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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。）

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（3）研究課題名（申請時に記載したものと同じ課題名を記入してください。）

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

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（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。

Selective killing of cancer cells using functional nanoparticles (NPs), while sparing healthy tissue, remains one of the central challenges in nanomedicine. Recent literature indicates that certain silica nanoparticles (SiO_2-NP) physicochemical profiles may induce selective toxicity toward cancer cells, suggesting the possibility of rationally designing silica-based nanomedicines that exploit cancer-specific vulnerabilities. To advance this direction, computational modeling capable of capturing subtle, nonlinear interactions between NP properties, biological contexts, and cellular responses is critically needed.

We expanded our previously published dataset, which includes 4124 samples from 115 publications, by manually curating and adding quantified cell viability (%) values. Using these quantified values, we developed an machine learning (ML)-based approach for the quantitative prediction of cytotoxicity for SiO_2-NPs, incorporating concentration dependencies that are vital for experimental researchers. However, it did not explore the model's potential to identify selectivity toward various cancer cells. Our new objective is to develop a new ML framework to identify selectively cytotoxic NPs, using SiO_2-NPs as a representative model case.

We have implemented sequential model-based optimization (SMBO) using extra-tree based optimizer to propose specific properties of SiO_2-NPs that show selective toxicity against cancer cells taking expected improvement (EI) as the acquisition function. We showed that high EI score could identify new sample point for cancer-selective properties, i.e., unmodified 20 nm SiO_2-NPs with 400 μg/mL against liver cells. Further validation with new experimental data provided by The University of Osaka is ongoing.