COMPUTATIONAL MODELING IN NANOTOXICOLOGY

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Abstract

Experimental in vitro and in vivo testing in modern toxicology might be significantly supported by the application of computational modeling (in silico studies). Such strategy helps to reduce cost, time and the use of laboratory animals.1, 2

Among various in silico techniques there are: (i) methods based on classical mechanics (i.e. molecular mechanics and molecular dynamics); (ii) methods based on quantum mechanics (i.e. ab initio, semiempirical and Density Fucntional Theory calculations); and (iii) chemoinformatic methods (i.e. Quantitative Structure-Activity Relationships modeling, grouping and read-across).1, 3, 4

Because of specific features and behavior of nanoparticles, computational methods originally developed for regular chemicals cannot always be applied explicite in nanotoxicology. Necessary adjustments have to be made.2, 5, 6 The lecture will discuss the current state-of-the-art and future needs in the development of computational modeling techniques for nanotoxicology.

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