



Taibah University  
**Journal of Taibah University Medical Sciences**

www.sciencedirect.com



Letter to the Editor

## Molecular and computational research in low- and middle-income countries: Development is close at hand

Nathalie Marina Pérez-Fontalvo, MD<sup>a</sup>, Mayra Alejandra De Arco-Aragón, MD<sup>a</sup>,  
Juranis del Carmen Jimenez-García, MD<sup>b</sup> and Ivan D. Lozada-Martinez<sup>c,\*</sup>

<sup>a</sup> Department of Medicine, School of Medicine, Universidad Libre, Barranquilla, Colombia

<sup>b</sup> Department of Medicine, School of Medicine, Universidad Metropolitana, Barranquilla, Colombia

<sup>c</sup> Department of Medicine, Medical and Surgical Research Center, School of Medicine, University of Cartagena, Cartagena, Colombia

Received 27 May 2021; accepted 30 June 2021; Available online 5 August 2021

To the Editor:

We read a recently published article by Umar et al. titled 'In-silico analysis of the inhibition of the SARS-CoV-2 main protease by some active compounds from selected African plants' with great interest. Through an in-silico study, the authors investigated the inhibitory effect of bioactive components of African plants on Mpro and predicted the pharmacological and toxicological profiles of these components, observing that these phytoconstituents possessed an antiviral potential against SARS-Cov-2, even greater than hydroxychloroquine.<sup>1</sup> We thank Umar et al.<sup>1</sup> for providing such valuable evidence. However, we would like to make some comments on the relevance of supporting such studies in low- and middle-income countries, and the impact they will have on their public health priorities in the near future.

Given the catastrophe that the COVID-19 pandemic has generated for public health and health systems globally,<sup>2–4</sup> there is an evident need to strengthen the funding and organization of biomedical research not only in high-income countries, but mainly in low- and middle-income countries, which have very high indicators of poverty, inequality, violence and burden of disease.<sup>5,6</sup> In-silico studies constitute a fundamental and innovative tool in the modeling of protein and molecular structures for the design and discovery of new drugs.<sup>1,7</sup> Recently, Murunga et al.<sup>8</sup>

reviewed the published evidence on knowledge, practice, and support of translational studies in low- and middle-income countries, finding that the participation from these countries on this type of studies was almost non-existent; hence, it is necessary to strengthen institutional guidelines, incentives, funding, and training to remove the barriers to perform this type of studies.<sup>8</sup> The same difficulties were exposed by Ahmed et al.,<sup>9</sup> who state that, due to barriers to access to updated state of the art, low participation in global meetings, difficulties in access to quality technologies and equipment, among others, there are currently many challenges for the development of studies in biomedicine.<sup>9</sup> For these reasons, observing the work and results of Umar et al.<sup>1</sup> generates much satisfaction and enthusiasm, since according to the requirements to perform these computational studies, it is expected that these simulations are performed almost entirely in developed countries. However, it is possible to perceive that the technological and scientific development in this group of countries is gradually being achieved.

More importantly, in the current context of the COVID-19 pandemic and considering the emergence of new SARS-Cov-2 strains with unpredictable behaviour,<sup>2,3</sup> it is imperative that each nation study the viral genotype to determine the degree of transmissibility and aggressiveness of the most prevalent strain at the local level in a personalized manner. Additionally, these studies are indispensable for the constant evaluation of therapeutic targets for other types of infectious diseases that are endemic in regions such as Latin America and the Caribbean or Africa (Tuberculosis or Malaria), and that can provide a solution sooner than expected.<sup>10</sup>

Although it was reported a decade ago that the strengthening of health policy and research systems was very low (4 % of the total publications on these topics came from authors from low- and middle-income countries),<sup>6</sup> GloPID-

\* Corresponding address: Medical and Surgical Research Center, University of Cartagena, Cartagena de Indias, Colombia.

E-mail: [ivandavidloma@gmail.com](mailto:ivandavidloma@gmail.com) (I.D. Lozada-Martinez)

Peer review under responsibility of Taibah University.



Production and hosting by Elsevier

R has recognized that the attempt to produce theoretical knowledge, treatment research, and design diagnostic tools for the solution of COVID-19 from low- and middle-income countries has been remarkable.<sup>11</sup> Therefore, it is expected that a significant increase in the number of molecular, clinical, and computational studies by these countries will be observed in the coming years, and that they will become a global reference. It is necessary to reinforce knowledge and specialized support networks that allow international collaborations that facilitate the search for solutions to regional and global public health problems. It is evident that the development of these countries on the part of science is getting closer and closer.

### Source of funding

This research did not receive any specific grant from funding agencies in the public, commercial, or not-for-profit sectors.

### Conflict of interest

The authors have no conflict of interest to declare.

### Ethical approval

The authors confirm that this letter had been prepared in accordance with COPE roles and regulations. Given the nature of the letter, the IRB review was not required.

### Authors' contributions

Every author contributed equally in all the parts of the research. All authors have critically reviewed and approved the final draft and are responsible for the content and similarity index of the manuscript.

### References

1. Umar HI, Josiah SS, Saliu TP, Jimoh TO, Ajayi A, Danjuma JB. In-silico analysis of the inhibition of the SARS-CoV-2 main protease by some active compounds from selected African plants. *J Taibah Univ Med Sci* 2021; 16(2): 162–176. <https://doi.org/10.1016/j.jtumed.2020.12.005>.
2. Bong CL, Brasher C, Chikumba E, McDougall R, Mellin-Olsen J, Enright A. The COVID-19 pandemic: effects on low-

- and middle-income countries. *Anesth Analg* 2020; 131(1): 86–92. <https://doi.org/10.1213/ANE.0000000000004846>.
3. Hopman J, Allegranzi B, Mehtar S. Managing COVID-19 in low- and middle-income countries. *J Am Med Assoc* 2020; 323(16): 1549–1550. <https://doi.org/10.1001/jama.2020.4169>.
4. Walker PGT, Whittaker C, Watson OJ, Baguelin M, Winskill P, Hamlet A, et al. The impact of COVID-19 and strategies for mitigation and suppression in low- and middle-income countries. *Science* 2020; 369(6502): 413–422. <https://doi.org/10.1126/science.abc0035>.
5. English KM, Pourbohloul B. Increasing health policy and systems research capacity in low- and middle-income countries: results from a bibliometric analysis. *Health Res Pol Syst* 2017; 15(1): 64. <https://doi.org/10.1186/s12961-017-0229-1>.
6. Adam T, Ahmad S, Bigdeli M, Ghaffar A, Røttingen JA. Trends in health policy and systems research over the past decade: still too little capacity in low-income countries. *PLoS One* 2011; 6(11):e27263. <https://doi.org/10.1371/journal.pone.0027263>.
7. Brogi S, Castro Ramalho T, Kuca K, Medina-Franco JL, Valko M. Editorial: in silico methods for drug design and discovery. *Front Chem* 2020; 612: 8. <https://doi.org/10.3389/fchem.2020.00612>.
8. Murunga VI, Oronje RN, Bates I, Tagoe N, Pulford J. Review of published evidence on knowledge translation capacity, practice and support among researchers and research institutions in low- and middle-income countries. *Health Res Pol Syst* 2020; 18(1): 16. <https://doi.org/10.1186/s12961-019-0524-0>.
9. Ahmed A, Daily JP, Lescano AG, Golightly LM, Fasina A. Challenges and strategies for biomedical researchers returning to low- and middle-income countries after training. *Am J Trop Med Hyg* 2020; 102(3): 494–496. <https://doi.org/10.4269/ajtmh.19-0674>.
10. Hogan AB, Jewell BL, Sherrard-Smith E, Vesga JF, Watson OJ, Whittaker C, et al. Potential impact of the COVID-19 pandemic on HIV, tuberculosis, and malaria in low-income and middle-income countries: a modelling study. *Lancet Glob Health* 2020; 8(9): e1132–e1141. [https://doi.org/10.1016/S2214-109X\(20\)30288-6](https://doi.org/10.1016/S2214-109X(20)30288-6).
11. Global Research Collaboration for Infectious Disease Preparedness (GLOPID-R). *COVID-19 research in low and middle income countries [Internet]*; 26 May 2021. Available in: <https://www.glopid-r.org/covid-19-research-in-low-and-middle-income-countries/>.

**How to cite this article:** Pérez-Fontalvo NM, De Arco-Aragón MA, Jimenez-García JdelC, Lozada-Martinez ID. Molecular and computational research in low- and middle-income countries: Development is close at hand. *J Taibah Univ Med Sc* 2021;16(6):948–949.