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A Review

Nanoinformatics - A newly introduced tool for research

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Research in the field of nanotechnology has witnessed rapid increase in the synthesis of Engineered nanoparticles (ENPs). This has even led to development of new discipline of Nanotoxicology. Advances in the field of Nanotoxicology further led to development of new domain-nanoinformatics. This new domain of nanoinformatics provides a computational perspective to biology and nanotechnology addressing multi level integration. Nanoinformatics not only helps in predicting nanoparticle structure, composition and behaviour but also covers raw data management, analysis of data derived from biomedical applications and simulation of nanoparticle interactions with biological systems. In addition, it accelerates nano-related research and applications into clinical practice. There are various computational models developed to study the key steps in nano-medicine like drug encapsulation and release, nanoparticle targeting, delivery and uptake and nanoparticle effects on cells and tissues. These prospects have opened up a large domain enabling possibilities of nanomedicine and frontiers for clinical practice and biomedical research in a cost-effective manner along with various applications including studies in clinical trials, toxicity assays, drug delivery systems. This review highlights new approaches for Engineered nanoparticles (ENP) risk assessment and regulation.

Keywords: Computational methods, Drug delivery system, Engineered nanoparticles (ENP), Nanoinformatics, Nanotoxicology, Risk assessment

Introduction

Nanoparticles (NPs) have wide applications in diverse fields and therefore there is an exponential increase in number of studies involvedusing the nanoparticles[1]. Last few years have seen an increase in the synthesis of engineered nanoparticles (ENPs) on an average of 10-10^5 tons per year[2]. Even the global market of nanoparticle-based products[3] indicatethe same fact. Although, the unique properties of nanomaterials hold promise for many applications, but at the same time it also raises safety concerns for human health. These ENPs exhibit the ability to penetrate the human cells and flow in bloodstream which may lead to undesirable effects on the metabolic systems[4]. ENPs can exert their toxic effects by interacting directly with DNA or other biomolecules as they enter the cells *via* penetration through cell membrane[5]. The damaging effects of ENPs were also observed on plant organs, changing the length of stem, root and affecting plant growth. Many reports have documented the effects of ENPs through food chain revealing toxicity in the ecosystem[6]. Hazardous properties of nanoparticles depend on particle size, surface area, surface chemistry, crystalline structure, aggregation in media, and purity of these NPs. The risk profile of these nanoparticles is becoming challenging and precarious taking their life cycle into consideration. Unexpected results further add to the challenges of risk assessment as they may lead to serious miscalculations. Enthusiastic research on nanoparticles led to their revolutionary usage without prior knowledge about their behavior and prospective toxic effects. Insurgent usage of nanoparticles can be alarming for human health[2]. It is imperative to check biological effects of nanoparticle-based products on human health and environment from production, transportation, and recycling till disposal.

The main concepts on nanotoxicology were developed around 2004[7] for careful evaluation regarding sustainability and risk production of nanoparticles. There are two main strategies for toxicological evaluation: a) To test every single type of nanoparticle produced b) Predicting nanoparticle behavior with regard to its structure and composition[8]. Assessing the safety of nanoparticles through experiments is time consuming, therefore, computational methods offer a better alternative. The predictive modelling of nanoparticle risk assessment

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