REVIEW ARTICLE

TECHNIQUES AND ALGORITHMS FOR STRUCTURE-BASED VIRTUAL SCREENING (SBVS): AN OVERVIEW

Raksha K. Rao[a]*, Somdatta Y. Chaudhari[a], Shailaja B. Jadhav[a], Pravin D. Chaudhari[b] and Ujwala B. Yedake[a]

(Received 21 January 2022) (Accepted 27 October 2022)

ABSTRACT

Today, the world of science is constantly challenged with new genomics, which in turn is responsible for new disease-causing targets. Hence, there is a need for developing drugs acting against such targets. Computational methods are proving to be a mainstay in the drug discovery process, mainly through virtual screening. This review discusses about the recent advancements in structure-based drug design with reference to Virtual Screening along with its procedures from ligand preparation and protein preparation, docking, scoring function, databases, and virtual (VS) algorithms. Application of Structure-based VS in combination with other virtual screening techniques has also been highlighted in this review.