The potential ecotoxicological impact of pharmaceutical and personal care products on humans and freshwater, based on USEtox™ characterization factors. A Spanish case study of toxicity impact scores

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HIGHLIGHTS

• Characterization factors (CFs) of 27 PPCPs widely used worldwide were estimated.
• CF can be used to generate impact score rankings.
• Emission to continental freshwater compartment showed the highest CFs values for human and ecotoxicological effects.
• Freshwater aquatic ecotoxicological CFs are much higher than human toxicity CFs.
• The values of CFs can be incorporated in Life Cycle Impact Assessment (LCIA) studies.

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ABSTRACT

Pharmaceutical and personal care products (PPCPs) are being increasingly included in Life Cycle Assessment studies (LCAs) since they have brought into evidence both human and ecological adverse effects due to their presence in different environmental compartments, wastewater facilities and industry. Therefore, the main goal of this research was to estimate the characterization factors (CFs) of 27 PPCPs widely used worldwide in order to incorporate their values into Life Cycle Impact Assessment studies (LCIA) or to generate a toxicity impact score ranking. Physicochemical properties, degradation rates, bioaccumulation, ecotoxicity and human health effects were collected from experimental data, recognized databases or estimated using EPI Suite™ and the USEtox™ software, and were subsequently used for estimating CFs. In addition, a Spanish toxicity impact score ranking was carried out for 49 PPCPs using the 27 newly calculated CFs, and 22 CFs already available in the literature, besides the data related to the occurrence of PPCPs in the environment in Spain. It has been highlighted that emissions into the continental freshwater compartment showed the highest CFs values for human effects (ranging from $10^{-9}$ to $10^{-3}$ Cases·kg$^{-1}$), followed by emissions into the air ($10^{-9}$ to $10^{-5}$ Cases·kg$^{-1}$), soil ($10^{-11}$ to $10^{2}$ Cases·kg$^{-1}$) and seawater ($10^{-12}$ to $10^{-8}$ Cases·kg$^{-1}$). CFs regarding the affectation of freshwater aquatic environments were the highest of those proceeding from emissions into continental freshwater (between $10^0$ PAF·m$^{-1}$·day·kg$^{-1}$emission) due to the direct contact between the source of emission and the compartment affected, followed by soil (among $10^{-3}$ to $10^0$ PAF·m$^{-1}$·day·kg$^{-1}$emission), and air (among $10^{-2}$ to $10^4$ PAF·m$^{-1}$·day·kg$^{-1}$emission) while the lowest were the CFs of continental seawater (among $10^{-28}$ to $10^{-28}$).
1. Introduction

In recent years, pharmaceutical and personal care products (PPCPs) have been found at different levels of concentration in all environmental compartments (air, water, and soil), and many of their impacts are still unknown or under analysis. The primary routes of pharmaceuticals into the environment are through human excretion, disposal of unused products and through agricultural usage, but high concentrations of pharmaceuticals have also been reported in treated industrial effluents or recipient waters, through direct discharge from manufacturing companies (Larsson et al., 2007; Larsson, 2014a). A wide range of pharmaceutical products have been detected in surface and groundwater, associated with wastewater disposal (Brausch and Rand, 2011; Ebele et al., 2017; Stuart et al., 2012) but can also be found in soil, sediments (Larsson, 2014b; Xu et al., 2009) and to a lesser extent possibly in the air (Larsson, 2014b).

There is a lot of research in this area, some of which was carried out by Ebele et al. (2017) who presented a review of the current state-of-knowledge on PPCPs in the freshwater aquatic environments (water, sediments and biota) of the five continents. Xu et al. (2009) studied the degradation and adsorption of selected PPCPs in agricultural soils, while Gaw et al. (2014) reviewed the sources, impacts and concentrations of pharmaceuticals in marine and coastal environments, among many others. In the specific case of personal care products (PCPs), Tolls et al. (2009) indicated that considerable amounts of these compounds are utilized each day, resulting in large quantities of chemical substances that could potentially reach environmental compartments, particularly water, but also soil and air.

Currently, there are thousands of PPCPs which are available on the market and are used daily, and they can be released into the environment individually, although in most cases they tend to be released in ever-changing mixtures, whose effects can be synergetic or antagonistic, so the possibility of knowing the potential impact that all these compounds and their mixtures might generate in nature is almost impossible, without spending a large amount of money, resources and time.

The effects of PPCPs in the environment are very diverse, these compounds can be persistent, bioaccumulable and can cause acute and chronic human and ecotoxicological damage. Therefore, the interest in knowing the ecotoxicological effects of PPCPs on the environment has increased in the last years. Some authors (Brausch and Rand, 2011; Cleuvers, 2003, 2004; Daughton and Brooks, 2010; Fent et al., 2006; Sanderson et al., 2004a; Santos et al., 2010; Vasquez and Fatta-Kassinos, 2013) have reported ecotoxicological data from different types of assays (for single PPCP or their mixtures) including different species (trophic levels), times of exposure (chronic, subchronic or acute) and endpoints (half maximal effective concentration, EC_{50}; concentration which causes the death of 50% of the sample population, LC_{50}; non-observed adverse effect level, NOAEL; lowest observed adverse effect level, LOAEL).

Although there is a great variety of analyses and tests to bring into evidence the negative effect of PPCPs on the environment, it is necessary to have different methods of predicting these effects, due to the large number of these types of compounds, and the diverse ways that they can be found in the environment.

A large number of tools for predicting the impact of a process, activity or contaminant in the environment are currently available. One of them is the Life Cycle Assessment (LCA), which allows the estimation of the potential impacts of such compounds on human health, ecosystems and resources. LCA has been extended to many aspects of production and consumption, including eco-design of products, cleaner production, environment labels, green purchase, resource management, waste management and environment strategy, etc. (Nie et al., 2010), and therefore, LCA is gradually gaining acceptance as an efficient tool for the environmental evaluation of the potential impact of chemicals and chemical processes. LCA does not substitute other methodologies (such as environmental risk assessment, or the ratio between predicted environmental concentration and the predicted no effect concentration etc.) since the different tools fulfill different purposes and they can, in fact, play complementary roles and benefit from each other (Muñoz et al., 2008). Kobayashi et al. (2015) proposed the combination of LCA and quantitative risk assessment (QRA) with different hybridization approaches, taking into account that LCA is useful in the evaluation of global impacts and QRA in local impacts.

The guidelines of LCA studies are established in the standard series of ISO 14040, and more specifically in the ISO 14040:2006 and 14044:2006 standards (ISO, 2006). LCA methodology can be a powerful tool: (i) to identify the type of impact (on renewable or non-renewable resources, global warming, ozone depletion, toxicity, acidification, energy and water use, among others) of diverse compounds in different environmental scenarios; (ii) to compare these impacts with those from other compounds; (iii) to implement preventive or corrective actions to minimize the potential or real adverse effect caused by them.

The life cycle impact assessment (LCIA) phase of a LCA study requires not only the data from the emissions inventory, but also the characterization factors (CFs, alternatively referred to as equivalency factors) to provide indicators in the context of various impact categories (such as global warming, stratospheric ozone depletion, tropospheric ozone creation, eutrophication/nitrification, acidification, toxicological impacts on humans, and toxicological impacts on ecosystems) (Pennington et al., 2004).

Knowledge of CFs is mainly essential for determining/estimating the human and ecological potential impact of chemicals on different environments (air, freshwater, seawater, natural soil, agricultural soil, etc.) and they must be included in the LCIA stage of LCA studies.

CFs are also used to determine the relative importance of a substance to toxicity related impact categories, such as human toxicity or ecotoxicity in LCA studies. The CFs accounts for the environmental persistence (fate), accumulation in the human food chain (exposure) and toxicity (effect) of a chemical. Fate and exposure factors can be calculated by means of "evaluative" multimedia fate and exposure models, while effect factors can be derived from ecotoxicity data on human beings and laboratory organisms (Huijbregts et al., 2005a).

In this sense, the USEtox™ model, which has been developed as a result of a Task Force on Toxic Impacts under the UNEP-SETAC Life Cycle Initiative, is a powerful tool for calculating CFs. It is a way to characterize human and ecotoxicological impacts in LCIA and comparative risk assessment (CRA) analysis. USEtox™ was designed to describe the fate, exposure and effects of chemicals (Huijbregts et al., 2010a).
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