AI for toxicology: in silico tools to reduce experimental testing

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The rapid development of nanotechnology in areas such as biomedicine, electronics, and advanced materials has significantly increased the need to understand the potential toxic effects of engineered nanomaterials. Assessing nanoparticle toxicity remains a complex challenge because their biological impact depends on a wide range of physicochemical properties, including size, surface chemistry, and experimental exposure conditions. Traditional toxicological evaluation, particularly in vivo testing, is often costly, time-consuming, and raises ethical concerns, highlighting the importance of complementary approaches that can help guide experimental work.

This work explores how data-driven methods can support nanotoxicology by identifying patterns between nanoparticle properties and biological responses. After briefly introducing the role of machine learning in toxicological research, I will present a case study focused on predicting the toxicity of nanoparticles from physicochemical descriptors.

The study uses an experimental dataset derived from in vitro assays evaluating the biological effects of iron oxide nanoparticles and cerium dioxide nanoparticles. Several machine learning classifiers were trained to predict cytotoxicity and genotoxicity outcomes using physicochemical characteristics and experimental variables. Feature selection methods were applied to identify the most informative attributes influencing toxicity.

The results show that predictive models can capture relevant relationships between nanoparticle properties and toxicological outcomes, highlighting key variables such as hydrodynamic size and exposure conditions. Beyond prediction, these models can help prioritize experiments, guide safer material design, and contribute to the development of alternative strategies that reduce the need for extensive experimental testing.

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