

Nutrigenetic and Bioinformatic Analysis of Rice Bran Bioactives for the Treatment of Lifestyle Related Disease Diabetes and Hypertension

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Abstract : Diabetes and hypertension are the major lifestyle related diseases. The α -amylase and angiotensin converting enzymes (ACE) are the key enzymes that regulate diabetes and hypertension. The aim was to develop a drug for the treatment of diabetes and hypertension. The Rice Bran (RB) sample (*Oryza sativa*; BRRI-Dhan-84) was collected from the Bangladesh Rice Research Institute (BRRI), and rice bran proteins were isolated and hydrolyzed by hydrolyzing enzyme alcalase and trypsin. In vivo experiment suggested that rice bran bioactives has an effect on regulating the expression of several key gluconeogenesis and lipogenesis-regulating genes, such as glucose-6-phosphatase, phosphoenolpyruvate carboxykinase, and fatty acid synthase. The above genes have a connection of regulating the glucose level, lipids profile as well as act as an anti-inflammatory agent. A molecular docking, bioinformatics and in vitro experiments were performed. We found rice bran protein hydrolysates significantly (<0.05) influence the peptide concentration in the case of trypsin, alcalase, and (trypsin + alcalase) digestion. The in vitro analysis found that protein hydrolysate significantly (<0.05) reduced diabetic and hypertension as well as oxidative stress. A molecular docking study showed that the YY and IP peptide have a significantly strong binding affinity to the active site of the ACE enzyme and α -amylase with -7.8Kcal/mol and -6.2Kcal/mol , respectively. The Molecular dynamics (MD) simulation and Swiss ADME data analysis showed that less toxicity risk, good physicochemical properties, pharmacokinetics, and drug-likeness with drug scores 0.45 and 0.55 of YY and IP peptides, respectively. Thus, rice bran bioactive could be a good candidate for the treatment of diabetes and hypertension.

Keywords : anti-hypertensive and anti-hyperglycemic, anti-oxidative, bioinformatics, in vitro study, rice bran proteins and peptides

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