Chapter 66
Quasi–SMILES for Nano–QSAR Prediction of Toxic Effect of Al$_2$O$_3$ Nanoparticles

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ABSTRACT

The level of malondialdehyde (MDA) in wet tissue of different organs is utilized as a measure of toxic effect. The numerical data on the concentration of MDA in wet tissue of liver, kidneys, brain, and heart of rat is examined as the endpoint which are impacted by different dose (mg/kg), exposure time (3 and 14 days) and single oral treatment of aluminium nano-oxide (Al$_2$O$_3$) with 30 nm or 40 nm. An attempt to develop predictive model for this endpoint has been carried out in this work. SMILES is a traditional tool to represent molecular structure for QSPRs/QSARs. In contrast to traditional SMILES, so-called quasi-SMILES can be a tool to build up quantitative features – property / activity relationships (QFPRs/ QFARs) for endpoints which are not defined by solely molecular structure, but by a group of physico-chemical and/or biochemical conditions. The quasi-SMILES is the representation of the above eclectic conditions whereas the QFPR/QFAR are models of endpoints which are modified under impacts of these eclectic conditions.

1. INTRODUCTION

The influence of various nanomaterials on the everyday life gradually increase owing to their high functional potential be very useful materials for different applications (Vanić and Škalko-Basnet, 2013; Ma et al., 2013; Singh and Gupta, 2014; Melagraki and Afantitis, 2014; Panneerselvam and Choi, 2014;

Potrč et al., 2015; Sauer et al., 2015; Speck-Planche et al., 2015). However, a tool to risk assessment for nanomaterials similar to quantitative structure – property /activity relationships (QSPRs/QSARs) (Toropova et al., 2012; Yilmaz et al., 2015) as research field is in an initial phase of the development (Muthu, 2012; Oksel et al., 2015). The solution of this task for regulatory purposes in the case of nanomaterials involved in the agriculture, food, cosmetics, drug discovery, etc. needs to be reached in the near future (Arts et al., 2014; Arts et al., 2015; Filon et al., 2015; Amenta et al., 2015).

In general, different measures of danger acting of nanomaterials upon cells are known (Long et al., 2009; Prabhakar et al., 2012; Diez-Ortiz et al., 2015; Toropova et al., 2015a; Hadrup et al., 2015). In particular, the level of malondialdehyde (MDA) in wet tissue of different organs is considered as a measure of toxic effect of nanomaterials (Long et al., 2009; Prabhakar et al., 2012).

Attempts which are aimed to build up models for such acting of nanomaterials using the traditional QSPR/QSAR approaches (De Abrew et al., 2015), as rule, are impossible excepting the cases of acting of small molecules together with a nanomaterial (Fourches et al., 2010; Toropov et al., 2013).

In the case of traditional materials where the molecular structure represented by SMILES is available to mathematical and computational analyses, the QSPR/QSAR is a tool to more or less satisfactory prediction of different endpoints (Veselinović et al., 2013; Achary, 2014a, 2014b; Comelli et al., 2014; Nesmerak et al., 2014; Worachartcheewan et al., 2014; Toropova and Toropov, 2014; Veselinović et al., 2015).

A possible way to build up such models can be expressed by paradigm: "Endpoint = f(SMILES)". In the case of nanomaterials where weak variation of molecular structure accompanied by intensive variation of conditions more appropriate paradigm is "Endpoint = f(Eclectic data)".

The quasi-SMILES can be the representation of eclectic data (Toropov and Toropova, 2015). The quasi-SMILES are analogies of traditional SMILES, but symbols involved in the quasi-SMILES are representations of features and/or conditions that are not representation of features of the molecular architecture only. (Toropova and Toropov, 2013; Toropov and Toropova, 2014; Toropova et al., 2015b).

The aim of this work is to build up models for level of MDA in wet tissue of different organs of rat under different action of Al_2O_3 nanoparticles.

2. METHOD

2.1. Data

The experimental data on the level MDA in wet tissue (nanomoles of MDA per gram wet tissue) of liver, kidneys, brain, and heart of rat under different conditions taken in the literature (Prabhakar et al., 2012). Table 1 contains the representation of different conditions of acting Al_2O_3 nanoparticles by quasi-SMILES. These data (quasi-SMILES together with endpoint values) were three times randomly split into the training, calibration, and validation set. The length of quasi-SMILES (the number of symbols) is important indicator for possibility of a model to be successful.

It is to be noted that length 1 for quasi-SMILES is nonsense, because in this case the prevalence of each attribute is zero in the training or in calibration set (the presence in both mentioned set is impossible), i.e. for each attribute, A, one can obtain:

$N_{training}(A) \times N_{calibration}(A) = 0$

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