ELSEVIER
Biophysical Chemistry 269 (2021) 106529
https://doi.org/10.1016/j.bpc.2020.106529

Phytochemical Profile, Antioxidant, α-amylase Inhibition, Binding Interaction and Docking Studies of Justicia carnea Bioactive Compounds with α-amylase

Akpovwehwee A. Anigboro, Oghenetega J. Avwioroko, Oghenenyore A. Ohwokevwo , Beruoritse Pessu , Nyerhovwo J. Tonukari

Abstract: The present study investigated the antioxidant and in vitro antidiabetic capacities of Justicia carnea aqueous leaf extract (JCAE) using α-amylase inhibition model. α-Amylase binding-interaction with JCAE was also investigated using fluorescence spectroscopy and molecular docking. Phytochemical screening and Gas ChromatographyMass Spectrometry (GC–MS) analysis indicated presence of bioactive compounds. Phenolic (132 mg GAE/g) and flavonoid contents (31.08 mg CE/g) were high. JCAE exhibited high antioxidant capacity and effectively inhibited α-amylase activity (IC50, 671.43 ± 1.88 μg/mL), though lesser than acarbose effect (IC50, 108.91 ± 0.61 μg/mL). α-Amylase intrinsic fluorescence was quenched in the presence of JCAE. Ultraviolet-visible and FTIR spectroscopies affirmed mild changes in α-amylase conformation. Synchronous fluorescence analysis indicated alterations in the microenvironments of tryptophan residues near α-amylase active site. Molecular docking affirmed non-polar interactions of compounds 6 and 7 in JCAE with Asp-197 and Trp-58 residues of α-amylase, respectively. Overall, JCAE indicated potential to prevent postprandial hyperglycemia by slowing down carbohydrate hydrolysis

Keywords: Justicia carnea, α-Amylase inhibition, Antioxidant, Binding interaction, Fluorescence quenching, Molecular docking