World Academy of Science, Engineering and Technology
International Journal of Pharmacological and Pharmaceutical Sciences
Vol:18, No:11, 2024

Screening of Phytochemicals Compounds from Chasmanthera dependens and Carissa edulis as Potential Inhibitors of Carbonic Anhydrases CA II (3HS4) Receptor using a Target-Based Drug Design

Authors : Owonikoko Abayomi Dele

Abstract : Epilepsy is an unresolved disease that needs urgent attention. It is a brain disorder that affects over sixty-five (65) million people around the globe. Despite the availability of commercial anti-epileptic drugs, the war against this unmet condition is yet to be resolved. Most epilepsy patients are resistant to available anti-epileptic medications thus the need for affordable novel therapy against epilepsy is a necessity. Numerous phytochemicals have been reported for their potency, efficacy and safety as therapeutic agents against many diseases. This study investigated 99 isolated phytochemicals from Chasmanthera dependens and Carissa edulis against carbonic anhydrase (ii) drug target. The absorption, distribution, metabolism, excretion and toxicity (ADMET) of the isolated compounds were examined using admet SAR-2 web server while Swiss ADME was used to analyze the oral bioavailability, drug-likeness and lead-likeness properties of the selected leads. PASS web server was used to predict the biological activities of selected leads while other important physicochemical properties and interactions of the selected leads with the active site of the target after successful molecular docking simulation with the pyrx virtual screening tool were also examined. The results of these study identified seven lead compounds; C49- alpha-carissanol (-7.6 kcal/mol), C13- Catechin (-7.4 kcal/mol), C45- Salicin (-7.4 kcal/mol), C6- Bisnorargemonine (-7.3 kcal/mol), C36- Pallidine (-7.1 kcal/mol), S4- Lacosamide (-7.1 kcal/mol), and S7- Acetazolamide (-6.4 kcal/mol) for CA II (3HS4 receptor). These leads compounds are probable inhibitors of this drug target due to the observed good binding affinities and favourable interactions with the active site of the drug target, excellent ADMET profiles, PASS Properties, drug-likeness, lead-likeness and oral bioavailability properties. The identified leads have better binding energies as compared to the binding energies of the two standards. Thus, seven identified lead compounds can be developed further towards the development of new anti-epileptic medications.

Keywords : drug-likeness, phytochemicals, carbonic anhydrases, metalloeazymes, active site, ADMET
Conference Title : ICMCDD 2024 : International Conference on Medicinal Chemistry and Drug Design
Conference Location : Kyoto, Japan
Conference Dates : November 18-19, 2024