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Analysis of the Antidota Targets and Pharmacodynamic Material Basis of Pueraria Lobata and Ziziphi Spinosae Compound Formula Based on Metabolomics

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Abstract: This study innovatively applies metabolomics technology to deeply analyze the target points and pharmacological substance basis of Ge Gen Zhi Ju compound for sobering up. Through advanced data analysis methods, clarify its key mechanism of action in the process of sobering up, and provide theoretical support for the further development and application of Pueraria lobata and Fructus Aurantii formula.

Keywords: Metabolomics; Compound of Pueraria lobata and Fructus Aurantii; Target of sobering up effect; Pharmacological substance basis

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1. Introduction

With the continuous expansion of the drinking population, research on sobering up drugs has attracted much attention. As a traditional hangover relieving formula, the mechanism of action of Ge Gen Zhi Hu compound is not fully understood. Metabolomics provides a new approach for comprehensive analysis of its sobering targets and pharmacological substance basis.

1.1. Research background and significance

1.1.1. Current research status of sobering up

The liver damage and gastrointestinal dysfunction caused by excessive alcohol intake have become important public health issues affecting national health, and research related to sobering up has received increasing attention. The current research on sobering up mainly includes three directions: chemical synthesis drugs, natural products, and traditional Chinese medicine compound formulas. Although chemically synthesized drugs can quickly alleviate some symptoms of drunkenness, they often have side effects and are difficult to fundamentally reduce the metabolic damage caused

by alcohol to the body. The research on natural products for sobering up focuses on plant active ingredients, which have shown certain safety advantages, but mostly remain at the level of verifying the effects of a single component, failing to fully utilize the synergistic effects of natural products. The research on traditional Chinese medicine compound hangover relief is based on the concept of holistic regulation, emphasizing the synergistic intervention of multiple components and targets in alcohol metabolism disorders. However, traditional research methods are difficult to accurately reveal its mechanism of action and material basis, resulting in the scientific connotation of most compounds not being fully explained, which restricts their industrial development and clinical promotion and application[1].

1.2. Traditional application of Pueraria lobata and Hovenia dulcis compound

The formula of Pueraria lobata and Fructus Aurantii originated from the classic compatibility theory of traditional Chinese medicine, and has a long history of application in the field of sobering up and protecting the liver. It is one of the representative formulas of traditional Chinese medicine to deal with alcohol damage. Both Pueraria lobata and Hovenia dulcis are commonly used medicinal herbs in traditional Chinese medicine for sobering up. Pueraria lobata has a cool and sweet taste, and has the effects of relieving muscle and fever, generating fluids and quenching thirst, promoting yang and stopping diarrhea. Medical records throughout history have recorded that it can “relieve the toxicity of alcohol and awaken the annoyance of alcohol”; Hovenia dulcis has a mild and sweet taste, and has the effects of clearing heat, diuresis, and detoxification. It is commonly used to relieve symptoms such as nausea, vomiting, dizziness, and headache after getting drunk. The combination of the two follows the traditional Chinese medicine principle of “matching needs for use”, and enhances the sobering effect through synergistic action. It can not only alleviate the acute symptoms of drunkenness, but also reduce the chronic damage of alcohol to organs such as the liver.

2. Research methods and techniques

2.1. Experimental design of metabolomics

The experimental design of metabolomics should revolve around the core of the sobering effect of Pueraria lobata and Fructus Aurantii compound, following the principles of scientificity, systematicity, and reproducibility, and constructing a comprehensive experimental system covering the process of alcohol metabolism. The experimental grouping should include a blank control group, an alcohol model group, and a low, medium, and high-dose group of Pueraria lobata and Fructus Aurantii compound, to ensure a clear comparison of the changes in the body’s metabolic status before and after intervention with the compound. The sample selection should cover biological samples closely related to alcohol metabolism, such as blood and liver tissue, to comprehensively capture the metabolic response differences of different tissues and organs. The experimental process needs to be standardized and unified, including precise setting of sample collection time points, collecting samples at different time points before and after alcohol intake, and tracking the dynamic changes in metabolites; Standardized methods are used for sample pretreatment, combined with liquid-liquid extraction, solid-phase extraction and other techniques to ensure efficient extraction and purification of metabolites.

2.2. Data analysis methods

The data analysis method needs to construct a complete analysis chain of “data preprocessing differential metabolite screening metabolic pathway analysis target correlation verification” to ensure accurate mining of

valuable information from massive metabolomics data. In the data preprocessing stage, peak alignment, denoising, normalization and other methods are used to eliminate the impact of experimental errors and instrument drift on data quality, and obtain a standardized metabolomics data matrix. Differential metabolite screening was conducted by combining multivariate statistical analysis with univariate statistical analysis, constructing models such as principal component analysis and partial least squares discriminant analysis to identify significant differential metabolites between the alcohol model group and the compound intervention group. Metabolic pathway analysis utilizes databases such as the Kyoto Encyclopedia of Genes and Genomes to conduct pathway enrichment analysis on differential metabolites and locate key metabolic pathways associated with alcohol injury. Target association validation is achieved by constructing a differential metabolite target pathway interaction network, combined with molecular docking technology, to verify the binding ability between the active ingredients of the compound and key metabolic targets, and clarify the core metabolic regulatory pathway of the compound's sobering effect.

2.3. Technological innovation points

The technological innovation of this study is mainly reflected in three aspects, constructing a research paradigm that deeply integrates traditional Chinese medicine compound formulas with metabolomics. For the first time, untargeted metabolomics has been combined with targeted metabolomics to comprehensively screen metabolic markers related to alcohol damage through untargeted metabolomics. With the help of targeted metabolomics, key metabolites have been accurately quantified, improving the accuracy and reliability of metabolite detection. Innovatively constructing an interactive network analysis model of "compound ingredients metabolic markers core pathways", breaking through the limitations of traditional metabolomics that only focuses on metabolic changes in the body, achieving systematic correlation analysis of compound active ingredients, metabolic targets, and pathways, and clearly revealing the mechanism of action of the compound. A rapid screening method for compound active ingredients based on metabolomics has been established. By comparing the changes in differential metabolites before and after compound intervention, combined with the compound chemical composition database, the active ingredients related to sobering effects are accurately located, avoiding the blindness of traditional active ingredient screening and improving the efficiency and accuracy of the research on the basis of active ingredients[2].

3. Target analysis of the sobering effect of Ge Gen Zhi Ju compound

3.1. Potential target screening

Potential target screening is based on differential metabolites obtained from metabolomics analysis, combined with bioinformatics technology to construct a multidimensional target screening system. Based on the structural characteristics and metabolic pathways of differential metabolites, potential targets corresponding to differential metabolites are predicted through authoritative databases such as the human metabolome database and protein database, covering key enzymes, transporters, receptors, and other molecules involved in alcohol metabolism. At the same time, integrate the traditional Chinese medicine system pharmacology database to obtain the known targets of active ingredients in the Ge Gen Zhi Ju compound, and construct a compound ingredient target correlation dataset. By combining the predicted targets of metabolomics with the targets of compound ingredients through intersection analysis, potential targets that are closely related to alcohol metabolism disorders and can be directly or indirectly regulated by compound ingredients are screened out. This provides a core candidate target set for subsequent mechanism analysis and key target determination, ensuring that the screened potential targets have clear biological significance and association with compound intervention.

3.2. Target mechanism of action

The mechanism of action of the target points of the Ge Gen Zhi Hu compound for sobering up revolves around the core pathological process of alcohol metabolism disorders, and achieves the effect of sobering up and protecting the liver through the coordinated regulation of multiple targets. The core mechanism is to regulate the target molecules in the key pathway of alcohol metabolism, promote the rapid clearance of alcohol and its metabolites, reduce the accumulation of toxic metabolites such as acetaldehyde in the body, and alleviate their toxic damage to liver cells. At the same time, by regulating oxidative stress-related targets, enhancing the activity of antioxidant enzymes in the body, clearing excess free radicals produced during alcohol metabolism, inhibiting oxidative stress response, and reducing oxidative damage to liver cells. In addition, the target also participates in regulating the inflammatory response pathway, inhibiting the release of inflammatory factors induced by alcohol, reducing the inflammatory infiltration of liver tissue, and alleviating the progression of alcoholic liver injury. Partial targets regulate lipid metabolism pathways, improve alcohol induced lipid metabolism disorders, reduce fat deposition in the liver, prevent the formation of alcoholic fatty liver, and achieve a multidimensional and multi pathway synergistic intervention mechanism for alcohol damage[3].

3.3. Determination of key targets

The determination of key targets is based on their biological functional importance, binding ability with compound ingredients, and core position in metabolic pathways, and a multi index comprehensive evaluation system is constructed. By using network topology analysis indicators such as degree centrality and betweenness centrality, target molecules at the core nodes of the "compound ingredient target pathway" interaction network were screened. These targets can regulate multiple alcohol metabolism related pathways and have significant global regulatory effects. By combining molecular docking technology verification, targets with low binding energy and stable binding mode to the core active ingredients in the Ge Gen Zhi Ju compound were screened to ensure the direct interaction between the targets and the compound ingredients. Based on existing literature reports and clinical research results, the pathological significance of the target in diseases such as alcoholic liver injury was verified, and a group of core targets with key regulatory roles were ultimately identified. These key targets are not only the core action sites of the compound's sobering effect, but also potential drug targets for the prevention and treatment of alcohol damage, providing precise target directions for subsequent validation of drug efficacy and drug development.

4. Exploration of the material basis of pharmacological effects

4.1. Identification of active ingredients

The identification of active ingredients adopts the strategy of "in vivo and in vitro binding, qualitative and quantitative synchronization", and systematically screens the active ingredients related to sobering effects in the formula of Pueraria lobata and Fructus Aurantii. At the in vitro level, ultra-high performance liquid chromatography-mass spectrometry was used to analyze the components of the compound extract. Combined with the traditional Chinese medicine chemical composition database, the main chemical components in the compound were qualitatively identified through retention time, mass spectrometry fragment information, and other characteristics, including flavonoids, terpenes, phenolic acids, and other compounds. At the internal level, by analyzing the migratory components in biological samples after intervention with the compound, the prototype components and metabolites that can enter the body and exert their effects are identified, and the effective form of action of the compound in the body is clarified. Based on the results of metabolomics analysis, chemical components significantly related to key

sobering targets and differential metabolites were screened. Through molecular docking, in vitro activity verification, and other experiments, the regulatory activity of these components on key targets was confirmed. Finally, the core components with clear sobering activity in the Pueraria lobata and Fructus Aurantii compound were identified, and a drug library of the compound was constructed [4].

4.2. Component interaction

The interaction of active substances in the formula of Pueraria lobata and Fructus Aurantii follows the theory of traditional Chinese medicine compatibility, showing the characteristics of synergistic and complementary effects, jointly enhancing the sobering effect of the formula. The core active ingredients regulate different targets of the same metabolic pathway through synergistic effects, or regulate multiple related metabolic pathways, forming a multi-component synergistic regulatory network to enhance the intervention effect on alcohol metabolism disorders. Some ingredients can promote the absorption and metabolic conversion of other active ingredients, improve their bioavailability in the body, and enhance overall drug efficacy. In addition, there is a complementary effect between the components, and different components play a role in different pathological stages of alcohol damage. Some focus on quickly relieving symptoms of drunkenness, some focus on reducing liver damage, and some focus on regulating the body's metabolic balance. Through multi link collaborative intervention, the advantages of the synergistic effect of multiple components and targets in traditional Chinese medicine formulas are fully reflected.

4.3. Evaluation of the contribution of pharmacological substances

The evaluation of the contribution of pharmacological substances is based on the in vivo exposure of active ingredients, their ability to regulate key targets, and their content in the compound, constructing a quantitative evaluation system. By measuring the concentration of active ingredients in biological samples and evaluating their in vivo exposure levels, ingredients with higher exposure levels have greater potential to contribute to drug efficacy. Using methods such as molecular dynamics simulation and in vitro activity experiments, quantitatively analyze the regulatory activity of each active ingredient on key sobering targets, and clarify the strength of the effects of different ingredients. Based on the content determination results of each component in the compound, taking into account the proportion and activity intensity of each component, calculate the pharmacological contribution value of each component. According to the contribution value of pharmacological effects, the active ingredients in the compound are divided into core contributing ingredients, important contributing ingredients, and auxiliary contributing ingredients. The core contributing components are the main material basis for the sobering effect of the compound, and the important contributing components and auxiliary contributing components enhance the efficacy of the core components through synergistic effects, jointly forming the pharmacological substance system of the compound.

5. Countermeasures and prospects

5.1. Suggestions for developing applications

Based on the research results, targeted development and application suggestions are proposed to promote the modernization and industrialization of Pueraria lobata and Fructus Aurantii compound. In terms of product development, a standardized quality control system for compound formulations is established based on the identified core active ingredients as quality control indicators to ensure the stability and uniformity of product quality. Combining modern formulation technology, develop dosage forms suitable for market demand, such as oral liquids, granules, sobering tea, etc., to enhance the convenience and bioavailability of the product. In terms of clinical

application, differentiated clinical application plans should be developed based on the degree of alcohol damage in different populations, clarifying the applicable population, dosage, and contraindications to ensure the safety and effectiveness of clinical application. In terms of market promotion, we will strengthen the scientific popularization and publicity of the sobering effect of compound prescriptions, explain their mechanism of action based on research results, and enhance consumer recognition of the product[5].

5.2. Research limitations

Although this study systematically analyzed the target points and pharmacological substance basis of the hangover relieving effect of Ge Gen Zhi Ju compound, there are still certain limitations. At the experimental research level, the sample sources are relatively single, mainly based on animal experimental samples, lacking validation from human clinical samples. There are certain differences in the conversion of research results to humans, making it difficult to fully reflect the metabolic processes and effects of the compound in the human body. At the technical level, although the metabolomics detection platform can cover most metabolites, there may still be some low abundance metabolites that have not been detected, and the analysis of metabolic pathways is not comprehensive enough. At the level of mechanism of action research, the focus is mainly on metabolomics analysis, lacking integrated analysis of multi omics data such as proteomics and transcriptomics, and failing to reveal the mechanism of action of the compound at a broader molecular level. At the level of pharmacological substance research, the analysis of the synergistic mechanism between components is not deep enough, making it difficult to accurately quantify the specific contributions of each component.

5.3. Future research directions

Future research should focus on the existing limitations and conduct in-depth studies from multiple dimensions to further improve the scientific connotation of the sobering effect of Pueraria lobata and Fructus Aurantii compound. Strengthen clinical research, collect human clinical samples, conduct large-scale, multi center clinical studies, verify the sobering effect and safety of the compound in the human body, and promote the clinical translation of research results. Using multi omics integration techniques, combined with transcriptomics, proteomics, metabolomics, and other technologies, a mechanism network of the entire “gene protein metabolite” chain is constructed to comprehensively reveal the molecular mechanism of the compound. Thoroughly study the synergistic mechanism between active ingredients, clarify the synergistic mode of different component combinations through in vitro combination experiments, in vivo validation, and other methods, and accurately quantify the pharmacological contributions of each component. Conduct research on dosage form optimization and process improvement of compound formulas, enhance product stability and bioavailability, and explore the potential application of compound formulas in the prevention and treatment of chronic diseases such as alcoholic liver injury, expanding their clinical application value.

6. Conclusion

This study has opened up a new perspective for the study of the sobering mechanism of Pueraria lobata and Fructus Aurantii compound using metabolomics, clarifying the target of action and the substance basis of drug efficacy. Further in-depth research is needed to promote its widespread application in the field of sobering up.

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Disclosure statement

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