ORIGINAL RESEARCH ARTICLES

PHYSICOCHEMICAL AND PHARMACOKINETIC ANALYSIS AND DOCKING OF DRUG REPOSITIONING AGAINST SARS-COV-2: AN *IN SILICO* STUDY

Jackson A. Pereira[a] and Eduardo D. Costa[a]*

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ABSTRACT

Studies on the development of effective and cost-effective oral drugs are the new priority of the pharmaceutical industry for the prevention and treatment of COVID-19. This work was based on the computational analysis of physicochemical parameters, pharmacokinetic and toxicological measurements, molecular docking and *in silico* measurement of the antiviral activity of 12 repositionable drugs. The Molinspiration platform (physical-chemical parameters), pkCSM® (absorption, distribution, metabolism and excretion), OSIRIS Property Explorer® (toxicological measurements), Seam® (Docking with the RdRp protein) and AVCpred server® (antiviral activity) were used. Considering the 12 selected repositionable drugs, molecular anchoring data with the RdRp protein, only the drug tilorone had lower binding energy than the control used in this study (Molnupiravir). Ledipasvir, daclatasvir and piperaquine showed the best percentage of antiviral inhibition considering the control pattern. ADME-Tox data showed that piperaquine has a high toxicological potential for mutagenesis, tumorigenesis and irritant effects. The findings of this study indicate that ledipasvir and daclatasvir showed greatest potential for inhibition RdRp and action against COVID-19.