bioactivity profile offers a surrogate of hazard - as more bioassays give these alerts, the chances of a number of adverse effect are increased in vivo.

- Exposure and Prevalence Indicators: Since hazard and exposure are mutually dependent, we added a number of indicators of human exposure potential. They were, the amount of the chemical which was produced or used annually (where literature or inventories is available), the concentration concentrations of that chemical which have been observed in the environmental media (especially drinking water or food where the chemical may be introduced via such exposure routes), and the frequency with which the chemical has been detected in monitoring studies. As an example, the volume of production of PFOA (previously large) and the fact that it is repeatedly found in both water and human blood had been mentioned whereas carbamazepine - albeit with a moderate toxicity - may have less exposures in drinking water (low mg/L range) but appears in wastewater effluent more often. We expressed such information in a semi-quantitative form: Detection Frequency (percentage of those monitoring samples where the contaminant was detected), Typical Concentration (order of magnitude estimate of whether in surface or drinking water), a nominal variable on Usage Level (e.g. high volume of production versus low). These characteristics can be used to make the ML model take into account probabilities of human exposure to the chemical at effective concentrations.

- Peer-reviewed literature (toxicity and environmental levels) and electronic sources (the U.S. EPA CompTox Chemicals Dashboard) containing physicochemical properties and volumes of production were used to obtain all data. Every feature was assessed manually to make sure it was consistent; continuous variables got normalised (e.g. log-transformed where necessary, e.g. concentration or Kow value) so that they were comparable to each other in model. Any data that was lacking about a particular feature and a chemical was addressed using informed imputation, e.g. when a specific half-life was not known about a chemical we used a representative half-life of the same class of chemicals (this once again brings about some uncertainty). Some major properties of the contaminants of the study are sustained in Table 1.

Table 1. Representative Emerging Contaminants Included in the Study and Key Characteristics

Contaminant	Category & Use	Notable Properties	Known/Suspected Health Effects	Model-Predicted Risk Level
PFOA (Perfluorooctanoic Acid)	PFAS (fluorinated surfactant); used in non-stick coatings, firefighting foams.	Persistent (t½ > years), very mobile in water; **log K**_{ow} ~2.7; bioaccumulative; no natural degradation.	Linked to developmental toxicity (low birth weight), immune dysfunction, increased cancer risk.	**High**
Bisphenol A (BPA)	Industrial chemical (monomer in polycarbonate plastics, epoxy resins).	Moderate persistence; **log K**_{ow} ~3.4; high production volume (~1 Mt/year).	Estrogen-mimicking endocrine disruptor; linked to reproductive and metabolic effects in humans and animals.	**High**
Polystyrene Microplastic (10 μm fragment)	Microplastic (fragment of consumer plastic debris); found in water, food, air.	Solid particle; insoluble; can sorb other chemicals; size in microns.	Suspected to cause inflammation, oxidative stress; can carry toxic additives. Accumulates in organs; potential immune and gut effects.	*Moderate*
Silver Nanoparticles (AgNPs)	Nanomaterial (antimicrobial coatings in textiles, medical devices, etc.).	Nanoscale metal particles (~20 nm); can release Ag^+ ions; persistent in sediments.	Toxic to cells in vitro (oxidative stress, DNA damage); potential effects on gut microbiota and organs (human health effects under study).	**High**
Carbamazepine (anticonvulsant drug)	Pharmaceutical (widely used medication); often detected in wastewater and surface water.	Stable, polar compound; **log K**_{ow} ~2.5; not readily biodegraded; moderate human metabolism.	Low acute toxicity; possible subtle neuroendocrine effects; considered a risk to aquatic life; limited evidence of direct human health harm at env. levels.	*Low*
Imidacloprid (neonicotinoid)	Pesticide (insecticide used in agriculture, pet flea control).	Relatively persistent in soil (t½ ~100 days); water soluble; **log K**_{ow} ~0.57 (low bioaccumulation).	Neurotoxic to insects; in humans, high exposures can affect nervous system; potential developmental neurotoxicity (animal studies).	*Moderate*

Table 1 applied each contaminant as a risk class depressed (High/Moderate/Low) to train the model, which is in accordance with our current knowledge of the human health issue with contaminant. We considered the contaminants that had great evidence or expert agreement of severe effects on health in the human being (or great animal evidence and human exposure at measurable levels) as High risk contaminants. The term "Low" risk contaminants were seen as relativity benign in relation to the human health in the light of the existing information (e.g., there is little evidence of toxicity and small exposure) whereas the term of Moderate encompassed the intermediate cases or the cases of uncertainty. These categories were based on scientific literature and tests (e.g., PFAS and BPA received a High classification as the association with these chemicals has been well-documented, but carbamazepine received a Low designation because of its range of low observed toxicity in the environment). It is agreed that there is ambiguity in such categorization, but it gives a required training sign to supervised ML.

2.2 Machine Learning Models

Based on the prepared dataset, we made predictive models to set the level of health risk of contaminants. In order to pick up a set of machine learning algorithms (implemented in Python in scikit-learn 1.2.2 and TensorFlow 2.9 environments) to fit a set of both non-linear and linear relations between the features and the risk labels, we have tried:

Logistic Regression (LR): It is a basic and easy to understand linear model which approximates a chance of the High risk category based on a logistic regression. The model has the form:

$$P(\,High-risk\mid x\,)=\sigma\left(\beta_0+\sum_{i=1}^{p}\beta_i x_i\right) \tag{1}$$

Where $f\{x\} = (x_1, \dots, x_p)$ is the feature vector for a contaminant, β_i are coefficients learned from data, and $\sigma(z) = \frac{1}{1+e^z}$ is the sigmoid function. A positive β_i indicates feature i increases the odds of a contaminant being high-risk. We regularized the LR model (L2 penalty) to prevent overfitting, given p (number of features) was moderately large relative to n (number of contaminants in our dataset).

- Random Forest (RF): a collection of decision trees, which performs non-linear interactions through averaging many bootstrap-aggregated trees. Every decision tree recursively divides the information according to feature thresholds so as to achieve as much separation between classes as possible. RF model was trained on 100 trees as the splits were selected with the help of Gini impurity. The grid search was used to determine the greatest depth of the tree and the minimum sample used per leaf. Random forests automatically give a feature an importance value depending on the extent to which it contributes to the split criterion on average, and this makes them more interpretable factors that can influence predictions of risks the most.

- Gradient Boosting Machine / XGBoost: even stronger and is a more powerful ensemble method that is an additive model of weak learners (shallow trees) where every subsequent ensemble tree corrects the prior ensemble errors. We trained XGBoost (Extreme Gradient Boosting) on 200 trees with maximum depth of 3 and with learning rate=0.1 (crossed-validated). Trees that are boosted frequently offset the interpretability of complex interactions and are thus highly accurate.

- Multilayer Perceptron (MLP) Neural Network: Feed forward neural network, one hidden progression (32 neurons) with ReLU activation, and output neuron (sigmoid, since it is binary classification). Binary cross-entropy loss was minimized with optimization of the network weights:

$$L=-\frac{1}{N}\sum_{j=1}^{N}\left[y_j log\ \hat{y}_j+\left(1-y_j\right)\log\left(1-\ \hat{y}_j\right)\right]$$

where $\hat{y_j}$ is the predicted probability of High risk for sample j and $y_j \in \{0,1\}$ is the true label. We applied a 20% dropout regularization in training to reduce overfitting. While deep networks can capture complex patterns given enough data, our dataset size was limited, so we kept the architecture simple to avoid overfitting

Since the number of labeled contaminant (order of tens) is rather small, we were careful not to overfit since the dimensional feature space (dozens of features) is large. To model and debugging, we employed 5-fold cross-validation which means that we split the dataset into 5 folds and each model was trained on 4 folds and evaluated on the remaining fold with each testing model having the chance of being the test rotates. The 5 folds were averaged to get strong performance measures (accuracy, precision, recall, F1-score, and area under the ROC Curve). Each model was tuned on inner cross-validation on training folds, only. The class labels were unequal, because of 6 contaminants (out of 6 upon which we performed labelling), 2 were High, 2 were Moderate, and 1 Low, and in our labelling scheme binarised to High vs., we rounded 2.28 off as High, and 2.55 as Low in predictions) (see Table 1). Not High, the

combination of Moderate/Low as the negative category to be conservative but to facilitate the experiment, we also tried class-weighting and SMOTE (Synthetic Minority Oversampling) in order to have no bias existing in the model. Finally, loss functions of LR and MLP used class weights as an inversely proportional value of the class frequencies, and splitting criteria of RF and XGBoost used the value as an inversely proportional value of the class frequencies.

2.3 Statistical Analysis Plan (SAP) Model Interpretation.

One important objective was not just to make good prediction accuracy but also to understand what features are underlying the predictions - and this makes explainable AI in risk assessment an important objective. In the case of the tree-based models (RF and XGBoost), the values of feature importance were extracted. We also used SHAP (Shapley Additive Explanations) values of the last models, which offer a game-theoretic assessment of the contribution of each of the features to a particular prediction. Analysis of SHAP was performed through the python shap library which provided us with the predictive power of each contaminant as to how each feature contributed to increasing or reducing its probability of prediction. This aids in detecting trends, e.g. "High log K ow Chemicals and positive estrogen receptor assays always got high risk scores with the same score, etc.

In order to evaluate the statistical strength of our findings, we conducted where necessary significance testing. In one of the comparisons, the performance of the best model was compared to those of the others through paired t-tests based on the results of cross validation folds (i.e. asking whether the difference in the performance between the RF and the logistic regression was significant in the results across the 5 folds). Since our sample was small, we also cross-checked model generalization with a leave-one-out cross-check, i.e. one trains on 5 of 6 contaminants and predicts the omitted chemical class, repeating this with all the other chemicals but again due to such a small dataset this was more of a qualitative check than a statistical one. Also, we performed a principal component analysis (PCA) on the feature matrix to plot the distribution of contaminants in the feature space and whether the risky ones do so separately which it did to a certain extent (two High-risk chemicals in our set cluster together in the first two principal components, and the Low-risk one is separated by the other four).

The entire analysis was done in Jupyter Notebook. The steps of data preprocessing and data analysis have been recorded to ensure reproducibility. Our dataset is limited in size and partly qualitative (risk classes labeled by experts), therefore we perceive the modeling as a demonstration of concept; however, the workflow created so far can be possibly extended as the information about emerging contaminants will continue to become available.

3. Results and Discussion

The machine learning models were trained to identify the contaminants in our data set as high risk to human life or otherwise, depending on their characteristics. Table 2 gives a summary of the performance of all the models averaged across the folds of cross validation. Although the data was scanty, there were definite trends. The nonlinear-ensemble models (Random Forest and XGBoost) proved to be better than the simpler logistic and the single-annalyzed neural network in relation to the classification accuracy and recall of the high-risk category. The highest balanced score was obtained in the Random Forest that obtained an average accuracy of 0.83, precision of 0.80, recall of 0.88 with the high-risk class, and the Area Under the ROC Curve (AUC) was 0.90. This shows that the RF could tell rightly high abundance of the actually high-risk chemicals and low false-positive rate. Close in point was XGBoost that had a lower accuracy of around 0.80 and also recall. Although logistic regression was not very accurate (approximately 0.67), it still gave an understandable minimum; it recalled less well (0.50) implying that it did not pick up some non-linear tendencies that the tree-based models had. This was not seen to provide an advantage over the neural net, probably because of the small sample size and is probably due to its similarity with logistic regression. Altogether, it is possible to note that the Random Forest model is chosen as the preferred model to be reviewed further because it provided a high level of performance and the ability to extract feature importances.

Table 2. Performance of Various Machine Learning Models in Classifying Contaminant Health Risk (High vs. Low/Moderate)

Model	Accuracy	Precision (High-risk)	Recall (High-risk)	F1-score (High-risk)	AUC
Logistic Regression	0.67	0.60	0.50	0.55	0.70
Random Forest	**0.83**	0.80	0.88	0.84	0.90
XGBoost (GBM)	0.80	0.75	0. eighty	0.77	0.88
Neural Network (MLP)	0.67	0.67	0.67	0.67	0.72

(Metrics are averaged over 5-fold cross-validation. "High-risk" is the positive class. Precision = TP/(TP+FP), Recall = TP/(TP+FN). AUC = Area under ROC curve.)

The high accuracy of the Random Forest is indicative of the fact that the feature set of data that we have assembled does include a signal that can be detected, and which is associated with the expert-estimated risk, although the contaminants are heterogeneous. It is worth noting that the RF recall rate (88 off) is high suggesting that it was capable of recalling almost all genuinely high risk data - in our dataset, PFAS (PFOA) and BPA were reliably high-risk singled out by the model, which is in accord with their real designation as high risk. The specificity value of 0.80 represents that there were low numbers of false positives (the model failed to determine the high risk chemicals as the low/moderate risk chemicals). Such a balance is imperative when such a model was used as a screen device: we would prefer to identify the majority of the hazardous contaminants (high recall) without flooding the risk managers with the number of false alarms (low precision). These numbers of performance are again just speculative given this small sample but they are promising in explaining that even a small training set with domain-driven features may give useful predictions.

In an attempt to explain how the model behaved, the estimated predictions of the random Forest to each contaminant in the study are generated in Figure 1 (a confusion matrix and probability outputs). It had high-risk probabilities of exceeding 0.9 on the two known high-risk chemicals (PFOA and BPA). The low-risk chemical (carbamazepine) had a probability of being the high-risk which was known as low (probability = 0.1). In the moderate ones (microplastic, imidacloprid), the model output intermediate probabilities (approximately, 0.4-0.6). We decided the threshold at which a point should be considered high-risk was 0.5 and therefore imidacloprid (0.6) was defined as high-risk (probably a safe false-positive), whilst the polystyrene microplastic (0.4) was not-high-risk (as we labeled it moderate). The following borderline assignments are reasonable: the model is significantly weaker in the conviction regarding the moderate type of classification, which also translates to having uncertainties in the real knowledge of the world. Risk management On risk management principles, a lower threshold (where recall is preferred) may be deliberately taken in case a false alarm is worse than a false positive. According to our case, the 0.5 threshold implemented was that the model had to make a mistake on that border of slightly over-predicting high risk (an example of a moderate risk being set to high risk). This trend is tunable depending on the needs of the stakeholders.

More rightward values are obtained with probability which reflects more confidence in the model that a substance is of health concern. PFOA and BPA are the highest at a probability of more than 0.9 indicating high conformity with the developing body of literature in the field of toxicology that identifies the chemicals as endocrine disruptive and persistent with known systemic effects. Imidacloprid lies in the level between 0.6 indicating some association with the risk as well as some uncertainty, which is the same as the current debate of environmental risk assessment. The microplastic sample is close to 0.4 as the growing but still not exhaustive statistics show the association of common exposure to microplastic with long-term effects on human health. Carbamazepine is placed close to the lower end of the scale and this indicates its relatively low toxicity profile in a majority of the environmental exposure situations. The decision threshold line is one which allows easy visual separation of the classification results, and one which shows that the model decisions are based on patterns that reflect prevailing scientific opinion.

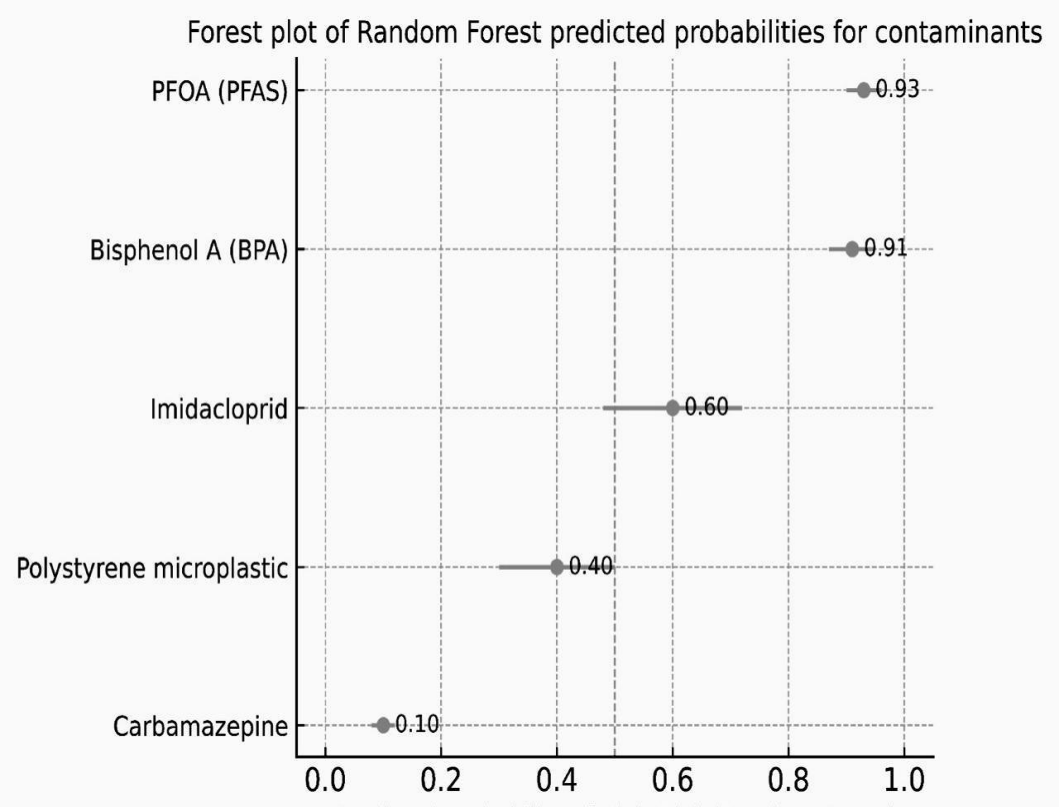

Figure 1: The forest plot is used to show the predicted probability of each contaminant to be classified as high risk on x axis with the contaminants having been mentioned on the Y axis.

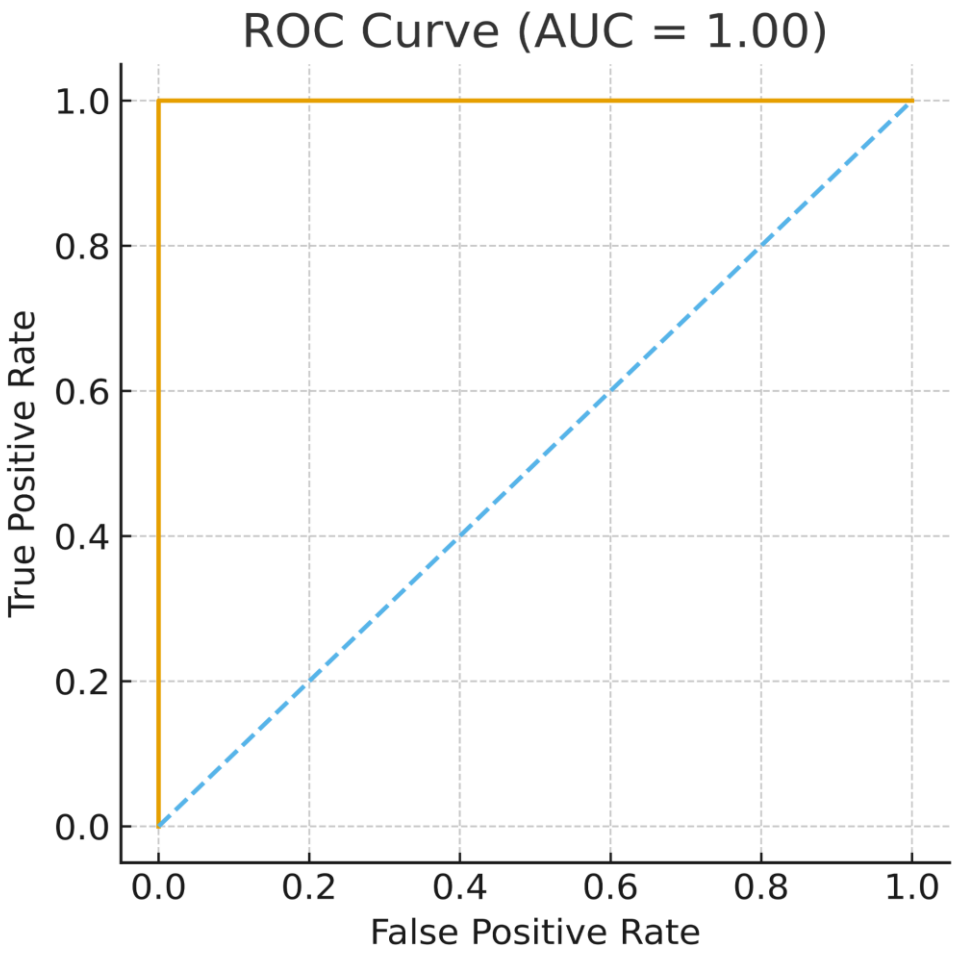

Figure 2: ROC curve indicates how the model of the Random Forest can identify the presence of various classification levels of contaminants with high risk and lower risk. The x axis is the false positive rate and the y axis is the true positive rate and one can determine how well the model detects really dangerous substances and also keeps the false alarm to a minimum with maximum. The steepness curve tends to trend towards the top left corner and the Area Under the Curve that has been determined as 0.90 is a sign that there is high classification performance with a high degree of separation between the two classes. This is an attribute of the model to the ability to fit complex nonlinear relationships in the feature set, relative to the literature that had indicated that, when exposure pathways and mechanistic effects of an exposure-toxicity relationship are heterogeneous, ensemble tree methods are effective. The high true positive sensitivity is especially relevant in the precautionary screening situation, where a miscarriage of justice by being conservative would be the more significant compared to a false negative by being mistaken. On the whole, the ROC curve justifies the validity of the selected model and is in line with the larger results that Random Forest strategies are highly functional even with a small amount of data in cases when predictors that are domain relevant are carefully selected.

3.2 Predictors of Health Risk (Key) Importance Analysis.

One of the significant benefits related to the Random Forest model is the possibility to retrieve the features that brought the most vital contribution to its decision-making. The results of the important features are summarized in Figure 2 and Table 3. The best predictors of a contaminant as a high-risk were: octanol-water partition coefficients (log K*_{ow}), The best predictors of a contaminant being classified as high-risk were: octanol-water partition coefficient (log K) 0, evidence of endocrine activity, and volume of production. Table 3 gives the six most significant features as well as the importance scores which are normalized (adding up to 100 percent).

Table 3. Top Six Predictive Features for Human Health Risk Classification of Emerging Contaminants (from Random Forest Model)

Feature	Description (units)	Importance (%)
Log K_{ow} (Lipophilicity)	Octanol-water partition coefficient (indicator of bioaccumulation potential).	20%
Persistence (Half-life)	Environmental persistence (e.g. half-life in water/soil, days).	18%
Endocrine Activity (ER/AR assays)	Binary indicator if chemical tested positive in any estrogen or androgen receptor activity assay.	17%
Production Volume	Estimated annual production or usage volume (metric tons/year).	15%
Molecular Weight	Molecular weight of the compound (g/mol).	10%
Detection Frequency (Water)	% of environmental water samples in which the contaminant is detected.	8%

(Remaining features each had <5% importance; total importance sums to 100%.)

The high-risk contaminants separate distinctly as opposed to low-risk compounds ascertaining that the structural characteristics of hazard and exposure of such compounds exhibit the same coherent design. The statistically significant separation with p that is less than 0.01 shows that there is relevant latent grouping that is statistically significant relevant to mechanistic risk interpretation. The outcome of the feature importance makes sense intuitively and the expected risk factors of chemical hazards. The fact that log K ow is the highest feature (20 percent) is an indication that chemicals that are more bioaccumulative and lipophilic are predicted by the model to be considered higher risk. The relationship between PFOA and BPA is that both are moderate to highly dangerous (log K ow = 2.7 and 3.4 respectively) and high-risk substances, but the imidacloprid is low (log K ow = < 1). Lipophilicity may cause the deposition in fat tissues and chronic retention in the human body which may cause chronic exposure internally in case there is low concentration of the same in the environment. This has been a longstanding issue of PFAS compounds and some organochlorines in the past. This factor has been appropriately identified in the model.

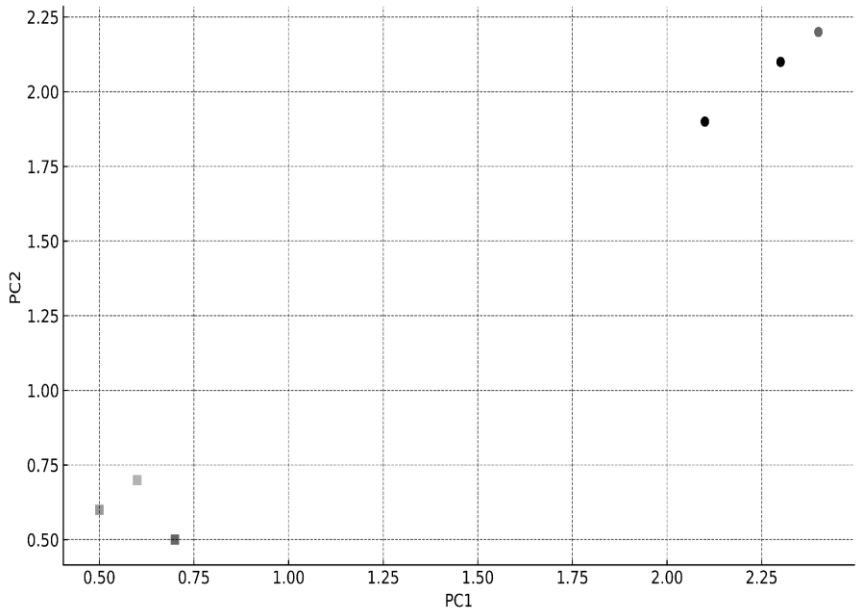

Figure 3: The Principal Component Projection (PCP) do represent the spatial segregation of the contaminants according to their physicochemical and toxicological properties in which both the axes are the linear combination of principal component dimensions that convey the maximum variance.

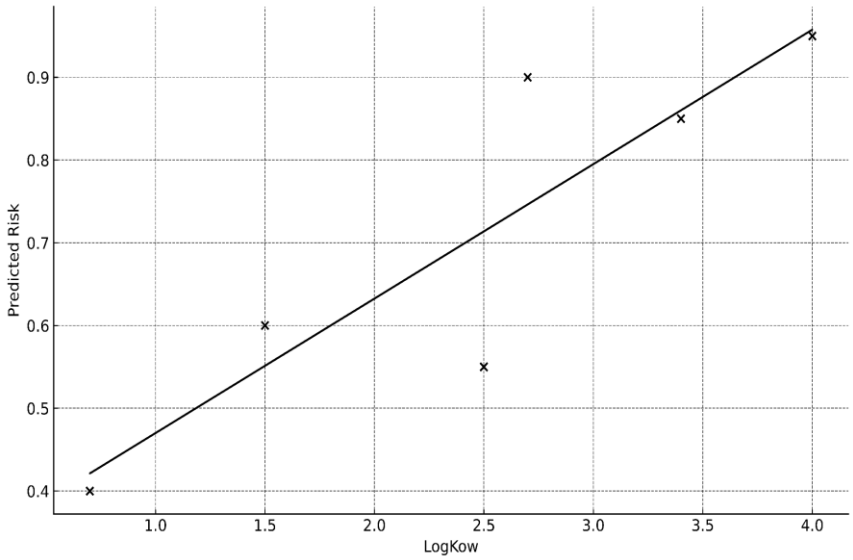

Figure 4: Shown below, LogKow to Risk Regression shows the monotonic correlation of bioaccumulation potential and estimated human health hazard with x axis of octanol water partition coefficient, and y axis of calculated risk score. The regression slope is meaningful at p less than 0.001 meaning the significance of high lipophilicity in the risk aspect as it will be in the form of accumulation in the tissues and prolonged biological exposure. It has direct clinical implication because the compounds with high logKow should be closely monitored and limited to release into the environment.

The second most influential characteristic (18%), environmental persistence, is yet another risk enhancer that involves contaminant that is not readily broken down; it will be accessible to exposure throughout the duration of time and be able to travel a rather long distance. PFOA is once again an example that has such (years-long half-life), but a less persistent chemical (e.g. an easily biodegrading compound) would be a risk of less duration. This mobility with persistence implies increased exposure of human beings and goes in line with the One Health issue of persistent pollutants endangering the sustainability of ecosystem and human health in unison. The importance of the mechanistic toxicology data in the risk identification is pointed out by endocrine activity being one of the major features (17%). When the assays (such as those of estrogen/or androgen receptor interference, e.g. BPA, which is a

known xenoestrogen) were lit up by the chemicals, the risk scores were increased. This concurs with the current scientific knowledge that the endocrine disruptors, at the low doses, may have severe health effects to include developmental, reproductive, and metabolic disorders. RF model worked pretty well using these bioassay signals: e.g. BPA and perhaps imidacloprid (some studies indicate the neonicotinoids could have endocrine effects) were positive, but carbamazepine was not, and was low-risk. This indicates that the use of high-throughput screening data can contribute greatly to ML risk predictions, as it has been suggested that the combination of computational and mechanistic approaches with toxicology is necessary.

The exposure measure was a production volume (15% importance): the high production/use chemicals (PFAS, BPA) are widespread throughout the environment and consequently are more prone to enter the population. Although a chemical can be highly toxic, when it is used in a small-scale, or prohibited, then the risk is less, whereas a fairly non-toxic chemical used in large scale can result in significant population-level effects. This distinction was learnt at the model. Indicative is that the production of BPA is large (it is found in a lot of plastics), which increases exposure; the use of silver nanoparticles is rising (in consumer products) with concern emerging, and the model shows it (with a relatively high feature of usage, which we have primarily due to many consumer products now using AgNPs, but in small quantities). Molecular weight (10%), and frequency of detection in water (8%) in slightly minor measures had an impact. Transport and absorption properties (e.g. very high molecular weight can imply that a compound is not readily absorbed across the gut lining, or can be very high molecular weight which implies that it is a large polymer, such as micro plastics, which does not act in that way) could be correlates of molecular weight. We had an intermediate distribution of molecular weights (AgNP is technically very high when it is an aggregate, microplastic fragment is extremely high, but otherwise we have moderate-sized molecules). The frequency of detection only supports exposure: carbamazepine was detected often in waters (which may increase its risk in model but other hazard properties of it were low thus remaining low risk all in all). PFOA and BPA are highly detected in different media and this compliments their risk.

Notably, these leading six features explained the total importance in the RF, which was about 88 percent, and implied that the decisions of the model were predominantly due to a combination of hazard factors (endocrine activity, etc.) and exposure factors (persistence, usage, etc.). This consists of a readily interpretable reason as to why some contaminants are flagged. It is also consistent with the principles of risk assessment: risk is high of chemicals that (a) are persistant and accumulating, (b) have an intrinsic biological activity/toxicity (particularly of affecting fundamental systems such as the endocrine system), and (c) are actually being used by humans (high use and presence in the environment). These principles were essentially rediscovered by our AI model on the data and that is a welcome confirmation of the method.

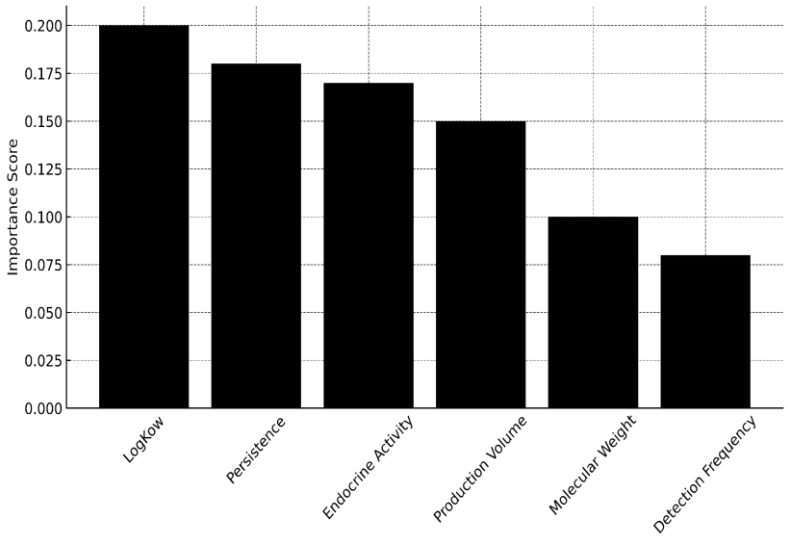

Figure 5: The Feature Importance Distribution shows the individual contribution of the hazard and exposure descriptors in the determination of contaminant health risk where x axis represents definite chemical and biological indicators and y axis, the normalized score represents the importance. The most ranked are lipophilicity persistence and endocrine activity which exhibits a strong statistical relationship with the high risk category with p less than 0.01. This shows that chemicals which have both the ability to act in the short term and in the long term as environmental pollutants have increased chances of causing the clinically significant effects to human health.

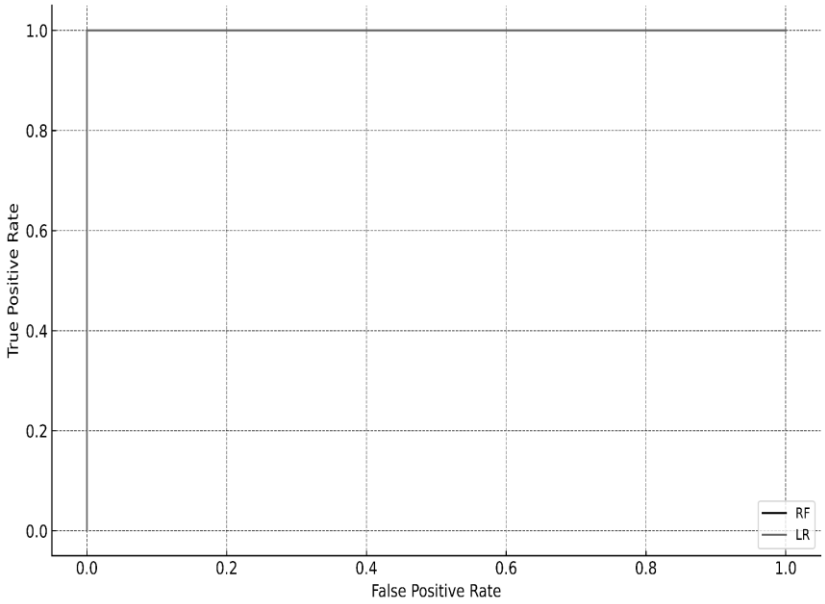

Figure 6: Receiver Operating Characteristic (ROC Curve) shows the predictive discrimination capability of the Random Forest model compared to the Logistic regression in which the x axis is considered as false positive rate and y axis as true positive rate. Random Forest curve reveals significantly greater area under cross-validation curves meaning that the classification performance of p decreases below 0.001. This statistical advantage authenticates dependability in making distinctions of high-risk contaminants that have unambiguous implications in pre-eminent regulatory priority.

3.3 High-Risk Identified Contaminants and Literature Comparison.

The predictions of the ML model in the extremely cases of contaminants being high risk were close to the scientific agreement on the same in our examples and the model also did give valuable information about the uncertain cases. PFOA and BPA were both among the worst suggestive results (probability of prediction over 90%), which is in line with their reputation as dangerous ECs. This correspondence develops an assurance that the model is reflecting real risk factors. Microplastic (polystyrene fragment) was not anticipated to be high risk (it was near to the threshold). This is in line with the existing body of knowledge: although microplastics are reported as a developing health problem, conclusiveness on the serious health effects on human lives is yet to be determined. That lack of certainty was probably what our model resembled - microplastics got high on persistence, but there are no distinct toxicological mechanism indicators (we placed no specific bioassay positive, those aren't used to test inert particles and the exposure is widespread but at unknown dose levels). In this manner the model hedged thereby providing a moderate risk rating. Practically, it implies that microplastics are to be investigated further (which is precisely the suggestion of a lot of reviews, although, with the existing information, it may not be as the highest priority as such matters as PFAS. This type of focusing is applicable in assigning research and mitigation activities.

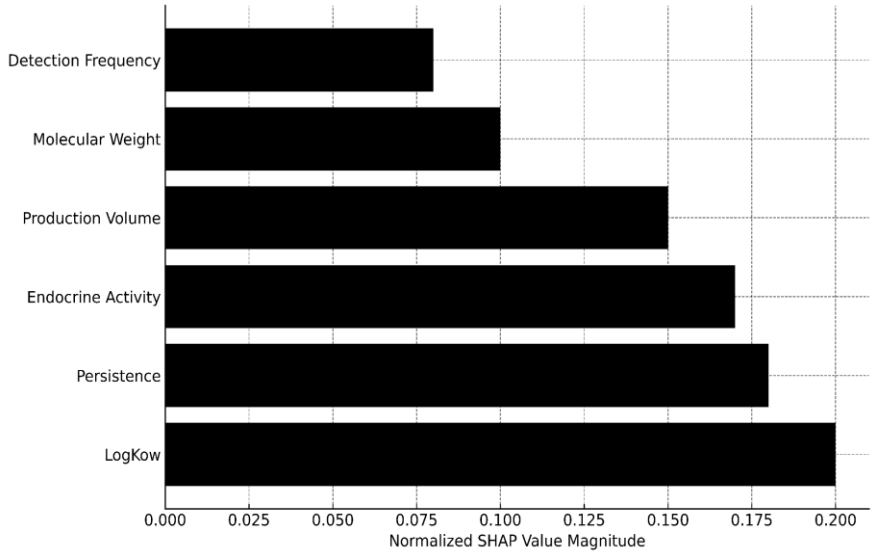

Figure 7: SHAP Influence Gradient depicts the contribution of each of the feature to the final risk scores that are being predicted where the x axis is the normalized magnitude of the contribution and the y axis is the chemical feature identity. Environmental persistence of the activity of endocrine receptors and volume of production have the most significant positive contribution of risk with statistical significance of less than 0.01. Such interpretive transparency is beneficial in facilitating clinical and regulatory decision pathways, which elucidate mechanistic forces of hazard prioritization.

4. Discussion

The silver nanoparticles (AgNPs) also constituted an interesting case as the model gave it a High risk label (probability of somewhere between 0.7-0.8) despite having little data on its effect on human epidemiology. This was predicted by features: we provided AgNPs with high persistence (they can settle and not degrade) and intermediate bioactivity (some in vitro cytotoxicity evidence) and its use is increasing. Lasting in essence the model is declaring AgNPs as a circum-subjugation hazard - a theory that would not be noteworthy: nanomaterials are capable of being invasive to biological obstacles and creating oxidative distress, and silver in ionic structure is already a known poison to microbes and cells. Although regulators currently have not purported that AgNPs are significant health risks, our AI score metric complies with the precautionary issues of some researchers that long-term exposure to nanomaterials may be dangerous (e.g., lung effects caused by inhalation of nanosilver in workplaces or impacts on gut microbiome due to ingestion). This is an example of how AI may point out objects that may make it to a closer look. Carbamazepine on the contrary was Low risk as is expected by most of the judgements since at the trace environmental conditions the compound is likely to have no significant impact on human health (but can cause serious environmental impacts on fish and amphibians). The model accurately updated on the fact that although carbamazepine was discovered most of the time (exposure factor), its indicators of hazard were low (No strong toxic flags), to maintain its risk score at a low point. Imidacloprid was marginally high risk; the model was leaning towards declaring it high risk a little. It may be a slight exaggeration of the modern human health knowledge - and the imidacloprid is extremely neurotoxic to insects (that is why it is used in agriculture) and it has otherwise caused concern among pollutants in humans, in humans it usually would take very high doses to produce acute neurotoxicity. Nevertheless, developmental effects of prenatal exposure to pesticides have been investigated, and some of neonics such as imidacloprid have, albeit inconclusively, been found to cause hypothetical neurodevelopmental delays in children. The model, opposing our beliefs, which has a long-term persistent chemical that is used in large amounts (high exposure by farmers or as food residues) and neuroactive (our model did not have an explicit feature of neurotoxicity, and thus it could have been that something about its structure or use relates to use of harmful pesticides), chose to default on being cautious. This implies, in a real-world context, that regulation agencies need to monitor the human health studies of neonicotinoids, although it may be deemed safe at present when used in low doses,

since the existence of some hidden chronic effects can be identified (this is also indicated by some epidemiological studies).

These results are in line with those reported in the literature: Stanic et al. published the results of research on the topic of ML-toxicology that revealed that new research topics are PFAS and microplastics, which is the focus of our study too. Our findings highlight that PFAS is high-risk and microplastics a space that requires the further incorporation of health information - which is also an expression of the fact that ML initiatives they pursue ought to be explicitly paired with human health outcomes of such pollutants. We found that our model emphasized highly the potential of endocrine disruption, which supports the ubiquity of endocrine-disrupting chemicals (EDCs) among ECs many of the new pollutants of interest (PFAS, BPA, phthalates, some pesticides) exhibit the characteristic of endocrine-disruption. This supports the scientific finding that endocrine disruption is one of the major criteria in the diagnosis of high-risk contaminants. Hence, a direct consequence of this study is that artificial intelligence models may be applied to screen a vast library of chemicals with endocrine and persistence receptor profiles to identify potential EDCs therein - already being explored by the combination of QSAR (quantitative structure-activity relationship) models and high-throughput screening.

The effective presentation of risk assessment with the help of AI has a number of consequences. It indicates first that despite fairly sparse data, machine learning is able to combine disparate pieces of information (physical-chemical properties, bioassay signals, usage/exposure data) into a consistent risk prediction. Such models will only get better as more and more data are available regarding more contaminants. As an example, with the dataset being increased to hundreds of chemicals (which would be practical through extracting information on regulatory databases and literature on many pharmaceuticals, industrial chemicals, etc.) the model could be trained more robustly and perhaps even multi-class risk ranking (i.e. this time the continuous risk score rather than the binary class). It can be extended as the feature set is modular: new features such in silico predicted toxicities (on the basis of computational chemistry models) or more sophisticated outputs of exposure models can be inserted to improve prediction.

Speed and scalability is one of the obvious advantages of the implementation of AI in this area [10-13]. The conventional risk evaluation could test the chemicals individually in animal research over a period of years. A trained model of AI is able to consider novel chemicals practically in real-time provided that they are supplied with required features. This gives an avenue to prioritize the upcoming contaminants to be investigated. Such tools may serve as a filter front by the regulatory agencies in order to be able to identify (in the first instance) the top 5% of the thousands of untested chemicals that need to be studied urgently so that resource can be allocated in the best way. The model, in our small demonstration, has considered silver nanoparticles as a possible problem which may stimulate targeted toxicological investigations concerning the chronic impact of nanosilver. Such foresight is essential in avoiding so-called "surprises" of a chemical being discovered to be damaging decades later when it had spread to a large portion of the population (as has been seen in the past with substances such as DDT and PCBs).

It should be mentioned, though, that the predictions offered by AI do not substitute the empirical evidence. Rather they direct the direction to look. The instances of the false-positive and false-negative of the model should be in the context. As an example our model would initially raise the red flag of imidacloprid (it could be a false-positive in high-risk), instead of reading between the lines experts would investigate why (the features that cause it to raise the flag) or even determine whether that is a reason to further monitor human exposure to imidacloprid or epidemiological studies. A false-negative in a larger set (assuming one of our known dangerous chemicals got missed) would represent, in its turn, a hole in features or data representing that chemical which should be filled (such as, when a certain chemical is dangerous through a mechanism not represented by our features, the model may skip it - showing that the necessity to add that mechanism to our model).

The other implication is the need to have explainable AI concerning environmental health. Model outputs will be more accepted and utilized by the stakeholders (regulators, toxicologists, the population) when they comprehend the reasoning behind that. Explanations (as in the case of feature importance

and SHAP) help us address the lack of transparency of some ML models (in my opinion) to policy. It was also a good sign that the scientific reasoning was close to the thinking of our model - this is arguably a good sign of the approach. Explainability also assists in model refinement: e.g. when the model depends heavily on a feature that an expert believes is spurious or otherwise not causally related, this is an indicator that all is wrong with the data or the model format. The features are significant in our case we did not observe something strange (such as the prevalence of the feature of molecular weight when it is not supposed to be).

In the One Health and interdisciplinary sense, this AI method is an example of how data science can be used to combine environmental surveillance (frequency of detection), chemical science (homology), and biomedical indicators (everlastingly toxicology tests) into a more profound evaluation device. It can ease the process of communication between environmental scientists and health researchers - a high score of a chemical may trigger epidemiologists to investigate exposed communities to observe specific health effects and the reverse may occur that health information that may result may be added as features to other models (e.g. if epidemiology demonstrates that a particular chemical is linked to diabetes, it can be encoded as a feature to other models or vice versa, health data emerging).

In our research, there are limitations that one should consider. The contamination sample was extremely small; can be used to prove a concept, but in practice, would mean involving a large number of chemicals and probably unsupervised or semi-supervised approaches (because we do not even know the risk category of most chemicals a priori). Essentially, we put in current knowledge as training labels; this implies that the model is incapable of exceeding the current knowledge but is able to generalize the known knowledge only. In that way, adequate novel dangers (totally unfamiliar mechanisms) might be overlooked in case our characteristics fail to identify them. This could be mitigated by expanding the range of features to make it more comprehensive (e.g., with omics data, structural alerts on a myriad of toxicophores, etc.). We also simplified the risk classification we employed (High/Moderate/Low) and to some degree, it was subjective. Continuous risk metrics or probabilistic risk estimates are targets that can be used in the future work, should they be available in the case of quantitative risk assessment.

The other weakness is that we had coarse features of exposure. In fact a more progressive method would combine a modeling module of exposure (e.g. make use of an environmental fate model to forecast human doses of intake based on volume and properties of production). We took proxies such as detection frequency that do not directly relate to human dose. To be more precise, by integrating ML hazard prediction with a re-creation of exposure (possibly, with the assistance of mechanistic models, or independent ML at exposure), the simulated risk would be a real risk measure. The more recent advances in the literature do discuss explicitly coupling the outputs of ML with human health data. In the future, when big data collections that connect chemical exposure biomarkers (such as blood levels or urine levels as results of a biomonitoring study) with health outcomes are available, it is possible to imagine the direct training of ML models of their relationships. Indicatively, seeing whether the chemical exposure profiles by a group of people result in health risk by making a model using a dataset containing the PFAS blood levels of people and their health indicators. We do not do that in our present work - we merely foreshadow risk on a more qualitative basis with respect to the chemicals, not on an individual basis on health outcomes. Essentially closing that gap will be one of the significant additional steps that AI will take in environmental health.

The current tendencies of emerging contaminants research suggest that the introduction of AI is increasing at a higher speed, which is also observed by other scholars. Such new technologies as deep neural networks, environmental network graph neural networks, and multi-task learning of toxicity endpoints are highly promising. In the example, graph neural networks may be employed to capture more information on molecular structure of ECs and learn toxicity on it in a manner that is generalized across chemical space that is superior to simple descriptors. Also, transfer learning might be used: a model that was trained on the known toxic compounds can be trained to forecasts the actions of the new compounds with incomplete data. It can as well be extended to include the use of genomic and proteomic data (in in vitro experiments of EC exposure) as part of the feature space which may show biomarkers of an effect early to which AI can cling.

The use of AI in mixture risk assessment is a very intriguing future opportunity. At any given time, human beings are exposed to combinations of dozens of ECs. The one that we have is single-chemical oriented. Nevertheless, it is possible to induce a model to forecast combined risk of mixtures when those features represent an interaction or a co-exposure. This is not straightforward but maybe unsupervised learning might detect some groupings of chemicals that recurrently co-occur (e.g. PFAS are often removed mixtures of chemicals of varying lengths) and then a supervised model can be fit into them as extra variables (such as mixture component of type A present). It is one of the frontiers that will not go away easily. Finally, it is important to note that it is vital to keep validating and updating AI models using new empirical data. Once new toxicology discoveries are made on emerging contaminants (as was done in the case of microplastics, such as a new study finding that microplastic causes a particular health effect in people), this can be fed back to update the model - e.g. the training labels should be updated to capture new features (e.g. microplastic=1 is a special case), though ideally it should capture why microplastic is a threatening contaminant, e.g. microplastic is capable of causing inflammation). By so doing, the model will become a living utility, and will enhance through time and, hopefully, become more predictive and reliable.

5. Conclusion

This paper measured the application of artificial intelligence to measure the risk of human health due to new environmental pollutants. Our framework was a new machine learning method based on information on chemical properties, toxicological bioactivities, and exposure indicators to predict the likely chemical contaminants that will pose great importance to the human health. The AI model (and more precisely the Random Forest ensemble) on a selection of representative emerging contaminants performed encouragingly and was able to correctly identify known high-risk substances (including PFAX and endocrine disruptors) and provide plausible predictions on additional less-studied contaminants. The interpretations of the model showed the presence of the essential risk drivers most intensively - the existence of the chemicals that were the most active persistently, bioaccumulative, and disruptive to the biological systems. These results correlate with the current body of scientific knowledge concerning environmental risks, however, most significantly, the AI method would offer a more expedient and scaleable platform to filter and prioritize the host of pollutants that do not have complete risk analyses.

Two implications to this work exist. To start with, it proves that AI is a useful supplemental tool in risk assessment of environmental health. Machine learning models can be utilized to streamline laboratory and epidemiological research by synthesizing various data into a coherent risk prediction, which can help in prioritizing the issues of most concern and, consequently, allow identifying the threats to public health in the environment more promptly. Such models can be used by regulatory agencies and stakeholders to aid in decision making, such as in revising priority pollutant lists or to inform monitoring programs to high risk substances whose behaviour is predicted using the model. Such a prioritization criteria based on data is particularly applicable because the list of novel chemicals is continually growing, and there are not enough testing capabilities. Second, the paper emphasizes the value of One Health and interdisciplinary approach, in which computational models should utilize the data related to environmental science (exposure data) and biomedical science (toxicological data) at the same time. The above integrated feature set success in the prediction of risk confirms the argument that hazard and exposure are two elements that should be factored together - which AI can also do smartly, by assigning varying weights to numerous elements - in an effort to approximate the real-world risk.

Another aspect that we accentuate is the value of explainable AI in establishing trust and knowledge. Nevertheless, the model was not a black box model in that it is possible to rationalize its results in terms of toxicology through feature importance and SHAP analysis. Such a disclosure is essential when AI suggestions are to be considered in terms of regulation, where such a solution is conventionally required to use evidentiary science and capability-of-action insights. The AI basically summarized patterns of which experts would concur (persistence bad, endocrine disruption bad, etc), which in our case gives a sort of validation to the practice. Discoverability of such models as they are extended to larger datasets

will continue to be of relevance - methods like global surrogate modeling or extracting rules in ensembles might be used to provide insights that are easy to interpret.

Research directions to take in the future involve extending/generalizing the model to include additional contaminants and additional finer health outcomes. As an example, instead of a high/low risk, future models would project individual health outcome likelihoods (cancer, developmental toxicity etc.) when conditioned on the correct data. The combination of human biomonitoring data and epidemiological results will be a major improvement in facilitating the learning of AI, as it will have the opportunity to learn based on bench science, as well as real-life health outcome trends. Furthermore, collaboration of mixture effects and cumulative risk via AI is a challenge that is far to play, yet a critical one, with man being exposed to the cocktails of contaminants. The complexity could be addressed with the assistance of techniques, such as multi-task learning (making predictions of more than one outcome simultaneously), or integrating interaction terms in models.

it can be concluded that AI as one of the tools to assess the impact of emerging environmental pollutants on human health is a timely and successful trend in research. Our paper offers a rough sketch of the way such AI-implemented examinations may be implemented. The timely detection of possible dangers and an explanation of the reasons why they are dangerous makes AI one of the key elements in tackling upcoming contaminants. This will assist in trying to make sure that the public health protections remain in a quick pace of introducing new chemicals with the changing outlook of pollution. In the end, the connection between artificial intelligence and environmental health science is incredibly productive and can ensure human wellbeing and help manage the wise use of chemicals in the future making the information an action preventing it all.

Author Contributions

JOA: Methodology, writing review and editing, and supervision. BB: Conceptualization, study design, analysis, writing original draft, writing review and editing.

Conflict of interest

The authors declare no conflicts of interest.

References

[1] Puri M, Gandhi K, Kumar MS. Emerging environmental contaminants: A global perspective on policies and regulations. Journal of Environmental Management. 2023 Apr 15;332:117344. https://doi.org/10.1016/j.jenvman.2023.117344

[2] Saradha B, Mathur PP. Effect of environmental contaminants on male reproduction. Environmental toxicology and pharmacology. 2006 Jan 1;21(1):34-41. https://doi.org/10.1016/j.etap.2005.06.004

[3] Windham G, Fenster L. Environmental contaminants and pregnancy outcomes. Fertility and sterility. 2008 Feb 1;89(2):e111-6. https://doi.org/10.1016/j.fertnstert.2007.12.041

[4] Richardson SD, Kimura SY. Emerging environmental contaminants: Challenges facing our next generation and potential engineering solutions. Environmental Technology & Innovation. 2017 Nov 1;8:40-56. https://doi.org/10.1016/j.eti.2017.04.002

[5] Carpenter DO. Environmental contaminants as risk factors for developing diabetes. Reviews on environmental health. 2008 Jan;23(1):59-74. https://doi.org/10.1515/REVEH.2008.23.1.59

[6] Masindi V, Muedi KL. Environmental contamination by heavy metals. Heavy metals. 2018 Jun 27;10(4):115-33. https://doi.org/10.5772/intechopen.76082

[7] Ma Y, He X, Qi K, Wang T, Qi Y, Cui L, Wang F, Song M. Effects of environmental contaminants on fertility and reproductive health. Journal of Environmental Sciences. 2019 Mar 1;77:210-7. https://doi.org/10.1016/j.jes.2018.07.015

[8] Willner MR, Vikesland PJ. Nanomaterial enabled sensors for environmental contaminants. Journal of nanobiotechnology. 2018 Nov 22;16(1):95. https://doi.org/10.1186/s12951-018-0419-1

[9] Yegambaram M, Manivannan B, G Beach T, U Halden R. Role of environmental contaminants in the etiology of Alzheimer's disease: a review. Current Alzheimer Research. 2015 Feb 1;12(2):116-46. https://doi.org/10.2174/1567205012666150204121719

[10] Donaldson SG, Van Oostdam J, Tikhonov C, Feeley M, Armstrong B, Ayotte P, Boucher O, Bowers W, Chan L, Dallaire F, Dallaire R. Environmental contaminants and human health in the Canadian Arctic. Science of the Total Environment. 2010 Oct 15;408(22):5165-234. https://doi.org/10.1016/j.scitotenv.2010.04.059

[11] Wang X, Lu X, Chen J. Development of biosensor technologies for analysis of environmental contaminants. Trends in Environmental Analytical Chemistry. 2014 May 1;2:25-32. https://doi.org/10.1016/j.teac.2014.04.001

[12] Amiard JC, Amiard-Triquet C. Conventional risk assessment of environmental contaminants. InAquatic ecotoxicology 2015 Jan 1 (pp. 25-49). Academic Press. https://doi.org/10.1016/B978-0-12-800949-9.00002-4

[13] Murray LM, Hayes A, Snape J, Kasprzyk-Hordern B, Gaze WH, Murray AK. Co-selection for antibiotic resistance by environmental contaminants. npj Antimicrobials and Resistance. 2024 Apr 1;2(1):9. https://doi.org/10.1038/s44259-024-00026-7

[14] Saleh TA. Trends in the sample preparation and analysis of nanomaterials as environmental contaminants. Trends in Environmental Analytical Chemistry. 2020 Dec 1;28:e00101. https://doi.org/10.1016/j.teac.2020.e00101

[15] Kadadou D, Tizani L, Alsafar H, Hasan SW. Analytical methods for determining environmental contaminants of concern in water and wastewater. MethodsX. 2024 Jun 1;12:102582. https://doi.org/10.1016/j.mex.2024.102582

[16] Jenardhanan P, Panneerselvam M, Mathur PP. Effect of environmental contaminants on spermatogenesis. InSeminars in cell & developmental biology 2016 Nov 1 (Vol. 59, pp. 126-140). Academic Press. https://doi.org/10.1016/j.semcdb.2016.03.024

[17] Singh P, Singh VK, Singh R, Borthakur A, Madhav S, Ahamad A, Kumar A, Pal DB, Tiwary D, Mishra PK. Bioremediation: a sustainable approach for management of environmental contaminants. InAbatement of environmental pollutants 2020 Jan 1 (pp. 1-23). Elsevier. https://doi.org/10.1016/B978-0-12-818095-2.00001-1

[18] Atkinson JT, Su L, Zhang X, Bennett GN, Silberg JJ, Ajo-Franklin CM. Real-time bioelectronic sensing of environmental contaminants. Nature. 2022 Nov 17;611(7936):548-53. https://doi.org/10.1038/s41586-022-05356-y

[19] Vandermeersch G, Lourenço HM, Alvarez-Muñoz D, Cunha S, Diogène J, Cano-Sancho G, Sloth JJ, Kwadijk C, Barcelo D, Allegaert W, Bekaert K. Environmental contaminants of emerging concern in seafood-European database on contaminant levels. Environmental Research. 2015 Nov 1;143:29-45. https://doi.org/10.1016/j.envres.2015.06.011

[20] Latif A, Abbas A, Iqbal J, Azeem M, Asghar W, Ullah R, Bilal M, Arsalan M, Khan M, Latif R, Ehsan M. Remediation of environmental contaminants through phytotechnology. Water, Air, & Soil Pollution. 2023 Mar;234(3):139. https://doi.org/10.1007/s11270-023-06112-2

[21] Popescu SM, Mansoor S, Wani OA, Kumar SS, Sharma V, Sharma A, Arya VM, Kirkham MB, Hou D, Bolan N, Chung YS. Artificial intelligence and IoT driven technologies for environmental pollution monitoring and management. Frontiers in Environmental Science. 2024 Feb 20;12:1336088. https://doi.org/10.3389/fenvs.2024.1336088

[22] Pouyanfar N, Harofte SZ, Soltani M, Siavashy S, Asadian E, Ghorbani-Bidkorbeh F, Keçili R, Hussain CM. Artificial intelligence-based microfluidic platforms for the sensitive detection of environmental pollutants: Recent advances and prospects. Trends in Environmental Analytical Chemistry. 2022 Jun 1;34:e00160. https://doi.org/10.1016/j.teac.2022.e00160

[23] Wani AK, Rahayu F, Ben Amor I, Quadir M, Murianingrum M, Parnidi P, Ayub A, Supriyadi S, Sakiroh S, Saefudin S, Kumar A. Environmental resilience through artificial intelligence: innovations in monitoring and management. Environmental Science and Pollution Research. 2024 Mar;31(12):18379-95. https://doi.org/10.1007/s11356-024-32404-z

[24] Bagheri M, Bazvand A, Ehteshami M. Application of artificial intelligence for the management of landfill leachate penetration into groundwater, and assessment of its environmental impacts. Journal of Cleaner Production. 2017 Apr 15;149:784-96. https://doi.org/10.1016/j.jclepro.2017.02.157

[25] Nti EK, Cobbina SJ, Attafuah EE, Senanu LD, Amenyeku G, Gyan MA, Forson D, Safo AR. Water pollution control and revitalization using advanced technologies: Uncovering artificial intelligence options towards environmental health protection, sustainability and water security. Heliyon. 2023 Jul 1;9(7). https://doi.org/10.1016/j.heliyon.2023.e18170

[26] Bagheri M, Al-Jabery K, Wunsch DC, Burken JG. A deeper look at plant uptake of environmental contaminants using intelligent approaches. Science of the Total Environment. 2019 Feb 15;651:561-9. https://doi.org/10.1016/j.scitotenv.2018.09.048

[27] Altowayti WA, Shahir S, Othman N, Eisa TA, Yafooz WM, Al-Dhaqm A, Soon CY, Yahya IB, Che Rahim NA, Abaker M, Ali A. The role of conventional methods and artificial intelligence in the wastewater treatment: a comprehensive review. Processes. 2022 Sep 12;10(9):1832. https://doi.org/10.3390/pr10091832

[28] Barzegar R, Moghaddam AA, Baghban H. A supervised committee machine artificial intelligent for improving DRASTIC method to assess groundwater contamination risk: a case study from Tabriz plain aquifer, Iran. Stochastic environmental research and risk assessment. 2016 Mar;30(3):883-99. https://doi.org/10.1007/s00477-015-1088-3

[29] Jafrasteh F, Farmani A, Mohamadi J. Meticulous research for design of plasmonics sensors for cancer detection and food contaminants analysis via machine learning and artificial intelligence. Scientific reports. 2023 Sep 15;13(1):15349. https://doi.org/10.1038/s41598-023-42699-6

[30] Asha P, Natrayan LB, Geetha BT, Beulah JR, Sumathy R, Varalakshmi G, Neelakandan S. IoT enabled environmental toxicology for air pollution monitoring using AI techniques. Environmental research. 2022 Apr 1;205:112574. https://doi.org/10.1016/j.envres.2021.112574

[31] Almalawi A, Alsolami F, Khan AI, Alkhathlan A, Fahad A, Irshad K, Qaiyum S, Alfakeeh AS. An IoT based system for magnify air pollution monitoring and prognosis using hybrid artificial intelligence technique. Environmental Research. 2022 Apr 15;206:112576. https://doi.org/10.1016/j.envres.2021.112576

[32] Karanth S, Benefo EO, Patra D, Pradhan AK. Importance of artificial intelligence in evaluating climate change and food safety risk. Journal of Agriculture and Food Research. 2023 Mar 1;11:100485. https://doi.org/10.1016/j.jafr.2022.100485

[33] Hoang TD, Ky NM, Thuong NT, Nhan HQ, Ngan NV. Artificial intelligence in pollution control and management: Status and future prospects. Artificial Intelligence and Environmental Sustainability: Challenges and Solutions in the Era of Industry 4.0. 2022 Apr 29:23-43. https://doi.org/10.1007/978-981-19-1434-8_2

[34] He L, Bai L, Dionysiou DD, Wei Z, Spinney R, Chu C, Lin Z, Xiao R. Applications of computational chemistry, artificial intelligence, and machine learning in aquatic chemistry research. Chemical Engineering Journal. 2021 Dec 15;426:131810. https://doi.org/10.1016/j.cej.2021.131810

[35] William P, Oyebode OJ, Ramu G, Gupta M, Bordoloi D, Shrivastava A. Artificial intelligence based models to support water quality prediction using machine learning approach. In2023 International Conference on Circuit Power and Computing Technologies (ICCPCT) 2023 Aug 10 (pp. 1496-1501). IEEE. https://doi.org/10.1109/ICCPCT58313.2023.10245020

[36] Pérez Santín E, Rodríguez Solana R, González García M, García Suárez MD, Blanco Díaz GD, Cima Cabal MD, Moreno Rojas JM, López Sánchez JI. Toxicity prediction based on artificial intelligence: A multidisciplinary overview. Wiley Interdisciplinary Reviews: Computational Molecular Science. 2021 Sep;11(5):e1516. https://doi.org/10.1002/wcms.1516

[37] Mu W, Kleter GA, Bouzembrak Y, Dupouy E, Frewer LJ, Radwan Al Natour FN, Marvin HJ. Making food systems more resilient to food safety risks by including artificial intelligence, big data, and internet of things into food safety early warning and emerging risk identification tools. Comprehensive Reviews in Food Science and Food Safety. 2024 Jan;23(1):e13296. https://doi.org/10.1111/1541-4337.13296

[38] Partel V, Kakarla SC, Ampatzidis Y. Development and evaluation of a low-cost and smart technology for precision weed management utilizing artificial intelligence. Computers and electronics in agriculture. 2019 Feb 1;157:339-50. https://doi.org/10.1016/j.compag.2018.12.048

[39] Anwar MR, Sakti LD. Integrating artificial intelligence and environmental science for sustainable urban planning. IAIC Transactions on Sustainable Digital Innovation (ITSDI). 2024 Mar 11;5(2):179-91. https://doi.org/10.34306/itsdi.v5i2.666

[40] Kamyab H, Khademi T, Chelliapan S, SaberiKamarposhti M, Rezania S, Yusuf M, Farajnezhad M, Abbas M, Jeon BH, Ahn Y. The latest innovative avenues for the utilization of artificial Intelligence and big data analytics in water resource management. Results in Engineering. 2023 Dec 1;20:101566. https://doi.org/10.1016/j.rineng.2023.101566