



# Metabolomics highlights pharmacological bioactivity and biochemical mechanism of traditional Chinese medicine



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## ARTICLE INFO

### Article history:

Received 31 March 2017  
Received in revised form  
13 May 2017  
Accepted 12 June 2017  
Available online 13 June 2017

### Keywords:

Natural product  
Traditional Chinese medicine  
Metabolomics  
Biochemical mechanism  
Pharmacodynamic mechanism

## ABSTRACT

Traditional Chinese medicine (TCM) has attracted increasing interest throughout the world because of its potential complementary therapy and an abundant source for new drug discovery. TCM possesses the significant bioactivity of the use of multi-component drugs and can act multiple targets by multiple components. Metabolomics is a holistic investigation of numerous metabolite responses of complex biology systems to pathological stimuli and drug treatments based on the global metabolic profiles in complex biological matrixes. It provides variation of systematic metabolic networks for characterizing pathological states in animal models and clinical studies. In agreement with the holistic thinking of TCM, metabolomics has shown potential in bioactivity evaluation and action mechanism of TCM as well as pharmaceutical research and development. Recently, different metabolomic technologies have been applied to the modernization of TCM and treatments of different diseases such as cardiovascular disease, kidney disease, liver disease and metabolic disease. Based on the reported literature, this paper introduced the application of metabolomics in efficacy evaluation of TCM and its biochemical action mechanism.

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## 1. Introduction

Natural medicine or traditional Chinese medicine (TCM) has been developed over thousands of years and has accumulated abundant clinical experience [1]. TCM becoming more popular because it is relatively inexpensive and widely available, and has

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fewer adverse effects. TCM is a unique medical system with the significant property of multi-component drugs. The therapeutic effects of TCM can usually be attributed to the combination of multiple elements of the herb or the formula acting together. Such complexity in TCM administration brings a great challenge in establishing suitable analytical approaches for the development of its modernization and standardization [2]. Although TCM has been effective in treating many illness especially chronic diseases, it lacks necessary well-defined molecular mechanism and sometimes even molecular basis. In agreement with the holistic thinking of TCM, metabolomics has shown potential in efficacy evaluation and its biochemical action mechanism of TCM.

Metabolomics was originally proposed as a method of functional genomics, an emerging subject of the post-genome era, which, together with genomics, transcriptomics and proteomics, jointly constitutes the ‘Systems Biology’ [3,4]. As a systemic approach, metabolomics adopts a “top-down” strategy to reflect the function of organisms from terminal symptoms of metabolic network and understand metabolic changes of a complete system caused by interventions in a holistic context [5,6]. As an emerging field of science in the post-genomics era, metabolomics has been broadly applied in many fields such as novel drug discovery [7], toxicological survey [8], clinical diagnostics and nutritional biochemistry [9]. Fig. 1 showed the information flow in the omics family and the classification of metabolomics [10]. The strategy of the metabolomics and its aim at grasping integral function has provided unprecedented enlightenment for the modern TCM. Additionally, Metabolomics is concerned with the quantitative understandings of the metabolite component of integrated living systems and its dynamic responses to the changes of both endogenous and exogenous factors and has many potential applications and advantages for the research of complex systems [11]. Recently, with metabolomic technology, the investigations have successively studied the key scientific issues in TCM including quality control, disease syndrome and differential treatment of the individual. For evaluating adequately the efficacy of TCM, metabolomics provides a valuable reference. Many research groups have used metabolomics for studying TCM in terms of efficacy evaluation [12–16]. In this review, we summarized several metabolomics techniques and data

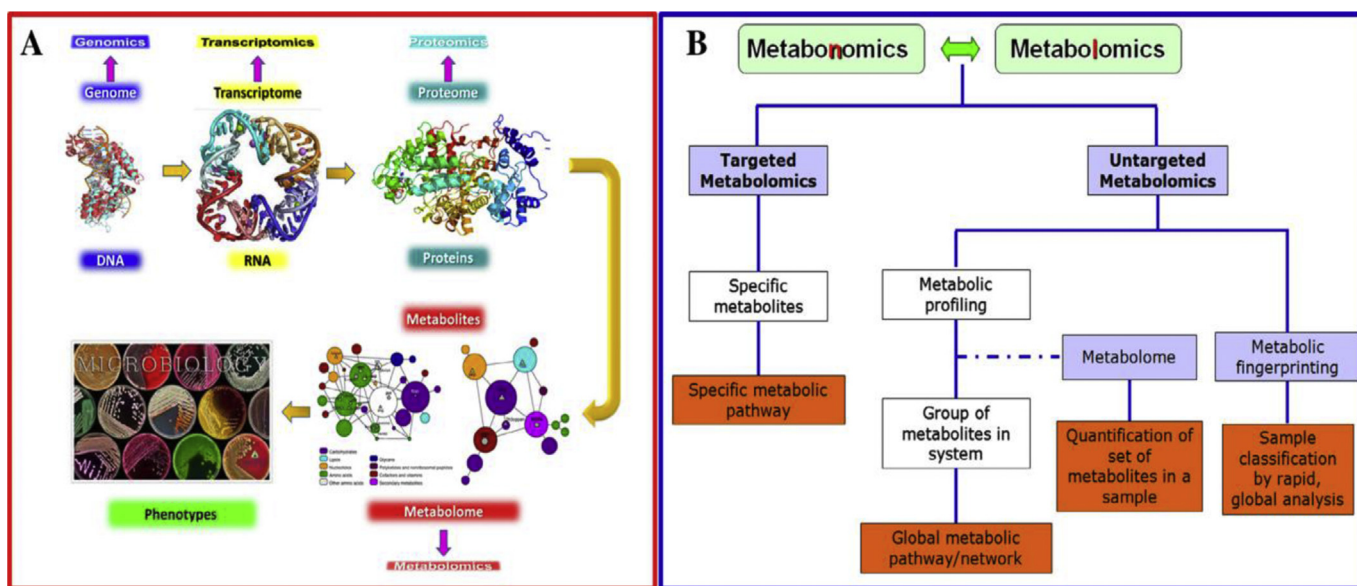
analysis methods. We supposed that the metabolomics platform to study the complex theoretical system of TCM is practicable.

## 2. Metabolomics technique

In the recent years, metabolomic technology has been widely used in the modern research of TCM. Modern technologies allow for qualitative and quantitative measurement of a vast number of metabolites in complex biological systems. Among these techniques, the main analytical techniques in metabolomics are proton nuclear magnetic resonance ( $^1\text{H}$  NMR) spectroscopy and mass spectrometry (MS) [17–19].  $^1\text{H}$  NMR is a non-destructive technique, although its sensitivity is less than that of MS, it is still popular in many applications due to its very rapidity, high throughput and easy operation.  $^1\text{H}$  NMR is widely used in chemistry, provides detailed information on molecular structure, both for pure compounds and in complex mixture as well as information on absolute or relative concentrations. The  $^1\text{H}$  NMR methods can also be used to probe metabolite molecular dynamics and mobility [20]. However, in most cases, MS is preferred because of its advantages of unparalleled sensitivity, super resolution and structural specificity. In practical applications, MS requires combining with different separation techniques such as gas chromatography (GC), liquid chromatography (LC), capillary electrophoresis (CE) and ultra performance liquid chromatography (UPLC) for a pre-separation [21]. Two-dimensional LC has applied in analysis of TCM and metabolomic investigation due to its enhanced selectivity, peak capacity and high resolution compared with one-dimensional LC [22]. Notably, electron ionization (EI) was usually used for GC-related techniques and electrospray ionization (ESI) was usually used for LC and CE-based mass spectrometry. Occasionally, atmospheric pressure chemical ionization (APCI) and atmospheric pressure photo ionization (APPI) are coupled to LC for detection of non-polar compounds [23,24].

## 3. Data processing and analysis

A flow chart of typical metabolomics experiment includes the experimental design, the extraction protocol, data acquisition, data



**Fig. 1.** Relationship of system biology and metabolomics. (A) In information flow in the omics family, the flow is from genes to transcripts to proteins to metabolites and to phenotype. (B) In classification of metabolomics and untargeted metabolomics are generally for discovery of metabolites or global metabolic pathways, whereas targeted metabolomics are tailored for specific metabolic pathway or metabolites.

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