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Nadia Morin-Crini
Eric Lichtfouse
Grégorio Crini *Editors*

Emerging Contaminants Vol. 1

Occurrence and Impact

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Editors

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Preface

Pollution is nothing but the resources we are not harvesting. We allow them to disperse because we've been ignorant of their value.

Buckminster Fuller

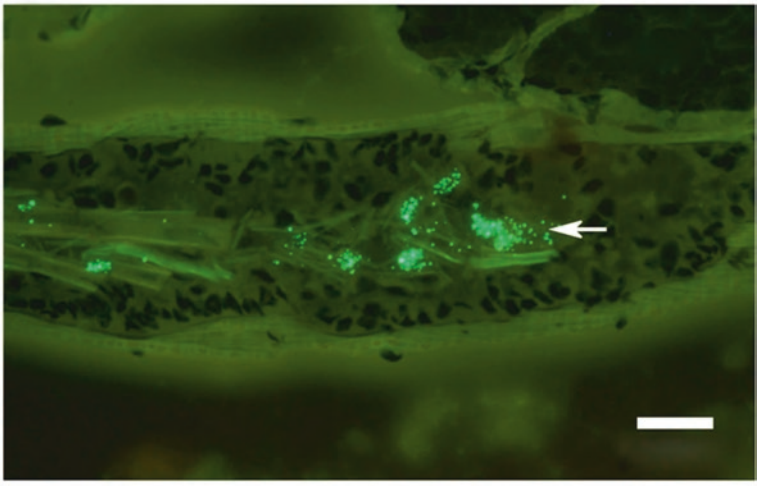

Figure. Fate of polyethylene beads and fragments after artificial ingestion by Antarctic krill, showing fragmentation and accumulation of beads in the midgut. White bar scale 50 μm. Reprinted from Dawson et al., Turning microplastics into nanoplastics through digestive fragmentation by Antarctic krill. Nature Communications 9, 1001 (2018). https://doi.org/10.1038/s41467-018-03465-9. Creative Commons CC BY

This book, entitled *Occurrence and Impact of Emerging Contaminants*, is the first volume on emerging contaminants published in the series Environmental Chemistry for a Sustainable World and written by 64 international contributors from 24 countries. In this volume, the chapters focus on the presence of emerging contaminants in the water compartment and their potential health effects.

The first chapter by Nadia Morin-Crini et al. summarizes the current state of knowledge on emerging contaminants, with focus on contaminants in aquatic systems. The second chapter by Anna Jurado et al. reviews the occurrence, fate, and associated risks of organic micropollutants included from the Watch List of the European groundwater bodies. Antimicrobial resistance is discussed in the next two chapters where Steffi Rocchi et al. disclose the emergence of pathogenic fungi resistant to triazole antifungal drugs in Chap. 3, and Charles P. Henriot et al. reveal the fate of antibiotic-resistant bacteria in the environment. In the last chapter, Ewa Konduracka and Paweł Rostoff discuss the relationship between outdoor air pollution and cardiovascular disorders in Chap. 5. The second volume focuses on methods for remediation of emerging contaminants.

The editors extend their thanks to all the authors who contributed to this book for their efforts in producing timely and high-quality chapters. The creation of this book would not have been possible without the assistance of several colleagues and friends deserving acknowledgment. They have helped by choosing contributors and reviewing chapters and in many other ways. Finally, we would like to thank the staff of Springer Nature for their highly professional editing of the publication.

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Abbreviations

ACE	acetamiprid
ADI	acceptable daily intake
AMX	amoxicillin
ARB	antibiotic-resistant bacteria
ARG	antibiotic resistance gene
AZY	azithromycin
BOD	biological oxygen demand
BPA	bisphenol A
BW	body weight
C_{max}	maximum concentration
CFU	colony-forming unit
CI	confidence interval
CIMT	carotid intima-media thickness
CIP	ciprofloxacin
CLA	clarithromycin
CLO	clothianidin
COD	chemical oxygen demand
D_{ow}	pH-dependent *n*-octanol-water distribution ratio
DDT	dichlorodiphenyltrichloroethane
DT_{50}	soil half-life
DWELs	drinking water equivalent levels
DWI	drinking water intake
E1	estrone
E2	17-beta-estradiol
EC	European Commission
EC_{50}	half-maximal effective concentration
EE2	17-alpha-ethinylestradiol
ERY	erythromycin
ESBL	extended-spectrum β-lactamase
FD	frequency of detection
GC-MS	gas chromatography coupled with mass spectrometry

GUS	groundwater ubiquity score
HPLC	high-performance liquid chromatography
HPLC-UV	high-performance liquid chromatography with UV detection
HQ	hazard quotient
HR	hazard ratio
IMD	imidacloprid
IQR	interquartile range
ISPRA	Italian National Institute for Environmental Protection and Research
K_{oc}	partition coefficient between soil organic carbon and water
K_{ow}	n-octanol-water partition coefficient
LC-MS/MS	liquid chromatography coupled with (tandem) mass spectrometry
LC_{50}	lethal concentration that kills 50% of the test animals during an observation period
LOD	limit of detection
LOQ	limit of quantification
LS	light source
MEC	measured environmental concentrations
MET	methiocarb
MFM	metaflumizone
n.d.	not detected
Non-STEMI	myocardial infarction without ST-segment elevation
OR	odds ratio
pK_a	the negative base-10 logarithm of the acid dissociation constant (K_a) of a solution
PM	particulate matter
PM_{10}	coarse particulate matter
$PM_{2.5}$	fine particulate matter
$PM_{0.1}$	ultrafine particulate matter
PNEC	predicted no-effect concentration
RQ	risk quotient
RR	removal rate
RR	relative risk
SCE	saturated calomel electrode
S_w	water solubility
SHE	standard hydrogen electrode
SS	stainless steel
STEMI	ST-segment elevation myocardial infarction
THI	thiacloprid
TMX	thiamethoxam
TOC	total organic carbon
VBNC	viable but non-culturable
WWTP	wastewater treatment plant

Chapter 1
Emerging Contaminants: Analysis, Aquatic Compartments and Water Pollution

Nadia Morin-Crini, Eric Lichtfouse, Guorui Liu, Vysetti Balaram, Ana Rita Lado Ribeiro, Zhijiang Lu, Friederike Stock, Eric Carmona, Margarida Ribau Teixeira, Lorenzo A. Picos-Corrales, Juan Carlos Moreno-Piraján, Liliana Giraldo, Cui Li, Abhishek Pandey, Didier Hocquet, Giangiacomo Torri, and Grégorio Crini

Abstract Over the past two decades, the presence of so-called emerging contaminants in various environmental compartments around the world, such as water, sediments, soils and atmosphere, and in a wide variety of consumer products has become a major concern for society, public health authorities, industry (namely food industry and water sector) and the agricultural sector. Some of these substances are endocrine disruptors and others are proven carcinogens and mutagens. In particular,

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there is a growing concern about the presence of emerging contaminants in water resources.

The list of substances and products is particularly long: pesticides, pharmaceuticals, drugs of abuse (including licit and illicit drugs), cosmetics, personal care products, surfactants, cleaning products, industrial formulations and chemicals, food additives, food packaging, metalloids, rare earth elements, nanomaterials, microplastics and pathogens. Most of these substances are found not only in domestic wastewater and industrial discharges, but also in surface and ground water, and consequently in drinking water and food sources. Therefore, emerging contaminants entering the aquatic compartment may cause known, unknown or suspected

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adverse effects on the ecosystems and/or human health. Many molecules have been classified in recent years as priority or priority hazardous substances, and thus, the industrial world and the municipal wastewater treatment plants are particularly concerned by the release of these substances by virtue of increasingly strict regulations. However, existing conventional municipal wastewater treatment plants and drinking water treatment plants were not designed for eliminating these new contaminants. In addition, most emerging contaminants are not yet routinely monitored either in industrial discharges or in the environment. From an academic point of view, emerging substances are also of great interest to the scientific community and receive special attention. The areas of research concern not only their effects on human health and their impact on environment, but also their sources, analysis and fate in the environment, as well as their remediation. Indeed, their behavior in the environment and their effects on all living organisms remain largely unknown. Many substances are difficult to remove by conventional water treatment processes. Thus, there is an intense research activity on all these topics.

The objective of this chapter is to present a recent state of knowledge on emerging substances and their presence in the aquatic environment. After general considerations on emerging contaminants, the first part is focused on chromatographic methods coupled to mass spectrometry for their analysis and detection, and on detection of microplastics in water and sediment. The presence of alkylphenols, rare earth elements and nanoparticles in the aquatic environment is then discussed. Finally, examples of contamination described from around the world, from China to Portugal, Mexico, Colombia and Brazil, are presented.

Keywords Emerging contaminants · Substances of global concern · Pharmaceuticals · Personal care products · Pesticides · Alkylphenols · Persistent organic pollutants · Microplastics · Rare earth elements · Nanoparticles · Biological agents · Analysis · Water pollution · Aquatic compartments

1.1 Introduction

Although water quality problems are largely associated with developing countries, they also persist in developed countries and include, for example, the loss of pristine water bodies, impacts related to changes in hydromorphology, the spread of invasive species, the loss of biodiversity, and the increasing occurrence of chemical substances (Morin-Crini and Crini 2017). The water quality problems are intimately linked to human activities, whether domestic, agricultural or industrial. Indeed, population growth, agricultural intensification, rapid urbanization, increased industrial production and climate change are beginning to impact on Nature's ability to provide safe and clean water for our essential uses and functions. One of the most important global environmental problems is water pollution by chemicals (Aristizabal-Ciro et al. 2017; Hernández-Padilla et al. 2017; Morin-Crini and Crini

2017; Botero-Coy et al. 2018; Crini and Lichtfouse 2018; Dong et al. 2018; Díaz-Casallas et al. 2019; Gallego-Schmid and Tarpani 2019; Kumar et al. 2019; Reichert et al. 2019; Deviller et al. 2020). We are all concerned about this problem and the anthropogenic sources are well-know, namely domestic discharges, hospital effluents, industrial wastewaters, runoff from agriculture, livestock and aquaculture, and landfill leachates. It is recognized that, due to insufficient chemical treatment abatement, the discharge of effluents from municipal wastewater treatment plants is an important route for the appearance of chemical substances such as pharmaceuticals in the aquatic environment (Hernández-Padilla et al. 2017; Botero-Coy et al. 2018; Crini and Lichtfouse 2018; Gallego-Schmid and Tarpani 2019; Inyinbor et al. 2019; Mohapatra and Kirpalani 2019; Patel et al. 2019).

Many chemical substances such as metals, dyes, phenols, pesticides, pharmaceuticals and other so-called emerging contaminants are indeed part of our daily lives as they are used in a wide variety of products and applications. For example, they are ubiquitously in every household: in food, energy drinks, medicines, household and cleaning products, personal care products, and cosmetics, paints, electronics and computers, furniture and even our clothes (Puzyn and Mostrag-Szlichtyng 2012; Mortimer 2013; Schrenk and Chopra 2013; Duedahl-Olesen 2013; Juliano and Magrini 2017). The vast majority of chemicals, called contaminants or pollutants depending on their toxicity and impact (Chapman 2007), end up in our discharges of wastewater treatment plants and ultimately in the aquatic compartments of the environment such as rivers, lakes, coastal and marine ecosystems, seawater and ice caps (Crini and Badot 2007, 2010; Kosma et al. 2014; Gee et al. 2015; Archer et al. 2017; Ebele et al. 2017; Peña-Guzmán et al. 2019; Xu et al. 2019). As a result, chemicals can be found not only in surface water and freshwater, but also in groundwater, which is the main source of drinking water in many countries (Dévier et al. 2013; Gee et al. 2015). The presence of chemicals in general, and particularly emerging substances, in water is a cause of concern and debate, as the risk they pose to human health and the environment is not yet fully understood. Biological agents are also widely found in the environment. They include bacteria, viruses, fungi (yeasts, molds) and parasites. The majority of these agents are harmless, but some may have potential to cause ill health. The bibliography on emerging chemical and biological contaminants is particularly abundant and many topics are of interest to the scientific community (Table 1.1). In particular, the presence, occurrence, transport of emerging contaminants in the water resources and their impact on water quality are documented in thousands of publications reported worldwide during the last two decades, demonstrating an increasing concern about them.

Due to their widespread use in our daily applications, chemicals are ubiquitous not only in water and sediments, but also in soils and the atmosphere, at concentrations between few ng/L and several µg/L (Salthammer 2014, 2020; Patel et al. 2019). In recent decades, thanks to significant advances in the analysis and detection of trace contaminants, emerging contaminants have also been detected in plants (due to soil and water pollution), food products, living organisms and protected species (*e.g.*, birds, polar bears), even in areas where there is no human activity (Datta et al. 2018; Routti et al. 2019). This demonstrates their uncontrolled

Table 1.1 Selected comprehensive reviews and papers on emerging contaminants published in the last five years

General topic	References
Alkylphenols	Careghini et al. 2015; Crini et al. 2016; Tuan Omar et al. 2016; Chokwe et al. 2017; Deshayes et al. 2017; Priac et al. 2017; Acir and Guenther 2018; Salgueiro-Gonzalez et al. 2017; Zaytseva and Medvedeva 2019; Olaniyan et al. 2020; Vargas-Berrones et al. 2020a, b
Aquatic toxicity	Harmon 2015; Priac et al. 2017; Acir and Guenther 2018; Koba et al. 2018; Lin et al. 2018a; Mearns et al. 2018; Mezzelani et al. 2018; Salgueiro-Gonzalez et al. 2018; de Marchi et al. 2019; Fekadu et al. 2019; Li et al. 2019b; Patel et al. 2019; Olaniyan et al. 2020
Aquifer	Moreau et al. 2019; Burri et al. 2019; Kurwadkar 2019; Daesslé et al. 2020; Sackaria and Elango 2020
Analysis	Lu and Gan 2014a; Gago-Ferrero et al. 2015; Löder and Gerdts 2015; Bijlsma et al. 2016; Jardak et al. 2016; Tuan Omar et al. 2016; Priac et al. 2017; Salgueiro-Gonzalez et al. 2017, 2018; Acir and Guenther 2018; Botero-Coy et al. 2018; Lorenzo et al. 2018; Patel et al. 2019; Sousa et al. 2019; de Oliveira et al. 2020; Kovalakova et al. 2020
Antibiotics	Botero-Coy et al. 2018; Dong et al. 2018; Gogoi et al. 2018; Mezzelani et al. 2018; Fekadu et al. 2019; Jurado et al. 2019; Kumar et al. 2019; Ng et al. 2019; Reichert et al. 2019; García et al. 2020; Khan et al. 2020; Patel et al. 2020; Wang and Zhuan 2020
Antibiotic resistance	Zad et al. 2018; Zhao et al. 2018; Kumar et al. 2019; Liu et al. 2019; Ng et al. 2019; Reichert et al. 2019; García et al. 2020
Behavior	Jardak et al. 2016; Ebele et al. 2017; Mearns et al. 2018; Li et al. 2019a; Houde et al. 2019; de Marchi et al. 2019; Patel et al. 2019; Starling et al. 2019; Yu et al. 2019
Bioaccumulation	Tuan Omar et al. 2016; Ebele et al. 2017; Damkjaer et al. 2018; Herrera-Melian et al. 2018; Jiang et al. 2018; Mauricio et al. 2018; Mearns et al. 2018; Mezzelani et al. 2018; Salgueiro-Gonzalez et al. 2018; Wang et al. 2018b; Houde et al. 2019; Patel et al. 2019; Xu et al. 2020
Biodegradation	Lu and Gan 2014a, b; Ebele et al. 2017; Couto et al. 2019; Cao et al. 2020; de Oliveira et al. 2020
Biomagnification	Mearns et al. 2018, 2019
Bisphenol A	Machado et al. 2016; Gogoi et al. 2018; Zhao et al. 2018; Xiao et al. 2020
Caffeine	Machado et al. 2016; Sodré et al. 2018; Montagner et al. 2019; Anastopoulos et al. 2020; Rigueto et al. 2020
Cosmetics	Juliano and Magrini 2017; Li et al. 2018a; Caldas et al. 2019
Disinfection by-products	Benitez et al. 2015; Nika et al. 2016; Zad et al. 2018; Gao et al. 2019; Ng et al. 2019; Khan et al. 2020
Drinking water	Gee et al. 2015; Hamza et al. 2016; Machado et al. 2016; Gwenzi et al. 2018; Sodré et al. 2018; Caldas et al. 2019; Gao et al. 2019; Patel et al. 2019; Starling et al. 2019; Iroegbu et al. 2020; Sousa et al. 2020
Ecotoxicology	Petrie et al. 2015; Cavalheiro et al. 2017; Kumar et al. 2019; Li et al. 2019b; Patel et al. 2019; Starling et al. 2019; Xu et al. 2019

(continued)

Table 1.1 (continued)

General topic	References
Ecological risk assessment	Gwenzi et al. 2018; Matich et al. 2019; Mezzelani et al. 2018; Pedrazzani et al. 2019; Xu et al. 2019
Endocrine disrupting compounds	Różalska et al. 2015; Ma et al. 2016; Murdoch and Sanin 2016; Tuan Omar et al. 2016; Archer et al. 2017; Acir and Guenther 2018; Dong et al. 2018; Gogoi et al. 2018; Liu et al. 2019; Ng et al. 2019; Olaniyan et al. 2020; Patel et al. 2020
Environmental fate	Cavalheiro et al. 2017; Monneret 2017; Priac et al. 2017; Archundia et al. 2018; Koumaki et al. 2018; Reichert et al. 2019; Yu et al. 2019
Exposure pathways	Chokwe et al. 2017; Koba et al. 2018; Mearns et al. 2018; Li et al. 2019b; Routti et al. 2019; Wu et al. 2020b; Xiao et al. 2020
Fate	Eggen and Vogelsang 2015; Katsigiannis et al. 2015; Noutsopoulos et al. 2015; Carr et al. 2016; Archer et al. 2017; Cavalheiro et al. 2017; Ebele et al. 2017; Datta et al. 2018; Gogoi et al. 2018; Zad et al. 2018; Zhao et al. 2018; Couto et al. 2019; de Marchi et al. 2019; Jurado et al. 2019; Mohapatra and Kirpalani 2019; Ng et al. 2019; Routti et al. 2019; Starling et al. 2019
Flame retardants	Hamza et al. 2016; Lin et al. 2018a; Zhao et al. 2018; Llompart et al. 2019; Li et al. 2019a; Peña-Guzmán et al. 2019; Tongue et al. 2019; Wang et al. 2020; Wu et al. 2020b; Zhou et al. 2020; Zuiderveen et al. 2020
Food additives	Careghini et al. 2015; Moreau et al. 2019; Peña-Guzmán et al. 2019
Hormones	Barbosa et al. 2016; Gogoi et al. 2018; Mezzelani et al. 2018; Zad et al. 2018; Fekadu et al. 2019; Montagner et al. 2019; Ng et al. 2019; Peña-Guzmán et al. 2019; Sousa et al. 2019
Illicit drugs	Bijlsma et al. 2016; Archer et al. 2017; Ng et al. 2019; Peña-Guzmán et al. 2019
Indoor pollutants	Salthammer 2014, 2020; Cretescu et al. 2019
Industrial wastewater	Petrie et al. 2015; Jardak et al. 2016; Archer et al. 2017; Chokwe et al. 2017; Priac et al. 2017; Botero-Coy et al. 2018; Dong et al. 2018; Montagner et al. 2019; Moreau et al. 2019; Ng et al. 2019; Patel et al. 2019; Peña-Guzmán et al. 2019; Tolboom et al. 2019; Zhang et al. 2019; Daesslé et al. 2020
Life cycle assessment	Gallego-Schmid and Tarpani 2019
Marine organisms	Lin et al. 2018a; Mearns et al. 2018, 2019
Metabolites	Petrie et al. 2015; Acir and Guenther 2018; Koba et al. 2018; Patel et al. 2019
Metabolomics	Matich et al. 2019
Microplastics	Löder and Gerdts 2015; Oberbeckmann et al. 2015; Thompson 2015; Carr et al. 2016; Avio et al. 2017; Juliano and Magrini 2017; Barboza et al. 2018; Datta et al. 2018; Lambert and Wagner 2018; Li et al. 2018b; Lin et al. 2018a; Wagner and Lambert 2018; Zad et al. 2018; da Costa et al. 2019; Guo and Wang 2019; Mishra et al. 2019; Ng et al. 2019; Prata et al. 2019; Stock et al. 2019; Amato-Lourenço et al. 2020; Guo et al. 2020; Iroegbu et al. 2020; Kumar et al. 2020; Möller et al. 2020; Tiwari et al. 2020; Wong et al. 2020; Xu et al. 2020

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Table 1.1 (continued)

General topic	References
Modeling	Wang et al. 2016c; Petrie et al. 2015; Peng et al. 2018; Li et al. 2019b; Moreau et al. 2019; Noutsopoulos et al. 2019; Sousa et al. 2019; Daesslé et al. 2020; Gibson 2020
Monitoring	Priac et al. 2017; Mearns et al. 2018; Sousa et al. 2018, 2019; Montagner et al. 2019; Moreau et al. 2019; Peña-Guzmán et al. 2019; Gibson 2020; Patel et al. 2020
Municipal wastewater	Bijlsma et al. 2016; Archer et al. 2017; Cavalheiro et al. 2017; Deshayes et al. 2017; Chokwe et al. 2017; Ebele et al. 2017; Hernández-Padilla et al. 2017; Priac et al. 2017; Dong et al. 2018; Gogoi et al. 2018; Gallego-Schmid and Tarpani 2019; Montagner et al. 2019; Peña-Guzmán et al. 2019; Starling et al. 2019
Nanoparticles/ nanomaterials	Hamza et al. 2016; Mearns et al. 2018; Zhao et al. 2018; de Marchi et al. 2019; Matich et al. 2019; Sousa and Teixeira 2020
Occurrence	Kosma et al. 2014; Annamalai and Namasivayam 2015; Careghini et al. 2015; Eggen and Vogelsang 2015; Hao et al. 2015; Petrie et al. 2015; Barbosa et al. 2016; Jardak et al. 2016; Hamza et al. 2016; Liu et al. 2016; Xu et al. 2016; Cavalheiro et al. 2017; Chokwe et al. 2017; Ebele et al. 2017; Priac et al. 2017; Acir and Guenther 2018; Amin et al. 2018; Botero-Coy et al. 2018; Gogoi et al. 2018; Herrera-Melian et al. 2018; Mezzelani et al. 2018; Zhao et al. 2018; Couto et al. 2019; Fekadu et al. 2019; Gao et al. 2019; Jurado et al. 2019; Li et al. 2019b; Patel et al. 2019; Ng et al. 2019; Starling et al. 2019; Xu et al. 2019; Yu et al. 2019; Xu et al. 2020
Pathogens	Ng et al. 2019
Parabens	Juliano and Magrini 2017; Mearns et al. 2018; Caldas et al. 2019; Salthammer 2020
Pesticides	Barbosa et al. 2015; Hamza et al. 2016; Machado et al. 2016; Dong et al. 2018; Mearns et al. 2018; Sodré et al. 2018; Caldas et al. 2019; Houde et al. 2019; Montagner et al. 2019; Moreau et al. 2019; Ng et al. 2019; Xu et al. 2019; Patel et al. 2020
Persistence	Ebele et al. 2017; Priac et al. 2017; Mezzelani et al. 2018; Houde et al. 2019; Li et al. 2019a; Gibson 2020
Persistent organic pollutants	Eggen and Vogelsang 2015; Harmon 2015; Kallenborn et al. 2015; Zeng 2015; Hamza et al. 2016
Personal care products	Eggen and Vogelsang 2015; Archer et al. 2017; Aristizabal-Ciro et al. 2017; Ebele et al. 2017; Juliano and Magrini 2017; Dong et al. 2018; Gogoi et al. 2018; Li et al. 2018a; Caldas et al. 2019; Liu et al. 2019; Moreau et al. 2019; Ng et al. 2019; Peña-Guzmán et al. 2019; Xu et al. 2019; Patel et al. 2020
Pharmaceuticals	Eggen and Vogelsang 2015; Tuan Omar et al. 2016; Roberts et al. 2016; Archer et al. 2017; Aristizabal-Ciro et al. 2017; Ebele et al. 2017; Botero-Coy et al. 2018; Dong et al. 2018; Gogoi et al. 2018; Koba et al. 2018; Mezzelani et al. 2018; Couto et al. 2019; Fekadu et al. 2019; Li et al. 2019b; Liu et al. 2019; Moreau et al. 2019; Ng et al. 2019; Peña-Guzmán et al. 2019; Xu et al. 2019; Yu et al. 2019; Patel et al. 2019, 2020

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Table 1.1 (continued)

General topic	References
Plasticizers	Llompart et al. 2019; Patel et al. 2020; Salthammer 2020; Wang et al. 2020
Perfluoroalkyl substances/ Polyfluoroalkyl compounds	DeWitt 2015; Xiao 2017; Dong et al. 2018; Lorenzo et al. 2018; Brusseau 2019; Klemes et al. 2019; Ng et al. 2019; Pan et al. 2020; Salthammer 2020
Radionuclides	Mearns et al. 2018; Zhang et al. 2019
Rare earth elements	Gwenzi et al. 2018; Mubashir 2018; Balaram 2019; Salthammer 2020
Reclaimed water	Gilabert-Alarcón et al. 2018; Sodré et al. 2018
Regulation	Barbosa et al. 2016; Acir and Guenther 2018; Dulio et al. 2018; Mearns et al. 2018; Jurado et al. 2019; Lapworth et al. 2019; Patel et al. 2019; Sousa et al. 2019
Remediation	Barbosa et al. 2016; Hamza et al. 2016; Jardak et al. 2016; Priac et al. 2017; Crini and Lichtfouse 2018; Ma et al. 2018; Couto et al. 2019; Crini et al. 2019; Kumar et al. 2019; Llompart et al. 2019; Liu et al. 2019; Patel et al. 2019, 2020; Serna-Galvis et al. 2019; Tolboom et al. 2019; Zaytseva and Medvedeva 2019; Zhang et al. 2019; Dhangar and Kumar 2020; Godage and Gionfriddo 2020; Khan et al. 2020; Mautner 2020; Pesqueira et al. 2020; Rasheed et al. 2020; Vara and Karnena 2020; Wang and Zhuan 2020; Yadav et al. 2020; Zaied et al. 2020
Risk assessment	Thomaidi et al. 2015; Osorio et al. 2016; Archer et al. 2017; Tahar et al. 2017; Gwenzi et al. 2018; Mearns et al. 2018; Mezzelani et al. 2018; Sodré et al. 2018; Jurado et al. 2019; Montagner et al. 2019; Patel et al. 2019; Pedrazzani et al. 2019; Xu et al. 2019; Wang et al. 2020
Sediments	Careghini et al. 2015; Petrie et al. 2015; Yang et al. 2015; Bradley et al. 2016; Jin and Zhu 2016; Ebele et al. 2017; Koumaki et al. 2017; Koba et al. 2018; Mearns et al. 2018; Salgueiro-Gonzalez et al. 2018; Li et al. 2019a; Stock et al. 2019
Soils	Careghini et al. 2015; Guo et al. 2020
Sources	Thompson 2015; Jardak et al. 2016; Chokwe et al. 2017; Deshayes et al. 2017; Sodré et al. 2018; Gogoi et al. 2018; Mezzelani et al. 2018; Patel et al. 2019
Surfactants	Hamza et al. 2016; Jardak et al. 2016; Xiao 2017; Llompart et al. 2019; Patel et al. 2020
Toxicity	Lu and Gan 2014a; Harmon 2015; Chokwe et al. 2017; Ebele et al. 2017; Priac et al. 2017; Acir and Guenther 2018; Guo et al. 2020; Olaniyan et al. 2020; Xiao et al. 2020
Tracers	Mearns et al. 2018; Moreau et al. 2019
Transport	Kallenborn et al. 2015; Ebele et al. 2017; Datta et al. 2018; Koba et al. 2018; Mearns et al. 2018; Zhao et al. 2018; Li et al. 2019b; Patel et al. 2019; Yu et al. 2019
Triclosan	Kosma et al. 2014; Juliano and Magrini 2017; Machado et al. 2016; Montagner et al. 2019
UV filters	Juliano and Magrini 2017; Mearns et al. 2018; Jurado et al. 2019; Peña-Guzmán et al. 2019; Sousa et al. 2019

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Table 1.1 (continued)

General topic	References
Wastewater treatment plants	Kosma et al. 2014; Hamza et al. 2016; Carr et al. 2016; Bijlsma et al. 2016; Archer et al. 2017; Hernández-Padilla et al. 2017; Botero-Coy et al. 2018; Gallego-Schmid and Tarpani 2019; Inyinbor et al. 2019; Mohapatra and Kirpalani 2019; Patel et al. 2019
Water compartment	Careghini et al. 2015; Koumaki et al. 2015; Machado et al. 2016; Archer et al. 2017; Aristizabal-Ciro et al. 2017; Ebele et al. 2017; Dong et al. 2018; Datta et al. 2018; Burri et al. 2019; Fekadu et al. 2019; Kurwadkar 2019; Li et al. 2019a; Montagner et al. 2019; Moreau et al. 2019; Peña-Guzmán et al. 2019; Starling et al. 2019; Stock et al. 2019; Xu et al. 2019; Daesslé et al. 2020; Kroon et al. 2020; Sackaria and Elango 2020; Wong et al. 2020
Water quality	Aristizabal-Ciro et al. 2017; Hernández-Padilla et al. 2017; Botero-Coy et al. 2018; Dong et al. 2018; Díaz-Casallas et al. 2019; Gallego-Schmid and Tarpani 2019; Kumar et al. 2019; Reichert et al. 2019; Deviller et al. 2020
Water management	Díaz-Casallas et al. 2019; Gilabert-Alarcón et al. 2018
Water reuse	Dulio et al. 2018; Ma et al. 2018; Sodré et al. 2018; Inyinbor et al. 2019; Deviller et al. 2020

movement in the global environment. Indeed, the issue of contaminants/pollutants and their impact on the environment (especially on water quality), society and human health is common to the entire World, making it a global concern at the present time. However, concentration levels are extremely variable from one continent to another, from one country to another and even from one region to another. Recently, Fekadu et al. (2019), comparing levels of contamination of pharmaceuticals such as carbamazepine and sulfamethoxazole in surface waters between Africa and Europe, observed that the maximum concentrations reported in Africa were 20,000 times higher than in Europe. The authors indicated that the variation in the consumption of pharmaceuticals, the partial removal of substances in wastewater treatment plants and the direct discharge of wastewater from livestock farms are among the reasons that may explain the observed differences (Fekadu et al. 2019). Other studies showed a correlation between the presence of emerging substances in the aquatic environment and discharges from wastewater treatment plants (Stackelberg et al. 2007; Kasprzyk-Hordern et al. 2008; Watkinson et al. 2009; Ort et al. 2010; Basile et al. 2011; Gonzalez et al. 2012; Machado et al. 2016; Priac et al. 2017; Gilabert-Alarcón et al. 2018; Mezzelani et al. 2018).

The vast majority of the anthropogenic substances are currently not regulated and some have been regulated only recently, namely certain pesticides and alkylphenols known as endocrine disruptors or endocrine-disrupting chemicals (Daughton 2004; Lu and Gan 2014a; Gee et al. 2015; Petrie et al. 2015; Barbosa et al. 2016; Morin-Crini and Crini 2017; Jurado et al. 2019; Sousa et al. 2019). For example, paraquat, an herbicide used worldwide since the 1960s that caused severe and fatal poisonings, was banned in the European Union in 2003 and withdrawn from the market in 2007. Another example is the organochlorine insecticide

chlordecone, introduced in 1958 and banned in 1978 in the US and in the early 1993 in the French West Indies (Rana et al. 2016). In 2000, a first list of 33 priority substances (several pesticides, the phthalate di(2-ethylhexyl)-phthalate, octylphenol, nonylphenol, solvents, among others) was established as a control measure for the next 15 years based on their significant risk to or *via* the aquatic environment (European Water Framework Directive 2000/60/EC; Decision 2455/2001/EC). In 2008, the Directive 2008/105/EC layed down the environmental quality standards (EQS) for the priority substances and certain other pollutants. Moreover, other groups of substances were also targeted to be reviewed for possible future prioritization (*e.g.*, bisphenol A, musk xylene, perfluorooctane sulphonic acid, dioxins, polychlorinated biphenyls), and in fact some of them were later included in the list of priority substances by Directive 2013/39/EU, which enlisted 45 priority subtances or group of substances. Additionally, this Directive preconized the launch of the first Watch List and recommended to include diclofenac, 17-β-estradiol and 17-α-ethinylestradiol. The non-steroidal anti-inflammatory drug diclofenac is often detected in European municipal wastewater treatment plants influents and effluents, surface water and groundwater. The first complete European watch list of substances of emerging concern (European Decision 2015/495/EU of 20 March 2015) was launched in 2015 and included three hormones (17-α-ethinylestradiol, 17-β-estradiol and estrone), four pharmaceuticals (diclofenac, azithromycin, clarithromycin and erythromycin), eight pesticides (methiocarb, oxadiazon, imidacloprid, thiacloprid, thiamethoxam, clothianidin, acetamiprid and triallate), a UV filter (2-ethylhexyl-4-methoxycinnamate) and an antioxidant (2,6-di-*tert*-butyl-4-methylphenol) commonly used as food additive (Morin-Crini and Crini 2017). This list is dynamic and the latest update was published in 2018 (*e.g.*, with the European Decision 2018/840/EU), by removing tri-allate, oxadiazon, 2,6-di-*tert*-butyl-4-methylphenol and diclofenac (due to the sufficient high-quality monitoring data already available, according to the Decision), as well as 2-ethylhexyl-4-methoxycinnamate (since data is needed for sediment rather than water), and by adding 3 candidates: the insecticide metaflumizone, and the antibiotics amoxicillin and ciprofloxacin. Recently, the substances propiconazole and 4-nonylphenol were banned in Europe in November 2018 and July 2019, respectively. Indeed, from a regulatory point of view, the situation is constantly evolving (Barbosa et al. 2016; Jurado et al. 2019; Sousa et al. 2019). The chronicle of European science, policy and legislation to develop a groundwater monitoring list can be found in the review by Lapworth et al. (2019). Water contamination by pesticides, pharmaceuticals and industrial chemicals has become a global environmental and health crisis (Morin-Crini and Crini 2017; Crini and Lichtfouse 2018; Patel et al. 2019; Tolboom et al. 2019). There is also a mobilization of the global scientific community on all subjects concerning emerging substances, from their analysis to their removal, their behavior in the environment and their impact on health (Table 1.1).

The objective of this chapter is to present a recent state of knowledge on emerging substances, considering several aspects presented in three parts. After general considerations on emerging contaminants, the first part is devoted to analysis and detection of emerging substances with the presentation of chromatographic

methods coupled to mass spectrometry for their analysis and detection. The detection of microplastics in water and sediments is also discussed. The second part of this chapter presents the occurrence, fate and toxicity of alkylphenols, rare earth elements and nanoparticles in the aquatic environment. The third part presents selected examples of contamination described from around the world, from China to Portugal, and Latin America.

1.2 General Considerations on Emerging Contaminants

1.2.1 Contamination and Pollution

Contamination/Pollution arises from all sectors of human activity, and is due to natural (petroleum, minerals, etc.) and anthropogenic causes (*e.g.*, sewage treatment sludge or persistent organic pollutants produced by waste incineration) and especially to synthetic substances produced by chemical industries (*e.g.*, dyes, fertilizers, pesticides, and so on). The terms contamination/pollution and contaminant/pollutant are often used in relation to subjects like environment, food and medicine (Crini and Badot 2007, 2010; Morin-Crini and Crini 2017). Both contaminant and pollutant refer to undesirable or unwanted substances. Pollutant refers to a harmful substance but contaminant is not necessarily harmful since contamination refers simply to the presence of a chemical substance where it should not be. This means that all pollutants are contaminants, but not all contaminants are pollutants. In this chapter, both these terms were used.

1.2.2 What Is an Emerging Contaminant?

A chemical pollutant is a substance toxic for flora, fauna and for humans, and present at concentrations such that, in Nature, has repercussions for the environment and/or on health in general (Crini and Badot 2007, 2010; Sauvé and Desrosiers 2014; Harmon 2015). Examples of pollutants/micropollutants known to the public are various, including nitrates, phosphates, pesticides such as glyphosate or atrazine, detergents (cleaning products), metals, dyes, pharmaceuticals such as diclofenac or ibuprofen, licit drugs (caffeine 1,3,7-trimethyl-3-7-dihydro-1H-purine-2,6-dione), illicit drugs (cocaine, amphetamines), synthetic (17-α-ethinylestradiol) and natural (17-β-estradiol) hormones, cosmetics and personal care products (parabens, triclosan, sunscreens and UV filters, domestic biocides, disinfectants), food derivatives and additives (nitrites, caffeine, artificial sweeteners), food packaging and containers (phthalates, other plasticizers), industrial substances (bisphenol A, surfactants, chlorinated solvents such as trichloroethylene, disinfection products, biocides, lubricants, silicones,

substances used in nonstick materials, ingredients used in paints), microbial pathogens, indoor pollutants, etc. Other substances, that are less known by the public, are considered substances of concern: estrogens (estriol), pesticides less known by the public but widely used such as methiocarb, triallate and oxadiazon, neonicotinoids (insecticides), 2,6-di-*tert*-butyl-4-methylphenol (anti-oxidant), UV filter (2-ethylhexyl-4-methoxycinnamate), macrolide antibiotics used in veterinary medicine and aquaculture, volatile organic compounds, polycyclic aromatic hydrocarbons, polychlorinated biphenyls, bromine-containing flame-retardants, perfluorinated compounds and perfluorinated alkyl substances, polybrominated diphenyl ethers, alkylphenols and alkylphenol polyethoxylates, rare earth elements, radionuclides, metalloids such as selenium, and many more (Kolpin et al. 2002; Daughton 2004; Tijani et al. 2016). The public is also increasingly aware of so-called emerging substances: antibiotics, analgesics, hormones and other drugs (anti-inflammatory, antidiabetic, antiepileptic), nanoparticles, bioterrorism and sabotage agents, and pathogens (cyanotoxins or algal toxins, mycotoxins, antibiotic-resistant organisms, etc.). The list of emerging substances and products is therefore particularly long (Tijani et al. 2016) and is also of great interest to the scientific community (Table 1.1).

The term "emerging contaminants/pollutants" refers primarily to those for which there are currently no regulations requiring monitoring or public reporting of their presence in our water supply or wastewaters. The US Environmental Protection Agency (EPA) defines an emerging pollutant as "a chemical or material which because of a recent source that it originates, or because of a new pathway that has developed, and for which a lack of published health standards exist poses a perceived, potential, or real threat to the human health or the environment" (source: US EPA 2012, Washington, DC). Their occurrence results from point (urban and industry) or diffuse (agriculture) contamination/pollution sources. Various other terms and definitions can be found in the literature. Indeed, there is no generally accepted definition, each definition and interpretation depending on the respective perspective and/or objective (Morin-Crini and Crini 2017; Salthammer 2020). In Europe, the term contaminant of emerging concern is a common term for chemicals that are currently not regulated (not submitted to a routine monitoring and/or emission control regime) but may be under scrutiny for future regulation (Dulio et al. 2018).

In the bibliography, there are several terms to denote emerging contaminants almost interchangeably such as emerging organic contaminants, emerging substances, substances of emerging concern, contaminants of emerging concern, emerging pollutants, emerging micropollutants and other similar terminologies (trace organic contaminants, micropollutants, trace organic compounds, trace pollutants, constituents of emerging concern, xenobiotic organic compounds, etc.). However, it is important to point out that all emerging pollutants are emerging contaminants, but not all emerging contaminants are emerging pollutants. This is often confuse in the literature. There are also terms that refer to subsets of emerging substances. All of these terms refer to many different types of chemicals, such as pharmaceuticals and drugs (medicines, non-prescription drugs, endocrine disrupting compounds), personal care products and cosmetics (soaps, fragrances, bisphenols, parabens, triclosan, endocrine disrupting compounds), household cleaning

products, industrial compounds (surfactants, flame/fire retardants, monomers and polymers, solvents), pesticides (new formulations), and other agricultural products (fertilizers, lawn care products) and biocides (Tijani et al. 2016; Morin-Crini and Crini 2017; Patel et al. 2019). Endocrine disruptors can be found in the pharmaceutical and/or cosmetic category. They also include a range of other compounds, including pesticides and phytocompounds, as well as industrial chemicals. Many researchers consider endocrine disruptors to be a narrower subclass of emerging substances. This term refers to specific substances that have been shown to have an effect on the endocrine system of aquatic organisms or that have been designed to act on the human hormone system. Other substances, products and new technologies of concern include UV filters, corrosion inhibitors (benzothiazoles), 3D-printing (thermoplastics, additives), E-cigarettes and E-shishas, nanomaterials and nanoparticles (new products of new anthropogenic processes, nanosprays), microplastics and nanoplastics (considered as truly "new" to the environment). Biological agents and other pathogens (pathogenic bacteria, multi-drug resistant microbes) can also be defined as emerging (Morin-Crini and Crini 2017; Crini and Lichtfouse 2018; García et al. 2020). Indeed, the literature also includes discussion of antibiotic-resistant microorganisms and antibiotic-resistance genes under the broad category of emerging contaminants. More recently, nanoparticles have also been included in the class of emerging substances (Mearns et al. 2018; Zhao et al. 2018; de Marchi et al. 2019; Matich et al. 2019).

Luo et al. (2014) proposed to classify emerging contaminants in five categories, namely personal care products (fragrances, disinfectants, UV filters and insect repellents), pharmaceuticals (non-steroidal anti-inflammatory drugs, antibiotics, lipid regulator, anticonvulsants, β-blockers), steroid hormones, industrial chemicals (plasticizers, fire retardants, bisphenol A, phthalates) and surfactants (cleaning products, alkylphenols), excluding pesticides. According to Norman network (2016), over 1000 emerging chemicals are recognized and classified in four main groups, *i.e.*, drugs, personal care products, endocrine disruptors and pesticides (Norman network 2016; Dulio et al. 2018). Another simplified classification for pharmaceuticals and personal care products proposed by Ebele et al. (2017) considers only one main family of endocrine disruptors, which is subdivided into three categories: (1) personal care products including cosmetics, disinfectants, conservation agents, fragrances and UV screens; (2) nonsteroidal drugs, including antibiotics, analgesics, and other pharmaceuticals (human and veterinary drugs); and (3) steroids (estrogens, etc.). Patel et al. (2020) recently proposed four groups of emerging contaminants (excluding pesticides), *i.e.*, pharmaceuticals, endocrine disruptors (including cosmetics, hormones, xenobiotics, plastics), personal care products (including cosmetics, UV filters, disinfectants, insect repellents such as triclosan, synthetic hormones, lipid regulators and steroids), and perfluorinated compounds. Other researchers and organizations have classified emerging substances into three broad categories: pharmaceuticals, personal care products and endocrine disrupting compounds, excluding pesticides. However, these classifications can be confusing because some personal care products are also endocrine-disrupting chemicals while other drugs are not (Darbre 2015; Gee et al. 2015). In reality, there is not yet an

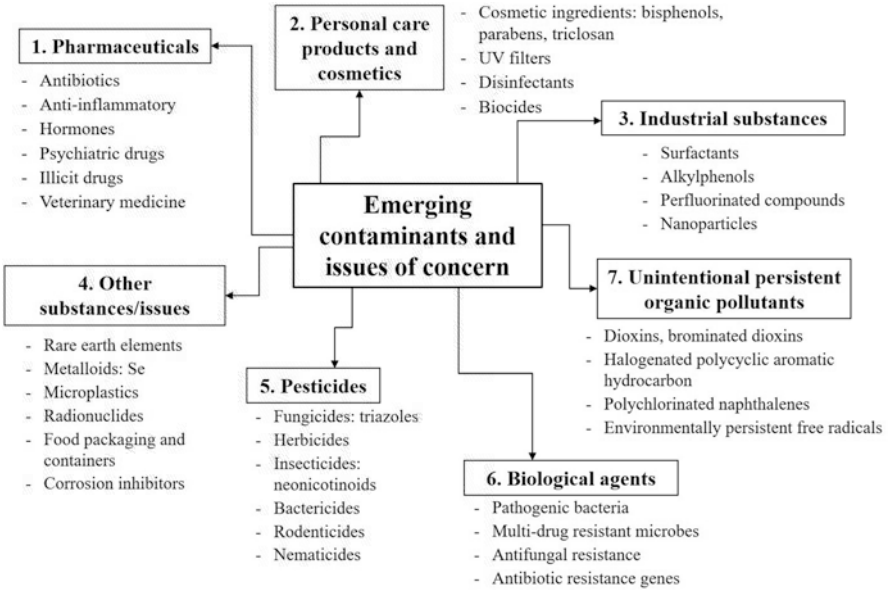

Fig. 1.1 Classification of emerging contaminants and issues of concern in water compartments

internationally recognized general classification for emerging substances. Nevertheless, many researchers agree with the definition given by the US EPA (Gogoi et al. 2018). Figure 1.1 provides a general classification of emerging contaminants and issues of concern in water compartments into seven categories, regardless of their risk to health or the environment.

1.2.3 Examples of Emerging Contaminants of Recent Concern

Polyfluoroalkyl or perfluoroalkyl, known by the abbreviation PFASs, are a family of emerging contaminants that have recently become a concern (Melzer et al. 2010; Gallo et al. 2012; Barry et al. 2013; Vestergren and Cousins 2013; DeWitt 2015; Xiao 2017; Dong et al. 2018; Lorenzo et al. 2018; Brusseau 2019; Ng et al. 2019; Klemes et al. 2019; Pan et al. 2020; Salthammer 2020). Perfluoroalkyl substances is a term used for a family of highly fluorinated chemicals (the term perfluorinated compounds can also be found in the literature). These substances contain fluorinated molecular chains that degrade very slowly in the environment and have a high bioaccumulation potential. They include subclasses such as perfluoroalkyl sulphonic acids (PFSAs) and perfluoroalkyl carboxylic acids (PFCAs). The list is particularly long as the Chemical Abstracts Service registers more than 4000 compounds.

These synthetic substances have been produced and widely used since the 1950s before their harmful health effects and persistence came to light. Today, they are still widely used in consumer products and for industrial uses, finding targeted applications in a wide variety of fields. For example, perfluoroalkyl substances (perfluoroalkyl sulfonates and perfluoroalkyl carboxylates) are widely used as polymer constituents in food containers and packaging (fast-food packaging, pizza boxes), processing aids in non-stick cookware (Teflon®), surface-active agents in waterproof clothing and stain-resistant carper (stain-resistant textiles, water-resistant textiles), and cleaning products. They are also used as individual ingredients in firefighting foams used in many military installations and airports, and in painting materials (Xiao et al. 2013; DeWitt 2015; Brusseau 2019; Pan et al. 2020). Other applications include coatings and metal plating, hydraulic fluids, medical devices, cosmetics (shampoos), pesticides, and photo imaging. The best known are perfluorooctanoic acid (PFOA) used as a repellent coating for textiles, paper products and cookware and perfluorooctanesulfonic acid (PFOS) used in fire fighting foams, carpet treatments, and mist suppressants in metal plating operations.

In 2009, perfluoroalkyl substances were listed in Annex B of the Stockholm Convention on Persistent Organic Pollutants (Stockholm Convention 2009: CN524-TREATIES 4, UNEP, Geneva) as substances of concern, restricted but not completely banned. Many substances are currently being considered for restriction under the 2015 Rome Directive (Stockholm Convention 2015: Decision POPRC-11/4, UNEP, Rome) and will be banned under the EU Chemicals Regulation from 2020. Indeed, perfluoroalkyl substances are chemicals considered to be persistent organic pollutants and long-range transported anthropic contaminants found at high concentrations in human and wildlife populations around the World, including in Arctic marine mammals. Their ubiquous persistence in the environment and their toxicity in animal models raise concerns about the effects on human health of chronic low-level exposure (Melzer et al. 2010; DeWitt 2015; Pan et al. 2020). Perfluoroalkyl substances have been linked to cancer, liver damage and thyroid disease (Melzer et al. 2010; Gallo et al. 2012; Barry et al. 2013; Vestergren and Cousins 2013). Klemes et al. (2019) recently reported that more than 16 million people in the United States were exposed to drinking water with perfluorinated alkyl substances concentrations exceeding 10 ng/L. Melzer et al. (2010) previously reported that higher concentrations of serum perfluorooctanoate and perfluorooctane sulfonate are associated with current thyroid disease in the general adult population in the United States. Gallo et al. (2012) demonstrated an association between concentrations of perfluorooctanoate and perfluorooctane sulfonate and serum levels of alanine of transaminase, a marker of hepatocellular damage. In another study, Barry et al. (2013) reported that exposure to perfluorooctanoic acid is associated with renal, pancreatic and testicular cancer in rats. Other examples can be found in the review by Vestergren and Cousins (2013).

The presence of perfluoroalkyl substances in tap water has become a priority. However, due to their chemical stability and composition, these substances are poorly or even not eliminated by conventional water treatment methods. Because they have no carbon-carbon double bonds and no functional groups, they are also