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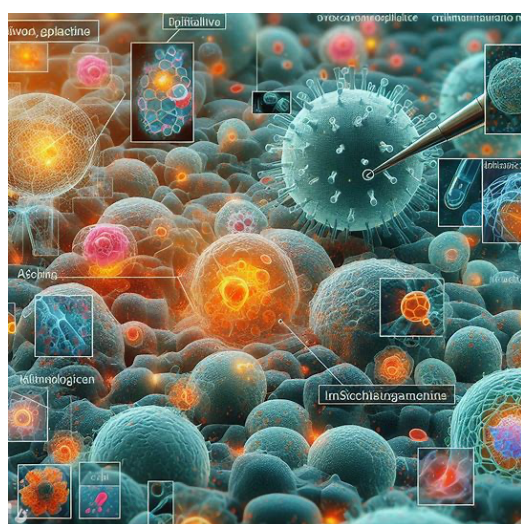
## Innovative Integration of Perturbation Theory into Machine Learning Models for Advanced Prediction in Nanotoxicology and Nanomedicine

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### Graphical Abstract



### Abstract.

The application of Perturbation Theory in machine learning (PTML) models was investigated to address various problems in nanotoxicology and nanomedicine. The article by Halder et al. (2020) proposes an in-silico model based on PTML to evaluate the genotoxicity of metal oxide nanoparticles, achieving high precision and predictive capacity, thus revolutionizing the safety evaluation of nanomaterials. Munteanu et al. (2021) applied PTML to predict the effectiveness of drug delivery systems in the treatment of glioblastoma, obtaining accurate results and

suggesting the applicability of this approach in nanomedicine. Finally, the study by Santana et al. (2020) used PTML in the design of drug delivery systems, highlighting its efficacy and specificity, with the PTML-RF model showing higher sensitivity and accuracy. These findings support the widespread utility of Perturbation Theory, and PTML in particular, as an advanced tool in the prediction and design of nanomaterials and drug delivery systems, with potential significant implications for the safety and efficacy of these technologies (Halder et al., 2020; Munteanu et al., 2021; Santana et al., 2020).

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