Human and ecotoxicological potential impact of pharmaceutical and personal care products from USEtox™ life cycle impact assessment characterization factors

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Background and objective: In the last years pharmaceutical and personal care products (PPCPs) have been found at different level of concentrations in all environmental compartment (air, water and soil), and many of their impacts are still unknown or they are under analysis. One tool used for estimated the potential impact of PPCPs in the environment is the life cycle assessment (LCA). PPCPs are being increasingly included in LCAs since they have evidenced ecological and human adverse effects and due to their presence in different environmental compartments, wastewater facilities and industry. In environmental LCAs, CFs (alternatively referred to as equivalency factors) are used to determine the relative importance of a substance to toxicity related impact categories, such as human toxicity and freshwater ecotoxicity (Huijbregts et al. 2005a). In this sense, the USEtox™ model is a powerful tool to calculate CFs. It is an environmental model for characterization of human and ecotoxicological impacts in life cycle impact assessment (LCIA) and comparative risk assessment (Huijbregts et al., 2010a). Despite the large number of substances which have been considered in the USEtox™ database (more than 3000 in the USEtox™ organic database 1.01) a small amount of PPCPs have been considered (approximately less than 2% of the organic database corresponds to this group of compounds). Accordingly, the CFs of many PPCPs have not been calculated. The main goal of this work is presenting the CFs estimates, using the USEtox™ model, of 27 wordwide used PPCPs, to incorporate these values in LCIA studies or to generate impact score rankings.

Methods and Results: In this work, an impact score ranking is propose for 49 PPCPs using the new CFs calculated, the CFs already available and also the data of PPCPs occurrence in the environment in Spain from a previously study (Ortiz et al., 2013). PPCPs from 14 different therapeutic classes have been considered in this study: analgesic/antipyretic, Angiotensin converting enzyme inhibitor, angiotensin receptor blockers, antibiotics, antidepressants, antiepileptics, anxiolytics, blood lipid regulators, cytostatics/cancer therapeutic, H_2 blocker, hormones, Platelet inhibitor, non-steroidal anti-inflammatory drugs (NSAIDs)/antirreumatics, X-ray contrast media and PCPs. Physicochemical properties, degradation rates, bioaccumulation, ecotoxicity and human health effects were collected from experimental data, recognized databases or estimated by EPI Suite™. The input parameters required by USEtox™ program were: molecular weight (MW), partition coefficient between octanol and water (K_{ow}), partition coefficient between organic carbon and water (K_{oc}), Henry law coefficient at 25ºC (K_H), vapor pressure at 25ºC (P_{vap}), solubility at 25ºC (Sol), degradation rate in air (K_{degA}), degradation rate in water (K_{degW}), bioaccumulation factor of the chemical (BAF), water ecotoxicity (chronic and acute) and human carcinogenic and non-carcinogenic effects. Emission of PPCPs to continental freshwater compartment showed the highest CFs for human effects (ranging on 10^{-9} to 10^{-3} cases kgemmited^{-1}), following emissions to air (10^{-9} to 10^{-5} cases kgemmited^{-1}), soil (10^{-11} to 10^{-5} cases kgemmited^{-1}) and sea water (10^{-12} to 10^{-4} cases kgemmited $^{-1}$). CFs of the affectation of freshwater aquatic environments were the highest from emission to continental freshwater (between 1 to 10^4 PAF m^3 d kg^{-1}) due to the direct contact between the source of emission and the compartment affected, followed by soil (from 10^{-1} to 10^4 cases kgemmited^{-1}), air (from 10^{-2} to 10^4 cases

kgemmited^{-1}) and the lowest were continental sea water CFs (from 10^{-28} to 10^{-3} cases kgemmited^{-1}).

Discussion: PPCPs with the highest impact scores are hormones, antidepressants, fragrances, antibiotics, angiotensin receptor blockers and blood lipid regulators, which have been already found in other ranking scores. In this study most antibiotics are located in the top 20 of the ecotoxicity impact score and for human toxicity impact score azithromycin and levofloxacin are in the top 10. Although it is not surprising that some of the compounds studied in this research occupy the top ranking (by previous researches) even their CFs was not known. The estimation of new CFs should be continued, either for compounds that are already marketed as for the new ones. These results, not available until now, are useful to do better LCIAs incorporating these pollutants in these studies or for assessing single hazard/risk environmental impact assessments.

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