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Preamble

Genetic testing in diagnosis is crucial for clinical practices. The diagnostic outcome needs to consider the familial pathological background collected before and after the genetic assessment of an individual. I specifically focus on metabolic and prenatal genetic tests that very well align with clinical diagnosis, with the cytogenetic proband, and that shows the probabilistic nature of genetic alterations leading to one should live with diseases throughout their life with the lifestyle modification and self-motivation support as guided by the genetic counselor. Taking into consideration the detailed pathological history of a family helps to detect or predict the inheritance patterns of disease between or within the family..

Genetic testing requires information on the disease phenotype from the individuals along with their family characteristics. Together it gives the highest accuracy for genetic testing that often helps to confirm the disease or the possibility of the disease inherited to their offspring. For instance, the inheritance patterns in complex diseases like Parkinson's disease reveal such familial connectivity of disease. Further, the information is useful in the differential diagnosis of Parkinson's disease from other phenocopies, such as essential tremor or supranuclear palsy, which are etiologically different based on the genetic hotspot. Apart from the benefits of differential diagnosis using genetic testing, a gene-specific analysis may provide innovations guiding towards disease-specific therapies and prognosis. Therefore, geneticist plays a vital role in detecting the individual or their offspring that may be susceptible to the disease based on the genetic polymorphism assessment. However, such polymorphic assessment during preimplantation, prenatal phases and in children may lead to conflicts in health insurance procedures.

In recent times, the utility of genetic testing on cardiac, metabolic, reproductive, and neurological diseases has increased significantly. Also, development in technologies and utilization of systems biology and multi-omics approach has moved towards multi-gene testing with microarray or next-generation sequencing panels. Such panels include hundreds of biomarker genes that can help in the early diagnosis of complex diseases.

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Preamble

Recent advancement in technologies has contributed enormously in medical research that develops precise diagnostic and personalized treatment strategies for complex diseases. Such technological improvement allows us to understand the behaviour of cells governed by a single molecule to complex molecular pathways. Particularly, new technologies enable us to characterize and understand the molecular basis of the system behind the physiological and pathological states. In essence, one can understand the behaviour of the system at the integrated levels of all omics like, genomics, epigenomics, proteomic, metabolomic and metallomics. The nuances of cellular activities will be uncovered at the levels of intermolecular interactions that share the required time and space in maintaining the molecular equilibrium for healthy living. Genome sequencing has un-raveled the genetic information hidden within a four-letter code "ATGC". This code not only identifies the behaviour of an organism but also its interactions with the environment. Simultaneously, the advancements in microscopy, imaging techniques, mass spectrometry, NMR, ICMS, protein array, and microarray have enabled real-time monitoring and visualization of molecular behaviour in body fluids, cells, and tissues. Data generated with the use of these techniques can be subjected to mathematical analyses with system biological platform.

Implementation of the precise diagnostic and treatment procedures in day-to-day medical practice is highly challenging due to the lack of molecular profiles of each individual in a population. Hence, there is an unmet need to generate large- molecular data, analyze and interpret for clinical translational actions. Such a clinical decision of drug selection is time-consuming and delays the translation process towards clinical practice. However, the rapid growth in the area of computational biology has provided access to the multi-omics of every individual in a population.

Systems biology has proven to delineate the molecular mechanisms causal to a disease which contributes to the development of a human disease model. Thus, systems biology is to identify diagnostic marker(s) and medicine for early precise diagnosis and treatment of an individual or a selected population based on the genetic make-up, metabolism, and environment.

This is a special issue that addresses the challenges in multi-disciplinary innovative research from different scientific disciplines such as bioinformatics, computing medicine, and genetic diagnosis.

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Preamble

Molecular modelling is an emerging area, which deals with the 3-dimensional structure of molecules. In general, understanding the 3D structure and dynamics of molecules, especially biomolecules, sheds light on the mechanism of action of those molecules. Such mechanistic insights are valuable to decode their role in the complex biological system and in the designing of drugs. In fact, recent drug discovery research often employs molecular modelling techniques at some stage(s) in the process. One of the important molecular modelling methods in drug research is protein structure prediction.

Proteins, being important functional molecules in the biological system, are often therapeutic targets. The proteins involved in a disease can be identified by various computational as well as experimental methods. Once the target is identified, the hunt is for a small molecule (lead) that binds with the target in a fairly specific manner. The small molecule that can bind and modulate the activity of a disease causing protein is known as a drug molecule. The designing of such a small molecule requires detailed knowledge of the target protein structure under investigation. The aim of protein structure prediction is to accurately model the structure of protein molecule, if experimental 3D structures are not available.

The following review article gives basic workflow, comprehensive latest information and practical guidelines in the research field of protein structure prediction for drug discovery applications.

Various resources (offline and online) that facilitate the accurate modelling is discussed in detail. Two original research articles highlight the use of computer-based molecular modelling methods in the design of novel therapeutic agents to treat hypertension and cystic fibrosis.