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Commentary

A Subtle but Effective Tool for Accelerating Drug Repurposing Against COVID-19 and Future Viral Eruptions

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ABSTRACT

The sense of emergency worldwide due to the COVID-19 pandemic alerted medical researchers to scramble for resources and rummage around for all possible armaments to fight the deadly pandemic.

Keywords: COVID-19; Pandemic; Vaccines

ABOUT THE STUDY

The author and many other scholars believe that attention to therapeutic approaches particularly using existing drugs was not given adequate leverage, and the majority of the global efforts went to the development of vaccines [1-3]. While the development of effective and safe vaccines is conceptually the ideal way forward, it encompasses risks of latent adverse effects and the possibility of gradual loss of efficacy due to ensuing viral mutations. Also, vaccines are administered to the general public including healthy subjects and this necessitates stringent safety studies as any unpredicted adverse effect may impart a huge health risk liability. Alternatively, developing totally new therapeutics needs extensive efforts and time from the discovery phase throughout animal safety studies, PK/PD and then clinical development phases. That is in addition to the risk of losing efficacy due to subsequent viral mutations as with the case of vaccines. As a result, there is an imperative need for an agile, fast and effective approach for drug discovery. In this instance, accelerated drug repurposing fits the bill and can be considered as the safest and most sensible approach provided that an actually fast way for screening and identifying effective drugs is realizable. The author recently published a report in SLAS Discovery that sheds light on a unique bioinformatics method for drug discovery called COMPARE analysis [4]. It works by applying the algorithm COMPARE on a publicly accessible drug database available from the NCI. The COMPARE algorithm and the NCI's drug data repository were originally created to enable drug screening to establish effective cancer treatments. The data repository includes the growth inhibitory profiles of more than 55000 drug molecules on a panel of 59 diverse cell lines. Each drug molecule stored in the data repository has a unique fingerprint on the cell panel depending on its interaction with each type of human cells. The role of COMPARE algorithm is to scan and identify molecules that share similar fingerprints. Interestingly, the author's study showed that this same approach is capable of uncovering active drugs against viral infections. Unlike pure in-silico approaches, the COMPARE approach is a hybrid of both informatics and actual biological interactions that take place between the cell growth machinery and tested drugs. Due to these features, relevant correlation within drugs of similar pharmacological modes can be identified regardless of their chemical structures. Only a few steps are needed to quickly identify effective drug candidates. The first step is to use the available state-of-the art clinical knowledge and observations to select compounds with ostensible antiviral effects. The selected drug molecules are then used as baits in COMPARE to fish for drugs that have similar growth inhibitory fingerprints. The fished drug molecules that have the highest correlation with the baits and are clinically approved, can be easily tested on animal models or on human volunteers because they have an established safety profile, dosing and PK/PD parameters. This would quickly increase the chances of identifying curative drugs without going through extensive and unguided laboratory-based screening. In case the initial screening cycle does not yield satisfactory drug candidates, more cycles of seeding and fishing can be repeated quickly until a curative therapeutic is identified. The described COMPARE approach is modular and can be used each time a novel infectious disease hits the population or manifests itself in a new mutation. It is highly recommended that this approach be part of the preparedness toolbox used to tackle current and future pandemics.

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