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Abstract

A Molecular Docking Study on Natural Compounds as Anxiolytics and Antidepressants †

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Abstract: Anxiety and depression are two conditions that had increased incidences in the context of COVID-19. The administration of current therapies based on anxiolytic and antidepressant drugs can result in adverse reactions and even potential dangers in the case of some patients, such as older adults and elderly patients. Aiming to identify safer treatments, we used molecular docking to screen twenty natural compounds against γ-aminobutyric acid A receptor (GABAA receptor), a major drug target in anxiety, and against serotonin transporter (SERT), a major drug target in depression. The list of compounds included molecules that were previously reported as beneficial in the two conditions. In the case of all molecules, we predicted their drug-likeness, bioavailability, and pharmacokinetic profiles. Molecular docking has shown that the top five molecules in terms of affinity for the GABAA receptor are luteolin, baicalein, myricetin, chrysin, and curcumin. In the case of SERT, the top five ligands were myricetin, luteolin, curcumin, apigenin, and fisetin. According to the predictions performed here, these molecules comply with drug-likeness rules, are bioavailable and non-toxic, present a high intestinal absorption, and are distributed to the central nervous system. Our results point toward luteolin, myricetin, and curcumin as common ligands for the GABAA receptor and SERT, suggesting their beneficial effects for both anxiety and depression.

Keywords: natural compounds; anxiolytics; antidepressants; molecular docking

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