Mini Review

Open Access

A review on application of nanoinformatics and bioinformatics in nanomedicine

Abstract

The field "Nanoinformatics" is emerged recently to analyze the requirement of computing applications at the scale of 10^-9. In this regard, initiatives were given in this review to identify challenges in implementation. The field of "nanomaterials" provided the possibility for the development of modern devices in medical industries to work in diagnosis, prevention and treatment of diseases. In this chapter, the application of nanoinformatics was discussed in detail with a focus on nanomedicine. Along with the existing applications of bioinformatics, efforts were also taken to incorporate the usage of the science behind informatics to extend the knowledge on basics of biological and clinical applications in nanoscience and nanotechnology.

Keywords: nanoainformatics, nanomaterials, nanomedicine, nanoscience, nanotechnology and bioinformatics

Volume 6 Issue 3 - 2020

Harishchander Anandaram, Aarthi Rashmi B
Department of Bioinformatics, Sri Krishna Arts and Science College, India

Correspondence: Harishchander Anandaram, Department of Bioinformatics, Sri Krishna Arts and Science College, Coimbatore, Tamilnadu, India, Tel +91-9940066227, Email harischandera@skasc.ac.in

Received: November 02, 2020 | **Published:** December 11, 2020

Introduction

Over the past decade many methods in computing based applications have been worked in the context of biomedicine to initiate research in the interdisciplinary areas such as bioinformatics, medical informatics and etc.[1–3] The application of informatics in the biomedical-related disciplines involves a wide range of technological and scientific approaches to solve complex problems on the basis of biomedical ontologies, integration methods and vocabularies. The basics of interdisciplinary fields work in the areas of data analytics, text mining and interoperability of systems. The applications of interdisciplinary research includes the sequencing of DNA and RNA, helps in analysis of clinical data, predicting the relationship between the mutations in the genes associated with diseases, the development of standard systems for the representation of data for exchange and the development of servers and tools for integrating the multilevel data with a multi-scale simulations of biomedical systems. The contribution of informatics in the above mentioned areas lead to obtain outstanding results in the projects of omics and human genome, the applications of using the advanced computers in clinical practice for decision support was active in the research of bioinformatics and medical informatics[4] to support various projects towards the development of the expert systems in clinical diagnosis.[5–9] In this context, the challenging and the unexplored concept is the application of computing to nanomedicine. Advancements in this research require the development of a knowledge based management system. The significant research areas in nanoinformatics are characterization of nano particles, modeling and simulation, imaging, development of terminologies, ontologies and standards, development of standards for data integration and exchange, interoperability of system, establishment of standards in big data analytics and machine learning, establishment of standard protocols to link the basic and the translational research in the science of nano-information to computerized medical records and to establish a networks of international researchers, projects and labs.[10,11] Nanoinformatics was recently emerged to analyze issues in processing information about the structure and the physico-chemical properties of nanomaterials and their interaction with the environment in the application of nanomedicine.[10,11] Such new applications emerge in a time where genomic and personalized medicine are still getting recognition, and promise additional future perspectives for biomedicine.

The term "nanoinformatics" in this chapter, is different from the related terms "nanomedical informatics" and "biomedical nanoinformatics". Nanoinformatics is also related to other applications of nanotechnology but in this chapter the term is referred for biomedical applications. Future aspects of challenges in nanoinformatics involve the understanding of the development of toxicity in therapeutics.[12–15] Nanomedicine includes a large number of practical aspects in the significant topics with a scientific impact on the early detection of diseases like cancer and the development of methods for a new molecular imaging based on the optical properties of nanoparticles to control the dosage by the application of nanorobots. In future, nanomedicine can overcome the limitations of solubility in the existing and new drugs.[8–14] Research in nanoinformatics involves efforts in managing the information of nanotechnology, like: (a) the lack of standard classifications for the nanomaterials, (b) the evolving knowledge of the complex biological, chemical and physical processes occurrences of molecular interactions at the nano scale, and c) the heterogeneity of the information content and structure of many scientific papers in the very diverse nano disciplines and subfields. All of these issues magnify the challenges of applying standard information extraction and retrieval methods to the literature without further additional knowledge of the specifics of the fields and subfields represented. New informatics approaches are needed to efficiently and effectively link information from nanomedicine, while addressing the various levels of complexity covered by research, development and translation in nanotechnology.

Knowledge and integration of data

The process of structuring the information in the field of nanomedicine is vital to initiate the advancements in research.[16–19] Though the term "nanoparticle" was introduced in the year 2007,[20–22] the controlled vocabulary was used in Pubmed for indexing and organizing the literature associated with the science behind the process of biomedical engineering. The process of structured vocabularies gave rise to the development of new ontology and taxonomies.[23–25] Other initiatives associated with nano technology include the

development of ontology for the discovery of new nanomaterials. The created ontology was named as the Nanotech Index Ontology. Proper annotation of nanoparticles in a web based system; allows professionals to access the information from a previous research and discover knowledge. These initiatives can expand the scope of ontologies in biomedical science and engineering like those included in the citations of the foundation of Open Biological and Biomedical Ontologies (OBO).[25]

Development of centre's

In the past decade, various research centre's were established to support inter disciplinary research like the Virtual Physiological Human (VPH) programme (Europe) and the National Centers for Biomedical Computing (NCBC,USA)[26–28] to support informatics and biomedical engineering in a global prospective. The research projects in VPH supports a large number of modeling and simulation of various systems, organs, tissues, cells of the body and their association to clinical applications. On the other hand, related efforts were taken in USA to match the research objectives. In both VPH and NCBC, basic and clinical researches were complement to each other. Many approaches in engineering and the development of tools for imaging, modeling signal processing, and simulation could be adapted in the future for the projects in nanoinformatics for modeling and simulating the behavior of nanoparticles to target the specific molecules within the human body or the development of a new imaging technique using quantum dots (QD) for clinical research and practice, as mentioned above. Various data repositories containing tools for modeling and simulation are already available for the applications of nanotechnology and the centre for data repository is called as the nanoHUB.[29] In contrast, the proprietary issues regarding the design and development of nanoparticle require an additional modification in computational approaches. The usage of open source softwares and tools in nanoinformatics could also facilitate linkage in future. In USA, the current facility is given in the cancer Nanotechnology Laboratory portal (caNanoLAB).[30] The nano hub includes applications for professional networking and development of interactive tools to perform simulation for nanotechnology. Similarly, the University of Talca, Chile in collaboration with the members of the Advanced Biomedical Computing Center, NCI-Frederick have developed a pilot database of the structures of nanoparticle as a part of the Collaboratory research unit for Structural Nanobiology (CSN).[31]

Establishment of standards

The ultimate requirement of a nanoinformatics infrastructure is to collect, curate, annotate, organize and archive the existing data. In addition to archiving the data, annotations and analysis from experts regarding its quality and extent of validity along with the federated system of layered access control to allow aggregation among public and private data. The development or expansion of tools, databases, software and repositories for nanoparticles, i.e. the information about their nanotoxicity, will allow the exchange of information about the actual 3-D structures of nanoparticles and nanomaterials. The data about the physical and chemical properties along with biomedical applications of nanoparticles will be present in the database.

Interoperability

The most important requirement of nanoinformatics is to federate the mostly isolated data in different institutions. caNanoLAB is a federated system, in this regard, the semantic interoperability of heterogeneous information systems containing a nano and other information will be a addressed as a key issue in nanoinformatics.[32] Similarly, the scientific literature related to nanomedicine is ill structured and hence the retrieval of information and extraction become a difficult task. Then, a related challenge involves the building of classifications for nanoparticles. Hence, the approaches in classification could be very helpful in creating new hierarchies and taxonomies based on actual characteristics of physical, chemical, clinical, toxic and spatial nature. Some scientists are currently working to develop a new taxonomy and ontology of "morphospatial" nature[33–35] by analyzing various examples from the images of biomedical studies. Current ontologies were based on the different types of data on the qualitative information but they cannot help in managing different, quantitative information on the shapes, forms and volumes for nanoparticles.

Virtual integration

The researchers in Biomedical Informatics have created a large number of tools to create models and perform simulation to aid the development of nanomedicine. Hence, the addition of significant information to understand the changes in the genotype induced by interaction of nanomaterials could possibly provide a new foundation for the analysis of phenotypical traits. Hence, a hypothetical "*nanotype*" could include a large catalog of biological targets, nanoparticles and their interactions along with the details of potential nanotoxicities and its relation to different diagnostic and therapeutic benefits in the field of medicine.[36–38]

Translational nanoinformatics

The field "nanomedicine" requires the next level of novel insights beyond the current technologies in informatics to focus on collecting, representing and linking the heterogeneous information. Another challenge is to develop a nomenclature for nanomaterials by analyzing the structures and information to incorporate new assumptions beyond the basic nomenclatures considered in biomedical instrumentations (BMI). Most of the current applications in nanoinformatics look very similar to the existing platforms built to develop bioinformatics but in nonoinformatics involves the analysis of nanomaterials of polymorphic and poly dispersed nature. Hence, there exist a substantial added requirement for the annotation and duration of data along with analyses by an expert to inform scientists about the quality and reliability of the data, along with the feasible test methods to analyze the models used in nanomedicine.

Nano information and electronic health record

The best challenge of nanoinformatics is to link the related data of nanomedicine to the EHRs of the patient. Development of a novel diagnostic and therapeutic methods based on the new nanomaterials can enhance the project proposals for the development of "personalized medicine" on the basis of advancements in OMICS. Management of the nano-related information requires the creation of potential tools for decision making along with the development of new models of EHRs. In order to accomplish the new extensions for current standards, tools such as SNOMED and HL7 must be developed to incorporate the terminologies and procedures of the nano-related information. Despite of the benefits of using nanoparticles for therapeutic purposes, the level of hazards for patient safety due secondary effects of nanoparticles should also be analyzed. In this context, the methods and techniques in nanoinformatics can contribute significantly to extract automatically to organize the specific information on nanotoxicology available in scientific papers. The extracted information can be used for various purposes, such as indexing and retrieving data in scientific papers with different entities to automatically finding relationships between the existing terms of

biomedical ontologies and nanoinformatics. Most of these researches actually address the challenges in (i) Data Management, (ii) Searches related to nano-ontologies and (iii) Extending traditional EHRs to include the nano-related information.

Conclusion

Fundamental issues still exist in understanding the new field of nanoinformatics. These include the applications of different techniques in computing in large number to cope with the different areas of nanotechnology. Recently, a large number of papers were already indexed in bibliographic databases for the development of nanomedicine and there are more number of companies along with nanotechnologists were working in the area of nanomedicine to advances in various aspects of biomedicine and understanding the ethical implications of research in nanomedicine. The importance of this field will allow the professionals to develop various computational approaches to address the challenges in nanoinformatics.

Future prospective

Data analysis in nanoinformatics involves the development of large databases to create standards for domain ontologies and mapping the related information to the computerized medical record and assimilating of new techniques medical imaging.

Requirement

In order to address the enormous challenges nanomedicine there is a requirement to make a significant investment to accelerate the current progress in research. The requirements of informatics are similar to the facilities provided for the genomic and post-genomic research projects that were transformed as biomedicine.

Funding details

No Funding was obtained to execute the project.

Acknowledgments

None.

Conflicts of interest

The author declares that there is no conflict of interest.

References

1. Altman RB. Bioinformatics in support of molecular medicine. Review. *Proc AMIA Symp*. 1998:53–61.
2. Kulikowski CA. The micro-macro spectrum of medical informatics challenges: from molecular medicine to transforming health care in a globalizing society. *Methods Inf Med*. 2002;41(1):20–24.
3. Kohane IS. Bioinformatics and clinical informatics: the imperative to collaborate. *J Am Med Inform Assoc*. 2000;7(5):512–516.
4. Maojo V, Kulikowski CA. Bioinformatics and medical informatics: collaborations on the road to genomic medicine? *J Am Med Inform Assoc*. 2003;10(6):515–522.
5. Maojo V, Iakovidis I, Martin-Sanchez F, et al. Medical informatics and bioinformatics: European efforts to facilitate synergy. *J Biomed Inform*. 2001;34(6):423–427.
6. Martin-Sanchez F, Iakovidis I, Nørager S, et al. Synergy between medical informatics and bioinformatics: facilitating genomic medicine for future health care. *J Biomed Inform*. 2004;37(1):30–42.
7. Kulikowski C, Weiss S. Computer-based Models of Glaucoma. Report no 3. Department of Computer Science, Computers in Biomedicine; New Brunswick, NJ. Rutgers University. 1971.
8. Kim BY, Rutka JT, Chan WC. Nanomedicine. *N Engl J Med*. 2010;363(25):2434–2443.
9. Doms A, Schroeder M. GoPubMed: exploring PubMed with the Gene Ontology. *Nucleic Acids Res*. 2005;33:W783–786.
10. Maojo V, Garcia-Remesal M, de la Iglesia D, et al. Nanoinformatics: developing advanced informatics applications for nanomedicine. In: Prokov A, editor. *Intracellular Delivery: Fundamentals and Applications (Fundamental Biomedical Technologies*. NY. Springer; 2011.
11. Maojo V, Martin-Sanchez F, Kulikowski C, et al. Nanoinformatics and DNA-based computing: catalyzing nanomedicine. *Pediatr Res*. 2010;67(5):481–489.
12. Freitas RA. Nanomedicine, Volume I: Basic Capabilities. Georgetown, Texas. Landes Bioscience; 1999.
13. Freitas RA. Nanomedicine, Volume IIA: Biocompatibility. Georgetown, Texas. Landes Bioscience; 2003.
14. Jain K. The handbook of Nanomedicine. NJ. Humana Press; 2008:161–192.
15. Thomas DG, Pappu RV, Baker NA. NanoParticle Ontology for cancer nanotechnology research. *J Biomed Inform*. 2011;44(1):59–74.
16. Rosse C, Mejino JVL. A reference ontology for biomedical informatics: the Foundational Model of Anatomy. *J Biomed Inform*. 2003;36:478–500.
17. Workshop on Nanoinformatics Strategies. Arlington, Virginia. National Science Foundation; 2007.
18. National Science Foundation. Arlington, Virginia (USA). Nanoinformatics 2010: A Collaborative Roadmaping Workshop; 2010.
19. Baker NA, Fritts M, Guccione S, et al. Nanotechnology Informatics White Paper. US Bethesda, MD. National Cancer Institute; 2009.
20. De la Iglesia D, Maojo V, Chiesa S, et al. International efforts in nanoinformatics research applied to nanomedicine. *Methods Inf Med*. 2011;50(1):84–95.
21. Kiberstis P, Roberts L. It's Not Just the Genes. *Science*. 2002;296(5568):685.
22. Green ED, Guyer MS. National Human Genome Research Institute Charting a course for genomic medicine from base pairs to bedside. *Nature*. 2011;470(7333):204–213.
23. PubMed. U.S. National Library of Medicine. National Institutes of Health.
24. Gordon N, Sagman U. Nanomedicine Taxonomy. Canadian Institute of Health Research & Canadian NanoBusiness Alliance. 2003.
25. Smith B, Ashburner M, Rosse C, et al. The OBO Foundry: coordinated evolution of ontologies to support biomedical data integration. *Nat Biotechnol*. 2007;25(11):1251–1255.
26. De la Calle G, García-Remesal M, Chiesa S, et al. BIRI: a new approach for automatically discovering and indexing available public bioinformatics resources from the literature. *BMC Bioinformatics*. 2009;10:320.
27. Viceconti M, Clapworthy G, Van Sint Jan S. The Virtual Physiological Human – A European initiative for in silico human modelling. *J Physiol Sci*. 2008;58(7):441–446.
28. Network for Computational Nanotechnology. National Science Foundation.
29. CaNanoLab. National Cancer Institute.
30. Collaboratory for Structural Nanobiology (CSN)

31. Munteanu CR. Convergence of Bioinformatics with Nanotechnology and Artificial Intelligence Technologies. *Current Bioinformatics*. 2011;6(2):144.
32. Gerstein M, Seringhaus M, Fields S. Structured digital abstract makes text mining easy. *Nature*. 2007;447(7141):142.
33. Maojo V, Crespo J, García-Remesal M, et al. Biomedical Ontologies: Toward Scientific Debate. *Methods Inf Med*. 2011;50(3):203–216.
34. Bewick S, Yang R, Zhang M. Complex mathematical models of biology at the nanoscale. *Wiley Interdisciplinary Reviews: Nanomedicine and Nanobiotechnology*. 2009;1(6):650–659.
35. O'Donoghue SI, Goodsell DS, Frangakis AS, et al. Visualization of macromolecular structures. *Nat Methods*. 2010;7(3):S42–55.
36. Berman H, Henrick K, Nakamura H. Announcing the worldwide Protein Data Bank. *Nat Struct Biol*. 2003;10(12):980.
37. Maojo V, Martín-Sánchez F. The ACTION-Grid White Paper: Linking Biomedical Informatics, Grid Computing and Nanomedicine. 2011.

Citation: Anandaram H, Rashmi AB. A review on application of nanoinformatics and bioinformatics in nanomedicine. *Adv Tissue Eng Regen Med Open Access*. 2020;6(3):53–56. DOI: 10.15406/atroa.2020.06.00118