Traditional medicine patents lead to enhanced drug discovery from natural products

John Zabilski
CAS Senior Product Manager
Spring 2011 ACS Meeting
**CAS supports the mission of the ACS**

**ACS Mission**

To advance the broader chemistry enterprise and its practitioners for the benefit of Earth and its people.

**CAS Mission**

To provide the world’s best digital research environment to search, retrieve, analyze, and link chemical information.
CAS has the most complete, high-quality chemistry databases

**CASREGISTRY℠**
- Organic and inorganic substances, sequences
- Substances reported in the literature back to 1802
- Updated daily with ~12,000 substances
- Substance information enriched with experimental and predicted property data, including more than 2.8 billion property values, data tags, and spectra

**CAplus℠**
- Journal articles, patents, and other reputable scientific sources
- More than 10,000 major scientific journals covered
- Patents from more than 60 patent offices
- Coverage back to early 1800s; cited references from 1997-present
- Updated daily with ~3,000 references

**CASREACT℠**
- Single- and multi-step reactions, synthetic preparations
- Extracted from journal articles and patents
- Coverage back to 1840; reaction conditions from 2003-present
- Updated weekly with ~30-50,000 reactions

**CHEMCATS℠**
- Chemical source information, including supplier addresses and pricing
- More than 1,000 suppliers
- More than 1,100 chemical catalogs
- Updated when new or revised catalogs are available

**MARPAT℠**
- Markush structures covering organic and organometallic substances in patents
- Coverage 1988-present
- Also 1961-1987 records derived from INPI data
- Updated daily with ~150-200 Markush structures
Three main services provide access to CAS content

STN
The premier network of sci-tech databases

SciFinder®
Essential content. Proven results.™

Science IP
The CAS search service
Agenda

• **World Traditional Medicine**
  – Success stories
  – Specific examples

• **World Traditional Medicine content in CAplus**
  – Coverage by country
  – Intellectually added indexing
  – CA Lexicon on STN®

• **Finding natural product pharmaceuticals with SciFinder®**
World Traditional Medicine (WTM): Everything old is new again

• Accelerated interest in mining the rich lode of traditional medical knowledge
  – Traditional Chinese Medicine (TCM)
  – Ayurveda – Traditional Indian Medicine (TIM)
  – Additional folk medicine remedies from other countries

• Alternative or complementary medicine is frequently used to supplement modern medical treatments

• Benefits of natural products may include
  – Reduced side effects
  – Effective alternatives to drug-resistant diseases
  – Decreased costs versus new drug development
Traditional medicine provides notable success stories for drug development

• **Artimisinin**
  – Became the preferred antimalarial treatment
  – Extracted from Sweet Wormwood *qinghao* (*Artemisia annua*)

• **Silybinin**
  – Originally used as hepatitic restorative
  – Milk thistle (*Silybum Marianum*)
  – Clinical studies as an antitumor agent

• **Taxol (Paclitaxel)**
  – Antitumor agent
  – Pacific yew (*Taxus brevifolia*)
  – Semisynthetic production
Qinghaosu -青蒿素 (Artemisinin) provides a traditional medicine alternative for treating drug-resistant malaria

Author(s): Li, Ying; Wu, Yu-Lin
Corporate Source: Shanghai Institute of Materia Medica, Shanghai Institutes for Biological Sciences, Chinese Academy of Sciences, Shanghai, 201203, Peop. Rep. China
Source: Current Medicinal Chemistry (2003), 10(21), 2197-2230
Publisher: Bentham Science Publishers Ltd.
Document Type: Journal; General Review
Language: English
OS.Citing Ref Count: 86 THERE ARE 86 CAPLUS RECORDS THAT CITE THIS RECORD
Reference Count: 265 THERE ARE 265 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT
Milk Thistle has led the way to natural product drug development as treatment for heptatoxicity.

*Silybum Marianum* provides a rich flavonoid antioxidant source traditionally used for treating liver disease.

**Silibinin**
(CAS RN 22888-70-6) has been extracted for additional clinical studies including antitumor activity.
Taxol reveals a model pathway for natural product drug development

• **Paclitaxel** was originally isolated from the bark of the rare Pacific yew tree
  – The extraction method destroyed the tree and produced insufficient quantities for treating all cancer patients that may have benefited
  – Additionally, Bristol-Myers Squibb (BMS) held the patent rights for Taxol derived from this natural product source

• **Pacific Yew alternatives** were developed by Robert A. Holton of Florida State University (FSU)
  – Semisynthetic process for production of paclitaxel
  – Improved metal alkoxide process to extract starting materials (10-deacetylbaccatin III) from other more common yew species
  – BMS signed a license agreement with FSU in 1990, giving the company the right to use the process
  – The Food & Drug Administration approved the semisynthesized drug for marketing in 1994
Improvements on the synthesis of taxol continue

"The interesting thing about [paclitaxel] is that fundamentally it's a diterpene skeleton, but it presents a variety of side chains on its surface. So there is more opportunity to make different molecules from [paclitaxel], I believe, than there has ever been with any cancer drug."

Robert A. Horton  C&EN Vol. 83, Issue 25 (6/20/05)
What makes CAS databases a rich source of WTM?

• Robust coverage of WTM content from multiple sources
• Continual enhancement of Asian coverage
• English translations of many “obscure” Asian-language patents and journal articles

• CAplusSM
  – 61 patent authorities, many smaller patent offices not always covered by others
  – 50,000 WTM patents added in recent years

• CAS REGISTRYSM
  – Links WTM to published substance information through CAS Registry Numbers®
CAS has added more than 50K World Traditional Medicine (WTM) patents to the CAplus database

- More than 50K additional WTM patents from 1985-2005 were added to CAplus/CA in recent years
  - Principally from the People’s Republic of China (60%)
  - Additional sources include Japan, Korea, Russia, United States, and European countries
  - Additional future entries from several countries are anticipated

- Supplements patent records already indexed

- Enhanced with
  - Supplemental terms derived from original document
  - Intellectually assigned controlled terms
  - English abstract text with details on preparation and composition
  - CAS Registry Numbers and Roles for specific substances
Asia has emerged as the premier region for World Traditional Medicine patents, with over 90% reported

- China: 60%
- Japan: 20%
- Republic of Korea: 10%
CAS indexing enhances the retrieval and understanding of the original document

- **Intellectually assigned indexing** by CAS scientists who are experts in the specific subject area of the original document
- Provides **consistent controlled terminology** to enhance retrieval
- **Precise terminology** focuses on the novel content reported in the original document
- Additional indexing provided for select equivalent family members
- **Correction of numbers, names, and chemical structures** that appeared erroneously in the original document
Chinese patent coverage in the CAplus database includes multiple publication types and family information

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<tr>
<td></td>
<td>C</td>
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<tr>
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<td>U</td>
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<td>Y</td>
<td>Granted Utility Model (2006 - April 6, 2010)</td>
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WTM patents include multi-stage and family information when available

```
=> FILE CAPLUS
COPYRIGHT (C) 2011 AMERICAN CHEMICAL SOCIETY (ACS)

=> S CN 1122711 A/PNK; D ALL
L1           1 CN 1122711 A/PNK
L20  ANSWER 1 OF 1  CAPLUS  COPYRIGHT 2011 ACS on STN
ACCESSION NUMBER:  2005:891632  CAPLUS
TITLE:                   A Chinese medicinal composition for treating hepatopathy, and its preparation method
INVENTOR(S):             Zhang, Yongpeng; Zhang, Yongfei; Zhao, Xuemei
PATENT ASSIGNEE(S):      Peop. Rep. China
SOURCE:                  Faming Zhuanli Shenqing, No pp. given
CODEN: CNXXEV

DOCUMENT TYPE:           Patent
LANGUAGE:                Chinese
FAMILY ACC. NUM. COUNT:  1

PATENT INFORMATION:

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<td>19950901</td>
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The PNK field allows a kind code to be searched with the patent number for accurate retrieval.
```
A Chinese medicinal composition, YIGANKANG, is prepared from Herba Artemisiae Scopariae, Radix Isatidis, Radix Astragali, Fructus Schisandrae Chinensis, Fructus Ligustri Lucidi, ant, Ganoderma, Radix Bupleuri, Radix Paeoniae Rubra, Lentinus Edodes, Cordyceps, and Radix Glycyrrhizae. The preparation method comprises pulverizing the raw materials, oven drying, mixing, pulverizing into powder, sterilizing, and making into honeyed pill or capsule; or comprises decocting, concentrating to soft extract, adding sugar powder, and making into granule. The composition has effects in removing toxic materials, preventing pestilence, supplementing qi, nourishing yin, regulating immunity, and reducing serum transaminase. The composition is used to treat acute and chronic hepatitis A, hepatitis B, hepatitis C, hepatitis D, hepatitis E, and hepatitis virus carrier due to autoimmunity deficiency.
Detailed indexing includes controlled terms, substance classes, and CAS Registry Numbers for specific compounds.

**CA Indexing includes:**
- Taxonomic terms
- Disease terms
- Substance Class terms
- Specific substances

### Indexed Terms

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<td>IT</td>
<td><strong>Ligusticum chuanxiong</strong></td>
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<td>IT</td>
<td>Liver disease</td>
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<td>IT</td>
<td>Manis</td>
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<td>IT</td>
<td>Natural products, pharmaceutical</td>
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<tr>
<td>IT</td>
<td>Abdominal disease</td>
</tr>
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<td>IT</td>
<td>(abdominal distention)</td>
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<td>IT</td>
<td>Disease, animal</td>
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<td>IT</td>
<td>(asthenia)</td>
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<td>IT</td>
<td>Medical goods</td>
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<tr>
<td>IT</td>
<td>(bags)</td>
</tr>
<tr>
<td>IT</td>
<td>Viral hepatitis</td>
</tr>
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<td>IT</td>
<td>(chronic)</td>
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</table>

**CAS Registry Number:** 507-70-0

- RL: BSU (Biological study unclassified); BIOL (Biological study)

### Image Descriptions

- **Ligusticum chuanxiong**
- **Borneol**

(CAS Registry Number 507-70-0)
Many natural products are being studied for multiple therapeutic uses

![Therapeutic Uses of Top Natural Products](image)

- **Astragalus**
- **Angelica sinensis**
- **Peony**
- **Sage**
- **Ligusticum chuanxiong**

Therapeutic Uses of Top Natural Products

**Number of Therapeutic Uses**

- **Neoplasm**
- **Hypertension**
- **Antibacterials**
- **Anti-inflammatory**
- **Analgesics**
The CA Lexicon provides a rich source for enhancing STN search strategies

- **The CA Lexicon** provides an online thesaurus of controlled terminology including
  - General subject terms
  - Chemical substance classes
  - Taxonomic hierarchies

- **Use the CA Lexicon to**
  - Identify new and useful subject and substance keywords
  - Acquire synonymous terms to enhance search retrieval
  - Refine searches with precise controlled terms
Controlled terminology in the CA Lexicon can enhance prior art searches

<table>
<thead>
<tr>
<th>CA Index Terms</th>
<th>Chemical Compound Classes</th>
<th>Taxonomic Vocabulary</th>
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<tbody>
<tr>
<td>• &gt; 16,200 subject headings (index terms)</td>
<td>• &gt; 11,280 frequently indexed substances</td>
<td>• &gt; 244,400 controlled taxonomic terms</td>
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<td>• &gt; 78,900 subject headings with linked terms</td>
<td>• Frequently cited substances from the past year</td>
<td>• Relationships between taxonomy and broader or non-taxonomic vocabulary</td>
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<tr>
<td>• Related concepts</td>
<td>• Broader terms for each substance</td>
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<tr>
<td>• Date ranges of use for each term</td>
<td>Synonyms</td>
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Expanding in the CA Lexicon reveals broader terms, narrower terms, and related terminology

=> E CHINESE CABBAGE+MAX/CT

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<th>Interpretation</th>
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<td>100276</td>
<td>BT3 Food/CT</td>
</tr>
<tr>
<td>E2</td>
<td>0</td>
<td>BT2 Plant-derived food (non-CA heading)/CT</td>
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<tr>
<td>E3</td>
<td>24742</td>
<td>BT1 Vegetable/CT</td>
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<td>E4</td>
<td>2711</td>
<td>--&gt; Chinese cabbage/CT</td>
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<tr>
<td>E5</td>
<td>0</td>
<td>OLD Brassica chinensis pekinensis/CT</td>
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<tr>
<td>E6</td>
<td>860</td>
<td>OLD Brassica pekinensis/CT</td>
</tr>
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<td>E7</td>
<td>1</td>
<td>OLD Pakchoi (Brassica chinensis pekinensis)/CT</td>
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<td></td>
<td>OLD Pakchoi (L) Brassica chinensis pekinensis/CT</td>
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<tr>
<td>E9</td>
<td>26</td>
<td>OLD Pe-tsai/CT</td>
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<tr>
<td>E10</td>
<td></td>
<td>UF BaiCai/CT</td>
</tr>
<tr>
<td>E11</td>
<td></td>
<td>UF Brassica campestris pekinensis/CT</td>
</tr>
<tr>
<td>E12</td>
<td></td>
<td>UF Brassica campestris pekinensis granaat/CT</td>
</tr>
<tr>
<td>E13</td>
<td></td>
<td>UF Celery cabbage/CT</td>
</tr>
<tr>
<td>E14</td>
<td></td>
<td>UF Napa cabbage/CT</td>
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<tr>
<td>E15</td>
<td></td>
<td>UF Pechay/CT</td>
</tr>
<tr>
<td>E16</td>
<td></td>
<td>UF Pekin cabbage/CT</td>
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<tr>
<td>E17</td>
<td></td>
<td>UF Petsai/CT</td>
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<tr>
<td>E18</td>
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<td>UF Sinapis pekinensis/CT</td>
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<td>703</td>
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<td>E24</td>
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<td>LT Chinese cabbage (L) kimchi/CT</td>
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******* END **********
CAplus highlights traditional medicine with several focused controlled terms

<table>
<thead>
<tr>
<th>=&gt;</th>
<th>E TRADITIONAL AND ALTERNATIVE MEDICINE+MAX/CT</th>
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<td>E1</td>
<td>11628 BT1 Medicine/CT</td>
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<td>E2</td>
<td>4274 --&gt; Traditional and alternative medicine/CT</td>
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<tr>
<td></td>
<td>HNTE Valid heading during volume 146 (2007) to present.</td>
</tr>
<tr>
<td></td>
<td>NOTE A broad category of treatment systems used in lieu of or in supplement to modern medicine.</td>
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<tr>
<td>E3</td>
<td>UF Alternative medicine/CT</td>
</tr>
<tr>
<td>E4</td>
<td>UF Complementary medicine/CT</td>
</tr>
<tr>
<td>E5</td>
<td>UF Complementary/alternative and traditional medicine/CT</td>
</tr>
<tr>
<td>E6</td>
<td>UF Complementary/alternative medicine/CT</td>
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<tr>
<td>E7</td>
<td>UF Ethnomedicine/CT</td>
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<tr>
<td>E8</td>
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</tr>
<tr>
<td>E9</td>
<td>UF Holistic medicine/CT</td>
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<tr>
<td>E10</td>
<td>UF Indigenous medicine/CT</td>
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<td>UF Oriental medicine/CT</td>
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<td>E12</td>
<td>UF Primitive medicine/CT</td>
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<tr>
<td>E13</td>
<td>UF Traditional medicine/CT</td>
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<tr>
<td>E14</td>
<td>130655 RT Natural products, pharmaceutical/CT</td>
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<tr>
<td>E15</td>
<td>2121 RT Traditional medicine diagnostic patterns/CT</td>
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<tr>
<td>E16</td>
<td>LT Traditional and alternative medicine (L) Ayurvedic medicine/CT</td>
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<tr>
<td>E17</td>
<td>LT Traditional and alternative medicine (L) Chinese medicine/CT</td>
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********** END **********
The majority of traditional medicine patents are indexed as “Natural products, pharmaceutical”

=> E E14+ALL
E4 130655 --> Natural products, pharmaceutical/CT
       HNTE Valid heading during volume 126
       (1997) to present.
E5   207    OLD   Extracts/CT
E6    1    OLD   Galenicals/CT
E7  3814    OLD   Pharmaceutical natural products/CT
E8     OLD   Pharmaceuticals (L) Oriental/CT

(continued on next slide)
Used For (UF) terms reveal additional general terminology

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<td>UF</td>
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<td>UF</td>
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<td>Chinese materia medica/CT</td>
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All Used For (UF) terms are accommodated by using the CA index term **Natural products, pharmaceutical/CT**
Related terms point to other hierarchies of interest

| E39 23256 RT | Dietary supplements/CT |
| E40 3066 RT  | Medicinal plants/CT     |
| E41 4274 RT  | Traditional and alternative medicine/CT |
| E42 2121 RT  | Traditional medicine diagnostic patterns/CT |

```
=>  E MEDICINAL PLANTS+NT/CT
E1  3066  -->  Medicinal plants/CT
E2    74  NT1  Acalypha indica/CT
E3      1  NT1  Aconitum officinalis/CT
E4      1  NT1  Agrimonia officinalis/CT
E5      1  NT1  Alchemilla officinalis/CT
E6   1960  NT1  Alisma orientale/CT
E7    52  NT1  Alliaria petiolata/CT
E8  6217  NT1  Allium sativum/CT
E9      1  NT2  Allium sativum japonicum/CT
E10     0  NT2  Allium sativum nipponicum/CT
E11     2  NT2  Allium sativum opioscorodon/CT
E12    15  NT2  Allium sativum pekinense/CT
E13     4  NT2  Allium sativum sativum/CT
E14  3792  NT1  Aloe barbadensis/CT
```
Linked terms include specific taxonomic terminology

E43 LT Natural products, pharmaceutical (L) An Zhong San/CT
E44 LT Natural products, pharmaceutical (L) AnGong NiuHuang Wan/CT
E45 LT Natural products, pharmaceutical (L) Anna Pavala Sindhooram/CT
E46 LT Natural products, pharmaceutical (L) BaiDai Wan/CT
E47 LT Natural products, pharmaceutical (L) Bawei Wan/CT
E48 LT Natural products, pharmaceutical (L) BingPeng San/CT
E49 LT Natural products, pharmaceutical (L) BuZhongYiQi Tang/CT
E50 LT Natural products, pharmaceutical (L) BuZhongYiQi Wan/CT
E51 LT Natural products, pharmaceutical (L) Byakkokaninjinto/CT
E52 LT Natural products, pharmaceutical (L) Canova medicine/CT
E53 LT Natural products, pharmaceutical (L) Catuama/CT
E54 LT Natural products, pharmaceutical (L) ChaiHu/CT
E55 LT Natural products, pharmaceutical (L) ChanSu/CT
E56 LT Natural products, pharmaceutical (L) ChenXiang LuBaiLu Pian/CT
E57 LT Natural products, pharmaceutical (L) Chuan Bei Jing/CT
E58 LT Natural products, pharmaceutical (L) Colla Corii Asini/CT
E59 LT Natural products, pharmaceutical (L) DaChengQi Tang/CT
E60 LT Natural products, pharmaceutical (L) DaHuang/CT
Several approaches can be used to find natural product pharmaceuticals in the CAS databases on SciFinder

- **Plant or organism name**
  - Genus species
  - Common name

- **Extracted chemical name**

- **Substance class**

- **Medical condition**
  - Specific name – Hepatitis C Virus
  - Affected organ – Liver disease

- **Therapeutic use**
  - Antitumor agents
  - Immunostimulants
A SciFinder search on *Ligusticum Chuanxiong* obtains more than 9,000 references.
In-depth traditional medicine indexing is revealed in the full display of the SciFinder record.

**17. Chinese medicine plaster for treating rheumatoid arthritis-associated pain and preparation method thereof**

By: Li, Guabin; Li, Xiaolong; Wang, Yuezhang
Assignee: Peop. Rep. China


The prepn. method comprises extg. above Chinese medicine materials in medical oil at 100°C for 30 min, cooling, and storing in basement for 30 days. The prepn. process comprises a preparation method comprising: a) preparing a medicinal material comprising the above-described Chinese medicine materials; b) adding the medicinal material to the medical oil to obtain a medal oil; c) storing the medal oil in a basement for 30 days; d) cooling the medal oil; and e) storing the cooled medal oil in a basement for 30 days. The prepn. method comprises extg. above Chinese medicine materials in medical oil at 100°C for 30 min, cooling, and storing in basement for 30 days. The prepn. method comprises extg. above Chinese medicine materials in medical oil at 100°C for 30 min, cooling, and storing in basement for 30 days.

**Patent Information**

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<th>Patent No.</th>
<th>Kind</th>
<th>Date</th>
<th>Application</th>
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<td>Mar 2, 2011</td>
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<td>Oct 28, 2010</td>
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**Indexing**

Pharmaceuticals (Section 63)

**Concepts**

Resins

Olibanum: process for prepn. of Chinese medical plaster contg. many traditional Chinese medicines for treating rheumatoid arthritis-asssocd. pain, with rapid onset of drug action, definite and stable therapeutic effect, no toxic and side effects

Medical goods

Plasters: process for prepn. of Chinese medical plaster contg. many traditional Chinese medicines for treating rheumatoid arthritis-asscocd. pain, with rapid onset of drug action, definite and stable therapeutic effect, no toxic and side effects

Achyranthes bidentata
Analgesics
Angelica dahuica
Angelica sinensis
Asarum sieboldii
Commiphora myrrha
Curcuma phaeocaulis
Glycyrrhiza uralensis
Lycopodium japonicum
Panax notoginseng
Pinellia ternata
Rheumatoid arthritis
Saposhnikovia divaricata

process for prepn. of Chinese medical plaster contg. many traditional Chinese medicines for treating rheumatoid arthritis-assocd. pain, with rapid onset of drug action, definite and stable therapeutic effect, no toxic and side effects
SciFinder analysis and refinement tools use CA indexing to focus search results to the specific area of interest.

Select Show More to see complete list of CA index terms.

- Rheumatic diseases
- Epimedium
- Topical drug delivery systems
- Saposhnikovia divaricata
- Manis
- Morus (plant)
- Dipsacus
- Chrysanthemum
Categorize provides a more in-depth breakdown of the CA indexing by organism name, medical terms, or substances.

Select additional natural products to be included in the composition.

Select drug delivery method or therapeutic use.
Use alternative names for comprehensive taxonomic search results

- **Supplement common name with Genus species name**
  - Pacific yew 193 references
  - *Taxus brevifolia* 459 references
  - Concept Topic Candidate includes both for 558 references

- **Include spelling/spacing/order variations when searching Chinese names**
  - Huang Qi 139 references
  - Huangqi 865 references

- **Save and combine answer sets for maximum retrieval**
Many natural products are studied as antitumor agents

1. Medical application of 15-benzylidene-14-deoxy-11,12-dehydroandrographolide derivative in preparing antitumor agents
   By Dai, Guifu; Xu, Huanyi; Liu, Hongmin; Dong, Rujing; Yan, Jingzhi; Zhu, Liping; Li, Weiren; Jiang, Zhiyong; Wang, Yanan; Wu, Fengquan
   From Faming Zhuani Shendeng (2011), CN 101972247 A. 20110216. Language: Chinese; Database: CAPLUS

2. Method for manufacturing total flavonoids of Ornithogalum caudatum used in antineoplastic agents, antiinflammatory agents and analgesics
   By Sun, Jiaming; Gao, Lijiu; Li, Laijun
   From Faming Zhuani Shendeng (2011), CN 101972385 A. 20110216. Language: Chinese; Database: CAPLUS

3. Extraction process of total saponins of Doellingeria scabra used as immunopotentiator or antineoplastic agent
   By Liu, Dongfeng; Guo, Qin; Yang, Chengdong
   From Faming Zhuani Shendeng (2011), CN 101972200 A. 20110216. Language: Chinese; Database: CAPLUS

4. Natural products for preventing and treating cancer
   By Park, JI Shin

5. Peptidic compound having antitumor effect, and use of same
   By Sueyoshi, Kiyotaka; Teruya, Toshik; Sasaki, Hiroshi
Refine by index term and use Get Substances to obtain molecular structures isolated from natural products.
View Substance Detail for complete names, formula, structure, properties, and related information.

**CAS Registry Number:** 1258385-27-1

**C₃₁ H₇₂ O₇**

β-D-Glucopyranoside, 5-hydroxy-1-methylhexyl

6-Hydroxy-2-O-β-D-glucopyranosylheptane

*Absolute stereochemistry. Currently available stereo shown.*

**Source of Registration:** CA
Summary

• CAS files are a rich source of natural product information
• Traditional Medicine patents from China and other countries are covered with detailed indexing of concepts and substances
• Powerful tools including STN and SciFinder can be used to efficiently extract out and organize information
• This information can lead to further developments in isolating active ingredients from natural products or creating synthetic pathways to important pharmaceuticals