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Trusting the Intangible: ecosystems monitoring and in silico techniques

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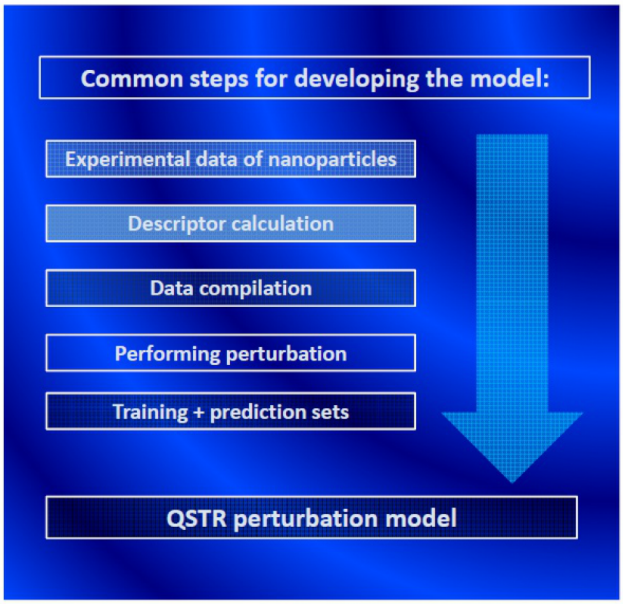
PURPOSE OF THE ABSTRACT

The toxicity prediction on sustainable nanoparticles (NP) /ecosystems interface in areas such as aquaculture or agriculture requires large experimental batteries of assays, due to the array of descriptors to assess. However, the experimental assessment of descriptors, such as composition or surface charge, is not only time consuming but also bearer of high economic costs. Several recently developed in silico models seemingly meet the needs of (1) short time results, (2) high efficiency in toxicity prediction, and (3) low economic costs, which are sought by industry and researchers alike. The present communication reviews the development of novel and feasible ecotoxicity prediction quantitative structure-activity/toxicity relationships (QSAR/QSTR) models in a wide range of ecosystems, including aqueous, and tested against several biotargets such as D. rerio embryos, microalga, RAW264.7 (Mouse) cells, or A549 (Human) cells, with experimental validation (i.e., determining the minimum percentage of correct classification for the predictive model) with results ranging from ninety-five percent and higher for the case of A549 (Human) cells [1-3]. These in silico models, which account for the NP pairs ecotoxicological profiles as consequence of intrinsic characteristics, experimental conditions and exposure time, represent the avenue for nanoparticle assessment regarding ecotoxicity and cytotoxicity.

FIGURES



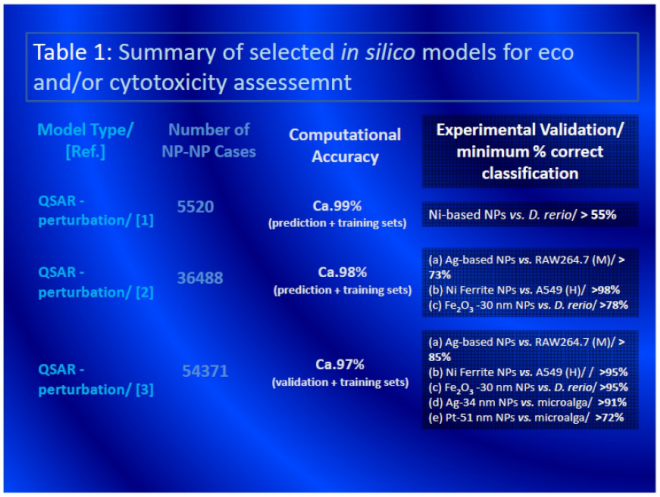


FIGURE 1

Development of the in silico model

Common steps in developing in silico models, namely QSAR-perturbation models, for environmental assessment

FIGURE 2

Synoptic Table

Summary of selected in silico models for eco and/or cytotoxicity assessment

KEYWORDS

in silico models | ecotoxicity | cytotoxicity | nanoparticles risk assessment

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