Jiaju Zhou · Guirong Xie · Xinjian Yan

Encyclopedia of Traditional Chinese Medicines

Molecular Structures, Pharmacological Activities, Natural Sources and Applications

Vol.1

Isolated Compounds A-C

Springer

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Encyclopedia of Traditional Chinese Medicines

Molecular Structures, Pharmacological Activities, Natural Sources and Applications

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Preface

A significant preoccupation of modern traditional Chinese medicine (TCM) research has been the characterization of TCM components, such as pertain to their isolation, purification, structural determination, and pharmacological activity. As a reference tool, this ***Encyclopedia of Traditional Chinese Medicines*** presents a comprehensive and integrative work on surveying TCM plant sources, chemistry, pharmacology and medicinal effects and indications in a systematic manner.

This encyclopedia is an integrated achievement of a long-term TCM research project by the authors at the Chinese Academy of Sciences [1–4], involving three parts and now organized in six volumes:

Part I (Volumes 1 to 4 and part of Volume 5) provides structural, physical, pharmacological and natural source information on 23,033 isolated chemicals captured from 5,535 references, basically up to year 2005. A great deal of effort has been paid on overlapping or contradictory data in order to provide readers with an accurate and reliable resource.

Part II (last part of Volume 5) describes 6,926 TCM plants and congeners, together with their medicinal effects and indications. The contents of Part I and Part II are all organized in alphabetical order.

Part III (Volume 6) includes seven indexes produced by a computer program. Based on the indexes, users can readily find concerned contents in multiple ways.

With this encyclopedia, the authors attempt to provide a bridge for the communication between the TCM system and Western medicinal systems, and a platform with multiple-subjects in support of research and development of the health sciences.

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[1] Xinjian Yan, Jiaju Zhou and Guirong Xie, *Traditional Chinese Medicines*: *Molecular structures, natural sources, and applications*, *1st edition*, Ashgate Publishing house, 1999

[2] Jiaju Zhou, Guirong Xie and Xinjian Yan, *Traditional Chinese Medicines*: *Molecular structures, natural sources, and applications*, *2nd edition*, Ashgate Publishing house, 2002

[3] Jiaju Zhou, Guirong Xie and Xinjian Yan, *Handbook of Chemical Components in Plant Origins of Traditional Chinese Medicines*, Chemical Industry Press, Beijing, 2004 (in Chinese)

[4] Jiaju Zhou, Guirong Xie and Xinjian Yan, *Data Collection of Chemical Components in Plant Origins of Traditional Chinese Medicines*, Vol 1–3, Science Press, Beijing, 2009 (in Chinese)

Introduction

This encyclopedia mainly consists two parts - compound and plant. Its core content is the structural and pharmacological information of 23,033 phytochemicals, as well as medical effects and indications of 6,926 plant species from which the phytochemicals were isolated. The compounds, i.e. phytochemicals, are ordered alphabetically, and their ordinal numbers are used as compound unique codes. The plant species are coded from T0001 to T6926. With this code system, the complicated "many to many" relationship between compounds and plants can be clearly expressed, and any individual compound or plant could be located easily in this 6 volumes book.

1. Compound Entry

Format of Compound Entry. A compound entry starts with a title line, in which there are two items: the compound's unique code and main name. Following the title line is the compound physical, pharmacological and source information, which may include 8 items:

> **Title line (code number, main name)**
> A. Synonyms of the compound (if any);
> B. CASRN number (if any);
> C. Formula (relative molecular mass);
> D. Physicochemical properties;
> E. Pharmacological data (if any);
> F. Source(s);
> G. Reference(s);
> H. Graphic structure.

Chemical Names and Synonyms. Generally, a compound may have one scientific name and several trivial names. In the encyclopedia, based on original articles, we select one name as the "main name" (appeared at the title line of each compound entry), and use it to alphabetically order the 23,033 compounds in the first 5 volumes. The main name is either a scientific name or a trivial name. All of other names of each compound, if any, are presented after the title line.

Stereochemistry of Chemical Structure. We protracted all compound structures down to atom-bond level including complicated glycosides, with stereo-chemical information based on the data in the original papers. For example, the structure with full stereochemistry of compound 22,834 (isolated from CHUAN XU DUAN *Dipsacus asperoides*) is:
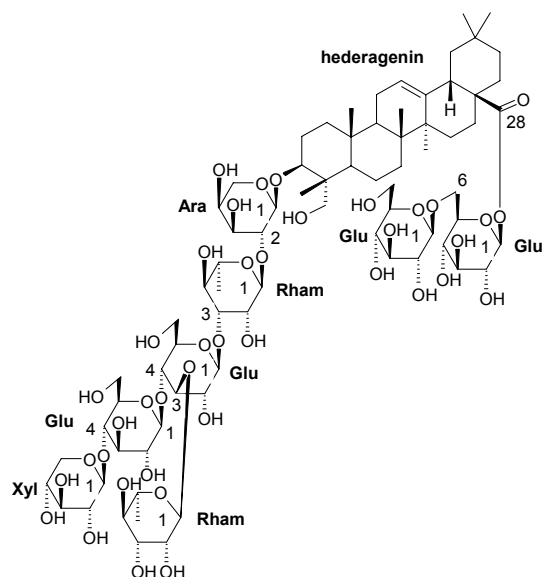
3-*O*-[*β-D*-**Xyl**opyranosyl**(1→4)**-*β-D*-**glu**copyranosyl**(1→4)**]
[*α-L*-**rham**nopyranosyl**(1→3)**]-*β-D*-**glu**copyranosyl**(1→3)**-
α-L-**rham**nopyranosyl**(1→2)**-*α-L*-**ara**binopyranosyl **hederagenin**-
28-*O*-*β-D*-**glu**copyranosyl**(1→6)**-*β-D*-**glu**copyranoside

Normalization of Pharmacological Data. More than 8,000 TCM components in this encyclopedia have a variety of pharmacological data, which are valuable not only for the study of TCM, but also for the development of Western medicine. Because different expressions are used for the same kind of data in different articles, we have to define and normalize thousands pharmacological terms, so that the data could be expressed by a unified way, and be easily understood by readers.

The pharmacological terms in the encyclopedia are presented by a multi-layered structure. In the top layer, there are around 20 types of pharmacological activity terms, they are cytotoxic (*in vitro* anticancer), antineoplastic (*in vivo* anticancer), antibacterial, antifungal, antiviral, anti-HIV, anti-inflammatory, antioxidant, antimalarial, enzyme inhibitors, NO production inhibitors, cardiovascular activity, smooth muscle relaxant and stimulant, toxin and medium lethal dose LD_{50}, and so forth. For each term there is a regulation about how to describe related pharmacological data. The following is an example:

> **Term name** (*in vitro/in vivo,*
> target cell **1**, quantitative data,
> control Compound, control's data;
> target cell **2**, quantitative data,
> control Compound, control's data;
> target cell **3**, quantitative data,
> control Compound, control's data;
> terse description of related mechanism if any).

Under the subtitle "Pharm:" of compound entry 248 (17-Acetoxylabda-7,12(E),14-triene), a set of bio-data is presented as follows:

Pharm: **Cytotoxic** (*in vitro*,
BT474 human galactophore cancer cell, IC_{50} = 4.7μg/mL,
control Doxorubicin hydrochloride, IC_{50} = 0.08μg/mL;
CHAGO human undifferentiated lung cancer cell, IC_{50} = 5.7μg/mL,
control Doxorubicin hydrochloride, IC_{50} = 2.3μg/mL;
HepG2 human liver cancer cell, IC_{50} = 6.5μg/mL,
control Doxorubicin hydrochloride, IC_{50} = 0.9μg/mL;
Kato3 human gastric cancer cell, IC_{50} = 5.3μg/mL,
control Doxorubicin hydrochloride, IC_{50} = 1.7μg/mL;
SW620 human colorectal adenocarcinoma cell, IC_{50} = 5.6μg/mL,
control Doxorubicin hydrochloride, IC_{50} = 1.1μg/mL).

In order to standardize abbreviations of cancer cells, such as BT474, CHAGO, etc., we defined and used 270 cancer cell codes (CCC) in the encyclopedia. For explanations of these codes, please see "Cancer Cell Codes in the Pharmacological Models" in Volume 1 of the encyclopedia.

By means of the formatted and structuralized methods, we normalized expressions of most pharmacological data appeared in the encyclopedia. For complete information of all 3367 normalized pharmacological activity terms, please see "Compound Pharmacological Activities Index" in Volume 6.

2. Plant Entry

One Species One Entry. Conventionally, a TCM name may include more than one plant species that have the same medical functions; therefore, a plant may not have an independent TCM entry and may be described under a TCM name. In this book, modern botany classification regulation is adopted and each plant species has an independent entry.

For example, traditional Chinese medicine DAN SHEN includes three species. They are equivalent in both effects and indications in TCM practice. In this encyclopedia, we defined three plant entries for each one of them.

T5680 *Salvia miltiorrhiza* (Lamiaceae); DAN SHEN; Danshen;
T5681 *Salvia miltiorrhiza* f. *alba* (Lamiaceae); BAI HUA DAN SHEN; Whiteflower Danshen;
T5688 *Salvia przewalskii* (Lamiaceae); GAN XI SHU WEI CAO; Przewalsk Sage.

With this method, we are able to smoothly link TCM information with that of modern botany.

Simplified Latin Name. For each TCM plant or TCM congener, four names are used in the encyclopedia. They are Latin name, English name, PIN-YIN name and Chinese

name, while the Chinese name only appears in TCM Plants PIN-YIN/Chinese Names Index" not in the main part of the book. For plant Latin name (e.g. scientific name), we use a simplified nomenclature, in which the nomenclator(s) information is not included. For example the Latin name of Chinese Angelica (DANG GUI) in the encyclopedia is *"Angelica sinensis"*, not "*Angelica sinensis* (Oliv.) Diels".

Family Name. According to the "International Code of Botanical Nomenclature" (2007), the following eight authoritative family names are used in the encyclopedia. The family names of long usage, which are not used in are the encyclopedia, indicated in parentheses:

> Apiaceae (Umbelliferae);
> Arecaceae (Palmae);
> Asteraceae (Compositae);
> Brassicaceae (Cruciferae);
> Clusiaceae (Guttiferae);
> Fabaceae (Leguminosae);
> Lamiaceae (Labiatae) and
> Poaceae (Gramineae).

PIN-YIN Name and Chinese Name. A simplified PIN-YIN name system is used in the encyclopedia. That is not to include the four-tone mark. However, there are exceptions. Among the thousand PIN-YIN names in the book, there are seven confusing cases. For each mistakable name, a superscript is attached to the name for indicating its four-tone in order to distinguish it from other plant species. For example: BAI MAO GEN[1] and BAI MAO GEN[4] are two different TCM plants:

> T3416 *Imperata cylindrica* var. *major* (Poaceae); BAI MAO GEN[1]; Lalang Grass Rhizome.
> T3309 *Hydrastis canadensis* (Ranunculaceae); BAI MAO GEN[4]; Golden-seal.

Other six cases are:

> T1449 *Cirsium japonicum* (Asteraceae); DA JI[4]; Japanese Thistle.
> T2608 *Euphorbia pekinensis* (Euphorbiaceae); DA JI[3]; Peking Euphorbia.
>
> T4124 *Matricaria chamomilla* [Syn. *Matricaria recutita*] (Asteraceae); MU[3] JU; Mayweed.
> T0197 *Aegle marmelos* (Rutaceae); MU[4] JU; Sepiaria.
>
> T1039 *Bruguiera gymnorrhiza* (Rhizophoraceae); MU LAN[3]; Common Bruguiera.
> T3423 *Indigofera tinctoria* (Fabaceae); MU LAN[2]; True Indigo.
>
> T6798 *Vitis vinifera* (Vitaceae); PU[2] TAO; European Grape.
> T6267 *Syzygium jambos* (Myrtaceae); PU[3] TAO; Roseapple.
>
> T2107 *Dendrobium nobile* (Orchidaceae); SHI HU[4]; Noble Dendrobium.
> T2646 *Evodia rutaecarpa* var. *officinalis* (Rutaceae); SHI HU[3]; Officinal Evodia.
>
> T1221 *Caryopteris divaricata* (Verbenaceae); YOU[2]; Divaricate Bluebeard.
> T1478 *Citrus grandis* (Rutaceae); YOU[4]; Pummelo.

Translation of TCM Effects Terms. In the Volume 5 of the encyclopedia, 6,926 TCM Plant entries list in alphabetical order of *Latin names*, including 2,923 original TCM plants (including few of animals)[R01-R04] and 4,003 congeners (including a few of non-TCM medicinal plants). For each TCM plant, two most important features are traditional TCM effects and indications.

For preparing this encyclopedia, one of the greatest challenges is how to correctly translate each TCM term into correspondent English, so that Western readers are able to understand the true meaning of the content in the book. After comparing several translation systems, we decided to use Wiseman's terminological system[R05-R07] for this book.

Wiseman's system obeys two most important principles: (1). The English-language terms should be faithful to the original concepts in traditional Chinese medicine. (2). The English-language TCM terminology should be flexible enough to allow modifications and extensions so that derivative effects can be described by a structuralized manner. For instance, the term "quicken blood" describes a general effect meaning "activating blood flow" or "promoting blood circulation". Elaboration of this term produces "quicken blood and transform stasis", "quicken blood and relieve pain", "quicken blood and regulate menstruation", and so on. The following illustrations an example of the structuralized expressions related to the term "quicken blood":

quicken blood and disinhibit water
quicken blood and dispel stasis
quicken blood and dispel wind
quicken blood and disperse swelling
quicken blood and disperse welling abscess
quicken blood and dissipate binds
quicken blood and dissipate stasis
quicken blood and free menstruation
quicken blood and free network vessels
quicken blood and free vessels
quicken blood and joint bones
quicken blood and move *qi*
quicken blood and move stasis
quicken blood and nourish heart
quicken blood and promote milk
quicken blood and quiet spirit
quicken blood and regulate menstruation
quicken blood and relieve pain
quicken blood and resolve toxin
quicken blood and settle pain
quicken blood and soothe sinews
quicken blood and stanch bleeding
quicken blood and strengthen sinews
quicken blood and transform stasis
quicken blood and vessels

Translation of TCM Indications Terms. Based on Wiseman's terminological system, *"Chinese-English Dictionary of Traditional Chinese Medicine"* compiled by Guangzhen Gao *et al.*[R08], *"An English-Chinese Medical Dictionary, Second Edition"* compiled by Weiyi Chen *et al.*[R09], and other reference dictionaries, we defined over 3,800 standard indication terms for translating TCM indications terms from Chinese to English. Among the 3,800 terms, 2,526 terms are actually used in the encyclopedia, in which 85% terms are traditional TCM terms and the rest 15% are common modern medicinal terms. Some typical examples of traditional TCM indication terms are as follows:

yin vacuity internal heat
yin vacuity lung dryness
yin vacuity tidal fever
chest impediment
chest impediment and heart pain
chest impediment and heart pain over back
chest oppression and pain
chest oppression with breathe hard
distention pain in rib-side
distention pain in stomach duct
distention pain in stomach duct and abdomen
externally contracted summer heat-damp
externally contracted wind evil
externally contracted wind-cold
externally contracted wind-heat
knocks and falls
sores
sores clove boil
swelling of sores and boils
sore scab and lichen
toxin swelling of sores

In summary, this encyclopedia provides a collection of more than 23,000 TCM chemical components isolated from natural resources and a large number of pharmacological activity data of these components. It may be used not only as a handbook to look for structures and pharmacological activities of TCM chemical components and source plant information, but also a fundamental platform for studying TCM with a systematic and integrative approach.