Screening of bioactive components of durian and mangosteen and analyzing their interactions with SARS-CoV-2 protein by computational studies

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ABSTRACT

Introduction: The COVID-19 pandemic has necessitated a global search for viable therapies and prevention methods. In this quest, computational investigations have played a key role by enabling rapid screening of potential therapeutic candidates. **Objective:** This research aimed to screen various bioactive compounds found in durian and mangosteen and analyze their interactions with SARS-CoV-2 using computational approaches. **Materials and Method:** Bioactive compounds of the durian and mangosteen were retrieved from PubChem, and Maestro Schrödinger sitemap was used to investigate the interactions and binding affinities of these possible compounds with the selected SARS-CoV-2 protein – 3CLpro. Furthermore, using SwissADME, an open-access tool, the pharmacokinetic, drug-like, and medicinal chemistry features of the selected compounds were predicted. **Results:** Following Lipinski's rule of five, 24 bioactive compounds from durian and mangosteen were shortlisted. After individual docking, compounds with the greatest interaction energies were chosen as lead compounds. Among the top bioactive compounds from durian, kaempferol had the highest docking score of -7.687 kcal/mol, with two hydrogen bond interactions. Chrysanthemin – the top bioactive compound from mangosteen – had a docking score of -7.311 kcal/mol, forming five hydrogen bond interactions with Asp 187, Thr 26, Hip 163, Asn 142, and Gly 143. **Conclusion:** Kaempferol and chrysanthemin are promising bioactive compounds that may inhibit SARS-CoV-2 protein targets and could serve as potential therapeutic candidates.