ECRONICON OPEN ACCESS

EC CLINICAL AND MEDICAL CASE REPORTS

Opinion

Recent Trends in Application of Artificial Intelligence in Prediction and Optimisation of Biomolecular Interactions

Harishchander A*

Centre for Excellence in Computational Engineering and Networking, Amrita Vishwa Vidyapeetham, Coimbatore, Tamil Nadu, India

***Corresponding Author:** Harishchander A, Centre for Excellence in Computational Engineering and Networking, Amrita Vishwa Vidyapeetham, Coimbatore, Tamil Nadu, India.

Received: October 13, 2021; **Published:** October 29, 2021

Keywords: *Bioinformatics; Computational Biology; Biomolecular Modeling; Simulation; Physiology; Pathology; Ligands; Alpha-Fold*

The AI applied inter-disciplinary fields, namely (i) Bioinformatics, (ii) Computational Biology, and (iii) Biomolecular Modeling and Simulation. The domain "Bioinformatics" involves the combination of technologies in bioscience and data analytics. Similarly, the field "Computational Biology" is the combination of "Biomolecular Characterization" and "virtual modeling." All the areas mentioned above do not work in isolation but as a combined network to understand the differences in biological processes in normal (Physiological) and abnormal (Pathological) conditions. The significant difference between bioinformatics and computational biology is the construction of virtual models to mimic a real-time system (Computational Biology) and the identification of various computational techniques to understand the dynamics of sensitivity specificity and precision of individual components and the working system in the virtual model (Bioinformatics) involves the application of Artificial Intelligence. Then concerning Biomolecular Modeling and simulation, the 3-D model of small molecules (ligands) can be constructed using various tools based on the Lamarcian Genetic Algorithm. Finally, Molecular Simulations can be static (simulation of molecules in a vacuum environment) and dynamic (simulation of molecules in water, buffer, and related ions involved in the system). Molecular docking is a static simulation where changes are observed only at the binding pose of the ligand and receptor in the vacuum environment. Interactions between biomolecules can be of Protein-DNA, Protein-Protein, Protein-Ligand, Protein-Peptide, etc. Most of the peptides carry therapeutic value, i.e. applied medicine and presently "Alpha-Fold" works well in predicting and optimizing biomolecular interaction.

Volume 4 Issue 11 November 2021