Network pharmacology and component analysis of four herbs decoction molecular mechanism in hypertension treatment

ABSTRACT

Traditional Chinese Medicines (TCM) are known for their curative effects on hypertension through a holistic approach. The molecular mechanisms of the formulation comprising Polygonum multiorum, Rehmannia glutinosa, Senna obtusifolia and Crataegus, used by Chinese practitioners in ameliorating hypertension, however remain a mystery. This initial study is thus aimed at unveiling the molecular mechanisms of this TCM formulation in treating hypertension. The methanolic extract compounds of the decoction were identied through Liquid chromatography mass spectrometry-mass spectrometry (LC-MS/MS). Oral bioavailability and drug likeness were then measured to lter out identied compounds. Several databases, such as the SwissTargetPrediction, STRING, OMIM and KEGG, were used to retrieve information on the predicted targets for the purpose of developing a network using Cytoscape Version 3.8. Enrichment analysis was then performed to elucidate the mechanisms of the decoction in hypertension mitigation. A total of 11 compounds identied were revealed to possess bioavailable and drug like characteristics, based on the Veber and Quantitative Estimation of Drug-likeness (QED) parameters. Pathway analysis showed enrichment of pathways such as cardiac muscle contraction, uid shear stress and atherosclerosis, dilated cardiomyopathy, renin-angiotensin system and hypertrophic cardiomyopathy (HCM), which are all strongly associated with hypertension. The network pharmacology analysis clearly shows that this TCM decoction ameliorates hypertension through several indirect pathways where most of the targets are involved in HCM, which is caused by hypertension.