MOL2NET, International Conference Series on Multidisciplinary Sciences
NANOMATJND-01: Jackson State University (JSU) and North Dakota State University (NDSU) Workshop Series on Nanotechnology and Material Sciences.

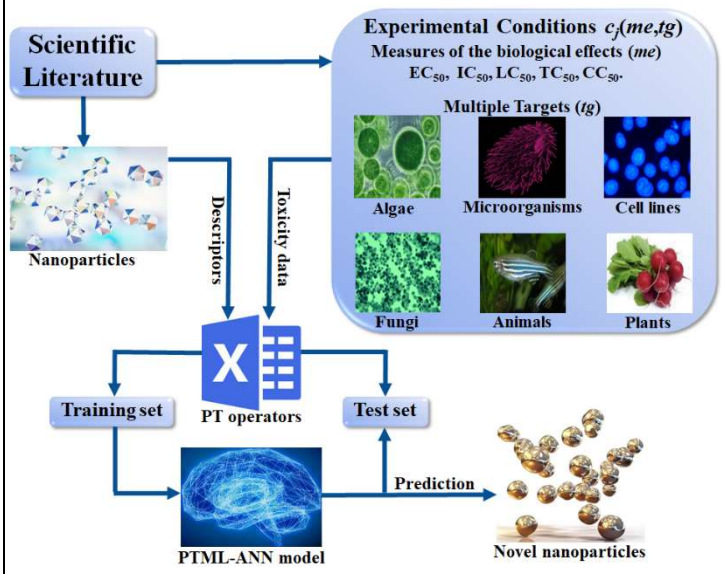
PTML-ANN Model for Simultaneous Prediction of Cytotoxic and Ecotoxic Effect of Nanoparticles

Valeria V. Kleandrova[a], Alejandro Speck-Planche[b].*

[a]Laboratory of Fundamental and Applied Research of Quality and Technology of Food Production, Moscow State University of Food Production, Volokolamskoe shosse 11, 125080, Moscow, Russian Federation
[b]Department of Chemistry, Institute of Pharmacy, I.M. Sechenov First Moscow State Medical University, Trubetskaya str., 8, b. 2, 119992, Moscow, Russian Federation

**Corresponding Author: Alejandro Speck-Planche (alejspivanovich@yahoo.es)*

Graphical Abstract



Abstract.

Biological data on the cytotoxic and the ecotoxic effects of coated and uncoated nanoparticles were retrieved from the scientific literature. The mathematical treatment of these data was based on the use of perturbation theory (PT) operators. This enabled the development of a model that combined perturbation theory concepts with artificial neural networks (PTML-ANN). New nanoparticles not reported during the generation of the PTML-ANN model were used in a virtual screening experiment. For these new nanoparticles, the predictions performed by the PTML-ANN model converged with the experimental results.

Keywords: Nanoparticles; PTML, ANN, cytotoxic; ecotoxic, virtual screening.

Introduction

Nanoparticles have a wide range of industrial applications.[1] Nevertheless, nanoparticles pose a threat to human health and the remarkable damages to the ecosystems.[2] Consequently, the development of predictive models for regulatory purposes in nanotechnology is of paramount importance. This communication reports a PTML-ANN focused on predicting the cytotoxic and ecotoxic profiles of coated and uncoated nanoparticles under diver experimental conditions.

Materials and Methods

Data set and descriptors

The data involving the different cytotoxic and ecotoxic endpoints of the nanoparticles were retrieved from the scientific literature.[3] The data included biological information regarding the targets (e.g., algae, microorganisms, animals, plants, etc.) and assay times. In addition, the data contained relevant chemical and/or physical information of the nanoparticles such as composition, shape, size, and conditions under which the size was assessed. Through the application of perturbation operators (PT), the data was mathematically pretreated, leading to the generation of sets of descriptors that considered chemical and biological information under which the nanoparticles were tested against the different targets.

Setting up the PTML-ANN model

The search for the best model was performed via artificial neural networks, where the most popular architectures were used, namely radial basis function (RBF) and multilayer perceptron (MLP). The statistical indices known as sensitivity and specificity were used to assess the performance of the model by checking its internal quality (training set) and predictive power (prediction set).

.

Results and Discussion

PTML-ANN model

The best model found was based on an ANN with the profile MLP 10-11-2. The PTML-ANN model exhibited a high performance, with sensitivities and specificities around 99% in both training and prediction sets. In addition to being validated by the external prediction set, a virtual screening experiment was carried out. New coated and uncoated nanoparticles (Ag, $NiFe_2O_4$, and Fe_2O_3) not reported during the generation of the PTML-ANN model were used as cases of study.[3] The experimental conditions of these new nanoparticles involved the assessment of cytotoxic and/or ecotoxic effects. The PTML model could accurately predict the different toxicity endpoints of the new nanoparticles.

Conclusions

The present PTML-ANN model is a computational tool that can be used to assess the regulatory used of different nanomaterials.

References

1. W.J. Stark, P.R. Stoessel, W. Wohlleben and A. Hafner, *Chem. Soc. Rev.*, 2015, **44**, 5793.
2. M. Ajdary, M.A. Moosavi, M. Rahmati, M. Falahati, M. Mahboubi, A. Mandegary, S. Jangjoo, R. Mohammadinejad and R.S. Varma, *Nanomaterials (Basel)*, 2018, **8**.
3. V.V. Kleandrova, F. Luan, H. Gonzalez-Diaz, J.M. Ruso, A. Speck-Planche and M.N.D.S. Cordeiro, *Environ. Sci. Technol.*, 2014, **48**, 14686.