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To reuse or not: is purified wastewater a non-toxic and sustainable resource for the future? (REASSURE)

Risks associated with hazardous pollutants in wastewater reuse and their mitigation

Uzair Akbar Khan, Cecilia Stålsby Lundborg, Lutz Ahrens, Karin Wiberg, Lars Sonesten, Claudia Von Brömssen, Foon Yin Lai

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Preface

In this report results from the project "To reuse or not: is purified wastewater a non-toxic and sustainable resource for the future? (REASSURE)" are presented.

The project is one of the four synthesis projects carried out within the research initiative Wastewater and Eutrophication.

With the four synthesis projects, the Swedish Environmental Protection Agency and the Swedish Agency for Marine and Water Management wanted to summarize and analyze the state of knowledge and knowledge needs in the areas of wastewater and eutrophication. The overall purpose of the syntheses was to contribute to policy development in sustainable water management so that we achieve the environmental objectives in the long term and that the state of the environment is improved. The call focused on three areas, one of which was wastewater as a resource.

The project has been financed with funds from the Swedish Environmental Protection Agency's environmental research grant.

The report was written by Uzair Akbar Khan, Lutz Ahrens, Karin Wiberg, Lars Sonesten, Claudia Von Brömssen and Foon Yin Lai (principal investigator), all from Swedish University of Agricultural Sciences SLU, with contribution from Cecilia Stålsby Lundborg from Karolinska Institutet.

The report has been reviewed for scientific quality by Åsa Davidsson (Lund university) as well as for practical relevance by Cezary Bose, Maximilian Lüdtke (the Swedish Environmental Protection Agency) and Margareta Lundin Unger (the Swedish Agency for Marine and Water Management).

The authors are responsible for the content of the report.

Stockholm, December 2024

Johan Bogren
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Summary

Innovative solutions, like safe reuse, are required in water and sludge management to achieve circular economy and to address the challenges of global water scarcity and soil nutrient loss. In the research project "REASSURE", the overall aim was to enhance the understanding of the potentiality and sustainability of using domestic wastewater as a resource in Sweden and abroad, with a focus on hazardous pollutants, metals and microplastics. The project had the following specific objectives:

1. Determine factors that influence or determine the reuse of wastewater and sludge across countries;
2. Characterize the current state of wastewater reuse in Sweden and the occurrence of hazardous pollutants as obstacles to its reuse;
3. Evaluate the effectiveness of different advanced treatment techniques against hazardous pollutants for a better effluent water quality;
4. Assess the risks of hazardous pollutants to environmental and health impacts associated with wastewater as a resource.

This literature synthesis project presents insights into the influencing factors for cross-national differences in the reuse of wastewater and sludge. Data on national wastewater and sludge reuse was compiled along with relevant national statistics. Sludge data is compiled in this report for cross-national comparison only. Wastewater reuse showed a positive correlation with fraction of wastewater treated, degree of urbanization, level of water stress, and GDP per capita. The project also discusses the situation of wastewater reuse in selected countries of interest, indicating that reuse practices, policies, and applications vary across these countries.

A comprehensive compilation of hazardous contaminants in effluent water for Swedish domestic and municipal wastewater, greywater, and blackwater was performed from literature. A workflow for literature review, meta-analysis and risk and hazard evaluation of contaminants (based on 14 parameters) in effluent wastewater was established. In addition, criteria for risk-based scoring, ranking, and prioritization of contaminants is also presented. This resulted in a priority list of 119 specific chemical contaminants of emerging concern (CECs) that can hinder sustainable wastewater reuse. Among the priority chemicals identified, 30 (primarily pharmaceuticals) had a risk quotient ≥ 1, indicating ecological risk. Additionally, 16 chemicals were flagged as environmental hazards due to their persistence and mobility, while approximately 60 chemicals were associated with positive predictions for at least four human health hazards. The 10 highest-priority chemicals were venlafaxine, bicalutamide, desvenlafaxine, diclofenac, amoxicillin, clarithromycin, diethyltoluamide, genistein, azithromycin, and fexofenadine. Although there can be a number of different potential options for wastewater reuse, this report has primary focus on agricultural irrigation for wastewater reuse, given that agriculture is the largest consumer of freshwater globally (United Nations, 2024). In Sweden, the reuse of treated municipal wastewater for irrigation could be especially advantageous for farmers in areas that experience significant water shortages during the growing season (Swedish Environmental Protection Agency, 2022).

The project also looks into available treatment technologies and their combinations for removal of these priority chemicals. Information on available advanced treatment technologies and their targeted chemical contaminants are compiled from the Swedish literature, and removal efficiencies of five selected technologies (granular activated carbon (GAC), ozonation, membrane bioreactor (MBR), nano-filtration (NF), and reverse osmosis (RO) for 38 priority chemicals, from international literature, were used to rank these technologies. Furthermore, it explores the link between advanced treatment technologies and the pollutant properties, and provides a cost analysis of these selected technologies. Considering its effectiveness to remove CECs and the lower cost, GAC, or a combination of technologies, may be used for safe wastewater reclamation.

The driving factors of wastewater and sludge reuse are useful for evaluating the potential of reusing such resources and development of new water management plans on recycling wastewater as sustainable water resource. Chemical pollutants identified as impediments to treated wastewater reuse can help in establishing criteria for the risk management plans under the EU regulation on wastewater reuse (Regulation (EU) 2020/741). The risk characterization and policy support, are greatly relevant to the Swedish Environmental Protection Agency for providing guidelines on reducing the spread of hazardous pollutants to the environment due to wastewater reuse. Advanced treatment options and strategies presented here will facilitate the municipalities' responsible for wastewater treatment facilities to consider modernizing their existing treatment facilities and even facilities on future plan to purify the wastewaters for reuse to a greater extent. Future policy briefs should consider to focus on reducing the presence of priority chemicals in effluent water by establishing concentration limits and mandating advanced treatment technologies, based on removal efficiency and ecological risk assessments. These should be integral to future regulations. As the dataset is derived from available literature, further studies and reanalysis using the meta-analysis workflow will be necessary to address potential unknown chemicals.

1. Introduction

In response to the global challenges of water scarcity and diminishing mineral resources, there is a growing consideration for using treated domestic wastewater as an alternative supply of water and nutrients. Water reuse and related issues are expected to impact world-wide crop production, and consequently the global food security (OECD, 2020). Water shortage is expected to affect a quarter of the world population by 2050 (United Nations, 2015). Nutrients taken up by food crops end up in wastewater and ultimately to receiving water bodies, resulting in nutrient loss from soil and disturbance to the ecosystem balance (Steffen et al., 2015). Therefore, closing the loop on resources in domestic wastewater is vital for sustainable water and agricultural managements in the future. In spite of these potential benefits, inadequate wastewater treatment especially for removing hazardous pollutants (Sörengård et al., 2019) undermines a safe wastewater reuse. The trade-off between wastewater reuse and the risk of hazardous pollutants leads to the research question: How safe and viable is wastewater as a resource for a non-toxic circular economy?

Reuse of domestic wastewater is made possible by its proper management and sanitation. Municipal effluents comprising wastewaters from different activities/sources and urban runoffs, is often the source of domestic wastewater for reuse. Reuse of municipal effluent stands at around 1 billion m^3 in Europe (European Commission, 2024). In Sweden, the southern county of Gotland, as an example, reuses 2.5 % of its municipal effluent for irrigation (Bio by Deloitte, 2015). However, the situation varies across countries and the differences may be explained by various factors, such as water availability and water requirement of industry and agriculture (Bio by Deloitte, 2015). Consumer perceptions and the economic incentive for the operators also influence among other parameters (Swedish Environmental Protection Agency, 2022). So far, it is unclear what factors drive adoption of reuse practices at a national level and identifying these factors can help sustainable management of these resources for reuse globally.

Despite the potential benefits of reuse for reaching a circular economy, previous studies indicate inadequacy of conventional treatment for removal of many hazardous pollutants present in domestic and municipal wastewater (Gago-Ferrero et al., 2017; Haalck et al., 2021; Sörengård et al., 2019). Many pollutants are hazardous for the environment and/or human health, e.g., antibiotics have public health concern linked to antimicrobial resistance (Richardson and Kimura, 2020).

The new EU regulation on wastewater reuse (Regulation (EU) 2020/741) mainly impose limits on microorganisms and traditional water quality parameters, but do not directly address hazardous pollutants in assessing effluent water quality. A comprehensive overview of the presence of commonly occurring hazardous pollutants in wastewaters and their implications for safe water reuse, their ecological risk and environmental and human health hazards, as well as new strategies to remove these pollutants for a sustainable reuse of such resources are, therefore, covered in this report of the REASSURE project, via a literature synthesis work striving for answering the following important questions:

1. What factors are the most relevant for explaining cross-national differences in the use of wastewater and sludge as a resource?

2. Are there spatial differences in wastewater reuse and which hazardous pollutants are of high concern in conventionally treated wastewaters in Sweden?
3. How can advanced treatment techniques help remove hazardous pollutants to facilitate safe reuse?
4. To what extent do hazardous pollutants pose environmental and human health risks in treated wastewaters?

2. Methodology

2.1 Cross-national comparison

In order to study factors affecting cross-national differences in wastewater and sludge reuse, various statistics are retrieved from different sources. Data on population, gross domestic product (GDP) per capita, degree of urbanization, agricultural irrigated land, level of water stress, and mean annual precipitation etc. were obtained from World Bank Open Data[1]. Annual mean surface air temperature (measured at 1.5–2 m height) data was obtained from World Bank Climate Change Knowledge Portal[2]. Linear regression was carried out between these parameters and fractions of wastewater reused. Spearman correlation coefficients (r_s) were also calculated. Data on national wastewater production, collection, treatment and reuse was taken from Jones et al. (2021) based on reported and predicted values. Fraction of wastewater reused (%) was calculated as the ratio of wastewater reused to wastewater produced. Data for production and reuse of sludge in Europe was obtained from Eurostat[3]. Fraction of sludge reused was calculated as ratio of sludge agricultural use to sludge production for 21 countries with available data. Most recent available data was used unless a much larger amount of data was available for near, previous years.

The top-four countries in the three categories of wastewater reuse, i.e., (1) total reuse of wastewater, (2) per capita reuse of wastewater, and (3) reuse as a percentage of total water extracted (Jimenez and Asano, 2008), were selected for further study in this project. This resulted in eight countries (China, Mexico, USA, Egypt, Qatar, Israel, Kuwait, and Singapore). Six other countries (Chile, Spain, Namibia, Cyprus, Australia, and Malta) are also considered so that it represents all major geographical regions of the world. These additional countries were selected from the top 20 in the three categories described above. Sweden was also included in the selection for comparison.

2.2 Characterization of hazardous pollutants in effluent water quality

2.2.1 Data compilation and pre-processing

A comprehensive literature review of scientific articles and grey literature was carried out on Web of Science, Scopus, DiVA portal, and Google scholar using carefully developed and validated search strings both in English and Swedish languages (Annex-I). Quality check of the search string was carried out using names of individual contaminants instead of group of contaminant. The results were validated by relevant key articles well-known to the authors. Abstract screening of the obtained

[1] https://data.worldbank.org/
[2] https://climateknowledgeportal.worldbank.org/
[3] https://data.europa.eu/en

scientific articles was carried out using Rayyan (Ouzzani et al., 2016). Literature published during January 2000 to October 2022 was included. List of scientific articles and gray literature included in the study is presented in Appendix-I. Extracted information and data from the selected articles and grey literature included contaminant name and group, concentrations in influent and/or effluent, detection/quantification limits, numbers of samples, wastewater type, treatment plant details, and sampling methods. In assessment of full texts, we divided hits (both scientific articles and grey literature) into three different categories: i) wastewater, ii) sludge, and iii) pilot studies with new technologies.

Data pre-processing included screening for duplicates with different names but same Chemical Abstract Service (CAS) numbers. A meta-analysis workflow adapted from Löffler et al. (2023) was developed based on occurrence and on risk and hazard assessment of chemical contaminants (Figure 1). For further data analysis and discussion, we focused on substances that had at least 20 quantifiable data points in the dataset and quantifiable frequency of more than 50 %. This resulted in 128 contaminants, comprising 119 chemical contaminants, five metals, and four linear alkylbenzene sulfonate compounds. The alkylbenzene sulfonate compounds were excluded from further risk and hazard assessment due to a lack of unique CAS numbers. Concentrations of linear and branched per- and polyfluoroalkyl substances (PFAS), when reported separately, were combined in the dataset for consistency.

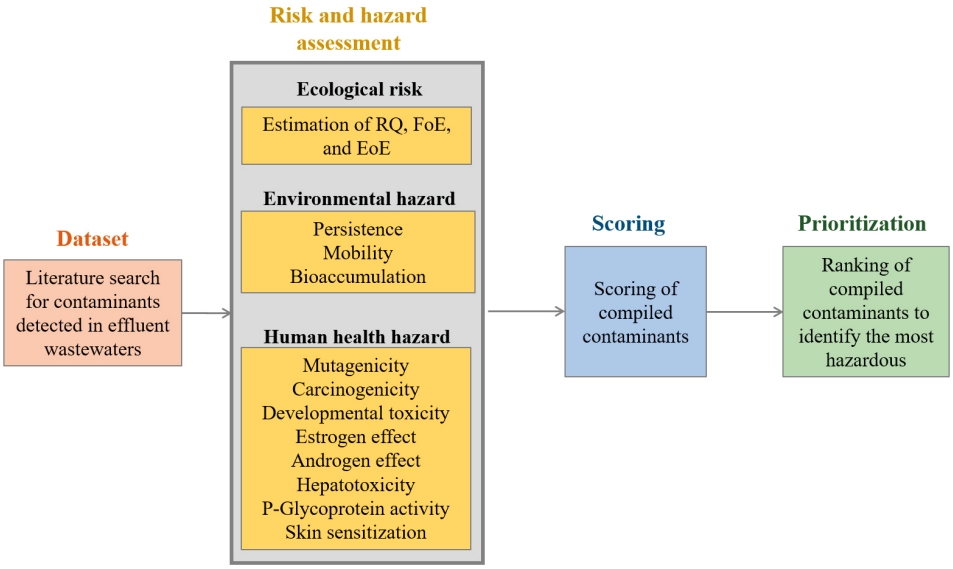


Figure 1: Meta-analysis workflow, comprising literature search, risk and hazard assessment, scoring, and prioritization of substances. RQ: risk quotient; FoE: frequency of exceedance; EoE: extent of exceedance. Adapted from Khan et al. (2024).

2.2.2 Ecological risk assessment and health hazard prediction

2.2.2.1 ECOLOGICAL RISK ASSESSMENT

Ecological risk assessment for each chemical was carried out by comparing the measured concentration in wastewater treatment effluent against predicted no-effect concentration (PNEC). Ecotoxicological data for chemicals was collected from sources such as the US EPA ECOTOX database (USEPA, 2023), the Swedish FASS pharmaceuticals database (FASS, 2023), the Pesticides Properties Database (PPDB, 2023), European Chemicals Agency (ECHA, 2023), and the scientific literature. PNECs were determined as per European guidelines for risk assessment (ECHA, 2008; EMA, 2018). For most sensitive species, an appropriate assessment factor was applied. Chronic ecotoxicity data from standard test species for algae, daphnids, and fish were applied by preference, but also data for non-standard species depending on data availability. Quantitative structure activity relationship (QSAR) data (ECOSAR, 2023) were obtained for data-poor chemicals and an assessment factor of 1000 was applied to the acute toxicity value for the most sensitive species.

Conventional ecological risk quotient (RQ) (Equation 1) was calculated for each chemical:

$$RQ = \frac{MEC_{eff,max}}{PNEC} \quad (1)$$

where $MEC_{eff,max}$ is measured environmental concentration, taken as the maximum effluent concentration in the dataset, and PNEC is the predicted no-effect concentration. As effluent water reuse provides an alternative to the common practice of using surface water, groundwater or drainage water for irrigation in some areas of Sweden (Swedish Agency for Marine and Water Management, 2022), assessment of effluent water quality in terms of ecological risk is carried out with a consideration of PNEC concerning aquatic organisms.

Frequency of exceedance (*FoE*) (Equation 2) and extent of exceedance (*EoE*) (Equation 3) (Alygizakis et al., 2019; Slobodnik et al., 2012), two additional risk parameters were also included:

$$FoE = \frac{n}{N} \quad (2)$$

$$EoE = \frac{MEC_{eff,95\%tile}}{PNEC} \quad (3)$$

where n is number of data points of effluent concentrations above PNEC, N is total number of data entries including both quantifiable and non-quantifiable data points, and $MEC_{eff,95\%tile}$ is measured effluent concentration of a chemical contaminant at the 95th percentile of the dataset.

A probabilistic risk assessment was also performed, adapting the methodology of Hanna et al. (2023). For this, reported concentrations were ranked in ascending order and percent rank (j) were assigned to them using the Weibull model (Equation 4), where i is the numerical rank and n is the number of data points. Linear regression was used to fit percent rank against the log transformed effluent concentrations. Regression coefficients were used to estimate the centile values corresponding to PNECs (Equation 5).

$$j = \frac{i * 100}{n + 1} \tag{4}$$

$$\text{centile value} = ((\text{slope} * log(\text{PNEC})) + \text{intercept}) \tag{5}$$

2.2.2.2 ENVIRONMENTAL HAZARD PREDICTION

Environmental hazard indicators, persistence (P), mobility (M), and bioaccumulation (B) were predicted using VEGA *in silico* platform (version 1.2.3), following Löffler et al. (2023). The following models were used: i) IRFMN (version 1.0.1) for persistence in water (half-life), ii) IRFMN (version 1.0.2) for water solubility, iii) Opera (version 1.0.1) for organic carbon-water partitioning coefficient, K_{OC}, and iv) CAESAR (version 2.1.15) for bioconcentration factor (BCF).

2.2.2.3 HUMAN HEALTH HAZARD PREDICTION

The concept for evaluating human health hazards used in this study was adapted from Bruks et al. (2022, 2021), Löffler et al. (2023), and Menger et al., (2023). The concept is based on using *in silico* approaches for predicting mutagenicity, carcinogenicity, developmental toxicity, skin sensitization, estrogen receptor effect, androgen receptor effect, hepatoxicity, and P-glycoprotein activity as proxies for human health hazards. The following models were used: Mutagenicity (Ames test) Consensus model (v.1.0.4), Carcinogenicity model (CAESAR) (v.2.1.10), Developmental Toxicity model (CAESAR) (v2.1.8), Skin Sensitization model (CAESAR) (v.2.1.7), Estrogen Receptor-mediated effect (IRFMN-CERAPP) (v.1.0.1), Androgen receptor-mediated effect (IRFMN-COMPARA) (v.1.0.1), Hepatoxicity model (IRFMN) (v.1.0.1), and P-Glycoprotein activity model (NIC) (v1.0.1).

Performance of environmental and human health hazard prediction models were evaluated by cross-checking inclusion of the priority list chemicals in the respective training and test datasets of the models. Most models included between 5 and 48 of the ranked chemical contaminants (Khan et al., 2024). However, skin sensitization model contained only one chemical from the list and P-glycoprotein activity model contained none, so estimates of these should be treated with caution.

2.2.3 Scoring and prioritization

The risk and hazard parameters were scored against criteria for ecological risk, and environmental and human health hazards (Table 1). Each parameter, except *FoE*, is given a score of either 0 when there is no risk or a negative hazard, or 1 when there is risk or a positive hazard. For FoE, the calculated numerical value was used as score.

The overall score of the ecological risk assessment ($Score_{Eco}$) (Equation 6) was calculated as:

$$Score_{Eco} = \frac{Score_{RQ} + Score_{EoE}}{2} + FoE \tag{6}$$

The overall score of predicted environmental hazard ($Score_{EH}$) (Equation 7) was estimated as:

$$Score_{EH} = \frac{\sum_{i=1}^{3} n_i}{3} \tag{7}$$

where n_i represents the scores for persistence, mobility, and bioaccumulation.

The overall score of human health hazard ($Score_{HH}$) (Equation 8) was calculated as:

$$Score_{HH} = \frac{\sum_{i=1}^{8} n_i}{8} \quad (8)$$

where n_i represents scores for mutagenicity, carcinogenicity, developmental toxicity, skin sensitization, estrogen receptor effect, androgen receptor effect, hepatoxicity, and P-glycoprotein activity.

Table 1: Parameters and related scoring criteria used when prioritizing chemical contaminants of emerging concern (CECs) in effluent wastewater (Khan et al., 2024).

	Parameter	Risk/hazard (score 1)	No risk/hazard (score 0)
Ecological risk	RQ	> 1	< 1
	EoE	> 1	< 1
	FoE	Not applicable	Not applicable
Environmental hazard	Persistence (half-life in water)	> 40 days	< 40 days
	Mobility (solubility and log K_{oc} (log L/kg))	> 0.15 mg/L and ≤ 4.5	< 0.15 mg/L and ≥ 4.5
	Bioaccumulation (log BCF) (log L/kg wet weight)	> 3.3	< 3.3
Human health hazard	Mutagenicity	Positive	Negative
	Carcinogenicity		
	Developmental toxicity		
	Skin sensitization		
	Estrogen receptor effect		
	Androgen receptor effect		
	Hepatoxicity		
	P-glykoprotein activity		

A final score (Equation 9) of each chemical contaminant was obtained:

$$Final\ score = Score_{Eco} + Score_{EH} + Score_{HH} \quad (9)$$

The final scores of each chemical were ranked in descending order to obtain a risk based priority list. Maximum score of $Score_{Eco}$ was 2 compared to 1 for $Score_{EH}$ and $Score_{HH}$ each, therefore $Score_{Eco}$ had a higher weight on the final score. The maximum final score was 4, representing the highest concern, and the minimum was 0, indicating the lowest concern.

2.3 Compilation of information on advanced treatment technologies

Information on available advanced treatment technologies and their targeted chemical contaminants are compiled from the Swedish literature (see 3.2.1). For simplicity and conciseness of these information, all membrane technologies were categorized as one technology, i.e., membrane filtration, which includes ultra-filtration, nano-filtration (NF) and reverse osmosis (RO), except for membrane bioreactor (MBR) as another category of membrane technology alone, and also both granular activated carbon (GAC) and powdered activated carbon (PAC) were categorized as activated carbon. For further detailed analysis (correlations), we focused on five commonly used technologies in water treatment, i.e., GAC, ozonation, MBR, NF, and RO. They also have different mechanisms in removals of contaminants, including adsorption and biodegradation for GAC, chemical reactions for ozonation, and size exclusion for MBR, NF and RO. Their maximum reported removal efficiency for the priority chemicals (n = 38, first quartile in the priority list and substances included in the proposed revisions to EU's Urban Waste Water Treatment Directive (UWWTD) (*COM(2022) 541 final*) (European Commission, 2022) was obtained from scientific literature. The search was conducted on Web of Science, Scopus, and Google Scholar by using keywords for the respective chemicals and treatment technologies. Based on the mean of maximum removal efficiencies for all the reported chemicals, individual advanced treatment technologies were ranked to show their adequacy to effectively remove these priority chemicals. The goal is to assess the maximum capability of the technology. This means we aim for studies that demonstrate the highest possible removal efficiency achievable with a specific technology. In other words, the maximum represents the highest performance threshold the technologically can reach, which is the key factor we are interested in when comparing different technologies. We also explored correlation (Spearman correlation coefficient) between physicochemical properties (octanol-water partitioning coefficient, log K_{ow}; water solubility; organic carbon-water partitioning coefficient, log K_{oc}; acid dissociation constant, pKa; and molecular weight) of these chemicals and their removal through the selected advanced treatment technologies. Molecular weight and pKa values were obtained from online sources (predominantly PubChem database) and the rest of the properties were determined using VEGA *in silico* platform (version 1.2.3). Capital, operation and maintenance, and energy costs of the advanced treatment technologies were also determined from literature and compared.

3. Results and Discussion

3.1 Cross-national differences in wastewater reuse

Global wastewater reuse is estimated to be around 41 billion m^3/year, representing only 11 % of the produced wastewater (Jones et al., 2021). The fraction highly varies between countries, with some reusing very high proportion of their produced wastewater (e.g., United Arab Emirates (UAE) (100 %), Israel (92 %), Kuwait (89 %), and Qatar (89 %)), while some others, mainly countries with low treatment levels or high availability of water resources, reusing very low proportions (Jones et al., 2021). Different factors that represent national climate, socio-economic conditions, and situation of water resources were explored to determine factors that can predict the potential of reusing treated wastewater in a country. Fraction of wastewater reused was positively correlated (Figure 2) with GDP per capita (r_s = 0.65), urbanization (r_s = 0.54), level of water stress (r_s = 0.47), agricultural irrigated land (r_s = 0.26) and fraction of wastewater treated (r_s = 0.76), and negatively correlated with average annual precipitation (r_s = −0.37) (figur 2). All these correlations were statistically significant ($p < 0.05$). However, linear and quadratic regression models did not provide a good fit to the data as indicated by the low R^2 values, suggesting that multiple variables should be taken into account to reliably predict wastewater reuse potential. For countries with missing data on wastewater reuse, estimations based on irrigation water scarcity, level of wastewater treatment, and desalination capacity per capita were used in the source dataset (Jones et al., 2021), therefore, these correlations should be treated with caution. GDP and water stress have been identified as the main influencing factors for wastewater treatment and reuse, respectively, in Asia (Liao et al., 2021). Almost all the countries with water stress levels well above 100 % (Kuwait, UAE, Saudi Arabia, Libya, Qatar) are located in the middle east, the region which accounts for 39 % of the global desalination capacity, indicating that it is severely constrained in terms of fresh water availability (Eke et al., 2020). These countries generally have very high rate of water reuse (89–100 %), except Libya and Saudi Arabia which reuse only 18 % and 33 % of their wastewater, respectively.

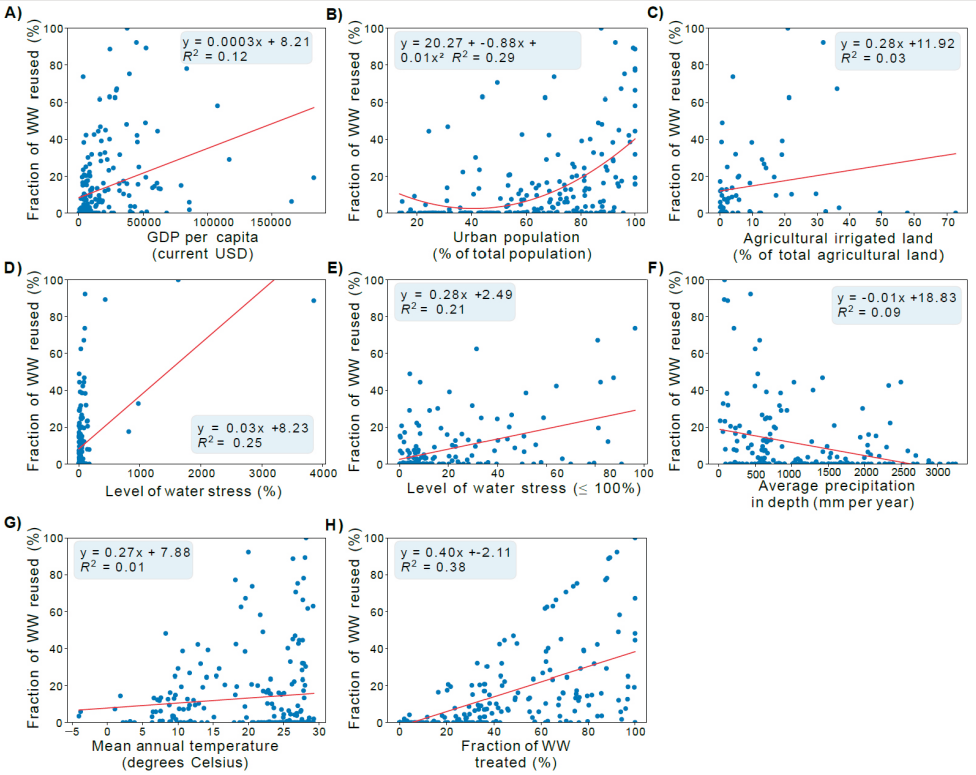


Figure 2. Regression analysis between the fractions of wastewater reused (ratio of the amount of wastewater reused to that of the wastewater produced in a country) and A) GDP per capita (current USD) (n = 208), B) urban population as a percentage of total population (n = 214), C) agricultural irrigated land as percentage of total agricultural land (n = 67), D) level of water stress represented by ratio of total freshwater withdrawn and total renewable freshwater resources (%) (n = 178), E) level of water stress (excluding countries with > 100 % water stress) (n = 161), F) average precipitation in depth (mm per year) (n = 182), G) mean annual temperature (°C) (n = 212), and H) fraction of wastewater treated (ratio of treated wastewater and produced wastewater) (%) (n = 214).

Factors affecting sludge reuse were only explored for Europe due to data availability. Only two factors, agricultural irrigated land (r_s = −0.47) and mean annual temperature (r_s = −0.74), had significant correlation with sludge reuse (Figure 3). Wastewater reuse and sludge reuse were inversely correlated (r_s = −0.35) (Figure 4), but the correlation was not significant (p = 0.1). This may be explained by differences in drivers and motivation for the adoption of sludge reuse and wastewater reuse. Water reuse is motivated by limited availability of fresh water resources while sludge reuse is rather driven by the agricultural requirement of nutrients. As droughts and warm periods are predicted to intensify under climate change (Vicente-Serrano et al., 2020), more and more countries will find it necessary to explore opportunities for wastewater reuse. Similarly, climate change induced alterations in nutrient cycling and availability (Brouder and Volenec, 2008) will also influence the future role of sludge in crop fertilization. For wastewater treatment plant operators, incentive to reusing sludge also comes from the high costs associated with sludge disposal (Domini et al., 2022).

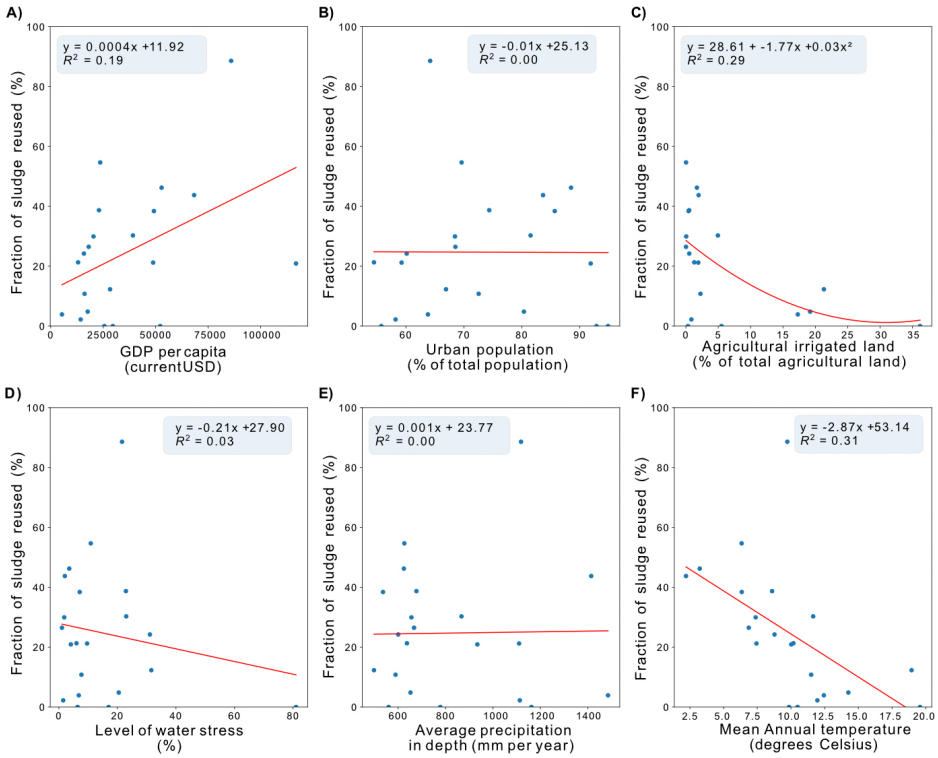


Figure 3. Regression analysis between the fraction of sludge reused (ratio of the amount of sludge reused to that of the sludge produced) and A) GDP per capita (current USD) (n = 21), B) urban population of total population (%) (n = 21), C) agricultural irrigated land of total agricultural land (%) (n = 19), D) level of water stress represented by ratio between total freshwater withdrawn and total renewable freshwater resources (%) (n = 21), E) average precipitation in depth (mm/year) (n = 21), F) and mean annual temperature (°C) (n = 21). Data covers countries in Europe.

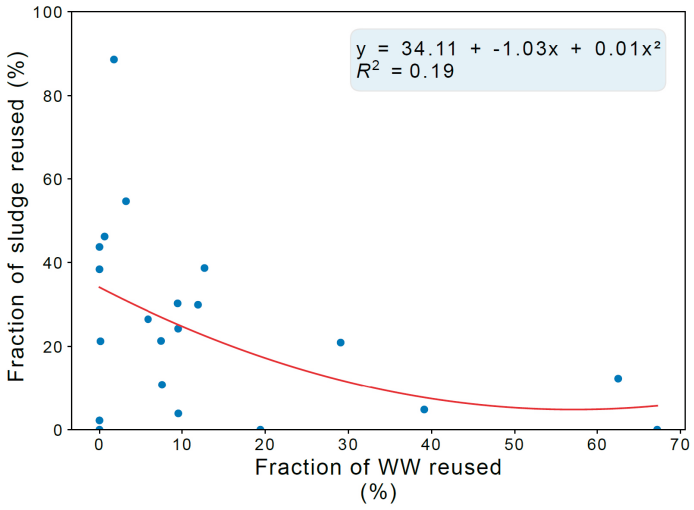


Figure 4. Regression analysis between the fraction of sludge reused and the fraction of wastewater reused (n = 21).

There are varying situations of wastewater reuse across the selected countries in this project (Table 2). In Sweden, ~ 80 % of the produced wastewater is treated but less than 1 % is reused (Jones et al., 2021) (Table 2). A very low level of water stress at 3.5 % appears to not incentivize reusing wastewater over freshwater extraction, unlike some other countries with high water stress, e.g., United Arab Emirates (1600 %), Qatar (431 %), and Israel (100 %). However, agricultural irrigated land makes up only 1.7 % of total agricultural land in Sweden and most of the crops are rain-fed (Grusson et al., 2021), therefore potential for wastewater reuse for agricultural irrigation exists during dry periods. In a recent report of the Swedish Environmental Protection Agency (2022) that analyzed measures for implementing EU regulation for water reuse (*Regulation (EU) 2020/741*), there are areas identified in the south where irrigation is needed during the growing seasons and hence have potential for reuse. Reuse in industry and irrigation of non-agricultural areas, e.g., golf courses, can also be a viable option. The study (Swedish Environmental Protection Agency, 2022) also concluded that public attitude towards irrigation with treated wastewater will be a decisive factor for the future of agricultural wastewater reuse in Sweden. In Sweden, the predominant water usage is for industry. Manufacturing industry accounts for 61 % of water consumption, followed by households at 23 %, other sectors at 13 %, and agriculture at 3 % (Swedish Agency for Marine and Water Management, 2022).

Cyprus and Malta are among the European countries with very high fraction of wastewater reuse, both reusing ~ 65 % (Table 2) of their wastewater (Duong and Saphores, 2015; Jones et al., 2021), although the level of water stress is quite different between the two countries, i.e., 32 % for Cyprus and 81 % for Malta. The countries are very similar in terms of climate (mean annual temperature and average precipitation, GDP per capita, and proportion of agricultural irrigated land). In addition, fraction of wastewater treated is also quite different, with Cyprus treating 62 % of wastewater while Malta treating 100 % (Jones et al., 2021).

In Spain, about a quarter of the produced wastewater is reused (Table 2) and more than 80 % of the total reuse takes place for agricultural irrigation and for urban irrigation (e.g., parks and recreational areas) (Jodar-Abellan et al., 2019; Jones et al., 2021). Demand for non-conventional water sources, like desalination and reclaimed water, are the highest in the southeastern region of the country, which has the lowest amount of available fresh water, and more than three quarters of agricultural irrigation reuse takes places in two southeastern river basin districts, i.e., Segura and Júcar (Jodar-Abellan et al., 2019). Spanish regulation for water reuse (Real Decreto 1620/2007) defines water quality limits for five classes (and 14 sub-classes) of intended water reuse. In all the classes, common parameters include intestinal nematodes, coliform bacteria (*Escimerichia Coli*), suspended solids, and turbidity. In addition, for most of the sub-classes, specific criteria, e.g., compliance with environmental quality standards for hazardous substances, are needed. However, a new legislation, i.e., urgent measures in agricultural and water matters (Real Decreto-Ley 4/2023) repealed any provisions of the previous regulation 1620/2007 in conflict with the recent EU water reuse regulation (*Regulation (EU) 2020/741*).

In Egypt, WWTPs are mostly located in urban areas and serve about 60 % of the population (Tawfik et al., 2021). Despite being illegal, reuse of untreated wastewater for irrigation is common in the Nile Delta, which takes place through discharge of untreated wastewater into the environment, including agricultural drains (Tawfik et al., 2021). This has led to increased concentrations of contaminants, such as metals in soil (Alnaimy et al., 2021). The relevant Egyptian code (ECP 501-2015)

prohibits reuse of treated wastewater for irrigating raw-eaten vegetables (Abdella Ahmed et al., 2022). For other irrigation uses, four categories of treated wastewater have been defined based on treatment levels to irrigate specific crops (Abdella Ahmed et al., 2022).

Qatar meets its entire water demand from seawater desalination (Ahmad and Al-Ghouti, 2020), although its fraction of wastewater reused accounts for ~ 90 % (Table 2). Around 39 % of treated wastewater in Qatar is used for agriculture, and other avenues of reuse have been identified, such as, in district cooling industries and construction sector etc. (Jasim et al., 2016). Groundwater is used at a rate four times its replenishing rate, indicating high water stress (Qatar Foundation, 2022). Treated wastewater is mostly used to recharge groundwater aquifers, as well as for irrigation of greenbelts, growing animal fodder, injected in deep aquifers, or discharged to lagoons and sea (Jasim et al., 2016; Qatar Foundation, 2022).

In Israel, the fraction of wastewater reused is ~ 90 % (Table 2). Treated wastewater fulfills ~ 50 % of the irrigation water demand and supports 25 % of all water demand (Fanack Water, 2023; Rahav et al., 2017). Around 80 % of the treated wastewater is used for irrigation, and most orchards in Israel are irrigated with treated wastewater (Rahav et al., 2017). Israel also relies heavily on desalination, which provides 50 % of the potable water supply (Fanack Water, 2023). There are special rules for granting permits for agricultural irrigation based on treatment level of the wastewater and barriers between wastewater and fruit. In addition, there are requirements such as field locations, warning signs, and measures to prevent contamination of drinking water (Ministry of Health, 2023). For irrigation of public gardens, there are also detailed guidelines for safe operation of co-existing double water systems, i.e., a drinking water system and a treated water system (Ministry of Health, 2023).

Kuwait gets its potable water through seawater desalination, but still treats and reuses ~ 90 % their wastewater (Table 2). One of the four WWTPs in Kuwait has a reverse osmosis and ultra-filtration based reclamation plant, the effluent of which is utilized for crop and natural reserve irrigation, while the others have conventional treatments up to a tertiary level for effluent water reuse for landscape and fodder irrigation (Aleisa, 2019).

The United States (US) produces around 62 billion gallons (234 million m^3) of treated wastewater everyday through 16 000 WWTPs (ASCE, 2021). The fractions of wastewater treated and reused in the US are 68 % and 13 %, respectively (Table 2) (Jones et al., 2021). In the guidelines for wastewater reuse by the US's Environmental Protection Agency (USEPA, 2012), reclaimed water quality is defined for various reuse categories, including urban, agricultural, environmental and industrial reuse, impoundments, groundwater recharge, and indirect potable reuse. Agricultural water reuse guidelines include pH, BOD[4], turbidity, fecal coliform and residual chlorine. In addition to the USEPA guidelines, many US states have their own guidelines and regulations (Shoushtarian and Negahban-Azar, 2020; USEPA, 2012).

In Mexico, around 63 % of the wastewater produced is treated and ~ 70 % of the treated flowrate is discharged into various water bodies according to Tabla-Vázquez et al. (2020). The rest (~ 30 %) is mainly used for irrigation in agricultural lands, golf courses etc. A similar estimate of 43 % wastewater reuse was provided in Jones et al. (2021) (Table 2). In addition to the treated wastewater, untreated wastewater is also

[4] Biochemical oxygen demand.

reused for agricultural irrigation. A study in the Mezquital valley reported 50 m^3/s of untreated wastewater irrigating 80 000 ha of agricultural land, leading to accumulation of hazardous contaminants, especially metals in the soil and crops (Ponce-Lira et al., 2020).

In Chile, more than 70 % of WWTPs provide treatment up to the secondary treatment stage and the wastewater can only be reused for irrigation of non-food crops (Villamar et al., 2018). Most of the wastewater is discharged into different water bodies and less than 1 % is reused for irrigating animal feed crops, grasslands etc. (Villamar et al., 2018).

China shows a steady increase in wastewater reuse during recent years, reaching around 13 billion m^3/year in 2019 (Qu et al., 2022). Even with these volumes, reclaimed water represents less than 1 % of the total water use (Zhu and Dou, 2018). Reuse is most widely practiced in Beijing and Tianjing. Most of the reclaimed water is used to improve urban landscape and ecology (Qu et al., 2022). Only 12 out of the 31 provinces in China use reclaimed water for agricultural irrigation, and only 5 provinces use it for groundwater recharge as there is a cautious attitude towards these practice due to perceived environmental risks (Zhu and Dou, 2018).

In Singapore, ~ 40 % of potable water comes from reclamation (Kog, 2020). Four reclaimed water plants, based on conventional wastewater treatment and membrane filtration (microfiltration/ultra-filtration/reverse osmosis) with UV disinfection, provide the treated wastewater for industrial reuse and indirect potable reuse after re-mineralization in reservoirs (Lefebvre, 2018). Options for direct potable reuse are also being explored as the next step.

Table 2. GDP per capita (current USD), agricultural irrigated land (%), level of water stress (%), average precipitation (mm/year), fraction of wastewater treated (%), and fraction of wastewater reused (%) for selected countries.

Region/ continents	Country	GDP/capita* (current USD)	Agricultural irrigated land of total agricultural land* (%)	Level of water stress* (%)	Average precipitation in depth* (mm/year)	Fraction of wastewater treated** (%)	Fraction of wastewater reused** (%)
Europe	Sweden	52 838	1.7	3.5	624	80	0.6
	Spain	26 984	14	40	636	71	24
	Cyprus	28 281	21	32	498	63	63
	Malta	29 598	36	81	560	100	67
Middle east/ North Africa	Egypt	3 572	NA	141	18	57	23
Middle east	Qatar	52 316	NA	431	74	89	89
	Israel	44 847	32	100	435	92	92
	Kuwait	24 298	NA	3 850	121	89	89
North America	United States	63 529	NA	28	715	68	13
	Mexico	8 895	5.8	45	758	43	20
South America	Chile	13 174	NA	9	1522	84	3.5
Asia	China	10 409	NA	44	645	49	14
Sydöstra Asien	Singapore	61 274	NA	82	2 497	100	44
Africa	Namibia	4 252	NA	0.86	285	21	21
Oceania	Australia	51 868	0.63	4.2	534	93	49

NA: not available; *World Bank Open Data; **based on Jones et al. (2021).

3.2 Current and future reuse needs in Sweden

According to the Swedish EPA report (2022), only a few Swedish counties have arrangements for wastewater reuse for irrigation, such as, Gotland, Kalmar, Skåne, and Uppsala. Combined risk of water shortage based on climate, storage capacity and water use is presented by Stensen et al. (2019), with higher risk observed in southern Sweden (Figure 5). Using this information, it can be seen that many more counties in addition to those mentioned above, such as Stockholm, Södermanland, and Västmanland could benefit from the availability of and access to treated wastewater for irrigation. There is around 1.2 billion m^3 of treated wastewater produced annually in Sweden[5] which can be used for this purpose. The reasons for limited reuse at the moment include public and farmer concern about hazardous pollutants in treated wastewater, similar to concerns around spreading wastewater sludge (Ekane et al., 2021) and uncertainty about future water quality regulations (Takman et al., 2023).

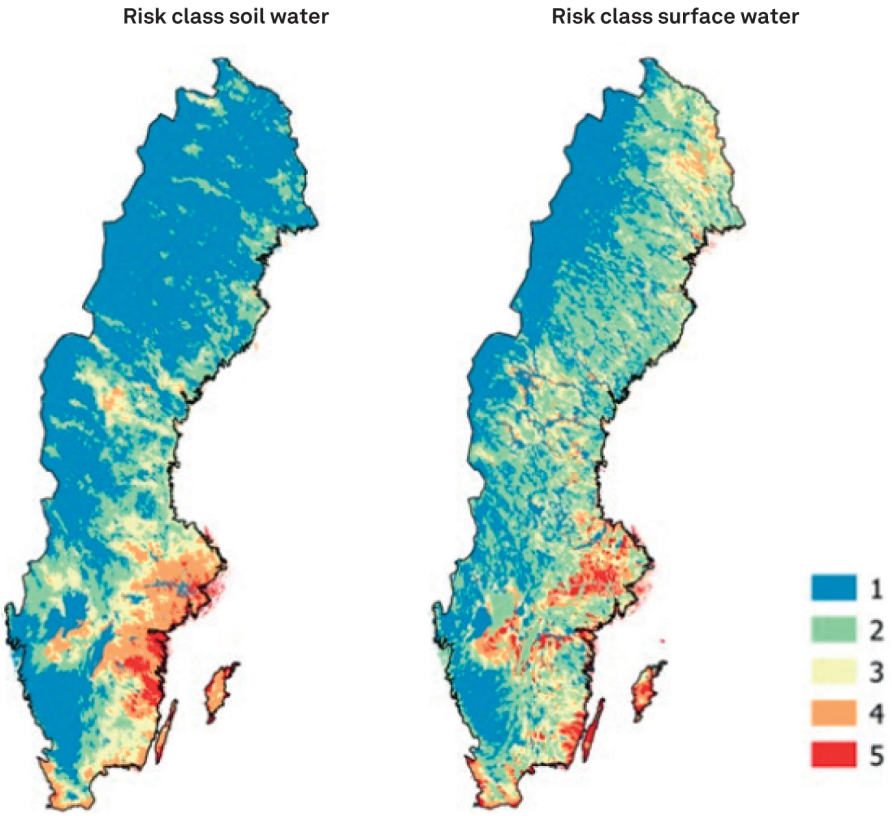


Figure 5. Risk of water scaricity in Sweden based on climate, storage capacity and individual water use. 1 represents lowest risk and 5 represents highest risk. Figure taken from Stensen et al. (2019).

[5] https://www.statistikdatabasen.scb.se/

3.3 Chemicals as impediments to reuse

A priority list of 119 chemicals (Figure 6) was obtained after scoring and ranking according to ecological risk and environmental and human health hazards (Table 1) (Khan et al., 2024). These chemicals can be considered as the main impediments to wastewater reuse in Sweden. Pharmaceuticals made a large part of the list with 69 chemicals, which is in line with the recent rise in concerns associated with pharmaceuticals and their risk (Chaturvedi et al., 2021; Wang et al., 2021). Top eighteen chemicals on the list had a final risk score of 2–3 out of a maximum score of 4. These include 15 pharmaceuticals, two personal care products, and an industrial chemical. Four antibiotics (amoxicillin, clarithromycin, azithromycin, and ciprofloxacin) are included in the top eighteen chemicals, and the risk quotient of antimicrobial resistance (RQ_{AMR}) was > 1 for three of these: ciprofloxacin (RQ_{AMR} = 17), clarithromycin (3.1), and amoxicillin (1.1). RQ_{AMR} was based on PNEC of resistance selection from a previous study (Bengtsson-Palme and Larsson, 2016). Two additional antibiotics, metronidazole and trimethoprim included in the list of 119 chemicals had RQ_{AMR} > 1. In addition, OH-metronidazole, a transformation product of metronidazole, also showed RQ_{AMR} > 1 based on $PNEC_{AMR}$ of the parent compound (Löffler et al., 2023). Predicted environmental concentrations in soil and crops with Swedish irrigation context can be found in Khan et al. (2024).

Figure 6. Final scores, score of ecological risks ($Score_{Eco}$), score of environmental hazards ($Score_{EH}$) and score of human health hazards ($Score_{HH}$) for high-priority chemical contaminants of concern (CECs) in effluent water (Khan et al., 2024).

Nine out of the 13 suggested chemicals in the proposed revisions to the EU urban wastewater treatment directive (UWWTD) (*COM(2022) 541 final*) (European Commission, 2022) are included in the list. These chemicals are diclofenac, clarithromycin, venlafaxine, benzotriazole, carbamazepine, citalopram, hydrochlorothiazide, irbesartan, and metoprolol. Four chemicals from the UWWTD are not in the list: amisulpride, candesartan, and two methylbenzotriazole isomers. Among the 119 prioritized compounds in this study, 31 are also included in the 53 priority compounds evaluated based on only ecological risk for recipient aquatic environments (Yang et al., 2022).

3.3.1 Ecological risk assessment

Thirty of the chemicals on the list had RQ ≥ 1, which included 26 pharmaceuticals, one food additive, one insect repellant, one antimicrobial agent, and one industrial chemical (Table A1). Clarithromycin had the highest RQ and EoE values of 390 and 79, respectively, followed by venlafaxine and diclofenac with RQ of 114 and 108, respectively, and EoE > 1. The number of chemicals showing risk was reduced from 30 to 24 for EoE > 1 (Table A1). Chemicals no longer showing ecological risk included bezafibrate, carbamazepine, codeine, metoprolol, thiabandazole, and tramadol. Highest concentration of some of these chemicals were measured in treated black water (carbamazepine and metoprolol) (Leven et al., 2016) or domestic wastewater treated in soil beds (thiabendazole) (Blum et al., 2017), which may be the reason for the difference between the highest concentration and the 95th percentile effluent concentration. For the other chemicals, sampling method, sampling season, or size and features of the WWTPs can be the reason for the difference. Some chemicals were almost always encountered in treated effluent in concentrations well above their respective PNECs as shown by their high FoE, e.g., bicalutamide (0.97) (Table A1). On the other hand, some rarely had concentrations above their PNECs, e.g., metoprolol and carbamazepine, which had the lowest FoE of 0.01. Highest overall ecological score was for bicalutamide ($Score_{ECO}$ = 1.97), followed by fexofenadine, diclofenac, venlafaxine, and amoxicillin (Figure 6). Influent and effluent concentration ranges along with the probabilistic risk assessment for all 119 priority chemicals are presented in Khan et al. (2024).

3.3.2 Environmental hazard assessment

A majority of chemicals had $Score_{EH}$ of 0.33, indicating that they exceeded the threshold for at least one of the three hazard criteria (persistence, mobility, bioaccumulation) (Figure 6, Table A2). 17 chemicals exceeded thresholds for two criteria ($Score_{EH}$ = 0.67), with 16 predicted to be persistent and mobile but not bioaccumulative, and one (perfluorohexanesulfonic acid) predicted to be mobile and bioaccumulative but not persistent. The only chemical with $Score_{EH}$ = 1 was PFOS, which is well known for its properties of being persistent, mobile and bioaccumulative (Brunn et al., 2023).

3.3.3 Human health hazard assessment

Around half of the 119 chemicals had positive predictions for at least four of the eight health hazard parameters (Figure 6, Table A3). Two chemicals (progesterone and tramadol) had positive predictions for seven out of the eight parameters, resulting in the highest $Score_{HH}$ of 0.88. These chemicals predicted negative only for mutagenicity. 59 chemicals had positive predictions for four to six health hazard parameters resulting in $Score_{HH}$ of 0.5–0.75. Most common parameters with positive predictions were skin sensitization, developmental toxicity, hepatoxicity, and carcinogenicity. Lowest $Score_{HH}$ was 0.12, which was for ramipril and salicylic acid.

3.4 Microplatics and metals as impediments to reuse

One of the major sources of microplastics in the environment are WWTPs (Murphy et al., 2016). In our literature study, microplastics data were reported by eight articles. Conventional WWTPs are generally considered effective in removing microplastics (Kelly et al., 2021; Murphy et al., 2016). For example, Rasmussen et al. (2021) reported 99 % removal of microplastics < 0.5 mm. However, there is still potential for release of large quantities of microplastics from WWTPs, especially from those with high flow rates (Kelly et al., 2021; Murphy et al., 2016). Microplastics are a concern for reuse of sewage water for irrigation because crops can take up microplastics (Li et al., 2020), leading to contamination of food chains. Direct transfer from soil to fauna can also happen (Huerta Lwanga et al., 2017). In marine species, microplastics can not only cause blockage of digestive tracts, but can also cause toxicity through bioaccumulation of toxic substances (Derraik, 2002). Microplastics are considered a concern in the revised UWWTD (*COM(2022) 541 fina*l) (European Commission, 2022) with mandatory monitoring in influent, effluent and sludge for agglomerations of 10 000 population equivalent and above.

A number of metals from various sources can make their way to WWTPs (Sörme and Lagerkvist, 2002). Five metals in our dataset fulfilled the criteria for selection (≥ 20 quantifiable data points and quantifiable frequency > 50 %), including cobalt (Co), nickel (Ni), copper (Cu), lead (Pb), and zinc (Zn). All of these, except Co, are also included in the EU sludge directive (*DIRECTIVE 86/278/EEC*) along with their limit values. In addition to these, the sludge directive also includes cadmium (Cd), mercury (Hg), and chromium (Cr). In the dataset, the removal efficiency of these metals were: Co (32 %), Ni (37 %), Cu (89 %), Pb (97 %), and Zn (87 %) (details presented in Khan et al. (2024)). Highly variable metal removal in WWTPs suggests that metal accumulation can take place in soil and crops irrigated with treated wastewater. Risk and hazard assessment for metal is more complicated compared to organic chemicals, especially when information about specition of metals is missing from the reported concentration, as speciation affects the toxic affects and hazard of metals (Uchimiya et al., 2020). Therefore, it is essential that information about speciation is included in monitoring plans, and/or determined by modeling and computational methods (Matheri et al., 2022).

3.5 Upstream source tracing

Managing the substances identified as obstacles to wastewater reuse is necessary for safe wastewater reuse. Management approaches can include removal in WWTPs and/or reducing inflows of these chemicals to WWTPs. The latter essentially requires upstream source tracing of these hazardous substances and employing approaches for reducing their production and for better handling/disposal to prevent their entry into municipal WWTPs (Fairbairn et al., 2016). For pharmaceuticals, that also comprise the majority of the priority chemicals on our list, production and sales data is usually maintained by pharmaceutical companies which can be used to track and control their sources. For other chemicals, sources within the catchment of individual WWTPs would need to be identified in the future and addressed based on levels of risk posed by them and available measures to mitigate the risk.

3.6 Advanced treatment technologies

In total, 31 technologies and related combinations were explored in the Swedish literature targeting various contaminants of emerging concern (Figure 7) in domestic and municipal wastewater. Major focus of these studies has been on pharmaceuticals, while some also explored microplastics and other organic micropollutants, such as PFAS and industrial chemicals. Ozonation and activated carbon along with their various combinations were the most frequently studied technologies (Figure 7).

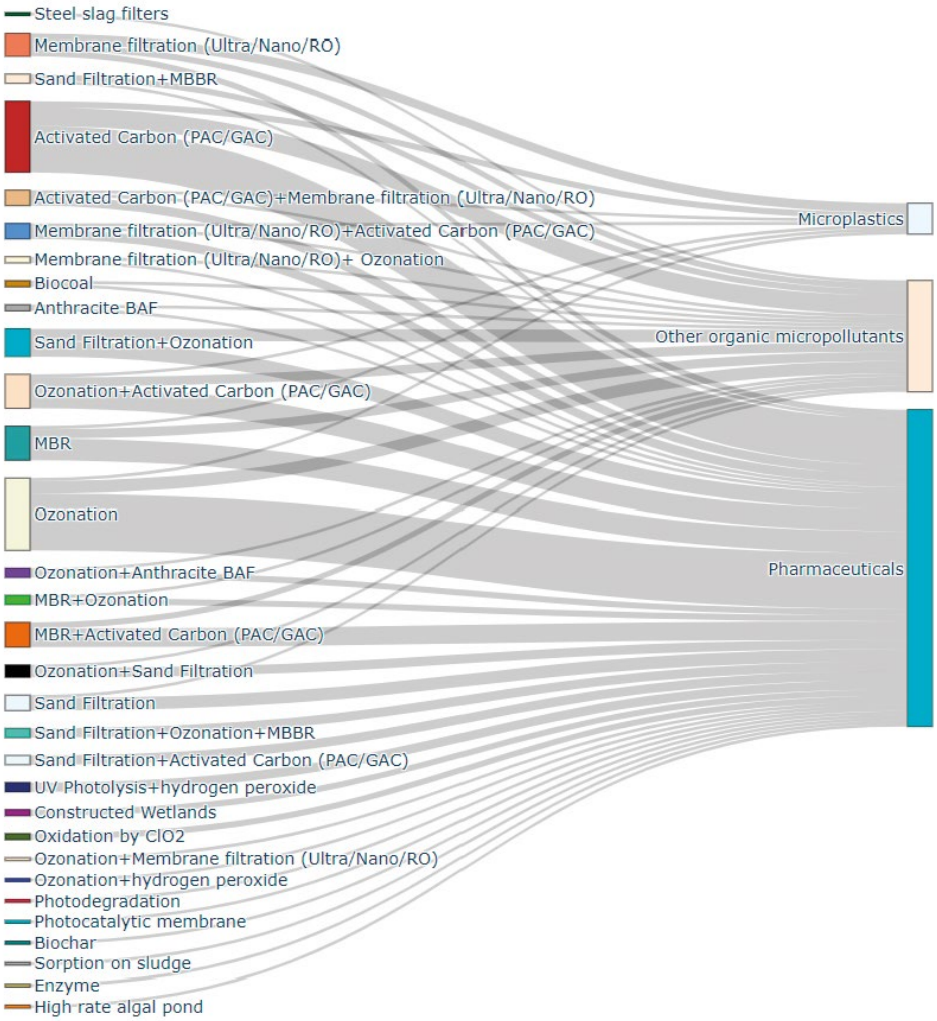


Figure 7. Illustration of techniques used to remove organic micropollutants in wastewater according to the studied literature from Sweden (see Appendix I for the list of references). RO: Reverse omosis. MBBR: Moving bed bioreactor. PAC: Powdered activated carbon. GAC: Granular activated carbon. BAF: Biologically active filtration. MBR: Membrane bioreactor. ClO2: Chlorine dioxide.

For the 38 selected chemicals (top 30 priority chemicals and 8 from the EU UWWTD; see Section 2.3) among the five selected advanced treatment technologies, average removal efficiency was the highest for GAC (94 %; data for 23 chemicals), followed by RO (92 %; 25 chemicals), NF (88 %; 24 chemicals), ozonation (86 %; 32 chemicals), and MBR (66 %; 30 chemicals) (Figure 8). Data on transformation products was especially scarce, for example, desvenlafaxine removal was only reported using MBR (64 % removal) (Hollman et al., 2020). Additionally, removal data on two chemicals (i.e., laureth-5 and daidzein) were not found for any of the technologies. RO generally has very high removal efficiency for organic micropollutants, which is also evident from our dataset; however, ketoprofen was an exception (15 % removal) (Rodriguez-Mozaz et al., 2015). Similarly, GAC performed well for all reported chemicals, except N,N-diethyl-m-toluamide (DEET, 17 % removal) (Yang et al., 2011). In recent years, converting existing bioreactors based on activated sludge process into submerged MBR have gained popularity, e.g., to achieve higher water quality for reuse appli-

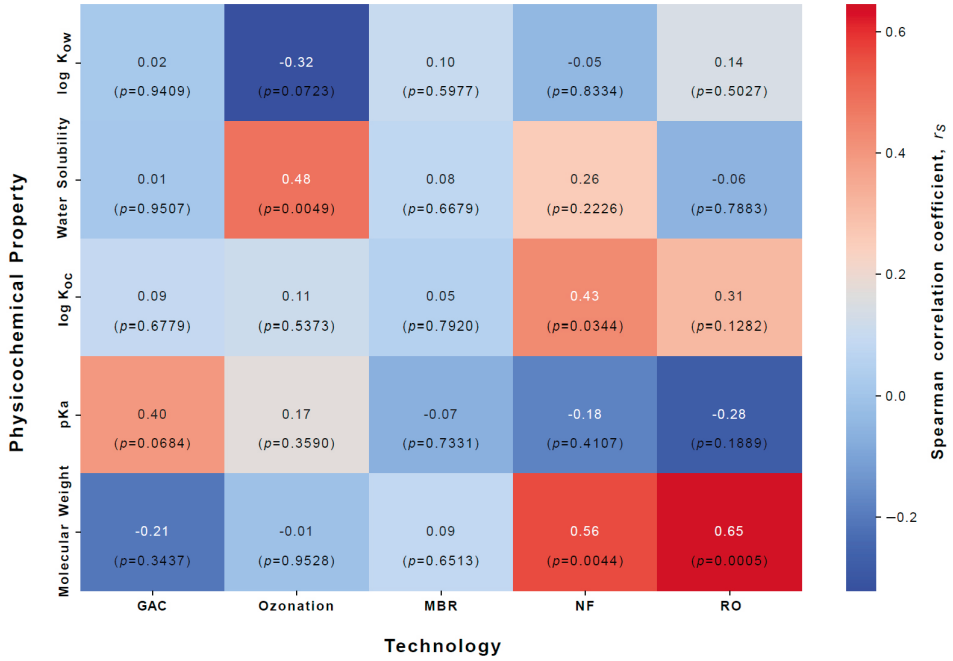
cations, due to their simplicity and low energy requirement (Obotey Ezugbe and Rathilal, 2020). However, MBR alone is not sufficient to effectively remove a large number of our priority chemicals, such as pharmaceuticals (Wang et al., 2018). Membranes used in MBR have a larger pore size (0.04–0.4 µm) (Mamo et al., 2016; Phan et al., 2014) than NF (0.001–0.01 µm retained diameter) and RO membranes (0.0001–0.001 µm retained diameter) (Obotey Ezugbe and Rathilal, 2020). Pharmaceutical molecules generally fall in the range 300–1 000 Da and require smaller pore sizes than MBR membranes; therefore, NF has been commonly used to remove pharmaceuticals from aqueous solutions (Sun et al., 2011). Our dataset also shows that NF has a good removal for a majority of our priority chemicals, with the exception of propranolol and benzotriazole (30 % and 17 % removal, respectively). Molecular weights of propranolol (260 Da) and benzotriazole (119 Da) can be too low for NF which generally has a molecular weight cut-off range of 200–10 000 Da[6]. RO membrane (molecular weight cut-off < 200 Da) were more effective for these chemicals. However, it should be noted that RO membranes operate at a higher pressure than NF membranes, resulting in higher energy costs.

Figure 8. Maximum removal efficiency (RE%) of 38 selected chemicals and average RE% (top row) using different advanced treatment technologies. GAC: granular activated carbon. MBR: membrane bioreactor. NF: nano-filtration. RO: reverse osmosis. Note: average RE were calculated after omitting chemicals with no data. See Appendix I for the list of references used to obtain removal efficiencies.

A number of physiochemical properties shows either positive or negative correlations with removal efficiency of different advanced treatment technologies (Figure 9). As expected, molecular weight of the chemicals was positively correlated with the removal efficiency of advanced treatment technologies which are based on

[6] https://www.lenntech.com/services/mwco.htm

physical separation (size exclusion mechanism), i.e., RO (r_s = 0.65, p < 0.05), NF (r_s = 0.56, p < 0.05), and to a much smaller extent, MBR (r_s = 0.09, p = 0.65) (Figure 9). Removal efficiency of GAC was positively correlated with pKa (r_s = 0.40, p = 0.07) and negatively correlated with molecular weight (r_s = −0.21, p = 0.3) of the chemicals. Chemicals can be either neutral (non-ionized) or ionized depending on the pKa of the chemical and pH of the solution; GAC generally adsorbs non-ionized species more effectively due to hydrophobic interactions. However, GAC types with surface charge can enhance removal of ionized species through ionic interaction. Removal efficiency of ozonation was positively correlated with water solubility (r_s = 0.48, p < 0.05) and negatively correlated with log K_{ow} (r_s = −0.32, p = 0.07). Other major correlations were observed for log K_{oc} *vs.* removal efficiency of NF (r_s = 0.43, p < 0.05) and RO (r_s = 0.3, p = 0.1). In view of these correlations, NF and RO can be the preferred choice for chemicals with high molecular weight and high log K_{oc}, such as clarithromycin. At the same time, chemicals with high pKa, such as benzotriazole, may be effectively targeted using GAC. For chemicals which are highly water soluble and have low K_{oc}, ozonation can be considered. However, there can be exceptions to these general correlations; for example, caffeine, which is highly water soluble with a low K_{ow}, was only 85 % removed through ozonation (Hollman et al., 2020). Ozonation generally requires a downstream treatment step to remove, among other impurities, organic transformation products potentially formed during ozonation. Therefore, a combination of ozonation and GAC can be considered a viable choice for a wide range of chemicals, including ozonation transformation products (Reaume et al., 2015). Even if organic micropollutants are effectively removed, in some cases, wastewater treated by NF may not be suitable as reclaimed water for irrigation, due to high levels of other impurities such as chloride, sodium, and calcium in NF effluent (Hafiz et al., 2021). On the other hand, both NF and ultra-filtration (the membrane used in MBR) membranes and ozonation, can remove *E. coli* below the limit of quantification, while GAC is also effective in *E. coli* removal below the EU requirement for water reuse (Bouchenak Khelladi et al., 2021; Gomes et al., 2019; Schwermer et al., 2017). *E. coli* concentration is an important parameter for the quality of reclaimed water and is one of the four parameters (*E. coli*, five-day biochemical oxygen demand, total suspended solids, and turbidity) included in the EU regulation on water reuse for agricultural irrigation (Regulation (*EU) 2020/741*).



Figur 9. Correlation matrix between physicochemical properties of chemicals (n = 38) and their removal efficiency through different advanced treatment technologies. GAC: granular activated carbon. MBR: membrane bioreactor. NF: nano-filtration. RO: reverse osmosis.

To better understand how cost-effective the selected technologies are, their capital, operating and energy costs are briefly compiled and compared (Table 3). GAC has the lowest costs for these aspects, followed by ozonation. MBR has the highest capital requirement. The reported range of capital investment required for MBR and for NF and RO overlap to some extent. Understandably, the energy requirement of membrane processes is many times higher than GAC, due to the application of high pressure that drives separation of water from pollutants across the membrane (Hafiz et al., 2021). Ozonation also closely follows membrane technologies, in terms of energy requirement, a major part of which is required for production of oxygen and generation of ozone from oxygen (Pistocchi et al., 2022). It should be noted that the approach adopted by different authors for calculation of these costs might vary, therefore this should be taken as a preliminary comparison only, e.g., the capital cost of MBR may include the cost of entire secondary treatment unit (activated sludge bioreactor) including the MBR screens. Similarly, the operating cost of GAC only includes the GAC regeneration cost. Furthermore, the actual cost of any system will also depend on operating conditions, e.g., operating pressure of NF and RO, and ozone dose in ozonation.

Table 3. Capital, operating and energy cost of different advanced treatment technologies.

	GAC		Ozonation		MBR		NF		RO	
	Cost	Reference	Cost	Reference	Cost	Reference	Cost	Reference	Cost	Reference
Capital cost (SEK/m³/day)	400	Pistocchi et al., 2022	1300*	Pistocchi et al., 2022	4 000–75 000**	Guo et al., 2014; Rahman et al., 2023; Xiao et al., 2019	5 000–26 000	https://samcotech.com/much-reverse-osmosis-nanofiltration-membrane-systems-cost/	5 000–26 000	https://samcotech.com/much-reverse-osmosis-nanofiltration-membrane-systems-cost/
Operating cost (SEK/m³)	0.15†	Pistocchi et al., 2022			1.4–2.5††	Xiao et al., 2019	0.9–7.5††	Abdel-Fatah, 2018; Shahmansouri and Bellona, 2015	1.09	Nazari Chamaki et al., 2023
Energy cost‡ (SEK/m³)	0.02	Pistocchi et al., 2022	0.20	Pistocchi et al., 2022	0.28–2.1	Rahman et al., 2023; Krzeminski et al., 2017	0.47–1.62‡‡	Hafiz et al., 2021	0.32–2.49	Hafiz et al., 2021; Nazari Chamaki et al., 2023

* Including downstream sand filter. Ozonation generally requires GAC treatment afterwards so the total cost would be 1300 + 400 = 1700 SEK.

** Cost calculation years 2007–2019.

† Only includes GAC regeneration cost.

†† Including energy cost (and membrane replacement cost in case of MBR), Cost for UF+NF setup for nano-filtration. Cost for 2014 onwards.

‡ Calculated using 2023 energy prices in Sweden and energy consumption data from the cited references.

‡‡ Calculated from specific energy consumption of nano-filtration for different experimental operating pressures.

Considering its effectiveness to remove CECs and the lower cost, GAC appears to be the most suitable technology for reclamation of treated municipal wastewater for agricultural irrigation. However, GAC may not be the best choice under all conditions, and it alone may not be able to remove all contaminants to a safe level, therefore, the decision on which technology or combination of technologies to use should be made after careful consideration of organic micropollutants present in the wastewater, their concentrations in the secondary (or tertiary) treated effluent, and the safe concentration in the reclaimed water based on the applicable PNEC values. Instead of a single technology, advanced treatment technologies can be used in tandem, e.g., ozonation and GAC, to broaden the range of organic micropollutants removed during the quaternary treatment steps. Removal efficiency can also vary over the lifetime of a technology such as GAC. Therefore, it should be considered for technology selection in the future.

4. Conclusions and Future Remarks

Situation of global water stress can worsen under a changing climate, and even countries like Sweden, which historically had a good access to water resources, may have to explore alternate supplies of water. Already, signs of water stress, such as decline in surface and ground water availability and rainfall deficits, have been observed in some parts of Sweden in recent decades (Grusson et al., 2021; Teutschbein et al., 2022). Treated municipal wastewater can be used as an alternate water resource especially in times and in areas experiencing water stress. Currently, only a handful of places in Sweden have arrangements for reusing treated wastewater. Since the annually available amount of treated wastewater in Sweden is considerable (1.2 billion m^3), there is substantial potential for expansion of wastewater reuse. For pursuing this, Sweden is also well placed in terms of socioeconomic conditions, as it ranks highly on three of the four factors (GDP per capita, urbanization, and fraction of wastewater treated) that were positively correlated with national wastewater reuse. The fourth factor is level of water stress; although, the overall level of water stress is low in Sweden at the moment, specific places already face water stress. A major factor in limited reuse is public and farmer concern about the presence of hazardous substances in treated wastewater and their associated risk. These concerns may be addressed by comprehensive and effective guidelines and regulations on water quality of treated effluent for reuse.

Current EU water reuse regulation (Regulation (EU) 2020/741) lacks any specific guidelines for CECs, and the proposed revisions to UWWTD (*COM(2022) 541 final*) (European Commission, 2022) only include 13 chemicals, inclusion of which is not risk-based. The EU water reuse regulation does, however, mandates risk management plans to address exposure risks to the environment, human health, and animal health under certain site-specific conditions. These measures are, however, insufficient as there are still significant gaps in ensuring that effluent water quality is safe for reuse, regarding risks of the hazardous pollutants. This is mainly because regulatory frameworks often fail to take into account the long-term ecological impacts and complex interactions of trace chemical residues. To address this issue and for future policy direction (e.g., policy briefs on the subject), defining and enforcing upper concentration limits for certain high-risk priority chemicals in effluent wastewater is required. Being one of the strengths of this work, the list of priority chemicals presented in this report and the underlying risk and hazard assessment methodology can be useful for this purpose and also for developing risk management plans for the Swedish environment. Preparation of policy brief should take into account the findings of this report, particularly the priority chemicals, and focus on reducing their occurrences in effluent water for reuse by providing limit concentraions, and making use of advanced treatment technologies mandatory. The limit concentrations should be determined by considering both removal efficiency of the employed technologies and ecological risk assessment of the resulting concentrations in effluent water. These should be essential components of any future regulation and legislation. It should be noted that,

because the dataset compiled is based on available literature, there can be other unknown chemicals which are not yet targeted in the past. Therefore, inclusion of additional literature and re-processing the data with our meta-analysis workflow would be beneficial in the future.

While evaluating effectiveness of different advanced treatment technologies, we have focused on high priority chemicals in our list and the compounds included in the proposed UWWTD. A similar approach can be used to define target compounds and chemical removal requirements for quaternary treatment, thereby expanding the list of 13 chemicals included in the proposed UWWTD. In addition, any regulation for safe reuse would not be complete without including mitigation measures to address the risk of transformation products. There are only a few transformation products (e.g., OH-metronidazole, desvenlafaxine, *N*-desmethylcitalopram) included in our list because of the limited focus on transformation products in the literature. This shortcoming would need to be addressed in future regulations. As this report only focuses on human health hazard predicted based on chemical stuctures, a potential knowledge gap to explore in the future is the human health risk assessment related to exposure to the priority chemicals through the consumption of crops irrigated with wastewater. In our evaluation, GAC turned out to be the most suitable technology although it may have to be used in tandem with other technologies for effective removal of all priority chemicals.

In addition to removal in wastewater treatment plants, an important component of the strategy to control exposure to hazardous chemicals is upstream source tracing and control. Our risk-based list of priority chemicals also serves as a list of target compounds for authorities to cost-effectively focus on for upstream source tracing and potential control of release.

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Appendix I

Search String for Web of Science

TS = (Swed* AND (wastewater OR sewage OR effluent* OR “black water” OR blackwater OR gr*ywater OR “grey water” OR “gray water” OR excreta OR sludge OR “source-separated” OR “source separated waste fraction*” OR “waste water”) AND (micropollutant* OR pharmaceutical* OR antibiotic* OR hormon* OR steroid* OR PFAS* OR PFAA* OR microplastic* OR “organic chemical*” OR “industr* chemical*” OR “persistent organic pollutant*” OR POP* OR NSAID* OR metal* OR nano* OR PPCP* OR “personal care product*” OR “contaminant* of emerging concern” OR contaminant* OR CEC* OR “New Emerging Risk Chemical*” OR NERC* OR “unwanted substance*” OR “unwanted chemical*” OR “antibiotic* resistance gene*”))

Search String for Scopus

TITLE-ABS-KEY (Swed* AND (wastewater OR sewage OR effluent* OR “black water” OR blackwater OR gr*ywater OR “grey water” OR “gray water” OR excreta OR sludge OR “source-separated” OR “source separated waste fraction*” OR “waste water”) AND (micropollutant* OR pharmaceutical* OR antibiotic* OR hormon* OR steroid* OR PFAS* OR PFAA* OR microplastic* OR “organic chemical*” OR “industr* chemical*” OR “persistent organic pollutant*” OR POP* OR NSAID* OR metal* OR nano* OR PPCP* OR “personal care product*” OR “contaminant* of emerging concern” OR contaminant* OR CEC* OR “New Emerging Risk Chemical*” OR NERC* OR “unwanted substance*” OR “unwanted chemical*” OR “antibiotic* resistance gene*”))

Table A1. Values of ecological risk parameters and their scores for the selected chemical contaminants. FoE: frequency of exceedance; EoE: extent of exceedance; RQ: risk quotient.

Contaminant	CAS Number	FoE	EoE	RQ	$Score_{RQ}$	$Score_{EOE}$	$(Score_{RQ}+Score_{EOE})/2$	$Score_{eco}$
bicalutamide	90357-06-5	0.97	6.0	8.0	1	1	1	1.97
fexofenadine	83799-24-0	0.94	65.3	66.7	1	1	1	1.94
diclofenac	15307-86-5	0.91	43.9	108.3	1	1	1	1.91
venlafaxine	93413-69-5	0.89	14.3	114.2	1	1	1	1.89
amoxicillin	26787-78-0	0.88	64.9	70.3	1	1	1	1.88
chlaritromycin	81103-11-9	0.86	78.4	390.0	1	1	1	1.86
DEET (N,N-diethyl-m-toluamide)	134-62-3	0.83	35.0	71.2	1	1	1	1.83
desvenlafaxine	93413-62-8	0.72	2.4	3.2	1	1	1	1.72
atorvastatin	134523-00-5	0.59	18.1	85.1	1	1	1	1.59
genistein	446-72-0	0.55	2.4	3.7	1	1	1	1.55
azithromycin	83905-01-5	0.51	4.3	8.9	1	1	1	1.51
triclosan	3380-34-5	0.50	8.0	11.5	1	1	1	1.5
gemfibrozil	25812-30-0	0.45	13.5	52.0	1	1	1	1.45
ranitidine	66357-35-5	0.31	2.8	4.5	1	1	1	1.31
daidzein	486-66-8	0.31	1.8	4.0	1	1	1	1.31
ketoprofen	22071-15-4	0.30	2.2	2.9	1	1	1	1.3
ibuprofen	15687-27-1	0.28	4.8	9.2	1	1	1	1.28
oxazepam	604-75-1	0.24	1.9	10.7	1	1	1	1.24
fluoxetine	54910-89-3	0.20	3.3	7.8	1	1	1	1.2
erythromycin	114-07-8	0.15	2.4	4.5	1	1	1	1.15
PFNA	375-95-1	0.14	1.6	7.6	1	1	1	1.14
propranolol	525-66-6	0.09	2.0	26.0	1	1	1	1.09
ciprofloxacin	85721-33-1	0.06	1.3	11.9	1	1	1	1.06
caffeine	58-08-2	0.05	1.1	3.6	1	1	1	1.05
thiabendazole	148-79-8	0.05	0.5	2.7	1	0	0.5	0.55
tramadol	27203-92-5	0.04	0.8	1.9	1	0	0.5	0.54
codeine	76-57-3	0.03	0.8	2.5	1	0	0.5	0.53
bezafibrate	41859-67-0	0.02	0.2	1.4	1	0	0.5	0.52
metoprolol	51384-51-1	0.01	0.4	1.1	1	0	0.5	0.51
carbamazepine	298-46-4	0.01	0.4	1.0	1	0	0.5	0.51

Contaminant	CAS Number	FoE	EoE	RQ	$Score_{RQ}$	$Score_{EOE}$	$(Score_{RQ}+Score_{EOE})/2$	$Score_{eco}$
metformin	657-24-9	0.00	0.8	0.9	0	0	0	0
sulfamethoxazole	723-46-6	0.00	0.7	0.9	0	0	0	0
2,4,7,9-tetramethyl-5-decyn-4,7-diol	126-86-3	0.00	0.1	0.9	0	0	0	0
sertraline	79617-96-2	0.00	0.1	0.9	0	0	0	0
sulisobenzone	4065-45-6	0.00	0.8	0.9	0	0	0	0
carbamazepine 10,11-epoxyde	36507-30-9	0.00	0.6	0.8	0	0	0	0
naproxen	22204-53-1	0.00	0.2	0.7	0	0	0	0
10,11-dihydro-10-hydroxycarbamazepine	29331-92-8	0.00	0.6	0.6	0	0	0	0
acetaminophen	103-90-2	0.00	0.2	0.5	0	0	0	0
loperamide	53179-11-6	0.00	0.1	0.5	0	0	0	0
losartan	114798-26-4	0.00	0.1	0.4	0	0	0	0
amitriptylin	50-48-6	0.00	0.1	0.4	0	0	0	0
furosemide	54-31-9	0.00	0.0	0.4	0	0	0	0
tris(2-chloroethyl)phosphate (TCEP)	115-96-8	0.00	0.2	0.3	0	0	0	0
nicotine	54-11-5	0.00	0.1	0.3	0	0	0	0
n-desmethylcitalopram	62498-67-3	0.00	0.2	0.2	0	0	0	0
tris(2-butoxyethyl)phosphate (TBEP)	78-51-3	0.00	0.2	0.2	0	0	0	0
memantine	19982-08-2	0.00	0.2	0.2	0	0	0	0
clindamycin	18323-44-9	0.00	0.1	0.2	0	0	0	0
phenazone	60-80-0	0.00	0.1	0.2	0	0	0	0
simvastatin	79902-63-9	0.00	0.1	0.2	0	0	0	0
terbutryn	886-50-0	0.00	0.1	0.2	0	0	0	0
citalopram	59729-33-8	0.00	0.0	0.1	0	0	0	0
laureth-5	3055-95-6	0.00	0.1	0.1	0	0	0	0
sotalol	3930-20-9	0.00	0.1	0.1	0	0	0	0
climbazole	38083-17-9	0.00	0.1	0.1	0	0	0	0
progesterone	57-83-0	0.00	0.0	0.1	0	0	0	0
3-(4-methylbenzylidene)camphor	36861-47-9	0.00	0.1	0.1	0	0	0	0
budesonide	51333-22-3	0.00	0.0	0.1	0	0	0	0
dibutyl phosphate	107-66-4	0.00	0.0	0.1	0	0	0	0
bisoprolol	66722-44-9	0.00	0.0	0.1	0	0	0	0

Contaminant	CAS Number	FoE	EoE	RQ	$Score_{RQ}$	$Score_{EOE}$	$(Score_{RQ}+Score_{EOE})/2$	$Score_{eco}$
clopidogrel	113665-84-2	0.00	0.1	0.1	0	0	0	0
benzotriazole	95-14-7	0.00	0.0	0.1	0	0	0	0
boscalid	188425-85-6	0.00	0.1	0.1	0	0	0	0
lidocaine	137-58-6	0.00	0.0	0.1	0	0	0	0
diuron	330-54-1	0.00	0.0	0.1	0	0	0	0
bisphenol A	80-05-7	0.00	0.0	0.0	0	0	0	0
lamotrigine	84057-84-1	0.00	0.0	0.0	0	0	0	0
fluconazole	86386-73-4	0.00	0.0	0.0	0	0	0	0
terbutaline	23031-25-6	0.00	0.0	0.0	0	0	0	0
clozapine	5786-21-0	0.00	0.0	0.0	0	0	0	0
mebendazole	31431-39-7	0.00	0.0	0.0	0	0	0	0
prothioconazole	178928-70-6	0.00	0.0	0.0	0	0	0	0
imazalil	35554-44-0	0.00	0.0	0.0	0	0	0	0
propiconazole	60207-90-1	0.00	0.0	0.0	0	0	0	0
tributyl citrate acetate	77-90-7	0.00	0.0	0.0	0	0	0	0
atenolol	29122-68-7	0.00	0.0	0.0	0	0	0	0
mirtazapine	85650-52-8	0.00	0.0	0.0	0	0	0	0
valsartan	137862-53-4	0.00	0.0	0.0	0	0	0	0
di-(2-ethylhexyl)phosphoric acid	298-07-7	0.00	0.0	0.0	0	0	0	0
benzophenone	119-61-9	0.00	0.0	0.0	0	0	0	0
albuterol (salbutamol)	18559-94-9	0.00	0.0	0.0	0	0	0	0
amidotrizoic acid	117-96-4	0.00	0.0	0.0	0	0	0	0
diltiazem	42399-41-7	0.00	0.0	0.0	0	0	0	0
verapamil	52-53-9	0.00	0.0	0.0	0	0	0	0
salicylic acid	69-72-7	0.00	0.0	0.0	0	0	0	0
zolpidem	82626-48-0	0.00	0.0	0.0	0	0	0	0
trimethoprim	738-70-5	0.00	0.0	0.0	0	0	0	0
BAM (dichlorobenzamide)	2008-58-4	0.00	0.0	0.0	0	0	0	0
telmisartan	144701-48-4	0.00	0.0	0.0	0	0	0	0
mono-n-butylphosphoric acid	1623-15-0	0.00	0.0	0.0	0	0	0	0
bupropion	34841-39-9	0.00	0.0	0.0	0	0	0	0

Contaminant	CAS Number	FoE	EoE	RQ	$Score_{RQ}$	$Score_{EOE}$	$(Score_{RQ}+Score_{EOE})/2$	$Score_{eco}$
theophylline	58-55-9	0.00	0.0	0.0	0	0	0	0
hydrochlorothiazide (HCTZ)	58-93-5	0.00	0.0	0.0	0	0	0	0
oxybenzone	131-57-7	0.00	0.0	0.0	0	0	0	0
amlodipine besylate	111470-99-6	0.00	0.0	0.0	0	0	0	0
primidone	125-33-7	0.00	0.0	0.0	0	0	0	0
mefenamic acid	61-68-7	0.00	0.0	0.0	0	0	0	0
PFOS	1763-23-1	0.00	0.0	0.0	0	0	0	0
6:2 FTSA	27619-97-2	0.00	0.0	0.0	0	0	0	0
sulfaclozine	102-65-8	0.00	0.0	0.0	0	0	0	0
ramipril	87333-19-5	0.00	0.0	0.0	0	0	0	0
irbesartan	138402-11-6	0.00	0.0	0.0	0	0	0	0
2,2'-dimorpholinyldiethylether	6425-39-4	0.00	0.0	0.0	0	0	0	0
oxycodone	76-42-6	0.00	0.0	0.0	0	0	0	0
sparfloxacin	110871-86-8	0.00	0.0	0.0	0	0	0	0
metronidazole	443-48-1	0.00	0.0	0.0	0	0	0	0
pyridoxine (vitamin b6)	65-23-6	0.00	0.0	0.0	0	0	0	0
PFHpA	375-85-9	0.00	0.0	0.0	0	0	0	0
PFPeA	2706-90-3	0.00	0.0	0.0	0	0	0	0
loratadine	79794-75-5	0.00	0.0	0.0	0	0	0	0
metronidazole-OH	4812-40-2	0.00	0.0	0.0	0	0	0	0
Cetirizine	83881-51-0	0.00	0.0	0.0	0	0	0	0
propamocarb	24579-73-5	0.00	0.0	0.0	0	0	0	0
tetraethylene glycol	112-60-7	0.00	0.0	0.0	0	0	0	0
PFHxS	355-46-4	0.00	0.0	0.0	0	0	0	0
PFHxA	307-24-4	0.00	0.0	0.0	0	0	0	0
PFOA	335-67-1	0.00	0.0	0.0	0	0	0	0
FOSA	754-91-6	0.00	0.0	0.0	0	0	0	0

Table A2. Values and scores of environmental hazard parameters for the selected chemical contaminants.

Substance name	CAS number	log BCF	Persistence water [days]	log Koc	Solubility [log (mol/L)]	BCF score	Persistence score	Mobility score	$Score_{EH}$
PFOS	1763-23-1	3.73	57	2.5	0.4	1	1	1	1
sertraline	79617-96-2	3.29	44	3.6	1.2	0	1	1	0.67
PFOA	335-67-1	3.12	57	3.2	1.6	0	1	1	0.67
clindamycin	18323-44-9	0.01	82	2.2	6 305.2	0	1	1	0.67
bisoprolol	66722-44-9	0.15	82	3.6	813.9	0	1	1	0.67
PFNA	375-95-1	2.58	57	3.5	0.3	0	1	1	0.67
mirtazapine	85650-52-8	1.25	44	2.8	156.3	0	1	1	0.67
amitriptyline	50-48-6	2.59	241	3.6	9.7	0	1	1	0.67
PFHxS	355-46-4	3.6	21	3.4	10.3	1	0	1	0.67
propiconazole	60207-90-1	1.78	44	3.4	110	0	1	1	0.67
cetirizine	83881-51-0	0.8	44	3	29.5	0	1	1	0.67
nicotine	54-11-5	0.4	141	2	10 492.8	0	1	1	0.67
ramipril	87333-19-5	0.56	82	2.7	49.6	0	1	1	0.67
sparfloxacin	110871-86-8	0.37	82	2.6	6 779.6	0	1	1	0.67
laureth-5	3055-95-6	−0.01	91	4.2	187	0	1	1	0.67
imazalil	35554-44-0	1.6	44	3.7	179.9	0	1	1	0.67
mono-n-butylphosphoric acid	1623-15-0	0.19	149	1.5	35 978.1	0	1	1	0.67
6:2 FTSA	27619-97-2	1.72	57	3	8.4	0	1	1	0.67
diclofenac	15307-86-5	2.7	0	3.8	2.4	0	0	1	0.33
naproxen	22204-53-1	1.42	7	2.7	15.9	0	0	1	0.33
oxazepam	604-75-1	0.83	22	2.6	141.9	0	0	1	0.33
trimethoprim	738-70-5	0.36	5	2.1	399.9	0	0	1	0.33
carbamazepine	298-46-4	1.35	15	2.8	112.1	0	0	1	0.33
citalopram	59729-33-8	1.63	23	3.4	24	0	0	1	0.33
ibuprofen	15687-27-1	1.62	8	2.1	21	0	0	1	0.33
fluconazole	86386-73-4	1.82	23	1.9	1104.7	0	0	1	0.33
metoprolol	51384-51-1	0.33	6	3.1	16 911.3	0	0	1	0.33
sulfamethoxazole	723-46-6	0.37	2	2	427.6	0	0	1	0.33
tramadol	27203-92-5	0.99	7	2.8	588	0	0	1	0.33
clarithromycin	81103-11-9	−1.6	82	4.7	2 470.7	0	1	0	0.33
ketoprofen	22071-15-4	1.49	15	2.8	51	0	0	1	0.33

Substance name	CAS number	log BCF	Persistence water [days]	log Koc	Solubility [log (mol/L)]	BCF score	Persistence score	Mobility score	$Score_{EH}$
atenolol	29122-68-7	0.08	6	2.5	13 289.3	0	0	1	0.33
erythromycin	114-07-8	–1.65	82	4.6	2 156.5	0	1	0	0.33
venlafaxine	93413-69-5	1.1	7	2.8	324.4	0	0	1	0.33
ciprofloxacin	85721-33-1	0.32	26	2.5	4 653.1	0	0	1	0.33
caffeine	58-08-2	0.02	5	1.8	7 974.7	0	0	1	0.33
losartan	114798-26-4	1.07	26	4.1	2.1	0	0	1	0.33
furosemide	54-31-9	–0.01	3	1.5	73	0	0	1	0.33
irbesartan	138402-11-6	1.1	23	4.3	0.4	0	0	1	0.33
sotalol	3930-20-9	0.37	10	2	2 180.2	0	0	1	0.33
diltiazem	42399-41-7	0.88	7	3.2	465.2	0	0	1	0.33
fluoxetine	54910-89-3	2.35	7	3.6	5.1	0	0	1	0.33
memantine	19982-08-2	1.95	2	3.7	119.5	0	0	1	0.33
tris(2-chloroethyl) phosphate (TCEP)	115-96-8	–0.18	36	1.2	1 302.2	0	0	1	0.33
propranolol	525-66-6	0.84	6	2.5	61.6	0	0	1	0.33
metformin	657-24-9	0.24	13	1	972	0	0	1	0.33
PFHxA	307-24-4	1.75	15	3	23.6	0	0	1	0.33
hydrochlorothiazide (HCTZ)	58-93-5	–0.06	2	1.7	722.6	0	0	1	0.33
azithromycin	83905-01-5	–1.58	82	4.6	1 293.6	0	1	0	0.33
metronidazole	443-48-1	0.15	6	1.8	9 494.1	0	0	1	0.33
lamotrigine	84057-84-1	0.61	16	2.3	2.5	0	0	1	0.33
valsartan	137862-53-4	0.8	26	2.8	18.9	0	0	1	0.33
zolpidem	82626-48-0	0.96	23	3.3	21.1	0	0	1	0.33
lidocaine	137-58-6	0.69	4	2.5	4 101.3	0	0	1	0.33
2,4,7,9-tetramethyl-5-decyn-4,7-diol	126-86-3	1.59	8	1.9	468.9	0	0	1	0.33
bezafibrate	41859-67-0	1.35	7	4.1	28.6	0	0	1	0.33
DEET (N,N-diethyl-m-toluamide)	134-62-3	0.38	8	2.3	685	0	0	1	0.33
desvenlafaxine	93413-62-8	1	4	2.7	594.7	0	0	1	0.33
climbazole	38083-17-9	1.38	7	3.1	42	0	0	1	0.33
salicylic acid	69-72-7	0.34	2	1.6	2 240.2	0	0	1	0.33
benzophenone	119-61-9	0.89	8	2.6	137	0	0	1	0.33

Substance name	CAS number	log BCF	Persistence water [days]	log Koc	Solubility [log (mol/L)]	BCF score	Persistence score	Mobility score	$Score_{EH}$
bicalutamide	90357-06-5	0.97	23	2.2	1.8	0	0	1	0.33
gemfibrozil	25812-30-0	1.67	7	2.3	45.3	0	0	1	0.33
terbutryn	886-50-0	1.09	26	2.9	25	0	0	1	0.33
diuron	330-54-1	0.93	23	2.4	42	0	0	1	0.33
PFPeA	2706-90-3	1.4	7	2	89.9	0	0	1	0.33
thiabendazole	148-79-8	0.41	6	3.2	50	0	0	1	0.33
clopidogrel	113665-84-2	1.52	7	3.2	13.5	0	0	1	0.33
acetaminophen	103-90-2	0.29	2	1.7	14 011.8	0	0	1	0.33
carbamazepine 10,11-epoxyde	36507-30-9	0.66	10	3.1	308.9	0	0	1	0.33
di-(2-ethylhexyl)phosphoric acid	298-07-7	0.64	23	3.2	182.2	0	0	1	0.33
phenazone	60-80-0	0.77	8	2	241.6	0	0	1	0.33
terbutaline	23031-25-6	0.32	4	2	2 947.4	0	0	1	0.33
10,11-dihydro-10-hydroxycarbamazepine	29331-92-8	0.83	26	2.8	116.2	0	0	1	0.33
3-(4-methylbenzylidene)camphor	36861-47-9	2.28	23	3.2	4	0	0	1	0.33
albuterol (salbutamol)	18559-94-9	0.21	4	1.9	4 639.7	0	0	1	0.33
BAM (dichlorobenzamide)	2008-58-4	0.73	7	0.5	2 727.9	0	0	1	0.33
dibutyl phosphate	107-66-4	0.75	13	1.3	17 207.4	0	0	1	0.33
n-desmethylcitalopram	62498-67-3	1.6	23	3	15.1	0	0	1	0.33
prothioconazole	178928-70-6	1.63	4	2.9	11.1	0	0	1	0.33
tetraethylene glycol	112-60-7	0.13	4	1	1 000 883.2	0	0	1	0.33
theophylline	58-55-9	0.05	8	1.6	3 333.1	0	0	1	0.33
tributyl citrate acetate	77-90-7	0.46	7	2.3	66	0	0	1	0.33
2,2'-dimorpholinyldiethylether	6425-39-4	−0.03	3	2.4	267 015.4	0	0	1	0.33
genistein	446-72-0	0.43	7	2.9	66.6	0	0	1	0.33
metronidazole-oh	4812-40-2	0.23	6	1.7	21 598.6	0	0	1	0.33
primidone	125-33-7	0.54	4	2	500	0	0	1	0.33
mefenamic acid	61-68-7	2.01	4	2.8	20	0	0	1	0.33
pyridoxine (vitamin b6)	65-23-6	0.08	2	1.9	63 524.7	0	0	1	0.33
mebendazole	31431-39-7	1.26	7	2.4	71.3	0	0	1	0.33
amidotrizoic acid	117-96-4	0.87	4	2.5	419.5	0	0	1	0.33

Substance name	CAS number	log BCF	Persistence water [days]	log Koc	Solubility [log (mol/L)]	BCF score	Persistence score	Mobility score	$Score_{EH}$
benzotriazole	95-14-7	0.37	6	1.7	19 817.9	0	0	1	0.33
loratadine	79794-75-5	1.61	7	3.6	0.4	0	0	1	0.33
oxybenzone	131-57-7	1.98	7	2.6	72.4	0	0	1	0.33
tris(2-butoxyethyl) phosphate (TBEP)	78-51-3	0.76	23	4.1	1100.2	0	0	1	0.33
bisphenol A	80-05-7	1.64	4	3.2	120.1	0	0	1	0.33
boscalid	188425-85-6	1.92	22	3.2	2.7	0	0	1	0.33
sulfaclozine	102-65-8	0.12	4	2.5	330.1	0	0	1	0.33
daidzein	486-66-8	0.63	7	2.9	64.4	0	0	1	0.33
bupropion	34841-39-9	1.02	22	2.1	275.4	0	0	1	0.33
clozapine	5786-21-0	0.96	3	2.7	26.3	0	0	1	0.33
loperamide	53179-11-6	1.13	23	4.5	12.8	0	0	1	0.33
PFHpA	375-85-9	2	23	3.3	8.6	0	0	1	0.33
amoxicillin	26787-78-0	0.35	10	1.7	1681.5	0	0	1	0.33
amlodipine*	111470-99-6	0.23	7	1.6	161.8	0	0	1	0.33
propamocarb	24579-73-5	0.37	2	2.5	894 754.3	0	0	1	0.33
sulisobenzone	4065-45-6	0.41	7	2.3	1561.3	0	0	1	0.33
besylate (bensensulfonic acid)*	111470-99-6	0.3	2	1.5	48 488.4	0	0	1	0.33
ranitidine	66357-35-5	0.16	3	3	654.3	0	0	1	0.33
FOSA	754-91-6	1.69	57	2.82	0.0 672	0	1	0	0.33
codeine	76-57-3	0.69	7	4.9	9 000.2	0	0	0	0
fexofenadine	83799-24-0	0.54	0	5.2	22.7	0	0	0	0
progesterone	57-83-0	1.91	23	5.7	8.8	0	0	0	0
atorvastatin	134523-00-5	0.35	26	5.4	28.3	0	0	0	0
telmisartan	144701-48-4	0.96	11	5.1	0.2	0	0	0	0
oxycodone	76-42-6	0.4	7	4.6	333.9	0	0	0	0
verapamil	52-53-9	0.64	7	5.2	0.8	0	0	0	0
budesonide	51333-22-3	0.56	26	4.7	40.8	0	0	0	0
simvastatin	79902-63-9	0.96	7	4.9	8.8	0	0	0	0
triclosan	3380-34-5	1.72	19	4.6	10	0	0	0	0

Table A3. Values and scores of human health hazard parameters for the selected chemical contaminants.

Substance name	CAS number	Mutagenicity	Carcinogenicity	Developmental toxicity	Estrogen receptor effect	Androgen receptor effect	Hepatoxicity	P-glycoprotein activity	Skin sensitization	Mutagenicity score	Carcinogenicity score	Developmental toxicity score	Estrogen receptor effect score	Androgen receptor effect score	Hepatoxicity score	P-glycoprotein activity score	Skin sensitization score	$Score_{HH}$
fluoxetine	54910-89-3	NON-mutagenic	NON-Carcinogen	Toxicant	Not	NON-active	Toxic	Inhibitor	Sensitizer	0	0	1	1	0	1	1	1	0.62
flukonazole	86386-73-4	NON-mutagenic	Carcinogen	Toxicant	NON-active	NON-active	Toxic	Non	Sensitizer	0	1	1	0	0	1	0	1	0.5
verapamil	52-53-9	NON-mutagenic	NON-Carcinogen	Toxicant	Active	NON-active	Toxic	Inhibitor	Sensitizer	0	0	1	1	0	1	1	1	0.62
bicalutamide	90357-06-5	NON-mutagenic	NON-Carcinogen	NON-Toxicant	NON-active	Active	Toxic	Substrate	Sensitizer	0	0	0	0	1	1	1	1	0.5
citalopram	59729-33-8	NON-mutagenic	Carcinogen	Toxicant	Not	NON-active	NON-Toxic	Non	Sensitizer	0	1	1	1	0	0	0	1	0.5
n-desmethyl-citalopram	62498-67-3	NON-mutagenic	NON-Carcinogen	Toxicant	Not	NON-active	NON-Toxic	Non	Sensitizer	0	0	1	1	0	0	0	1	0.38
clozapine	5786-21-0	NON-mutagenic	Carcinogen	Toxicant	NON-active	NON-active	Unknown	Inhibitor	Sensitizer	0	1	1	0	0	1	1	1	0.62
metformin	657-24-9	NON-mutagenic	NON-Carcinogen	Toxicant	Not	NON-active	Unknown	Non	Sensitizer	0	0	1	1	0	1	0	1	0.5
memantine	19982-08-2	NON-mutagenic	NON-Carcinogen	Toxicant	NON-active	NON-active	NON-Toxic	Non	Sensitizer	0	0	1	0	0	0	0	1	0.25
2,2'-dimor-pholinyl-diethyl-ether	6425-39-4	NON-mutagenic	NON-Carcinogen	NON-Toxicant	Possible	NON-active	Unknown	Non	Sensitizer	0	0	0	1	0	1	0	1	0.38
climbazole	38083-17-9	NON-mutagenic	NON-Carcinogen	Toxicant	NON-active	NON-active	Unknown	Non	Sensitizer	0	0	1	0	0	1	0	1	0.38
loperamide	53179-11-6	NON-mutagenic	NON-Carcinogen	NON-Toxicant	NON-active	Active	NON-Toxic	Inhibitor	NON-Sensitizer	0	0	0	0	1	0	1	0	0.25
zolpidem	82626-48-0	Mutagenic	Carcinogen	Toxicant	NON-active	NON-active	Toxic	Inhibitor	Sensitizer	1	1	1	0	0	1	1	1	0.75
atenolol	29122-68-7	NON-mutagenic	NON-Carcinogen	Toxicant	NON-active	NON-active	NON-Toxic	Non	Sensitizer	0	0	1	0	0	0	0	1	0.25
carbamazepine	298-46-4	NON-mutagenic	Carcinogen	Toxicant	NON-active	NON-active	Toxic	Non	Sensitizer	0	1	1	0	0	1	0	1	0.5
carbamazepine 10,11-epoxyde	36507-30-9	Mutagenic	Carcinogen	Toxicant	NON-active	NON-active	Toxic	Non	Sensitizer	1	1	1	0	0	1	0	1	0.62
10,11-dihydro-10-hydroxy-carbamazepine	29331-92-8	NON-mutagenic	NON-Carcinogen	Toxicant	NON-active	NON-active	Toxic	Non	Sensitizer	0	0	1	0	0	1	0	1	0.38

Substance name	CAS number	Mutagenicity	Carcinogenicity	Developmental toxicity	Estrogen receptor effect	Androgen receptor effect	Hepatoxicity	P-glycoprotein activity	Skin sensitization	Mutagenicity score	Carcinogenicity score	Developmental toxicity score	Estrogen receptor effect score	Androgen receptor effect score	Hepatoxicity score	P-glycoprotein activity score	Skin sensitization score	$Score_{HH}$
BAM (dichlorobenzamide)	2008-58-4	NON-mutagenic	NON-Carcinogen	Toxicant	Possible	NON-active	Unknown	Non	Sensitizer	0	0	1	1	0	1	0	1	0.5
clindamycin	18323-44-9	Mutagenic	Carcinogen	NON-Toxicant	NON-active	NON-active	Toxic	Inhibitor	NON-Sensitizer	1	1	0	0	0	1	1	0	0.5
lidocaine	137-58-6	NON-mutagenic	NON-Carcinogen	NON-Toxicant	NON-active	NON-active	Toxic	Non	Sensitizer	0	0	0	0	0	1	0	1	0.25
acetaminophen	103-90-2	NON-mutagenic	NON-Carcinogen	NON-Toxicant	NON-active	NON-active	Toxic	Non	Sensitizer	0	0	0	0	0	1	0	1	0.25
diuron	330-54-1	Mutagenic	NON-Carcinogen	Toxicant	NON-active	NON-active	Toxic	Non	Sensitizer	1	0	1	0	0	1	0	1	0.5
boscalid	188425-85-6	NON-mutagenic	NON-Carcinogen	Toxicant	NON-active	NON-active	Toxic	Non	Sensitizer	0	0	1	0	0	1	0	1	0.38
gemfibrozil	25812-30-0	NON-mutagenic	NON-Carcinogen	Toxicant	NON-active	NON-active	Unknown	Non	Sensitizer	0	0	1	0	0	1	0	1	0.38
PFNA	375-95-1	NON-mutagenic	Carcinogen	NON-Toxicant	NON-active	NON-active	Unknown	Non	NON-Sensitizer	0	1	0	0	0	1	0	0	0.25
PFOA	335-67-1	NON-mutagenic	Carcinogen	NON-Toxicant	NON-active	NON-active	Unknown	Non	Sensitizer	0	1	0	0	0	1	0	1	0.38
PFHpA	375-85-9	NON-mutagenic	Carcinogen	NON-Toxicant	NON-active	NON-active	Unknown	Non	Sensitizer	0	1	0	0	0	1	0	1	0.38
PFHxA	307-24-4	NON-mutagenic	Carcinogen	NON-Toxicant	NON-active	NON-active	Unknown	Non	Sensitizer	0	1	0	0	0	1	0	1	0.38
PFPeA	2706-90-3	NON-mutagenic	Carcinogen	NON-Toxicant	Possible	NON-active	Unknown	Non	Sensitizer	0	1	0	1	0	1	0	1	0.5
valsartan	137862-53-4	NON-mutagenic	Carcinogen	Toxicant	NON-active	NON-active	Toxic	Non	Sensitizer	0	1	1	0	0	1	0	1	0.5
bezafibrate	41859-67-0	NON-mutagenic	Carcinogen	Toxicant	Possible	NON-active	Toxic	Non	Sensitizer	0	1	1	1	0	1	0	1	0.62
fexofenadine	83799-24-0	NON-mutagenic	NON-Carcinogen	Toxicant	NON-active	NON-active	NON-Toxic	Inhibitor	Sensitizer	0	0	1	0	0	0	1	1	0.38
ibuprofen	15687-27-1	NON-mutagenic	NON-Carcinogen	Toxicant	NON-active	NON-active	Toxic	Non	Sensitizer	0	0	1	0	0	1	0	1	0.38
naproxen	22204-53-1	NON-mutagenic	NON-Carcinogen	Toxicant	NON-active	NON-active	Unknown	Non	Sensitizer	0	0	1	0	0	1	0	1	0.38
ketoprofen	22071-15-4	NON-mutagenic	NON-Carcinogen	Toxicant	NON-active	NON-active	Unknown	Non	Sensitizer	0	0	1	0	0	1	0	1	0.38

Substance name	CAS number	Mutagenicity	Carcinogenicity	Developmental toxicity	Estrogen receptor effect	Androgen receptor effect	Hepatoxicity	P-glycoprotein activity	Skin sensitization	Mutagenicity score	Carcinogenicity score	Developmental toxicity score	Estrogen receptor effect score	Androgen receptor effect score	Hepatoxicity score	P-glycoprotein activity score	Skin sensitization score	$Score_{HH}$
sparfloxacin	110871-86-8	Mutagenic	NON-Carcinogen	Toxicant	NON-active	NON-active	Toxic	Substrate	Sensitizer	1	0	1	0	0	1	1	1	0.62
ciprofloxacin	85721-33-1	Mutagenic	NON-Carcinogen	Toxicant	NON-active	NON-active	Toxic	Substrate	Sensitizer	1	0	1	0	0	1	1	1	0.62
ramipril	87333-19-5	NON-mutagenic	NON-Carcinogen	NON-Toxicant	NON-active	NON-active	Toxic	Non	NON-Sensitizer	0	0	0	0	0	1	0	0	0.12
amoxicillin	26787-78-0	NON-mutagenic	Carcinogen	NON-Toxicant	NON-active	NON-active	Toxic	Non	Sensitizer	0	1	0	0	0	1	0	1	0.38
atorvastatin	134523-00-5	NON-mutagenic	NON-Carcinogen	Toxicant	NON-active	NON-active	Toxic	Substrate	NON-Sensitizer	0	0	1	0	0	1	1	0	0.38
cetirizine	83881-51-0	NON-mutagenic	NON-Carcinogen	Toxicant	NON-active	NON-active	Unknown	Non	Sensitizer	0	0	1	0	0	1	0	1	0.38
diclofenac	15307-86-5	NON-mutagenic	NON-Carcinogen	Toxicant	NON-active	NON-active	Toxic	Non	Sensitizer	0	0	1	0	0	1	0	1	0.38
amidotrizoic acid	117-96-4	NON-mutagenic	Carcinogen	Toxicant	NON-active	NON-active	NON-Toxic	Non	Sensitizer	0	1	1	0	0	0	0	1	0.38
salicylic acid	69-72-7	NON-mutagenic	NON-Carcinogen	Toxicant	NON-active	NON-active	NON-Toxic	Non	NON-Sensitizer	0	0	1	0	0	0	0	0	0.12
furosemide	54-31-9	NON-mutagenic	NON-Carcinogen	Toxicant	NON-active	NON-active	Toxic	Non	Sensitizer	0	0	1	0	0	1	0	1	0.38
mefenamic acid	61-68-7	NON-mutagenic	Carcinogen	Toxicant	Possible	NON-active	Toxic	Non	Sensitizer	0	1	1	1	0	1	0	1	0.62
telmisartan	144701-48-4	Mutagenic	NON-Carcinogen	Toxicant	Possible	NON-active	Unknown	Non	NON-Sensitizer	1	0	1	1	0	1	0	0	0.5
tributyl citrate-acetate	77-90-7	NON-mutagenic	NON-Carcinogen	NON-Toxicant	NON-active	NON-active	Toxic	Inhibitor	NON-Sensitizer	0	0	0	0	0	1	1	0	0.25
clopidogrel	113665-84-2	NON-mutagenic	NON-Carcinogen	NON-Toxicant	NON-active	NON-active	Toxic	Inhibitor	Sensitizer	0	0	0	0	0	1	1	1	0.38
amlodipine*	111470-99-6	NON-mutagenic	NON-Carcinogen	Toxicant	NON-active	NON-active	NON-Toxic	Inhibitor	Sensitizer	0	0	1	0	0	0	1	1	0.38
mebendazole	31431-39-7	Mutagenic	Carcinogen	Toxicant	NON-active	NON-active	Toxic	Inhibitor	Sensitizer	1	1	1	0	0	1	1	1	0.75

Substance name	CAS number	Mutagenicity	Carcinogenicity	Developmental toxicity	Estrogen receptor effect	Androgen receptor effect	Hepatoxicity	P-glycoprotein activity	Skin sensitization	Mutagenicity score	Carcinogenicity score	Developmental toxicity score	Estrogen receptor effect score	Androgen receptor effect score	Hepatoxicity score	P-glycoprotein activity score	Skin sensitization score	$Score_{HH}$
diltiazem	42399-41-7	NON-mutagenic	NON-Carcinogen	NON-Toxicant	NON-active	NON-active	Toxic	Inhibitor	NON-Sensitizer	0	0	0	0	0	1	1	0	0.25
loratadine	79794-75-5	Mutagenic	Carcinogen	NON-Toxicant	NON-active	NON-active	NON-Toxic	Substrate	Sensitizer	1	1	0	0	0	0	1	1	0.5
propamocarb	24579-73-5	Mutagenic	NON-Carcinogen	Toxicant	NON-active	NON-active	Unknown	Non	Sensitizer	1	0	1	0	0	1	0	1	0.5
DEET (N,N-diethyl-m-toluamide)	134-62-3	NON-mutagenic	NON-Carcinogen	Toxicant	NON-active	NON-active	NON-Toxic	Non	Sensitizer	0	0	1	0	0	0	0	1	0.25
bupropion	34841-39-9	NON-mutagenic	Carcinogen	Toxicant	NON-active	NON-active	Unknown	Non	Sensitizer	0	1	1	0	0	1	0	1	0.5
sulisobenzone	4065-45-6	Mutagenic	Carcinogen	Toxicant	NON-active	NON-active	NON-Toxic	Inhibitor	Sensitizer	1	1	1	0	0	0	1	1	0.62
oxybenzone	131-57-7	Mutagenic	Carcinogen	Toxicant	Possible	NON-active	NON-Toxic	Non	Sensitizer	1	1	1	1	0	0	1	1	0.75
benzophenone	119-61-9	NON-mutagenic	NON-Carcinogen	Toxicant	Possible	NON-active	Unknown	Substrate	Sensitizer	0	0	1	1	0	1	1	1	0.62
genistein	446-72-0	NON-mutagenic	NON-Carcinogen	Toxicant	Active	NON-active	Toxic	Non	Sensitizer	0	0	1	1	0	1	0	1	0.5
daidzein	486-66-8	NON-mutagenic	Carcinogen	Toxicant	Active	NON-active	Toxic	Non	Sensitizer	0	1	1	1	0	1	0	1	0.62
phenazone	60-80-0	NON-mutagenic	Carcinogen	NON-Toxicant	NON-active	NON-active	Unknown	Non	Sensitizer	0	1	0	0	0	1	0	1	0.38
budesonide	51333-22-3	NON-mutagenic	Carcinogen	Toxicant	NON-active	NON-active	NON-Toxic	Inhibitor	NON-Sensitizer	0	1	1	0	0	0	1	0	0.38
oxycodone	76-42-6	NON-mutagenic	Carcinogen	Toxicant	Possible	NON-active	NON-Toxic	Non	Sensitizer	0	1	1	1	0	0	0	1	0.5
irbesartan	138402-11-6	NON-mutagenic	NON-Carcinogen	Toxicant	NON-active	NON-active	Toxic	Inhibitor	Sensitizer	0	0	1	0	0	1	1	1	0.5
oxazepam	604-75-1	NON-mutagenic	NON-Carcinogen	Toxicant	NON-active	Active	Toxic	Non	Sensitizer	0	0	1	0	1	1	0	1	0.5
3-(4-methyl-benzylidene)camphor	36861-47-9	NON-mutagenic	Carcinogen	Toxicant	Possible	Active	NON-Toxic	Non	Sensitizer	0	1	1	1	1	0	0	1	0.62
primidone	125-33-7	Mutagenic	NON-Carcinogen	Toxicant	Possible	NON-active	Toxic	Non	Sensitizer	1	0	1	1	0	1	0	1	0.62

Substance name	CAS number	Muta-genicity	Carcino-genicity	Develop-mental toxicity	Estrogen receptor effect	Androgen receptor effect	Hepa-toxicity	P-glyco-protein activity	Skin sensiti-zation	Muta-genicity score	Carcino-genicity score	Develop-mental toxicity score	Estrogen receptor effect score	Androgen receptor effect score	Hepa-toxicity score	P-glyco-protein activity score	Skin sensiti-zation score	$Score_{HH}$
theophylline	58-55-9	NON-mutagenic	NON-Carcinogen	Toxicant	NON-active	NON-active	Toxic	Non	Sensi-tizer	0	0	1	0	0	1	0	1	0.38
caffeine	58-08-2	NON-mutagenic	NON-Carcinogen	NON-Toxicant	NON-active	NON-active	Toxic	Non	Sensi-tizer	0	0	0	0	0	1	0	1	0.25
erythromycin	114-07-8	NON-mutagenic	NON-Carcinogen	Toxicant	NON-active	NON-active	Toxic	Substrate	NON-Sensi-tizer	0	0	1	0	0	1	1	0	0.38
clarithromycin	81103-11-9	NON-mutagenic	NON-Carcinogen	Toxicant	NON-active	NON-active	Toxic	Substrate	NON-Sensi-tizer	0	0	1	0	0	1	1	0	0.38
azithromycin	83905-01-5	NON-mutagenic	Carcinogen	Toxicant	NON-active	NON-active	Unknown	Substrate	NON-Sensi-tizer	0	1	1	0	0	1	1	0	0.5
simvastatin	79902-63-9	NON-mutagenic	Carcinogen	Toxicant	NON-active	NON-active	Toxic	Inhibitor	NON-Sensi-tizer	0	1	1	0	0	1	1	0	0.5
progesterone	57-83-0	NON-mutagenic	Carcinogen	Toxicant	Possible	Active	Toxic	Inhibitor	Sensi-tizer	0	1	1	1	1	1	1	1	0.88
mono-n-butyl-phosphoric acid	1623-15-0	NON-mutagenic	Carcinogen	Toxicant	Not	NON-active	Unknown	Non	Sensi-tizer	0	1	1	1	0	1	0	1	0.62
di-(2-ethylhexyl) phosphoric acid	298-07-7	NON-mutagenic	NON-Carcinogen	Toxicant	NON-active	NON-active	Unknown	Inhibitor	Sensi-tizer	0	0	1	0	0	1	1	1	0.5
dibutyl phosphate	107-66-4	NON-mutagenic	Carcinogen	Toxicant	Not	NON-active	Unknown	Non	Sensi-tizer	0	1	1	1	0	1	0	1	0.62
tris(2-chloroethyl) phosphate (TCEP)	115-96-8	NON-mutagenic	Carcinogen	Toxicant	NON-active	NON-active	Unknown	Non	Sensi-tizer	0	1	1	0	0	1	0	1	0.5
tris(2-butoxyethyl) phosphate (TBEP)	78-51-3	NON-mutagenic	NON-Carcinogen	Toxicant	NON-active	NON-active	Unknown	Non	Sensi-tizer	0	0	1	0	0	1	0	1	0.38
hydrochlorothiazide (HCTZ)	58-93-5	NON-mutagenic	NON-Carcinogen	Toxicant	NON-active	NON-active	Toxic	Non	Sensi-tizer	0	0	1	0	0	1	0	1	0.38
sotalol	3930-20-9	NON-mutagenic	Carcinogen	NON-Toxicant	NON-active	NON-active	NON-Toxic	Non	Sensi-tizer	0	1	0	0	0	0	0	1	0.25
sulfaklozine	102-65-8	NON-mutagenic	NON-Carcinogen	Toxicant	NON-active	NON-active	Toxic	Non	Sensi-tizer	0	0	1	0	0	1	0	1	0.38
sulfamethoxazole	723-46-6	NON-mutagenic	NON-Carcinogen	Toxicant	NON-active	NON-active	Toxic	Non	Sensi-tizer	0	0	1	0	0	1	0	1	0.38
PFOS	1763-23-1	NON-mutagenic	Carcinogen	NON-Toxicant	NON-active	NON-active	Unknown	Non	NON-Sensi-tizer	0	1	0	0	0	1	0	0	0.25

Substance name	CAS number	Mutagenicity	Carcinogenicity	Developmental toxicity	Estrogen receptor effect	Androgen receptor effect	Hepatoxicity	P-glycoprotein activity	Skin sensitization	Mutagenicity score	Carcinogenicity score	Developmental toxicity score	Estrogen receptor effect score	Androgen receptor effect score	Hepatoxicity score	P-glycoprotein activity score	Skin sensitization score	$Score_{HH}$
PFHxS	355-46-4	NON-mutagenic	Carcinogen	NON-Toxicant	NON-active	NON-active	Unknown	Non	Sensitizer	0	1	0	0	0	1	0	1	0.38
6:2 FTSA	27619-97-2	NON-mutagenic	Carcinogen	NON-Toxicant	NON-active	NON-active	Unknown	Non	Sensitizer	0	1	0	0	0	1	0	1	0.38
besylate (benzensulfonic acid)*	111470-99-6	NON-mutagenic	NON-Carcinogen	Toxicant	Not	NON-active	Unknown	Non	NON-Sensitizer	0	0	1	1	0	1	0	0	0.38
ranitidine	66357-35-5	NON-mutagenic	NON-Carcinogen	NON-Toxicant	NON-active	NON-active	Unknown	Non	Sensitizer	0	0	0	0	0	1	0	1	0.25
metronidazole	443-48-1	Mutagenic	Carcinogen	NON-Toxicant	NON-active	NON-active	Toxic	Non	Sensitizer	1	1	0	0	0	1	0	1	0.5
metronidazole-OH	4812-40-2	Mutagenic	NON-Carcinogen	NON-Toxicant	NON-active	NON-active	Unknown	Non	Sensitizer	1	0	0	0	0	1	0	1	0.38
2,4,7,9-tetramethyl-5-decyn-4,7-diol	126-86-3	NON-mutagenic	NON-Carcinogen	NON-Toxicant	NON-active	NON-active	Unknown	Non	Sensitizer	0	0	0	0	0	1	0	1	0.25
metoprolol	51384-51-1	NON-mutagenic	NON-Carcinogen	Toxicant	NON-active	NON-active	NON-Toxic	Non	Sensitizer	0	0	1	0	0	0	0	1	0.25
bisoprolol	66722-44-9	NON-mutagenic	NON-Carcinogen	Toxicant	Possible	NON-active	NON-Toxic	Non	Sensitizer	0	0	1	1	0	0	0	1	0.38
propranolol	525-66-6	NON-mutagenic	NON-Carcinogen	Toxicant	Possible	NON-active	Toxic	Non	Sensitizer	0	0	1	1	0	1	0	1	0.5
prothioconazole	178928-70-6	Mutagenic	Carcinogen	Toxicant	NON-active	NON-active	NON-Toxic	Non	Sensitizer	1	1	1	0	0	0	0	1	0.5
venlafaxine	93413-69-5	NON-mutagenic	Carcinogen	Toxicant	Possible	Active	Unknown	Non	Sensitizer	0	1	1	1	1	1	0	1	0.75
codeine	76-57-3	NON-mutagenic	NON-Carcinogen	Toxicant	Possible	NON-active	Toxic	Non	Sensitizer	0	0	1	1	0	1	0	1	0.5
tramadol	27203-92-5	NON-mutagenic	Carcinogen	Toxicant	Not	Active	Unknown	Inhibitor	Sensitizer	0	1	1	1	1	1	1	1	0.88
tetraethylene glycol	112-60-7	NON-mutagenic	Carcinogen	Toxicant	NON-active	NON-active	Unknown	Non	Sensitizer	0	1	1	0	0	1	0	1	0.5
laureth-5	3055-95-6	NON-mutagenic	NON-Carcinogen	Toxicant	Possible	NON-active	Unknown	Inhibitor	Sensitizer	0	0	1	1	0	1	1	1	0.62
losartan	114798-26-4	NON-mutagenic	NON-Carcinogen	Toxicant	Not	NON-active	Toxic	Substrate	Sensitizer	0	0	1	1	0	1	1	1	0.62
pyridoxine (vitamin b6)	65-23-6	NON-mutagenic	Carcinogen	NON-Toxicant	NON-active	NON-active	Toxic	Non	Sensitizer	0	1	0	0	0	1	0	1	0.38

Substance name	CAS number	Muta-genicity	Carcino-genicity	Develop-mental toxicity	Estrogen receptor effect	Androgen receptor effect	Hepa-toxicity	P-glyco-protein activity	Skin sensiti-zation	Muta-genicity score	Carcino-genicity score	Develop-mental toxicity score	Estrogen receptor effect score	Androgen receptor effect score	Hepa-toxicity score	P-glyco-protein activity score	Skin sensiti-zation score	$Score_{HH}$
terbutaline	23031-25-6	NON-mutagenic	Carcinogen	NON-Toxicant	NON-active	NON-active	NON-Toxic	Non	Sensi-tizer	0	1	0	0	0	0	0	1	0.25
desvenlafaxine	93413-62-8	NON-mutagenic	Carcinogen	Toxicant	Possible	Active	Unknown	Non	Sensi-tizer	0	1	1	1	1	1	0	1	0.75
bisphenol A	80-05-7	NON-mutagenic	NON-Carcinogen	Toxicant	Active	Active	Unknown	Non	Sensi-tizer	0	0	1	1	1	1	0	1	0.62
albuterol (salbutamol)	18559-94-9	NON-mutagenic	Carcinogen	Toxicant	NON-active	NON-active	NON-Toxic	Non	Sensi-tizer	0	1	1	0	0	0	0	1	0.38
triclosan	3380-34-5	NON-mutagenic	Carcinogen	Toxicant	NON-active	Active	NON-Toxic	Non	Sensi-tizer	0	1	1	0	1	0	0	1	0.5
amitriptyline	50-48-6	NON-mutagenic	NON-Carcinogen	Toxicant	Not	Active	Toxic	Inhibitor	Sensi-tizer	0	0	1	1	1	1	1	1	0.75
sertraline	79617-96-2	NON-mutagenic	NON-Carcinogen	Toxicant	NON-active	Active	Unknown	Inhibitor	Sensi-tizer	0	0	1	0	1	1	1	1	0.62
benzotriazole	95-14-7	Mutagenic	NON-Carcinogen	Toxicant	NON-active	NON-active	Toxic	Non	Sensi-tizer	1	0	1	0	0	1	0	1	0.5
terbutryn	886-50-0	NON-mutagenic	NON-Carcinogen	Toxicant	NON-active	NON-active	Unknown	Non	Sensi-tizer	0	0	1	0	0	1	0	1	0.38
trimethoprim	738-70-5	Mutagenic	NON-Carcinogen	Toxicant	NON-active	Active	Toxic	Substrate	Sensi-tizer	1	0	1	0	1	1	1	1	0.75
nicotine	54-11-5	NON-mutagenic	NON-Carcinogen	NON-Toxicant	NON-active	NON-active	Toxic	Non	Sensi-tizer	0	0	0	0	0	1	0	1	0.25
mirtazapine	85650-52-8	NON-mutagenic	Carcinogen	Toxicant	NON-active	NON-active	Toxic	Inhibitor	Sensi-tizer	0	1	1	0	0	1	1	1	0.62
imazalil	35554-44-0	NON-mutagenic	NON-Carcinogen	Toxicant	NON-active	Active	NON-Toxic	Non	Sensi-tizer	0	0	1	0	1	0	0	1	0.38
propiconazole	60207-90-1	NON-mutagenic	Carcinogen	NON-Toxicant	NON-active	Active	Toxic	Non	Sensi-tizer	0	1	0	0	1	1	0	1	0.5
thiabendazole	148-79-8	Mutagenic	NON-Carcinogen	Toxicant	NON-active	NON-active	Toxic	Non	Sensi-tizer	1	0	1	0	0	1	0	1	0.5
lamotrigine	84057-84-1	Mutagenic	NON-Carcinogen	Toxicant	NON-active	NON-active	Toxic	Non	Sensi-tizer	1	0	1	0	0	1	0	1	0.5
FOSA	754-91-6	NON-mutagenic	Carcinogen	NON-Toxicant	NON-active	NON-active	Unknown	Non	NON-Sensi-tizer	0	1	0	0	0	1	0	0	0.25

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To reuse or not: is purified wastewater a non-toxic and sustainable resource for the future? (REASSURE)

Risks associated with hazardous pollutants in wastewater reuse and their mitigation

In the REASSURE research project, the researchers have investigated the risks associated with hazardous pollutants in wastewater reuse and their mitigation. The aim of the research synthesis is to improve knowledge about the potential and sustainability of using treated domestic wastewater both in Sweden and internationally, with a focus on the adverse impacts by hazardous pollutants in the wastewater.

There are major differences between countries, both in practice and in how they view wastewater reuse, as well as the health risks it poses to people and the environment. Researchers have also evaluated the potential of advanced treatment technologies for hazardous pollutants.

The removal efficiency of chemical contaminants was summarized for five selected technologies. The results show that a combination of different technologies may be used to achieve acceptable wastewater treatment.

The project has been financed with funds from the Swedish Environmental Protection Agency's environmental research grant, which finances research to support the knowledge needs of the Swedish Environmental Protection Agency and the Swedish Agency for Marine and Water Management.

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