

### **List of Publications:**

1. Identification of Novel Inhibitors of Cancer Target Telomerase Using a Dual Structure-based Pharmacophore Approach to Virtually Screen Libraries, Molecular Docking and validation by Molecular Dynamics Simulations – **Accepted in Journal of Biomolecular structure and Dynamics (IF 4.1)**  
**Acceptance Letter Attached (Below)**
2. Targeting telomerase using structure-based drug repurposing approach: A therapeutic strategy to investigate anti-cancer potential of FDA approved drugs. (**Manuscript under submission**)
3. Design and development of machine learning model to identify small molecules as inhibitors of multifarious cancer targets. (**Manuscript under submission**)
4. Harnessing Drug Repurposing to Discover and Validate PCSK9-LDLR Disruptors: A Promising Strategy for Lipid Lowering and Cardiovascular Therapeutic Development. (**Manuscript under submission**)

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**Fwd: Journal of Biomolecular Structure & Dynamics - Decision on Manuscript ID TBSD-2024-1091.R2**

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**Madhu Chopra** <mchopradu@gmail.com>

Thu, Jun 27, 2024 at 6:05 PM

To: divpreetkaur96@gmail.com, Daman Chilana &lt;dsalujach1959@gmail.com&gt;, Prakash Jha &lt;prakash424@hotmail.com&gt;

Congratulations to the team.

Regards

----- Forwarded message -----

From: **Journal of Biomolecular Structure & Dynamics** <onbehalf@manuscriptcentral.com>

Date: Thu, Jun 27, 2024, 5:57 PM

Subject: Journal of Biomolecular Structure & Dynamics - Decision on Manuscript ID TBSD-2024-1091.R2

To: <mchopradu@gmail.com>

27-Jun-2024

Dear Professor Madhu Chopra,

Ref: Identification of Novel Inhibitors of Cancer Target Telomerase Using a Dual Structure-based Pharmacophore Approach to Virtually Screen Libraries, Molecular Docking and validation by Molecular Dynamics Simulations

Our referees have now considered your paper and have recommended publication in Journal of Biomolecular Structure & Dynamics. We are pleased to accept your paper in its current form which will now be forwarded to the publisher for copy editing and typesetting. The referee comments are included at the bottom of this letter, along with those of the editor who coordinated the review of your paper.

Within weeks, your paper will be published online ahead of print as a 'Latest Article', which can be cited using the DOI.

You will receive proofs for checking, and instructions for transfer of copyright in due course.

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If you have any questions about the status of your manuscript, please contact the Journal Editorial Office ([TBSD-peerreview@journals.tandf.co.uk](mailto:TBSD-peerreview@journals.tandf.co.uk)).

Thank you for your contribution to Journal of Biomolecular Structure & Dynamics and we look forward to receiving further submissions from you.

Sincerely,  
Dr Freddie Salsbury  
Associate Editor Journal of Biomolecular Structure & Dynamics  
[salsbufr@wfu.edu](mailto:salsbufr@wfu.edu)

Referee(s)' Comments to Author:

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**Journal of Biomolecular Structure and Dynamics**

**Identification of Novel Inhibitors of Cancer Target Telomerase Using a Dual Structure-based Pharmacophore Approach to Virtually Screen Libraries, Molecular Docking and validation by Molecular Dynamics Simulations**

<b>Submission ID</b>	244042521
<b>Article Type</b>	Research Article
<b>Keywords</b>	Drug discovery, Telomerase, Virtual Screening, Molecular dynamics simulation, Small molecule inhibitors
<b>Authors</b>	Divpreet Kaur, Daman Saluja, Madhu Chopra