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研究成果報告書

(1) 事業名（下記より該当事業名を選択し、ほかは削除してください。）

共同研究員

(2) 研究代表者

氏名： MARTIN

所属機関名・部局名・職名： 北海道大学 化学反応創成研究拠点 博士研究員

(3) 研究課題名（申請時に記載したものと同一課題名を記入してください。）

Machine Learning-Assisted Design for Cellular Toxicity Profiles of Amorphous Silica Nanoparticles

(4) 蛋白質研究所受入担当教員

教員名： Kenji MIZUGUCHI

（研究室名： Laboratory for Computational Biology）

(5) 研究成果の概要

*背景および目的、方法と結果について、公開して差し支えない範囲で記載。

Nanoparticles (NPs) are valued for their unique properties across industries like cosmetics, paints, textiles, and electronics. Despite their benefits, NP toxicity to human health requires careful assessment. Although NP *in vitro* toxicity studies have been ongoing, a comprehensive evaluation of cell sensitivity across different systems and organs is lacking due to the associated time and cost.

Our work has pioneered a cost-effective and efficient *in silico* prediction model, using machine learning (ML) and literature data mining, to assess amorphous silica nanoparticle (SiO₂-NP) safety by predicting whether a SiO₂-NP at a given condition is cytotoxic or not. However, our previous binary model lacked the concentration nuances crucial for experimental work. Our new goal is to develop a ML-based method for quantitative prediction, establishing SiO₂-NP toxicity profiles across various cell types.

We have enhanced our dataset with quantified cell viability (%) values by manual curation and created a regressor model for cell viability (%) with an R-squared value of 0.89 and an RMSE of 10.32% through split-sample internal validation, and an R-squared value of 0.52 and an RMSE of 20.77% through external validation. This regressor model provides experimental researchers with the chance to conduct entirely *in silico* toxicity screening for candidate substances, reducing the need for many labor-intensive experiments and allowing a rapid development of safe SiO₂-NPs for biomedical applications.