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**Nano-QSAR in cell biology: Model of cell viability as a mathematical function of available eclectic data**Alla P. Toropova<sup>\*</sup>, Andrey A. Toropov

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**ABSTRACT**

The prediction of biochemical endpoints is an important task of the modern medicinal chemistry, cell biology, and nanotechnology. Simplified molecular input-line entry system (SMILES) is a tool for representation of the molecular structure. In particular, SMILES can be used to build up the quantitative structure – property / activity relationships (QSPRs/QSARs). The QSPR/QSAR is a tool to predict an endpoint for a new substance, which has not been examined in experiment. Quasi-SMILES are representation of eclectic data related to an endpoint. In contrast to traditional SMILES, which are representation of the molecular structure, the quasi-SMILES are representation of conditions (in principle, the molecular structure also can be taken into account in quasi-SMILES). In this work, the quasi-SMILES were used to build up model for cell viability under impact of the metal-oxides nanoparticles by means of the CORAL software (<http://www.insilico.eu/coral>). The eclectic data for the quasi-SMILES are (i) molecular structure of metals-oxides; (ii) concentration of the nanoparticles; and (iii) the size of nanoparticles. The significance of different eclectic facts has been estimated. Mechanistic interpretation and the domain of applicability for the model are suggested. The statistical quality of the models is satisfactory for three different random distribution of available data into the training (sub-training and calibration) and the validation sets.

**Keywords:** quasi-SMILES; Nano-QSAR; Nano-QFAR; Monte Carlo method; CORAL software

**1. Introduction**

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