

# A local search approach to predict and optimize nanomaterial toxicity in early stage nanomaterial design

[Kostas Blekos](#)<sup>1</sup>, [Effie Marcoulaki](#)<sup>1</sup>

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## 1. Introduction

The rapid advancement of nanotechnology has led to the development of a wide range of engineered nanomaterials with unique properties and applications. Potential risks associated with human health and the environment remain largely unknown (Marcoulaki2021, Mancardi2023). To address this challenge, we propose a novel approach that utilizes local search techniques to predict and optimize nanomaterial toxicity during the early stages of nanomaterial design.

## 2. Nanomaterial Representation

Our approach leverages our recently proposed general and extendable representation for nanomaterials (Blekos2023), to greatly facilitate similarity assessments between components, which is crucial for calculating nanomaterial affinities. This representation forms the backbone of our local search methodology, which utilizes existing data on nanomaterial composition, structure, and toxicity to drive the identification and design of new nanomaterials with optimized safety profiles.

## 3. Local Search Approach

The local search approach is particularly well-suited for the complex and high-dimensional design space of nanomaterials. By efficiently exploring the neighborhood of known nanomaterials with desirable safety profiles, the algorithm can identify promising candidates that strike a balance between functionality and reduced toxicity. This targeted search strategy allows for the rapid discovery of safer nanomaterial designs, reducing the need for extensive experimental testing and accelerating the development process.

## 4. Bayesian-based Predictive Model

By integrating this local search framework with a Bayesian-based predictive model, we forecast the toxicological profiles of novel nanomaterials but also guide the iterative design process towards safer alternatives. As new data on nanomaterial toxicity becomes available, the model can be updated to refine its predictions and guide the search towards increasingly safer designs. This iterative feedback loop between the local

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<sup>1</sup> National Centre for Scientific Research "Demokritos", Greece; [mplekos@upatras.gr](mailto:mplekos@upatras.gr)

search algorithm and the predictive model ensures that the approach remains robust and responsive to the latest advancements in nanotoxicology research.

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## 6. References

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