Authors' Response To Peer Reviews

Authors' Response to Peer Reviews of "Discovery of Novel Inhibitors of HMG-CoA Reductase Using Bioactive Compounds Isolated From Cochlospermum Species Through Computational Methods: Virtual Screening and Algorithm Validation Study"

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JMIRx Bio 2025;3:e78093; doi: 10.2196/78093

Keywords: HMGR; statins; hypercholesterolemia; cochlospermum; phytochemicals; molecular docking

This is the authors' response to the peer-review report for "Discovery of Novel Inhibitors of HMG-CoA Reductase Using Bioactive Compounds Isolated From Cochlospermum Species Through Computational Methods: Virtual Screening and Algorithm Validation Study."

My profound appreciation goes to the reviewers [1] for their thoughtful, constructive, and actionable feedback on my manuscript [2]. I'm grateful for the opportunity to revise and improve my work based on the graceful comments provided. Here are the details of my responses to the reviewers' comments and the changes made to the manuscript.

Concerns and Feedback

Reviewers appreciated the depth and thoroughness of the search through the literature of peer-review research. Some reviewers were surprised about the date (1991) of some studies related to the high-performance liquid chromatography–UV analysis of phytochemicals identified in the ethanolic and methanolic extract of Cochlospermum tinctorium and wondered whether there may be more recent studies to also consider.

Response: Thank you for your kind comments and the concern raised. However, just like I mentioned during the live review session, studies related to the isolation and identification of some bioactive compounds from *C tinctorium* are quite old and indigenous with limited data available, but I was still able to pull more recent data from 2012.

To increase the reproducibility of the study, some reviewers wondered if it would be possible to make the data and code used to analyze the data openly available.

Response: The data file and details used for the analysis have now been made available in the manuscript and can be found in Multimedia Appendix 6.

The figures and tables are comprehensive and clearly presented, with well-written descriptions. If feasible, reviewers would suggest ways to visually highlight key compounds listed in tables using colors, bold text, or labels.

Furthermore, incorporating chemical structures directly within the relevant tables or as supplementary figures would further enhance the understanding of their molecular characteristics and potential interactions.

Response: The phytochemicals analyzed in this study had already been narrowed down to 10 top-ranked compounds and are contained in Tables 1 and 3 of the manuscript. Also, I have incorporated their chemical structures and a few additional details including those of statins (Table 4) to enhance readers' understanding. For information regarding their molecular characteristics and potential binding interactions, kindly check Multimedia Appendices 2-5.

While the author acknowledges the need for in vitro and in vivo validation studies, explicitly addressing potential computational limitations—such as docking inaccuracies, semirigid approach versus more flexible ones, or the absence of dynamic modeling—would further strengthen the discussion.

Response: Of course, computational studies have their own share of limitations especially molecular docking studies, and I'm well aware of certain docking inaccuracies and the advantage that more flexible docking and molecular dynamics simulations algorithms hold over semirigid docking. Nevertheless, a pragmatic approach had already been taken to ascertain the accuracy and validity of the "PyRx AutoDock Vina" algorithm used in this docking study. The details of this submission are in the "Methods" section of the manuscript under the subheading "Molecular Docking Analysis."

Some reviewers suggested adapting the part of the study that identified the compounds through literature review into a systematic review.

Response: This suggestion has been taken into consideration, and a systematic review has now been included as part of the manuscript title. Many thanks to the reviewers for their insightful comments.

Additional revisions have been made to the manuscript in response to the editorial team's valuable feedback, but are not highlighted in my responses above.

I trust that these revisions will address the issues raised by the reviewers and improve the quality of the manuscript.

Artificial intelligence disclosure: The author attests that there was no use of generative artificial intelligence technology in the generation of text, figures, or other informational content of this manuscript.

References

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2. Olatoye TI. Discovery of novel inhibitors of HMG-CoA reductase using bioactive compounds isolated from cochlospermum species through computational methods: virtual screening and algorithm validation study. JMIRx Bio. 2025;3:e71675. [doi: 10.2196/71675]

Edited by Amy Schwartz; This is a non–peer-reviewed article; submitted 26.05.2025; accepted 26.05.2025; published 10.07.2025

Please cite as:
Olatoye TI
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JMIRx Bio 2025;3:e78093
URL: https://bio.jmirx.org/2025/1/e78093
doi: 10.2196/78093