

Exploring the inhibitory role of *Persicaria hydropiper* bioactive compounds against 2KID protein associated with *Staphylococcus aureus* biofilm formation: Molecular docking, dynamic simulation and pharmacological property analysis

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The current communication states the role of *Persicaria hydropiper* (L.) bioactive compounds in the inhibition of *Staphylococcus aureus* sortase A through bioinformatic approaches. The *P. hydropiper*-derived phytochemicals (kaempferol, winterin, isalpinin, quercitrin and confertifolin) 3D structures (on retrieval from PubChem) were docked to *Staphylococcus aureus* sortase A (2KID) protein, using AutoDoc Vina. Pharmacological properties of the phytochemical ligands were determined through Lipinski's rule of 5 and ADMET analysis and bioavailability score prediction. All the ligands displayed good affinity to 2KID protein, displaying binding energy ranging from -8.0 kcal/mol (kaempferol) to 7.1 kcal/mol (confertifolin), compared to a conventional antibiotic, ciprofloxacin (binding energy: -6.7 kcal/mol). Because of its highest affinity to 2KID protein, kaempferol was subjected to molecular dynamic simulation study, which along with the binding free energy calculation will help characterize the stability of 2KID- kaempferol interaction. Hence, *P. hydropiper* phytochemicals might be useful in the development of drugs for the treatment against infection caused with biofilm forming *Staphylococcus aureus*.

Biography

Shyamapada Mandal is Professor and Head of the Department of Zoology, and Dean (Science), University of Gour Banga, India. He is interested on infectious diseases, probiotics, and genomics and bioinformatics research. He did pre-PhD, PhD, and post-PhD research under the guidance of Professor Nishith Kumar Pal at Calcutta School of Tropical Medicine, India. He has published 118 articles with eight book chapters. He is life member of IAMM and IASR, India and fellow member of SASS, India. Eight national academic and research awards have been conferred to him. He has guided 52 post graduate students; supervised three MPhil and three PhD students, and supervising 6 PhD and one MPhil students. Professor Mandal is among the world's top 2% scientists as per the survey of the Stanford University, published in PLOS (Public Library of Science) Biology (October, 2020). He is featured in the top 2% world scientists list for second consecutive time as published by the Stanford University-Elsevier BV (October, 2021).

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