Abstract

Nature as a treasure trove of potential anti-SARSCoV drug leads: a structural/mechanistic rationale

The novel Coronavirus disease 2019 (COVID-19) caused by SARS-CoV-2 is a potential factor for fatal illness and a tremendous concern for global public health. The COVID-19 pandemic has entered a dangerous new phase. In the context of drug discovery, the structurally-unique and chemically-diverse natural products have been valuable sources for drug leads. In this review, we report for potential candidates derived from natural sources with well-reported in vitro efficacy against SARS-CoV during the last decade. Additionally, a library of 496 phenolic metabolites was subjected to a computer-aided virtual screening against the active site of the recently reported SARS-CoV Main protease (Mpro). Analysis of physicochemical properties of these natural products has been carried out and presented for all the tested phenolic metabolites. Only three of the top candidates, viz. acetylglucopetunidin (31), isoxanthohumol (32) and ellagic acid (33), which are widely available in many edible fruits, obey both Lipinski’s and Veber’s rules of drug-likeness and thus possess high degrees of predicted bioavailability. These natural products are suggested as potential drug candidates for the development of anti-SARSCoV-2 therapeutics in the near future.