MINISTRY OF EDUCATION AND SCIENCE OF UKRAINE
KYIV NATIONAL UNIVERSITY OF TECHNOLOGIES AND DESIGN
Faculty of Chemical and Biopharmaceutical Technologies
Department of Biotechnology, Leather and Fur

QUALIFICATION THESIS

on the topic **Biotechnological study of *Taraxacum mongolicum* function mechanisms**

First (Bachelor's) level of higher education

Specialty 162 "Biotechnology and Bioengineering"

Educational and professional program "Biotechnology"

Completed: student of group BEBT-20
Zhang HUAZHI

Scientific supervisor
Olga IUNGIN, Ph.D., Assoc. Prof.

Reviewer
Olga ANDREYEVA, Dr. Sc., Prof.

Kyiv 2024

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Educational and professional program Biotechnology

APPROVE
Head of Department of Biotechnology,
Leather and Fur, Professor,
Doctor of Technical Science
Olena MOKROUSOVA

_____
«___»_____2024

ASSIGNMENTS
FOR THE QUALIFICATION THESIS
Zhang Huazhi

1. Thesis topic **Biotechnological study of *Taraxacum mongolicum* function mechanisms**
Scientific supervisor Olga Iungin, Ph.D., Assoc. Prof.

approved by the order of KNUTD "____"_____2024, №____

2. Initial data for work: assignments for qualification thesis, scientific literature on the topic of qualification thesis, materials of Pre-graduation practice

3. Content of the thesis (list of questions to be developed): literature review; object, purpose, and methods of the study; experimental part; conclusions

4. Date of issuance of the assignments_____

EXECUTION SCHEDULE

№	The name of the stages of the qualification thesis	Terms of performance of stage	Note on performance
1	Introduction	From 01 April 2024 to 11 April 2024	
2	Chapter 1. Literature review	From 06 April 2024 to 20 April 2024	
3	Chapter 2. Object, purpose, and methods of the study	From 21 April 2024 to 30 April 2024	
4	Chapter 3. Experimental part	From 01 May 2024 to 10 May 2024	
5	Conclusions	From 07 May 2024 to 12 May 2024	
6	Draw up a bachelor's thesis (final version)	From 20 May 2024 to 25 May 2024	
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8	Submission of bachelor's thesis to the department for review (14 days before the defense)	27 May 2024	
9	Checking the bachelor's thesis for signs of plagiarism (10 days before the defense)	31 May 2024	
10	Submission of bachelor's thesis for approval by the head of the department (from 7 days before the defense)	03 June 2024	

I am familiar with the task:

Student _____Zhang HUAZHI

Scientific supervisor _____Olga IUNGIN

SUMMARY

Huazhi Zhang. Biotechnological study of *Taraxacum mongolicum* function mechanisms– Manuscript.

Hyperuricemia, as a common metabolic disease, has a rising incidence in recent years, which seriously threatens human health. Dandelion, as a traditional Chinese herbal medicine, has attracted more and more attention for its potential in treating hyperuricemia. Based on network pharmacology and molecular docking technology, this study deeply explored the mechanism of dandelion in treating hyperuricemia. The active components and their targets in Taraxacum mongolicum were screened by network pharmacology, and the potential targets of Taraxacum mongolicum in treating hyperuricemia were determined by combining with the related targets. In this process, we synthesized a variety of database resources, made a comprehensive analysis of the chemical components of Taraxacum mongolicum, and predicted the possible targets of these components through bioinformatics. The drug- ingredient-target-pathway-disease network diagram was constructed, and the interaction between active ingredients of Taraxacum mongolicum and hyperuricemia-related targets was intuitively displayed. On this basis, we further analyzed the interaction network of potential targets, and revealed the key targets involved in the treatment of hyperuricemia by dandelion and their interaction mechanisms. In order to deeply understand the biological process and signal pathway of dandelion in the treatment of hyperuricemia, we carried out GO function enrichment analysis and KEGG signal pathway enrichment analysis. These analyses not only reveal the important role of

dandelion active components in regulating the biological processes related to hyperuricemia, but also provide us with the potential mechanism of dandelion in treating hyperuricemia. The interaction between core active components and key targets of Taraxacum mongolicum was verified by molecular docking technology. Through molecular docking simulation, we determined the binding mode of dandelion active components and targets, which further confirmed the effectiveness of dandelion in treating hyperuricemia.

The results of this study show that the active components in dandelion participate in the treatment of hyperuricemia by regulating several key targets. These targets involve uric acid metabolism, inflammatory reaction and other aspects, which together constitute the mechanism of dandelion in treating hyperuricemia. This discovery provides a scientific basis for the application of dandelion in the treatment of hyperuricemia, and also provides a new idea for developing new anti-hyperuricemia drugs. This study not only revealed the mechanism of dandelion in treating hyperuricemia, but also verified the application value of network pharmacology and molecular docking technology in Chinese herbal medicine research. Through the comprehensive application of modern pharmacology and bioinformatics, we can dig deeper into the pharmacological mechanism of Chinese herbal medicine and promote the modernization and scientific development of Chinese medicine.

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INTRODUCTION

Thyperuricemia, as a common metabolic disease, has a rising incidence in recent years, which seriously threatens human health. Dandelion, as a traditional Chinese herbal medicine, has attracted more and more attention for its potential in treating hyperuricemia. Based on network pharmacology and molecular docking technology, this study deeply explored the mechanism of dandelion in treating hyperuricemia. The active components and their targets in Taraxacum mongolicum were screened by network pharmacology, and the potential targets of Taraxacum mongolicum in treating hyperuricemia were determined by combining with the related targets. In this process, we synthesized a variety of database resources, made a comprehensive analysis of the chemical components of Taraxacum mongolicum, and predicted the possible targets of these components through bioinformatics. The drug- ingredient-target-pathway-disease network diagram was constructed, and the interaction between active ingredients of Taraxacum mongolicum and hyperuricemia-related targets was intuitively displayed. On this basis, we further analyzed the interaction network of potential targets, and revealed the key targets involved in the treatment of hyperuricemia by dandelion and their interaction mechanisms. In order to deeply understand the biological process and signal pathway of dandelion in the treatment of hyperuricemia, we carried out GO function enrichment analysis and KEGG signal pathway enrichment analysis. These analyses not only reveal the important role of dandelion active components in regulating the biological processes related to hyperuricemia, but also provide us with the potential mechanism of dandelion in treating hyperuricemia. The interaction between core active components and key

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Purpose of study. As a common metabolic disease, hyperuricemia (HUA) has become an important problem threatening human health. Hyperuricemia not only causes joint diseases such as gout, but also is closely related to a variety of diseases such as cardiovascular disease and kidney disease. Therefore, in-depth study of the pathogenesis of hyperuricemia and exploration of effective treatment methods have important clinical significance and social value.

High uric acid hematic disease treatment plan is still to be quick and convenient

for the characteristics of western medicine is given priority to, but the reference state drug administration's statement, the long-term use of such as not cloth company he pieces, benzene bromine Malone pieces and mainstream high uric acid hematic disease treatment, all can cause the different degree of damage of liver function and cardiovascular and cerebrovascular damage. Although most of the components of health drugs used in the adjuvant treatment of high-frequency uricemia are extracted from natural plants, their treatment cycle is long, the price is generally high, and the market is narrow.

Object of study. Dandelion, Chinese medicine also known as yellow flower diding, dandelion grass, Asteraceae perennial herbaceous plants. It was first recorded in Bencao Tujing (Illustrated Classic of Materia Medica). Its main functions are: clearing heat and detoxifying, removing swelling and dispersing knots, diuresis and diuresis. It is used for red eyes, sore throat, jaundice of dampness and heat, astringent pain and so on. The whole grass, dandelion sterols, choline, inulin and pectic substances.

Subject of study. Screening and effects of urate-lowering functional components from Dandelion

Key words: dandelion; Hyperuricemia; Network pharmacology; Molecular docking; Active ingredients; Over-Representation Analysis; mechanism of action

CHAPTER 1

LITERATURE REVIEW

1.1 Overview of network pharmacology

Network pharmacology, an emerging research field, has attracted extensive attention from researchers in recent years. It integrates the theory and technology of bioinformatics, systems biology, pharmacology and other disciplines, and provides a powerful tool for us to explore the interaction between drugs and organisms from a new perspective. Traditional drug research often focuses on the relationship between drugs and a single target. However, with the rapid development of modern biotechnology, people gradually realize that the interaction between drugs and organisms is actually a complex and multivariate network [1]. Based on this understanding, network pharmacology considers drugs and organisms as part of a complex network system, and reveals the interaction mechanism between drugs and organisms by constructing and analyzing these networks.

In the field of drug research and development, the application of network pharmacology provides us with new ideas and methods. It can help us to understand the mechanism of action of drugs more comprehensively, predict the potential efficacy and side effects of drugs, and provide guidance for the optimization and improvement of drugs. At the same time, network pharmacology can also be used for drug target discovery. By constructing a drug-target network, we can identify the main targets of drugs, which provides a basis for subsequent target verification and drug design.

Network pharmacology also plays an important role in the development of disease treatment strategies. By constructing the drug-disease network, we can reveal

the complex relationship between drugs and diseases, and provide theoretical support for the development of personalized treatment plans. Therefore, the emergence of network pharmacology not only enriches our understanding of the mechanism of drug action, but also provides new ideas and methods for drug development and disease treatment.

1.2 Overview of molecular docking technology

Molecular docking technology is a computational chemistry method to simulate the interaction between molecules. It predicts the binding mode and binding ability between receptors and ligands by simulating the binding process between them. Molecular docking technology has important application value in drug design and optimization, target discovery and verification.

The basic principle of molecular docking is based on the "lock-key model" and the "induced fit" theory. During docking, spatial and energy matching between molecules need to be considered. Spatial matching refers to the mutual adaptation of geometry and size between receptors and ligands. Energy matching refers to the interaction between the receptor and the ligand that can bring the system to the lowest energy stable state. The best binding mode can be found by continuously optimizing and adjusting the relative position and conformation between molecules [2].

1.3 Overview of hyperuricemia

Hyperuricemia is a metabolic disorder characterized by an increase in the concentration of uric acid in the blood. Uric acid is the end product of purine metabolism and is mainly excreted by the kidneys. Hyperuricemia occurs when excessive production or excretion of uric acid is reduced[3]. Hyperuricemia is closely

related to a variety of diseases, such as gout, kidney stones, cardiovascular diseases, etc. Long-term high uric acid levels can also cause kidney damage and affect renal function [4].

1.4 Research on network pharmacology and molecular docking of dandelion in the treatment of diseases

1.4.1 Current status of network pharmacology in Dandelion

In recent years, with the rise of network pharmacology, the pharmacological mechanism of dandelion has been studied more deeply. Network pharmacology can systematically reveal the interaction between drugs and organisms by constructing a drug-target-disease network. In the study of Dandelion, network pharmacology methods have been widely used to analyze the association between its active ingredients and a variety of diseases.

In his research, Yao Jiangqi [5] (2022) not only developed dandelion craft beer, but also deeply explored the inhibitory effect of dandelion on the increase of uric acid in mice. Through network pharmacology, he revealed the interaction between various active components of dandelion and uric acid metabolism-related targets, which provided theoretical support for the application of dandelion in the treatment of hyperuricemia.

Zou Chuanzong et al. [6] (2020) focused on the protective effect of dandelion on the kidney of rats with acute hyperuricemia. Using network pharmacology techniques, they analyzed the potential link between dandelion components and targets related to kidney protection, providing new ideas for the application of dandelion in the treatment of kidney-related diseases.

Li Yanni [7] (2023), in his research, focused on the identification and interaction mechanism of phenolic components inhibiting urease in Dandelion. Through network pharmacology, she systematically analyzed the interaction between the phenolic components and urease in Dandelion, revealed the potential mechanism of dandelion in inhibiting urease, and provided an important basis for the application of dandelion in related fields.

In general, the current research on network pharmacology of Taraxacum has made some progress. Through different research angles and methods, scholars have revealed the pharmacological mechanism of Taraxacum in many aspects, which provides strong support for the clinical application and drug research and development of Taraxacum. However, the pharmacological mechanism of dandelion still needs to be further studied in order to discover more potential therapeutic targets and drug candidates.

1.4.2 Molecular docking research status of Dandelion

Molecular docking, as a computational method to simulate interactions between molecules, has also been widely used in the study of dandelion. Through molecular docking, the binding mode and affinity between the active components of Dandelion and biological macromolecules can be predicted, thus revealing the pharmacological mechanism of action.

Sun Ying et al[8] used network pharmacology and molecular docking methods to analyze the mechanism of action of dandelion and Prunella vulgaris in the treatment of granulomatous mastitis. They used molecular docking technology to simulate the binding of the active ingredients in dandelion and prunella to mastitis related targets,

and found that these ingredients can effectively bind to the target to exert therapeutic effects. This study provides a theoretical basis for the combined use of dandelion and prunella vulgaris in the treatment of granulomatous mastitis. Some studies have used molecular docking technology to predict the binding of dandelion components to other disease-related proteins, such as anti-inflammatory proteins and antioxidant enzymes. These studies provide important clues to reveal the mechanism of action of dandelion in the treatment of other diseases.

1.4.3 Combined network pharmacology and molecular docking study of dandelion in the treatment of hyperuricemia

As a traditional Chinese medicine, dandelion has gradually attracted the attention of researchers in the treatment of hyperuricemia. The combined application of network pharmacology and molecular docking technology provides a new perspective and idea for revealing the mechanism of action of dandelion in the treatment of hyperuricemia.

Network pharmacology can systematically analyze the interaction between dandelion and hyperuricemia by constructing a drug-target-disease network model. In his research, Yao Jiangqi explored the development of dandelion craft beer and initially studied its inhibitory effect on the increase of uric acid in mice, which provided a preliminary experimental basis for the application of dandelion in the treatment of hyperuricemia [9]. However, there is still a lack of in-depth research on the specific mechanism of dandelion in the treatment of hyperuricemia.

Molecular docking technology can simulate the interaction between the active components of Dandelion and the targets related to hyperuricemia, and predict their

binding mode and affinity. Through molecular docking, we can gain a deeper understanding of the binding of dandelion components to uric acid metabolism-related enzymes or receptors, and thus reveal the mechanism of action of dandelion in the treatment of hyperuricemia. Zou Chuanzong et al. found that dandelion had a protective effect on the kidney of rats with acute hyperuricemia, which may be related to the interaction between dandelion components and targets related to uric acid metabolism[10].

Combining network pharmacology and molecular docking technology, we can more comprehensively reveal the mechanism of action of dandelion in the treatment of hyperuricemia. Firstly, through network pharmacology analysis, we could identify the key active components and targets in Dandelion that are relevant for the treatment of hyperuricemia. Then, using molecular docking technology, we can model the interaction of these active ingredients with the target and predict the binding mode and affinity. This will help us to understand the pharmacological mechanism of dandelion in the treatment of hyperuricemia, and provide a more scientific basis for the clinical application of dandelion.

However, the current research on the combination of network pharmacology and molecular docking of dandelion in the treatment of hyperuricemia is still in its infancy, and there are still many challenges and limitations. For example, the active ingredients in Dandelion are complex and diverse, and their interactions may involve multiple targets and pathways. Therefore, more in-depth studies are needed to understand the regulatory mechanism of their network. In addition, the prediction results of molecular docking technology still need further experimental verification to ensure its accuracy

and reliability.

1.5 Significance of topic selection

As a common metabolic disease, hyperuricemia (HUA) has become an important problem threatening human health. Hyperuricemia not only causes joint diseases such as gout, but also is closely related to a variety of diseases such as cardiovascular disease and kidney disease. Therefore, in-depth study of the pathogenesis of hyperuricemia and exploration of effective treatment methods have important clinical significance and social value.

As a traditional Chinese herbal medicine, dandelion has the effects of clearing heat, detoxifying, diuresis and dampness, and is widely used in the treatment of various diseases among people. In recent years, with the development of modern pharmacology and bioinformatics, the pharmacological mechanism of dandelion has been gradually revealed, and its potential in the treatment of hyperuricemia has gradually attracted attention. Based on network pharmacology and molecular docking technology, this study aims to explore the mechanism of dandelion in the treatment of hyperuricemia. Through the network pharmacology method, the active ingredients and their action targets in Taraxacum chinensis were screened, and the potential action targets of taraxacum chinensis in the treatment of hyperuricemia were analyzed combined with the related targets of hyperuricemia. At the same time, molecular docking technology was used to verify the interaction between the active components of Dandelion and key targets, so as to reveal the mechanism of action of dandelion in the treatment of hyperuricemia.

This study is helpful to understand the pharmacological mechanism of dandelion

in the treatment of hyperuricemia, and provide theoretical basis for the clinical application of dandelion. By uncovering the interactions between the active components of dandelion and the key targets of hyperuricemia, we can provide a scientific basis for the application of dandelion in the treatment of hyperuricemia, and help promote the modernization and internationalization of traditional Chinese herbs such as dandelion. The results can provide new ideas and directions for the treatment of hyperuricemia. Exploring the active components and their targets in Taraculum dandelion can provide candidate components and targets for the development of new anti-hyperuricemia drugs, and help to solve the problems such as the limited number of current drugs for the treatment of hyperuricemia and the large side effects. Research can also promote the application of network pharmacology and molecular docking technology in TCM research. Through the combination of modern pharmacology and bioinformatics methods with the theory of traditional Chinese medicine, the pharmacological mechanism of traditional Chinese medicine can be further explored, and the modernization and scientific development of traditional Chinese medicine can be promoted.

Conclusions to chapter 1

As a traditional Chinese herbal medicine, dandelion has the effects of clearing heat, detoxifying, diuresis and dampness, and is widely used in the treatment of various diseases among people. In recent years, with the development of modern pharmacology and bioinformatics, the pharmacological mechanism of dandelion has been gradually revealed, and its potential in the treatment of hyperuricemia has gradually attracted

attention. Based on network pharmacology and molecular docking technology, this study aims to explore the mechanism of dandelion in the treatment of hyperuricemia. Through the network pharmacology method, the active ingredients and their action targets in Taraxacum chinensis were screened, and the potential action targets of taraxacum chinensis in the treatment of hyperuricemia were analyzed combined with the related targets of hyperuricemia. At the same time, molecular docking technology was used to verify the interaction between the active components of Dandelion and key targets, so as to reveal the mechanism of action of dandelion in the treatment of hyperuricemia.

CHAPTER 2

OBJECT, PURPOSE AND METHODS OF THE STUDY

2.1 Object and purpose of study

Object of study. Dandelion, Chinese medicine also known as yellow flower diding, dandelion grass, Asteraceae perennial herbaceous plants. It was first recorded in Bencao Tujing (Illustrated Classic of Materia Medica). Its main functions are: clearing heat and detoxifying, removing swelling and dispersing knots, diuresis and diuresis. It is used for red eyes, sore throat, jaundice of dampness and heat, astringent pain and so on. The whole grass, dandelion sterols, choline, inulin and pectic substances.

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2.2 Screening of active ingredients and targets of Dandelion

According to the five principles of lipinski, the screening conditions (① Molecular weight (MW) of molecules should not exceed 500 daltons) were selected from herb (http://herb.ac.cn/) database. This is because large molecular weights may lead to poor absorption of molecules in the gut. ② The number of hydrogen bond donors (such as hydroxyl groups, amino groups, etc.) in the compound structure should not exceed 5. Hydrogen bond donors can form hydrogen bonds with amino acids in proteins and affect the interaction between drug molecules and proteins. ③ The number of hydrogen bond receptors in the compound should not exceed 10. Hydrogen bond receptors may affect the binding ability of drug molecules when they interact with proteins. ④ The fat-water partition coefficient (logP) of the compound should be between -2 and 5. This parameter measures the equilibrium distribution of molecules between water and fat, and a higher LogP value may mean that the molecule is too hydrophobic or too lipophilic. ⑤ The number of rotatable bonds in the compound should not exceed 10. This helps maintain the shape of the molecule for better binding to targets in the organism). The action targets related to the active ingredients in dandelion were retrieved, and the action targets of each ingredient were saved in EXCEL in the form of a table. Subsequently, these active ingredients were imported into TCMSP for target prediction. The UniProt database (http: / /www.uniprot.org) was used to obtain the target genes.

To ensure the accuracy of the data, we also used PubChem database and SwissTargetPrediction database to perform format conversion and target prediction of active ingredients. Finally, targets from multiple sources were deduplicated and

merged to obtain the main action component targets of Dandelion.

2.3 Screening of targets related to hyperuricemia

Using GeneCards (https://www.genecards.org/), OMIM (https://omim.org/) and DrugBank (https://www.drugbank.com/), and other authoritative database, "Hyperuricemia" or "High uric acid" was used as the key word to collect the disease targets related to hyperuricemia. Similarly, the collected targets were de-reprocessed and taken union to ensure the comprehensiveness and accuracy of the targets.

2.4 Screening of potential targets of dandelion in the treatment of hyperuricemia

The intersection analysis of the action targets of the active ingredients of dandelion and the targets related to hyperuricemia was performed to reveal the potential action targets of dandelion in the treatment of hyperuricemia. This analysis process using Venny2.1 (https://bioinfogp.cnb.csic.es/tools/venny), the summary of overlap gene and map Wayne. The intersection between the active components of dandelion and the targets of hyperuricemia can be visually displayed.

2.5 Drawing of protein interaction network (PPI)

The screened potential targets of dandelion in the treatment of hyperuricemia were transferred into the STRING online analysis platform (https://string-db.org/) for protein interaction analysis. The analysis data were transferred into Cytoscape 3.7.2 software, and the PPI network was drawn to reveal the interaction between the active component targets of Dandelion and the hyperuricemia targets, and the topological calculation was performed to obtain the key targets.

2.6 Enrichment analysis

Using microscopic letter platform (https://www.bioinformatics.com.cn/) to

select the intersection of targets for enrichment of KEGG pathways and GO function analysis. The analysis data were imported into ImageGP and GraphPad Prism 8.0 software for visualization, and enrichment analysis maps were drawn to reveal the mechanism of action of dandelion in the treatment of hyperuricemia.

2.7 Molecular docking analysis

In order to verify whether the effective components of Dandelion can be successfully combined with the key targets in space, molecular docking verification is needed. PDB files of key targets as receptor molecules were downloaded from the RCSB PDB database. mol2 format files of the active components of dandelion used as ligands by the docking process were searched by TCMSP, and the structure was optimized using Chem 3D software. Finally, the use of CB - DOCK2 (https://cadd.labshare.cn/cb-dock2) online molecular docking platform for molecular docking analysis, obtained the dandelion effective components and key target combination mode and the affinity between the score. These results provide strong evidence to verify the potential mechanism of dandelion in the treatment of hyperuricemia

Conclusions to chapter 2

This study mainly utilized Screening of active ingredients and targets of Dandelion, screening of active ingredients and targets of Dandelion, screening of potential targets of dandelion in the treatment of hyperuricemia, enrichment analysis and molecular docking analysis.

CHAPTER 3

EXPERIMENTAL PART

3.1 Exploration of active compounds in Dandelion (Dandelion)

After exhaustive literature research, the chemical composition of dandelion has been comprehensively sorted out. This process not only referred to the authoritative data of the Pharmacopoeia of the People's Republic of China (2020 edition), but also combined the research data of high performance liquid chromatography (HPLC), Chinese Medicine System Pharmacology Database Analysis Platform (TCMSP) (http: / / ibts.Hkbu.edu.hk/LSP/tcmsp.php), biological information credits on molecular mechanisms of traditional Chinese Medicine, and a large number of review articles to ensure that the information obtained is accurate and comprehensive. Through this series of analyses, 116 compounds closely related to dandelion were successfully identified, which covered a variety of chemical types, fully demonstrating the complexity and diversity of dandelion.

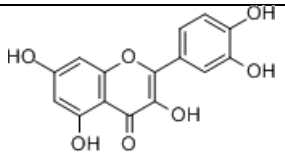
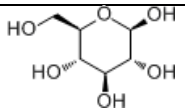
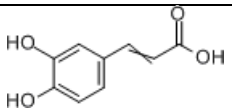
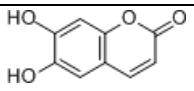
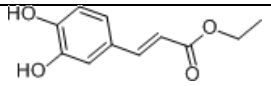
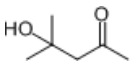
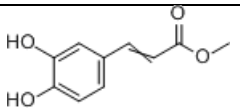
Among the active ingredients of dandelion, flavonoids are particularly prominent, including luteolin, quercetin, hesperidin, apigenin and other components. Due to their unique biological activities, these flavonoids play a key role in the medicinal effects of Dandelion. In addition, phenolic acids are also important components of Dandelion, and the presence of vanillic acid, p-coumaric acid, caffeic acid and other phenolic acids further enriches the pharmacological effects of dandelion.

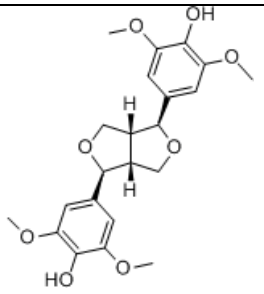
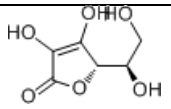
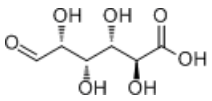
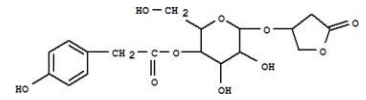
In addition to the above two compounds, dandelion also contains terpenes, pigments, phytosterols, sesquiterpene lactones, coumarins and fatty acids. These

compounds have their own characteristics and together constitute the basis of the medicinal effect of dandelion.

The structural information of these 11 active compounds is listed in detail in Table 3-1, which provides an important reference basis for subsequent in-depth research. Through the in-depth study of these compounds, we are expected to reveal the pharmacological mechanism of taraxacum and provide a more scientific basis for the clinical application of taraxacum.

Table 3-1 11 active compounds of Dandelion

Herb ID	Chemical compound	Molecular formula	CAS	Chemical structure
HBIN041495	Quercetin	C15H1007	117-39-5	
HBIN043442	Scopoletin	C10H804	492-61-5	
HBIN019298	Caffeic acid	C9H8O4	331-39-5	
HBIN025796	Seven pages Pavilion	C9H604	305-01-1	
HBIN025897	Ethyl caffeinate	C11H1204	102-37-4	
HBIN0010490	Diacetone alcohol	C6H1202	123-42-2	
HBIN035129	Methyl caffeic acid	C21H2008	3843-74-1	

HBIN045261	(+) -eugenol	C22H2608	21453-69-0	
HBIN048047	D-ascorbic acid	C6H806	10504-35-5	
HBIN039022	B-d-galacturonic acid	C6H1007	18968-14-4	
HBIN045521	Dandelion side	C18H22010	98449-40-2	

In order to better screen the most active compounds in dandelion, we adopted the Lipinski's five principles of drugs. According to the lipinski's five principles of screening criteria (molecular weight, the number of hydrogen bond receptors in the compound, the number of hydrogen bond donors in the compound structure, the lipid-water partition coefficient of the compound, and the number of rottable bonds in the compound), the evaluation method was used. After comprehensive evaluation of these compounds, 11 active compounds were finally selected. These compounds not only have good pharmacological activities, but also show good performance in absorption, distribution, metabolism and excretion in human body, so they are of great research value and application prospect.

3.2 Construction and interpretation of drug-active ingredient-target-pathway-disease network diagram

In the process of in-depth research on the mechanism of taraxacum, the DAVID database was used to find the top 20 pathways associated with hyperuricemia, and the

targets of these pathways were listed one by one. Cytoscape software was used to visualize the target genes of these pathways and the corresponding targets of 11 key active ingredients of taraxacum. Finally, 62 potential targets associated with it were successfully identified, and the drug-active ingredient-target-pathway-disease network diagram was constructed (as shown in Figure 3-1). Through this network diagram, we can clearly see how the active ingredients of dandelion are linked to hyperuricemia through common target genes, Its compounds HBIN041495(quercetin), HBIN45521 (taraxoside) and HBIN25796 (esculetin) as the main active components are linked to hyperuricemia through common target genes, which provides a strong theoretical support for our understanding of the mechanism of its drug action.

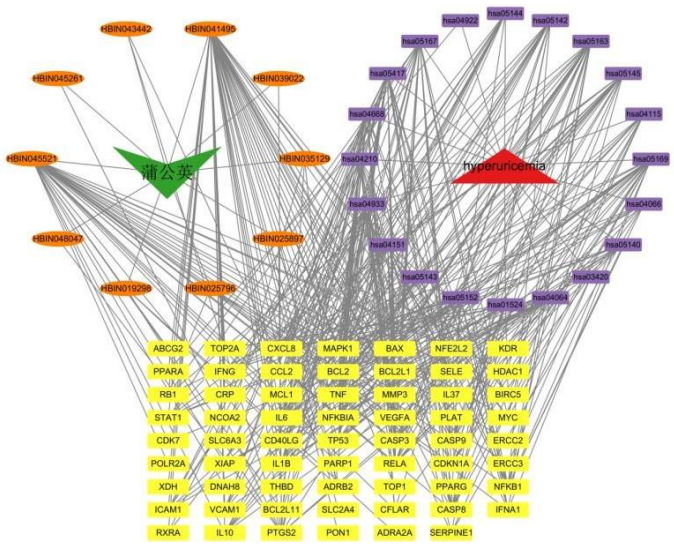


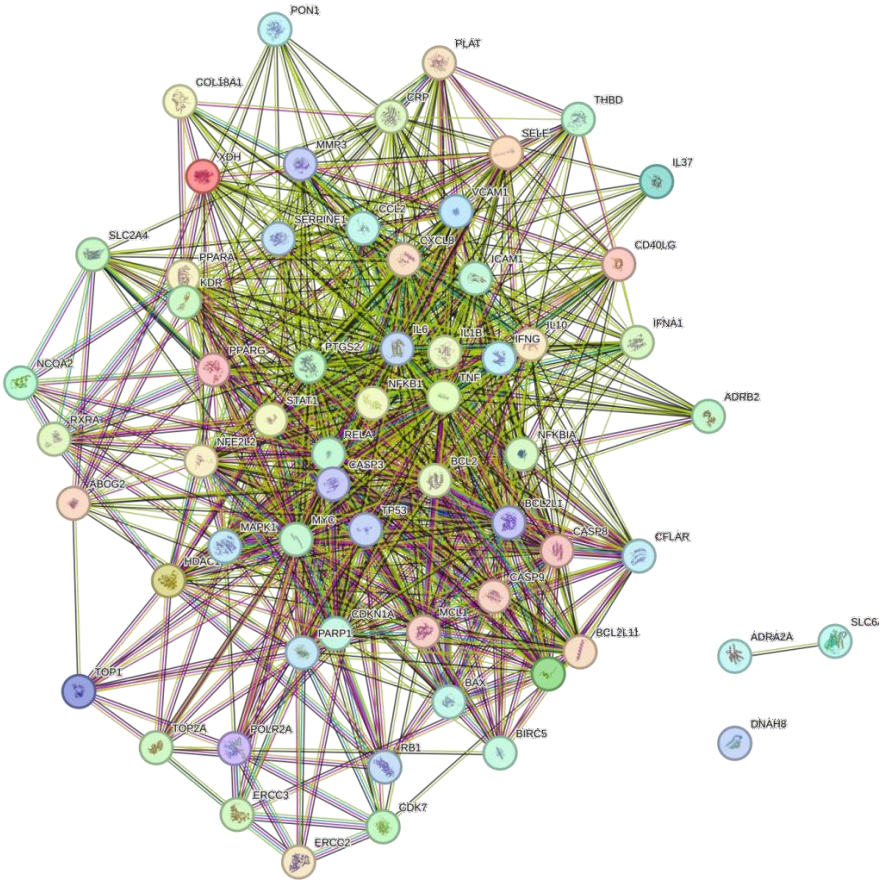
Figure 3-1 "Drug-active ingredient-target-pathway-disease" network

3.3 Construction and analysis of potential target interaction network

To further explore the potential mechanism of action of dandelion in the

treatment of hyperuricemia, we searched 907 potential therapeutic targets for hyperuricemia through GeneCards, OMIM, TTD and other authoritative databases. Furthermore, we compared these targets with the targets of drugs, and finally identified 62 common intersection targets. In order to further study the interaction of these intersection targets in the process of dandelion treatment of hyperuricemia, we used the STRING platform and Cytoscape software to draw the PPI (protein-protein interaction) network diagram (as shown in Figure 3-2). This network graph involves a total of 62 nodes and 820 edges, and the size of nodes is closely related to their degree value in the network (i.e. the degree of connectivity). By using the Cytoscape plugin cytoHubba for topological calculation analysis, we found that MYC, TP53, IL6 and other targets (as shown in Figure 3-3) played a central role in the process of dandelion pair treatment of hyperuricemia, and the correlation between them and other targets was particularly significant. These findings provide important clues and basis for us to further reveal the therapeutic mechanism of dandelion in the treatment of hyperuricemia.

Figure 3-2 Interaction network of potential targets in Dandelion



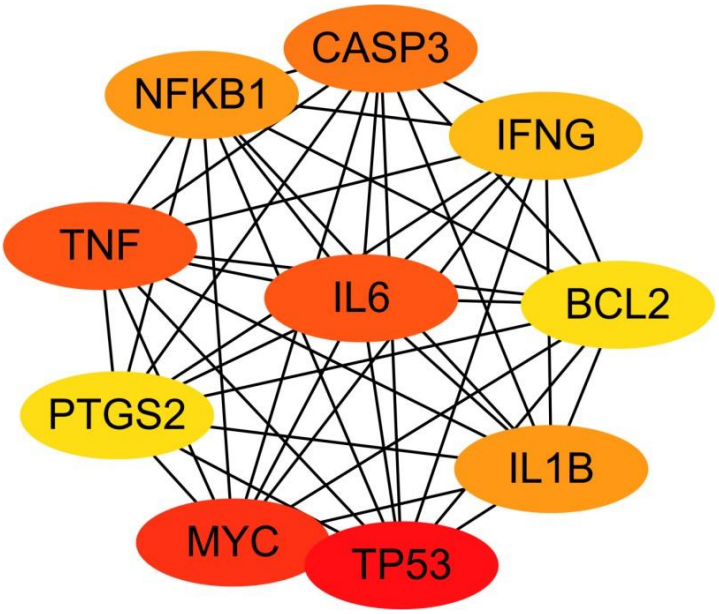


Figure 3-3 cytoHubba core gene mining results

3.4 GO functional enrichment analysis and KEGG signaling pathway enrichment analysis

In order to further explore the mechanism of action of dandelion in the treatment of hyperuricemia, we used DAVID database and Omicshare cloud platform to perform detailed GO functional enrichment analysis and KEGG signaling pathway enrichment analysis of 62 previously identified potential targets. By drawing a bubble map, We observed that these targets were mainly involved in biological processes (GO-BP) including response to lipopolysaccharide, response to molecue of bacteria oriain, and response to oxygen evels, response to oxidative stress, celular response to chemica stress, etc., these processes are closely related to the treatment of hyperuricemia (FIG. 3-4).

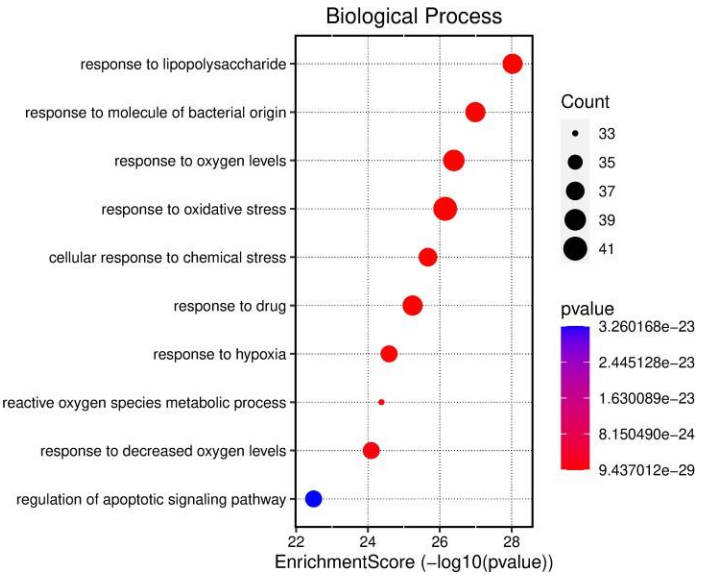
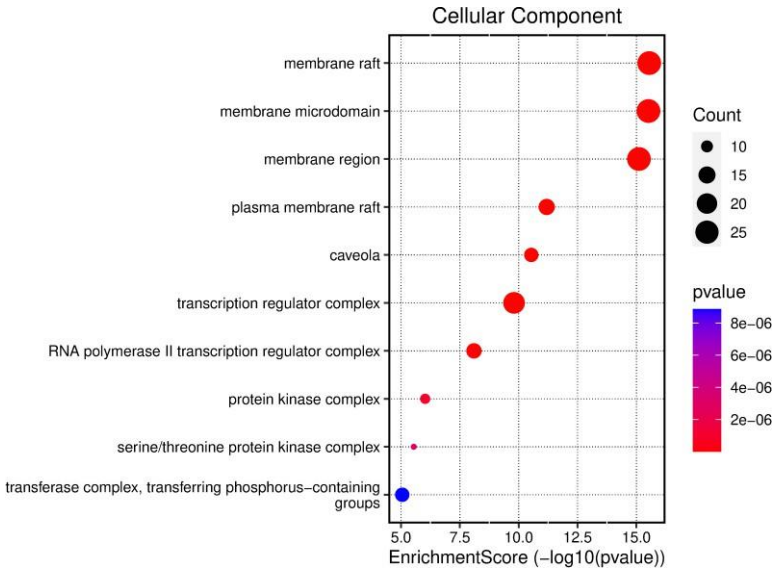


Figure 3-4 GO-BP enrichment analysis

Meanwhile, the results of cell composition (GO-CC) analysis showed that These targets were mainly involved in key processes such as memorane raft, membrane microdomain, memorane redion, plasma membrane raft, and caveola (FIG. 3-5).

Figure 3-5 GO-CC enrichment analysis



At the same time, the results of molecular function (GO-MF) analysis showed

that These targets are mainly involved in DNA-binding transcription factor binding, repressing transcription factor pinding, and RNA polymerase ll-specific Key functions such as DNA-binding transcription factorbinding, cytokine receptor binding, and cytokine activity (FIG. 3-6).

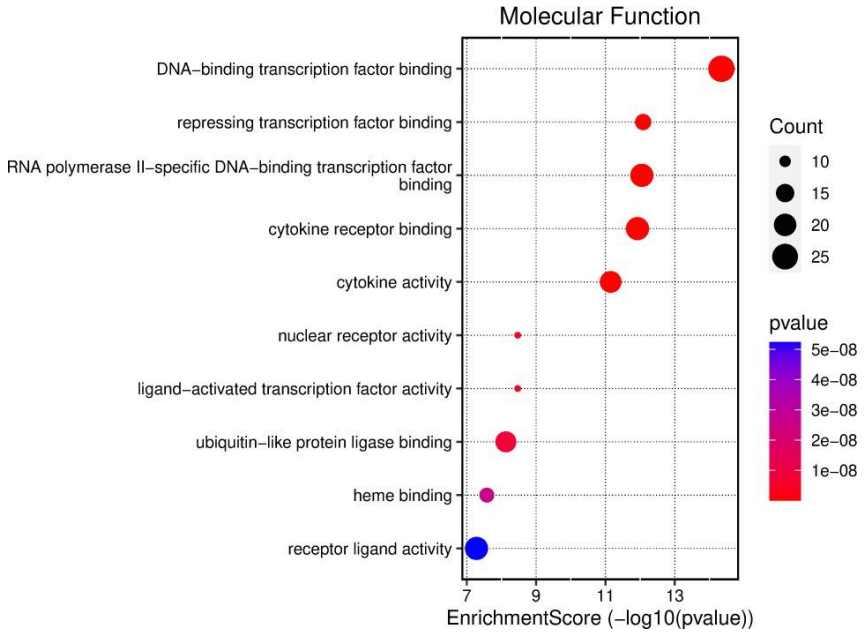
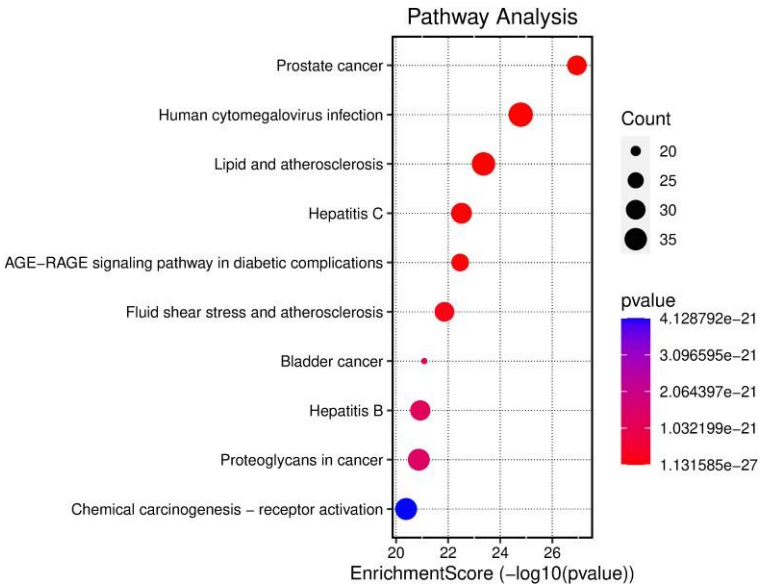


Figure 3-6 GO-MF enrichment analysis

In KEGG pathway enrichment analysis, the results mainly included the following pathways: Prostate cancer, Human cytomegalovirus infection, Lipid and atheroscerosis, Hepatitis C, AGE-RAGE signaling pathway in diabetic complications, Fuid shear stress and atherosclerosis, Bladder cancer, Hepatitis B, Proteoglycans in cancer, Chemica carcinoma-receptor activation, etc. (Figure 3-7). These signaling pathways play important roles in inflammatory response and immune regulation, which further supports the potential efficacy of dandelion in the treatment of hyperuricemia.

All the above results were subjected to rigorous statistical analysis ($P < 0.05$), and the top 10 most representative results were selected.

FIG. 3-7 KEGG pathway enrichment analysis



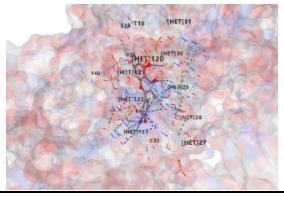
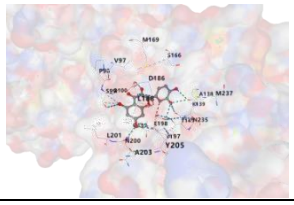
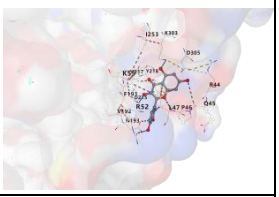
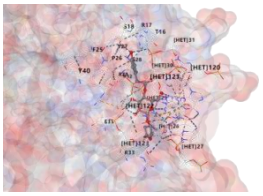
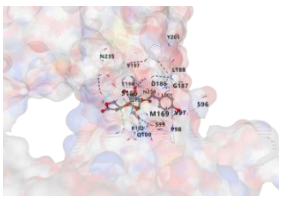
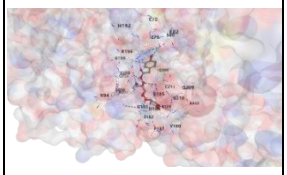
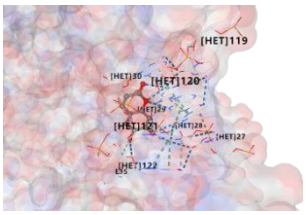
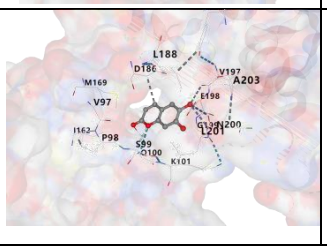
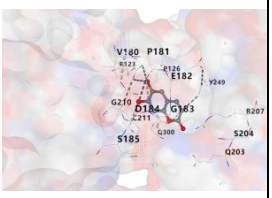
3.6 Molecular docking to verify the interaction between core active ingredients and targets

To further verify the interaction between the core active components and the core targets, we performed molecular docking studies using the CB-DOCK2 online molecular docking platform. We selected the core active ingredients of dandelion, quercetin, taraxin, and esculetin, and performed molecular docking with the core targets MYC, TP53, and IL-6 (Tables 3-2, 3-3). The results showed that the binding energies of these active ingredients with the target proteins were all lower than -5.0 kcal • mol-1, suggesting that they had good binding activities with the target proteins, which further confirmed the potential efficacy of dandelion in the treatment of hyperuricemia in the spatial structure calculus.

Table 3-2 Binding energy between core active ingredients and core targets

Active ingredient	Binding energy(kcal • mol－1)		
	MYC	TP53	IL-6
Quercetin	-9.7	-7.5	-8.2
The Buckeye Pavilion	-7.7	-6.2	-7.1
Dandelion side	-9.5	-6.9	-8.4

Table 3-3 Molecular docking results

	MYC	TP53	IL-6
Quercetin			
Dandelion side			
The buckeye pavilion			

Conclusions to chapter 3

GO through enrichment and KEGG pathway enrichment analysis function, we reveal the dandelion potential molecular mechanisms for the treatment of high uric acid hematic disease. The role of dandelion is mainly involved in the positive regulation of nitric oxide synthesis, inflammatory response, cellular response to lipopolysaccharide, immune response and other biological processes.Molecular docking was used to verify the interaction between the core active components of Dandelion and key targets. Through simulating molecular docking process, we determine the dandelion the

combination of active ingredients and target mode and affinity, further confirmed the effectiveness of dandelion in the treatment of high uric acid hematic disease.In this study, the mechanism of action of dandelion in the treatment of hyperuricemia was explored by comprehensive application of network pharmacology and molecular docking technology. We found that dandelion exerted anti-inflammatory and immunomodulatory effects through a variety of active ingredients and targets and multiple signaling pathways, thereby achieving effective treatment of hyperuricemia. The research results not only for the dandelion in the application of high uric acid hematic disease treatment provides a scientific basis, for TCM modernization and scientific development provides a new thought and method.

CONCLUSIONS

Based on network pharmacology and molecular docking technology, this study conducted a comprehensive and in-depth study on the mechanism of action of dandelion in the treatment of hyperuricemia. Through comprehensive analysis of the active ingredients, targets of action and the related molecular mechanisms of hyperuricemia in dandelion, we have come to a series of innovative and practical conclusions.

1. A variety of active components in dandelion, such as quercetin, aesculin, and

taraxacin, have been confirmed to have significant anti-inflammatory and immunomodulatory functions. These active ingredients can act on multiple targets related to hyperuricemia, including inflammatory factors and immune-related receptors, so as to play a therapeutic role. This finding not only explains the potential mechanism of dandelion in the treatment of hyperuricemia, but also provides a strong scientific support for the application of dandelion in the modernization and internationalization of traditional Chinese medicine.

2. Through GO functional enrichment analysis and KEGG pathway enrichment analysis, we revealed the potential molecular mechanism of dandelion in the treatment of hyperuricemia. The role of dandelion is mainly involved in the positive regulation of nitric oxide synthesis, inflammatory response, cellular response to lipopolysaccharide, immune response and other biological processes. These biological processes are closely related to the occurrence and development of hyperuricemia, and dandelion achieves effective treatment of hyperuricemia by regulating these processes.

3. Dandelion exerts anti-inflammatory and immunomodulatory effects by regulating key pathways such as Toll-like receptor signaling pathway, TNF signaling pathway and NOD-like receptor signaling pathway. Regulation of these pathways is essential for the control of inflammatory response and immune imbalance in hyperuricemia.

4. In this study, molecular docking was also used to verify the interaction between the core active components of Dandelion and key targets. By simulating the molecular docking process, we determined the binding mode and affinity of the active components of Dandelion to their targets, further confirming the efficacy of dandelion

in the treatment of hyperuricemia. The application of this technology not only improves the accuracy and reliability of the research, but also provides an important reference for subsequent drug development and optimization.

5. The present study explored the mechanism of action of dandelion in the treatment of hyperuricemia by integrated application of network pharmacology and molecular docking technology. We found that dandelion exerted anti-inflammatory and immunomodulatory effects through a variety of active ingredients and targets and multiple signaling pathways, thereby achieving effective treatment of hyperuricemia. This research result not only provides a scientific basis for the application of dandelion in the treatment of hyperuricemia, but also provides new ideas and methods for the modernization and scientific development of traditional Chinese medicine. However, this study still has some limitations. Firstly, although the potential mechanisms of action of dandelion in treating hyperuricemia were predicted by network pharmacology and molecular docking techniques, these predictions still need to be further verified by experiments. Secondly, there are many active ingredients in dandelion. This study only conducted in-depth discussions on some of the main ingredients, and future research can further expand the research on other ingredients. In addition, this study mainly focused on the anti-inflammatory and immunomodulatory effects of Taraxacum, and other mechanisms such as its regulation of uric acid metabolism can be further explored in the future.

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APPENDIX

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NATIONAL RESEARCH & DEVELOPMENT INSTITUTE FOR TEXTILES AND LEATHER (INCDTP) - DIVISION LEATHER AND FOOTWEAR RESEARCH INSTITUTE (ICPI)

ICAMS 2022

ADVANCED MATERIALS AND SYSTEMS

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NANOPIGMENTS FOR LEATHER FINISHING COATINGS

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The work is focused on obtaining nanopigments by adsorption of anionic dyes on positively charged montmorillonite. The effect of sequential modification of aqueous dispersions of montmorillonite with cationic and anionic compounds on the structural and charge characteristics of mineral dispersions was studied. The effect of chemical dispersion of agglomerates of aqueous montmorillonite dispersions after adding carbonate solutions was shown. The treatment of dispersions of original montmorillonite with sodium carbonate provides maximum dispersion of mineral aggregates by penetrating into the interstructural space of aluminosilicate packets, moving them apart and separating them. It was found that the modification of montmorillonite dispersed by sodium carbonate by adding basic chromium sulfate is accompanied by a change in the surface chemistry of the mineral and structural transformations. Structural changes are manifested by the formation of a developed structure of cationic montmorillonite. The cationic surface charge of montmorillonite and high specific surface of montmorillonite are important factors for ensuring effective adsorption of anionic dyes on the surface of the mineral. The efficiency of adsorption of anionic dyes on cationic montmorillonite is investigated. It was shown that the adsorption of dyes dependent on the pH of the medium. The scheme of obtaining nanopigments, which were characterized by good covering power, saturated and intense colour was proposed.

Keywords: montmorillonite, pigment, leather finishing coating

INTRODUCTION

Traditional leather finishing involves applying a covering composition to the surface of leather. The finishing coating provides protection of leather from external atmospheric and mechanical impacts (Covington, 2009).

The type of leather coating depends on the content of pigments and can be (Covington, 2017; Zhuravsky *et al.*, 1996; Kanyan, 2019): aniline – a transparent coating without the use of pigments; semi-aniline – characterized by a small content of pigments to provide, mainly, a shade of color; and pigmented – with a significant content of pigments for complete coverage of the surface of leather with a colored covering layer.

Pigments provide color and covering power to the finishing coating (Winter *et al.*, 2017). Organic or inorganic pigments are used in the finishing coating of leathers. Covering compositions with organic pigments provide leather with shine, bright and intense color, but have low light fastness and heat resistance. Inorganic pigments create a high-quality coating with good light fastness and water resistance, but are characterized by a high tendency to sedimentation and are limited in color and brightness (Winter *et al.*, 2017; Osgood, 1990).

The ability of the coating to form a uniform coating stable composition with required thickness depends on the properties of the pigment, the origin of their surface, and the size of the particles.

The use of nanopigments provide improved physical and mechanical indexes of the leather finishing coating (Bondaryeva and Mokrousova, 2020; Bondaryeva *et al.*, 2021).

The aim of the work was to describe the scientific basis of patterns of anionic dyes adsorption on positively charged montmorillonite to obtain nanopigments for leather finishing coatings.

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EXPERIMENTAL

Materials

Bentonite clay from the Cherkassky deposit (Ukraine), after thorough purification and washing was used as a basis for obtaining nanopigments. The main mineral was montmorillonite, the content was 85±3 %. The value of the exchange capacity was 72 mg-eq/100 g of clay. Humidity – 27 ± 3 %.

The sodium carbonate, basic chromium sulfate (III) and anionic dyes were used to modify dispersions of montmorillonite.

Methods

The nanopigments were obtained by sequential treatment of aqueous montmorillonite dispersions (100 g/l) with sodium carbonate, basic chromium sulfate and anionic dyes.

Firstly, 6,0% of sodium carbonate from weight of dry montmorillonite was used, and then the cationic form of montmorillonite was obtained by modifying the dispersion of Na^+-montmorillonite with chromium compound. For this purpose, the basic chromium sulfate was used – $Cr_2(SO_4)_m(OH)_{6-2m}$, chromium oxide (III) content was 25.6 %. A solution of basic chromium sulfate in the amount of 10.0% Cr_2O_3 (by weight of the montmorillonite) was added to the dispersion of Na^+-montmorillonite (MMT–Na^+). Mixing was continued until a homogeneous mass of gray colour was obtained. The pH value of the modified dispersion of cationic montmorillonite (MMT-Cr^{3+}) was 4.5-5.2.

The nanopigments were prepared by gradually mixing the cationic form of montmorillonite with the anionic dyes. Mixing was performed using a mechanical mixer (30–40 min, 40–45°C) to obtain time-stable dispersions in the form of nanopigments of saturated deep colour. The consumption of anionic dyes in a ratio of 1:1 according to the mineral component. The nanopigments were obtained as the colored modified dispersions of montmorillonite.

A laser-correlation spectrometer "ZetaSizer-3" (Malvern Instrument, USA) with a Multi Computing Correlator type 7032 CE was used to study the dispersion of mineral systems.

The adsorption of dyes from aqueous solutions on the cationic form of montmorillonite was determined by measuring the light transmittance of dye solutions of different concentrations.

The electrokinetic potential was determined by microelectrophoresis.

RESULTS AND DISCUSSION

In montmorillonite modification, molecules of polar liquids (for example, sodium carbonate) can freely penetrate into the interpackets space of montmorillonite, push them apart and increase the distance between packets. As a result, montmorillonite particles disperse spontaneously in water, their number per unit volume increases significantly, and the number of direct contacts for further interactions increases.

It is shown that treatment of dispersions of native montmorillonite with sodium carbonate provides maximum dispersion of mineral aggregates by penetrating into the interstructural space of aluminosilicate packets, moving them apart and separating them.

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