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Computational methods for predicting genotoxicity of metal oxide nanomaterials (A classification and regression tree model for predicting comet assay results)

Nazanin Golbamaki[1], Aggelos Avramopoulos[2], Azadi Golbamaki[1], Bakhtiyor Rasulev[3], Mark Cronin[4], Antonio Cassano[4], Emilio Benfenati[1] and Jerzy Leszczynski[3]

[1]The Mario Negri Institute, Italy
[2]National Hellenic Research Foundation, Greece
[3]Jackson State University, USA
[4]Liverpool John Moores University, UK

Nanotechnology is currently utilized in many areas of industry, medicine, and military applications. Nanomaterials can be viewed as a new type of "atom" with size dependent physicochemical, optical and electronic properties that make them suitable for a wide variety of applications. The same properties that make these particles exciting for technological research and development may also make them problematic from a toxicological perspective. Due to the rapid growth in the nanotechnology industry there, is an urgent need to define hazard identification and risk management strategy for nanomaterials. Developing rapid methods for predicting the toxic behaviour and environmental impact of these nanomaterials is therefore important and timely. Computational methods such as Quantitative Structure-Activity Relationships (Q-SAR) and Read-Across to screen and prioritize chemicals in both the development and safety assessment stages are promoted by different chemical legislations (e.g. REACH legislation). There are many open questions in the field of QSAR models for nanomaterials, among which the choice of appropriate descriptors to the nanomaterials. Molecular descriptors are at the very core of the QSAR analysis, since they establish a causal link between the chemical structure and the observed property, by mapping the structure of the compound into a set of numerical or binary values representing various molecular properties that are important for explaining the activity or property of the molecule. Based on a collection of genotoxicity profiles performed by the authors, we developed a data set containing 15 nano metal oxides, for which results of the genotoxicity test comet were available in the literature. In this work we performed quantum chemical calculations on these metal oxides and found descriptors that are highly correlated with the observed genotoxicity in the comet assay. An initial pool of about thirty descriptors for each NP was built and used to build a QSAR model. A predictive model based on Classification and Regression Tree (CART) was developed. CART analysis is a recursive partitioning method that builds classification and regression trees for predicting continuous dependent variables (regression) and categorical predictor variables (classification). The current model shows a good correlation between selected quantum chemical descriptors and genotoxicity which can be useful in predicting the genotoxicity of new and untested metal oxide nanoparticles.

nazanin.golbamaki@marionegri.it