In silico phytochemical repurposing of natural molecules as entry inhibitors against RBD of the spike protein of SARS-CoV-2 using molecular docking studies

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Abstract

The receptor binding domain (RBD) of Spike-protein (S-protein) is responsible for virus entry via interaction with host protein ACE2 (angiotensin-converting enzyme 2), present on the cell surface of humans. Therefore, S-protein is an important target to block the entry of the SARS-CoV-2 into the cell for further growth. In the present study, phytochemical repurposing of natural molecules: narirutin, naringin, neohesperidin and hesperidin were performed against the RBD S-protein/ACE2 interface as well as the RBD of the S-protein using molecular docking. These natural molecules were found to have structural similarity to each other and had binding potential against the viral infections. It is first time reported here that the naringin and narirutin are having binding potential against both RBD S-protein/ACE2 interface and active site of RBD of S-protein using binding mode analysis. Hence, this study will open avenues for multitargeting similar natural molecules binding against the SARS-CoV-2 proteins as all reports are made in this single study.

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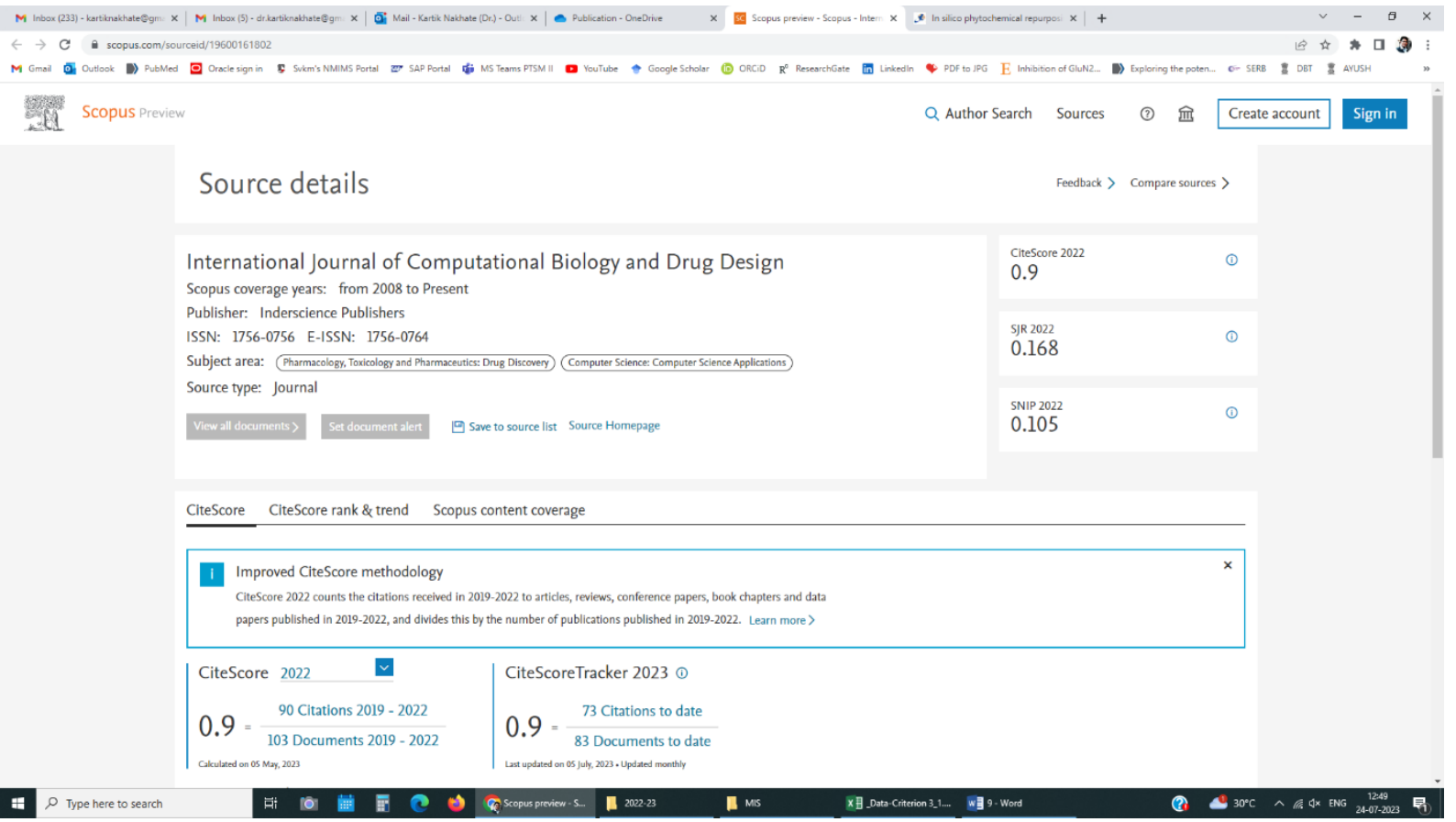
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