

Artificial intelligence in COVID-19 drug repurposing

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Abstract

Drug repurposing or repositioning may be a technique whereby existing drugs are used to treat emerging and challenging diseases, including COVID-19. Drug repurposing has become a promising approach due to the chance for reduced development timelines and overall costs. The artificial intelligence (AI) pioneers of the 1950s foresaw building machines that would sense, reason, and think like people—a proof-of-concept referred to as general AI. The increasing cost of drug development is thanks to the massive volume of compounds to be tested in preclinical stages and therefore the high proportion of randomised controlled trials (RCTs) that don't find clinical benefits or with toxicity issues. This Review provides a robust rationale for using AI-based assistive tools for drug repurposing medications for human disease, including during the COVID-19 pandemic. Drug repurposing may be a convenient alternative when the necessity for brand spanking new drugs in an unexpected medical scenario is urgent, as is the case of emerging pathogens. In recent years, approaches supported network biology have demonstrated to be superior to gene-centric ones. Mechanistic models of pathways provide a natural bridge from variations at the size of gene activity (transcription) to variations in phenotype (at the extent of cells, tissues, or organisms). Interestingly, the notion of causality provided by the mechanistic model of the COVID-19 disease map are often exploited beyond the own pathways modeled.

Introduction

Actually, mechanistic models of human signaling pathways are successfully used to uncover specific molecular mechanisms behind different diseases, to reveal modes of action of medicine, and to suggest personalized treatments. Interestingly, the notion of causality provided by the mechanistic model of the COVID-19 disease map are often exploited beyond the own pathways modeled.

Consequently, this potential modulator capacity could make them suitable candidates to become therapeutic targets. Among the drugs predicted to possess a relevant effect, a number of them are currently under clinical trials. Interestingly, these drugs define different functional profile templates, which can be useful to take a position similar consequences for other drugs with similar patterns of influence over the signaling circuits that define the disease hallmarks..

Analysis

Chloroquine and ciclosporin are representative of two different modes of action by either affecting massively to most COVID-19 disease map circuits or only affecting a couple of specific ones, respectively. In fact, a recently published compilation of medicine currently in clinical trials allowed to validate many predictions. The results presented here, although promising, are often considered only a subset of the potential drug candidates for repurposing, as long as the detailed definition of the COVID-19 disease map is still an on-going effort..

Although novel chemical and biologic entities are being evaluated as potential therapeutics for SARS-CoV-2 infection, the repositioning and off-label use of existing agents approved for unrelated conditions is widely advocated as a therapeutic approach against COVID-19 as it offers more rapid, actionable interventions against the virus.

Conclusion

The outbreak of the novel coronavirus disease COVID-19, caused by the SARS-CoV-2 virus has spread rapidly round the globe during the past 3 months. As the virus infected cases and deathrate of this disease is increasing exponentially, scientists and researchers everywhere the planet are relentlessly working to know this new virus along with possible treatment regimens by discovering active therapeutic agents and vaccines. So, there's an urgent requirement of latest and effective medications which will treat the disease caused by SARS-CoV-2.