# *In silico* identification of new antiviral pharmacophores from the floral biodiversity and approved phytochemicals in the fight against COVID-19 – (PHYTO-COVID)

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Currently, there is no specialized approved treatments and/or drugs available for the treatment of COVID-19 and several clinical explorations relevant to the therapies of COVID-19 are on-going. The recognition of plant-derived compounds (phytochemicals) as attractive targets to inhibit COVID-19 replication has emerged resulting in an investigation of existing drugs to target the viral protease. Existing approved drugs are being investigated against COVID-19 treatment – *via* drug repurposing. With the support of bioinformatic tools, commonly used in rational drug design, we aimed to assess African herbal medicine along with existing approved drugs, in an endeavour to contribute to a global solution against COVID-19. The main aims are: (1) to identify potential inhibitors for SARS-CoV-2 through existing approved and plant-derived compounds with viral proteins using *in silico* molecular docking; (2) to perform advanced quantum and molecular dynamic simulation to elucidate the inhibition affinity of the most active compound(s) and (3) to explore the possibility to develop nutraceuticals/functional foods and register and/or patent potent plant-derived compound against COVID-19.
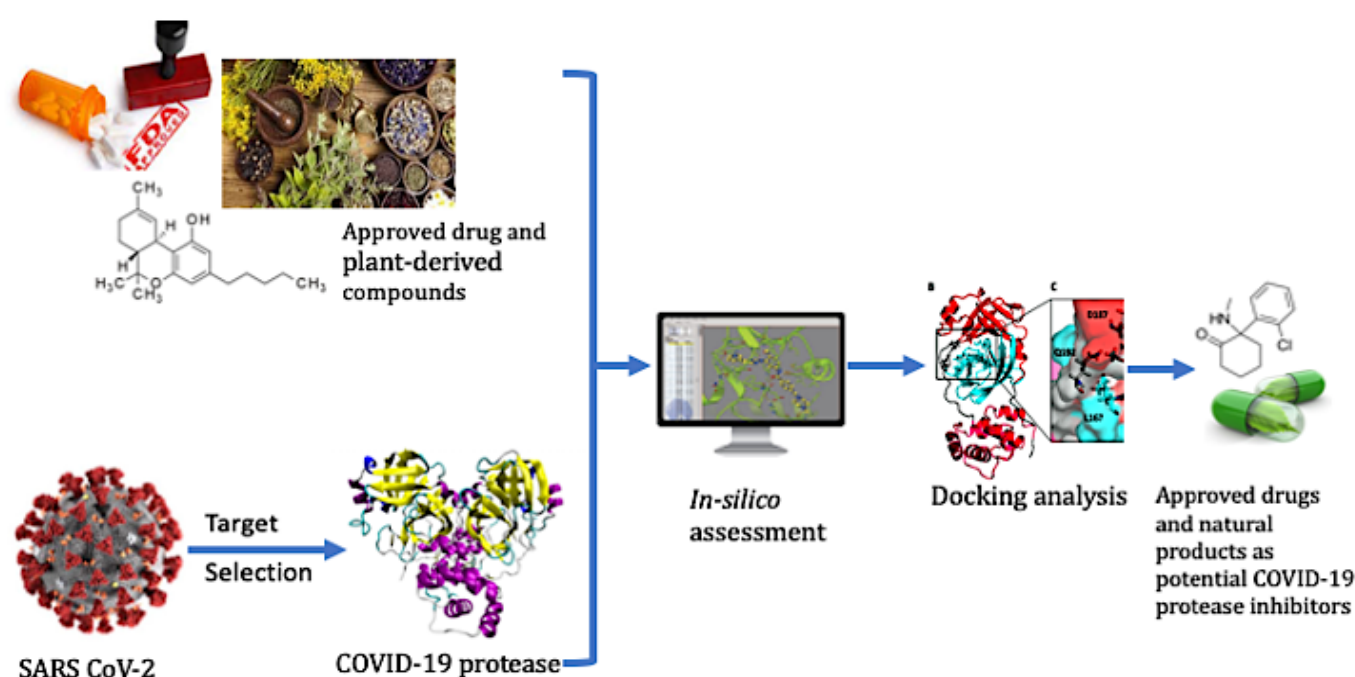
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