

## Article

# Evaluation of the Pathway of Contaminants in the Environment: A Case Study of Different Aquatic Environmental Compartments

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**Abstract:** The occurrence of contaminants of emerging concern (CECs) in several environmental compartments has raised significant concern given the extensive array of compounds and their consistent detection across various environmental matrices. Monitoring all potentially harmful compounds and identifying their sources is nearly impossible. However, providing data on their occurrence is crucial and lays the groundwork for decision makers to craft mitigation strategies toward a more sustainable water policy. Hence, the primary aim of this study was to conduct an evaluation study on CECs occurrence in the environment. The main novelty relies on understanding their specific pathway in three different environmental aquatic compartments. For that, a combined study of a systematic review and systemic analysis was performed. Initially, the five most common types of CECs found in aquatic ecosystems (groundwater and surface water) and wastewater were considered. For each group of CECs, five contaminants were identified. A bibliographic portfolio was generated through the application of a systematic review. Finally, a systemic analysis of the bibliographic portfolio was conducted. All classes of contaminants studied were identified in the environmental compartments evaluated. Except for pesticides, the degree of contamination by CECs followed a sequence based on the aquatic compartment (i.e., WW–SW–GW).

**Keywords:** pollutants; contaminant dispersion; pharmaceutical; water pollution



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## 1. Introduction

The occurrence of contaminants of emerging concern (CECs) in several environmental compartments has raised significant concern given the extensive array of compounds and their consistent detection across various environmental matrices [1]. CECs refer to substances that occur naturally, are manufactured, or are of human origin—chemicals/materials—that are suspected to be present or have been recently identified in various environmental compartments [2]. The American Chemical Society's global Chemical Abstracts Service has registered more than 142 million chemicals [3]. Additionally, a recent report from the United Nations Environment Program and the International Council of Chemical Associations indicated that more than 350,000 chemicals and mixtures are commercially used worldwide [4]. These substances possess characteristics that could potentially pose risks to both biota and humans [5].

The main types of CECs found in wastewater samples and aquatic ecosystems are pesticides, hormones, pharmaceuticals, industrial chemicals (including illicit drugs, plasticizers, and lifestyle compounds such as caffeine), and personal care products [2,6].

Pesticides are chemical substances used to preventing, destroying, repelling, or mitigating any pest and diseases in agriculture, forestry, and public health [7]. They include herbicides, insecticides, fungicides, and rodenticides. These compounds can enter aquatic ecosystems through runoff from agricultural fields, urban areas, and residential areas, posing as a significant threat to aquatic organisms due to their toxicity, persistence, and potential to bioaccumulate in the food chain [7,8]. Common pesticide contaminants in aquatic environments include atrazine, glyphosate, chlorpyrifos, and diazinon [9]. Studies have shown adverse effects on aquatic organisms such as fish, amphibians, and invertebrates as well as potential risks to human health through consumption of aquatic organisms and contaminated water [7].

Hormones are naturally occurring chemicals produced by organisms to regulate various physiological functions. Also, hormones can be synthetic substances with an effect similar to that of an animal or plant hormone [2]. In aquatic environments, hormones of concern include endogenous hormones produced by animals (such as estrogen, progesterone, and testosterone) as well as synthetic hormones used in pharmaceuticals and animal husbandry (such as estradiol, ethinylestradiol, and testosterone). These hormones can enter water bodies through discharge from wastewater treatment plants, agricultural runoff, and animal waste [10,11]. Even at minimal doses, they can disrupt the endocrine systems of aquatic organisms. Furthermore, there are concerns about the potential for these hormone-disrupting compounds to accumulate in the environment and affect human health through drinking water and seafood consumption [10,12].

Pharmaceuticals are medicinal drugs used to prevent, diagnose, or treat diseases in both humans and animals [13]. Common pharmaceutical contaminants found in aquatic environments include antibiotics, analgesics, antidepressants, antihistamines, and contraceptives. These compounds can enter water bodies through excretion by humans and animals, improper disposal of unused medications, and discharge from pharmaceutical manufacturing facilities and healthcare facilities [14,15]. While pharmaceuticals are designed to have specific biological effects, their presence in aquatic ecosystems at trace levels can lead to unintended consequences. Chronic exposure to pharmaceutical contaminants has been associated with adverse effects on aquatic organisms, including altered behavior, growth, reproduction, and immune function [16]. In addition, there are also concerns about the development of antibiotic resistance in bacteria exposed to subtherapeutic levels of antibiotics in the environment [17,18].

Industrial chemicals comprise a wide range of synthetic compounds used in manufacturing, processing, and various industrial activities. These include heavy metals, organic solvents, flame retardants, plasticizers, and surfactants [19]. Industrial chemicals can enter aquatic ecosystems through direct discharge from industrial facilities, atmospheric deposition, and runoff from contaminated sites [20,21]. Many industrial chemicals are persistent and bioaccumulative, posing long-term risks to aquatic organisms and human health. Exposure to industrial chemical contaminants has been linked to a range of adverse effects, including developmental abnormalities, reproductive disorders, neurotoxicity, and carcinogenicity. Some industrial chemicals, such as polychlorinated biphenyls (PCBs) and dioxins, are regulated as persistent organic pollutants due to their environmental persistence and toxicity [22].

Personal care products are consumer goods used on various external parts of the body. These products are utilized to cleanse, protect against harmful germs, and maintain the overall health and condition of these body parts [23]. They include ingredients such as fragrances, preservatives, UV filters, antimicrobial agents, and plasticizers. Personal care product contaminants can enter aquatic environments through wastewater discharge from households and recreational activities (e.g., swimming) [24,25]. While individual personal care product ingredients are typically present at low concentrations, their cumulative effects and interactions with other contaminants in aquatic ecosystems are a growing concern [26]. Some ingredients in personal care products, such as triclosan and phthalates, have been identified as potential endocrine disruptors and environmental contaminants of emerging concern. Studies have shown adverse effects on aquatic organisms, including

algae, fish, and invertebrates, as well as potential risks to human health through exposure via recreational water activities and consumption of contaminated water/food [25].

These compounds are frequently manufactured to fulfill society's daily requirements and are subsequently introduced into the environment. Their presence has consistently been detected at low concentrations in the majority of cases (i.e.,  $\text{ng L}^{-1}$ – $\mu\text{g L}^{-1}$ ) [6]. However, even at trace concentrations, when in contact with living organisms, CECs may induce the above-mentioned adverse effects, including decreased fish reproduction caused by endocrine system disruption, reduced invertebrate populations due to sublethal toxicity, and the spread of antibiotic-resistant bacteria (ARB) and antibiotic-resistant genes (ARGs) [17,18,27].

Urban wastewaters represent a significant source of CECs into the environment, as conventional technologies employed in urban wastewater treatment plants (WWTPs) often lack the efficiency to completely eliminate them. Another pathway for the release of CECs is the practice of reusing wastewater, which leads to the widespread presence of CECs in agroecosystems and their subsequent entry into the soil and food chain. Furthermore, CECs may also be introduced into nature directly from the skin and/or urine human contamination during activities such as swimming or bathing.

Monitoring all potentially harmful compounds in the environment and identifying their sources is nearly impossible. However, providing data on their occurrence is crucial and lays the groundwork for decision makers to craft mitigation strategies toward a more sustainable water policy. Hence, the main objective of this work was to conduct an evaluation study on the occurrence of CECs in the environment and their pathway. For that, a combined study of a systematic review and systemic analysis was performed. Initially, the five most common types of CECs found in aquatic ecosystems (groundwater and surface water) and wastewater were considered. One of the main novelties of the research work relies on understanding the pathway of the determined contaminants in the three different aquatic environmental compartments. For each group of CECs, five contaminants were identified. A bibliographic portfolio was generated through the application of a systematic review. Finally, a systemic analysis of the bibliographic portfolio was conducted, and the main observations were highlighted.

## 2. Materials and Methods

### 2.1. Systematic Review

The bibliographic portfolio (BP) was obtained through systematic exploratory research and using the ProKnow-C (*Knowledge Development Process—Constructivist*) instrument. The methodology used can be consulted elsewhere [28]. This approach is designed to delineate works through a series of phases for the creation of a bibliographic portfolio. It involved a systemic analysis of the content of the works and a comparative study to map and investigate the primary outcomes achieved by the authors. To achieve this objective, specific criteria were applied during the search stage: (i) inclusion of scientific works published in indexed journals from the Scopus and Web of Science databases; (ii) consideration of works from 2000 to 2020; and (iii) inclusion of works available in English and in full format. The entire process was structured into four distinct stages: (1) identification, (2) triage, (3) eligibility, and (4) inclusion.

For the identification stage, the five most common types of CECs found in aquatic ecosystems (groundwater and surface water) and wastewater were considered: pharmaceuticals, personal care products, synthetic/natural hormones, pesticides, and industrial chemicals. The identification involved the selection of keywords, categorized into two distinct thematic axes and amalgamated using Boolean operators (OR, AND), resulting in the creation of the search string ("*emerging pollutants*" OR "*emerging contaminants*" OR "*pharmaceutical*" OR "*personal care product*" OR "*hormone*" OR "*pesticide*" OR "*industrial chemical*" AND "*groundwater*" OR "*surface water*" OR "*wastewater*").

During the triage phase, the works were uploaded to a designated folder within a bibliographic management system. They underwent filtration after a meticulous review

of the titles, leading to the exclusion of duplicate documents and those not in alignment with the research objectives. To validate their eligibility, the works were organized on a spreadsheet and categorized based on their citation count in the Google Scholar database, serving as a measure of their scientific relevance. Following this, the abstracts of the pertinent works were re-evaluated, leading to the exclusion of those that did not align with the research criteria. For each group of CEC, the five most identified contaminants were included in the BP. Additionally, their detection was described, if possible, in two aquatic ecosystems, i.e., groundwater (GW) and surface water (SW), and in wastewater (WW) samples. In the last step, during the inclusion phase, a comprehensive assessment of the entire repository was conducted after ensuring the full availability of each work's content online. This involved a thorough examination, and any work not aligning with the research scope was excluded. The retained works, deemed to align with the research objectives, remained on the list and constituted the bibliographic portfolio (BP).

Through this portfolio, it was possible to carry out a systemic analysis of articles aligned with the theme, i.e., the presence and pathways of CECs in the environment.

## 2.2. Systemic Analysis of the BP

The selected works from the BP were analyzed individually regarding the main characteristics: group of contaminant and concentration detected, molecular formula, and environmental compartment detected.

## 2.3. Comparison Analysis

The works were divided according to the group of contaminants and the environmental compartment in which the CEC was found. The five top CECs of each group of contaminants were identified. Their behavior and pathways in the environment were evaluated in order to identify tendencies.

## 3. Results

### 3.1. Systematic Review and Creation of the Bibliographic Portfolio

CECs have been consistently reported to occur in the environment at low concentrations (e.g.,  $\text{ng L}^{-1}$ – $\mu\text{g L}^{-1}$ ). Tables 1–5 present a thematic synthesis of the BP publications, categorized according to (i) the contaminant group (i.e., pesticides, hormones, pharmaceuticals, industrial chemicals, and personal care products); (ii) molecular formula; (iii) environmental compartment detected (i.e., groundwater (GW), surface water (SW), and wastewater (WW)); and (iv) concentration detected.

**Table 1.** Bibliographic portfolio on pesticides detection in the environment.

Group	CEC (Molecular Formula)	Environmental Compartment Detected	CEC Concentration Detected ( $\mu\text{g L}^{-1}$ )	Reference
Pesticides	Carbofuran ( $\text{C}_{12}\text{H}_{15}\text{NO}_3$ )	GW	0.1–10.4	[29,30]
		SW	0.95–1.67	[31]
	Atrazine ( $\text{C}_8\text{H}_{14}\text{ClN}_5$ )	GW	0.03–0.7	[32–35]
		SW	0.06 *	[36]
	Clomazone ( $\text{C}_{12}\text{H}_{14}\text{ClNO}_2$ )	GW	0.8–10.8	[30,35]
		SW	3.2	[35]
	Iprodione ( $\text{C}_{13}\text{H}_{13}\text{Cl}_2\text{N}_3\text{O}_3$ )	GW	0.06	[33]
		SW	0.01–0.03	[37,38]
	Carbendazim ( $\text{C}_9\text{H}_9\text{N}_3\text{O}_2$ )	GW	1.6	[33]
		SW	0.1	[36]
WW		0.014–0.078	[39]	

\* Average value.

**Table 2.** Bibliographic portfolio on hormones detection in the environment.

Group	CEC (Molecular Formula)	Environmental Compartment Detected	CEC Concentration Detected ( $\mu\text{g L}^{-1}$ )	Reference
Hormones	Estriol ( $\text{C}_{18}\text{H}_{24}\text{O}_3$ )	GW	$0.16 \times 10^{-3}$	[40]
		SW	$1.9 \times 10^{-3}$	[40]
		WW	$4.9 \times 10^{-3}$ *	[41]
	17 $\beta$ -estradiol ( $\text{C}_{18}\text{H}_{24}\text{O}_2$ )	GW	$0.1 \times 10^{-3}$	[42]
		SW	0.01–0.2	[43,44]
		WW	1.1–1.2	[45]
	Estrone ( $\text{C}_{18}\text{H}_{22}\text{O}_2$ )	GW	$1.1 \times 10^{-3}$	[42]
		SW	$4.6 \times 10^{-3}$	[40]
		WW	0.01–0.18	[45,46]
	Progesterone ( $\text{C}_{21}\text{H}_{30}\text{O}_2$ )	GW	$2.8 \times 10^{-3}$ – $4.1 \times 10^{-3}$	[47]
		SW	$1.15 \times 10^{-3}$ –0.2	[44,47,48]
	Testosterone ( $\text{C}_{19}\text{H}_{28}\text{O}_2$ )	GW	$4.3 \times 10^{-3}$ – $6 \times 10^{-3}$	[47]
SW		$2.8 \times 10^{-3}$ –0.21	[44,47]	

\* Average value.

**Table 3.** Bibliographic portfolio on pharmaceuticals detection in the environment.

Group	CEC (Molecular Formula)	Environmental Compartment Detected	CEC Concentration Detected ( $\mu\text{g L}^{-1}$ )	Reference
Pharmaceutical	Azithromycin ( $\text{C}_{38}\text{H}_{72}\text{N}_2\text{O}_{12}$ )	SW	0.06–0.1	[49]
		WW	0.06–2.5	[16,50]
	Oxytetracycline ( $\text{C}_{22}\text{H}_{24}\text{N}_2\text{O}_9$ )	SW	0.02–0.34	[44,51]
		WW	0.35	[52]
	Ibuprofen ( $\text{C}_{13}\text{H}_{18}\text{O}_2$ )	GW	0.05	[53]
		SW	1.0	[44]
		WW	1.3–4.1	[16,54]
	Amoxicillin ( $\text{C}_{16}\text{H}_{19}\text{N}_3\text{O}_5\text{S}$ )	SW	0.2–0.3 *	[52,55]
		WW	0.33–6.9	[52,56]
	Diclofenac ( $\text{C}_{14}\text{H}_{11}\text{Cl}_2\text{NO}_2$ )	GW	0.04 *	[34]
SW		0.14–0.31	[57]	
WW		0.6–2.43	[16,54]	

\* Average value.

**Table 4.** Bibliographic portfolio on industrial chemicals detection in the environment.

Group	CEC (Molecular Formula)	Environmental Compartment Detected	CEC Concentration Detected ( $\mu\text{g L}^{-1}$ )	Reference
Industrial chemicals	Caffeine ( $\text{C}_8\text{H}_{10}\text{N}_4\text{O}_2$ )	GW	$6 \times 10^{-3}$ –0.045	[29,58]
		SW	6.0	[44]
		WW	66	[54]
	Cotinine ( $\text{C}_{10}\text{H}_{12}\text{N}_2\text{O}$ )	GW	0.06–0.4	[34,59]
		SW	0.9	[44]
		WW	0.7–2.6	[60]

Table 4. Cont.

Group	CEC (Molecular Formula)	Environmental Compartment Detected	CEC Concentration Detected ( $\mu\text{g L}^{-1}$ )	Reference
Industrial chemicals	Nicotine ( $\text{C}_{10}\text{H}_{14}\text{N}_2$ )	GW	0.041 *	[34,61]
		WW	–8.07 1.1–14.6	[54,60]
	bis(2-ethylhexyl) phthalate ( $\text{C}_{24}\text{H}_{38}\text{O}_4$ )	GW	0.39–46	[32,33]
		SW	20	[44]
		WW	61	[62]
Cocaine ( $\text{C}_{17}\text{H}_{21}\text{NO}_4$ )	GW	1.2	[61]	
	WW	0.29–3.7	[60,63]	

\* Average value.

Table 5. Bibliographic portfolio on personal care products detection in the environment.

Group	CEC (Molecular Formula)	Environmental Compartment Detected	CEC Concentration Detected ( $\mu\text{g L}^{-1}$ )	Reference
Personal care products	Triclosan ( $\text{C}_{12}\text{H}_7\text{Cl}_3\text{O}_2$ )	GW	$2 \times 10^{-3}$	[29]
		SW	$1.9 \times 10^{-3}$ *	[44,64]
		WW	–2.3 0.18–4.4	[65]
	Octocrylene ( $\text{C}_{24}\text{H}_{27}\text{NO}_2$ )	GW	$8.4 \times 10^{-3}$	[34]
		SW	0.05 *	[36]
		WW	13	[66]
	Celestolide ( $\text{C}_{17}\text{H}_{24}\text{O}$ )	SW	$2.5 \times 10^{-3}$ *	[67]
		WW	0.03–0.05	[54,66,68]
	Galaxolide ( $\text{C}_{18}\text{H}_{26}\text{O}$ )	GW	0.043	[34]
		SW	0.02–4.8	[67,69]
WW		1.1–25	[54,66]	
Tonalide ( $\text{C}_{18}\text{H}_{26}\text{O}$ )	GW	$7.5 \times 10^{-3}$	[34]	
	SW	0.1 *–0.95	[67,69]	
	WW	0.04–1.95	[46,54,66]	

\* Average value.

### 3.2. Analysis of the Contaminants

The BP-listed studies identified five contaminants of each group of contaminants.

Regarding pesticides, the following contaminants were identified: carbofuran, atrazine, clomazone, iprodione, and carbendazim. Carbofuran is a potent carbamate insecticide and nematicide extensively employed in agriculture to manage pests in crops of rice, corn, and potatoes, among others. It poses a significant risk to aquatic ecosystems due to its high water solubility and potential for runoff into water bodies [70]. Atrazine is a broad-spectrum herbicide commonly used in agriculture to control weeds in crops such as corn, sugarcane, and sorghum. It is known for its persistence in the environment and ability to leach into groundwater and surface water [71]. Clomazone is a selective herbicide used to control grass and broadleaf weeds in crops such as soybeans, cotton, and peanuts. It has the potential to contaminate aquatic environments through runoff and drift during application [72]. Iprodione is a fungicide commonly applied in agriculture to control fungal diseases in crops such as fruits, vegetables, and ornamentals [73]. Carbendazim is a systemic fungicide used to control fungal diseases in crops such as fruits, vegetables, and cereals. It is known for its persistence in soil and water and has the potential to accumulate in aquatic organisms [74].

Considering hormones, estriol, 17 $\beta$ -estradiol, estrone, progesterone, and testosterone were detected. Estriol is a naturally occurring estrogen hormone produced by the ovaries during pregnancy. It is also found in smaller amounts in non-pregnant individuals, primarily as a metabolic product of estradiol [12]. 17 $\beta$ -Estradiol, commonly known as estradiol, is the primary female sex hormone and the most potent naturally occurring estrogen. It regulates the menstrual cycle, fertility, and secondary sexual characteristics in females [12]. Estrone is an estrogen hormone and one of the three main naturally occurring estrogens in humans, along with estradiol and estriol. It is primarily produced by the ovaries in females and by the testes in males as well as by conversion from other hormones in peripheral tissues [75]. Progesterone is a type of steroid hormone involved in the menstrual cycle, embryogenesis in females, and pregnancy. It is primarily produced by the ovaries following ovulation and by the placenta during pregnancy [76]. Testosterone is the primary male sex hormone and an androgen steroid hormone. It plays a crucial role in the development of male reproductive tissues, secondary sexual characteristics, and sperm production [76].

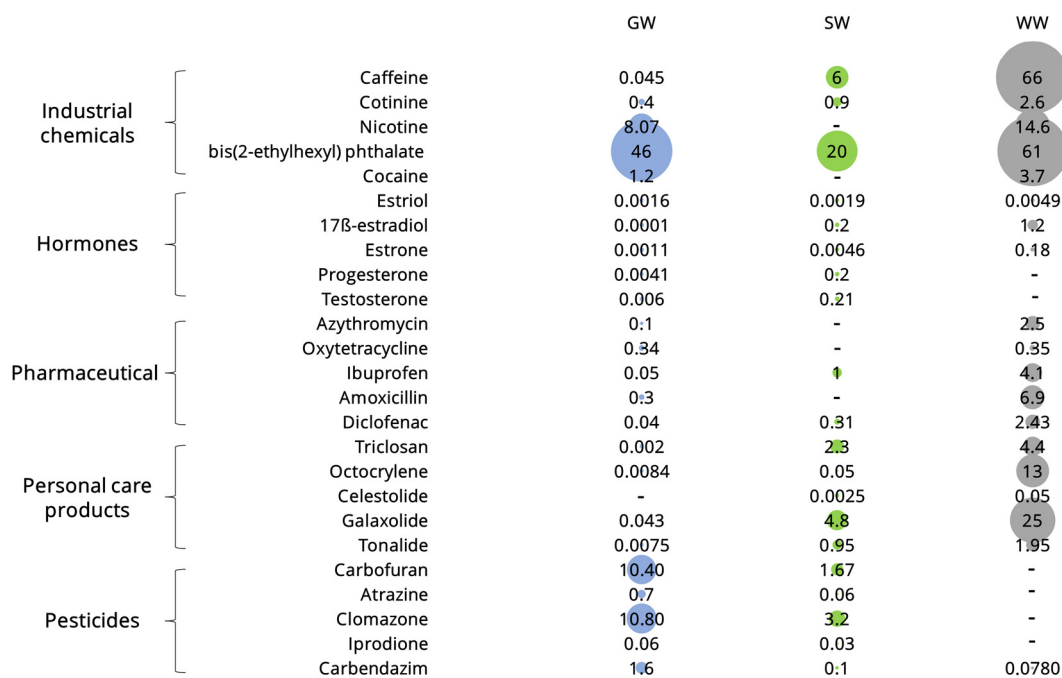
For pharmaceuticals, azithromycin, oxytetracycline, ibuprofen, amoxicillin, and diclofenac were detected. Azithromycin is a broad-spectrum antibiotic used to treat a variety of bacterial infections in humans and animals. It belongs to the class of macrolide antibiotics and is commonly prescribed for respiratory tract infections, skin infections, and sexually transmitted diseases [77]. Oxytetracycline is a broad-spectrum antibiotic belonging to the tetracycline class. It is widely used in veterinary medicine to treat bacterial infections in livestock and aquaculture as well as in some human medications [78]. Ibuprofen is an anti-inflammatory drug commonly employed to relieve pain, lower fever, and reduce inflammation. It is widely available over-the-counter and is one of the most commonly used pharmaceuticals worldwide [79]. Amoxicillin is a broad-spectrum penicillin antibiotic used to treat bacterial infections in humans and animals. It is commonly prescribed for respiratory tract infections, urinary tract infections, and skin infections [80]. Diclofenac is also an anti-inflammatory drug used to relieve pain, reduce inflammation, and treat various inflammatory conditions in humans and animals. It is available in both prescription and over-the-counter formulations [80].

In the case of industrial chemicals, caffeine, cotinine, nicotine, bis(2-ethylhexyl) phthalate, and cocaine were identified. Caffeine is a stimulant compound found in various beverages (e.g., coffee, tea, and energy drinks) as well as in certain medications and dietary supplements [81]. Cotinine is a metabolite of nicotine, formed in the body following the metabolism of nicotine from tobacco products [82]. Nicotine is a highly toxic alkaloid found in tobacco plants and tobacco smoke [82]. Bis(2-ethylhexyl) phthalate (DEHP) is a plasticizer commonly used in the production of polyvinyl chloride (PVC) plastics to impart flexibility and durability [83]. Cocaine is a potent stimulant drug derived from the leaves of the coca plant [84].

Finally, considering personal care products, the following contaminants were detected: triclosan, octocrylene, celestolide, galaxolide, and tonalide. Triclosan is an antimicrobial agent commonly used in personal care products such as toothpaste and deodorants as well as in household cleaning products. Triclosan is considered an environmental contaminant of concern due to its persistence and bioaccumulative potential [85]. Octocrylene is an organic compound used as an ultraviolet (UV) filter in sunscreen and skincare products to absorb UV radiation and protect the skin from sun damage [86]. Celestolide, also known as synthetic musk fragrance, is a synthetic compound used in personal care products such as perfumes, colognes, and lotions to impart a musky scent [87]. Galaxolide, also known as HHCB (1,3,4,6,7,8-hexahydro-4,6,6,7,8,8-hexamethylcyclopenta[g]-2-benzopyran), is a synthetic musk fragrance used in personal care products such as perfumes, lotions, and laundry detergents to provide a long-lasting scent [88]. Tonalide, also known as AHTN (7-acetyl-1,1,3,4,4,6-hexamethyl-1,2,3,4-tetrahydronaphthalene), is a synthetic musk fragrance used in personal care products such as perfumes, lotions, and cosmetics to provide a sweet, floral scent [88].

### 3.3. BP Systemic Analysis

The BP-listed studies aimed at various topics in the areas of chemical/environmental sciences, for example, water treatment, water reuse, agriculture, and analytical methods, among others. The contaminants were categorized into five classes, namely pharmaceuticals, personal care products, hormones, pesticides, and industrial chemicals, and delineated based on their detected concentrations. All classes were identified in the three types of water compartments assessed in this study (i.e., groundwater, surface water, and wastewater). Figure 1 presents the graphical bubble chart view for the results obtained from the bibliographic portfolio.



**Figure 1.** Bubble chart of contaminants included in the bibliographic portfolio and their respective concentrations detected in aquatic systems and wastewater. Value concentration of CEC is expressed in  $\mu\text{g L}^{-1}$ .

## 4. Discussion

Following the findings of the bibliographic portfolio, an analysis of the detection of the contaminants in the different aquatic environmental compartments and their pathway was conducted. Firstly, the main findings regarding each environmental compartment were described. Subsequently, insights into the pathway of contaminants in the environment and possible future research directions were discussed.

### 4.1. Groundwater

All classes of contaminants studied were identified in groundwater samples. Their concentration varied from 0.0001 to 46  $\mu\text{g L}^{-1}$ .

Hormones were detected in a lower concentration when compared with the other groups of CECs, in the range of  $10^{-3}$   $\mu\text{g L}^{-1}$ . This fact is due to the pathway in which these contaminants are introduced into the environment, which will be discussed further. Oppositely, pesticides were detected with greater intensity, as these compounds are applied directly to the soil, facilitating their path to groundwater.

### 4.2. Surface Water

Contaminants from all groups of CECs, within the studied ones, were detected in surface water samples. Their concentration ranged from 0.002 to 20  $\mu\text{g L}^{-1}$ .

Industrial chemicals were detected in a higher concentration when compared with the other groups of CECs. This is probably due to the fact that the treatment used in most of the sewage treatment plants are not able to efficiently remove these CECs, leading to their release into receiving surface water bodies, and/or to the incorrect release of industrial effluents directly to water bodies.

#### 4.3. Wastewater

All groups of CECs, within the studied ones, were detected in wastewater samples. Their concentration varied from 0.005 to 66  $\mu\text{g L}^{-1}$ .

Industrial chemicals were detected in a higher concentration when compared with the other groups of CECs. This fact is probably due to the higher dose in which these compounds are used and due to the incorrect release of industrial effluents directly to sewage treatment plants. On the other hand, pesticides were not widely found in wastewater samples. Within the studied contaminants, carbendazim was the only one that was detected in WW samples at a relative low concentration, 0.078  $\mu\text{g L}^{-1}$ .

#### 4.4. Pathways

Within the studies evaluated, industrial chemicals, hormones, pharmaceuticals, personal care products, and pesticides were detected in the range of 0.045–66, 0.0001–1.2, 0.04–6.9, 0.002–25, and 0.03–10.8  $\mu\text{g L}^{-1}$ , respectively. Except for pesticides, the degree of contamination by CECs followed a sequence based on the aquatic compartment (GW < SW < WW) (Figure 2). Contrary to the expected result, one study showed a high concentration of an industrial chemical in groundwater samples. The authors attributed the high concentration of Bis(2-ethylhexyl)phthalate in the groundwater, namely 46  $\mu\text{g L}^{-1}$ , to solid waste leachate infiltration [32].

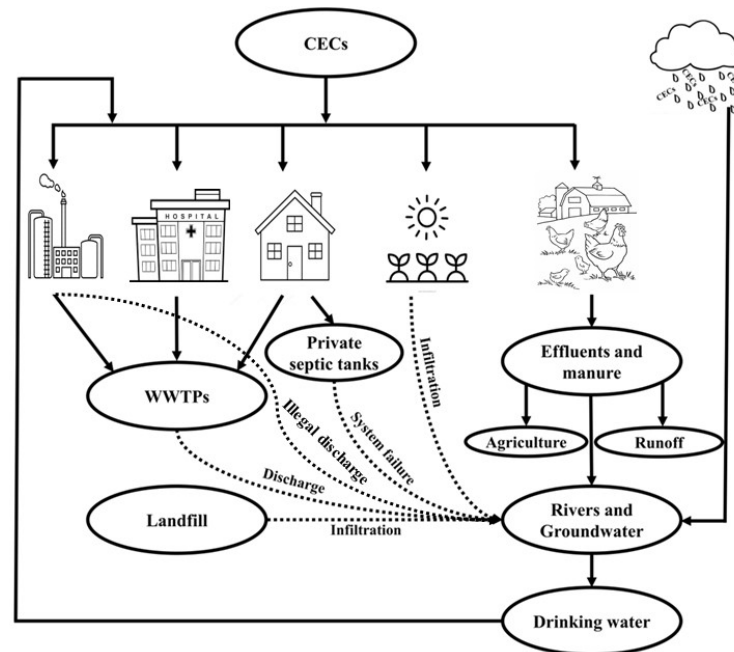


**Figure 2.** Degree of CEC contamination within the aquatic compartments across the studies analyzed in the BP. \* Contamination may vary significantly due to soil contamination.

The observed trend in CEC concentration depicted in Figure 2 is attributed to the pathway through which pollutants enter the environment (Figure 3).

The primary contributors to the release of industrial chemicals, hormones, pharmaceuticals, and personal care products into natural aquatic environments are wastewater treatment plants (WWTPs), from which the compounds are transported to the receiving surface water bodies and then to groundwater. These compounds enter wastewater primarily through various pathways related to human activities (Figure 3). Many of these compounds are used in households and are subsequently washed down drains or flushed down toilets. This includes pharmaceuticals (from medications), personal care products (e.g., shampoos, soaps, and cosmetics), and household cleaning agents. In addition, industrial facilities can release a variety of chemicals into wastewater through their manufacturing processes. These chemicals may include solvents, heavy metals, and other substances used in industrial processes. Similarly, hospitals, clinics, and research laboratories may discharge

pharmaceuticals and other chemicals directly into the wastewater system due to improper disposal practices or incomplete removal during treatment. Finally, rainfall can carry pollutants from urban areas (such as roadways, parking lots, and industrial sites) into storm drains that ultimately connect to wastewater treatment plants.



**Figure 3.** Pathway of CECs into the environment.

Once these compounds enter the wastewater system—whether from houses, hospitals, industries, agriculture, or other sources—they are transported to WWTPs. Conventional wastewater treatment plants are often not equipped to effectively remove all trace amounts of emerging contaminants. As a result, some of these compounds can still be detected in effluent discharged from treatment plants, which then enters surface water bodies (like rivers, lakes, or oceans) and can eventually impact groundwater through infiltration or surface water–groundwater interactions.

Conversely, numerous studies indicate the pervasive presence of pesticides on both groundwater and surface water. These compounds are frequently used in agriculture, which means direct use on the soil, and can be carried into nearby surface water bodies through runoff or leach into groundwater.

The atmosphere is also recognized as a potential origin for various volatile CECs. These substances enter the atmosphere through emissions, during manufacturing or incineration processes, and through volatilization from wastewater or surface water. Additionally, these compounds may return to aquatic compartments through precipitation.

Although a distinct pattern in the degree of CEC contamination in aquatic compartments is evident, the concentration of CECs may vary significantly according to the environmental compartment situation. In this sense, contamination by industrial activities, underground aquifers located close to sources of contamination (hospitals, industries), chemical accidents, and intensive agriculture, among other factors, may influence the distribution of CECs between environmental compartments.

#### 4.5. Future Research Directions

Taking into account the findings of the current study, several future research directions can be identified to address knowledge gaps and improve management strategies. Some potential areas for future research are the following:

- (i) Understanding the fate/transport of CECs: Research efforts should focus on improving the understanding of the fate and transport mechanisms of pollutants in different

- environmental compartments. This includes studying the processes of degradation, sorption, volatilization, and bioaccumulation to predict the behavior of contaminants in aquatic ecosystems more accurately;
- (ii) Monitoring and surveillance: There is a need for enhanced monitoring and surveillance programs to track the occurrence, distribution, and trends of CECs in aquatic environments. This includes developing sensitive analytical methods for detecting low concentrations of contaminants, establishing biomonitoring programs to assess exposure in aquatic organisms, and implementing integrated monitoring approaches to evaluate temporal and spatial variability;
  - (iii) Source identification and mitigation: Research should focus on identifying the primary sources of contaminants in aquatic ecosystems and implementing effective mitigation measures to reduce their input into the environment. This includes promoting best management practices in agriculture to minimize pesticide runoff, enhancing wastewater treatment technologies for the removal of pharmaceuticals and personal care products, and investigating green chemistry methods to minimize the production and utilization of hazardous industrial chemicals.

## 5. Conclusions

In this study, the occurrence of several contaminants of emerging concern in three different environmental compartments and their pathway were assessed and discussed. The presence of CECs in the environment has been continuously reported at low concentrations ( $\text{ng L}^{-1}$ – $\mu\text{g L}^{-1}$ ), and all the classes of CECs, within the studied ones, were detected in the three types of water compartment considered in this work (groundwater, surface water, and wastewater). Within the studies evaluated, industrial chemicals, hormones, pharmaceuticals, personal care products, and pesticides were detected in the range of 0.045–66, 0.0001–1.2, 0.04–6.9, 0.002–25, and 0.03–10.8  $\mu\text{g L}^{-1}$ , respectively.

Based on the information reported in the bibliographic portfolio and on the analysis of the detection of CECs in the three different environmental compartments, it was possible to infer that, apart from pesticides, the degree of contamination by CECs followed a sequence based on the aquatic compartment (GW < SW < WW). This observation is an interesting finding of the work that had not yet been reported in the literature considering the five classes of contaminants and the three selected environmental compartments. This phenomenon is attributed to the fact that the primary contributors to the release of industrial chemicals, hormones, pharmaceuticals, and personal care products into natural aquatic environments are wastewater treatment plants (WWTPs), from which the compounds are transported to the receiving surface water bodies and then to groundwater. On the other hand, pesticides are commonly utilized in agriculture, which means their direct use on the soil; thus, they can be carried into nearby surface water bodies through runoff or leaching into groundwater.

It is worth pointing out that although a clear trend was observed in the level of contamination by CECs according to the aquatic compartment, CECs concentration can vary significantly according to the environmental compartment situation. Therefore, research efforts should focus on improving our understanding of the fate and transport mechanisms of contaminants. This includes studying the processes of degradation, sorption, volatilization, and bioaccumulation to predict the behavior of contaminants in aquatic ecosystems more accurately.

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