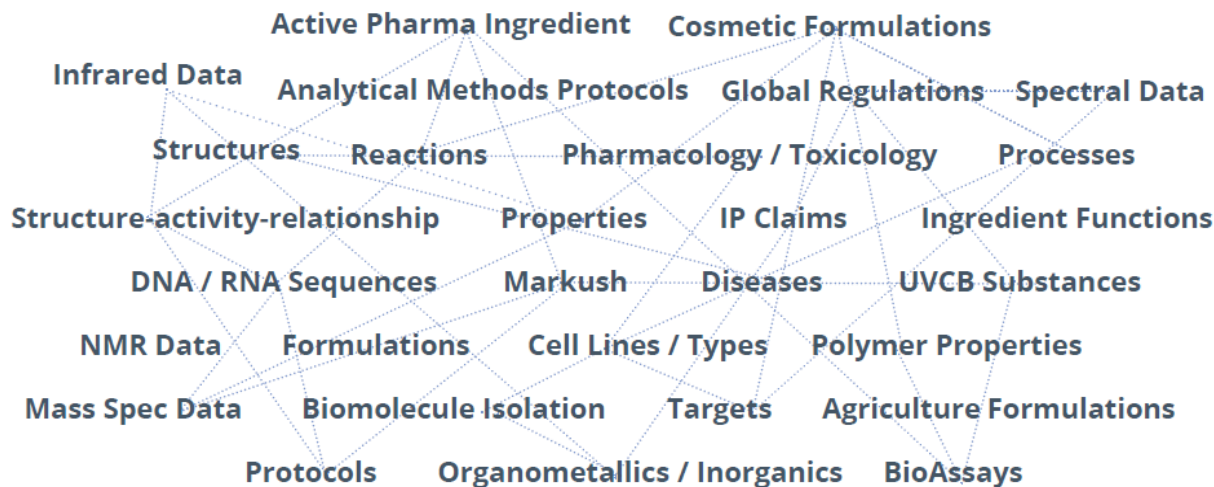
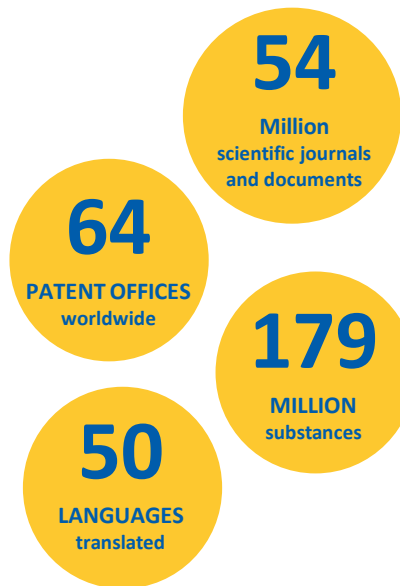


钱欣博士
cqian@acs-i.org
美国化学文摘社

SciFinderⁿ在天然药物化学研究方面的应用

SciFinderⁿ涵盖内容的独特性



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- 化学物质数量全球领先。目前收录的化学物质数量已超过1.79亿个，是进行新化合物确认的唯一可用资源。
- 生物大分子数量全球领先。目前收录来自期刊和专利中的约5.8亿条序列（包括蛋白、核酸）
- 由CAS创建的CAS登记号是化学物质的黄金标准；是对物质进行确认的唯一身份识别号；是在进行化学品进出口交易时，必须向相关国家管控机构提供的身份识别号；是在申报课题项目时，需向评议组提供的身份识别号
- CAS几乎收录了从高分子聚合物到纳米颗粒的所有类别的物质，包括有机物、无机物、聚合物、合金、矿物质、配合物、混合物、生物序列等

Sources: <https://www.cas.org/about/cas-content>

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- CAS不但收录专利中报道的确定结构的物质，还收录专利中的通式结构（马库什结构），帮助用户在使用CAS的数据后能够最大程度的避免专利法律风险
- 化学反应数量全球领先，目前收录的化学反应数量超过1.34亿条，是确认新的化学反应、工艺和方法时必不可缺的资源
- 近千名科学家每天阅读来自全球的科技文献，并根据CAS制定的规则 and 标准、从信息专家和科学家的角度对原文中重要的信息进行改写和标引，从而节省CAS的用户花在阅读、理解、总结科技原文文献所需的时间，将更多的时间投入到其他的工作中



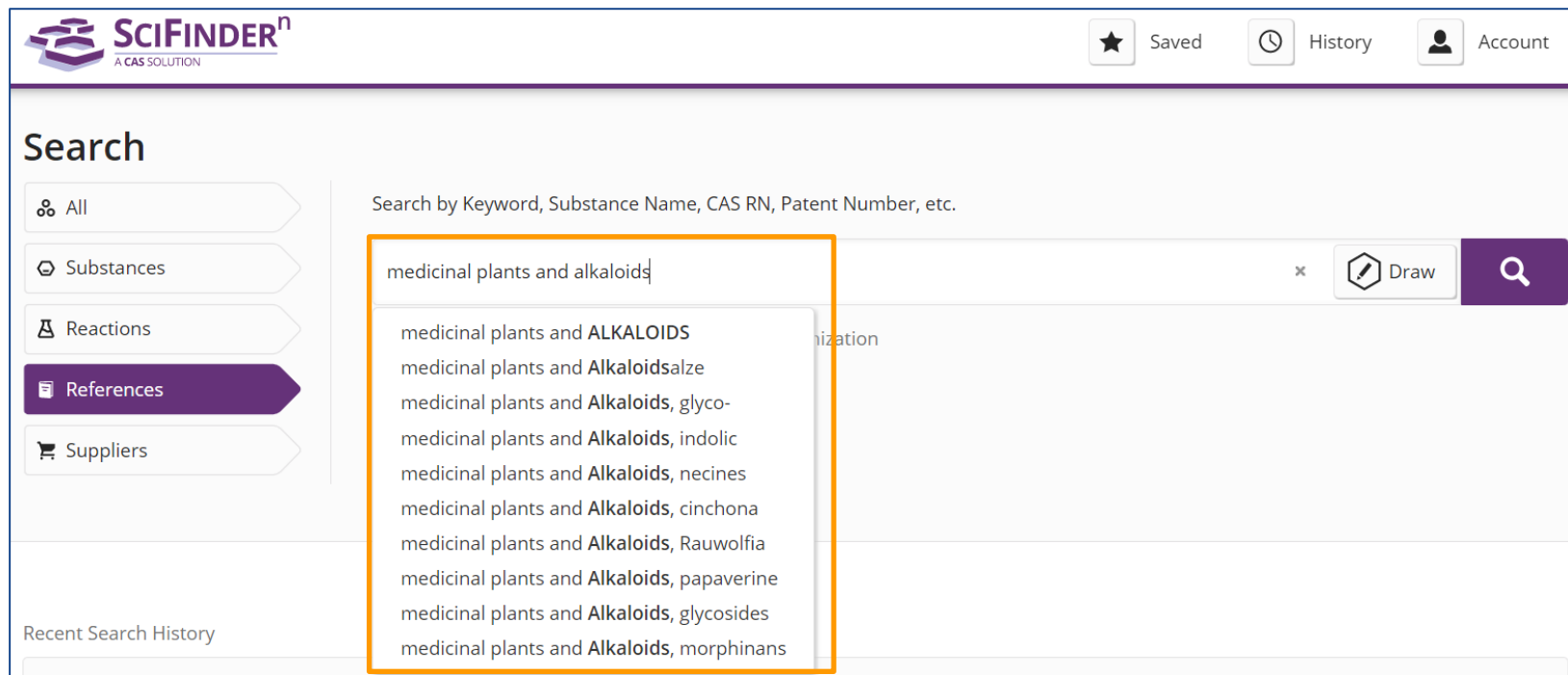
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大纲

- 天然活性成分的提取分离和活性研究
- 根据谱图信息来分析物质结构
- 骨架结构新颖性的确定
- 具有生物活性的衍生化结构检索
- 结构改造与合成

优选布尔逻辑运算符支持的文献主题检索，充分利用提示词启发检索思路



The screenshot displays the SciFinder search interface. On the left, a sidebar contains navigation options: All, Substances, Reactions, References (highlighted in purple), and Suppliers. The main search area features a text input field with the query "medicinal plants and alkaloids". A dropdown menu is visible below the input field, listing several search suggestions: "medicinal plants and ALKALOIDS", "medicinal plants and Alkaloidsalze", "medicinal plants and Alkaloids, glyco-", "medicinal plants and Alkaloids, indolic", "medicinal plants and Alkaloids, necines", "medicinal plants and Alkaloids, cinchona", "medicinal plants and Alkaloids, Rauwolfia", "medicinal plants and Alkaloids, papaverine", "medicinal plants and Alkaloids, glycosides", and "medicinal plants and Alkaloids, morphinans". The top of the interface includes the SciFinder logo, a "Saved" button, a "History" button, and an "Account" button. The bottom right corner features the CAS logo and the text "A DIVISION OF THE AMERICAN CHEMICAL SOCIETY".

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References medicinal plants and alkaloids

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References (29,838)

Sort: Relevance View: Partial Abstract

Substances Reactions Cited By

1

Alkaloid biosynthesis-the basis for metabolic engineering of medicinal plants

By: Kutchan, Toni M.
Plant Cell (1995), 7(7), 1059-70 | Language: English, Database: CPlus

A review with many references on the progress that has been made in the title area as a result of the fusion of alkaloids chem., enzymol., and mol. biol., as well as some perspectives for future developments.

Full Text Substances (0) Reactions (0)

2

Phytochemical constituents of some Nigerian medicinal plants

By: Edeoga, H. O.; Okwu, D. E.; Mbaebie, B. O.
African Journal of Biotechnology - ONLINE (2005), 4(7), 685-688 | Language: English, Database: CPlus

Alkaloids, tannins, saponins, steroid, terpenoid, flavonoids, phlobatannin and cardiac glycosides belonging to different families were assessed and compared. The medicinal plants studied were Emilia coccinea, Euphorbia heterophylla, Physalis angulata, Richardia spigelia anthelmia, Stachytarpheta cayennensis and Tradax procumbens. All the plants contained tannins and flavonoids except for the absence of tannins in S. acuta and flavonoids in Tradax procumbens.

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3

Medicinal plants and antimicrobial activity

By: Rios, J. L.; Recio, M. C.
Journal of Ethnopharmacology (2005), 100(1-2), 80-84 | Language: English, Database: CPlus

medicinal plants and alkaloids

41

Direct analysis of alkaloid profiling in plant tissue by using matrix-assisted laser desorption/ionization mass spectrometry

By: Wu, Wei; Liang, Zhitao; Zhao, Zhongzhen; Cai, Zongwei
Journal of Mass Spectrometry (2007), 42(1), 58-69 | Language: English, Database: CPlus

A method for the direct determination of alkaloid profiling in plant tissues by using matrix-assisted laser desorption/ionization time-of-flight mass spectrometry (MALDI-TOFMS) was developed. The alkaloid profiles of the herbs were obtained without the need for complicated sample preparation Exptl. results demonstrated that the direct MALDI-TOFMS anal. allowed rapid and reliable characterization of the components in plant tissues. Four commonly used Chinese medicinal herbs were studied, including Aconitum Carmichaeli Debx. (Fuzi in Chinese) and Processed Fuzi for herb differentiation and authentication.

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References ▾ "medicinal plants" and alkaloids × Draw 🔍 ★ ⌚ 👤

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一键获取文献中涉及的重要物质

☐ 1

Alkaloid biosynthesis-the basis for metabolic engineering of medicinal plants

By: Kutchan, Toni M.
Plant Cell (1995), 7(7), 1059-70 | Language: English, Database: CAPLUS

A review with many references on the progress that has been made in the title area as a result of the fusion of **alkaloids** chem., enzymol., and mol. biol., as well as some perspectives for future developments.

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☐ 2

Phytochemical constituents of some Nigerian medicinal plants

By: Edeoga, H. O.; Okwu, D. E.; Mbaebie, B. O.
African Journal of Biotechnology - ONLINE (2005), 4(7), 685-688 | Language: English, Database: CAPLUS

Alkaloids, tannins, saponins, steroid, terpenoid, flavonoids, phlobatannin and cardiac glycoside distribution in ten **medicinal plants** belonging to different families were assessed and compared. The **medicinal plants** investigated were Cleome nutidosperma, Emilia coccinea, Euphorbia heterophylla, Physalis angulata, Richardia bransitensis, Scopolia dulcis, Sida acuta, Spigelia anthelmia, Stachytarpheta cayennensis and Tridax procumbens. All the plants were found to contain **alkaloids**, tannins and flavonoids except for the absence of tannins in *S. acuta* and flavonoids in *S. cayennensis* resp. The signif...

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☐ 3

Medicinal plants and antimicrobial activity

By: Rios, J. L.; Recio, M. C.
Journal of Ethnopharmacology (2005), 100(1-2), 80-84 | Language: English, Database: CAPLUS

A review. In the present paper, we analyze the past, present and future of **medicinal plants**, both as potential antimicrobial

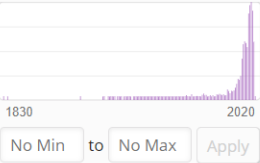
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- ☐ Alkaloids (3,425)
- ☐ Flavonoids (1,858)
- ☐ Tannins (1,591)
- ☐ Medicinal plants (1,494)
- ☐ Saponins (1,479)

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2

Phytochemical constituents of some Nigerian medicinal plants

By: Edeoga, H. O.; Okwu, D. E.; Mbaebie, B. O.
African Journal of Biotechnology - ONLINE (2005), 4(7), 685-688 | Language: English, Database: CPlus

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3

Medicinal plants and antimicrobial activity

By: Rios, J. L.; Recio, M. C.
Journal of Ethnopharmacology (2005), 100(1-2), 80-84 | Language: English, Database: CPlus

A review. In the present paper, we analyze the past, present and future of medicinal plants, both as potential antimicrobial crude drugs as well as a source for natural compounds that act as new anti-infection agents. In the past few decades, the search for new anti-infection agents has occupied many research groups in the field of ethnopharmacol. When we reviewed the number of articles published on the antimicrobial activity of medicinal plants in PubMed during the period between 1966 and 1994, we found 115; however, in the following decade between 1995 and 2004, this number more than doubled...

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Top Count Alphanumeric Search

6 Selected

<input checked="" type="checkbox"/> Alkaloids (3,425)	<input type="checkbox"/> Polyphenols (nonpolymeric) (229)	<input type="checkbox"/> Mineral elements (101)
<input type="checkbox"/> Flavonoids (1,858)	<input type="checkbox"/> Seed (206)	<input checked="" type="checkbox"/> Molecular structure (101)
<input type="checkbox"/> Tannins (1,591)	<input type="checkbox"/> Bark (200)	<input type="checkbox"/> Salmonella typhi (100)
<input type="checkbox"/> Medicinal plants (1,494)	<input type="checkbox"/> Klebsiella pneumoniae (185)	<input type="checkbox"/> Inflammation (99)
<input type="checkbox"/> Saponins (1,479)	<input type="checkbox"/> Bacillus subtilis (183)	<input type="checkbox"/> Lignroine (93)
<input type="checkbox"/> Pharmaceutical natural products (1,232)	<input type="checkbox"/> Fungicides (176)	<input type="checkbox"/> Oils (93)
<input checked="" type="checkbox"/> Steroids (986)	<input type="checkbox"/> Flower (174)	<input type="checkbox"/> Rhizome (91)
<input type="checkbox"/> Leaf (961)	<input checked="" type="checkbox"/> Antidiabetic agents (173)	<input type="checkbox"/> Gums and Mucilages (89)
<input checked="" type="checkbox"/> Terpenes (939)	<input type="checkbox"/> Plants (170)	<input type="checkbox"/> Metabolism, plant, second (89)
<input type="checkbox"/> Glycosides (925)	<input type="checkbox"/> Reducing sugars (161)	<input type="checkbox"/> Secondary metabolism, p (89)
<input type="checkbox"/> Carbohydrates (777)	<input type="checkbox"/> Essential oils (159)	<input type="checkbox"/> Resins (88)
<input type="checkbox"/> Phenols (745)	<input type="checkbox"/> Phytosterols (158)	<input checked="" type="checkbox"/> Antiviral agents (84)

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extract **Search**

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<input type="checkbox"/> Catharanthus roseus Linn. extract (1)	<input type="checkbox"/> Malt extract (1)	<input type="checkbox"/> Rosemary extract (1)
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<input type="checkbox"/> Grape seed extract (1)	<input type="checkbox"/> plant extract, Bidens pilosa (1)	<input type="checkbox"/> Yeast extract (3)
<input type="checkbox"/> Liver Extracts (1)	<input type="checkbox"/> Plant extracts (388)	

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extraction

3 Selected **萃取方法**

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<input type="checkbox"/> Extraction (57)	<input type="checkbox"/> Micro-matrix solid phase dispersive extraction (1)	<input type="checkbox"/> Soxhlet extraction (3)
<input type="checkbox"/> Extraction apparatus (1)	<input type="checkbox"/> Microwave extraction (3)	<input type="checkbox"/> Supercritical extraction (8)
<input type="checkbox"/> Liquid-liquid extraction (2)	<input checked="" type="checkbox"/> Solid phase extraction (7)	<input checked="" type="checkbox"/> Ultrasonic extraction (6)

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Concept ×

Top Count Alphanumeric **Search**

Concept Name
structure

3 Selected **分子结构, 构效关系等**

<input type="checkbox"/> Amorphous structure (1)	<input type="checkbox"/> Quantitative structure-activity relationship (1)	<input type="checkbox"/> Structure-activity relationship, bactericidal (1)
<input type="checkbox"/> Crystal structure (15)	<input type="checkbox"/> Quantitative Structure-Activity Relationship (1)	<input type="checkbox"/> Structure-activity relationship, cardiotoxic (1)
<input checked="" type="checkbox"/> Molecular structure (101)	<input type="checkbox"/> Secondary structure (2)	<input type="checkbox"/> Structure-activity relationship, enzyme-inhibiting (2)
<input checked="" type="checkbox"/> Molecular structure determination methods (1)	<input type="checkbox"/> Soil structure (1)	<input type="checkbox"/> Structure-activity relationship, leishmanicidal (1)
<input type="checkbox"/> Molecular structure determination methods, NMR spectrometric (1)	<input type="checkbox"/> Structure-activity relationship (37)	<input type="checkbox"/> Structure-activity relationship, toxic (1)
<input checked="" type="checkbox"/> Molecular structure, natural product (142)	<input type="checkbox"/> Structure-activity relationship, analgesic (1)	<input type="checkbox"/> Structure-activity relationship, vasodilating (1)
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 - Medicinal plants (1,494)
 - Saponins (1,479)
 - ☒ Molecular structure (101)
 - ☒ Molecular structure determination methods (1)
 - ☒ Molecular structure determination methods, NMR spectrometric (1)

References (103) Sort: Relevance ▾ View: Partial Abstract ▾

☐ Substances ▾ ☐ Reactions ▾ ☐ Cited By ▾

☐ 1

Pharmacological properties of some structurally related indole alkaloids contained in the Asian herbal medicines, hirsutine and mitragynine, with special reference to their Ca²⁺ antagonistic and opioid-like effects

By: Watanabe, Kazuo; Yano, Shingo; Horie, Syunji; Yamamoto, Leonardo Tomo; Takayama, Hiromitsu; Aimi, Norio; Sakai, Shin-ichiro; Ponglux, Dhavadee; Tongroach, Pavich; Shan, Jie; et al
Edited by Watanabe, Hiroshi; Shibuya, Takeshi
Pharmacological Research on Traditional Herbal Medicines No Source data available (1999), 163-177 | Language: English, Database: CAPLUS

The authors studied the pharmacol. properties of alkaloids isolated from the Chinese herbal medicine *Uncaria Ramulus* et *Uncaria rhynchophylla*. The authors were interested in the similarity of the chem. structure of mitragynine to those of *Uncaria alkaloids* such as hirsutine and dihydrocorynantheine. The structure requirements for analgesic action were received and a neuropharmacol. anal. of the mode of action of these indole alkaloids with such unique pharmacol. properties was performed.

☐ 2

Simultaneous HPLC determination of three bioactive alkaloids in the Asian medicinal plant *Stephania rotunda*.

By: Bory, Sothavireak; Bun, Sok-Siya; Baghdikian, Béatrice; Mabrouki, Fathi; Cheng, Sun Kaing; Elias, Riad; Bune, Hot; Ollivier, Evelyne
Natural product communications (2010), 5(6), 877-82 | Language: English, Database: MEDLINE

A reliable high-performance liquid chromatography (HPLC) method coupled with photodiode array detection has been developed and validated for the determination of three major alkaloids: cepharanthine, tetrahydropalmatine and xylopinine in *Stephania rotunda* Lour. (Menispermaceae) collected in Cambodia. The chromatographic separation was carried out on a

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Conference
Source

Pharmacological Research on Traditional Herbal Medicines
Pages: 163-177
Conference
1999

Database Information
Company/Organization

AN: 2000:4413
CAN: 132.273830
Capius

Faculty of Pharmaceutical Sciences
Chiba University
Chiba 263-0022
Japan

Publisher
Language

Harwood Academic Publishers
English

Pharmacological properties of some structurally related indole alkaloids contained in the Asian herbal medicines, hirsutine and mitragynine, with special reference to their Ca²⁺ antagonistic and opioid-like effects

By: Watanabe, Kazuo; Yano, Shingo; Horie, Syunji; Yamamoto, Leonardo Tomo; Takayama, Hiromitsu; Aimi, Norio; Sakai, Shin-Ichiro; Ponglux, Dhavadee; Tongroach, Pavich; Shan, Jie; et al
Edited by Watanabe, Hiroshi; Shibuya, Takeshi
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Abstract: The authors studied the pharmacol. properties of **alkaloids** isolated from the Chinese herbal medicine Uncariae Ramulus et Uncus (Uncaria rhynchophylla). The authors were interested in the similarity of the chem. structure of mitragynine to those of Uncaria **alkaloids** such as hirsutine and dihydrocorynantheine. The structure requirements for analgesic action were received and a neuropharmacol. anal. of the mode of action of these indole **alkaloids** with such unique pharmacol. properties was performed.

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Concepts

Calcium channel blockers

Calcium channels
Role: Biological Study, Unclassified

Indole alkaloids
Role: Adverse Effect, Including Toxicity, Biological Activity or Effector, Except Adverse; Biological Study, Unclassified; Properties; Therapeutic Use

Medicinal plants

Mitragyna

Molecular structure

Opioid receptors
Role: Biological Study, Unclassified

Pharmaceutical natural products
Role: Adverse Effect, Including Toxicity, Biological Activity or Effector, Except Adverse; Biological Study, Unclassified; Properties; Therapeutic Use

Signal transduction

Structure-activity relationship, analgesic

Uncaria rhynchophylla

Vascular smooth muscle

Vasodilation

Substances

7440-70-2

Ca
Calcium

Role: Biological Study, Unclassified, Biological Study

57-27-2

C₁₇H₁₉NO₃
Morphine

Role: Adverse Effect, Including Toxicity, Biological Use, Unclassified, Biological Study, Uses

7729-23-9

C₂₂H₂₈N₂O₃
Hirsutine

Role: Adverse Effect, Including Toxicity, Biological Activity or Effector, Except Adverse, Biological Study, Unclassified, Properties, Therapeutic Use, Biological Study, Uses

50439-68-4

C₂₂H₂₈N₂O₃
Dihydrocorynantheine

Role: Adverse Effect, Including Toxicity, Biological Activity or Effector, Except Adverse, Biological Study, Unclassified, Properties, Therapeutic Use, Biological Study, Uses

Search Within Results

× analysis

4

In vitro antimicrobial activity and phytochemical analysis of some indian medicinal plants

By: Parekh, Jigna; Chanda, Sumitra V.

Turkish Journal of Biology (2007), 31(1), 53-58 | Language: English, Database: CAPlus

| [MethodsNow: Analysis](#)

The antibacterial effect of some selected Indian medicinal plants was evaluated on bacterial strains like *Bacillus cereus* ATCC11778, *Staphylococcus aureus* ATCC25923, *Enterobacter aerogenes* ATCC13048, *Escherichia coli* ATCC25922 and *Klebsiella pneumoniae* NCIM2719. The solvents used for the extraction of plants were water and methanol. The in vitro antibacterial activity was performed by agar disk diffusion and agar well diffusion method. The most susceptible Gram-pos. bacteria was *B. cereus*, while the most susceptible Gram-neg. bacteria was *K. pneumoniae*. The extracts of *Abrus precatorius*, *Cardi...*

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Reactions (0)

Cited By (194)

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5

Separation and identification of Aconitum alkaloids and their metabolites in human urine

By: Zhang, Hong-Gui; Sun, Ying; Duan, Ming-Yu; Chen, Yu-Juan; Zhong, Da-Fang; Zhang, Han-Qi

Toxicol (2005), 46(5), 500-506 | Language: English, Database: CAPlus

| [MethodsNow: Analysis](#)

To study the safety of Aconitum medicinal herbs in clinic and identify Aconitum alkaloids poisoning in forensic medicine, Aconitum alkaloids and their metabolites were separated and identified in human urine by liquid chromatog.-electrospray ionization-multi-stage mass spectrometry (LC-ESI-MSⁿ) and chem. pathway of metabolism was investigated. The alkaloids and their metabolites in the urine sample were extracted with solid-phase cartridges and separated by HPLC with acetonitrile-water-formic acid (40:60:0.5) mobile phase. Structures of five metabolites and three parent Aconitum alkaloids were...

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Substances (8)

Reactions (0)

Cited By (67)

Citation Map

6

Qualitative and quantitative analysis of phytochemicals of Taraxacum officinale

By: Mir, M. Amin; Sawhney, S. S.; Jassal, M. M. S.

Wudpecker Journal of Pharmacy and Pharmacology (2013), 2(1), 1-5 | Language: English, Database: CAPlus

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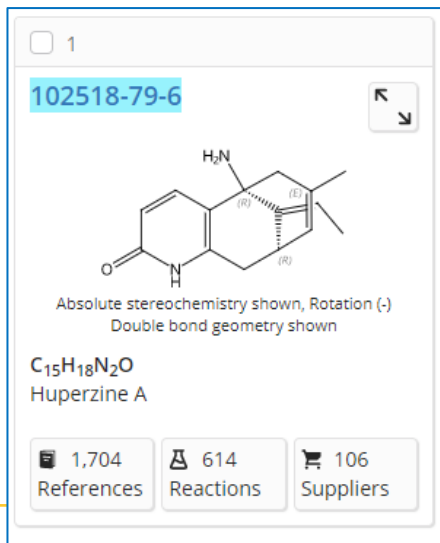
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☐ Report (2)

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Substance Role

☐ Adverse Effect (48)

☐ Analytical Study (123)

☐ Biological Study (1,417)

☐ Formation (3)

☐ Miscellaneous (1)

☐ Nanoscale (7)

☐ Occurrence (47)

☐ Preparation (258)

☐ Process (57)

☐ Properties (112)

☐ Reactant or Reagent (45)

☐ Uses (1,096)

[View Fewer](#)

References (1,704)

Sort: Relevance View: Full Abstract

☐ Substances ☐ Reactions ☐ Cited By

☐ 1

Structure of acetylcholinesterase complexed with the nootropic alkaloid, (-)-huperzine A

By: Raves, Mia L.; Harel, Michal; Pang, Yuan-Ping; Silman, Israel; Kozikowski, Alan P.; Sussman, Joel L.
Nature Structural Biology (1997), 4(1), 57-63 | Language: English, Database: CAPLUS and MEDLINE

(-)-Huperzine A (HupA) is found in an extract from a club moss that has been used for centuries in Chinese folk medicine. Its action has been attributed to its ability to strongly inhibit acetylcholinesterase (AChE). The crystal structure of the complex of AChE with optically pure HupA at 2.5 Å resolution shows an unexpected orientation for the inhibitor with surprisingly few strong direct interactions with protein residues to explain its high affinity. This structure is compared to the native structure of AChE devoid of any inhibitor as determined to the same resolution. An anal. of the affinities of structural analogs of HupA, correlated with their interactions with the protein, shows the importance of individual hydrophobic interactions between HupA and aromatic residues in the active-site gorge of AChE.

Full Text

Substances (2)

Reactions (0)

Cited By (355)

Citation Map

☐ 2

Efficacy of tablet huperzine-A on memory, cognition, and behavior in Alzheimer's disease

By: Xu, Si-Sun; Gao, Zhi-Xu; Weng, Zheng; Du, Zun-Ming; Xu, Wei-An; Yang, Jian-Shen; Zhang, Ming-Lian; Tong, Zhen-Hua; Fang, Yong-Sheng
Zhongguo Yaoli Xuebao (1995), 16(5), 391-5 | Language: English, Database: CAPLUS and MEDLINE

The aim of the study was to evaluate the efficacy and safety of tableted huperzine-A (Hup) in patients with Alzheimer's disease. Using a multicenter, prospective, double-blind, parallel, placebo controlled and randomized method, 50 patients were administered orally 0.2 mg (4 tablets) Hup and 53 patients were given po 4 tablets of placebo bid for 8 wk. All patients were evaluated with Wechsler memory scale, Hasegawa dementia scale, mini-mental state examination scale, activity of daily living scale, treatment emergency symptom scale, and measured with BP, HR, ECG, EEG, ALT, AKP, BUN, Cr, Hb, WBC, and urine routine. About 58% (29/50) of patients treated with Hup showed improvements in their memory ($P < 0.01$), cognitive ($P < 0.01$), and behavioral ($P < 0.01$) functions. The efficacy of Hup was better than placebo (36%, 19/53) ($P < 0.05$). No severe side effect was found. Hup is a promising drug for symptomatic treatment of Alzheimer's disease.

Full Text

Substance (1)

Reactions (0)

Cited By (105)

Citation Map

7

通过Concept，快速聚焦关注的技术领域，获取所需信息

Filter by

- Document Type
- Substance Role
- Language
- Publication Year
- Available at My Institution
- Author
- Organization
- Publication Name
- Concept**
 - Alkaloids (508)
 - Cholinesterase inhibitors (478)
 - Homo sapiens (465)
 - Human (465)
 - Alzheimer disease (449)
 - [View All](#)
- CAS Solutions
- Formulation Purpose
- Database
- Search Within Results

References (1,704)

☐ Substances ☐ Reactions

1

Structure of acetylcholinesterase con
By: Raves, Mia L.; Harel, Michal; Pang, Yuan-Ping; Nature Structural Biology (1997), 4(1), 57-63 | Lar

(-)-Huperzine A (HupA) is found in an extract from has been attributed to its ability to strongly inhibi optically pure HupA at 2.5 Å resolution shows an interactions with protein residues to explain its h inhibitor as determined to the same resolution Å interactions with the protein, shows the importan the active-site gorge of AChE.

Full Text

2

Efficacy of tablet huperzine-A on mer
By: Xu, Si-Sun; Gao, Zhi-Xu; Weng, Zheng; Du, Zun Sheng Zhongguo Yaoli Xuebao (1995), 16(5), 391-5 | Lar

The aim of the study was to evaluate the efficacy Using a multicenter, prospective, double-blind, pa orally 0.2 mg (4 tablets) Hup and 53 patients were Wechsler memory scale, Hasegawa dementia sca emergency symptom scale, and measured with B of patients treated with Hup showed improve

Concept

Top Count Alphanumeric Search

Concept Name

extraction

提取

Search

☐ Select All on Page

<input type="checkbox"/> Countercurrent extraction (2)	<input type="checkbox"/> Extraction apparatus (32)	<input type="checkbox"/> Solvent extraction (30)
<input type="checkbox"/> DNA extraction (1)	<input type="checkbox"/> Liquid-liquid extraction (1)	<input type="checkbox"/> Supercritical extraction (3)
<input type="checkbox"/> Extraction (40)	<input type="checkbox"/> Solid phase extraction (1)	<input type="checkbox"/> Ultrasonic extraction (10)

Concept

Top Count Alphanumeric Search

Concept Name

process

工艺

Search

☐ Select All on Page

<input type="checkbox"/> Coating process (4)	<input type="checkbox"/> Drying process (7)	<input type="checkbox"/> Spray drying process (14)
<input type="checkbox"/> Concentration (process) (5)	<input type="checkbox"/> Fluidized-bed coating process (1)	<input type="checkbox"/> Vacuum drying process (4)
<input type="checkbox"/> Dehydration process (7)	<input type="checkbox"/> Process automation (1)	

Concept

Top Count Alphanumeric Search

Concept Name

HPLC

HPLC

Search

☐ Select All on Page

<input type="checkbox"/> Affinity HPLC (1)	<input type="checkbox"/> HPLC-tandem mass spectrometry (2)	<input type="checkbox"/> Reversed phase HPLC stationary phases (1)
<input type="checkbox"/> HPLC (57)	<input type="checkbox"/> Preparative HPLC (1)	<input type="checkbox"/> Reversed-phase ion pair HPLC (1)
<input type="checkbox"/> HPLC stationary phases (1)	<input type="checkbox"/> Reversed-phase HPLC (15)	

大纲

- 天然活性成分的提取分离和活性等研究
- 根据谱图信息来分析物质结构
- 骨架结构新颖性的确定
- 具有生物活性的衍生化结构检索
- 结构改造与合成

例1：已知质谱和核磁谱图信息，分析天然活性成分的结构

Substance Property

Select Property

Molecular Weight

Enter Value

399 to 401

Results based on predicted properties only.

46.07
125 to 350
>300

Add Another Property

— AND —

Experimental Spectra

Select Spectrum

Carbon-13 NMR


Enter Value

158, 139.6, 128.9, 79.4

(Search includes allowance of ± 2 ppm)

Example: 152.3, 127.6, 133.1
155.02 to 207.59
187

Add Another Spectra



Clear All

根据example中提供的格式，输入谱峰值或者数值范围。



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点击CAS RN查看具体的谱图信息; 根据Experimental Spectra查看其他谱图研究信息

Filter by

Commercial Availability

☐ Available (2)
 ☐ Not Available (2)

Reaction Role

☐ Product (4)
 ☐ Reactant (1)

Reference Role

☐ Biological Study (1)
 ☐ Preparation (4)
 ☐ Properties (1)
 ☐ Reactant or Reagent (2)
 ☐ Uses (1)

Stereochemistry

Number of Components

Substance Class

Isotopes

Metals

Molecular Weight

Experimental Spectrum

☐ Carbon-13 NMR (4)
 ☐ Mass (2)
 ☐ Proton NMR (1)

Regulatory Information

Bioactivity Indicator

Search Within Results


Substances (4)

Sort: Relevance

View Partial

1

245726-48-1



Relative stereochemistry shown
Double bond geometry shown

C₂₅H₃₄N₂O₃

rel-(aZ)-a-[(4R,5S)-4,5-Dihydro-4-methyl-5-phenyl-1H-pyrazol-3-yl]methylene]-2-...

2

References

1


Reaction

0

Suppliers

2

1374017-64-7



Absolute stereochemistry shown

C₂₄H₃₂NO₄

Pyridine, 2,4-dimethoxy-5-phenyl-3-[(2R,3R,5S,6R)-tetrahydro-3,5-dimethyl-6-[[1R...]]methylene]-2-pyridine

1

Reference

1

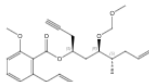
Reaction

1

Suppliers

3

850715-38-7



Absolute stereochemistry shown, Rotation (+)

C₂₄H₃₂O₅

Benzoic acid, 2-methoxy-6-(2-propen-1-yl)-, (1S,3R,4S)-3-(methoxymethoxy)-4-meth...

1

Reference

12


Reactions

0

Suppliers

4

198267-89-9



Double bond geometry shown

C₂₂H₂₂NO₆

2-Butenedioic acid, 2-[(4-methoxyphenyl)(2-methoxy-2-phenylethyl)amino]-, 1,4-di...

1

Reference

1

Reaction

1

Suppliers

Carbon-13 NMR Spectrum Detail (1 of 1)

Chemical Structure: Cc1ccc(cc1)-c2cc3c(cc2)cc4c(c3)ccccc4
 Relative stereochemistry shown
 Double bond geometry shown

CAS Registry Number: 245726-48-1
Formula: C₂₀H₁₄N₂O₃

CAS Name: *rel*-(2*Z*)-α-[(4*R*,5*S*)-4,5-Dihydro-4-methyl-5-phenyl-1*H*-pyrazol-3-yl]methyl-2-hydroxy-6-phenylmethoxybenzenemethanol

Spectrum Summary		Conditions	
Spectrum ID	6TETB99_117.C	Working Frequency	75 MHz
Peak Data	157.9, 157.1, 148.4, 144.7, 140.9, 136.9, 128.7, 128.6, 128.5 (2C), 128.3 (2C), 128.1, 127.7 (2C), 126.5 (2C), 110.3, 107.0, 105.9, 103.1, 77.5, 70.8, 37.5, 14.2 ppm	Solvent	Chloroform- <i>d</i> (855-49-6)
Source	Spectral data were obtained from Advanced Chemistry Development, Inc.		

再通过Bioactivity Indicator, 查看对应的活性研究信息

- Stereochemistry
- Number of Components
- Substance Class
- Isotopes
- Metals
- Molecular Weight
- Experimental Spectrum
- Regulatory Information
- Bioactivity Indicator**
 - Anti-infective agents (1)
 - Antitumor agents (1)
- Search Within Results

850715-38-7

Absolute stereochemistry shown, Rotation (+)

C₂₄H₃₂O₅
Benzoic acid, 2-methoxy-6-(2-propen-1-yl)-, (1S,3R,4S)-3-(methoxymethoxy)-4-methoxy-...

1

12

0

Reference

Reactions

Suppliers

1374017-64-7

Absolute stereochemistry shown

C₂₄H₃₃NO₄
Pyridine, 2,4-dimethoxy-5-phenyl-3-[(2R,3R,5S,6R)-tetrahydro-3,5-dimethyl-6-[[1R...]]

1

1

1

Reference

Reaction

Supplier

245726-48-1

Relative stereochemistry shown, Double bond geometry

C₂₅H₂₄N₂O₃
rel-(αZ)-α-[[[(4R,5S)-4,5-Dihydro-5-methyl-1H-pyrazol-2-yl]methylene]-2-...

2

1

References

Reaction

198267-89-9

Double bond geometry shown

C₂₂H₂₅NO₆
2-Butenedioic acid, 2-[(4-methoxyphenyl)(2-methoxy-2-phenylethyl)amino]-, 1,4-di-...

4

Filter by

- Commercial Availability
- Reaction Role
- Reference Role
- Stereochemistry
- Number of Components
- Substance Class
- Isotopes
- Metals
- Molecular Weight
- Experimental Spectrum
- Regulatory Information
- Bioactivity Indicator**
 - Anti-infective agents (1)
 - Antitumor agents (1)
- Search Within Results

Substances (1)

References

Reactions

Suppliers

1

1374017-64-7

Absolute stereochemistry shown

C₂₄H₃₃NO₄
Pyridine, 2,4-dimethoxy-5-phenyl-3-[(2R,3R,5S,6R)-tetrahydro-3,5-dimethyl-6-[[1R...]]

1

1

1

Reference

Reaction

Supplier

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23

一键获得对应的研究文献

The screenshot displays the SciFinder web interface. At the top, there is a search bar with the text 'Substances' and 'Enter a query...'. To the right of the search bar are icons for 'Draw', a magnifying glass, a star, a clock, and a user profile. Below the search bar, there is a 'Return to Home' link. On the left side, there is a 'Filter by' section with various categories: Commercial Availability, Reaction Role, Reference Role, Stereochemistry, Number of Components, Substance Class, Isotopes, Metals, Molecular Weight, Experimental Spectrum, Regulatory Information, and Bioactivity Indicator. The 'References' dropdown menu is highlighted with a yellow box, showing options for 'All Results' and 'Selected Results'. The main content area is titled 'Substances (4)' and shows three search results. Each result includes a chemical structure, a title, a molecular formula, and a list of references, reactions, and suppliers.

Substances (4)

Sort: Relevance View Partial

References

Get References for Substances

All Results Selected Results

1374017-64-7

Absolute stereochemistry shown, Rotation (+)

$C_{24}H_{32}O_5$
Benzoic acid, 2-methoxy-6-(2-propen-1-yl)-, (1S,3R,4S)-3-(methoxymethoxy)-4-meth...

1 Reference 12 Reactions 0 Suppliers

245726-48-1

Relative stereochemistry shown
Double bond geometry shown

$C_{25}H_{24}N_2O_3$
rel-(αZ)- α -[[[(4R,5S)-4,5-Dihydro-4-methyl-5-phenyl-1H-pyrazol-3-yl]methylene]-2-...

2 References 1 Reaction 0 Suppliers



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根据文献详情判断文献主旨

Filter by

Document Type

☐ Journal (5)
 ☐ Review (1)

Substance Role

☐ Biological Study (1)
 ☐ Preparation (5)
 ☐ Properties (1)
 ☐ Reactant or Reagent (2)
 ☐ Uses (1)

Language

☐ English (5)

Publication Year

1997

2012

No Min

to

No Max

Apply

References (5)

Sort: Relevance View: Partial Abstract

☐ Substances
 ☐ Reactions
 ☐ Cited By

☐ 1

Antiprotozoal and Antimicrobial Compounds from the Plant Pathogen *Septoria pistaciarum*

By: Kumarihamy, Mallika; Khan, Shabana I.; Jacob, Melissa; Tekwani, Babu L.; Duke, Stephen O.; Ferreira, Daneel; Nanayakkara, N. P. Dhammika
 Journal of Natural Products (2012), 75(5), 883-889 | Language: English, Database: CAPLUS

1

R₁

CH₃

2

CH₃

R₂

CH₂OH

3

CH₃

R₃

H

4

CH₃

R₄

CH₃

5

R₁

H

6

R₂

H

7

OAc

8

OAc

Four new 1,4-dihydroxy-5-phenyl-2-pyridinone alkaloids, 17-hydroxy-N-(O-methyl)septoriamycin A (1), 17-acetoxy-N-(O-methyl)septoriamycin A (2), 13-(S)-hydroxy-N-(O-methyl)septoriamycin A (3), and 13-(R)-hydroxy-N-(O-methyl)septoriamycin A (4), together with the known compounds (+)-cercosporin (5), (+)-14-O-acetylcerosporin (6), (+)-di-O-acetylcerosporin (7), lumichrome, and brassicasterol, were isolated from an Et acetate extract of a culture medium of *Septoria pistaciarum*. Methylation of septoriamycin A (8) with diazomethane yielded three di-O-Me analogs, two of which existed as mixtures of...

View More

Full Text

Substances (14)

Reactions (2)

Cited By (16)

Citation Map

Synthesis and molecular structure of 3-(2-benzyloxy-6-hydroxyphenyl)-5-styrylpyrazoles.



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Reference Detail (1 of 5)

Substances (14)

Reactions (2)

Cited By (16)



Citation Map



Save

Journal

Source

Journal of Natural Products

Volume: 75

Issue: 5

Pages: 883-889

Journal

2012

DOI:

[10.1021/jp200940b](https://doi.org/10.1021/jp200940b)

Database Information

AN: 2012:611017

CAN: 156:583096

CAPUS

[View MEDLINE Reference](#)

Company/Organization

National Center for Natural Products Research, Research Institute of Pharmaceutical Sciences, and Department of Pharmacognosy, School of Pharmacy
The University of Mississippi
University, Mississippi 38677
United States

Publisher

American Chemical Society-
American Society of
Pharmacognosy

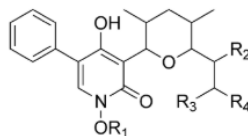
Language

English

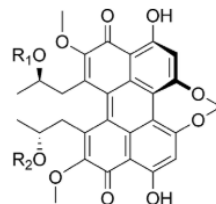
Antiprotozoal and Antimicrobial Compounds from the Plant Pathogen *Septoria pistaciarum*

By: Kumarihamy, Mallika; Khan, Shabana I.; Jacob, Melissa; Tekwani, Babu L.; Duke, Stephen O.; Ferreira, Daneel; Nanayakkara, N. P. Dhammika

Abstract: Four new 1,4-dihydroxy-5-phenyl-2-pyridinone alkaloids, 17-hydroxy-N-(O-methyl)septoriamycin A (1), 17-acetoxy-N-(O-methyl)septoriamycin A (2), 13-(5)-hydroxy-N-(O-methyl)septoriamycin A (3), and 13-(R)-hydroxy-N-(O-methyl)septoriamycin A (4), together with the known compounds (+)-cercosporin (5), (+)-14-O-acetylcercosporin (6), (+)-di-O-acetylcercosporin (7), lumichrome, and brassicasterol, were isolated from an Et acetate extract of a culture medium of *Septoria pistaciarum*. Methylation of septoriamycin A (8) with diazomethane yielded three di-O-Me analogs, two of which existed as mixtures of rotamers. We previously reported antimalarial activity of septoriamycin A. This compound also exhibited significant activity against *Leishmania donovani* promastigotes. Compounds 5-7 showed moderate in vitro activity against *L. donovani* promastigotes and chloroquine-sensitive (D6) and -resistant (W2) strains of *Plasmodium falciparum*, whereas compound 5 was fairly active against methicillin-sensitive and methicillin-resistant strains of *Staphylococcus aureus*. Compounds 5-7 also displayed moderate phytotoxic activity against both a dicot (lettuce, *Lactuca sativa*) and a monocot (bentgrass, *Agrostis stolonifera*) and cytotoxicity against a panel of cell lines.



	R ₁	R ₂	R ₃	R ₄
1	CH ₃	CH ₂ OH	H	CH ₃
2	CH ₃	CH ₂ OAc	H	CH ₃
3	CH ₃	CH ₃	OH (S)	CH ₃
4	CH ₃	CH ₃	OH (R)	CH ₃
8	H	CH ₃	H	CH ₃
9	CH ₃	CH ₃	H	CH ₃



	R ₁	R ₂
5	H	H
6	OAc	H
7	OAc	OAc

Full Text

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▼ Concepts

▼ Substances

▼ Citations

文献详情



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浏览概念词库和物质列表，获取文献中关键的研究点和物质对应的研究角色

Substances

Substances (14)

74-88-4



CH₃I
Methyl iodide

Role: Reactant, Reactant or Reagent

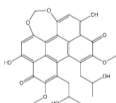
334-88-3



CH₂N₂
Diazomethane

Role: Reactant, Reactant or Reagent

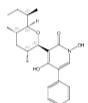
150132-90-4



C₂₉H₂₆O₁₀
(13bR)-5,12-Dihydroxy-8,9-bis[(2R)-2-hydroxypropyl]-7,10-dimethoxyperylol[1,12-def]-1,3-dioxepin-6,11-dione

Role: Pharmacological Activity, Properties, Purification or Recovery, Therapeutic Use, Biological Study, Preparation, Uses

1234619-27-2

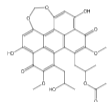


Absolute stereochemistry shown, Rotation (+)

C₂₂H₂₅NO₄
1,4-Dihydroxy-5-phenyl-3-[(2R,3R,5S,6R)-tetrahydro-3,5-dimethyl-6-[(1R)-1-methylpropyl]-2H-pyran-2-yl]-2(1H)-pyridinone

Role: Pharmacological Activity, Purification or Recovery, Reactant, Therapeutic Use, Biological Study, Preparation, Reactant or Reagent, Uses

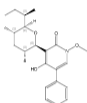
62574-07-6



C₃₁H₂₈O₁₁
(13bR)-8-[(8R)-2-(Acetyloxy)propyl]-5,12-dihydroxy-9-[(2R)-2-hydroxypropyl]-7,10-dimethoxyperylol[1,12-def]-1,3-dioxepin-6,11-dione

Role: Pharmacological Activity, Properties, Purification or Recovery, Therapeutic Use, Biological Study, Preparation, Uses

1234619-28-3



Absolute stereochemistry shown, Rotation (+)

C₂₃H₃₁NO₄
4-Hydroxy-1-methoxy-5-phenyl-3-[(2R,3R,5S,6R)-tetrahydro-3,5-dimethyl-6-[(1R)-1-methylpropyl]-2H-pyran-2-yl]-2(1H)-pyridinone

Role: Properties, Synthetic Preparation, Preparation

Concepts

天然产物、结构和活性

Agrostis stolonifera	Lettuce
Antimalarials	Methicillin-resistant Staphylococcus aureus
Antimicrobial agents	Molecular structure, natural product
Antitumor agents	Mycosphaerella pistaciarum
Cytotoxicity	Natural products
Lactuca sativa	Phytotoxicity
Leishmania donovani	Plasmodium falciparum
Leishmanicides	Staphylococcus aureus



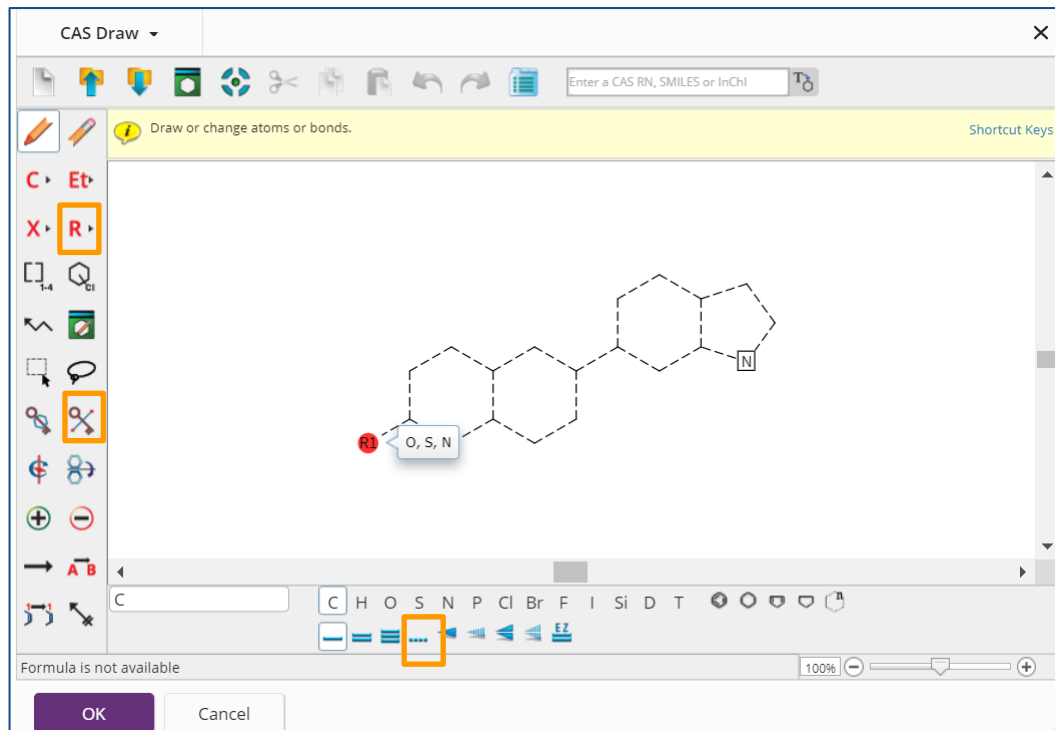
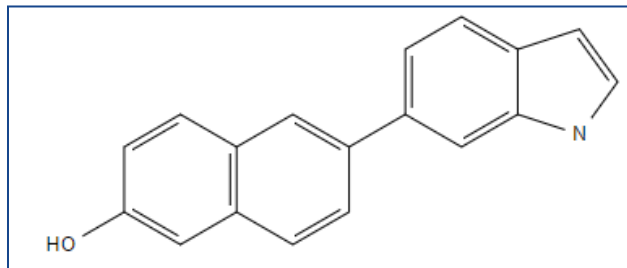
CAS

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大纲

- 天然活性成分的提取分离和活性等研究
- 根据谱图信息来分析物质结构
- **骨架结构新颖性的确定**
- 具有生物活性的衍生化结构检索
- 结构改造与合成

根据已知结构来绘制并检索同一环系骨架结构的物质



一次检索，同时获得精确结构、亚结构和相似结构结果

SCI FINDERⁿ
A CAS SOLUTION

Substances ▾ Enter a query... Edit ▴

← Return to Home

Structure Match

- As Drawn (1)
- Substructure (22)
- Similarity (3)

Analyze Structure Precision

Filter by

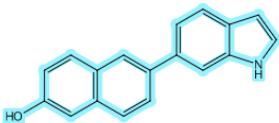
- Commercial Availability
 - Available (1)
- Reaction Role
 - Product (1)
- Reference Role
 - Biological Study (1)

Substances (1)

References ▾ Reactions ▾ Suppliers ▾

1

1027786-51-1



C18H13NO
2-Naphthalenol, 6-(1H-indol-6-yl)-

1 Reference 2 Reactions 2 Suppliers

Edit Drawing Remove

Search Patent Markush



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浏览亚结构检索结果，完善检索结构

Structure Match

As Drawn (1)

Substructure (22)

Similarity (3)

Analyze Structure Precision

Filter by

Commercial Availability

☐ Available (3)

☐ Not Available (19)

Reaction Role

☐ Product (21)

☐ Reactant (10)

Reference Role

☐ Biological Study (7)

☐ Preparation (21)

☐ Reactant or Reagent (10)

☐ Uses (11)

Stereochemistry

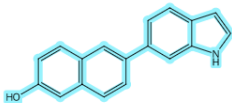
Number of Components

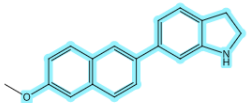
Substance Class

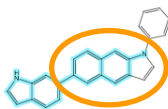
Substances (22)

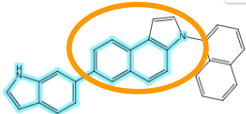
Sort: Relevance View: Partial

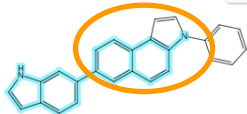
References Reactions Suppliers

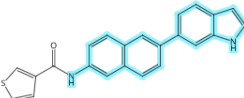
1 1027786-51-1

C18H13NO
2-Naphthalenol, 6-(1H-indol-6-yl)-
1 Reference 2 Reactions 2 Suppliers

2 1770587-88-6

C19H17NO
1H-Indole, 2,3-dihydro-6-(6-methoxy-2-naphthalenyl)-
0 References 0 Reactions 1 Supplier

3 1656292-63-5

C26H18N2
1H-Benz[7]indole, 6-(1H-indol-6-yl)-1-phenyl-
1 Reference 5 Reactions 0 Suppliers

4 1656292-48-6

C30H20N2
3H-Benz[e]indole, 7-(1H-indol-6-yl)-3-(1-naphthalenyl)-
0 References 0 Reactions 0 Suppliers

5 1656292-46-4

C26H18N2
3H-Benz[e]indole, 7-(1H-indol-6-yl)-3-phenyl-
0 References 0 Reactions 0 Suppliers

6 919362-71-3

C23H16N2OS
N-[6-(1H-indol-6-yl)-2-naphthalenyl]-3-thiophenecarboxamide
0 References 0 Reactions 0 Suppliers

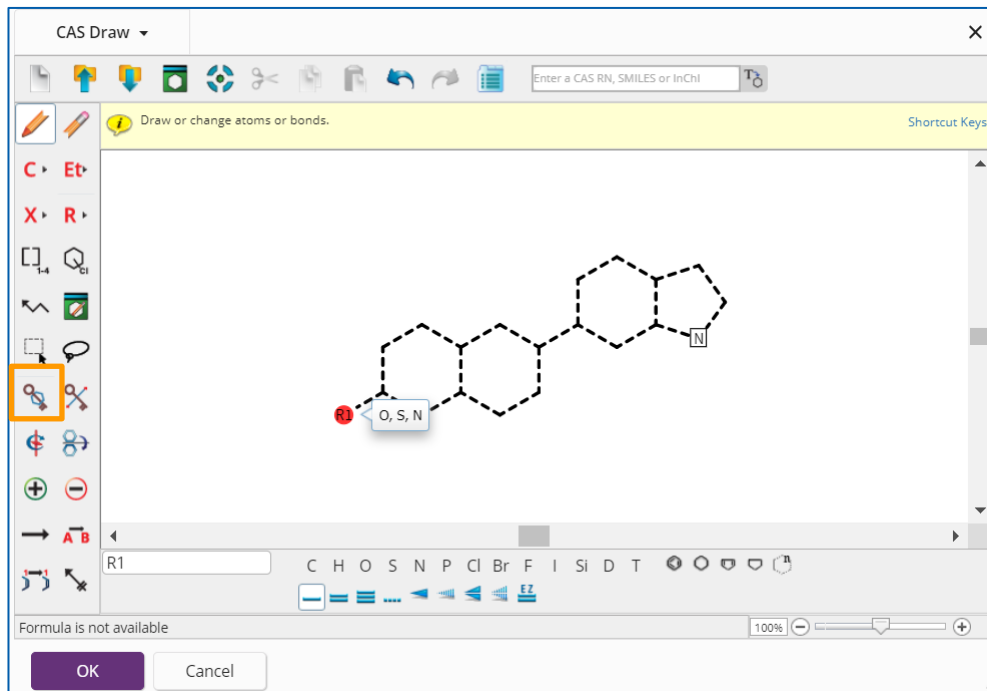
如果不希望母核上出现并环，
可使用环锁定工具修改检索
结构



CAS[®]

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进一步修改检索结构式



可进一步通过左侧聚类项，分析物质的理化属性、生物活性和研究角色等信息

Structure Match

As Drawn (1)

Substructure (8)

Similarity (3)

Analyze Structure Precision

Filter by

- > Commercial Availability
- > Reaction Role
- > Reference Role
- > Stereochemistry
- > Number of Components
- > Substance Class
- > Isotopes
- > Metals
- > Molecular Weight
- > Regulatory Information
- > Bioactivity Indicator
- > Target Indicator
- > Search Within Results

Substances (8)

Sort: Relevance ▾ View Partial ▾

[+] [References ▾] [Reactions ▾] [Suppliers ▾]

<input type="checkbox"/> 1 1027786-51-1 C₁₀H₁₃NO 2-Naphthalenol, 6-(1 <i>H</i> -indol-6-yl)- [Reference 1] [Reactions 2] [Suppliers 2]	<input type="checkbox"/> 2 1770587-88-6 C₁₉H₁₇NO 1 <i>H</i> -Indole, 2,3-dihydro-6-(6-methoxy-2-naphthalenyl)- [References 0] [Reactions 0] [Supplier 1]	<input type="checkbox"/> 3 919362-71-3 C₂₃H₁₆N₂O₅ <i>N</i> -[6-(1 <i>H</i> -indol-6-yl)-2-naphthalenyl]-3-thiophenecarboxamide [Reference 1] [Reactions 3] [Suppliers 3]
<input type="checkbox"/> 4 919362-59-7 C₂₃H₁₆N₂O₅S 3-Thiophenecarboxamide, <i>N</i> -[[6-(2,3-dihydro-2-oxo-1 <i>H</i> -indol-6-yl)-2-naphthalenyl]- [Reference 1] [Reactions 3] [Suppliers 3]	<input type="checkbox"/> 5 1275029-06-5 C₄₂H₅₂N₆O₇ L-Prolinamide, <i>N</i> -(methoxycarbonyl)-L-valyl-, <i>N</i> -[6-{2-[(2 <i>S</i> ,3 <i>S</i>)-2-(methoxycarbonyl)]-1-[(2 <i>S</i> ,3 <i>S</i>)-2-(methoxycarbonyl)propanamido]ethyl}phenyl]- Absolute stereochemistry shown [Reference 1] [Reactions 3] [Suppliers 3]	<input type="checkbox"/> 6 1275019-44-7 C₄₂H₅₂N₆O₇ Carbamic acid, <i>N</i> -[[1(1 <i>S</i> ,2 <i>S</i>)-1-[[[(2 <i>S</i> ,2'-[6-{[[[(3 <i>S</i>)-1-[(2 <i>S</i>)-2'-(methoxycarbonyl)]]]]]]]]]]]]]]] Absolute stereochemistry shown [Reference 1] [Reactions 3] [Suppliers 3]



SciFINDERⁿ
A CAS SOLUTION

Substances ▾ Enter a query...

Edit ▾ 🔍 ★ ⌚ 👤

← Return to Home

Patent Markush Match

As Drawn (7) **Substructure (95)**

Filter by

Patent Office

- ☐ World Intellectual Property Organization (4)
- ☐ China (1)
- ☐ European Patent Organization (1)
- ☐ United States (1)

Patent Markush (7)

References ▾

1

CN107082775

Patent claim 6

PATENTPAK ▾ Full Text ▾

536,537,541,543,546,549: opt. substd. by G2

2

WO2016111140

Patent claim 1

PATENTPAK ▾ Full Text ▾

739,740,744,746,749,752: opt. substd. by 1 or more G2

Edit Drawing Remove

☒ Search Patent Markush

Sort: Relevance ▾

📄 ✉️ ★ Save

同时需要进行
Markush结构检索，
尽可能全面地获取
公开的结构信息

根据匹配的结构结果、取代
关系和原文匹配位置描述，
再通过**PatentPak**进入原文定
位处仔细分析专利风险。



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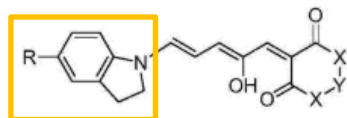
专利原文中匹配的结构展示

CN 107082775 A

权利要求书

1/2 页

1. 一种光致变色化合物, 其结构如式A所示,



A

其中, R是荧光基团, 为取代的或未取代的萘, 蒽, 芘, 1,8-萘酰亚胺, 氧吡喃酮, R上的取代基为C₁₋₄烷基、卤素、羟基、C₁₋₄烷氧基或C₁₋₄烷基胺基;

X是氧, Y是C(CH₃)₂; 或者

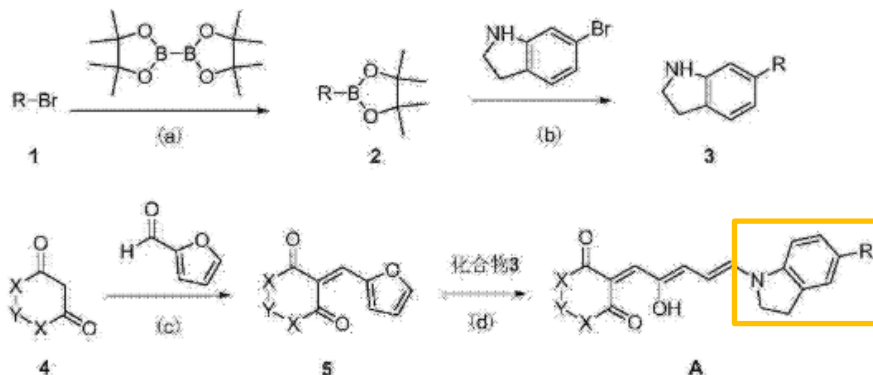
X是N(CH₃), Y是C(O).

CN 107082775 A

权利要求书

2

6. 制备权利要求1或2所述的光致变色化合物的方法, 合成路线如下:



其中, R, X和Y的定义如权利要求1或2所述; 合成过程包括步骤:

- 在钯催化和碱条件下化合物1与联硼酸频那醇酯反应得到化合物2;
- 在钯催化和碱条件下化合物2与5-溴吲哚啉通过suzuki偶联反应得到化合物3;
- 化合物4与糠醛反应得到化合物5;
- 化合物5和化合物3反应得到目标产物A。



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大纲

- 天然活性成分的提取分离和活性等研究
- 根据谱图信息来分析物质结构
- 骨架结构新颖性的确定
- 具有生物活性的衍生化结构检索
- 结构改造与合成

衍生化结构检索的目的

新颖性：天然产物提取物可能是全新的化合物，也有可能已被现有文献报道。

生物活性：提取物可能具有显著的生物活性，也有可能没有足够的生物活性特征。

稳定性：很多提取物稳定性并不理想。

还有**生物利用度**和**毒性**等各种直接成药的缺陷。

无论是为了提高天然提取物的生物活性、生物利用度、增强稳定性、降低毒性，还是为了创造新分子等，都可以尝试通过研究结构衍生化来实现。

例：青蒿素的生物利用度低，需要通过结构改造来研究其衍生化合物

SCIFINDERⁿ A CAS SOLUTION

Substances qinghaosu

Substances (1)

Filter by

- Commercial Availability
 - Available (1)
- Reaction Role
 - Product (1)
 - Reactant (1)
 - Reagent (1)
 - Catalyst (1)
 - Solvent (1)
- Reference Role
 - Adverse Effect (1)
 - Analytical Study (1)
 - Biological Study (1)
 - Formation (1)
 - Miscellaneous (1)

1

63968-64-9

Absolute stereochemistry shown

C15H22O5
Qinghaosu

8,079 References 2,724 Reactions 101 Suppliers

SCIFINDERⁿ A CAS SOLUTION

Substances qinghaosu

63968-64-9

CAS RN 63968-64-9

CAS Name Artemisinin

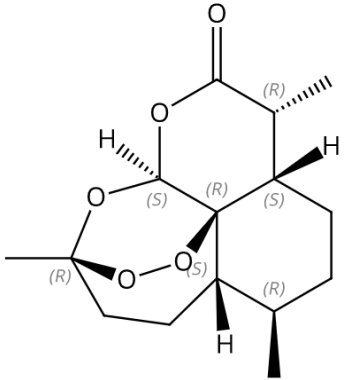
Substance Detail

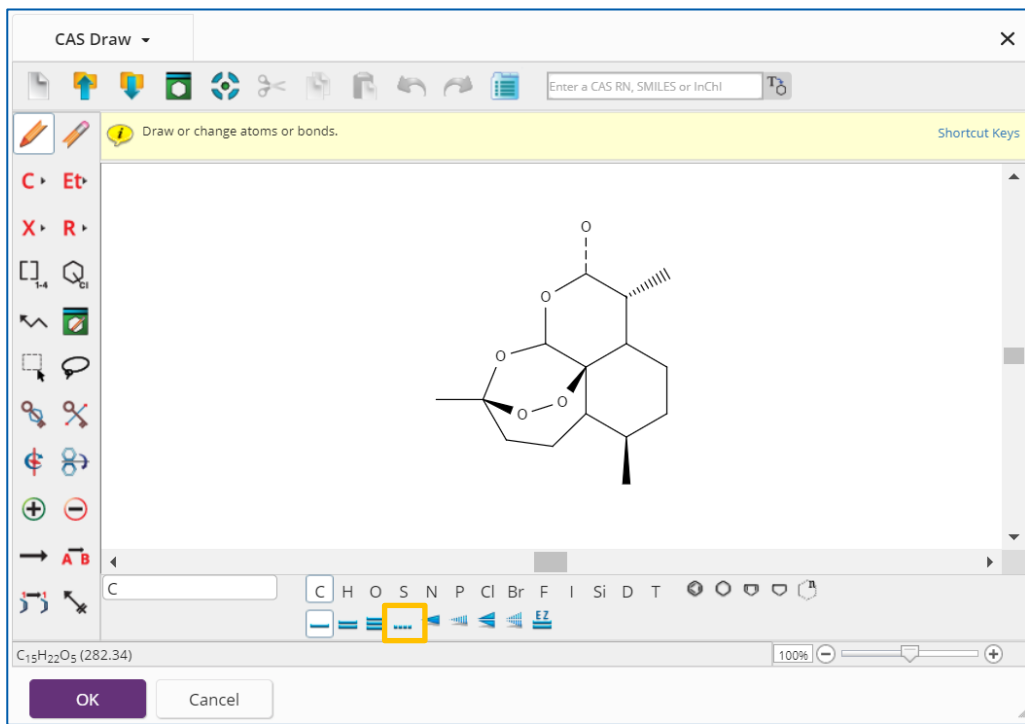
- Reactions (2,724)
- Synthesize (2,284)
- Create Retrosynthesis Plan
- References (8,079)
- Suppliers (101)

Edit Structure

Reset

Absolute stereochemistry shown





根据需要，通过CAS Draw中的绘图工具修改母核结构

考虑从何处着手衍生化，
然后限定结构检索式

结构编辑器使用指南

https://scifinder-n.cas.org/help/#t=Drawing_Search_Queries%2FDrawing_with_CAS_Draw.htm



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通过亚结构结果获取含有同一母核的结构

Structure Match

As Drawn (129)

Substructure (4,310)

Similarity (11K)

Analyze Structure Precision

Filter by

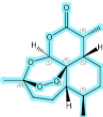
- Commercial Availability
- Reaction Role
- Reference Role
- Stereochemistry**
 - ☒ Absolute Stereo Match (1,423)
 - ☒ Absolute Stereo Mirror Image (1)
 - ☒ Relative Stereo Match (3)
 - ☐ Stereo that Doesn't Match Query (136)
 - ☐ No Stereo in Answer Structure (190)

Substances (1,427)

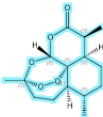
Sort: Relevance View Partial

References Reactions Suppliers

1 63968-64-9

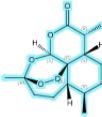

Absolute stereochemistry shown
C15H22O5
Artemisinin
8,079 References 2,724 Reactions 101 Suppliers

2 2231322-39-5


Absolute stereochemistry shown, Rotation (-)
C15H22O5
3,12-Epoxy-12H-pyrano[4,3-j]-1,2-benzodioxepin-10(3H)-one, octahydro-3,6,9-trime...
1 Reference 35 Reactions 0 Suppliers

3 1015079-59-0

85536-03-4
Image Not Available


Absolute stereochemistry shown
C15H22O5.Unspecified
Components: 2
3,12-Epoxy-12H-pyrano[4,3-j]-1,2-benzodioxepin-10(3H)-one, octahydro-3,6,9-trime...
1 Reference 0 Reactions 0 Suppliers

根据Stereochemistry获取各类相关手性的物质结果

根据Bioactivity Indicator, 筛选感兴趣的生物活性

Number of Components

Substance Class

Isotopes

Metals

Molecular Weight

Experimental Property

Experimental Spectrum

Regulatory Information

Bioactivity Indicator

☒ Anti-infective agents (1,427)

☐ Antitumor agents (1,388)

☐ Pharmaceutical immune agents (137)

☐ Cytotoxic agents (77)

☐ Antiproliferative agents (61)

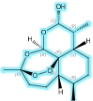
[View All](#)

Target Indicator

Search Within Results

4

71939-50-9



Absolute stereochemistry shown

$C_{15}H_{24}O_5$
Dihydroartemisinin

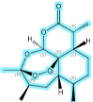
2,355
References

821
Reactions

91
Suppliers

7

849366-16-1

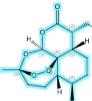


Absolute stereochemistry shown

$C_{16}H_{24}O_5$
3,12-Epoxy-12H-pyrano[4,3-f]-1,2-benzodioxepin-10(3H)-one, octahydro-3,4,6,9-tet...

5

139727-21-2



Absolute stereochemistry shown, Rotation (+)

$C_{16}H_{24}O_5$
(3R,5aS,6R,8aS,9R,12S,12aR)-9-Ethyl octahydro-3,6-dimethyl-3,12-epoxy-12H-pyrano...

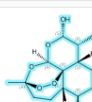
15
References

4
Reactions

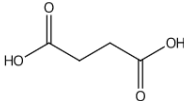
0
Suppliers

8

847591-39-3

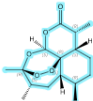


Absolute stereochemistry shown



6

849366-17-2



Absolute stereochemistry shown

$C_{16}H_{24}O_5$
3,12-Epoxy-12H-pyrano[4,3-f]-1,2-benzodioxepin-10(3H)-one, octahydro-3,4,6,9-tet...

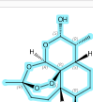
1
Reference

0
Reactions

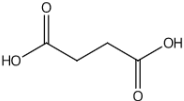
0
Suppliers

9

1392514-35-0

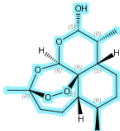


Absolute stereochemistry shown



4

71939-50-9



Absolute stereochemistry shown

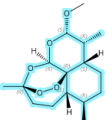
$C_{15}H_{24}O_5$
Dihydroartemisinin

2,355
References

821
Reactions

32

71963-77-4



Absolute stereochemistry shown, Rotation (+)

$C_{16}H_{26}O_5$
Artemether

2,719
References

147
Reactions

88
Suppliers

药效更高, 但稳定性不高

药效和稳定性更高的结构

CAS

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41

Structure Match

As Drawn (129)

Substructure (4,310)

Similarity (11K)

Filter by

- Similarity
 - ☒ 95-98 (4)
 - ☒ 90-94 (18)
 - ☒ 85-89 (56)
 - ☐ 80-84 (155)
 - ☐ 75-79 (212)
 - [View All](#)
- Commercial Availability
- Reaction Role
- Reference Role
- Stereochemistry
- Number of Components
- Substance Class
- Isotopes
- Metals
- Molecular Weight
- Experimental Property
- Experimental Spectrum
- Regulatory Information
- Bioactivity Indicator
 - ☐ Anti-infective agents (285)
 - ☒ Antitumor agents (78)
 - ☐ Receptor antagonists (8)


Substances (78)

Sort: Relevance View Partial

References Reactions Suppliers

1

63968-64-9




Absolute stereochemistry shown

$C_{15}H_{22}O_5$
Artemisinin

8,079 References 2,724 Reactions 101 Suppliers

2

71939-50-9




Absolute stereochemistry shown

$C_{15}H_{24}O_5$
Dihydroartemisinin

2,355 References 821 Reactions 91 Suppliers

3

2250435-24-4



Absolute stereochemistry shown

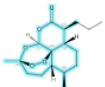
9000-69-5
Image Not Available

$C_{15}H_{24}O_5 \cdot x\text{Unspecified}$
Components: 2

1 Reference 1 Reaction 0 Suppliers

4

391618-54-5




Absolute stereochemistry shown

$C_{17}H_{26}O_5$
3,12-Epoxy-12H-pyrano[4,3-j]-1,2-benzodioxepin-10(3H)-one, octahydro-3,6-dimethyl-...

1 Reference 1 Reaction 1 Supplier

5

613233-62-8



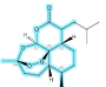
Absolute stereochemistry shown

$C_{16}H_{22}O_5$
(3R,5aS,6R,8aS,12R,12aS)-Decahydro-3,6-dimethyl-3,12-epoxy-12H-pyrano[4,3-j]-1,2-...

2 References 1 Reaction 0 Suppliers

6

255730-29-1




Absolute stereochemistry shown

$C_{16}H_{26}O_5$
3,12-Epoxy-12H-pyrano[4,3-j]-1,2-benzodioxepin-10(3H)-one, octahydro-3,6-dimethyl-...

1 Reference 7 Reactions 0 Suppliers


7

391618-68-1




8

150358-72-8



9

613233-63-9



通过Similarity的结果，获取更广泛的相似骨架结构；并继续通过Bioactivity Indicator，发现其对应的潜在功效



CAS[®]

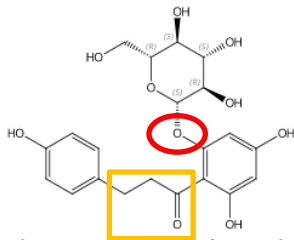
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大纲

- 天然活性成分的提取分离和活性等研究
- 根据谱图信息来分析物质结构
- 骨架结构新颖性的确定
- 具有生物活性的衍生化结构检索
- 结构改造与合成

例1：提高稳定性的结构改造

60-81-1

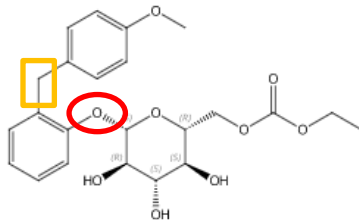


Absolute stereochemistry shown

$C_{21}H_{24}O_{10}$
Phloridzin

天然提取物根皮苷

408504-26-7

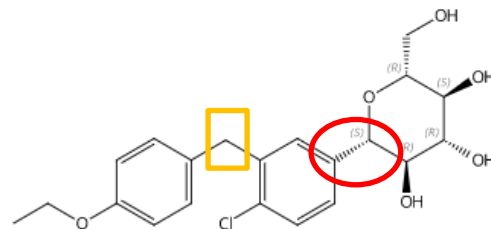


Absolute stereochemistry shown

$C_{23}H_{28}O_9$
Sergliflozin etabonate

结构改造物A

461432-26-8




Absolute stereochemistry shown, Rotation (+)

$C_{21}H_{25}ClO_6$
Dapagliflozin

结构改造物B


快速纵览最优逆合成反应路线，并锁定关键起始原料和反应类型


 **Retrosynthesis** [Edit Plan Options](#)

Overview

Steps

Step Key

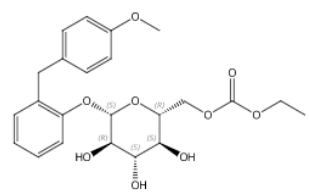
\Rightarrow  Experimental

\Rightarrow  Predicted ☒

Plan Information

Estimated Yield: **45%**
Overall Price: **\$266.81**
(USD per 100 grams)
Commercially Available:
A, B, C, E, F, G, H, I, J




408504-26-7



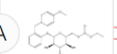
Absolute stereochemistry shown

$C_{23}H_{28}O_9$
Sergliflozin etabonate

Powered by **ChemPlanner®**

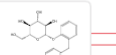
   Save

A




Suppliers (16)

B




Suppliers (7)

C




Suppliers (48)

D




Suppliers (28)

E




Suppliers (93)

F




Suppliers (28)

G




Suppliers (144)

H




Suppliers (9)

I



Suppliers (79)

J



Suppliers (88)

Max. Yield: 82%

Max. Yield: 87%

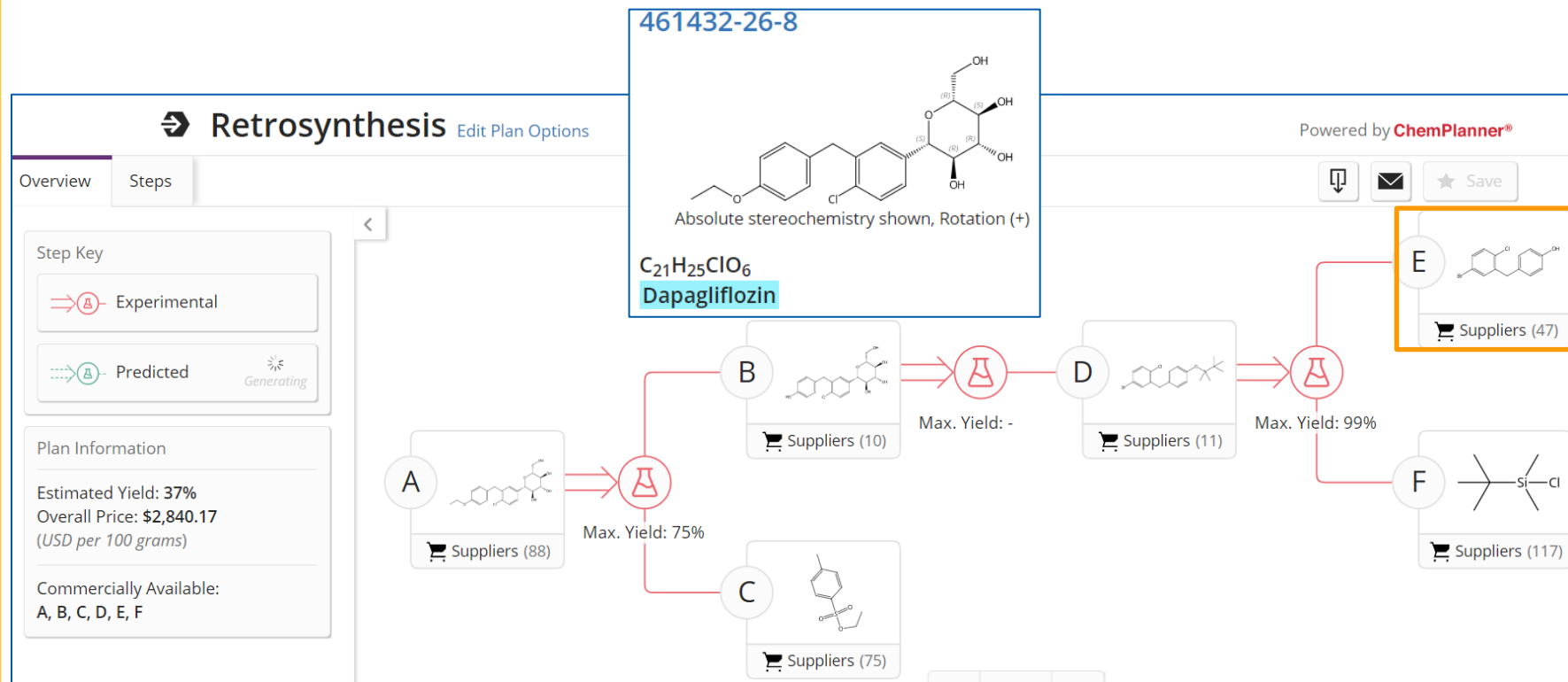
Max. Yield: 90%

Max. Yield: 72%

Max. Yield: 97%

点击每个试剂瓶查看实验条件等更为详细的合成信息

快速纵览最优逆合成反应路线，并锁定关键起始原料和反应类型



点击每个试剂瓶查看实验条件等更为详细的合成信息



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例2：通过Non-Participating Functional Groups, 查看反应前后没有发生变化的官能团列表

Structure Match

As Drawn (48)

Substructure (4,118)

Similarity (617)

Filter by

- Yield
- Number of Steps
- Non-Participating Functional Groups**
 - Ether (316)
 - Amine (293)
 - Tertiary amine (285)
 - Imine (135)
 - Amide (130)
 - [View All](#)

Reactions (4,118)

View Expanded

References

Scheme 1 (47 Reactions) Steps: 1 Yield: 92-96%

Suppliers (97)

Suppliers (119)

Reaction Summary Steps: 1 Yield: 96%

1.1 Reagents: Butyllithium
Solvents: Pentane, Tetrahydrofuran; 45 min, -78 °C

1.2 Reagents: Trimethyl borate; 1 h, -78 °C; -78 °C → rt; 3 h, rt

1.3 Reagents: Hydrochloric acid
Solvents: Ethyl acetate, Water

[View Reaction Detail](#)

The synthesis and application of 2-acetyl-6-(1-naphthyl)-pyridine oxime as a new ligand for palladium precatalyst in suzuki coupling reaction

By: Zhou, Yongchang; et al
Journal of Heterocyclic Chemistry (2009), 46(1), 116-118

[Full Text](#)

点击View All查看所有的Non-Participating Functional Groups

浏览同时共存的官能团，并根据拟采用的原料结构选择不参与反应的官能团

Non-Participating Functional Groups

By Count Alphanumeric

<input type="checkbox"/> Ether (316)	<input type="checkbox"/> Nitro (16)	<input type="checkbox"/> Cyclic ketone (4)
<input type="checkbox"/> Amine (293)	<input type="checkbox"/> Phenyl halide (14)	<input type="checkbox"/> Primary amine (3)
<input type="checkbox"/> Tertiary amine (285)	<input type="checkbox"/> Secondary alcohol (12)	<input type="checkbox"/> Unsaturated ester (3)
<input type="checkbox"/> Imine (135)	<input type="checkbox"/> Acetal (11)	<input type="checkbox"/> Urea (3)
<input type="checkbox"/> Amide (130)	<input type="checkbox"/> Acyclic alkene (10)	<input type="checkbox"/> Phosphonate (2)
<input checked="" type="checkbox"/> Halide (121)	<input type="checkbox"/> Diene (10)	<input type="checkbox"/> Sulfone (2)
<input type="checkbox"/> Sulfide (92)	<input type="checkbox"/> Ketone (10)	<input type="checkbox"/> Tertiary alcohol (2)
<input type="checkbox"/> Carboxamidine (54)	<input type="checkbox"/> Alkyl halide (8)	<input type="checkbox"/> Acid halide (1)
<input type="checkbox"/> Alkene (50)	<input type="checkbox"/> Alkyne (8)	<input type="checkbox"/> Azide (1)
<input type="checkbox"/> Cyclic alkene (40)	<input type="checkbox"/> Aldehyde (7)	<input type="checkbox"/> Cyclic ester (1)
<input type="checkbox"/> Alcohol (31)	<input type="checkbox"/> Acyclic ketone (6)	<input type="checkbox"/> Cyclopentadienyl metal (1)
<input type="checkbox"/> Nitrile (26)	<input type="checkbox"/> Primary alcohol (6)	<input type="checkbox"/> Organometal (1)

Apply Cancel

查看筛选后的结果

Structure Match

As Drawn (48)

Substructure (4,118)

Similarity (617)

Filter by

Yield

Number of Steps

Non-Participating Functional Groups

☐ Ether (316)

☐ Amine (293)

☐ Tertiary amine (285)

☐ Imine (135)

☐ Amide (130)

☒ Halide (121)

[View All](#)


Experimental Protocols

☐ MethodsNow: Synthesis (15)

Reactions (121)

☐ References


Scheme 1 (3 Reactions)



[Suppliers \(70\)](#) [Suppliers \(14\)](#)

[Expand Scheme](#)


Scheme 2 (1 Reaction)



[Suppliers \(92\)](#) [Suppliers \(17\)](#)


[Expand Scheme](#)

Scheme 7 (4 Reactions)




[Expand Scheme](#)

Scheme 8 (1 Reaction)



[Expand Scheme](#)

Scheme 9 (1 Reaction)



[Expand Scheme](#)

对F, Cl和Br有选择性，
且可控制Br的反应当量



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例3：已知天然产物结构，获取其衍生物及合成信息

- 以石杉碱甲为例：CAS No. 102518-79-6
- 执行相同检索策略：结构式检索

SciFinder[®]结果

← Return to Home

Structure Match

As Drawn (47)

Substructure (291)

Similarity (1,760)

Analyze Structure Precision

Filter by

Commercial Availability

☐ Available (31)

☐ Not Available (260)

Reaction Role

☐ Product (215)

☐ Reactant (17)

☐ Catalyst (1)

Reference Role

☐ Adverse Effect (9)

☐ Analytical Study (16)

☐ Biological Study (255)

☐ Formation (1)

☐ Miscellaneous (1)

[View All](#)

Stereochemistry

Number of Components

Substance Class

Isotopes

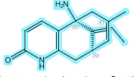
Metals

Substances (291)

Sort: Relevance View: Partial

References Reactions Suppliers

1 102518-79-6

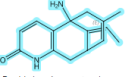


Absolute stereochemistry shown, Rotation (-)
Double bond geometry shown

$C_{15}H_{18}N_2O$
Huperzine A

1,704 References 614 Reactions 106 Suppliers

2 120786-18-7

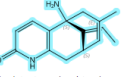


Double bond geometry shown

$C_{15}H_{18}N_2O$
(11E)-5-Amino-11-ethylidene-5,6,9,10-tetrahydro-7-methyl-5,9-methanocycloocta[b]pyridine

43 References 134 Reactions 44 Suppliers

3 130791-77-4

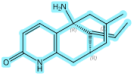


Absolute stereochemistry shown
Double bond geometry shown

$C_{15}H_{18}N_2O$
(+)-Huperzine A

79 References 8 Reactions 8 Suppliers

4 92138-20-0

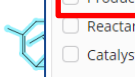


Absolute stereochemistry shown, Rotation (-)
Double bond geometry shown

$C_{15}H_{18}N_2O$
(5R,9R,11Z)-5-Amino-11-ethylidene-5,6,9,10-tetrahydro-7-methyl-5,9-methanocycloocta[b]pyridine

4 References 12 Reactions 4 Suppliers

5 1895931-35-7



Absolute stereochemistry shown, Rotation (-)
Double bond geometry shown

$C_{15}H_{18}N_2O$
(5R,9R,11Z)-5-Amino-11-ethylidene-5,6,9,10-tetrahydro-7-methyl-5,9-methanocycloocta[b]pyridine

2 References 2 Reactions 2 Suppliers

SciFinder[®] 共检索到衍生物291个，
合计反应1177个


Filter by

Reactions (1,177)

Group: By Scheme View: Expanded

References

Scheme 1 (1 Reaction) Steps: 1 Yield: 100%



Absolute stereochemistry shown

Absolute stereochemistry shown, Rotation (-)

Reaction Summary Steps: 1 Yield: 100%

1.1 Reagents: Hydrogen bromide

Divergent Total Synthesis of the Lycopodium Alkaloids
Huperzine A, Huperzine B, and Huperzine U

在线学习资源

1.CAS官网上的培训资料

<https://www.cas.org/support/training/scifinder-n>

2.SciFinder-n Help使用指南

https://scifinder-n.cas.org/help/#t=Searching_in_SciFinder-n%2FIntroduction_to_searching.htm

3.SciFinder-n What's New功能更新动态

https://scifinder-n.cas.org/help/#t=About_SciFinder-n%2FSciFinderN_Release_Notes%2FSciFinderN_Release_Notes.htm



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