Since January 2020 Elsevier has created a COVID-19 resource centre with free information in English and Mandarin on the novel coronavirus COVID-19. The COVID-19 resource centre is hosted on Elsevier Connect, the company's public news and information website.

Methods 206 (2022) 99–100

Contents lists available at ScienceDirect

Methods

journal homepage: www.elsevier.com/locate/ymeth

Editorial

Computational methods and strategies for combating COVID-19

The special issue collects the original research papers on computational methods and strategies for combating the COVID-19 pandemic. We proposed to cover the theoretical studies related to computational drug discovery, drug repurposing and related therapeutic aspects of COVID-19, such as computational techniques for detecting COVID-19, vaccination and treatment strategies, and novel forecasting models for SARS-COV-2 providing a deeper understanding of issues related to co-morbidity etc. We also invited contributions on virus genome phylogenetic studies identifying the novel mutations influencing the spread of the virus, detailed biophysical prediction of binding affinities allowing for the tissue specificity of virus-host protein-protein interactions, and the description of the universe of protein-protein host-pathogen interactions.

After a thorough review, we accepted eight papers in this special issue covering most of the targeted areas mentioned above. In general, we have classified the papers into three major categories: 1) Socio-demographic analysis, 2) Host-Pathogen interaction networks, and 3) Drug Repurposing studies (Fig. 1).

In the first category, we group together three works on the socio-demographic analysis of the spread of the COVID-19 pandemic. The work by Ghosh et al. [1] is on the phylogenetic analysis of COVID-19, a detailed study of multiple sequence alignment of 18,392 SARS-CoV-2 genomes for 71 countries. Mutation points as single nucleotide polymorphisms (SNPs) are identified in each virus clade detected through this phylogenetic analysis. These global dataset analyses further reveal that climatic and socio-demographic conditions have a more significant role in the spread of COVID-19, highlighted in the following works of Chatterjee et al. [2] and Gogolewski et al. [3]. In the work of Chatterjee et al. [2], the relationship of socio-demographic conditions, such as temperature, humidity, and population density of the regions, with the region-specific outbreak intensity of COVID-19 has been identified by the application of fuzzy association rule mining on COVID and social data collected from different countries. While in the work of Gogolewski et al. [3], case fatality rates (CFR) for COVID-19 have been extensively studied based on the historical data regarding mortality in Poland during the first six months of the pandemic, when no SARS-CoV-2 variants of concern were present among infected. It leads to the CFR's exploration to find its decreasing trend in time.

In the second category, host-pathogen interaction networks of COVID-19 have been exploited in two works by Barman et al. [4] and Saha et al. [5] since these networks are always considered one of the significant resources for identifying potential drug targets. In the work of Barman et al. [4], a combination of essential network centrality measures and functional properties of the human proteins have been utilized to identify the critical human targets of SARS-CoV-2 from the host-pathogen interaction networks. As a result, four human proteins, *viz.*, PRKACA, RHOA, CDK5RAP2, and CEP250, have emerged as the best therapeutic targets, of which another group also found PRKACA and CEP250 as potential candidates for drug targets in COVID-19. In the work of Saha et al. [5], the COVID-19-Human Interaction network is generated by a fuzzy affinity function. In addition, spreader nodes and edges through which infection of COVID-19 gets mediated from one protein to another are also highlighted in the developed interaction network by applying the spreadability index.

In the third category, drug repurposing studies have been highlighted in the works of Hwang et al. [6], Lazniewski et al. [7], and Saha et al. [8]. Hwang et al. [6] developed a computational drug repurposing platform to detect unique therapies for patients infected with coronaviruses. It utilizes virus-host interactions and differential proteins expressed 24 h after infection to be known from wet lab data. It leads to identifying 196 approved drugs as the probable repurposed drugs of COVID-19. They have also used an artificial neural network to explain the action mechanisms of the specified 196 drugs. In the work of Lazniewski et al. [7], molecular interactions of various potential anti-blocking molecules against the SARS-CoV-2 spike protein (approved drugs, *in vivo*, tested compounds) have been studied through multiple computational methods, including molecular docking, ADME predictions, and molecular dynamics simulations coupled with MM/PBSA. The results of these computational experiments highlight that the most favourable COVID-19 inhibitors are zafirlukast, pranlukast, candesartan, cilexetil, saquinavir, and simeprevir. Finally, Saha et al. [8] did a detailed exploration of the protein-protein interaction network and symptom-based gene-protein mapping of approved and experimental drugs from DrugBank in an *in-silico* Human-nCoV interaction network. The results are further analyzed, and a drug consensus algorithm has been applied from which Fostamatinib/R406 emerges as one of the potential contenders for combatting COVID-19. The result is also validated by a docking study on COVID-19 crystal structures: 6LU7, 6M2Q, 6W9C, 6M0J, 6M71, and 6VXX.

Overall, our special issue summarises the current computational strategies and methods for combating the COVID-19 pandemic. Listed manuscripts under this special issue show immense promise and report exciting findings in this direction. We hope some of these groups will also engage with clinical collaborators for effective validation of the methods and will help address the immediate societal needs to curb the ongoing menace emanating from this pandemic.

https://doi.org/10.1016/j.ymeth.2022.08.011

Available online 24 August 2022

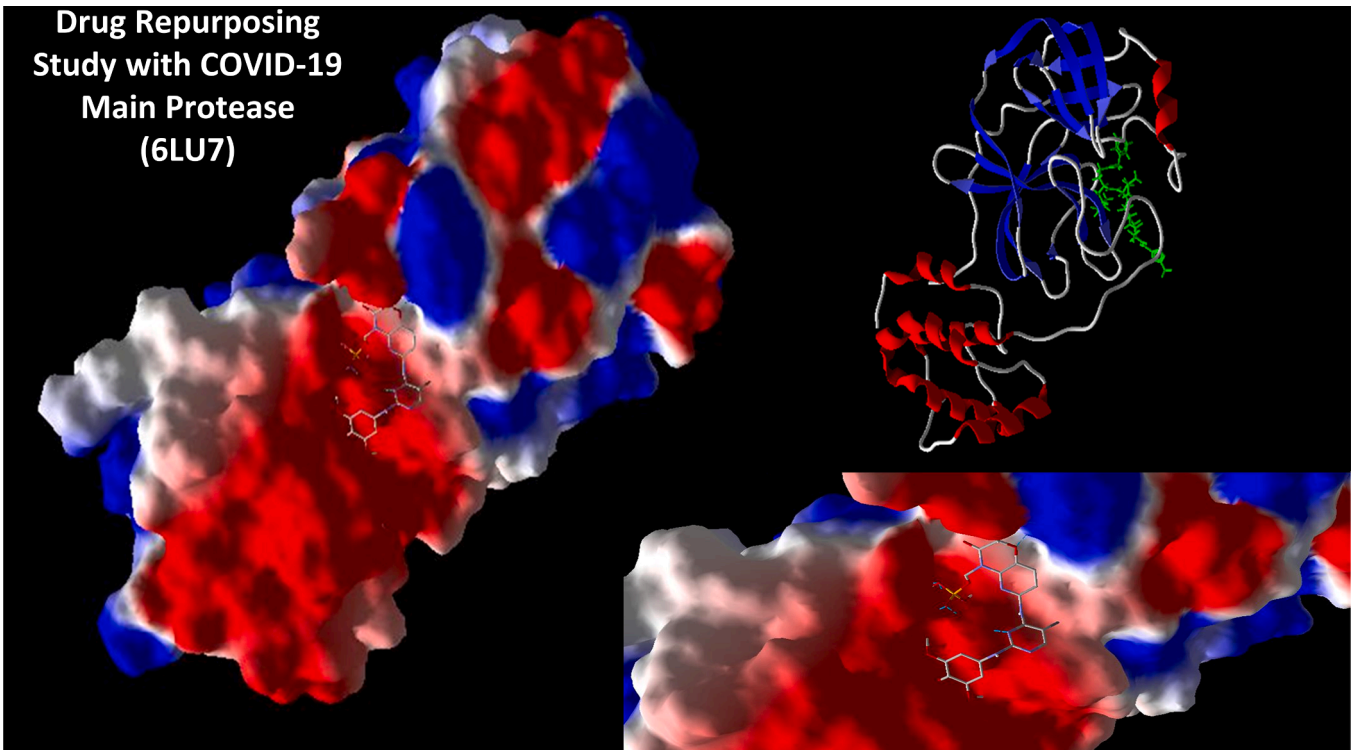

Fig. 1.

References

[1] N. Ghosh, I. Saha, S. Nandi, N. Sharma, Characterization of SARS-CoV-2 clades based on signature SNPs unveils continuous evolution, Methods 203 (2022) 282–296.
[2] S. Chatterjee, D. Chakrabarty, A. Mukhopadhyay, Fuzzy association analysis for identifying climatic and socio-demographic factors impacting the spread of COVID-19, Methods 203 (2022) 511–522.
[3] K. Gogolewski, B. Miasojedow, M. Sadkowska-Todys, M. Stepień, U. Demkow, A. Lech, E. Szczurek, D. Rabczenko, M. Rosińska, A. Gambin, Data-driven case fatality rate estimation for the primary lineage of SARS-CoV-2 in Poland, Methods 203 (2022) 584–593.
[4] R.K. Barman, A. Mukhopadhyay, U. Maulik, S. Das, A network biology approach to identify crucial host targets for COVID-19, Methods 203 (2022) 108–115.
[5] S. Saha, A.K. Halder, S.S. Bandyopadhyay, P. Chatterjee, M. Nasipuri, S. Basu, Computational modeling of human-nCoV protein-protein interaction network, Methods 203 (2022) 488–497.
[6] W. Hwang, N. Han, Identification of potential pan-coronavirus therapies using a computational drug repurposing platform, Methods 203 (2022) 214–225.
[7] M. Lazniewski, D. Dermawan, S. Hidayat, M. Muchtaridi, W.K. Dawson, D. Plewczynski, Drug repurposing for identification of potential spike inhibitors for SARS-CoV-2 using molecular docking and molecular dynamics simulations, Methods 203 (2022) 498–510.
[8] S. Saha, A.K. Halder, S.S. Bandyopadhyay, P. Chatterjee, M. Nasipuri, D. Bose, S. Basu, Drug repurposing for COVID-19 using computational screening: Is Fostamatinib/R406 a potential candidate? Methods 203 (2022) 564–574.

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