Chapter 50
Quantitative Nanostructure–Activity Relationship Models for the Risk Assessment of NanoMaterials

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ABSTRACT

In the last few decades, nanotechnology has been deeply established into human's everyday life with a great number of applications in cosmetics, textiles, electronics, optics, medicine, and many more. Although nanotechnology applications are rapidly increasing, the toxicity of some nanomaterials to living organisms and the environment still remains unknown and needs to be explored. The traditional toxicological evaluation of nanoparticles with the wide range of types, shapes, and sizes often involves expensive and time-consuming procedures. An efficient and cheap alternative is the development and application of predictive computational models using Quantitative Nanostructure-Activity Relationship (QNAR) methods. Towards this goal, researchers are mainly focused on the adverse effects of metal oxides and carbon nanotubes, but to date, QNAR studies are rare mainly because of the limited number of available organized datasets. In this chapter, recent studies for predictive QNAR models for the risk assessment of nanomaterials are reported and the perspectives of computational nanotoxicology that deeply relies on the intense collaboration between experimental and computational scientists are discussed.

INTRODUCTION

Due to their small size, nanoparticles, exhibit unique physicochemical properties compared to their bulk counterparts and have already found numerous applications in several biomedical and consumer products. Since the production of nanomaterials increases day by day, the probability that they could

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cause adverse effects to human health and the environment rapidly rises. In order to reduce the cost and time demanded for the experimental evaluation of toxicity, computational methods, such as Quantitative Structure-Activity Relationships (QSARs) are being used to predict the potential toxic effects of nanoparticles. In this chapter, the use of Quantitative Nanostructure-Activity Relationship (QNAR) modeling is discussed as a useful tool to predict the biological and toxicological effects caused by diverse types of manufactured nanoparticles (MNPs). Recent studies are reported summarizing the available predictive QNAR models for the risk assessment of nanomaterials (NMs). Finally, the perspectives and the future of computational nanotoxicology that strongly depend on the intense collaborations between experimental and computational scientists are discussed.

BACKGROUND

According to the U.S. National Nanotechnology Initiative (NNI), nanotechnology is defined as the understanding and control of matter at dimensions of roughly 1 to 100 nanometers, where unique phenomena enable novel applications. At this level, the physical, chemical, and biological properties of materials differ in fundamental and variable ways from the properties of individual atoms and molecules or bulk matter (NNI, 2000).

Nanotechnology has become one of the most promising areas of science and it has fairly emerged as one of the central new technologies in the 21st century, drawing worldwide attention (Haase, Tentschert, & Luch, 2012; Fourches, Pu, & Tropsha, 2011). Hitherto, nanotechnology is an important industrial sector in industrialized countries and it has been referred to as the next industrial revolution. The first national nanotechnology program (NNI) was launched in USA in 2000, to serve as the central point of communication, cooperation, and collaboration for all Federal agencies engaged in nanotechnology research, bringing together the expertise needed to advance this broad and complex field (Bondarenko, 2013). Nanotechnology has found numerous applications in materials science, medicine, cosmetics, or clothing, bioimaging, sensing and electronics (Fourches et al., 2011; Makarucha, Todorova, & Yarovsky, 2011). Nanomedicine, for instance, an emerging application of nanotechnology, provides the possibility of delivering small drug molecules to specific cells, by developing novel diagnostics and therapeutics (Wang, Byrne, Napier, & DeSimone, 2011).

Up to date, several classifications of nanomaterials have been proposed. According to the European Committee for Standardization (CEN) Technical Specification, nanomaterials can be classified into two broad categories, namely nanoobjects and nanostructured materials (Figure 1) (Haase et al., 2012).

According to Hansen, Larsen, Olsen and Baun (2007) and depending on the location of the nanoscale structure in the system, nanomaterials are organized into three broad categories, as it depicted in Figure 2.

For simplicity, nanomaterials can generally be organized into four types (Messina, Olsina, & Stege, 2013):

1. Carbon-based materials,
2. Metal-based materials, including metal oxides and quantum dots,
3. Dendrimers, and
4. Composites.