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Title: A comprehensive SARS-CoV-2 genomic analysis identifies potential targets for drug repurposing

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SARS-CoV-2 Keywords:

genomic analysis

Issue Date: 2021

Publisher: **PLOS** 

Citation: PLoS ONE, 16(3).

Abstract:

The severe acute respiratory syndrome coronavirus 2 (SARS-CoV-2) which is a novel human coronavirus strain (HCoV) was initially reported in December 2019 in Wuhan City, China. This acute infection caused pneumonia-like symptoms and other respiratory tract illness. Its higher transmission and infection rate has successfully enabled it to have a global spread over a matter of small time. One of the major concerns involving the SARS-COV-2 is the mutation rate, which enhances the virus evolution and genome variability, thereby making the design of therapeutics difficult. In this study, we identified the most common haplotypes from the haplotype network. The conserved genes and population level variants were analysed. Non-Structural Protein 10 (NSP10), Nucleoprotein, Papain-like protease (Plpro or NSP3) and 3-Chymotrypsin like protease (3CLpro or NSP5), which were conserved at the highest threshold, were used as drug targets for molecular dynamics simulations. Darifenacin, Nebivolol, Bictegravir, Alvimopan and Irbesartan are among the potential drugs, which are suggested for further pre-clinical and clinical trials. This particular study provides a comprehensive targeting of the conserved genes. We also identified the mutation frequencies across the viral genome.

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URI: https://doi.org/10.1371/journal.pone.0248553 (https://doi.org/10.1371/journal.pone.0248553)

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