

## **SciForum** MOL2NET Nanoparticles mutagenicity: search for matches and potential limitations of Comet assay and Ames test

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## Abstract

One of main problems of nanotoxicology is related to difficulty in selection of the most appropriate mutagenicity test. For instance, it is an open question, whether or not Ames test is relevant for nanoparticles. The major principles and mechanisms of action supposed to be different, because Ames test is based on prokaryotic responses, while other available methods are based on eukaryotic cells. Mutagenicity of 28 silica- and metal oxide nanoparticles was evaluated by means of combination of supervised and unsupervised learning techniques. Classification models were developed for mutagenicity of nanoparticles in Ames and Comet tests. Quantitative comparison of results was followed by self-organizing map modeling. Self-organizing maps were employed to find topology of a whole data set on the basis of developed classification models and known endpoints. It was found, that ionic characteristics were responsible for mutagenicity. Data visualization technique was helpful to understand specific interactions between important descriptors in different models. For series of untested NPs mutagenicity/safety were predicted.

## Keywords

Nanoparticles, Ames test, Comet, classification, modeling, QSAR, toxicity, mutagenicity