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In silico antimalarial drug designining

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Malaria is an infection caused by mosquitoes to the human beings. Among the known five species of Plasmodium, the majority of the deaths are caused by P. Falciparum and P. Vivax. The enzyme plasmodium falciparum dihydrofolate reductase is a well known malarial drug target. The aim of the present study is to use Quassinoids as the ant malarial drug and to dock it with the plasmodium falciparum dihydrofolate reductase by the protein-ligand docking. The known scaffold of Quassinoid is taken and is substituted with the chemical compounds at "Y" position. 12 Quassinoid ligands were drawn in chemsketch and their sterioisomers were created. These were then docked with the protein 4dpd. The dock results showed three Quassinoid models to be the potential ligands. Among the three Quassinoids, Quassinoid model 1 showed the highest dock score with 40.728.

Biography

R.D. Shailima Vardhini is currently working as the Head of the Department-Biochemistry, St. Mary's College, Yousufguda, Hyderabad, AP, India. She has published research articles in various reputed international journals and is also on the Reviewer and Editorial Board of reputed Journals. Her research interests include Cancer Biology, Nanotechnology and Bioinformatics.

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