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Plasma metabolomics combined with personalized diagnosis guided by Chinese medicine reveals subtypes of chronic heart failure

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KEYWORDS

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Abstract *Background:* Chronic heart failure (CHF) is characterized by insufficient blood supply from heart to meet the body's metabolic demands. Integrating Western and traditional Chinese medicine to treat CHF has proved a validated therapeutic approach. In recent years, metabolomics has been regarded as a potential platform to provide biomarkers for disease-subtypes.

Objective: To examine 38 patients, combined NMR plasma metabolomics and traditional Chinese medicine diagnosis in order to identify diagnostic biomarkers for two CHF syndrome subtypes.

Methods: After processing the spectra, orthogonal partial least square discriminant analysis was performed, and the contributing NMR signals were analyzed using Y-scrambling statistical validation with good reliability.

Results: Plasma metabolic patterns of yin deficiency and yang deficiency patients were clearly discriminated. The yin-deficiency group had increased level of lactate, glycoprotein, lipoprotein and lower levels of glucose, valine and proline. The yang-deficiency group had higher levels of lactate, glycoprotein and pyruvic acid, and lower levels of glucose and lipoprotein.

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Potential biomarkers of CHF based on the two traditional Chinese medicine syndromes indicated alternative modes of metabolites and metabolic pathways in the disease, e.g. dysfunction of energy utilization and disturbance in fatty acids, amino acids.

Conclusion: This study suggests that combining metabolomics with traditional Chinese medicine diagnosis can reveal metabolic signatures for CHF syndrome subtypes. The plasma metabolites identified might be of special clinical relevance for subtypes of CHF, which could lead to further understanding of mechanisms involved and an improvement in personalized treatment for CHF.

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Introduction

Chronic heart failure (CHF), a progressive clinical syndrome characterized by the inability of the heart to adequately pump blood to meet metabolic demands of the body. It represents the final common pathogenesis in various causes of heart damage.¹ Despite a substantial improvement in the survival rate after the onset of CHF because of increasing use of pharmacological interventions, the mortality of patients suffering from CHF remains high. It is well recognized that the incidence and prevalence of CHF is expected to increase further with the aging population, better strategies for the prevention and treatment of CHF is required.

With progress in bioinformatics and medical science, the focus on health and disease in Western life sciences has shifted from standard protocol-based disease management to personalized medicine. Based on personalized health and systematical diagnostic principles, traditional Chinese medicine (TCM) has proved clinically effective at restoring the self-regulatory ability of the human system for thousands of years. Using integrated TCM and Western medicine to treat CHF has been reported to enhance heart function and reduce related clinical symptoms, including expiratory dyspnea and chronic fatigue, and subsequently improve echocardiographic measures, the 6-min walking distance test and patients' quality of life.² TCM physicians also pay increased attention to overall maladjustments of the functional status called 'syndrome type'.³ It is not simply an assemblage of the signs and symptoms of diseases, but also a functional status caused by the reaction to, or interaction with, environmental changes and pathogenic factors.⁴ The essence of TCM 'syndrome type' is the disturbance in biological metabolism networks, and changes in concentration and relative proportions of metabolomics biomarkers resulting from an imbalance in the human system.

Metabolomics, an important component of systematical biology, can be used to perform dynamic studies on non-injured tissues and organs in vivo and in vitro using non-invasive approaches under nearly physiological conditions.⁵ Therefore, metabolomics detection and analysis of biological samples may contribute to understand the biochemical changes associated with the progression of diseases. And identification of disease-associated metabolic biomarkers could allow early diagnosis of disease and establishment of predictive diagnostic systems. It is reported that metabolomics gives unparalleled advantage to the most common

cardiovascular condition encountered in clinical practice, heart failure.⁶ Metabolomics has also shown significant potential in TCM studies in recent years. And several studies^{7,8} combining metabolomics techniques and TCM syndrome types have demonstrated fingerprints of metabolic changes that characterize Western medicine diagnosed diseases, which highlight the potential of metabolomics in the evaluation of disease condition and TCM-guided personalized treatment.

As one of the most used metabolomics analysis platforms, nuclear magnetic resonance (NMR) spectroscopy has been widely applied to metabolomics research as it provides the advantages of high resolution and high sensitivity. Thus, NMR is useful for revealing systematically the metabolomics pathways and mechanisms involved in CHF through exploring TCM syndromes and therapies.

The current research was a parallel comparative study that analyzed plasma metabolites of 38 CHF patients using NMR spectroscopy to examine:

- (1) potential metabolic biomarkers contributing to discriminate TCM syndrome types (yang-deficiency vs. non-yang-deficiency, and yin-deficiency vs. non-yin-deficiency); and
- (2) similarities and differences in TCM syndrome-related biomarker patterns. We hypothesize that combining TCM diagnosis with metabolomics could provide quantitative biological evidence for TCM diagnosis by identifying CHF subtypes with related plasma metabolic patterns.

Materials and methods

Participants and study design

The study was designed as an explorative study without intervention. Patients with a history of coronary heart disease that met the CHF diagnostic criteria in accordance with the Guidelines for the Diagnosis and Management of Chronic Heart Failure established by the Chinese Society of Cardiology of the Chinese Medical Association in 2007 were enrolled. Eligibility criteria were age ≥ 45 years and left ventricular ejection fraction $< 50\%$. All patients were in New York Heart Association (NYHA) classes II–IV. All patients underwent our standardized recruitment and

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