CHAPTER 1

Recent Advances and Role of Computational Chemistry in Drug Designing and Development on Viral Diseases

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Abstract: The growing number of contagious viral diseases among different geographic regions has become a threat to human health and the economy on a global scale. Various viral epidemics in the past have caused huge casualties due to lack of effective vaccine, the recent outbreak of COVID-19 is a good example of it. Drug designing and development is a lengthy, tedious and expensive process that is always associated with a high level of uncertainty as the success rate of their approval as a drug is very low. Computer-aided drug designing by utilizing *in silico* methods has shown prominent ways to develop novel drugs in a cost-efficient manner and has evolved as a rescue in the past few years. Interestingly, the highest FDA approval reached a maximum (59 drugs) in 2018 for which a lot of credit goes to the successful development of computational chemistry tools for drug designing in the last two decades. These methods provide better chances of getting hit compounds in a far more accurate and faster way. Drug designing is a cyclic optimization process that involves various steps like creating a molecule, selecting the target for this molecule, analysing the binding pattern and estimating the pharmacokinetics of the molecule. The final development of a drug candidate is cumulative of positive results obtained in each aforementioned step. Various computational techniques/approaches such as molecular dynamic studies, homology modelling, ligand docking, pharmacophore modelling and QSAR can be utilized in each phase of the drug discovery cycle. In this chapter, we aim to highlight the recent advances that have taken place in developing tools and methodologies that lead to *in silico* preparation of novel drugs against various viral infections like Ebola, Zika, Hepatitis C and Coronavirus.

Keywords: Computational chemistry, Homology modeling, *In Silico*, Ligand-based drug designing, Ligand docking, Multi target drug designing, Pharmacophore modeling, Protein target, Quantum mechanics, Structure-based drug designing, Viral infection, Virtual screening.

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