Risk Assessment of Cosmetic Preservatives Using QSAR: QSAR of Cosmetic Preservatives

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ABSTRACT

Cosmetic manufacturers need to demonstrate the safety and efficacy of the products against microbial contamination to assure consumer safety and to improve shelf-life. The preservation strategies include chemical, physical, or physiological strategies. The most common is the use of antimicrobial agents. The toxicity assessment of preservatives used in cosmetic products is essential. It can be done by computational methods such as quantitative structure-activity relationship (QSAR) using several software such as ADME-Tox, TOPKAT, Dragon, T.E.S.T., and ECOSAR. The present manuscript elaborates a detailed view on cosmetic preservatives, regulatory aspects and application of computational strategies for toxicity prediction.

KEYWORDS

Antimicrobial Synthetic Agents, Computational Studies, Cosmetic Preservatives, QSAR, Risk Assessment, Toxic Effects

INTRODUCTION

Cosmetic products have a history of thousands of years for enhancing appearance and protection. The term ‘Cosmetics’ is derived from the Greek “Kosmtikos” meaning ‘having the power to arrange, skilled in decoration’, to give “kosmein”, to adorn, and “kosmos”, order, harmony (Ayenimo et al., 2010). The Council of European Union regulation gave the following definition: “cosmetic product means any substance or mixture intended to be placed in contact with the external parts of the human body (epidermis, hair system, nails, lips, and external genital organs) or with the teeth and the mucous membranes of the oral cavity with a view exclusively or mainly to cleaning them, perfuming them, changing their appearance, protecting them, keeping them in good condition, or correcting body odor” (Rothe et al., 2011; Yeomans et al., 2012). Cosmetic ingredients are acquired from natural (plants, animals and mineral), synthetic as well as semi-synthetic sources (Talapatra et al., 2016). Cosmetics can be classified as leave-on, rinse-off hair, skin care, face care and oral care products (Bremer et

DOI: 10.4018/IJQSPR.2020010103

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al., 1991; Chiller et al., 2001; Prabhamanju et al., 2009; Davies et al., 2010; Easley et al., 2016; U.S. Code. Regulations: 2016, Easley et al., 2016; Dos Santos et al., 2017). Now-a-days, the market for cosmetic products has become vast and customary throughout the world, although the extent of their popularity and use may vary with countries.

Cosmetic products containing water and organic/inorganic compounds require preservation against microbial contamination to ensure consumer’s safety and to enhance a product’s shelf-life. The main goal of microbiological safety is to protect consumer against potentially pathogenic microbial contamination, together with the prevention of biological and physiochemical degradation of products (Halla et al., 2018). As cosmetic/personal care and beauty products are biodegradable in nature, the product gets expired and become unsafe for consumers. The chemical additives used in cosmetics exhibit human body toxicity (cytotoxicity, genotoxicity, mutagenicity, neurotoxicity, oestrogenicity), mild hypersensitivity to anaphylaxix/lethal intoxication (Bilal and Iqbal, 2019). Among the other additives, preservatives are antimicrobial substances added to cosmetic formulations to ensure safety by inhibiting the microbial growth and reducing the load of microbial contaminants (Amasa et al., 2012). In addition to the preservatives, the other ingredients used in cosmetics may be of major health concern, and they are becoming emerging pollutants for the environment (Juliano and Magrini, 2017). In comparison to pharmaceuticals, cosmetics are used in larger quantities and throughout the course of life. Additionally, the external applications rule out the metabolic transformation, and they enter the environment unaltered during washing, showering or bathing (Ternes et al., 2004). Therefore, the toxicity assessment of preservatives used in cosmetic products is essential to ensure environmental and animal and human life safety. Studies have been carried out which warrant requirement of use of environment friendly cosmetic ingredients during manufacture (L’Haridon et al., 2018).

Due to lack of ecotoxicological data for effect of pharmaceuticals and cosmetics on the environment, European Medicines Agency (EMA) has released guidelines for the risk assessment. Various parameters to assess impact of cosmetic ingredients on aquatic environments are released by the international organizations (Environmental Protection Agency (EPA), Cradle to Cradle (C2C), European legislation (European Regulation 1272/2008)) (Vita et al., 2018). As per the guidelines issued by various regulatory organizations, to reduce animal use in experimentation, computational methods such as quantitative structure-activity relationship (QSAR), ADME-Tox, expert systems such as TOPKAT, T.E.S.T., and ECOSAR can be used for toxicity and risk assessment (Figure 1). These are elaborated as follows:

Figure 1. Role of QSAR/QSTR in toxicity/risk assessment of cosmetic preservatives
Multilayer Perceptron Model for Predicting Acute Toxicity of Fungicides on Rats