Editorial

Molecular Docking: A Shortcut to Defeat COVID-19?

The current COVID-19 pandemic created a significant challenge for all human life aspects including the health sector. One of the most important challenges was how to find treatment for the disease. Till now, a long list of pharmaceuticals has been tested; mostly disappointing. However, the virus' incursion continues (1).

All the currently available pharmaceuticals used for the treatment of COVID-19 are repurposed ones (2); while, none have been promising yet and emerging drugs are inevitable. Molecular docking is a shortcut to the discovery of emerging repurposed drugs (3). In this issue of the Journal of Cellular and Molecular Anesthesia, Saidijam et al. have proposed three main SARSCoV-2 NTPase/Helicase inhibitors as potential pharmaceuticals for the treatment of COVID-19, using molecular docking and dynamics simulation approach (4). These three phenolic compounds (i.e. amentoflavone, theaflavin 3'-gallate, and procyanidin) have been discovered from a long list of 52 phenolic compounds (mostly flavonoids) using a drug discovery method (i.e. a molecular docking) to analyze their binding affinity to SARS-CoV-2 NTPase/helicase.

There are some Pro and Con viewpoints regarding such drug discovery techniques. One of them is that in such studies no clinical or preclinical studies are needed to discover these compounds since the methodology of the study is a fast-track shortcut to find the potential pharmaceuticals in emergent cases like COVID-19. Besides, these potential therapies have been emerged using bioinformatics prediction models and molecular docking approaches with a relatively sound and logical rationale. On the other hand, these compounds defect proofs and need trials to be documented as therapeutic agents.

The COVID-19 era has ruled us through paths that were not well experienced. COVID-19 has taught us new paradigms not learned before; in other words, we are learning a paradigm shift in our medicine; however, a long path is ahead of us and many other new lessons should be learned.

References

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