Finding drug discovery clues from the informatics analysis of traditional medicines

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The discovery of Artemisinin by Tu YouYou gives a good example of drug discovery based on the clues from the traditional medicines. A question is whether Tu's miraculous discovery tale can be repeated by the modern informatics analysis of the traditional medicines. We investigated this question by examining to what extent the known drug-productive herbs in the traditional Chinese medicine (TCM) can be indicated by comparative analysis of the traditionally described medicinal functions with respect to the targeted therapeutic symptoms. We found that the drug-productive herbs may be indicated at lower false rate by coupling the analysis of the TCM functions together with theknowledge of the phylogenetically clustered distribution patterns of drug-productive species. Traditional medicines also offer new therapeutic approaches based on synergistic combination of low-potency natural products. We quantitatively studied the potency gaps between the approved drugs and the natural products of the same therapeutic classes, and evaluated the questions of whether, at what probability, and by what mechanisms these potency gaps can be overcome by the synergistic combinations of the natural products.

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Biochemical approaches for diabetic management

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Diabetes mellitus is the most prevalent metabolic syndrome worldwide, characterized by hyperglycemia (increase in glucose level) resulting in various short-term metabolic changes in lipid and protein metabolism and long-term irreversible vascular changes. When proteins are exposed to elevated levels of glucose a series of non-enzymatic chemical reactions occur that lead to the gradual build-up of advanced glycation end products (AGEs) in body tissues that cause various complications in the body. Hyperglycemia, affects eyes (cataract), blood vessels (atherosclerosis), nerves (neuropathy), kidney (nephropathy) and cause impaired wound healing. Postprandial hyperglycemia is an independent risk factor for cardiovascular diseases. Non-enzymatic models for anti-glycation i.e., (BSA-MG) and enzymatic model α-glucosidase inhibition will be discussed. In glycation, reactive intermediate methylglyoxal (MG) binds with amino acid more easily than its carbohydrate precursor. Serum albumin, which is 80% of blood protein, is more prone to non-enzymatic glycation. Inhibition of protein glycation due to hyperglycemia is therefore an important and attractive approach towards the prevention and management of late diabetic complications. α-Glucosidase is an enzyme responsible for the conversion of complex carbohydrates to glucose. Keeping this in view, our group is working for investigation of novelanti-glycating agents. Based on virtual screening results, we have synthesized several classes of compounds and evaluated them for their in vitro and in vivoα-glucosidase inhibitory potential and methylglyoxal binding potential. All these interesting results will be discussed in detail during talk.

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