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Type	Oral communication
Session	Bioinformatics challenges in the SARS-Cov-2/COVID-19 pandemic
Title	SciKi: Science Wiki: An In Silico Drug Discovery approach to Combat COVID-19
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Motivation

Multi-disciplinary open science has emerged as a powerful mechanism to accelerate science and fight the rapidly evolving worldwide COVID-19 pandemic [1]. Indeed, the current pandemic has raised the need for efficient and effective identification of potential drug candidates for COVID-19, thus creating an urgency for spreading knowledge and innovation on host response to SARS-CoV-2 infection. However, what is currently known about such a pathogen remains limited, with very few drugs approved to date.
Recently, in the context of the RxCovEA framework [2], we introduced a novel methodology [3] for the in-silico modeling of SARS-CoV-2 infection in host cells by leveraging the power of our PHENotype SIMulator (PHENSIM) [4]. This method allows us to determine the viral effects on cellular host-immune response with high sensitivity and specificity. Furthermore, such predictions help to narrow down promising repurposable therapeutic strategies, leading to novel potential candidates for therapeutic targeting. Additionally, disseminating the results through a more collaborative environment allows the verification of hypotheses, namely by detecting contradictions, validating sources, and filtering fake data, such a tool is critically needed.

Methods

In this context, here we introduce SciKi (Scientific Wiki), a toolbox developed to interpret and disseminate the results obtained by using our drug-discovery framework.
The tool has been designed to interact with open science communities innovatively by helping researchers search for candidate drugs based on publications, wikis, leader-boards, and comments and machine-generated “interpretations” for successful (e.g., thresholded by statistical significance) candidates.

Results

Powered by this tool, coupled with domain expertise, we have identified several potential COVID-19 drugs, including methylprednisolone and metformin, and further discern key cellular SARS-CoV-2-affected pathways as potential new druggable targets in COVID-19 pathogenesis.

Info

References

1. Kadakia, Kushal T., et al. "Leveraging open science to accelerate research." New England Journal of Medicine (2021).
2. Bischof, Evelyne, et al. "ANERGY TO SYNERGY– THE ENERGY FUELING THE RXCOVEA FRAMEWORK." International Journal for Multiscale Computational Engineering 18.3 (2020).
3. Maria, Naomi, et al. "Rapid Identification of Druggable Targets and the Power of the PHENotype SIMulator for Effective Drug Repurposing in COVID-19." (2021).
4. Alaimo, Salvatore, et al. "PHENSIM: Phenotype Simulator." bioRxiv (2020); Plos Comp Bio (Under

Review).	
Figure	
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Availability	-
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