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Predictive safety assessment of engineered nanomaterials

With the rapid development and numerous applications of engineered nanomaterials (ENMs) in science and technology, their impact on environmental health and safety should be considered carefully. This requires an effective platform to investigate the potential adverse effects and hazardous biological outcomes of numerous nanomaterials and their formulations. We consider predictive toxicology a rational approach for this effort, which utilizes mechanism-based in vitro high-throughput screening (HTS) to make predictions on ENMs adverse outcomes in vivo. Moreover, this approach is able to link the physicochemical properties of ENMs to toxicity that allows the development of structure activity relationships (SARs). To build this predictive platform, extensive analytical and bioanalytical techniques and tools are required. Herein, we described the predictive toxicology approach and the accompanying analytical and bioanalytical techniques. In addition, we elaborated several successful examples as a result of using the predictive approach.

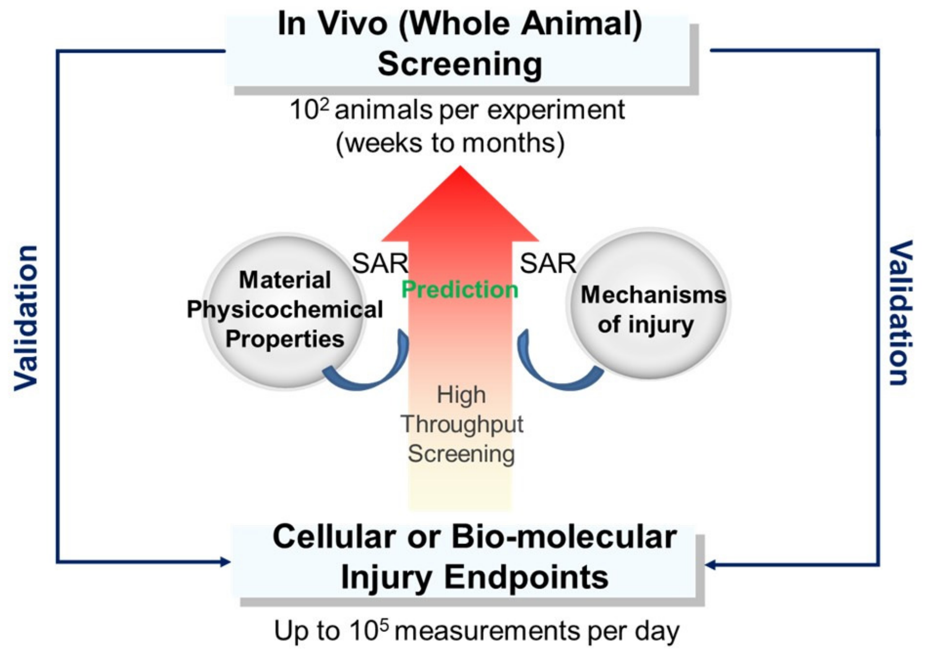

Fig. 1. The predictive toxicological paradigm for ENM hazard testing. This approach includes establishment of ENM libraries, in vitro cellular or bio-molecular assays using high throughput screening technique. Limited but focused in vivo animal studies are used to validate the in vitro results. The quantitative structure-activity relationships (SAR) could be established through data analysis.

Predictive toxicological approach includes the establishment of systematic ENM library, the in vitro cellular or bio-molecular injury mechanisms capable of predicting potential human and environmental hazard, and validation by limited but focused animal studies. These robust scientific paradigms, characterized by screening of multiple toxicants concurrently, was recommended to be an alternative testing approach to reduce costly animal studies examining one toxicant at a time. Consequently, this platform will facilitate design of safer ENMs for sustainable development of nano-applications.

Fundamental elements to establish a predictive toxicological paradigm

Four elements were necessary for establishing this predictive toxicological paradigm: (1) synthesis of compositional and combinational ENM libraries; (2) comprehensive physicochemical characterizations of ENMs; (3) use of in vitro high content and rapid throughput screening method and platform to assess the biological effects of nanomaterials and their related properties with the goal to link the properties to biological injury, and (4) validation of in vitro prediction through limited but focused in vivo studies to establish SARs.

Successful case studies of using predictive toxicology paradigms and HTS approach

We reviewed five cases of mechanism-based toxicological paradigms using established HTS and predictive toxicology approaches (Fig. 2). The first example is the study of toxicological profile of metal oxide (MOx) nanoparticles. The second example is the toxicity assessment for SiO_2 nanoparticles. The third example is the work with the engineered carbonaceous nanomaterials (ECNs), which includes carbon nanotubes (CNTs). Another example of ECN is the 2-dimension (2D) carbonaceous nanomaterials, e.g. graphene and graphene oxide (GO). The fifth example is the development of predictive toxicology paradigm for rare earth oxide nanomaterials (REO).

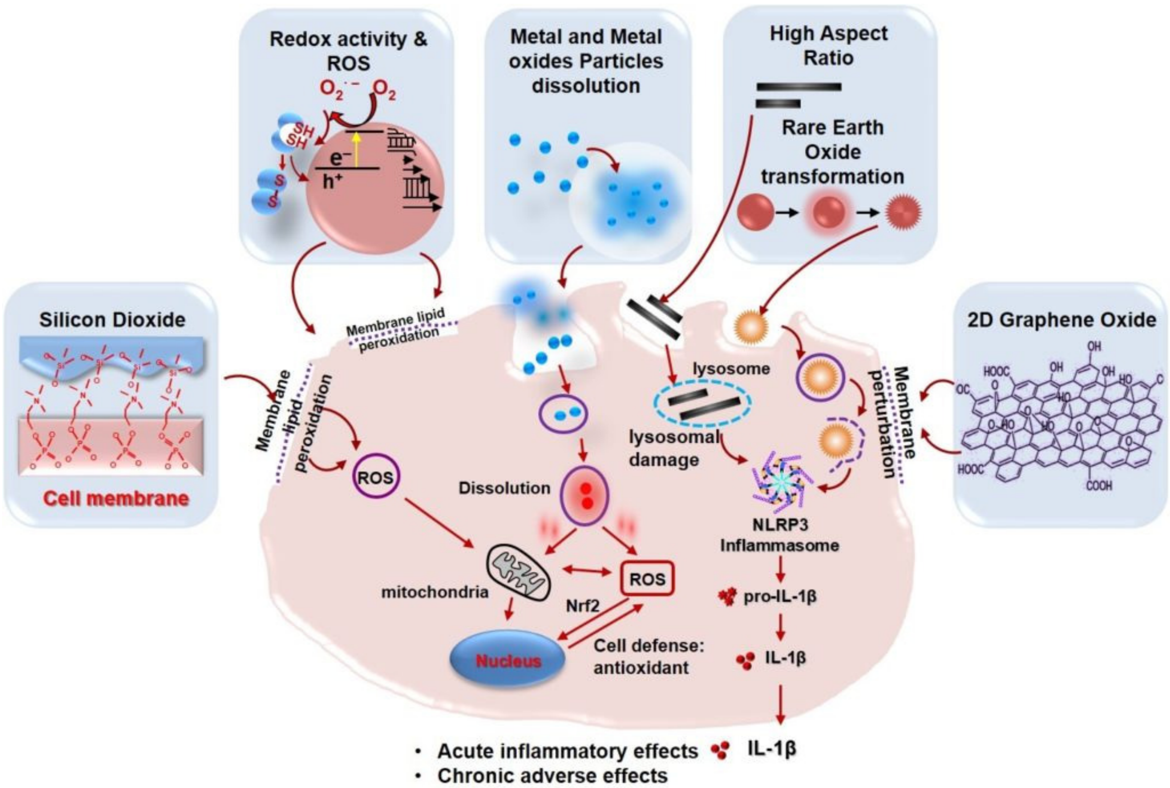

Fig. 2. Examples of mechanistic injury responses for HTS, including metal oxide nanomaterials, silica-based nanomaterials, carbon nanotubes, graphene oxide, and rare earth oxide.

Robust analytical techniques and assays are available for characterization of nanomaterial physicochemical properties abiotically, in vitro and in vivo effects, which are especially important to link to their properties to toxicity and build the structure activity relationships. Ultimately, the creative use of optimal techniques, and the toxicity screening approach we advocate, will provide valuable guidance for designing safer nanomaterials for their future applications.

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