



OPEN ACCESS

EDITED AND REVIEWED BY
Daniel Salamango,
Stony Brook University, United States

*CORRESPONDENCE

Deepti Parashar
✉ deeptiparasharster@gmail.com
Sarah Cherian
✉ sarahcherian100@gmail.com

[†]These authors have equally contributed to this work

RECEIVED 20 May 2023

ACCEPTED 22 May 2023

PUBLISHED 23 June 2023

CITATION

Kasabe B, Ahire G, Patil P, Punekar M, Davuluri KS, Kakade M, Alagarasu K, Parashar D and Cherian S (2023) Corrigendum: Drug repurposing approach against chikungunya virus: an *in vitro* and *in silico* study. *Front. Cell. Infect. Microbiol.* 13:1226054. doi: 10.3389/fcimb.2023.1226054

COPYRIGHT

© 2023 Kasabe, Ahire, Patil, Punekar, Davuluri, Kakade, Alagarasu, Parashar and Cherian. This is an open-access article distributed under the terms of the [Creative Commons Attribution License \(CC BY\)](https://creativecommons.org/licenses/by/4.0/). 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.

Corrigendum: Drug repurposing approach against chikungunya virus: an *in vitro* and *in silico* study

Bhagyashri Kasabe^{1†}, Gunwant Ahire^{2†}, Poonam Patil², Madhura Punekar², Kusuma Sai Davuluri², Mahadeo Kakade², Kalichamy Alagarasu², Deepti Parashar^{2*} and Sarah Cherian^{1*}

¹Bioinformatics Group, Indian Council of Medical Research (ICMR)-National Institute of Virology, Pune, Maharashtra, India, ²Dengue & Chikungunya Group, Indian Council of Medical Research (ICMR)-National Institute of Virology, Pune, Maharashtra, India

KEYWORDS

chikungunya virus (CHIKV), drug repurposing, structural and non-structural proteins, *in silico* screening, *in vitro* validation

A corrigendum on

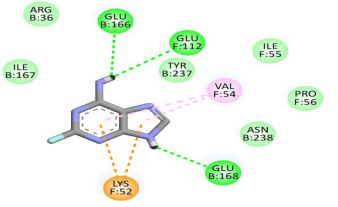
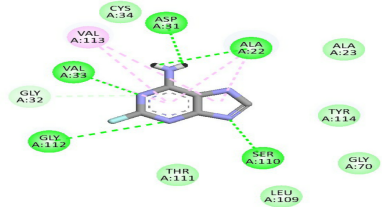
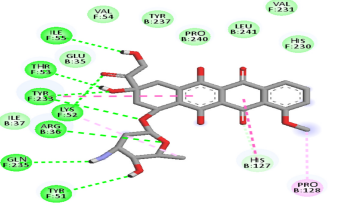
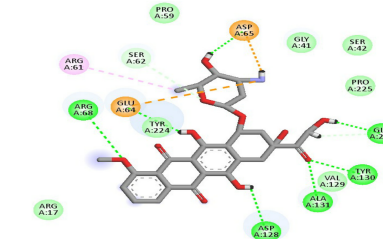
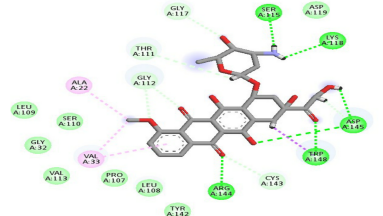
Drug repurposing approach against chikungunya virus: an *in vitro* and *in silico* study

by Kasabe B, Ahire G, Patil P, Punekar M, Davuluri KS, Kakade M, Alagarasu K, Parashar D and Cherian S (2023) *Front. Cell. Infect. Microbiol.* 13:1132538. doi: 10.3389/fcimb.2023.1132538

In the published article, there was an error in [Table 4](#) as published. The target for metyrapone was listed twice while the target for lomibuvir was missed. The corrected [Table 4](#) and its caption [Molecular docking interactions of the nine FDA approved drugs with CHIKV structural and non-structural proteins based on the binding affinity values and best pose] appear below.

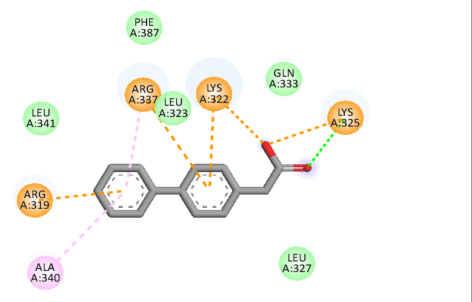
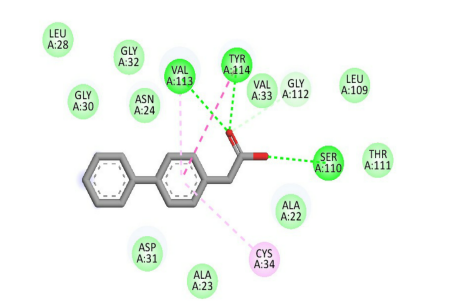
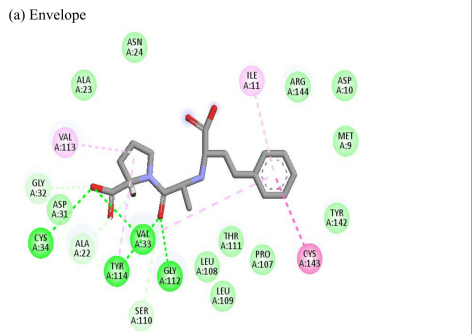
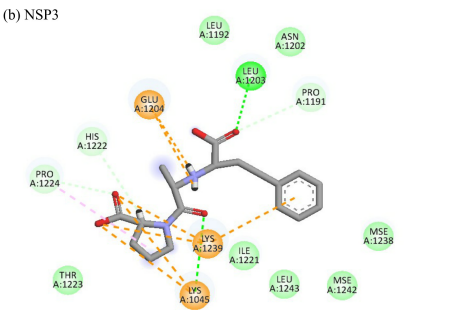
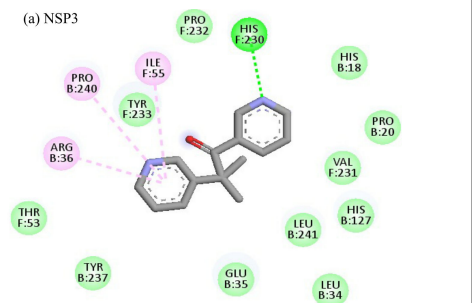
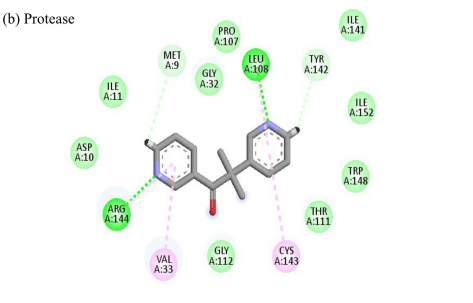
The authors apologize for this error and state that this does not change the scientific conclusions of the article in any way. The original article has been updated.

TABLE 4 Molecular docking interactions of the nine FDA approved drugs with CHIKV structural and non-structural proteins based on the binding affinity values and best pose.

| Compound | Potential binding viral targets | Docking score | Binding energy (kcal/mol) | Ligand Efficiency (kcal/ mol) |
|----------------|--|------------------------------------|----------------------------|-------------------------------|
| 2-Fluroadenine | (a) NSP3  | (a)-6.966 (b)-2.958 | -37.69 -25.51 | -11.091 -5.632 |
| | (b) Envelope  | | | |
| Doxorubicin | (a) Envelope  | (a)-4.76 (b)-6.069 (c)-3.547 | -77.88 -77.55 -77.21 | -13.179 -15.343 -13.297 |
| | (b) MTase  | | | |
| | (c) NSP3  | | | |

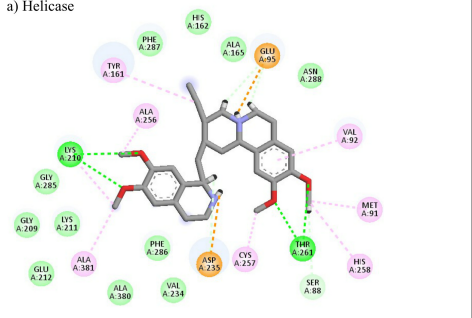
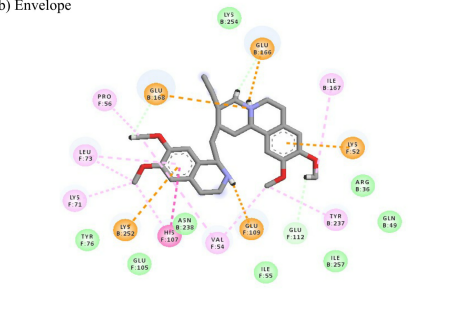
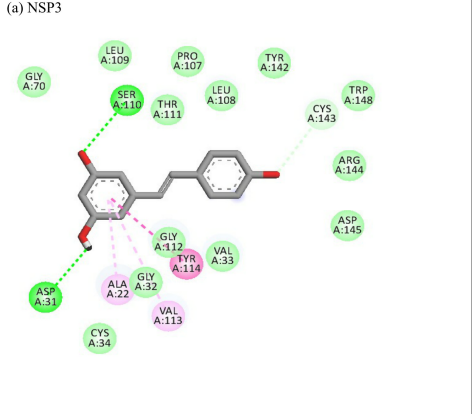
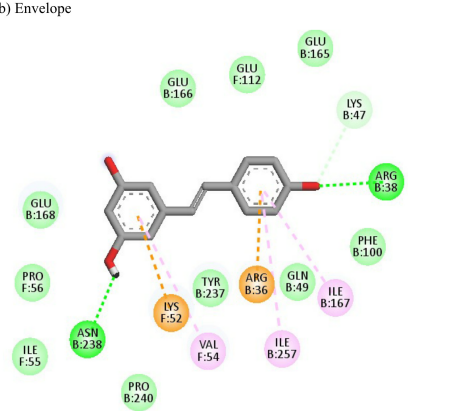
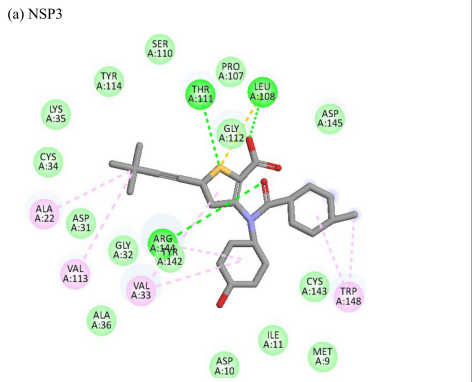
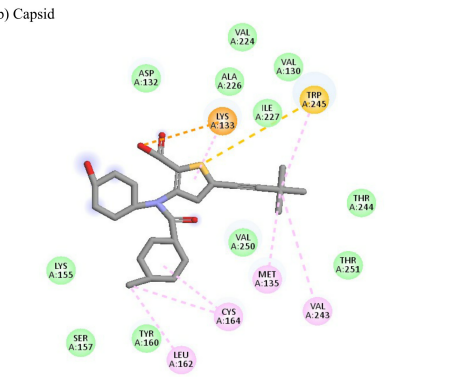
(Continued)

TABLE 4 Continued

| Compound | Potential binding viral targets | Docking score | Binding energy (kcal/mol) | Ligand Efficiency (kcal/ mol) | |
|-------------|--|--|---------------------------|-------------------------------|--------------------|
| Felbiac | (a) RdRp  | (b) NSP3  | (a)-4.332 (b)-6.115 | -44.3 -39.72 | -11.74 -10.529 |
| | (a) Envelope  | (b) NSP3  | (a)-4.358 (b)-6.498 | -51.12 -50.81 | -12.521 -13.255 |
| Enalaprilat | (a) NSP3  | (b) Protease  | (a)-7.476 (b)-4.02 | -60.97 -55.33 | -14.452 -11.234 |

(Continued)

TABLE 4 Continued

| Compound | Potential binding viral targets | | Docking score | Binding energy (kcal/mol) | Ligand Efficiency (kcal/ mol) |
|-------------|---|--|------------------------|---------------------------|-------------------------------|
| Emetine | a) Helicase | (b) Envelope | (a)-4.086 (b)-4.238 | -74.25 -71.81 | |
| |  |  | | | |
| Resveratrol | a) NSP3 | (b) Envelope | (a)-6.22 (b)-4.675 | -56.45 -47.43 | -14.72 -11.734 |
| |  |  | | | |
| Lombubivir | a) NSP3 | (b) Capsid | (a)-5.573 (b)-4.759 | -81.13 -78.83 | |
| |  |  | | | |

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.