**Systematic investigation of the multi-scale mechanisms of herbal medicine on treating ventricular remodeling: theoretical and experimental studies**

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**Abstract:**

*Background*: To explore the underlying molecule mechanism of herbal medicine in preventing ventricular remodeling (VR), we take a herbal formula that is clinically effective for preventing VR as an example, which composed of Pachyma hoelen Rumph, Atractylodes macrocephala Koidz., Cassia Twig and Licorice. Due to multi-components and multi-targets in herbal medicine, it is extremely difficult to systematically explain its mechanisms of action.

*Methods:* An innovative systematic investigation framework which combines with pharmacokinetic screening, target fishing, network pharmacology, DeepDDI algorithm, computational chemistry, molecular thermodynamics, *in vivo* and *in vitro* experiments was performed for deciphering the underlying molecular mechanisms of herbal medicine for treating VR.

*Results:* ADME screening and SysDT algorithm determined 75 potentially active compounds and 109 corresponding targets. Then, systematic analysis of networks reveals the crucial active ingredients and key targets in herbal medicine. Additionally, transcriptomic analysis identifies 33 key regulators during VR progression. Moreover, PPI network and biological function enrichment present four crucial signaling pathways, *i.e.* NF-κB and TNF, PI3K-AKT and C-type lectin receptor signaling pathways involved in VR. Besides, both molecular experiments at animal and cell levels revealing the beneficial effect of herbal medicine on preventing VR. Finally, MD simulations and binding free energy validate the reliability of drug-target interactions.

*Conclusion:* Our novelty is to build a systematic strategy which combines various theoretical methods combined with experimental approaches. This strategy provides a deep understanding for the study of molecular mechanisms of herbal medicine on treating diseases from systematic level, and offers a new idea for modern medicine to explore drug interventions for complex diseases as well.

**Keywords:** Herbal Medicine; Ventricular Remodeling; Mechanisms of Action; MD simulations; Experimental Validation

**Biography: Jinghui Wang** is graduated from Dalian University of Technology with a doctorate in Chemical Engineering and Technology on December 2017 and he is a master tutor. In 2018, he joined in the Institute of Integrated Traditional Chinese and Western Medicine, Anhui University of Traditional Chinese Medicine. His research area is the intersection of artificial intelligence and medicine. He published several papers about Machine learning, CADD and Cancer biomarkers. Additionally, he presided over a National Natural Science Foundation of China, a high-level talent project of Anhui University of Traditional Chinese Medicine, and won the third prize of the Natural Achievement Award of Liaoning Province. Besides, his researches were reported by Metz Medicine alone, providing a new way for modern medicine to treat complex diseases.

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