Combining Features of Metal Oxide Nanoparticles: Nano-QSAR for Cytotoxicity

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ABSTRACT

A poor applicability of classic 2D descriptors for representation of metal oxide nanoparticles is briefly discussed. The combination of 1D descriptors with previously calculated size-dependent descriptors is utilized to represent the structural features of nanoparticles in QSAR modeling. For this purpose, descriptors based on the fundamental characteristics of atoms (nuclear charge, oxidation level, electronegativity, ionic radius, ionic refraction etc.) were combined with those derived from structural formula (doublets – A2, AB, …; triplets – A3, A2B, ABC, … etc.) and “liquid drop model” derived size-dependent parameters. Nano-QSAR models are developed for cytotoxicity of metal oxide nanoparticles against E. coli and HaCaT cells. Two developed nano-QSAR models are discussed in terms of cluster analysis.

KEYWORDS

Combinatoric, Descriptors, Nano-QSAR, Oxidative Stress, PLS

INTRODUCTION

The understanding of relationships between structure of chemicals and their properties is of the general interest and allows to make accurate predictions of properties for untested materials based on their structural data. During the recent decades, the creation of new classes of chemicals (materials, reagents, drugs, etc.) is almost always accompanied with Quantitative Structure-Activity/Properties Relationships (QSAR/QSPR) analysis. A strict formal methodology (the basic principles and rules for implementation) has been developed for the solution of QSAR/QSPR tasks (Cherkasov et al., 2014). The majority of QSAR/QSPR studies are conducted for organic compounds and aimed in creating new drugs (Wang et al., 2017). Obviously, the structural specificity of organic compounds is different compared to inorganic compounds. Organic compounds are built from a limited types of elements (organogeneres), while inorganic compounds could contain any element of the periodic system. Moreover, typical inorganic compounds are less diverse in topology (molecular graphs).
Based on that, it is clear, that fundamental differences between organics and inorganics should be taken in account during computational modeling.

The majority of developed descriptors are applicable only to organic compounds (Todeschini and Consonni, 2009). In this paper, we intend to draw attention to the suitability of classic two-dimensional (2D) descriptors for inorganic structures. In fact, some studies reported the application of 2D descriptors to represent the structural features of inorganic compounds for QSAR/QSPR modeling (Mu, et al., 2006; Mu, et al., 2007; Sizochenko et al., 2014; Isayev et al., 2017).

2D descriptors could be generated using structural formula of the molecule (Todeschini and Consonni, 2009). Back to mid-nineteenth century, the initial concept of the structural formula introduced the theory of valence developed by A. Butlerov and his predecessors A.S. Cooper and F.A. Kekule. Hence, the specific language of structural formula represents a natural way of describing organic substances. Likewise, this language was adopted for description of inorganic compounds; but for many ionic inorganic crystals it is not correct to use this language. A general example is presented in Figure 1.

In accordance with the rules of valence, there could be possible variations in topological connections for each structural formula. However, in the case of inorganic crystals, these variations do not seem to be correct (Figure 1). Based on that, we state that the classic 2D descriptors are not entirely correct in the case of inorganic crystals. The simplest alternative is the application of 1D descriptors. Despite the very primitive way of structural representation, such approach is potentially useful (Diller et al., 2007). As our team has previously demonstrated, the amount of information related to a specific compound can be significantly increased with combinatorial calculations applied to the brutto formula (Kuz’m in et al., 2005; Kuz’m in et al., 2008).

The objective of the current paper is the adaptation of 1D approach to study properties of inorganic nanoparticles. Models for the toxicity of metal oxide nanoparticles against E. Coli and HaCaT cells were developed and discussed.

MATERIALS AND METHODS

In this study, \textit{in vitro} cytotoxicity data (pEC_{50} and pLC_{50}) of metal oxide nanoparticles (ZnO, CuO, V_{2}O_{3}, Y_{2}O_{3}, Bi_{2}O_{3}, In_{2}O_{3}, Sb_{2}O_{3}, Al_{2}O_{3}, Fe_{2}O_{3}, SnO_{2}, ZrO_{2}, TiO_{2}, CoO, NiO, Cr_{2}O_{3}, La_{2}O_{3}) towards bacteria \textit{Escherichia coli} and human keratinocyte cell line HaCaT (Puzyn et al., 2011; Gajewicz et al., 2015) was used for testing of proposed modeling approach.

\textbf{Figure 1. Modeling the structure of inorganic compounds}
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