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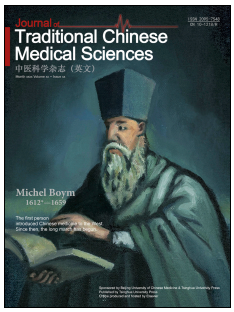

Structural similarity-based prediction of the potential active ingredients and mechanism of action of traditional Chinese medicine formulations used to anti-aging

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Structural similarity-based prediction of the potential active ingredients and mechanism of action of traditional Chinese medicine formulations used to anti-aging

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Abstract

Objective: To predict the potential active ingredients (PAIs) and mechanism of action of traditional Chinese medicine formulations used to delay aging.

Methods: We incorporated the use of quantum-chemistry calculations and machine learning to predict the active ingredients of some Chinese herbal medicines used to delay aging. Then, a network-pharmacology approach was used to uncover how these PAIs delayed aging.

Results: Twelve PAIs with anti-aging effects were discovered: androsterone, MHP, cortisone, propyl methyl trisulfide, retinol, retinal, cortisol, 11-*cis*-Retinol, (2R, 3R)-3-hydroxyproline, 4,5alpha-Dihydrocortisone, (2S)-2-ammonio-6-ureidohexanoate and17alpha, 21-Dihydroxy-5beta-pregnane-3,11,20-trione. Enrichment analyses indicated that a putative compound target and aging target were significantly associated with: regulation of the immune system; insulin receptor signaling pathway; regulation of the mitotic cell cycle; response to nutrient levels; response to oxidative stress; release of cytochrome c from mitochondria; learning or memory; inflammatory response.

Conclusions: A novel method was proposed to predict the PAIs of anti-aging herbal medicines by incorporating quantum-chemistry calculations and machine learning. Then, a network-pharmacology approach was used to uncover how these PAIs delay aging. The information provided by our study on PAIs may aid the discovery of anti-aging drugs.

KEYWORDS

Quantum chemistry calculations; Machine learning; Active ingredients; Mechanism; Aging