ISSN: 2640-5571

Short communication

Advances in Nanoscience and Nanotechnology

Computational Modelling: A New Era to Predict Nanotoxicity

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Submitted: 16 Jan 2019; **Accepted:** 22 Jan 2019; **Published:** 05 Feb 2019

Nanotechnology is the use of technology in a nanoscale level, which involves figment of matter within 1 to 100 nanometers at least in one dimension. Materials in nanoscale size exhibit different properties when compared to macro scale counterparts, enabling them to be used in unique ways. Nanomaterials have very small size but high surface area, and have several advantages over bulk materials. Therefore they are suitable for widespread application in commercial products.

Since early 1990s nanotechnology is being used in commercial products. Due to their unique properties, engineered nanomaterials (ENMs) are being used in nearly all sectors of manufacturing. For example, there are several consumer products and industrial applications of nanotechnology comprising nanoelectronics, nanomedicine, molecular assemblies, tissue engineering, antibiotics, nanocomposites, personal care items, cosmetics, paints, textiles, pesticides, electronic materials, food items, sports tools, water purification modules and many more. Initially there were about 800 commercially available nanoproducts globally, which increased to 1700 by 2014, and expected to exceed 3000 by 2020 [1].

Although the engineered nanomaterials (ENMs) are beneficial in several aspects, increasing production of engineered nanoproducts and their applications have increased concerns of their impacts on living organisms and on the environment. It is very important to have knowledge on subsequent toxic effect of nanomaterials on living organisms and on environment before its application. From several evidences on toxic effects of engineered nanomaterials (ENMs), it was found that some of them impose detrimental toxic hazards on living organisms even on humans. These studies necessitate development of scientific research on the subject- nanotoxicology as evidences indicated more toxic effects of ENMs than their naturally occurring counterparts.

One of the most important aspects of the nanotoxicological research is the lack of standard methods for testing and evaluating their observed effects on different organisms and the environment. There are no specific criteria to study nanotoxicity; researchers are used to set the parameters according to their convenience. Mainly *in vitro* and *in vivo* approaches have been taken to measure toxicity of ENMs. But recent studies have shown a small relation of the *in vitro* study with *in vivo* toxicity of engineered nanomaterials (ENMs). *In vitro* tests cannot predict probable toxico-kinetic of the materials in the body system that can be accepted as indicators of toxicity. Where as *In vivo* tests can predict the real world scenario, but they are time-consuming, expensive, and may evoke ethical issues.

On the contrary if we can develop some in silico modelling methods, by which we can predict toxicity of a newly synthesized nanomaterial by computer simulation, it can save our time and money. Development of computer simulated models to predict nanotoxicity has started from the mid 2000s; most of them are based on structure-activity relationships.

The engineered nanomaterials (ENMs) have specific structural properties, therefore they show specific characters, and toxicity is one of them. Their properties vary with their particle size, particle shape, size distribution, zeta potential, surface area and crystalline structure etc. Quantitative structure–activity relationships, referred to as QSARs, is a computational technique which endeavour to predict the biological activity of a compound by considering its relation to a set of physical and compositional properties (such as particle size, particle shape, size distribution, zeta potential, surface area and crystalline structure etc.) . The basic principle behind the QSAR studies relates with different types of nanotoxic effects with measurable or calculable physico-chemical parameters. QSAR models can predict the unknown activities (such as toxicity) of a newly synthesized nanomaterial, by relating the structure and respective activity using a suitable computer simulated mathematical model.

At first structure of engineered nanomaterials (ENMs) and their related activities are summarized from ongoing research papers. Several databases are also available, from where data on nanotoxicity can be obtained (e.g. - ISA-TAB Nano, eNanoMapper, Nano Material Registry etc.) [2]. In QSAR model, the mathematical objects, which are called molecular descriptors, are clearly described. These descriptors must have calculable values and they are related with some properties of nanoparticles: such as particle shape, size, surface area, particle surface property, ionization potential, zeta potential etc. They can be derived from semi empirical methods or from commercial softwares. These molecular descriptors can provide a great variety of information and helps to understand the relationship between molecular characteristics and biological activities. At the same time, a subset of the identifiers associated with toxic properties (e.g. cell apoptosis, cell death, metabolic changes, developmental disorders etc.) is selected and modelled using mathematical techniques. Multivariate linear regression model

is the choice to discover QSARs between different physicochemical properties of a given material and assessment of the responses of exposed biological system. By using these models the probable effects of a newly synthesized nanomaterial can be predicted easily. Finally, the accuracy of the model is assessed using statistical cross-validation techniques.

The computer based QSAR models not only save time, but also save money and do not evoke ethical issues. They are fast and cost effective. Though the QSAR models regarding nanotoxicity is still in developing stage, but the results are promising [3-9].

The future of computational modelling to predict nanotoxicity is very promising. But the only problem is the lack of standard methods for testing and evaluating their observed effects. The nano QSAR models will be more fruitful, if all the researchers use the same kind of determinants for quantifying the nano characters and properties. Several databases are also available regarding nano toxicological studies, but they are not customized for a wide variety of use. The databases also need to be standardized. It requires interaction and data sharing between different researchers globally. Development of a universal protocol for nanotoxicology research will make this kind of research more effective. Using the universal protocol any researcher will be able to predict the potential toxic effects of engineered nanomaterials (ENMs) before their manufacture and use.

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