

Could traditional Chinese medicine hold an answer to the obesity problem?

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Obesity might be a very modern problem, but a team of scientists from Taiwan and China is turning to the age-old principles of traditional Chinese medicine (TCM) to help fight it. Breaking research published in the *Journal of Biomolecular Structure and Dynamics* indicates a possible new direction for the treatment of metabolic syndrome.

Metabolic syndrome, a collective disorder characterised by obesity and multiple clinical disorders, is on the rise. Obesity itself is an endocrine disease caused by the body's inability to handle excessive energy intake. It can lead to serious <u>chronic diseases</u> like hypertension, osteoarthritis, cardiovascular disease, sleep apnea, stroke and type-2 diabetes.

Peroxisome proliferator-activated receptors (PPARs) are key regulators of lipid and <u>carbohydrate metabolism</u>; they are involved in regulating many physiological functions initiated by nutrients, nutraceuticals and phytochemicals. There are three subtypes of PPARs – PPAR-a, PPAR-g and PPAR- ∂ –which all play important roles. Because of these roles, the three are also important <u>drug targets</u> for treating metabolic syndrome.

TCM compounds have long been recognised as potential lead candidates in creating anti-viral, anti-tumour and anti-inflammation agents. To see whether they might also be used to design agonists targeting PPAR-a, PPAR-g, and PPAR-∂ in the fight against metabolic disease, the researchers consulted the TCM Database@Taiwan, which lists more than 30,000 small-molecule compounds of TCM origin. The team ran a series of models and simulations to virtually screen the database, establishing



structure-based pharmacore models for each PPAR protein in order to identify the key actions during docking; molecular dynamics simulation and homology modelling were also performed. The results, published in the *Journal of Biomolecular Structure and Dynamics*, identify two TCM compounds as potential lead compounds in developing agonists targeting multiple PPARs: (S)-tryptophan-betaxanthin and berberrubine. Further research is needed, but the current study points to an exciting new direction for the treatment of metabolic syndrome.

More information: Chen, K. et al. Three-in-one agonists for PPAR-α, PPAR-γ, and PPAR-δ from traditional Chinese medicine, *Journal of Biomolecular Structure and Dynamics*, Volume 30, Issue 6, 2012, DOI: 10.1080/07391102.2012.689699

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