Abstract

In 2019, a new virus spread in Wuhan, China, causing fever-like symptoms. It was later identified as Coronavirus disease 2019 (COVID-19), and in March 2020, it was announced as a pandemic. As of 2024, the COVID-19 pandemic has been confirmed in 774 million cases and has resulted in over seven million fatalities, according to a World Health Organization (WHO) report. To date, finding a single, highly effective drug for COVID-19 is still a challenge. In this regard, a drug repurposing strategy is one of the best approaches to finding new treatment in a short time. Herein, we suggest drug repurposing tactics to find a treatment for the COVID-19 pandemic using already-approved antibiotics. A database of 108 β-lactam antibiotics was built and screened against the main protease (M^{pro}) enzyme using molecular docking and molecular dynamic simulation techniques. Standard precision (SP) docking revealed that Aspoxicillin, Ceforanide, Azlocillin, Cefpiramide, Mezlocillin, Doripenem, Piperacillin, Cefoperazone, Amdinocillin, and Cefbuperazone have good docking scores. Molecular dynamics simulations were performed for 300 ns on frontrunner antibiotics to evaluate the docking results and to determine the stability of these antibiotics within the active site of the M^{pro} protein. The molecular dynamics simulation showed that Cefoperazone was more stable compared to a co-crystal (N3 peptide) inhibitor, which made it a possible treatment for COVID-19.

Keywords: COVID-19, Docking, MD, main protease