

REVIEWER'S REPORT

Manuscript No.: IJAR-52056

Date: 04-06-2025

Title: Physicochemical Feature-Driven Nanotoxicity Prediction Using Supervised Machine Learning Algorithms

Recommendation:

Accept as it is.....**YES**.....
 Accept after minor revision.....
 Accept after major revision
 Do not accept (*Reasons below*)

Rating	Excel.	Good	Fair	Poor
Originality		√		
Techn. Quality		√		
Clarity			√	
Significance			√	

Reviewer's Name: Mr Bilal Mir

Reviewer's Decision about Paper: **Recommended for Publication.**

Comments (*Use additional pages, if required*)

Reviewer's Comment / Report

General Overview:

The manuscript presents a data-driven machine learning framework for predicting the toxicity of metal oxide nanoparticles using physicochemical features. The study addresses a critical need in nanotoxicology for faster, cost-effective, and scalable assessment methods. By evaluating multiple supervised learning models and identifying key predictive features, the work contributes meaningfully to the integration of computational approaches in nanomaterial risk assessment.

Abstract Evaluation:

The abstract is concise, informative, and clearly outlines the research problem, methodology, key results, and implications. The mention of specific nanoparticles and algorithms gives context and scope, while performance metrics and feature importance provide concrete evidence of the study's effectiveness.

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Introduction Evaluation:

The introduction effectively contextualizes the importance of metal oxide nanoparticles in various industries and the urgent need for improved toxicity assessment methods. It references relevant applications and physicochemical attributes that underpin nanoparticle utility, setting a strong foundation for the study's focus on machine learning-driven prediction.

Methodology and Data:

The study employs a well-structured approach using nine physicochemical descriptors and six distinct supervised learning algorithms. The choice of algorithms reflects a good balance between interpretability and predictive power. The inclusion of multiple performance evaluation metrics (accuracy, ROC curves, precision-recall, confusion matrices) demonstrates rigorous model validation.

Results and Interpretation:

The Decision Tree model's superior accuracy and interpretability are clearly presented and justified. Feature importance analysis highlights biologically and chemically relevant factors—dosage, number of oxygen atoms, electron affinity—which aligns well with established scientific understanding of nanoparticle toxicity.

Scientific Merit and Relevance:

This research contributes to advancing predictive toxicology by leveraging machine learning techniques, thereby potentially reducing reliance on traditional in vitro and in vivo assays. The findings hold practical significance for nanomaterial design and regulatory frameworks.

Clarity and Organization:

The manuscript is well-organized, with a logical flow from introduction through methodology to results. The language is precise and technical, suitable for an audience familiar with nanotoxicology and computational modeling. Key terms are well-defined, and explanations are coherent.

Terminology and Language Use:

Scientific terminology is appropriately used throughout, reflecting current literature and domain standards. The manuscript maintains formal academic language with clarity, avoiding ambiguity.

Conclusion:

The study effectively demonstrates the feasibility and advantages of using physicochemical descriptors coupled with supervised machine learning algorithms for nanotoxicity prediction. The clear identification of influential features and model robustness supports its potential application in safer nanomaterial development.

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Overall Assessment:

The manuscript presents a valuable, methodologically sound, and clearly articulated contribution to the field of nanotoxicology and computational toxicology. It meets academic standards and is well-suited for publication in a relevant scientific journal.