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Review Article

Construction and Application of Traditional Chinese Medicine Minerals Database

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Abstract: Mineral drugs are rich in resources in China and have distinct curative effects, and are an irreplaceable component of traditional Chinese medicine (TCM). So, this makes minerals drugs become a research hotspot in the medical and geological fields, and a large number of related literatures have emerged. However, there are still some problems in mineral medicine research, mainly reflected in the qualitative and quantitative detection method is not mature, ignoring the importance of mineral properties for the study of pharmacological effects, and the studies on mineral drugs from the perspective of mineralogy are few at present. Chemical constituents of mineral drugs are the main source for the study of Pharmacological action. Therefore, it is meaningful to study mineral drugs by combining mineralogy with pharmacology. In this paper, a comprehensive classification system of mineral drugs is summarized, and the modern detection techniques (Infrared and Raman spectroscopy) for studying qualitative and quantitative analysis of mineral drugs are discussed. In addition, the design and application of TCM minerals database is also described. Here, we hope that this will provide a useful reference for the classification and analysis of mineral drugs from the perspective of mineralogy, and the digitization construction and application of Traditional Chinese Medicine minerals database.

Keywords: Traditional Chinese Medicine Minerals Database, The Perspective of Mineralogy, Infrared and Raman Spectroscopy, Classification of Mineral Drugs, Digitization Construction

1. Introduction

From time immemorial, mineral drugs have been the carrier of Chinese civilization and have contributed the unique strength to the cause of people's health. Mineral medicine, same as animal medicine and botanical medicine, is an indispensable part of Traditional Chinese medicine, playing an irreplaceable role in treating difficult miscellaneous diseases and protecting human health. The earliest record of mineral drug can be traced back to the Shan Hai Jing in the Warring States Period [1, 2]. Medicinal minerals refer to natural mineral rocks, including minerals, rocks, soil, fossils, organic matter, ore, etc., which should be used as medicinal materials for making Chinese patent medicines or traditional Chinese medicine prescriptions in clinical application of TCM. Such as realgar, cinnabar, quartz, amber, spirifer's fossil shell [3].

Medical mineralogy is an interdiscipline of geology, mineralogy and medicine. From the perspective of mineralogy, it is mainly used to study the physical properties, chemical composition and trace elements of various rocks and minerals used for medicinal purposes. From the perspective of medicine, the pharmacological properties, functions, main therapeutic effects, processing methods are studied to be mineral drugs and prescriptions [4]. In China, mineral have played a significant role not only in clinical

application, but also in medical treatment and health care as drugs, because of their constant source and obvious therapeutic effect. TCM Mineral resources is an important material basis for the original innovation of science and technology, the development of social economy and the improvement of national scientific literacy. It has the characteristics of public benefit, basic, longterm and strategy.

With the in-depth study of TCM minerals, many medical scholars have studied their pharmacological effects, efficacy and quality detection owing to the unique clinical effect of mineral drugs in recent years. However, relevant researches that compare the pharmaceutical properties of mineral drugs with the mineralogical properties are few at present, ignoring the importance of mineralogical properties to the pharmaco-logical effects of mineral drugs. This paper aims to construct a TCM minerals database based on medicinal mineral data, which systematically and scientifically collects and sorts out the mineral drug information (medicinal properties, mineral properties, and typical spectral characteristics) and realizes the data sharing, so as to standardize the name of medicinal minerals from the perspective of mineralogy and pharmacology, provide evidence for identification, and furnish guidance and demonstration for the digital construction and sharing of TCM mineral resources in China.

2. Classification of Traditional Chinese Medicine Minerals

Ancient books and records have witnessed the development and changes of mineral drug history, and there are different opinions on the specific types of mineral drugs. For example, there are 41 kinds of mineral drugs included in the earliest pharmaceutical native Shennong Bencao in China, 46 kinds of mineral drugs were recorded in the Tang Bencao compiled by the government of the Tang Dynasty, and 129 kinds of mineral drugs were recorded in the Compendium of Materia Medica written by Li Shizhen in the Ming Dynasty. In modern times, there are less than 30 kinds of mineral drugs included in Chinese Pharmacopoeia 2020. Due to the long history of mineral drugs, the medicinal value of some mineral drugs has not been studied and known by pharmaceutical and mineral scholars. According to the related literature and Chinese Pharmacopoeia, 55 kinds of commonly used medical materials in traditional Chinese medicine minerals were included in the traditional Chinese medicine minerals database.

2.1. Classification of Traditional Chinese Medicine Minerals Based on Traditional Chinese Pharmacology

There are many ways of classification in TCM minerals. Because it is essentially a mineral, it should be classified from two aspects of pharmacy and mineralogy. In terms of traditional Chinese medicine, according to the different sources, processing methods and raw material properties of mineral drugs, mineral drugs were divided into three types: natural minerals with medicinal value, mineral processed products and mineral pharmaceutical preparations. Among them, natural minerals such as cinnabar, gypsum, realgar, fossils of animals or animal bones (keels, stone swallows), and amber. The processed products of minerals include light powder, red powder, alum and so on. mineral pharmaceutical preparations include xiaolingdan, baihu decotion, Huanglong pills, etc. [5, 6].

Then according to the clinical function be divided into five types: sedation and tranquility, hemostatic, antidote, pesticide and other [7]. The author refers the classification of mineral drugs in Traditional Chinese pharmacology [8], and classifies them from the perspectives of efficacy (Table 1).

Table 1. *Classification of Mineral Drugs Based on Pharmacological Action.*

Pharmacological action		Mineral medicine	Clinical role
Diaphoretic Drug	wind-cold-dispersing	Gypsum	relax muscles and promote sweating, it is used to disperse exterior evils and relieve exterior symptoms. Most of them are products of pungent powder, which has the characteristics of pungent powder, rising and floating, walking and dredging.
Antipyretics Drug	heat-clearing and fire-purging liver-clearing and eyesight heat clearing antipyretic-detoxicate heat-clearing and dampnessdrying asthenic-fever clearing	Gypsum, Hanshuishi, Calcite Azurite, Marcylite Halite Orpiment, Sulphur, Maifanite, Amber Gypsum, Anhydrite, Orpiment, Arsenopyrite	The property of the medicine is cold, mainly used for febris, dysentery, carbuncles and sores, redness, sore throat and other symptoms.
Diarrhea Drug	offensive drugs lubricant purgation potentpur gatives for elimination of retained body fluid	Anhydrous Sodium Sulfate, Mirabilite	The main function is to defecate, clear heat and reduce fire and edema, so as to exclude the intestinal food stagnation, dry stool and subside edema.
Water and Dampness-eliminating Drug		Talc, Saltpeter	It can facilitate urination, eliminate the pathogenic factors of water and dampness in the body, relieve various diseases caused by water and dampness retention.
Damp Dispersing Drug		Chalcanthite	It is suitable for dampness obstructing spleen-stomach, body burnout, abdominal distension and tightness, mouth sweet and salivating tongue coating white greasy and other symptoms.
Antirheumatic Drug		Realgar, Orpiment	It is suitable for rheumatism arthralgia, limb adverse, acid numbness and weakness of waist and knee.

Pharmacological action		Mineral medicine	Clinical role
Qi-regulating Drug		Maifanite	It is suitable for spleen and stomach qi stagnation, chest qi stagnation, chest pain, liver qi stagnation, hypochondrium distending pain, breast pain or lump, irregular menstruation.
Invigorating Blood Circulation and Eliminating Stasis Drug		Pyrite, Ophicalcitum	It should be applied to chest pain caused by blood stasis, rheumatic arthralgia, sore swelling and pain caused by falling pain, irregular menstruation, menstruation, dysmenorrhea, postpartum stasis and abdominal pain.
Hemostatic Drug		Halloysite, Kaolin, Hydromuscovite	Hemostatic is mainly used in various parts of the bleeding syndrome, such as hemoptysis, bleeding, hematemesis, urinary bleeding, bloody stool, purpura, traumatic bleeding, collapse and leakage.
Digestive Drug		Green vitriol, Salammoniac, Halitum Purpureum, Pyrolusite	Digestive drug is mainly used for abdominal distension, nausea and vomiting, regardless of diet, diarrhea or constipation.
Anthelmintic Drug		Borax, Azurite	The insecticide drug can remove or kill parasites in the intestine.
Expectorant Cough Suppressant and Snti-asthmatic Drug	warming and resolving cold-phlegm	Stalactite, Sulphur	Phlegm drug can be used not only for cough and asthma caused by phlegm, but also for gall tumor, epilepsy and convulsions.
	clearing away heat to resolve phlegm	Chloriteschist, Pumice	
	relieving cough and asthma	Malachite, Galena, Stalactite	
Cold-expelling Drug		Maifanite, Hanshuishi	It can dispel coldness, for the treatment of cold syndrome.
Resuscitation Drug			It is good at walking, opening and closing the orifices, awakening consciousness. It is mainly suitable for fever and coma, as well as convulsion, epilepsy, stroke and other diseases.
Drug for suppressing hyperactive liver for calming endogenous wind		Fluorite, Quartz, Hematite, Fossil	It is suitable for hyperactivity of liver yang, dizziness of head and eye, liver-wind stirring and convulsion.
Sedative Drug	zhongzhen anshen	Magnet, Cinnabar, Amber, Margarita, Native Gold, Native silver, Vermiculite, Selenite	Sedative Drug is suitable for yang-energy agitation, palpitation, insomnia, convulsive epilepsy and irritability.
Tonic Drug	yangxin anshen		Tonic drug is mainly used for asthenia, with the effect of tonifying deficiency and strengthening weakness, and function in the treatment of human deficiency.
	energen-invigorating drugs	Asbestos	
	yang-tonifying		
	blood nourishing	Stalactite	
	nourishing yin	Hematite, Ophicalcitum	
Astringent Drug		Red Halloysite, Limonite, Alum	It can treat all kinds of spondylolisthesis, with astringent sweats, antidiarrheal, solid essence, reduce stool, hemostasis, cough and other effects.

2.2. Classification of Traditional Chinese Medicine Minerals Based on Mineralogy

From the perspective of mineralogy, the classification method of gold, jade, stone and halogen in Li Shizhen 's Compendium of Materia Medica in Ming Dynasty is the earliest classification form of mineral drugs, which lays the foundation for the classification of modern mineral medicines [9]. There are three main types of traditional mineralogy classification: geochemical classification based on the geochemical properties of elements in minerals; genetic classification based on occurrence and formation conditions of minerals; classification based on crystal chemistry [10]. Since the chemical composition of mineral drugs contain trace elements to ensure the normal operation of human mechanism, most of literatures on the pharmacological effects of mineral drugs are also mostly based on their chemical constituents. Classification on chemical constituents of mineral drugs can effectively study their pharmacological effects. Combined with the literature and the illustrated handbook of Chinese Mineral Medicine [11], the main cationic species of mineral drugs mainly were divided into: silicon compound, calcium compounds, sodium compound, mercury and its compound, arsenic compound, aluminum compound, copper and its compound, iron and its compound, lead compound, etc. (Table 2) [12].

Table 2. *Classification of Mineral Drugs Based on Chemical Composition.*

Compound	Mineral medicine	Pharmacological effects and mechanism
Silicon compound	Quartz, Agate, Chlorite-schist, Vermiculite, Actinolite, Pumice, Talc, Asbestos	Talc, quartz, for example, are silicate minerals, talc $Mg_3[Si_4O_{10}](OH)_2$ has a protective effect on skin mucosa and antibacterial. Quartz SiO_2 has sedative, antitussive and antiasthmatic effects [12].
Calcium compound	Gypsum, Feldspar, Calcite, Dolonite,, keel	Calcium-containing mineral drug is mainly composed of oxides, carbonates and calcium fluoride. The drug has anticonvulsant and soothing effects, which are clinically used for epilepsy mania [12].

Compound	Mineral medicine	Pharmacological effects and mechanism
Sodium compound	Halite, Mirabilite, Anhydrous sodium sulfate, Borax, Saltpeter	It can reduce local leukocyte infiltration, regulate body immunity and prevent postoperative infection. Mirabilite is sodium sulfate containing water, it has anti-inflammatory and laxative effects, and borax has anticorrosion and anticonvulsant effects [12].
Arsenic compound	White arsenic, Arsenolite, Realgar Orpiment, Arsenopyrite	Arsenic is toxic and has high medical value. Realgar mainly contains arsenic sulfide, it has antibacterial effect and resistance to schistosomes [12, 13].
Mercury and its compound	Cinnabar, Mercurous chloride	Mercury dissociates and reacts with biological molecules such as amino acids to form complexes with strong physiological activity and low toxicity. Such as cinnabar can act on the central nervous system, with hypnotic, brain protection, effects [12].
Aluminum compound	Alum, Kaolin, Red halloysite, Hydromuscovite	Alum and red halloysite are commonly used in clinical practice. Alum is mainly used for external use to treat various skin diseases and inflammation. Alum and red halloysite can treat enteritis and other diseases [14].
Copper and its compound	Malachite, Azurite, Chalcanthite, Marcylite	Cu has a certain effect on cardiovascular, bone marrow, central nervous system and erythropoiesis. $CuSO_4 \cdot 5H_2O$ is the main component of sulfur compounds and has good antibacterial effect. For example, azurite and marcylite [12, 15].
Iron and its compound	Magnet, Hematite, Limonite, Limonite nodule, Pyrite, Fibroferrite	Fe is the most abundant and important hematopoietic element in human body. Iron-containing drugs mainly exist in the form of iron sulfide, iron element, iron oxide or iron sulfate. The mineral is clinically used for iron deficiency anemia, treatment of convulsions, swelling toxins. Mineral drugs have magnetite, hematite, natural copper, etc. [12].
Lead and its compound	Minium, Galena	Pb has high toxicity, which is mainly used for external use as a common basic raw material for surgery. Minium is rarely used alone in clinical practice. It is often compatible with other TCM and plays a great role in detoxification [16].
Au, Ag	Native gold, Native silver	Au and Ag are toxic to some extent and should be paid attention to in clinical application.
Others	Sulphur, Amber, Hanshuishi, Sal ammoniac, Pyrolusite, Calamine, Fluorite, Maifanite	Amber is an organic substance, which can calm panic, blood stasis, diuretic. Maifanite stone is commonly used as health care products.

3. Application of Spectroscopy Technology in TCM Minerals

Nowadays, the qualitative and quantitative research on mineral drugs has become a research hotspot owing to the imperfect standard system of mineral drugs. Compared with botanical medicine and animal medicine, the chemical structure of mineral medicine is simple, but mineral drugs have similar appearance and many common associated minerals [17]. In addition, their name and usage are slightly different in different times, resulting in the phenomenon that mineral drugs have many names, which increases the difficulty of mineral drug identification and quality inspection. At present, the research on mineral drugs is relatively weak, and the quality standards need to be improved. Traditional identification methods and modern analytical techniques (Infrared spectroscopy, Raman spectroscopy, and X-ray diffraction) should be studied in the identification, quality control, determination and quantitative analysis of mineral drugs.

3.1. Infrared Spectroscopy Test and Identification of Mineral Medicine

As a new analytical method, Infrared spectroscopy has distinct characteristics: it does not damage the sample, does not damage the overall unity of the four flavors and five tastes of single Chinese medicine, and does not damage the compatibility integrity of the prescription; less preprocessing can reduce the factors that cause the detection error; rapid and effective detection to ensure the quality of traditional Chinese medicine production process and provide new technology for rapid detection; strong characteristic, which can enrich the chemical components with difference. In the later stage, the spectral fingerprint, first derivative spectroscopy, second derivative spectrum and two-dimensional spectrum get more results for solving the complexity and similarity of Chinese medicinal materials [18].

3.1.1. Near Infrared Spectroscopy

Near infrared light (NIR) is an electromagnetic wave between visible light (VIS) and medium infrared light (MIR). ASTM defines its wavelength at 780~2526 nm [19]. Near infrared spectroscopy has the advantages of simple operation and fast analysis, and has been widely used in agriculture [20], chemical industry [21], food [22] and medical examination [23]. The application research in the field of analysis of traditional Chinese medicine minerals is also gradually carried out [23-32]. In recent years, there have been many reports on the research of near-infrared spectroscopy in the field of traditional Chinese medicine minerals. Chen et al. (2016) tested and analyzed the NIR characteristic spectral bands of 51 common mineral drugs with different anion types, proving that most mineral drugs have their typical NIR characteristic spectral bands. Based on the characteristic NIR spectral band, the characteristics of mineral drugs from different origins, raw and forging products, genuine and counterfeit goods can be identified, providing a scientific basis for the rapid identification of mineral drugs by NIR [17]. Song et al. (2019) collected the near infrared spectrum of borax samples, calculated the correlation coefficient between the sample spectrum and the reference spectroscopy with the first derivative as the pretreatment method, and carried out qualitative analysis. The partial least squares (PLS) method was used to establish the quantitative analysis model, which provided a new rapid analysis method for the quality control of borax [24]. In addition, in the determination and analysis of similar components in mineral drugs, Yuan et al. (2014) used NIR combined with OPUS

chemical software, with ethylenediaminetetraacetic acid titration (EDTA) method as a reference, and used partial least squares method to establish quantitative analysis models for $CaCO_3$ of eight kinds of mineral drugs, including calcite, calamine, stone flower, fossil crab, spirifer's fossil shell, stalactite, yellow croaker earstone and tubular stalactite. The results showed that NIR quantitative model could be used to rapidly determine the content of $CaCO_3$ in TCM minerals [25]. But this method has large error and complicated operation, the indicator discoloration and titration end point are susceptible to subjective factors. Through literature research, it is found that near-infrared quantitative analysis technology has broad application prospects for the study of mineral drugs, and the research range and content have been expanded. However, it is also found in the study that NIR technology still has shortcomings. For example, (1) there is a lack of operational standards that cannot provide data support for NIR modeling; (2) The source of mineral drug is complex, and it is difficult to obtain samples that can represent the characteristics of all samples for NIR modeling because the composition and property characteristics of the same medicinal material from different origins vary widely; (3) The research on the processing and preservation of medicinal mineral materials is relatively blank; (4) The NIR characteristic spectroscopy of some mineral drugs is not obvious, which is not suitable for variety identification with NIR [17, 23].

3.1.2. Mid-infrared Spectroscopy

The wavelength range of mid-infrared spectroscopy is 250~5000nm, and the wavenumber range is 4000~400cm^{-1}. Generally, the wavelength range of mid-infrared spectrum is used for most infrared spectrum test. Because of the advantages of fast analysis speed, simultaneous analysis of various components, nonpolluting analysis and no special pretreatment of samples, it has indispensable applications in medical, geological and mineral products, materials and other fields.

Yan et al. (2015) identified different sulfate minerals by mid-infrared spectroscopy. The sulfate specific SO_4^{2-} of sulfate minerals can be seen at 1200-400 cm^{-1}. In addition, due to the formation principle and the peak shape, peak number and transmittance of cations is different, it is effective that different types of sulfate mineral drugs are distinguished by infrared spectroscopy. The infrared derivative spectra of Xuanming powder and anhydrous sodium sulfate are different, providing reference for the quality control [26]. Li et al. (2014) used FTIR to compare seven kinds of calcium carbonate medicinal materials. It is concluded that the infrared spectra of pearl, nacre and abalone shell is similar, the infrared spectra of stalactite and oyster is similar, and the infrared spectra of stamen and keel is obviously different, which can be distinguished from other medicinal materials. It provides a reference for the identification and differentiation of carbonate mineral drugs [27]. Chen et al. (2011) used Infrared spectroscopy to analyze 29 batches of samples from different origins. Finally, it was concluded that there were differences in the 3618cm^{-1} and 3695cm^{-1} infrared spectra waves of different sources of red halloysite, so as to effectively distinguish red halloysite and kaolinite [28]. Cao et al. (1990) determined infrared spectra of more than 280 samples of 95 kinds of mineral medicines, and indicated that infrared spectroscopy could be popularized as a new method for the identification of mineral medicines [29].

3.2. Raman Spectroscopy Test and Identification of Mineral Medicines

Raman spectroscopy can reflect the internal information of molecules, which is used to reflect the structural characteristics of a single or mixture system, and has its unique role in the qualitative analysis and identification of substances [30]. Raman spectroscopy was used for non-destructive testing to make up for the absorption peaks or very weak peaks that were not shown in the infrared spectrum.

Zhang et al. (2001) studied the pearl layer and pearl of the main pearl oyster (mussel) shells in China by laser Raman spectroscopy. From the characteristic Raman spectroscopy, it was concluded that the organic matter in the pearl layer and pearl of the pearl oyster shell originated from the formation of aragonite structure, and the Raman peak of complex organic matter was detected in the pearl layer of Pteria penguin, so it was deduced that the organic matter was the main reason for the color of Pteria penguin and pearl layer [31]. Lei et al. (2016) used Raman spectroscopy to test six kinds of sulfate-containing mineral medicines and gypsum processed products, and combined with OPUS software to summarize and analyze the characteristic spectral lines of mineral drugs, so as to qualitatively identify sulfate-containing mineral drugs, reflect the differences before and after processing of mineral drugs, and lay the foundation for the application of Raman spectroscopy in the analysis of mineral drugs [32]. In addition, Raman spectroscopy can be used for supplementary test and analysis of some mineral drugs (such as quartz, cinnabar, realgar) that have no response to infrared spectroscopy or are affected by large adsorption water [17].

Infrared spectroscopy and Raman spectroscopy are emerging nondestructive rapid analysis techniques for mineral and medicinal materials. They are simple, economical and practical, but there are also some defects. For Raman spectroscopy, the characteristic peaks are sharp and strong, and the response to water is weak, when the sample with deep color is tested, the fluorescence interference is strong and the map effect is poor. However, the Infrared spectroscopy is mostly characterized by wide peaks and strong response to water, which is not significantly affected by the sample color [17]. Combining the test results of the two methods with complementary advantages can systematically identify mineral drugs, which provides a new direction for the authenticity identification, qualitative and quantitative analysis and quality control of mineral drugs.

3.3. Infrared and Raman Spectral Data Information of Samples from TCM Minerals Database

Based on the importance of Infrared and Raman spectroscopy in the identification of mineral drugs. By

referring to the RRUFF database of California, the database of traditional Chinese medicine minerals innovatively and systematically tests and collects the Infrared and Raman spectra of mineral medicine samples, and analyzes the composition and structure of the samples, so as to realize the rapid and nondestructive identification of mineral medicines, provide available and referenced Infrared and Raman data (Figures 1, 2) for professionals engaged in this field, and further realize the perfect combination of traditional Chinese medicine culture connotation and modern detection methods.

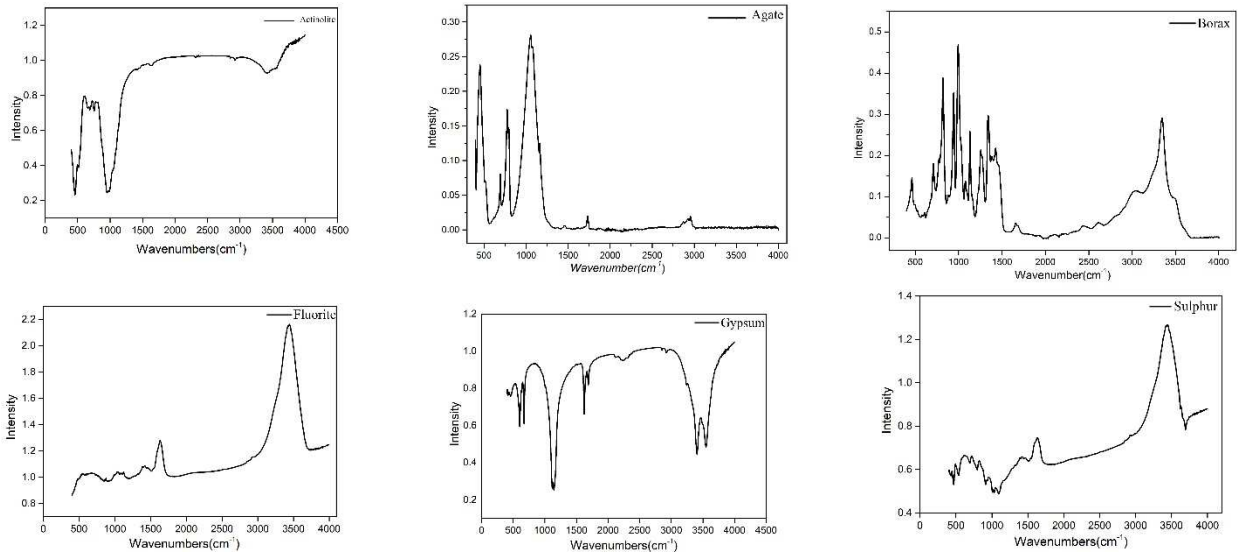


Figure 1. *Infrared Spectrogram of Some Mineral Drugs in Database.*

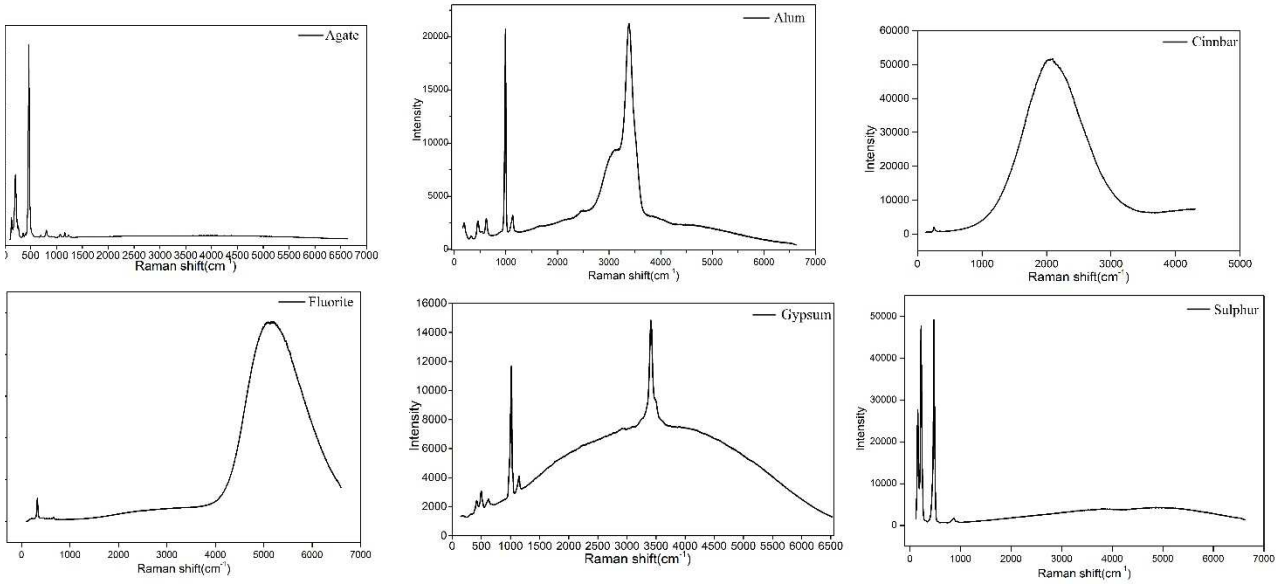


Figure 2. *Raman Spectrogram of Some Mineral Drugs in Database.*

4. Application and Practice of TCM Minerals Database

4.1. Structure and Design of TCM Minerals Database

The Database of Traditional Chinese Medicine Minerals system is mainly composed of business layer and user layer [33].

The business layer is composed of front-end website and back-end database management system of traditional Chinese medicine minerals. The most popular back-end separation technology architecture (Vue, Element+ SpringBoot, Mybatis, Mysql) is used to develop and construct. Background management system mainly realizes the input and management of traditional Chinese medicine mineral data, and provides external data access interface; the front-end website is deployed by Nginx, and the web publishing and sharing of traditional Chinese medicine mineral data are realized by linking the back-end interface.

The user layer is part of the sharing function of database resources that enables all types of users of the platform to obtain the required data through the browser, such as get the

specimen information, obtaining the spectrum information, and understanding the relevant knowledge of traditional Chinese medicine minerals.

Figure 3. *Homepage of traditional Chinese Medicine Minerals Database.*

4.2. Introduction of Database Home Page

Traditional Chinese medicine minerals database is divided into six parts: database overview, mineral information index, mineral pictures, mineral classification, historical allusions and related information. Classification of traditional Chinese medicine minerals are divided into oral use, external use and health care three parts according to their medicinal effects and made into a classification tree. Traditional Chinese medicine mineral historical allusions are displayed on the front page as popular science articles. 55 pictures of fine traditional Chinese medicine minerals [34, 35] were collected on the home page of the database. The information page on mineral details of traditional Chinese medicine minerals contains pharmaceutical properties, mineral information characteristics, typical spectral data and so on (Figure 3).

4.3. Specimen Information and Source of the Database

According to the relevant literature, Chinese Pharmacopoeia 2020 and related websites, a total of 52 kinds of Chinese medicine minerals and 3 kinds of Chinese medicine rock data are recorded and collected in the database of traditional Chinese medicine minerals. The specimen information is mainly composed of medicinal properties, mineralogical properties and spectral information.

The pharmacal properties of traditional Chinese medicine minerals include their medicinal properties, chemical constituents, physical properties, and the Infrared spectroscopy and Raman spectroscopy data commonly used as standard reference for rapid analysis of mineral composition and purity by quality inspection institutions. The data of 16963 physical specimens of traditional Chinese medicine minerals from different sources are included, which provides professional knowledge, rapid identification methods and data of traditional Chinese medicine minerals for practitioners, improves the public's understanding of traditional Chinese medicine minerals, and inherits and develops traditional Chinese medicine culture.

4.3.1. Common Specification for Description of TCM Mineral Specimen Resources

The common description specification stipulates that the common information of rock and mineral specimens of traditional Chinese medicine should have passport information, medicinal properties and mineralogical properties, including 50 data items. Based on this, the common information table of rock and mineral specimens of traditional Chinese medicine is formulated as the input standard of specimen data in database [33].

Data items of Common information are as follows:

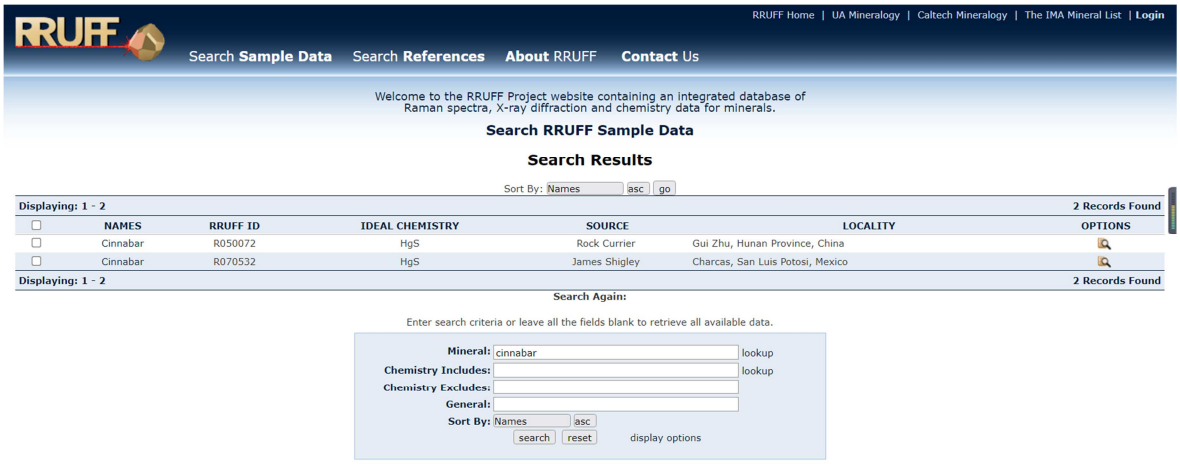
1. Passport information: medicinal name, other names, English name, medicinal type, mineral type.
2. Pharmaceutical properties: taste and meridian distribution, features of decoction pieces, pharmacological effects, efficacy and Indications, dosage and usage, processing methods, precautions.
3. Chemical properties: chemical formula, chemical composition.
4. Crystallographic properties: crystal morphology, crystal system, crystal type, symmetry symbol, space group, lattice parameter a0/b0/c0/z, cell parameter α/β/γ, X-ray powder diffraction, crystal structure.
5. Optical properties: color, luster, transparency, streak, polychromatism, dispersion, refractive index, axial and light character, reflectivity.
6. Mechanical properties: hardness, relative density, cleavage, fracture, brittleness, flexibility, elasticity.
7. Genetic occurrence and associated minerals: genetic occurrence, associated minerals.

8. Spectral information: Infrared spectroscopy, Raman spectroscopy.
9. Typical specimens.
10. References.

4.3.2. Typical Specimen Sources

Based on the National Infrastructure of Mineral Rock and Fossil Resources for Science and Technology and RRUFF database of the University of California (Figure 4), 16963 samples of traditional Chinese medicine minerals from different origins were included in the database. The Infrared spectroscopy and Raman spectroscopy of mineral samples with uniform composition were analyzed in the National Infrastructure of Mineral Rock and Fossil Resources for Science and Technology [35, 36].

(a)



(b)

Figure 4. *National Infrastructure of Mineral Rock and Fossil Resource for Science and Technology (a), RRUFF Database of University of California (b).*

4.4. Historical Allusions and Related Information of Traditional Chinese Medicine Minerals

The mineral historical allusion section of traditional Chinese medicine shows five mineral historical allusions with high importance and familiarity. Such as dragon's bone, Lead oxide, danqiushi, alum, sulfur (Figure 5).

Relevant information section shows the national current affairs of traditional Chinese medicine (Figure 5), such as the relevant interpretation of White Paper, the relevant measures for the development of traditional Chinese medicine, and the international exchange of traditional Chinese medicine.

Users can enter the historical allusions and related information section through the home page to understand the relevant knowledge of traditional Chinese medicine minerals and national policies, so as to have a deeper understanding of traditional Chinese medicine minerals.

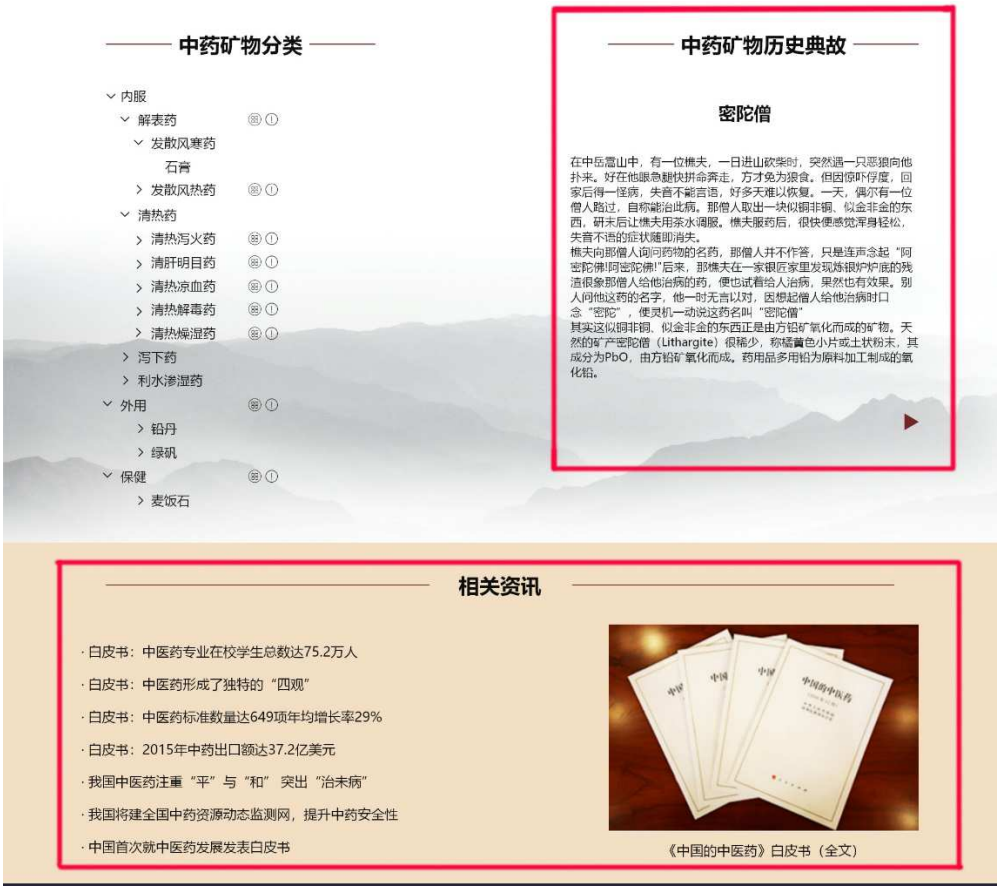


Figure 5. *Historical allusions and related information sections.*

4.5. Detail Information of Database Specimen — A Case Study of Cinnabar (Chen Sha)

Taking the common Chinese medicine mineral around us—cinnabar (Chensha) as an example there are many ways to query the detailed information of the Chinese medicine mineral on the front page of the website.

Users can directly search the mineral name, medicinal name or English name of the mineral drug in the search box, and can also choose to enter the mineral details page from the mineral classification tree of traditional Chinese medicine (Figure 6).

Cinnabar [8, 10, 11, 37, 38]: also called zhusha and dansha in traditional Chinese medicine.

Pharmacological characteristics: clear heart and calm mind detoxification. It is suitable for palpitations, insomnia, dreaminess, epilepsy, infantile convulsions, blurred vision, sore mouth, sore throat, sore swelling poison.

Species Study: In the ancient Chinese pharmacy masterpiece Kai Bao Ben Cao also marked: Cinnabar, from Chenzhou, Jinzhou, the highest medicinal value, followed by other effects.

Chemical Properties: the main chemical composition is mercury sulfide (HgS), the natural ore.

Crystallographic Characteristics: red, adamantine to metallic luster, belongs to trigonal crystal system, and it is homogeneous polymorphism with the black cinnabar of isometric system, shape of rhombohedron and short prismatic, penetrate twin, aggregates are granular or massive.

Optical Properties: bright red or dark red, color of containing impurities is brown red. Strips is red to brown, glossy, the pure cinnabar is gold luster.

Mechanical properties: Mohs hardness is 2.5, density is 8.10. Good cleavage with parallel cylindrical surface.

Genetic occurrence and associated minerals: occurring in limestone, slate and sandstone. The name of Chensha comes

directly from its origin-Chenzhou (now Yuanling, Hunan), which is the earliest place to discover Chensha in China. Tongren in Guizhou, Chenxi, Yuanling and Mayang in Hunan are the main producing areas of Chensha. In addition, Sichuan and Guangxi are also produced. Chensha is a typical low-temperature hydrothermal mineral, and its genesis is related to modern volcanism. China is the main producing country of Chensha, mainly from Xinhuang in Hunan and Tongren in Guizhou.

Typical specimens: a total of 340 specimens.

Spectroscopic data: infrared spectroscopy, Raman spectroscopy (download).

Figure 6. *The detailed page of traditional Chinese medicine mineral.*

5. Conclusion

This paper introduces the classification of traditional Chinese medicine minerals, the platform design of traditional Chinese medicine mineral database, and the advantages of Infrared and Raman spectroscopy in identifying mineral drugs. Due to the proposal of "Healthy China" strategy and COVID-19's unexpected attack, the thousands of years of TCM thinking concept of "preventing disease" and the experience of fighting "epidemic", once again show its unique cultural charm and medical value to the world. The construction of TCM minerals database is the result of urgent development of TCM minerals under big data. Facing the new situation and new requirements of database development, the construction of traditional Chinese medicine minerals database still needs to be further improved and perfected, mainly from the following three aspects.

5.1. Inheritance of TCM Culture

Traditional Chinese medicine embodies profound philosophical wisdom and thousands of years of health concept and practical experience of the Chinese nation. Chinese medicine as a treasure in the cultural treasure, it is significant to protect, inherit and spread TCM thought, culture and concept, especially don 't forget mineral medicine is one of the TCM. The Traditional Chinese Medicine Minerals Database has sorted out the precious wealth of predecessors and carried out an orderly induction, aiming to promote human cognition and future innovation of traditional Chinese medicine minerals, improve the public's understanding of traditional Chinese medicine minerals, make every effort to inherit and carry forward the culture of traditional Chinese medicine, and finally strive to construct a database of traditional Chinese medicine minerals that integrates science popularization, publicity and interdisciplinary integration.

5.2. Promoting Interdisciplinary Integration of TCM and Mineralogy

The medicinal mineralogy is a new frontier subject with mineral medicinal materials and medical mineral raw materials as the research object [39]. Mineral drugs are the interdisciplinary integration of traditional Chinese medicine and mineralogy, and also an important part of TCM culture. Because mineral resources are widespread and have unique curative effects, the development of medicinal mineralogy is experiencing an unprecedented opportunity, standardizing the classification of mineral drugs and providing the identification evidence are still needed to be studied. Besides, promoting the interdisciplinary integration of TCM and mineralogy, and realizing the combination of traditional Chinese medicine culture connotation and modern detection methods still needs a lot of exploration.

5.3. Improving the Relevant Content of TCM Minerals Database

With the rapid development and application of big data and artificial intelligence, the application of new information technology in pharmaceutical mineralogy and the use of mathematical models to solve more pharmaceutical mineralogy problems have become one of the many methods of medicine, geology and mineralogy. The construction of database is to apply information technology to the integration, management and sharing of mineral drug specimen resources [40]. The database of traditional Chinese medicine minerals is still in the initial stage of exploration. In order to promote the

protection and sharing of mineral specimen resources of TCM and improve the utilization rate of existing resources, it is necessary to further improve the content of the database, deepen technical means and increase its popularization of science. The standardization, digitization and networking of collection, collation, preservation and utilization of mineral specimen resources of traditional Chinese medicines are needed to realized. TCM Minerals database will further provide strong scientific and technological support for scientific research, scientific and technological innovation, professional teaching and scientific popularization in the field of pharmaceutical mineralogy.

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