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Exploring the possible phytochemical treatment of black fungus by ADMET profiling and molecular docking study targeting rhizopuspepsin and lipase from *Rhizopus microsporus*

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Mucormycosis is a rare but serious fungal infection caused with mucormycetes (*Rhizopus oryzae* (or *Rhizopusmicrosporus*), *Mucor* species, *Lichtheimia corymbifera* and *Rhizomucor pusillus*) and is currently associated COVID-19 as 'black fungus' causing high mortality. This communication states the inhibition of target proteins of *Rhizopusmicrospores* by some bioactive phytochemicals following *in silico* approaches. Therefore, we have docked the phytochemical ligands (retrieved from <u>https://www.rcsb.org/</u>): cajanone, diosgenin and piperine, along with the standard treatment isavuconazole to X-ray diffraction structure (obtained from RCSB Protein Data Bank) of two target proteins rhizopuspepsin and lipase from *Rhizopus microsporus* var. chinensis, in order to determine the binding affinity of the ligands to the receptors. The four ligands cajanone, diosgenin, piperine and isavuconazole had respective binding energy of –9.1, –8.7, –7.8 and –7.3 kcal/mol to rhizopuspepsin and –7.6, –8.1, –6.6 and –7.1 kcal/mol, displaying hydrogen bonds and/or hydrophobic interactions. The drug-likeness, bioavailability and ADMET properties were determined for the ligands intended to be utilised as the candidate drugs against Mucorales infection and thereby preventing 'black fungus' during COVID-19 pandemic.

Biography

Shyamapada Mandal, Professor, Department of Zoology and Dean (Faculty of Science) University of Gour Banga, India, He is interested on infectious diseases, probiotics and genomics, bioinformatics and in silico drug development 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 117 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. 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).