OBJECTIVE: A new research model “revealing disease nature by the comprehensive application of Metabonomics and Serum Pharmacocchemistry of Chinese Medicine, explaining prescription effective material basic and mechanism of action on the basis of the relevance between the prescription chemical component and disease nature” is proposed in this thesis. The following results and conclusions are achieved by the study on the Xiaoyao Powder as the research template.

METHODS: 10 batches Xiaoyao Powder HPLC fingerprints were established, 22 common peaks were determined, the similarity of every batch and common models was above 0.99. 10 batches Xiaoyao Powder volatile components GC-MS fingerprints were established, 29 common peaks were determined, the similarity of every batch and common models was above 0.99. The Wistar rat model was established by immobilization stress using bound and fatigue stimulation and solitary ways lasting for 21 days. The model was recognized as model of syndrome of stagnation of liver qi and spleen deficiency from animal characterization, food intake, bodyweight, open field test, novelty suppressed feeding test, sucrose preference test, as well as effect of Xiaoyao powder. The hematuria and biochemical indexes such as D-xylose excretion rate, AST, ALB and CHE was measured and liver injury pathology was observed by HE dye. Furthermore, metabolomics analysis to compare the change trend of metabolic products with normal group.

RESULTS: They showed that established fingerprints were featured by abundant information, distinct features, high stability and good repeatability, which can effectively monitor the quality of Xiaoyao Powder. 14 blood migration components were identified, No. 3, 9, 10, 14 are the inherent components in blood, the content in blood was increased significantly after taking Xiaoyao Powder. Regarding serum chromatographic fingerprint as direction, relevant drugs were identified from liver tissue pathology results, comparing with normal group, hepatic lobule structure disorder occurs among liver qi stagnation and spleen qi deficiency syndrome group rats and liver injury group rats showed that their expression was tired, their hair scattered, dull yellow and easily fall, they liked gathering together and less activity, listless, their stool was shaped and thin pond. Viewing from liver tissue pathology results, comparing with normal group, hepatic lobule structure disorder occurs among liver qi stagnation and spleen qi deficiency syndrome group rats and liver injury group rats decreased, AST increased, ALB and CHE decreased. Furthermore, metabolomics analysis to compare the change trend of metabolic products with normal group.

CONCLUSION: The common physiology, pathology and metabolic network basis exist in liver qi stagnation and spleen qi deficiency syndrome and liver injury. Xiaoyao Powder effective parts that formed by serum pharmacocchemistry of Chinese Medicine chemical method can intervene liver qi stagnation and spleen qi deficiency syndrome and liver injury simultaneously, especially repairing liver cells injury, regulating the content of AST, ALB, and CHE. Metabolomics shows that Xiaoyao Powder plays the role of protecting liver by the regulating of one carbon unit, special metabolism of sulfur contained in amino acids, aromatic amino acids, and three tricarboxylic acid cycle. Metabolomics can build up the nature relationship between prescription internal chemical components and syndrome, disease, serum pharmacocchemistry of Chinese Medicine chemical method can build up the relationship between prescription internal chemistry components and prescription. Therefore, the combination application of metabolomics and serum pharmacocchemistry of Chinese Medicine can explain the nature relationship of prescription, syndrome and disease, which embodies distinguished advantage in the research of prescription effective material basic and mechanism of action.

Keywords: Xiaoyao Powder; Liver qi Stagnation and Spleen qi Deficiency Syndrome; Liver Injury; Metabonomics; Serum Pharmacocchemistry of Chinese Medicine

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THE DEMONSTRATIVE STUDY OF MATERIAL BASE AND MECHANISM OF TCM XIAOYAO SAN BASED ON UNDERSTANDING THE ESSENTIAL RELATION OF A TCM PRESCRIPTION AND SPECIAL DISEASE/SYNDROMES

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CONCLUSION: The common physiology, pathology and metabolic network basis exist in liver qi stagnation and spleen qi deficiency syndrome and liver injury. Xiaoyao Powder effective parts that formed by serum pharmacocchemistry of Chinese Medicine chemical method can intervene liver qi stagnation and spleen qi deficiency syndrome group rats and liver injury group rats increased simultaneously, the content of Octadecadienoic acid and Oleic acid decreased simultaneously. Xiaoyao Powder effective parts that formed by serum pharmacocchemistry of Chinese Medicine chemical method can improve liver qi stagnation and spleen qi deficiency syndrome rats behavioristics, liver tissue pathology results, comparing with normal group, hepatic lobule structure disorder occurs among liver qi stagnation and spleen qi deficiency syndrome group rats and liver injury group rats decreased, AST increased, ALB and CHE decreased.

Viewing from metabolomics analysis, comparing with normal group, Glycine, Butanediol acid, Propanoic acid, Methionine, Glutamine and Phenylalanine in serum of liver qi stagnation and spleen qi deficiency syndrome group rats and liver injury group rats increased simultaneously, the content of Octadecadienoic acid and Oleic acid decreased simultaneously. Xiaoyao Powder effective parts that formed by serum pharmacocchemistry of Chinese Medicine chemical method can improve liver qi stagnation and spleen qi deficiency syndrome and liver injury rats behavioristics, liver tissue pathology and hematuria and biochemical indexes, they can callback the change trend of metabolic products. 

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