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Convergence of nanoinformatics nanobiotechnology and bioinformatics

Abstract

Deploying tools in bioinformatics and computational chemistry to standardize, analyse and store nanobiotechnological information has gained rapid prominence after the discovery and application of DNA genomics in therapeutics. The current and traditional principles of nanobiotechnology, together with bioinformatics and analytical computational chemistry have converged into an exciting biomedical field called nanoinformatics. This review looks at this emerging sub-discipline of nanoinformatics and its intersection with nanobiotechnology in medical science in general.

Keywords: nanobiotechnology, nanoinformatics, bioinformatics

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Introduction

The medical applications of information systems sciences (i.e. informatics) have gained prominence as essential sciences in nanobiotechnology research, and have become particularly suitable in generating the appropriate research design frameworks. While these two concepts rely on computational and DNA analyses as well as protein sequencing, nanoinformatics specifically relates to the characterization of particles with applications in nanobiotechnology using strategies in computational and analytical chemistry. The introduction and application of contemporary information science techniques in solving problems in nanobiotechnology is likely to accelerate the discovery of tailored treatments, markedly reduce their side effects, and generally enhance their therapeutic efficacy. The conglomerate of these varied advantages has precipitated the concept of nanomedicine, which has also advanced exponentially in recent years. The discussions below will look at the convergence of nanobiotechnology and nanoinformatics by dissecting the disciplines into key thematic areas, followed by a discussion of the challenges, applications and future prospects in empirical nanobiotechnology and bioinformatics.

Intersection of nanobiotechnology and nanomedicine

Nanomedicine today has branched into various sub-disciplines, with a focus on manipulating nanosized structures at the molecular level, all geared towards deriving new and more benefits to medicine.[1] These sub-disciplines have primarily focused on monitoring and evaluating the myriad of emerging methods for drug administration and treatment.[2,3] The exponential generation of nanoscale data have also enabled multiband interdisciplinary disciplines to harness skills in creating new nanoparticles with relevant biomedical applications. The generation of this data, however, demands a thorough analysis, not only of their physicochemical properties, but also extensive structural characterization,[2] requiring massive input and utilization of computational skills and resources.

For these reasons, the field of nanoinformatics has emerged to develop both the computational tools and skills required to support the empirical analysis of the massive information generated in the field.[4]

In this regard, the Bio-Informatics Resource Inventory (BIRI) has become a useful initiative in indexing bioinformatics resources. This inventory is currently deployed in the European Commission-funded Action Grid Project (AGP). Earlier studies have established a network of bio-links where the disciplines and sub-disciplines converge in a complex biomedical system as shown in Figure 1 below.[5]

The field of nanomedicince is broad and complex, requiring the need to extract, process, analyze, and evaluate massive information arising out of informatics. With this in mind, the new challenges associated with biomedical informatics (BMI) will have to be resolved by converging nanoinformatics with techniques primarily around information and communication technologies (ICTs).[6,7] Further, bioinformatics (databases/-omics), information technology and computational chemistry using modeling and simulation can be employed to evaluate the different nanosystems in therapy and diagnostics. Currently, this area has not been rigorously exploited not only due to the complexities of the various biological systems, but also because of the skills, expertise, as well as the multidisciplinary efforts required to derive new complex models for elucidating the varied phenomena at the nanoscale level.[8]

Computational techniques and challenges in nanoinformatics

During the early stages of nanoscale project development, a computational approach comes in very handy. As a powerful technique, it can be used in designing transport systems for drugs and molecular devices.[3] In recent years, the stoichiometry of new nanomaterials has been successfully utilized in conjunction with the increasing use of computational molecular design techniques;[9,10] this has been possible because of the increased capacity, and the convergence of a number of methodologies utilizing computational chemistry.[10] Computational chemistry has also helped in the design, modeling and simulation, of nanomaterials,[11] nanoparticles,[12] metallic nanoparticles,[13] nanospheres,[14] nanocapsules,[15] and quantum dots.[16] These nanosized particles are currently being used as carrier for early diagnosis in nanomedicine.[16] In modeling and simulation, the application of molecular dynamics requires an accurate characterization of the physico-chemical properties[17,18] of the nanosystem, in order to obtain accurate results about the structural dynamics at the atomic level.
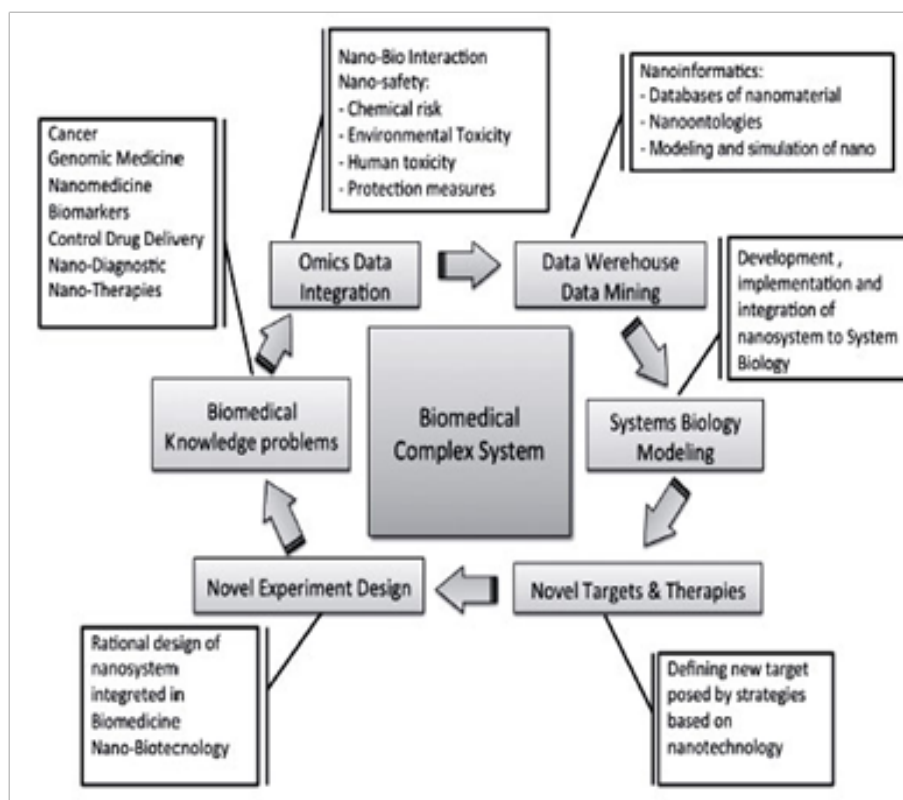
Figure 1 Schematic illustration for the convergence of different nanoscale disciplines and sub-disciplines from biomedicine to nanobiotechnology in a biomedical system.

Analytical computational mechanics can be deployed in determining the optimized structure of nanomaterials. This method uses a molecular model where spheres and springs depict inter-spatial atoms and bonds respectively.[19] Hence, modeling at the nanoscale level requires accurate coordinates for both the organic and inorganic components of the nanostructures.[18] These characteristics are extremely important in the 3-dimensional structural representation of nanostructures. Computational molecular chemistry also deploys quantum mechanics to predict the structure of nanomaterials, and to quantify the different descriptors that depend on the electronic nomenclature of the system.[18] Notwithstanding the appropriateness of these methods, they are limited by the time required for the calculations.[19] For this reason, quantum mechanics would require new methods or an adaptation of the traditionally used techniques in order to become relevant in contemporary nanoinformatics.

Over the past 30 years, the different approaches in computational chemistry used for designing nanoparticles have been very diverse. For example, some earlier researchers have used modeling and simulation techniques to study the size, structure, and characteristics of nanoparticles.[19] Such characteristics posit an essential role when deployed as carriers in systemic transport. Another classic example of advanced computational chemistry is the use of a biopolymeric membrane in designing a drug delivery vehicle.[20] Overall, it seems reasonable to point out, that designing suitable nanosystems requires contemporary and analytical computational chemistry, or adaptation of the available traditional ones, in order to generate workable procedures or protocols.

Conclusion

The evolution and rapid emergence of bioinformatics around biotechnology-related problems has helped in exploring complex biomedical and biophysical challenges, from genomics to protein structure. While the intersection of biotechnology and nanotechnology seems to pose new challenges to modeling designs, a number of concepts developed over the last three decades in computational chemistry could be merged in order to facilitate speedy research and understanding in the emerging fields of nanobiotechnology and nanomedicine. While admitting that the applications of nanomedicine and biotechnology requires sophisticated approaches to manipulate data at the molecular level; these complex approaches could best be handled through the creation of networks of geographically distant research scientists via "nano web seminars", in disseminating and discussing the information and knowledge generated. In designing accurate nanosystems, concepts such as ontologies, genomics and bioinformatics, could be merged with computational chemistry, to generate the sub-discipline of nanoinformatics. It is expected that most of the computer-related techniques in nanobiotechnology and nanoinformatics would accelerate discoveries specific for biomedical treatments in a bottom-up approach.[21]

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Conflict of interest

The author declares no conflict of interest.

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