

Traditional medicine patents lead to enhanced drug discovery from natural products

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Spring 2011 ACS Meeting



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Markush structures covering organic and organometallic substances in patents

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Three main services provide access to CAS content



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

- **Artemisinin**
 - Became the preferred antimalarial treatment
 - Extracted from Sweet Wormwood *qinghao* (*Artemisia annua*)
- **Silybinin**
 - Originally used as hepatic 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

ANSWER 1 OF 1 CAPLUS COPYRIGHT 2011 ACS on STN
ACCESSION NUMBER: 2003:816610 CAPLUS
DOCUMENT NUMBER: 140:228088
TITLE: An over four millennium story behind qinghaosu
(artemisinin)-a fantastic antimalarial drug from a
traditional chinese herb
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
CODEN: CMCHE7; ISSN: 0929-8673
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

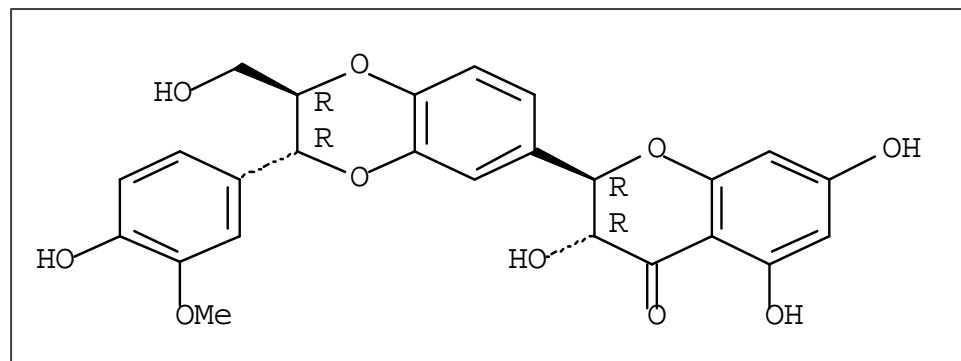
Milk Thistle has led the way to natural product drug development as treatment for hepatotoxicity



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

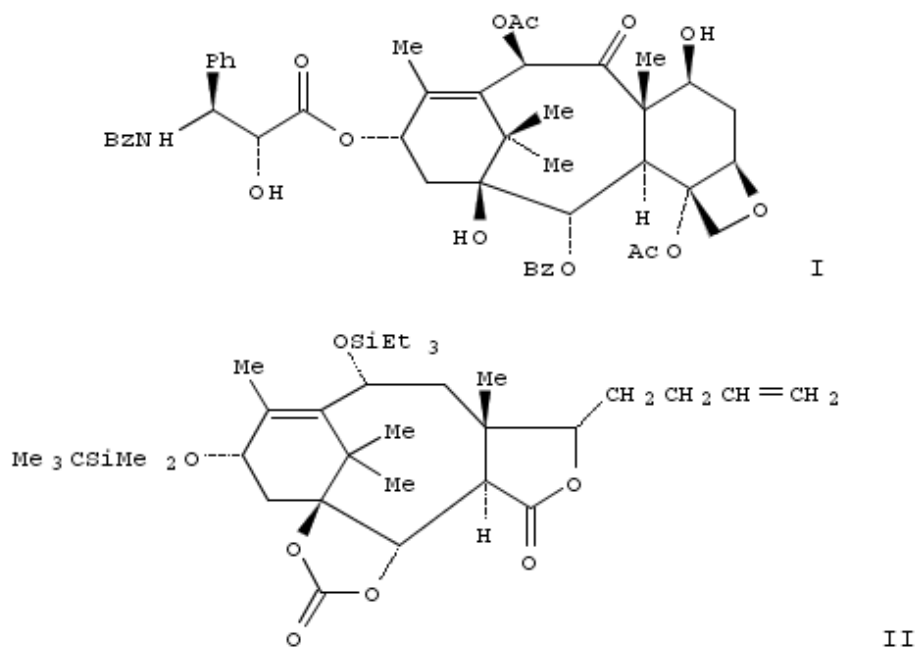
- **Paclitaxel** was originally isolated from the bark of the rare Pacific yew tree
 - The extraction method destroyed the tree and produced insufficient quantities for treating all cancer patients that may have benefited
 - Additionally, Bristol-Myers Squibb (BMS) held the patent rights for Taxol derived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

103. First total synthesis of taxol. 2. Completion of the C and D rings

By Holton, Robert A.; Kim, Hyeong Baik; Somoza, Carmen; Liang, Feng; Biediger, Ronald J.; Boatman, P. Douglas; Shindo, Mitsuru; Smith, Chase C.; Kim, Soekchan; et al. From *Journal of the American Chemical Society* (1994), 116(4), 1599-1600. Language: English, Database: CAPLUS

Completion of a total synthesis of the anti-tumor agent taxol (I) is described. These stages result in the conversion of the intermediate II having three rings in which six stereocenters of the natural product are set to taxol. Methods for cyclization of the C and D rings and final functionalization of taxol are described.



“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?

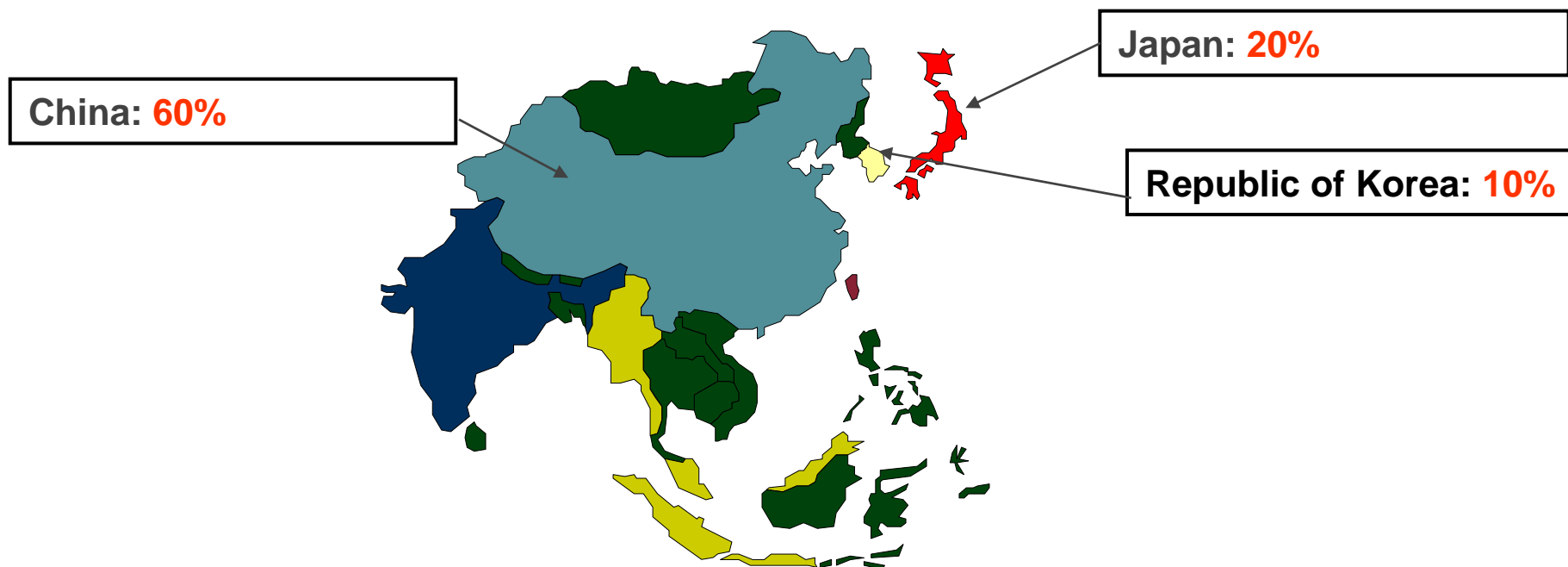
- Robust coverage of WTM content from multiple sources
- Continual enhancement of Asian coverage
- English translations of many “obscure” Asian-language patents and journal articles
- **CAplusSM**
 - 61 patent authorities, many smaller patent offices not always covered by others
 - 50,000 WTM patents 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



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

China, People's Republic of (CN)	Patent Kind Code	Publication Type
	A	Unexamined Application
	B	Examined Application
	C	Granted Patent
	U	Granted Utility Model (Starting April 7, 2010)
	Y	Granted Utility Model (2006 - April 6, 2010)

WTM patents include multi-stage and family information when available

=> FILE CAPLUS

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=> S CN 1122711 A/PNK; D ALL

L1 1 CN 1122711 A/PNK

The PNK field allows a kind code to be searched with the patent number for accurate retrieval.

L20 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2011 ACS o

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:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
-----	-----	-----	-----	-----
CN 1122711	A	19960522	CN 1995-108879	19950901 <--
CN 1056071	C	20000906		
PRIORITY APPLN. INFO.:			CN 1995-108879	19950901

Abstract text provides composition details which are reflected in the indexing

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

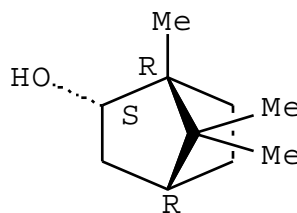
IT Analgesics
 Ascites
 Aspongopus
 Astragalus
 Atractylodes macrocephala
 Aucklandia
 Bupleurum
 Cirrhosis
 Edema
 Epimedium
 Fallopia japonica
 Hepatitis
 Ipomoea
 Tsatis
Ligusticum chuanxiong
 Liver disease
 Manis
 Natural products, pharmaceutical
 ●●●
 IT Abdominal disease
 (abdominal distention)
 IT Disease, animal
 (asthenia)
 IT Medical goods
 (bags)
 IT Viral hepatitis
 (chronic)
 ●●●
 IT **507-70-0**
 RL: BSU (Biological study unclassified);
 BIOL (Biological study)

CA Indexing includes:

- Taxonomic terms
- Disease terms
- Substance Class terms
- Specific substances



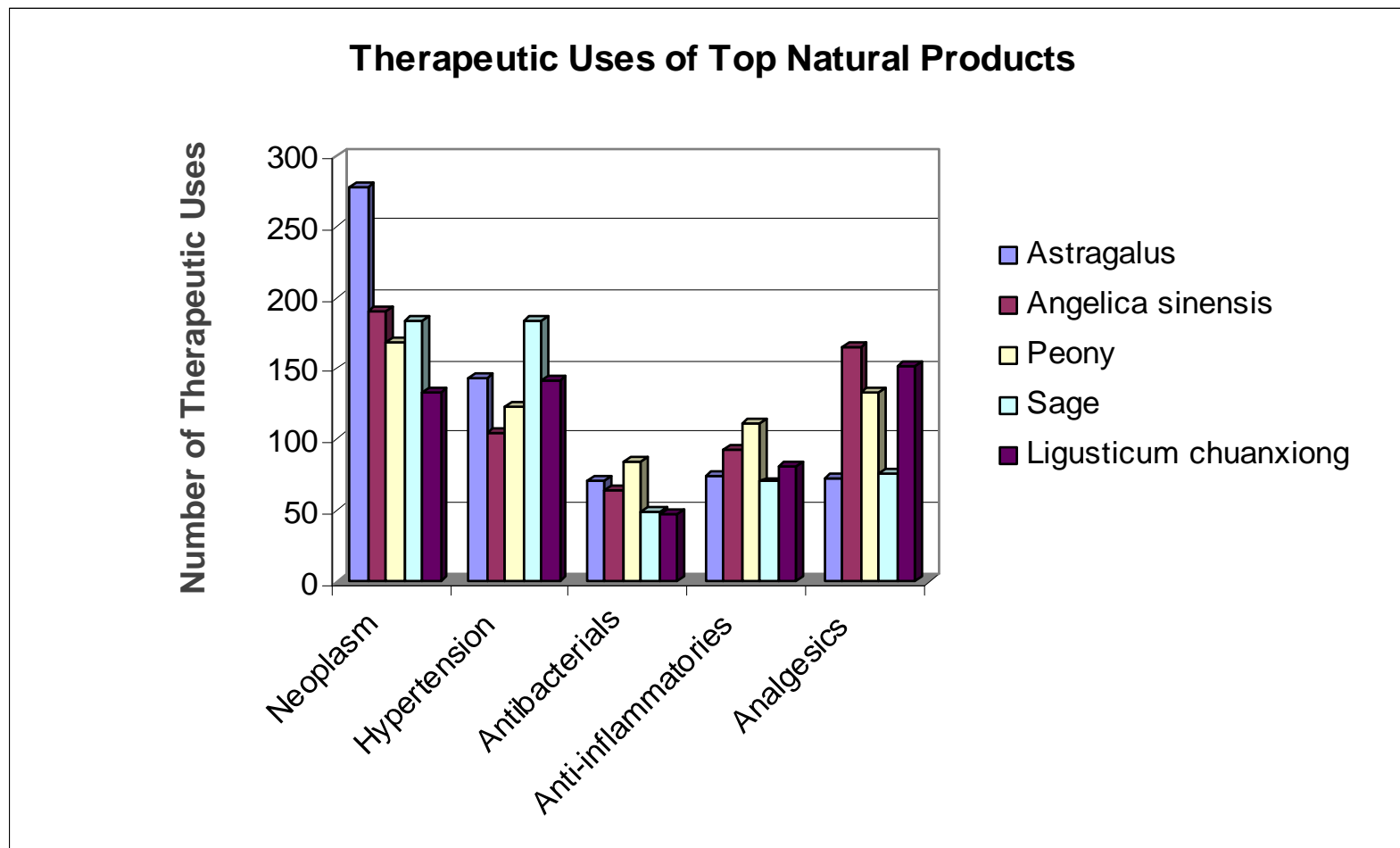
*Ligusticum
chuanxiong*



Borneol

(CAS Registry Number 507-70-0)

Many natural products are being studied for multiple therapeutic uses



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

CA Index Terms	Chemical Compound Classes	Taxonomic Vocabulary
<ul style="list-style-type: none"> • > 16,200 subject headings (index terms) • > 78,900 subject headings with linked terms • Related concepts • Date ranges of use for each term 	<ul style="list-style-type: none"> • > 11,280 frequently indexed substances • Frequently cited substances from the past year • Broader terms for each substance 	<ul style="list-style-type: none"> • > 244,400 controlled taxonomic terms • Relationships between taxonomy and broader or non-taxonomic vocabulary
<p style="text-align: center;">← Synonyms →</p>		

Expanding in the CA Lexicon reveals broader terms, narrower terms, and related terminology

```

=> E CHINESE CABBAGE+MAX/CT
E1      100276   BT3  Food/CT
E2      0       BT2  Plant-derived food (non-CA heading)/CT
E3      24742   BT1  Vegetable/CT
E4      2711    -->  Chinese cabbage/CT
                   HNTE Valid heading during volume 86 (1977) to present.
E5      0       OLD  Brassica chinensis pekinensis/CT
E6      860     OLD  Brassica pekinensis/CT
E7      1       OLD  Pakchoi (Brassica chinensis pekinensis)/CT
E8      0       OLD  Pakchoi (L) Brassica chinensis pekinensis/CT
E9      26      OLD  Pe-tsai/CT
E10     0       UF   BaiCai/CT
E11     0       UF   Brassica campestris pekinensis/CT
E12     0       UF   Brassica campestris pekinensis granaat/CT
E13     0       UF   Celery cabbage/CT
E14     0       UF   Napa cabbage/CT
E15     0       UF   Pechay/CT
E16     0       UF   Pekin cabbage/CT
E17     0       UF   Petsai/CT
E18     0       UF   Sinapis pekinensis/CT
E19     0       UF   ZiSu/CT
E20     1       NT1  Brassica pekinensis cylindrica/CT
E21     0       NT1  Brassica pekinensis dentata/CT
E22     3511    RT   Brassica oleracea capitata/CT
E23     703     RT   Brassica rapa chinensis/CT
E24     0       LT   Chinese cabbage (L) kimchi/CT
***** END *****

```

CPlus highlights traditional medicine with several focused controlled terms

```

=> E TRADITIONAL AND ALTERNATIVE MEDICINE+MAX/CT
E1      11628  BT1  Medicine/CT
E2      4274  --> Traditional and alternative medicine/CT
          HNTE Valid heading during volume 146 (2007) to present.
          NOTE A broad category of treatment systems used in lieu
                of or in supplement to modern medicine.
E3      UF    Alternative medicine/CT
E4      UF    Complementary medicine/CT
E5      UF    Complementary/alternative and traditional
                medicine/CT
E6      UF    Complementary/alternative medicine/CT
E7      UF    Ethnomedicine/CT
E8      UF    Folk medicine/CT
E9      UF    Holistic medicine/CT
E10     UF    Indigenous medicine/CT
E11     UF    Oriental medicine/CT
E12     UF    Primitive medicine/CT
E13     UF    Traditional medicine/CT
E14     130655 RT    Natural products, pharmaceutical/CT
E15     2121  RT    Traditional medicine diagnostic patterns/CT
E16     LT    Traditional and alternative medicine (L)
                Ayurvedic medicine/CT
E17     LT    Traditional and alternative medicine (L)
                Chinese medicine/CT

***** END *****

```

The CA Lexicon is an online thesaurus of controlled terminology available on STN

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          207   OLD Pharmaceuticals (L) Oriental/CT
```

(continued on next slide)

Used For (UF) terms reveal additional general terminology

E9	UF	Ayurvedic drugs/CT
E10	UF	Ayurvedic herbal medicine/CT
E11	UF	Ayurvedic herbs/CT
E12	UF	Ayurvedic medicine/CT
E13	UF	Chinese drugs/CT
	UF	Chinese herbal medicine/CT
	UF	Chinese materia medica/CT
	UF	Chinese medicine/CT
	UF	Chinese medicines/CT
	UF	Effective fractions/CT
	UF	Galenic pharmaceuticals/CT
	UF	Herbal drugs/CT
	UF	Herbal medicines/CT
E21	UF	Kampo/CT
E22	UF	Kampo/CT
E23	UF	Kampo pharmaceutical natural products/CT
E24	UF	Natural drugs/CT
E25	UF	Natural pharmaceuticals/CT
E26	UF	Natural product pharmaceuticals/CT
E27	UF	Oriental drugs/CT
E28	UF	Oriental pharmaceuticals/CT
E29	UF	Pharmaceuticals natural products/CT
E30	UF	Traditional Chinese medicines/CT
E31	UF	Traditional medicines/CT
E32	UF	

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

SciFinder - Research Topic Candidates - Windows Internet Explorer

https://scifinder.cas.org/scifinder/view/scifinder/scifinderExplore.jsf

Live Search

SciFinder - Research Topic Candi...

Explore References | Explore Substances | Explore Reactions

Welcome John A Zablski | Sign Out

Create Keep Me Posted | Research Topic "Ligusticum Chuanxiong"

Research Topic Candidates

2 Topics 1 Selected

Select All Deselect All

Research Topic Candidates	References
<input type="checkbox"/> 9335 references were found containing "Ligusticum Chuanxiong" as entered.	9335
<input checked="" type="checkbox"/> 9380 references were found containing the concept "Ligusticum Chuanxiong".	9380

Get References

Analysis Refine

Analyze by: Author Name

Click bar to view only those references within the current answer set

Wang Xinsuo	117
Wang Feng	103
Zheng Yongfeng	86
Wang Wenkui	74
Li Yongqiang	55
Wang Lijuan	43
Liu Lu	42
Yan Lijun	41
Yin Kehua	41
Li Xu	38

Show More

Categorize

More detailed analysis based on CAS indexing

4. Method for manufacturing traditional chinese medicine preparation for treating alopecia
By Ge, Deju; Zhou, Bing

Internet 100%

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, Guibin; Li, Xiaolong; Wang, Yuezhang

Assignee: Peop. Rep. China

Title Chinese medicine plaster is prepd. from *Ailanthus altissima* twig, *Salix b* twig, *Prunus persica* twig, *Angelica dahurica*, *Angelica sinensis*, *Paeonia rubra*, *glutinosa*, *Cinnamomum cassia*, *Rheum officinale*, *Momordica cochinchinensis*, *Commiphora myrrha*, *Ferula sinkiangensis*, *Glycyrrhiza uralensis*, *Curcuma longa*, **Ligusticum chuanxiong**, *Angelica pubescens*, *Achyranthes bidentata*, *Acanthop*, *Trogopterus xanthipes feces*, *Curcuma phaeocaulis*, *Asarum sieboldii*, each 2g, *Panax notoginseng* 30g; *Lycopodium japonicum*, *Astragalus membranaceus*, *S* g. 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 for treating rheumatoid arthritis-assocd. pain, with simple prepn. process, convenience in use, rapid effect, low curative cost, short curative duration, etc.

Patent Information

Patent No.	Kind	Date	Application
CN 101982195	A	Mar 2, 2011	CN 2010-10522519

Priority Application

CN 2010-10522519	Oct 28, 2010
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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-assocd. 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-assocd. pain, with rapid onset of drug action, definite and stable therapeutic effect, no toxic and side effects

<i>Achyranthes bidentata</i>	Analgesia
Analgesics	<i>Angelica dahurica</i>
<i>Angelica pubescens</i>	<i>Angelica sinensis</i>
<i>Asarum sieboldii</i>	<i>Astragalus membranaceus</i>
<i>Commiphora myrrha</i>	<i>Curcuma longa</i>
<i>Curcuma phaeocaulis</i>	<i>Ferula sinkiangensis</i>
<i>Glycyrrhiza uralensis</i>	Ligusticum chuanxiong
<i>Lycopodium japonicum</i>	Natural products, pharmaceutical
<i>Paeonia officinalis</i>	<i>Panax notoginseng</i>
<i>Pinellia ternata</i>	<i>Rheum officinale</i>
Rheumatoid arthritis	<i>Sanguisorba officinalis</i>
<i>Saposhnikovia divaricata</i>	<i>Scrophularia ningpoensis</i>

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

Analysis **Refine**

Analyze by: 

Index Term 

Click bar to view only those references within the current answer set


Ligusticum chuanxiong	6689
Natural products, pharmaceutical	6198
Angelica sinensis	3288
Salvia miltiorrhiza	1857
Glycyrrhiza	1458
Angelica dahurica	1334
Astragalus	1334
Rehmannia	1199
Carthamus	1187
Human	1147

Show More

Categorize


More detailed analysis based on CAS indexing

Categorize

Analysis - Index Term 

Only 1,000 Terms are displayed.

6434 Items 1 Selected

Sort by: **Frequency** 

Select bars to view only those references within the current answer set.

<input type="checkbox"/>	Pheretima	406
<input type="checkbox"/>	Panax notoginseng	404
<input checked="" type="checkbox"/>	Rheumatic diseases	404
<input type="checkbox"/>	Epimedium	401
<input type="checkbox"/>	Topical drug delivery systems	397
<input type="checkbox"/>	Saposhnikovia divaricata	395
<input type="checkbox"/>	Manis	392
<input type="checkbox"/>	Morus (plant)	392
<input type="checkbox"/>	Dipsacus	389
<input type="checkbox"/>	Chrysanthemum	385

Apply **Cancel**

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

Categorize provides a more in-depth breakdown of the CA indexing by organism name, medical terms, or substances

Categorize ⓘ

1. Select a heading and category. 2. Select index terms of interest.

Category Heading ⓘ	Category ⓘ	Index Terms ⓘ	Selected Terms ⓘ
All	Organisms (3096)	1 2 3 4 ... 31 Select All Deselect All	Click 'x' to remove the category from 'Selected Terms'
Biology	Animal pathology (356)	<input type="checkbox"/> Ligusticum chuanxiong 6694	<input checked="" type="checkbox"/> Biology > Organisms (2 Terms)
Biotechnology	Substances in biology (1752)	<input checked="" type="checkbox"/> Angelica sinensis 3282	
General chemistry	Anatomy (291)	<input type="checkbox"/> Sage (Salvia miltiorhiza) 1864	
Polymer chemistry	Processes & systems (153)	<input checked="" type="checkbox"/> Angelica dahurica 1334	
Technology	Immunology (82)	<input type="checkbox"/> Astragalus 1334	
Analytical chemistry	Substances in adverse effects (229)	<input type="checkbox"/> Rehmannia 1199	
Environmental chemistry	Endocrinology (100)	<input type="checkbox"/> Carthamus 1183	
Genetics & protein chemistry		<input type="checkbox"/> Cinnamomum 1875	
Synthetic chemistry			
Physical chemistry			
Catalysis			

Biology > Organisms > 2 Index Term(s) Selected

Select additional natural products to be included in the composition

Categorize ⓘ

1. Select a heading and category. 2. Select index terms of interest.

Category Heading ⓘ	Category ⓘ	Index Terms ⓘ	Selected Terms ⓘ
All	Medicine (206)	1 2 3	Click 'x' to remove the category from 'Selected Terms'
Biology	Substances in medicine (2095)	Select All Deselect All	<input checked="" type="checkbox"/> Biotechnology > Medicine (1 Term)
Biotechnology	Food (240)	<input type="checkbox"/> Anti-inflammatory agents 288	
General chemistry	Substances in biological uses (625)	<input type="checkbox"/> Drug delivery systems, powders 280	
Polymer chemistry	Substances in food chemistry (283)	<input type="checkbox"/> Immunostimulants 261	
Technology	Agriculture (39)	<input type="checkbox"/> Anesthesia 157	
Analytical chemistry	Substances in adverse effects (229)	<input type="checkbox"/> Antibacterial agents 148	
Environmental chemistry	Toxicology & forensics (23)	<input type="checkbox"/> Health products 144	
Genetics & protein chemistry	Substances in agriculture (87)	<input type="checkbox"/> Cardiovascular agents 132	
Synthetic chemistry		<input type="checkbox"/> Drug delivery systems, ointments 113	
Physical chemistry		<input type="checkbox"/> Cytoprotective agents 103	
Catalysis		<input checked="" type="checkbox"/> Drug delivery systems, transdermal 90	
		<input type="checkbox"/> Antirheumatic agents 82	
		<input type="checkbox"/> Antiviral agents 82	

Biotechnology > Medicine > 1 Index Term(s) Selected

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

SciFinder®

Explore References | Explore Substances | Explore Reactions

Welcome John A Zablski | Sign Out

Create Keep Me Posted | Research Topic "antitumor agents from natural ..." > references (1567) > refine "Patents only" (321)

References | Get Substances | Get Reactions | Get Cited | Get Citing | Get Full Text | Combine Answer Sets

321 References | 0 Selected | Keep Selected | Remove Selected | Remove Duplicates | Add Tags | Save | Print | Export

Select All | Deselect All | Sort by: Accession Number | Answers per Page [20] | 1 2 3 4 5 6 ... 17 | Display: [icon]

- 1. Medical application of 15-benzylidene-14-deoxy-11,12-dehydroandrographolide derivative in preparing antitumor agents**
By Dai, Guifu; Xu, Haiwei; Liu, Hongmin; Dong, Ruijing; Yan, Lijun; Zhu, Liping; Li, Weiyei; Jiang, Zhiwen; Wang, Yanan; Wu, Fengjuan
From Faming Zhuanli Shenqing (2011), CN 101972247 A 20110216. Language: Chinese, Database: CAPLUS
Substances Reactions Citing Full Text Link 0 Comments 0 Tags
- 2. Method for manufacturing total flavonoids of Ornithogalum caudatum used in antineoplastic agents, antiinflammatory agents and analgesics**
By Sun, Jiaming; Gao, Lu; Xiu, Laigui
From Faming Zhuanli Shenqing (2011), CN 101972385 A 20110216. Language: Chinese, Database: CAPLUS
Substances Reactions Citing Full Text Link 0 Comments 0 Tags
- 3. Extraction process of total saponins of Doellingeria scaber used as immunopotentiator or antineoplastic agent**
By Liu, Dongfeng; Guo, Qin; Yang, Chengdong
From Faming Zhuanli Shenqing (2011), CN 101972290 A 20110216. Language: Chinese, Database: CAPLUS
Substances Reactions Citing Full Text Link 0 Comments 0 Tags
- 4. Natural products for preventing and treating cancer**
By Park, Ui Sin
From Repub. Korean Kongkae Taeho Kongbo (2011), KR 2011014061 A 20110210. Language: Korean, Database: CAPLUS
Substances Reactions Citing Full Text Link 0 Comments 0 Tags
- 5. Peptidic compound having antitumor effect, and use of same**
By Suenaga, Kiyotake; Teruya, Toshiaki; Sasaki, Hiroaki
From PCT Int. Appl. (2011), WO 2011013612 A1 20110203. Language: Japanese, Database: CAPLUS
Substances Reactions Citing Full Text Link 0 Comments 0 Tags

Analysis | Refine

Analyze by: Index Term

Click bar to view only those references within the current answer set

Antitumor agents	299
Natural products, pharmaceutical	200
Human	110
Neoplasm	84
Solvent extraction	65
Lung, neoplasm	55
Drug delivery systems	52
Molecular structure, natural product	51
Mammary gland, neoplasm	46
Carcinoma	41

Refine by index term and use Get Substances to obtain molecular structures isolated from natural products

References **Get Substances** Get Reactions Get Cited Get Citing Get Full Text Combine Answer Sets

321 References 0 Selected Keep Selected Remove Selected Remove Duplicates Add Tags Save Print Export

51 references with the Index Terms **Molecular structure, natural product** are displayed Keep Analysis Clear Analysis

Select All Deselect All Sort by: Accession Number ↓ ↓ Answers per Page [20] 1 2 3 Display: [icon]

7. **Novel Streptomyces, macrocyclic compounds produced thereby, and antitumor agents, tumor cell invasion inhibitors, and antibacterial agents containing them**
By Igarashi, Yasuhiro; Iida, Takako; Miyanochi, Koji; Sudo, Yuri
From Jpn. Kokai Tokkyo Koho (2011), JP 2011010586 A 20110120. Language: Japanese, Database: CAPLUS
+Substances ▲Reactions 📄Citing

49. **Neobieslactone compound for application thereof**
By Zhang, Weidong; Su, Juan; Shan, Lei; Liu, ...
From Faming Zhuanli Shenqing Gongkai Shuor...
+Substances ▲Reactions 📄Citing

61. **Novel C8 side-chain hydrogen... prepare the medical preparations**
By Jiang, Xifei; Zheng, Jin
From Faming Zhuanli Shenqing Gongkai Shuor...
+Substances ▲Reactions 📄Citing

66. **Preparation of novobiocin ana disorders, autoimmune disorders,**
By Blagg, Brian
From U.S. Pat. Appl. Publ. (2009), US 20090...
+Substances ▲Reactions 📄Citing

Get Substances ⓘ

Retrieve substances for:

All references
 Selected references

Limit results to:

Adverse Effect, including toxicity Prophetics in Patents
 Analytical Study Preparation
 Biological Study Process
 Combinatorial Study Properties
 Formation, nonpreparative Reactant or Reagent
 Miscellaneous Uses
 Occurrence

Searching...

Analysis Refine

Analyze by: ⓘ

Index Term [v]

Click bar to view only those references within the current answer set

Antitumor agents	299
Natural products, pharmaceutical	200
Human	110
Neoplasm	84
Solvent extraction	65
Lung, neoplasm	55
Drug delivery systems	52
Molecular structure, natural product	51
Mammary gland, neoplasm	46

View Substance Detail for complete names, formula, structure, properties, and related information

Substance Detail [Get References](#) [Get Reactions](#) [Get Commercial Sources](#) [Get Regulatory Information](#)

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CAS Registry Number: 1258385-27-1

C₁₃ H₂₆ 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**

