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Discovery and development of innovative drug from traditional medicine by integrated chinmedomics strategies in the post-genomic era

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ABSTRACT

Traditional medicine which consisted of multiple herbal drugs and its complexity greatly limited the new drug discovery from traditional medicine in the post-genomic era. Natural products discovery approach affords no information about compound structure or pharmacological activities until late in the discovery process and leads to low probabilities of finding compounds with unique biological properties. Therefore, by integrating serum pharmacochemistry-based screening with high-resolution metabolomics analysis, we have developed a new platform, termed chinmedomics which is capable of directly discover the bioactive constituents. By analyzing the correlation between the endogenous biomarker of diseases or TCM syndrome and exogenous constituents to find the highly associated constituents with efficacy of formulae as the effective substances, and further clarifying the activities of effective substances, and may discover lead compounds and make the innovative drug discovery based on clinical experiences. It will significantly advance the drug discovery from traditional medicine in the post-genomic era.
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Contents

1. Introduction

Phytomedicine is a part of health care systems around the world. The World Health Organization (WHO) estimates that 80% of the world's people rely on herbs for their primary health care needs [1]. Traditional Chinese medicine (TCM) is one of the oldest phytomedicine systems of health care, and it has been used in Asian countries such as China, Japan, and Korea for thousands of years [2]. For improving health, practitioners often prescribe a combination of herbs called *formulae* based on an over-all symptoms and signs of syndrome, and work together harmoniously to achieve ideally therapeutic effects (Fig. 1A). Single herb already contains thousands of compounds, formulae consisting of multi-herb has become the chemical composition giant system (Fig. 1B). Compared to chemical drugs, TCM have multi-component, -targets and -pathway characteristics and possess unparalleled advantages when faced with miscellaneous diseases [3,4]. That means to say, the efficacy of TCM

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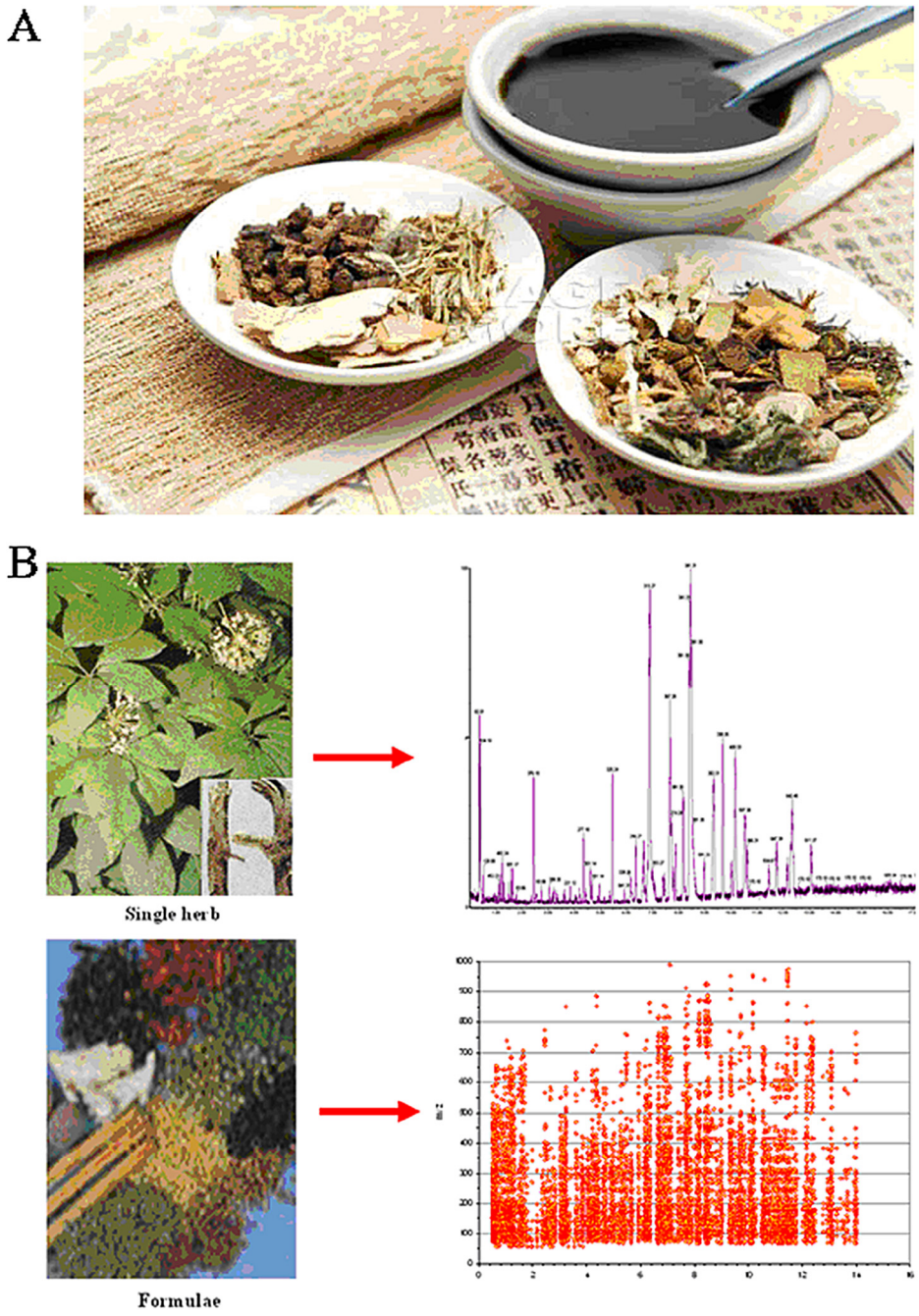

Fig. 1. The characteristics of TCM. A, TCM formulae is a combination of herbs. B: formulae consisting of multi-herb with multi-components.

depends on the combined action of multiple herbs because it usually contains a lot of ingredients and exert synergistic therapeutic efficacies. However, this can cause many difficulties in the search for the effective substances of TCM.

Syndrome and formulae are two important parts of TCM and the premise for effective substances of TCM [5]. However, vagueness of syndrome and complexity of formulae greatly limited the diagnosis syndromes and evaluation of effective substances of formulae. TCM is so complicated that it's almost impossible to explore the molecular mechanism and effective substances thoroughly. Tremendous progress has been made in the TCM and it's time-consuming and laborious to explore the efficacy of each compound. Moreover, compounds in TCM exert therapeutic effects in combination rather than as individuals. In early 1990s, we firstly established the theory and method on Serum Pharmacochemistry of TCM (SPT), providing methodology for the discovery of active constituents *in vivo* from TCM, solving the efficacy and effectiveness of TCM [6]. Syndrome is a basic description of the disease in TCM, and formulae are corresponding drugs against syndrome. Due to lack of objective criteria for syndrome diagnostics, and thus it is difficult to properly evaluate the efficacy of formulae. From the point of modern system medicine, TCM syndrome is a functional state that caused by the body's metabolic imbalances (Fig. 2). Metabolomics and TCM have some similar characteristics such as entirety, comprehensiveness and dynamic changes, *etc* [7–9].

In the 21st century, we have made SPT integrated with metabolomics, developed a system method called Chinmedomics,

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