



OPEN ACCESS

EDITED AND REVIEWED BY

Lars Kaderali,
Universitätsmedizin Greifswald, Germany

*CORRESPONDENCE

Samuel Ken-En Gan
samgan@apdskeg.com
Evangelia Georgia Kostaki
ekostakh@med.uoa.gr

RECEIVED 05 September 2023

ACCEPTED 11 September 2023

PUBLISHED 22 September 2023

CITATION

Gan SK-E and Kostaki EG (2023)

Editorial: Methods in bioinformatic and predictive virology.

Front. Virol. 3:1288953.

doi: 10.3389/fviro.2023.1288953

COPYRIGHT

© 2023 Gan and Kostaki. This is an open-access article distributed under the terms of the [Creative Commons Attribution License \(CC BY\)](#). The use, distribution or reproduction in other forums is permitted, provided the original author(s) and the copyright owner(s) are credited and that the original publication in this journal is cited, in accordance with accepted academic practice. No use, distribution or reproduction is permitted which does not comply with these terms.

Editorial: Methods in bioinformatic and predictive virology

Samuel Ken-En Gan^{1,2*} and Evangelia Georgia Kostaki^{3*}¹Antibody & Product Development (APD) Lab, Wenzhou-Kean University, Wenzhou, Zhejiang, China,²James Cook University, Singapore, Singapore, ³Department of Hygiene, Epidemiology and Medical Statistics, Medical School, National and Kapodistrian University of Athens, Athens, Greece

KEYWORDS

viruses, virology, prediction, bioinformatics, mixed-methods, viral mutations, escape mutations

Editorial on the Research Topic

Methods in bioinformatic and predictive virology

Viruses were cast under the international spotlight due to the global COVID-19 pandemic in the early 2020s, renewing interests and applications in the field. With the pandemic still ongoing at the time of writing due to escape variants and subvariants, there is renewed interest in studying, developing, or applying predictive methods from other viruses unto SARS-CoV-2. There is much to cross-fertilize, especially when there are ongoing viral infections that continue to plaque the world apart from COVID-19.

Given the great resources to experimentally work on pathogenic viruses that few scientists have access to, such as access to samples, higher biosafety facilities, the tools and applications from bioinformatics was a great welcome, particularly in prediction.

Applications from ongoing viral pathogens, particularly ongoing old viral infections like the human immunodeficiency virus (HIV) (1) had provided a lot of transferable knowledge in the treatment of COVID-19 (2–5). Using HIV as a model, mutations have been studied experimentally (6) to allow computational modelling to study drug cross-resistances (7, 8), and viral fitness (9) towards the development of interventions (10–12).

Incorporating both experimental and computational methods, it is possible to build frameworks for future pandemic preparedness through the understanding of how mutations enable zoonotic transmissions from animal reservoirs as gleaned from H5N8 avian influenza (13). There is certainly much that methods in the computational analysis towards predicting zoonoses and cross-drug resistance can contribute to healthcare now and in the future.

Given the attention to COVID-19, there has been a large amount of literature on the virus released since year 2020. Within this topic of Methods in Bioinformatic and Predictive Virology, we have examples of the potential of such methods, both

computational and experimental towards the application in COVID-19. We have the building of OrthoVirae Tree, an analysis software on the relatedness of Orthornavirae from the RNA-dependent RNA polymerase (RdRp) gene sequence (Cheng et al.) that allows the potential informing of viral relatedness and by extension, guide the possible cross-use of existing antivirals to newly discovered viruses.

Similarly, we have SARSNTdb, a database to study the conservation of regions in SARS-CoV (Orgera et al.) that can allow the identification of conserved target regions for long-lasting vaccines and interventions that not only is relevant to COVID-19, but future coronavirus-related infections.

Similarly, the ability to predict the activity of neutralizing antibodies to new mutations in the SARS-CoV-2 spike (Ford et al.) will shed light on how effective interventions would be in the appearances of novel mutations and new variants. The Research Topic covered important areas in tracing, targeting, and evaluation required in pandemic preparedness in years to come.

Author contributions

SG: Conceptualization, Funding acquisition, Investigation, Resources, Writing – original draft, Writing – review & editing.
EK: Writing – original draft, Writing – review & editing.

References

- Johnson A. M. (2023). Pandemic HIV and its legacy for medicine and global health. *Clin Med (London, England)* 23(2):106–14. doi: 10.7861/clinmed.ed.23.2.harv
- Brown DA, O'Brien KK, Josh J, Nixon SA, Hanass-Hancock J, Galantino M, et al. Six lessons for COVID-19 rehabilitation from HIV rehabilitation. *Phys Ther* (2020) 100 (11):1906–9. doi: 10.1093/ptj/pzaa142
- Eaton LA, Kalichman SC. Social and behavioral health responses to COVID-19: lessons learned from four decades of an HIV pandemic. *J Behav Med* (2020) 43(3):341–345. doi: 10.1007/s10865-020-00157-y
- Edelman EJ, Aoun-Barakat L, Villanueva M, Friedland G. Confronting another pandemic: lessons from HIV can inform our COVID-19 response. *AIDS Behav* (2020) 24(7):1977–1979. doi: 10.1007/s10461-020-02908-z
- Logie CH. Lessons learned from HIV can inform our approach to COVID-19 stigma. *J Int AIDS Soc* (2020) 23(5):e25504. doi: 10.1002/jia2.25504
- Yeo JY, Koh DW-S, Yap P, Goh G-R, Gan SK-E. Spontaneous mutations in HIV-1 gag, protease, RT p66 in the first replication cycle and how they appear: insights from an *in vitro* assay on mutation rates and types. *Int J Mol Sci* (2021) 22(1):370. doi: 10.3390/ijms22010370
- Su CT-T, Ling W-L, Lua W-H, Haw Y-X, Gan SK-E. Structural analyses of 2015-updated drug-resistant mutations in HIV-1 protease: an implication of protease inhibitor cross-resistance. *BMC Bioinf* (2016) 17(S19):500. doi: 10.1186/s12859-016-1372-3
- Chiang R-H, Gan S-E, Su C-T. A computational study for rational HIV-1 non-nucleoside reverse transcriptase inhibitor selection and the discovery of novel allosteric pockets for inhibitor design. *Bioscience Rep* (2018) 38(2). doi: 10.1042/bsr20171113
- Samsudin F, Gan SK-E, Bond PJ. The impact of Gag non-cleavage site mutations on HIV-1 viral fitness from integrative modelling and simulations. *Comput Struct Biotechnol J* (2021) 19:330–42. doi: 10.1016/j.csbj.2020.12.022
- Su CT-T, Kwoh C-K, Verma CS, Gan SK-E. Modeling the full length HIV-1 Gag polyprotein reveals the role of its p6 subunit in viral maturation and the effect of non-cleavage site mutations in protease drug resistance. *J Biomolecular Structure Dynamics* (2017) 36(16):4366–77. doi: 10.1080/07391102.2017.1417160
- Phua S-X, Chan K-F, Su CT-T, Poh J-J, Gan SK-E. Perspective: The promises of a holistic view of proteins—impact on antibody engineering and drug discovery. *Bioscience Rep* (2019) 39(1):BSR20181958. doi: 10.1042/bsr20181958
- Gan SK-E, Phua S-X, Yeo JY. Sagacious epitope selection for vaccines, and both antibody-based therapeutics and diagnostics: tips from virology and oncology. *Antibody Ther* (2022) 5(1):63–72. doi: 10.1093/abt/tbac005
- Yeo JY, Gan SK-E. Peering into Avian Influenza A(H5N8) for a Framework towards Pandemic Preparedness. *Viruses* (2021) 13(11):2276. doi: 10.3390/v13112276

Acknowledgments

We thank the publisher, the contributing authors, the reviewers, and associated editors in their effort to make this Research Topic possible to our readers.

Conflict of interest

The authors declare that the research was conducted in the absence of any commercial or financial relationships that could be construed as a potential conflict of interest.

The author(s) SG, EK declared that they were editorial board members of Frontiers, at the time of submission. This had no impact on the peer review process and the final decision.

Publisher's note

All claims expressed in this article are solely those of the authors and do not necessarily represent those of their affiliated organizations, or those of the publisher, the editors and the reviewers. Any product that may be evaluated in this article, or claim that may be made by its manufacturer, is not guaranteed or endorsed by the publisher.