

# CPMCP: a database of Chinese patent medicine and compound prescription

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## Abstract

Although several traditional Chinese medicine (TCM)-related databases have emerged, they focus on researching single medicinal materials, which is far from sufficient for clinical research and application. In comparison, compound prescriptions are more informative and meaningful in TCM, for they embody the information on the compatibility of TCM besides the relatively isolated information about single medicinal materials. The compatibility information is essential in TCM because it conveys not only what components are involved to treat special diseases but also how to combine these single medical materials. We established a database of Chinese patent medicine and compound prescription (CPMCP). It demonstrates the prescription information of Chinese patent medicines (CPMs) and ancient Chinese medicine prescriptions (CMPs). CPMCP reports their comprehensive and standardized information such as the components, indications and contraindications. It is worth mentioning that we organized relevant experts and spent lots of time manually mapping the functions of compound prescriptions in ancient Chinese to the standardized TCM symptom vocabularies, obtaining a total of 71 414 associations between compound prescriptions and TCM symptoms. In this way, CPMCP established the associations between TCM and modern medicine (MM) according to the associations between TCM symptoms and MM symptoms. In addition, to further exhibit the compatibility mechanism of compound prescriptions, CPMCP summarizes a set of common drug combination principles by analyzing the existing prescriptions. We believe that CPMCP can promote the modernization of TCM and make greater contributions to MM.

Database URL: <http://cpmcp.top>

### Key points

- Chinese patent medicine and compound prescription (CPMCP) is an online database for traditional Chinese medicine (TCM).
- CPMCP promotes the modernization of TCM.
- CPMCP helps to reveal the compatibility mechanism of compound prescriptions.

## Introduction

Traditional Chinese medicine (TCM) is an empirical science summed up by ancient Chinese based on thousands of

years of clinical experience (1–3). Today, TCM still plays an irreplaceable role in maintaining the daily health of Chinese people (4). The doctors of TCM treat diseases by using natural medicinal materials (i.e. natural herbs, animals or minerals) (5, 6). For example, *Artemisia annua* was widely used to treat malaria in ancient China. In 1972, Tu *et al.* successfully extracted artemisinin (C<sub>15</sub>H<sub>22</sub>O<sub>5</sub>), a colorless crystal, from *A. annua* (7). It was confirmed that artemisinin is the main active ingredient in *A. annua* for the treatment of malaria. This infers that TCM and modern medicine (MM) share the same theoretical basis at the molecular level. That is, compounds treat diseases by regulating the activity of molecular targets (8–10). However, treating disease with a single natural material may cause serious side effects due to the complex ingredients of that material (11). Therefore, Chinese medicine practitioners try to treat diseases by flexibly combining a

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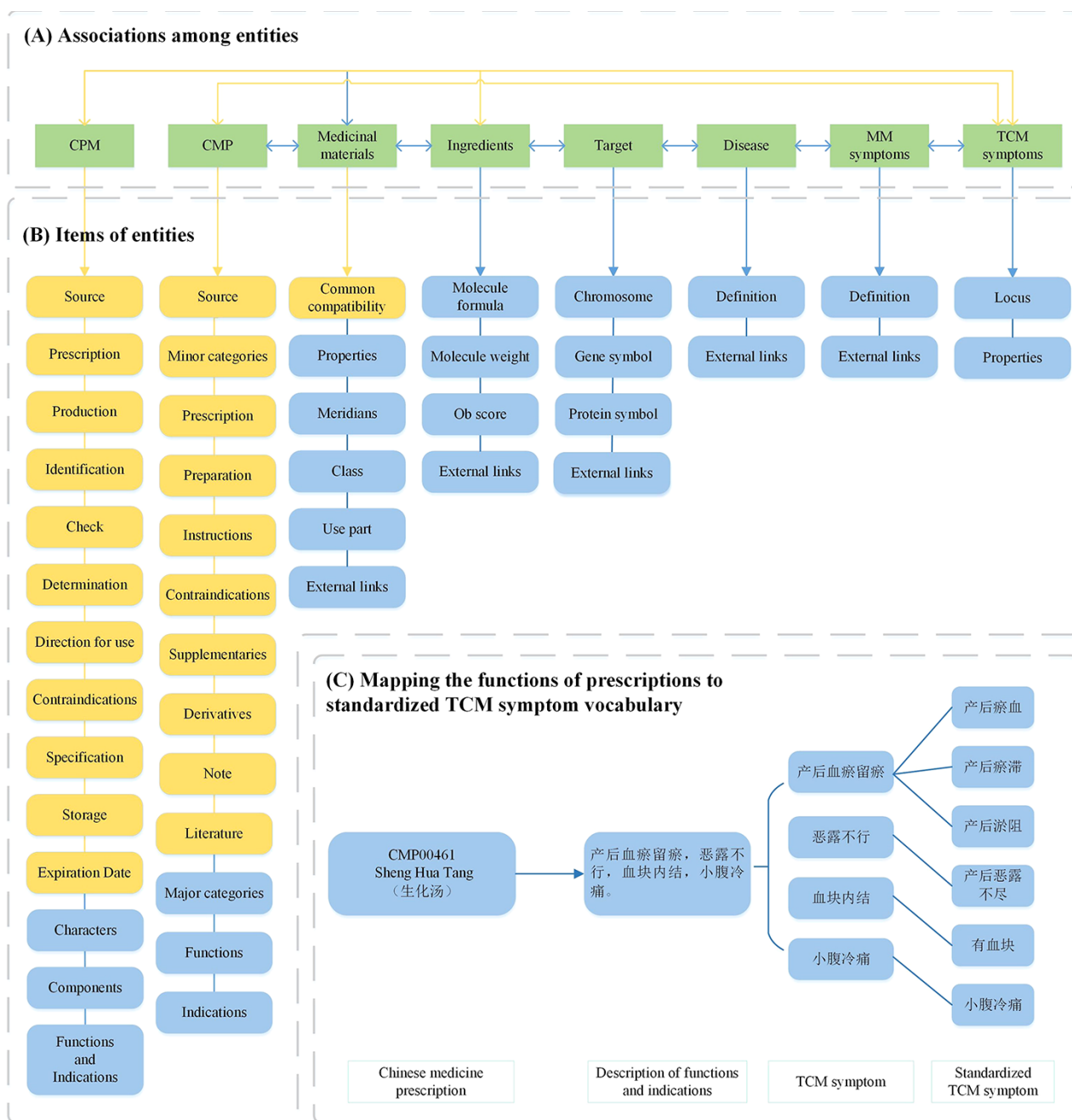
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variety of natural medicines to form compound prescriptions (8). For example, the alkaloids in *Pinellia* (a natural herb) can treat hiccups and belching. However, taking unprocessed *Pinellia* orally will inhibit the secretion and release of PGE2, a protective mediator of the gastric mucosa, thereby injuring the gastric mucosa (which can be seemed as the side-effect of *Pinellia*). Ginger, another herb for treating hiccups and belching, can effectively antagonize the inhibition of *Pinellia* to protect the gastric mucosa with its active ingredient, 6-gingerol. Therefore, TCM practitioners try to combine *Pinellia* and

ginger, which not only can enhance the curative effect of the herbs but also can alleviate the side effects caused by *Pinellia* (12, 13). The compound prescription has the characteristics of multicomponent, multi-approach and multi-target. Multiple components in the prescription can act synergistically on multiple targets and regulate different signal pathways, thereby treating complex diseases.

Since 2019, the novel coronavirus (severe acute respiratory syndrome coronavirus 2), which broke out in more than 200 countries, has caused the novel coronavirus disease



**Figure 1.** Information and relationships of entities in CPMCP. Boxes and lines with highlights refer to the novel information and functions in CPMCP compared with other available TCM-related databases, including SymMap, ETCM and HERB. (A) Relationships between the entities in CPMCP. (B) Details of entities. (C) Example to show how to construct the association between a compound prescription and standardized TCM symptom vocabularies.

**Table 1.** Number and sources of various entities in CPMCP

Entities	Number	Source
CPMs	1469	Compendium of National Standards for Chinese Patent Medicines
CMPs	656	Various Chinese Medicine Works
Medicinal materials	1557	Chinese Pharmacopoeia
Ingredients	26 341	TCMID, TCMSP, and TCM-ID
Targets	20 965	HIT and TCMSP
Diseases	14 086	OMIM and Orphanet
MM symptom	1148	MeSH, SIDER, and Unified Medical Language System (UMLS)
TCM symptoms	2285	Chinese Pharmacopoeia, Research on the Standardization of TCM Terminology, and Pathology Terminology Standardization

(COVID-19), a highly contagious and pathogenic viral pneumonia (14). Up to now, there are still no related specific medicines developed in the world. However, several TCM compounds have been proven to be effective in relieving the symptoms and pain of patients with COVID-19. In the COVID-19 diagnosis and treatment plan (trial version 7) of China, Qingfei Paidu Decoction (QPD) is used in the clinical treatment of mild, routine and severe patients. Zhao *et al.* analyzed the mechanism of QPD in the treatment of COVID-19 from the perspective of network pharmacology. QPD can be used as an antiviral agent to inhibit the translation of

viral messenger RNA by targeting ribosomal proteins which are necessary for viral replication (15). Xu *et al.* believe that the main active ingredients in QPD against COVID-19 are quercetin, luteolin, kaempferol, naringin and isorhynchon (16). These five components can regulate COVID-19-related targets such as Mitogen-activated protein kinase 1 (MAPK1) and interleukin-6 and signaling pathways such as tumor necrosis factor and NF-kappa-B through compound-target interactions. Through interaction, these components can inhibit the inflammatory response, regulate immune function, reduce lung damage and thus treat COVID-19. Yao *et al.* also found that the main active components of QPD are well binding to targets such as RNA-dependent RNA polymerase (RdRp) and Papain Like protease (PLpr), thereby regulating a variety of related signaling pathways to treat symptoms such as fever and cough caused by COVID-19 (17). These works suggest that TCM is an important and effective medical science that can provide an important reference for the development and improvement of MM.

In recent years, several online databases related to TCM have emerged, such as HIT (18), TCMID (10), SymMap (19) and HERB (20). They reported the active components and targets of natural medicine and try to associate them with modern diseases. However, these works focus on a single medicinal material, ignoring the more clinically valuable TCM compound prescriptions.

In light of the above facts and to further facilitate clinical research and application, we established a database

**Figure 2.** Home page of CPMCP.

of Chinese patent medicine and compound prescription (CPMCP). It reports the prescription information of Chinese patent medicines (CPMs) and ancient Chinese medicine prescriptions (CMPs), including comprehensive and standardized information such as the combination of medicinal materials, indications and contraindications (the detailed and innovative information of CPMCP is shown in Figure 1A and B). Due to the relevant descriptions of prescriptions being recorded in ancient Chinese, we have organized relevant experts to manually map and verify the functions and indications of prescriptions to 2285 standardized TCM symptom vocabulary (as shown in Figure 1C), obtaining a total of 71 414 associations between compound prescriptions and TCM symptoms. In this way, CPMCP establishes the associations between TCM and MM according to the associations between TCM symptoms and MM symptoms. Finally, CPMCP reports the relevant information of eight categories of entities collected from different data sources, including (i) CPMs, (ii) ancient CMPs, (iii) natural medicinal materials, (iv) chemical ingredients, (v) targets, (vi) diseases, (vii) TCM symptoms and (viii) MM symptoms. The associations between these entities are also reported in our database (as shown in Figure 1A). The number and sources of various entities in CPMCP are shown in Table 1.

Since TCM prescriptions involve the use of a variety of medicinal materials, the compatibility mechanism between medicinal materials is important (21). CPMCP summarizes a set of common drug combination principles by analyzing the combination of medicinal materials in existing prescriptions. We believe that CPMCP can promote the modernization of TCM and make greater contributions to MM.

## Materials and Methods

### Tool implementation and usage

CPMCP is built on Python 3.9 and its framework Flask 2.0 and front-end framework React 17.0. Front-end pages are developed based on Material UI 5.0 which follows Google's Material Design. State management is designed based on MobX 6.3. As for routing, we use React-Router 5.3. Front-end and back-end interactions are handled by axios 0.24. All front-end data's visualization is rendered using ECharts 5.3. All data are stored and managed by MariaDB 10.7.3, an open source relational database, and the object-relational mapping middleware is Flask-SQLAlchemy 2.5.1. The operating system is based on Ubuntu 20.04 LTS version, and the web server is deployed using Nginx 1.21. All services are managed using Docker 20.10.16. The database has been tested in multiple operating systems, browsers and network environments to ensure its stability.

### Data sources of CPMCP

The data sources of CPMCP can be divided into two categories: online databases and existing publications. For publications, CPMCP obtained 2202 TCM compound prescriptions, which consist of 1484 CPMs and 718 CMPs. The information on CPMs was extracted from the "Compendium of National Standards for Chinese Patent Medicines" (2002 edition), which is approved by the State Drug Administration

of China. The details of CMPs were collected from various classical TCM-related works. CPMCP shows the names, components, usages, applications and contraindications of these prescriptions. According to the components and the applications of these prescriptions, CPMCP extracted 1557 natural medicinal materials and 2285 TCM symptoms from the Chinese Pharmacopoeia (2015 edition). The names of TCM symptoms were standardized according to an authoritative TCM publication named "Research on the Standardization of TCM Terminology" (2016 Edition) and a published TCM terminology integration platform. According to "Pathology Terminology Standardization" (2015 edition), the CPMCP obtained information on the definitions, loci and attributes of these symptoms.

In terms of database, CPMCP collected MM symptom terms from MeSH database (2015 version) (22) and SIDER database (2016 version) (23). According to the annotations in the SymMap database (19), the TCM symptoms were mapped to MM symptoms. After that, we extracted the chemical ingredient information of natural medicinal materials from TCMID (10), TCMSP (24), and TCM-ID databases (25) and obtained the target genes of these ingredients from HIT (18) and TCMSP databases. Diseases in CPMCP were gotten from OMIM (26) and Orphanet databases (27). The disease-gene associations were obtained from HPO (28), DrugBank (29) and National Center for Biotechnology Information (NCBI) databases (30). The number and sources of various entities in CPMCP are shown in Table 1.

## Results

### Search for information that interests you

On the home page (Figure 2), you can search for the content you are interested in by selecting different filters, including CPMs, CMPs, medicinal materials, targets, diseases, TCM symptoms and MM symptoms (in this step, fuzzy search is supported). The specific items contained in each type of entity

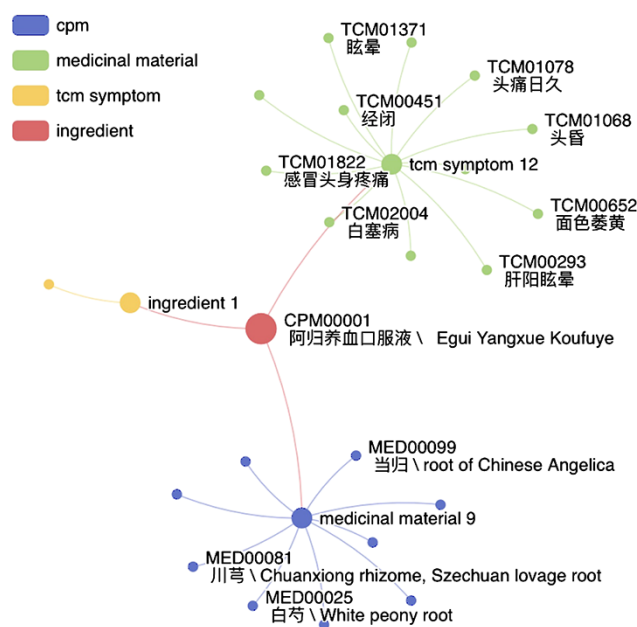


Figure 3. Associations between a CPM and other entities.



are given in Figure 1B. For each type of entity, we have provided some samples below the search box for users' reference. If you want to browse all entries for a certain type of entity, you can click the search button directly by specifying the filter type.

### The associations between entities are visualized

According to the different types of associations among the entities, CPMCP constructed and visualized the heterogeneous graph for each entity. Taking the CPM, Egui Yangxue Koufuye, as an example (as shown in Figure 3), its components (medicinal materials and ingredients) and related TCM symptom are demonstrated intuitively.

It is worth noting that the functions and indications of CPMs and CMPs are described in ancient Chinese, which brings difficulties to practitioners of TCM in the process of using them. We organized relevant experts to manually map the functions of compound prescriptions in ancient Chinese to the standardized TCM symptom vocabularies (as shown in Figure 1C), obtaining a total of 71 414 associations between compound prescriptions and TCM symptoms. In this way, CPMCP established the association between compound prescription and disease through the meta-path: compound prescriptions → TCM symptoms → MM symptoms → diseases. This function of CPMCP contributes to the modernization of TCM. Moreover, CPMCP established another meta-path:

compound prescriptions → medical materials → ingredients → targets → diseases. This meta-path can explain how a prescription treats a specific disease from the perspective of MM. It provides much valuable information for the interpretability of TCM.

### CPMCP summarized the common compatibility of medicinal materials

The compatibility information is essential in TCM because it conveys not only what components are involved to treat special diseases but also how to combine these single medicinal materials. Therefore, when TCM practitioners construct a TCM compound prescription, they need to check the compatibility mechanism of the medicinal materials involved in the prescription. CPMCP summarizes a set of common drug combination principles by analyzing the combination of medicinal materials in existing prescriptions.

For each medicinal material, CPMCP built a doughnut chart to demonstrate the nine most common compatibilities (Figure 4). Complete compatibility information was given in the form of a table sorted by their frequency (Figure 5). For example, in Figure 5, we can intuitively see that Baishao has appeared together with Danggui 63 times. It can be inferred from this that Baishao and Danggui are often used together. In this way, CPMCP revealed the habits and taboos of collocation among medicinal materials.

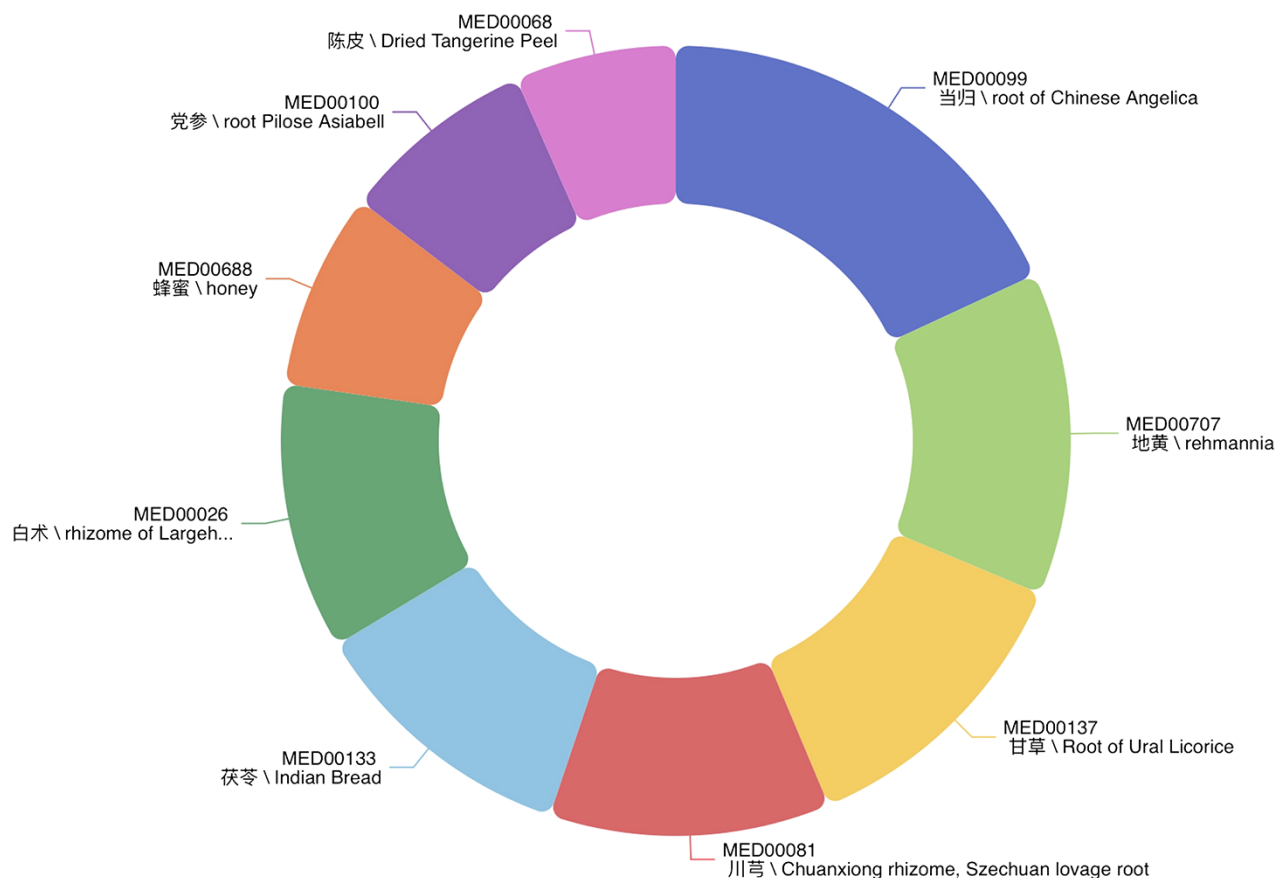


Figure 4. Nine most common compatibilities of a medicinal material named Baishao.

ID	Name chinese	Name pinyin	Name latin	Frequency
MED00099	当归	Danggui	Radix Angelicae Sinensis,Angelicae Sinensis Radix	63
MED00707	地黄	Dihuang	Rehmanniae Radix	46
MED00137	甘草	Gancao	Glycyrrhizae Radix Et Rhizoma, Radix Glycyrrhizae	43
MED00081	川芎	Chuanxiong	Chuanxiong Rhizoma, Radix Chuanxiong; Rhizoma Chuanxiong	40
MED00133	茯苓	Fuling	Poria	39
MED00026	白术	Baizhu	Atractylodis Macrocephalae Rhizoma, Rhizoma Atractylodis Macrocephalae	38
MED00688	蜂蜜	Fengmi	Mel	28
MED00100	党参	Dangshen	Codonopsis Radix, Radix Codonopsis Pilosulae	28
MED00068	陈皮	Chenpi	Citri Reticulatae Pericarpium, Pericarpium Citri Reticulatae	23
MED00191	黄芪	Huangqi	Astragali Radix, Radix Astragali	23
MED00436	香附	Xiangfu	Rhizoma Cyperi, Cyperi Rhizoma	21
MED00344	肉桂	Rougui	Cortex Cinmomi, Cinnamomi Cortex	20
MED00062	柴胡	Chaihu	Radix Bupleuri, Bupleuri Radix	19
MED00455	延胡索	Yanhusuo	Rhizoma Corydalis, Corydalis Rhizoma	19
MED00363	山药	Shanyao	Rhizoma Dioscoreae, Dioscoreae Rhizoma	16
MED00296	木香	Muxiang	Radix Aucklandiae, Aucklandiae Radix	15
MED00097	丹参	Danshen	Radix Salviae Ligulioabae, Salviae Miltiorrhizae Radix Et Rhizoma	15
MED00192	黄芩	Huangqin	Scutellariae Radix, Radix Scutellariae	14
MED00288	牡丹皮	Mudanpi	Cortex Moutan, Moutan Cortex	14
MED00308	牛膝	Niuxi	Radix Achyranthis Bidentatae, Achyranthis Bidentatae Radix	14
MED00600	阿胶	Ejiao	Asini Corii Colla	14
MED00359	砂仁	Sharen	Amomi Fructus, Fructus Amomi	13
MED00460	益母草	Yimucao	Herba Leonuri, Leonuri Herba	13
MED00147	枸杞子	Gouqizi	Lycii Fructus, Fructus Lycii	13
MED00541	炙甘草	Zhigancao	Glycyrrhizae Radix Et Rhizoma Praeparata Cum Melle	13

Figure 5. All of the common compatibilities of Baishao.

## Conclusion

In this work, a TCM-related database, CPMCP, was proposed. CPMCP reports the comprehensive and standardized information of CPMs and ancient CMPs, such as their components, indications and contraindications. To promote the modernization of TCM, CPMCP mapped the instructions of TCM compound prescriptions to the standardized TCM symptom vocabularies manually. In this way, CPMCP established the associations between the TCM compound prescriptions and diseases. Since the compatibility information is essential in TCM, CPMCP summarized the common compatibility of medicinal materials by analyzing the existing TCM compound prescriptions. This function is helpful for revealing the habits and taboos of collocation among medicinal materials. We believe that CPMCP can promote the modernization of TCM and make greater contributions to MM.

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## Conflict of interest

The authors have declared no competing interests.

## Authors' contributions

C.S. wrote the manuscript, R.T. collected and processed the data, J.H. developed the website, C.S., J.H. and M.L. assisted

data processing, H.Y and Y.W. verified the data and J.-M.W. and J.L. conceived the study.

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