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In vivo and in silico analysis of inhibition of rice (Oryza sativa) bran lipase with guava leaf (Psidium guineense swartz) extract

A. M. S. C. Sooriyawansha¹, R. Munaweera¹, N. Jayathilaka^{1*} and K. N. Seneviratne¹

¹Department of Chemistry, Faculty of Science, University of Kelaniya, Sri Lanka njayathi@kln.ac.lk*

Rice (Oryza sativa) bran (RB) is one of the most important co-products in the rice milling industry. It is frequently utilized in animal feed or discarded as waste. After milling, the majority of RB cells are ruptured, and the bran layer is removed from the endosperm. Due to that, the RB lipids encounter highly reactive rice bran lipase (RBL) enzymes which hydrolyze the RB lipids into free fatty acids. Hence RB has a short shelf life. This is the major drawback of using RB as an animal feedstock. This study focused on inhibiting the RBL activity using natural potent inhibitors and determining the mechanism of inhibition to increase the shelf life of RB. The RBLs were isolated by ion-exchange chromatography at pH 10.0 buffer. Guava (Psidium guineense swartz) leaf ethanol: water extracts were tested for inhibition of RBLs. Orlistat, a human gastric and pancreatic lipase inhibitor was used as a positive control. The percent RBLs inhibitory activities were assessed using phenyl acetate assay and the guava leaf ethanol: water extract inhibited the RBL activity ($47.81\% \pm 9.44\%$). The in vivo data were validated by computational analysis. Homology-modeling of RBLs size in 40 kDa and 32 kDa, and molecular docking (AUTODOCK4) were carried out with the lactone or listat to determine the best docking poses with the lowest estimated Gibbs free energy values (ΔG) for the mechanism of inhibition. Or listat lactone ring carbon bound covalently to the serine residue in the characteristic GXSXG pentapeptide sequence (where X=any amino acid) in the catalytic site of the RBLs enzyme. Therefore, lactones present in guava leaf ethanol: water extract has the potential to inhibit the activity of RBLs with a similar mechanism of orlistat. Our finding suggests that guava leaf ethanol: water extract can be applied as a natural solution to increase the shelf life of RB.

Keywords: Rice bran, *Oryza sativa*, *Lipase*, Orlistat, *Psidium guineense swartz*