Identifying Potential SARS-CoV-2 Protease (PLpro) Inhibitors through in silico Virtual Screening and Text Mining: An Analysis of Toxicity and Interaction Effects.

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Abstract

At the end of 2019 a new coronavirus surfaced in China, SARS-CoV-2, responsible for the ongoing pandemic. There is a need for novel and stable therapies to help patients of COVID-19. Drug repositioning is a strategy to quickly find medicines already used to treatment to another pathology. In this work, we used the PLpro as molecular target for it being responsible for cleaving other viral proteins and interfering with the immune system. In the Brazilian Pharmacopeia is described many different Active Pharmaceutical Ingredients (API) used in Brazil and the world. Using the in silico techniques of virtual screening, the top 44 API pass through Toxicity prediction, where 36 API prove to not be mutagenic. Using molecular weight, distance to the protein, and literature information 19 API go through prediction of chemical interactions, we determine the top 6 APIs with the best chance of interacting with the PLpro. With this result, we determine new possible API that will be tested in vitro to determine its ability to inhibit SARS-CoV-2's PLpro, and could be readily made available to the infected populous.

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