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Repurposing of antiparasitic drugs for Candidate SARS-CoV-2 Main Protease Inhibitors by combined *in silico* Method

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Abstract

The SARS-CoV-2 outbreak that is spreading rapidly around the world requires urgently effective treatments. Therefore, *in silico* drug repurposing represents a powerful strategy to enable the acceleration of the identification of drug candidates with already known safety profiles. The SARS-CoV-2 main protease is essential for viral replication and an attractive drug target. This study used the virtual screening protocol with both long-range and short-range interactions to select candidate SARS-CoV-2 main protease inhibitors. The Informational spectrum method developed for small molecules was first applied for searching the Drugbank database of antiparasitic agents and further followed by molecular docking. After *in silico* screening of drug space, we propose several drugs as potential SARS-CoV-2 main protease inhibitors for further experimental testing.

Keywords:

SARS-CoV-2, main protease, virtual screening, drug repurposing, antiparasitics

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