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University of Aveiro & Ordem dos Engenheiros

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Edited by:
João Araújo Pereira Coutinho
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SCIENTIFIC PROGRAM

Time	Tuesday, 2/10	Wednesday, 3/10	Thursday, 4/10
8:00 – 8:15	Registration		
8:15 – 8:30			
8:30 – 8:45			
8:45 – 9:00			
9:00 – 9:15		Plenary Lecture (PL3) Rajamani Krishna	Plenary Lecture (PL5) Gabriele Centi
9:15 – 9:30			
9:30 – 9:45	Welcome Session		
9:45 – 10:00			
10:00 – 10:15	Plenary Lecture (PL1) Nien-Hwa Linda Wang	O-BB07 O-EE01 O-IM03	O-RS11 O-EE10 O-BS05
10:15 – 10:30		O-BB08 O-EE02 O-IM04	O-RS12 O-EE11 O-BS06
10:30 – 10:45		O-BB09 O-EE03 O-IM05	O-RS13 O-EE12 O-BS07
10:45 – 11:00		O-BB10 O-EE04 O-IM06	O-RS14 O-EE13 O-BS08
11:00 – 11:15	Coffee-break	O-BB11 O-EE05 O-IM07	O-RS15 O-EE14 O-BS09
11:15 – 11:30		Coffee-break	Coffee-break
11:30 – 11:45	O-RS01 O-BS01 Bondalti		
11:45 – 12:00	O-RS02 O-BS02 O-MP01	O-BB12 O-EE06 O-ME01	Plenary Lecture (PL6) Nikolaos Hadjichristidis
12:00 – 12:15	O-RS03 O-BS03 O-MP02	O-BB13 O-EE07 O-ME02	
12:15 – 12:30	O-RS04 O-BS04 Prio	O-BB14 O-EE08 O-ME03	
12:30 – 12:45	O-RS05 O-BB01 O-IM01	O-BB15 O-EE09 O-ME04	
12:45 – 14:15	Lunch	Lunch	Lunch
14:15 – 14:30	Keynotes (KN1 and KN2) João Rocha Rosa Quinta-Ferreira	Keynotes (KN3 and KN4) Adélio Mendes José António Teixeira	Keynotes (KN5 and KN6) Maria Ascensão Reis Ramesh Gardas
14:30 – 14:45			
14:45 – 15:00			
15:00 – 15:15	O-RS06 O-BB02 BB&G	Plenary Lecture (PL4) María José Cocero	O-RS16 O-EE15 O-IM11
15:15 – 15:30	O-RS07 O-BB03 O-MP03		O-RS17 O-EE16 O-IM12
15:30 – 15:45	O-RS08 O-BB04 BP		O-RS18 O-EE17 O-IM13
15:45 – 16:00	O-RS09 O-BB05 O-MP04		O-MP05 O-IM09 O-IM14
16:00 – 16:15	O-IM02 O-BB06 O-RS10	Poster Session and Coffee-break P-BB, P-RS, P-MP, P-ME	O-IM08 O-IM10 O-IM15
16:15 – 16:30	Plenary Lecture (PL2) Paul Christakopoulos		Awards and Closing Session
16:30 – 16:45			
16:45 – 17:00			Multibiorefinery Project Meeting (Coffee-break) CHEMPOR participants are welcome
17:00 – 17:15			
17:15 – 17:30	Formal Session with Minister of Economy	Bus to Vista Alegre Museum Visit	
17:30 – 17:45			
17:45 – 18:00			
18:00 – 18:15	Poster Session and Coffee-break P-BS, P-IM, P-EE		
18:15 – 18:30			
18:30 – 18:45			
18:45 – 19:00			
19:00 – 19:15			
19:15 – 19:30			
19:30		Conference Dinner	

[PL] - Plenary Lecture
[KN] - Keynote Presentation
[RS] - Reaction and Separation Processes
[BS]- Biorefinery and Sustainability
[MP] - Modeling, Synthesis and Integration of Chemical Processes

[BB] - Biological Engineering and Biotechnology
[IM] - Innovative Materials and Applications
[EE] - Energy and Environment
[ME] - Multiscale and Multidisciplinary Engineering Education

Monitoring of emerging micropollutants in hydric media in Bragança district

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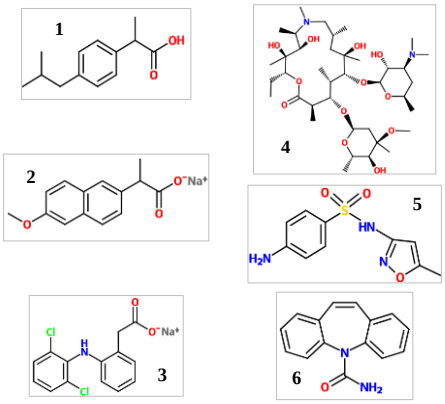

1 Ibuprofen, 2 Diclofenac Sodium, 3 Naproxen Sodium, 4 Azithromycin, 5 Sulfamethoxazole, 6 Carbamazepine

This work aims to develop and validate a method for the quantification and monitoring of emerging micropollutants belonging to the class of pharmaceuticals and personal care products (PPCP´s) in several hydric media from Bragança district, Portugal. Six pharmaceutical drugs were selected for this study, namely, ibuprofen, diclofenac, naproxen, azithromycin, sulfamethoxazole and carbamazepine and belongs to three different subclasses that were worldwide prescribed: three anti-inflammatory, two antibiotics and one antiepileptic, respectively. These compounds were chosen after searching which compounds could be more frequently medical prescribed in Bragança, based on related studies associated with regions with similar socioeconomic data. The next step will be the selection of an extraction and an instrumental method of analysis, as well as the selection of the samples collection points in Bragança and to perform some preliminary monitoring of the referred emerging micropollutants.

Introduction

The water is an extremely important substance for life. It is used in distinct metabolic functions of the body and even to produce energy in hydroelectric stations [1]. The ingestion and contact with contaminated water may cause harmful effects to living beings and are related to most of the main diseases that affect global population [2]. It is well known that with the increase of the human action and the industrial activities, the quality of this resource has been strongly affected [1].

The recent advances of the analytical techniques allowed the identification of new compounds in the environment. The emerging pollutants are substances found in different media and that are not considered as pollutants until now. When found in very small concentrations, as micrograms or nanograms per liter, these substances are named as emerging micropollutants [3].

These contaminants may cause damaging effects even in low quantities, but as this fact was recently found, some of them are not yet legislated. For this reason, toxicity, bioaccumulation and health effects studies are important to indicate whether it is necessary or not to legislate about these substances [4].

In the European Union, for example, the Directive 2008/105/CE presents a list of 33 priority substances and their maximum concentrations allowed in nature. These substances are pollutants known for decades. The Directive 2013/9/EU included other 12 compounds in this list and created a vigilance list with 10 substances that could indicate risk to the aquatic matrix and that did not have enough data to their monitoring [5].

Emerging micropollutants have been found in different groups of substances, as pharmaceutical drugs, beauty and cleaning products and illegal drugs. Due to the lack of legislation, there is no specific classification for these substances, but the most common classification found in literature divides them among: persistent organic pollutants (POP's), endocrine disrupting compounds (EDC's) and pharmaceuticals and personal care products (PPCP's) [4].

The PPCP's are known as pseudo-persistent pollutants, because despite not being totally resistant to degradation, such as POP's, they are continually reintroduced to the environment, keeping significant concentrations in hydric media [6].

Despite of their importance to society avoiding and treating diseases, medical drugs may cause undesired effects to health when consumed in wrong quantities or ways. It is believed that the main cause of wrong ingestion of these products is self-medication, but the contact with contaminated water is another relevant cause supported during the previous decades by the recent advances of the analytical techniques [7].

Another important concerning about PPCP's is the fact that they are logically developed with a high pharmacological potency, which means that they can cause the desired effects in a significant way, even at low concentrations while retaining their physicochemical properties long enough to serve the medical purpose developed [3]. Because of these and other factors, PPCP's are substances excreted in relevant quantities by the human body and that are not effectively removed from water in sewage treatment plants [4].

Objectives

Because these are compounds present in very low concentrations, their analysis and study are not easy tasks. Sophisticated instrumental methods of analysis are needed to measure substances concentrations at the micrograms and nanograms orders of magnitude. Portugal, like many other countries from the European Union, does not have legislation for PPCP's micropollutants yet.

Therefore, it is necessary to develop effective methods for quantification and consequent maintain a serious monitoring of these substances in different hydric media.

The aim of this study is to develop a method of analysis to quantify and to monitor the concentration of several PPCP´s in aqueous media. These compounds are present in pharmaceutical drugs, such as the main active principles, of different classes that are believed to be found in the hydric media from the Bragança district.

Methods

In order to select what substances will be analyzed in this study, it was necessary to investigate which, among several types of drugs, would be found most frequently in hydric media from Bragança.

The first step was to search for works with a similar objective performed in the north region of Portugal and the second step

was to search for studies carried out in places like the region of interest, considering socioeconomic data. Among the characteristics taking into account to select these studies were: to be a small or medium city, maximum 180000 habitants per wastewater treatment plant (WWTP), with a WWTP that receives predominantly domestic discharges, which can include sewage from a hospital. These locations may have agricultural and service activities, but not industrial activities in significant quantities.

Results and Conclusions

After a preliminary screening, six pharmaceutical drugs were selected: ibuprofen, diclofenac, naproxen, azithromycin, sulfamethoxazole and carbamazepine. The first three are anti-inflammatory, followed by two antibiotics and one antiepileptic, respectively. Table 1 presents the results of some studies that quantified these substances in different hydric media. Concentrations for the same place are expected to be higher in the raw sewage, followed by the influent, effluent and groundwater. In the table, this correlation does not happen because the samples are from different aqueous matrices and different locations, which explains the significant variability of the data showed. Moreover, the results presented are average values for each one of the collection sites.

The next step will be to select an extraction/concentration technique and the instrumental method of analysis. The main alternatives for extraction/concentration considered in this study are Solid Phase Extraction (SPE) and Solid Phase Micro Extraction (SPME). The SPE uses cartridges filled with sorbents, which retains the analytes according to the polarity and consequent affinity to their molecules. SPME is a technique which uses a silica fiber covered by a thin layer of a polymer or a solid adsorbent, chosen according to the desired purpose. The coated fiber is wrapped inside the needle of a microsphere inserted into the sample for extraction of the analytes [4].

For the methods of instrumental analysis, the possibilities that are considered are High Performance Liquid Chromatography coupled with mass spectrometry (HPLC-MS) or Gas Chromatography coupled with mass spectrometry (GC-MS).

After the development and validation of the method with real samples, it will be possible to detect and quantify this type of pollutants in some of the hydric media in the district of Bragança.

Table 1. Pharmaceutical drugs quantified in some published studies.

Compound	Average concentration (ng/L)	Hydric media	Method of analysis	Reference
Ibuprofen	110	Effluent	SPE-GC-MS	[7]
	87.1	Groundwater	SPE-LC-MS	[8]
	84000	Influent	SPE-GC-MS	[9]
Diclofenac	100	Raw sewage	SPE-HPLC-MS	[4]
	290	Effluent	SPE-GC-MS	[7]
	75.3	Groundwater	SPE-LC-MS	[8]
	1500	Influent	SPE-GC-MS	[9]
Naproxen	410	Effluent	SPE-GC-MS	[7]
	0.43	Groundwater	SPE-LC-MS	[8]
Azithromycin	96.3	Groundwater	SPE-LC-MS	[8]
Sulfamethoxazole	13	Raw sewage	SPE-HPLC-MS	[4]
	15.3	Groundwater	SPE-LC-MS	[8]
Carbamazepine	440	Effluent	SPE-LC-MS	[7]
	44.32	Groundwater	SPE-LC-MS	[8]
	350	Influent	SPE-GC-MS	[9]

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