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Novel therapeutic effects of sesamin on type-1 diabetes-induced cardiac dysfunction

Tran Duong Thuy
Ton Duc Thang University, Vietnam

Type-1 diabetes (T1D) is also called insulin-dependent diabetes or autoimmune diabetes. In particular, the pancreas produces insufficient insulin or because cells do not use insulin which makes blood glucose and urine glucose increase. Diabetes is a risk factor to increase the occurrence and severity of cardiovascular events. According to statistics, cardiovascular complications are the leading cause of death of 3/4 of the number of diabetic patients over 40 years old. Sesame (*Sesamum indicum*) is one of natural medicine which has been known with many functions for good health. Sesamin is a lignan extracted from the sesame seed, has many beneficial effects such as hypoglycemia, ameliorate lipid metabolism, antioxidant and hypolipidemic activity, reduced cholesterol and anti-inflammatory activity. In this study, after oral administration of Sesamin extract for four week, all the diabetes subjects underwent to blood glucose test, heart rate (HR), electrocardiography (ECG), blood pressure, hematoxylin and eosin stain to observe the effect of Sesamin on diabetes. Sesamin consuming slightly improved blood glucose levels in rats with type-1 diabetes. But it significantly ameliorated HR, blood pressure (BP) and QT interval in male diabetes rats. This indicated that Sesamin has a positive effect on reducing cardiovascular complications in diabetic animals.

duongthuy1108@gmail.com

In silico screening peptide bond-containing compounds for hepatitis C virus (HCV) NS3/4A protease inhibitors

Nhung Thi Tuyet Tran
Ton Duc Thang University, Vietnam

Hepatitis C virus (HCV) infection is a global health burden with over 180 million people infected worldwide and without vaccine available currently. The HCV NS3 (Non-structural) protein is an essential protease for viral polyprotein processing. For full activity, the NS3 protease requires a NS4A protein as a co-factor. NS3 and its recombinant protease are regarded currently as a potential target for anti-viral drugs. Thus, specific inhibitor of its enzyme activity is highly important. To screen inhibitors against NS3 protease, software of molecular docking model (Autodock version 4.2) was used to evaluate the free energy after NS4A/NS3 protease was docked with ligands from chemical library (chemical compounds bank). After checking the docking score of 50,000 peptide bond-containing compounds, three compounds with free energy <-10 Kcal/mol were obtained (Candidate 1, 2 and 3). A natural inhibitor, hexapeptide DEMEEC was used to examine the inhibitory potency. One of candidates, Candidate 1 was found to have high inhibition effect against NS4A/NS3 protease. The inhibitory parameters, IC50 and Ki of NS4A-GSGS-NS3 against Candidate 1 were 61.1 μM and 7.88 μM respectively. The Lineweaver-Burk plot of inhibitory kinetics showed that candidate 1 acted as a competitive manner which suggested that it competes with substrate to bind into active sites. Interaction between Candidate 1 and NS3 protease domain simulated by PyRx software that showed binding affinity of candidate 1 with His57 and Ser139 (catalytic triad). The inhibition activity of Candidate 1 is not good enough but it could be further modified on its chemical structure to improve the inhibitory activity and to be a better inhibitor.

tranthituyetnhung2906@gmail.com