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Dual targeting in prostate cancer with phytoconstituents as a potent lead: a computational approach for novel drug discovery

Sachin A. Dhawale[a], Pallavi Bhosle[b], Sadhana Mahajan[c], Geetanjali Patil[a], Sachin Gawale[a], Mangesh Ghodke[a], Ganesh Tapadiya[a] and Azim Ansari[d]

[a]Department of Pharmaceutical Chemistry, Shreeyash Institute of Pharmaceutical Education and Research, Aurangabad, India; [b]Pharmacology, Shrinath College of Pharmacy, Aurangabad, India; [c]K.B.H.S.S Institute of Pharmacy, Nashik, India; [d]S.V.K.M Institute of Pharmacy, Dhule, India

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ABSTRACT

Prostate Cancer (PCa) is an abnormal cell growth within the prostate. This condition is the second most widespread malignancy in elderly males and one of the most frequently diagnosed life-threatening conditions. The Androgen receptor signaling pathway played a crucial role in the initiation and spread to increase the risk of PCa. Hence, targeting the AR receptor signaling pathway is a key strategy for a therapeutic plan for PCa. Our study focuses on recognizing potential inhibitors for dual targeting in PCa by using the *in-silico* approach. In this study, we target the two enzymes that are CYP17A1 (3RUK) and 5α-reductase (3G1R) responsible for PCa, with the help of phytoconstituents. The natural plant contains various phytochemical types produced from secondary metabolites and used as a medical treatment. The *in-silico* investigation of phytoconstituents and enzymes was done by approaching molecular docking, ADMET analysis, and high-level molecular dynamic simulation used to assess the stability and binding affinities of the protein-ligand complex. Some phytoconstituents, such as Peonidin, Pelargonidin, Malvidin and Berberine show complex has good molecular interaction with protein. The reliability of the docking scores was examined using a molecular dynamic simulation, which revealed that the complex remained stable throughout the simulation, which ranged from 0 to 200 ns. The selected hits may be effective against CYP17A1 (3RUK) and 5α-reductase (3G1R) (PCa) using a computer-aided drug design (CADD) method, which further enables researchers for upcoming in-vivo and in-vitro research, according to our *in-silico* approach.

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CONTACT Sachin A. Dhawale sdhawale021@gmail.com Department of Pharmaceutical Chemistry, Shreeyash Institute of Pharmaceutical Education and Research, Aurangabad 431010, Maharashtra, India

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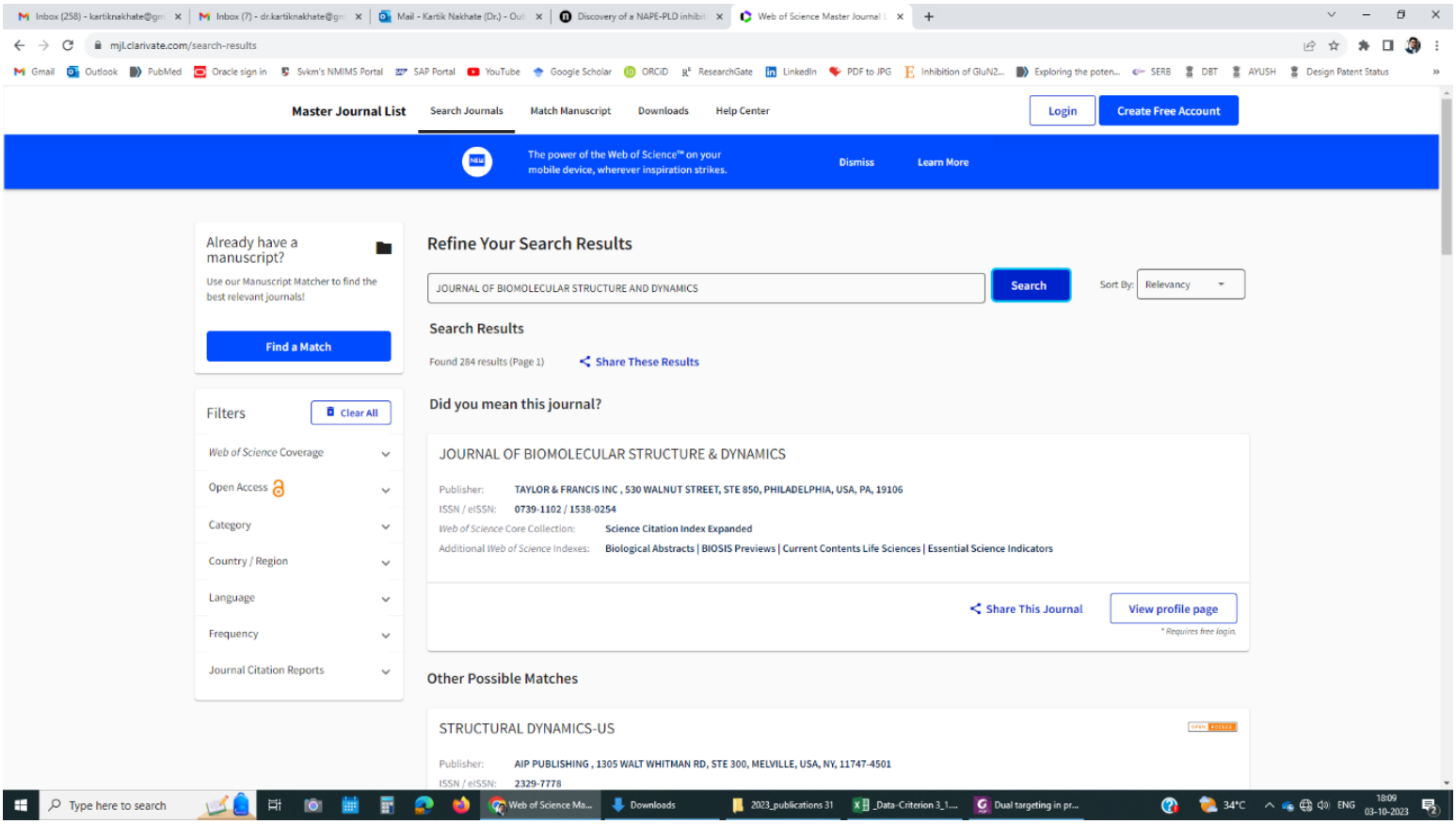
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