Host-directed FDA-approved drugs with antiviral activity against SARS-CoV-2 identified by hierarchical in silico/in vitro screening methods

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Abstract

The unprecedent situation generated by the COVID-19 global emergency has prompted us to actively work to fight against this pandemic by searching for repurposable agents among FDA approved drugs to shed light into immediate opportunities for the treatment of COVID-19 patients. In the attempt to proceed toward a proper rationalization of the search for new antivirals among approved drugs, we carried out a hierarchical in silico/in vitro protocol which successfully combines virtual and biological screening to speed up the identification of host-directed therapies against COVID-19 in an effective way. To this end a multi-target virtual screening approach focused on hostbased targets related to viral entry, followed by the experimental evaluation of the antiviral activity of selected compounds, has been carried out. As a result, five different potentially repurposable drugs interfering with viral entry-cepharantine, clofazimine, metergoline, imatinib and efloxate-have been identified.

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