Evidence-based prediction of cellular toxicity for amorphous silica nanoparticles

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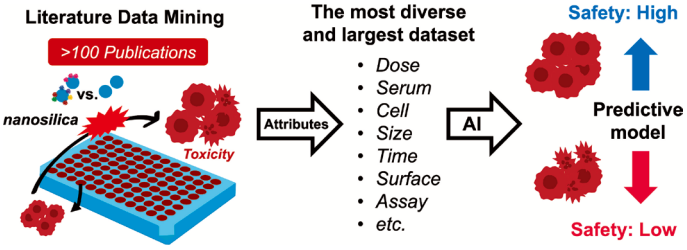
Abstract

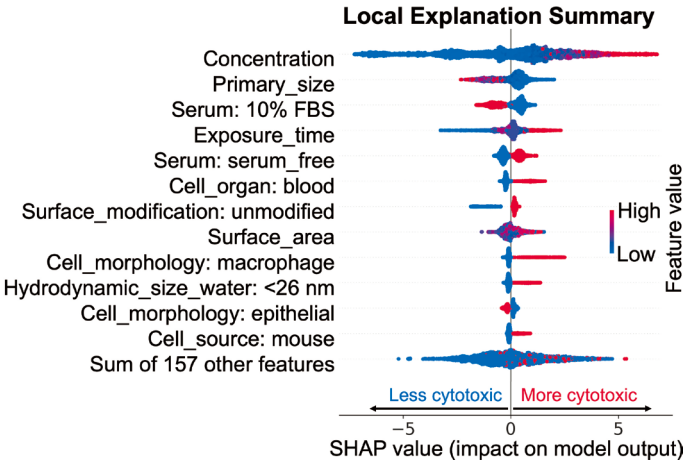
Our research group has established a new method using artificial intelligence for safer design of nanosilicas, a type of nanoparticle, by combining literature data mining and machine learning. The method established in this study is expected to contribute to the development of safer nanoparticle materials in various industrial fields.

Background & Results

The exponential growth in scientific literature, exemplified by the annual increase in publications, including last year's 34,000 papers in the nanomaterials field alone, as indexed in PubMed, underscores the sheer magnitude of knowledge being generated. This surge in information has reached a point where it transcends the capacity of any single individual to efficiently read and comprehensively understand. To harness the immense potential of this wealth of literature for nanomaterials, Artificial Intelligence (AI) emerges as a powerful tool that can significantly accelerate the process of designing safe and functional nanoparticles.

Our group has established a new method using AI to design nanosilicas (SiO2-NPs), a type of nanoparticle with diameter less than 100 nanometers or less, more safely. Specifically, by carefully collecting information from over 100 scientific papers and utilizing an advanced AI algorithm (CatBoost), we established a generic *in silico* prediction model for evaluating the safety of nanosilicas by combining literature data mining and machine learning. This research revealed several important factors that affect the safety of nanosilicas, including concentration, presence of serum, size, exposure time, and surface properties. The results showed that modifying the surface of nanosilicas and using them at low concentrations can significantly improve their safety.





Significance of the research and Future perspective

The motivation behind this research is to address the critical gap in considering the safety implications of nanoparticles' design conditions. While their widespread use has revolutionized various industries, including cosmetics, paints, textiles, and electronics, safety has not received adequate attention. By establishing a new evidence-based method using AI, researchers can distinguish between cytotoxic and noncytotoxic nanoparticles, thereby bearing significant implications to improve the safety of nanoparticles and enhance consumer confidence in everyday uses of nanomaterials. Through generation of nano-databases by literature data mining, future research can conduct high-throughput *in silico* screening to massive targeted discovery of functional nanoparticles such as selectivity towards cancer cells.

Patent
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