

利用 CAS SciFinder Discovery Platform™

高效获取科技信息



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美国化学文摘社 (CAS) 北京代表处

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CAS

A division of the
American Chemical Society

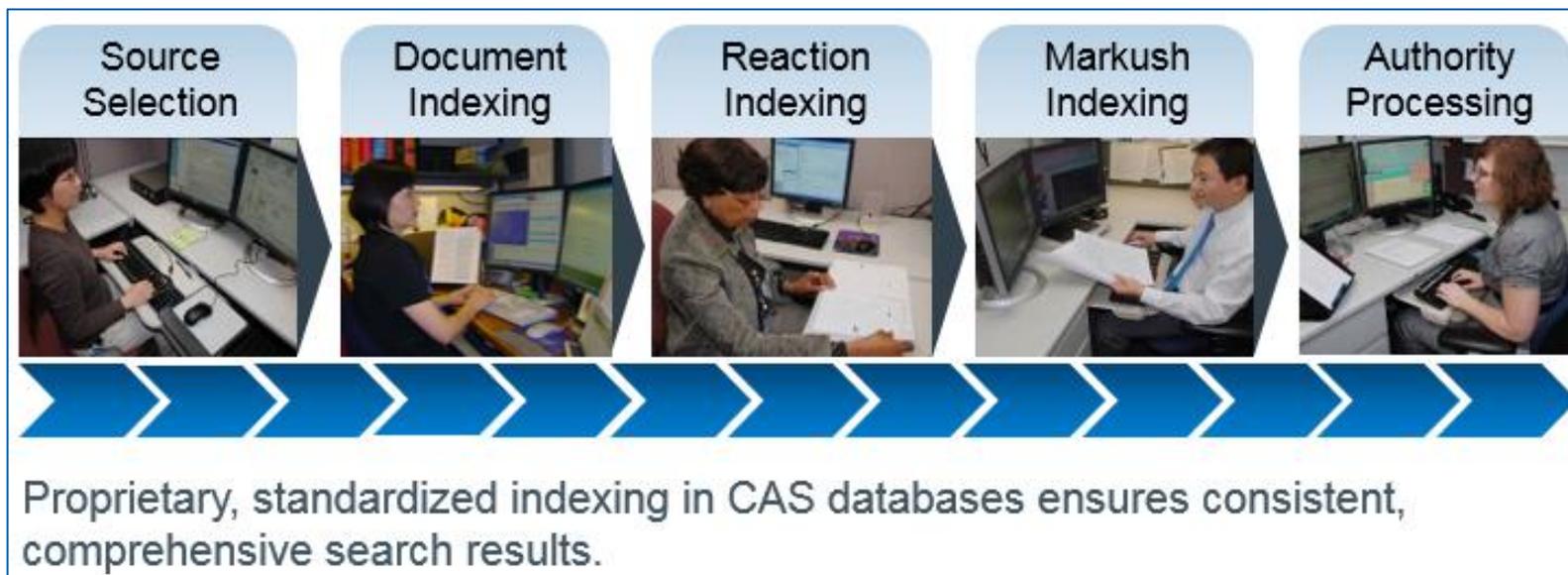


大纲

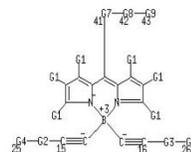
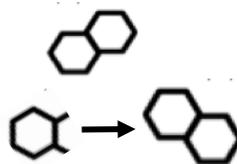
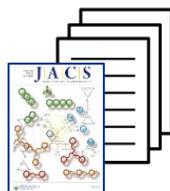
- CAS 与 CAS SciFinder Discovery Platform 简介
- 科研信息的高效查阅
 - 如何拓展文献调研?
 - 如何调研某类物质?
 - 如何调研反应信息?
 - 怎么查、怎么选具体的实验方案?
- 常见问题



CAS 科学家智力标引



Data
pre-repository



Androst-4-en-3-one,
17-hydroxy-17-
methyl-, (17β)-

CAS 科学家利用人类智慧对公开内容进行揭示，使相关信息更容易被挖掘

CAS 具有最全面的学科连接内容合集



Over
50K
scientific journals
and documents
> 50k 科学期刊

Over
279
million substances
> 2.79亿独特物质

Over
50
languages
translated
> 50种语言

109
patent offices
worldwide
109家专利局

CAS SciFinder Discovery Platform 涵盖的 工作流程解决方案



新一代的权威科学研究工具，是化学及相关学科智能研究平台，提供全球全面、可靠的化学及相关学科研究信息和分析工具



专业的制剂/配方数据库，助力制剂/配方研究科学家快速评估配方、寻找可替代供应商和探索监管信息



独特的分析方法详情数据库，有助于分析科学家快速获取详尽的分析方法信息、直接用于实验，并启发新方法的建立

如何获取 CAS SciFinder 账号

(登录学校图书馆网站, 扫描二维码填写个人信息)

1. 网页方式, IP地址+用户名+密码登录, 无并发用户限制。CAS SciFinder Discovery Platform (Academic) 登录账号注册须知:

(1) 读者在使用CAS SciFinder Discovery Platform各解决方案之前须用邮箱(推荐使用学校邮箱)注册账号密码。新读者扫描下方二维码填写个人信息后在48小时内查收邮箱收到的注册链接, 使用邮箱收到的链接中注册

(2) 2023年试用CAS SciFinder阶段注册的用户可以使用原账号密码登录, 如果登陆有疑问请邮箱联系CAS中国客服(客服邮箱: China@acs-i.org)



点击激活链接后注册成功; 之后直接
点击 <https://scifinder-n.cas.org> 访问

<https://lib.cmc.edu.cn/info/1006/2275.htm>

CAS SciFinder 登录

<https://scifinder-n.cas.org>



Log in to SciFinder®

Username or Email Address

Next

[Create an account.](#) | [Can't log in?](#)



Log in to SciFinder®

Welcome, [Not You?](#)

Password

Log In

Keep me signed in

[Create an account.](#) | [Can't log in?](#)

CAS SciFinder 主界面

The screenshot shows the CAS SciFinder main interface. On the left, a sidebar menu is highlighted with a yellow box, containing categories like 'CAS SCIFINDER DISCOVERY PLATFORM', 'CAS SciFinder', 'CAS Analytical Methods', 'CAS Formulus', 'STN IP PROTECTION SUITE', 'CAS STNext', 'CAS Scientific Patent Explorer', 'REGULATORY', 'CAS Chemical Compliance Index', 'ACCOUNT MANAGEMENT', and 'CAS Profile'. Below this sidebar, the text 'CAS 解决方案' is present. The main interface features a top navigation bar with the CAS SciFinder logo, a notification bell, a chat icon, and a user profile icon. A dropdown menu for the user profile is open, showing options like 'What's New?', 'Help and Support', 'My CAS Profile', 'Settings', 'Log Out', and '账户信息'. Below the navigation bar, there's a 'Good Morning,' greeting and a search bar with tabs for 'All', 'Substances', 'Reactions', 'References', and 'Suppliers'. The search bar includes a 'Draw' button and a search icon. Below the search bar, there's a dropdown menu for 'Author Name' and a text input field with the placeholder 'Enter last name, first name middle name.' and an 'Example: Schubert, J A'. A '+ Add Advanced Search Field' button is also visible. The main content area features three cards: 'Retrosynthetic Analysis', 'Search CAS Lexicon', and 'Search CAS Sequences'. Below these cards, the text '历史记录' is present. At the bottom, there's a 'Recent Search History' section with a 'View All Search History' link and a date 'October 8, 2024'. The CAS logo is in the bottom right corner.

大纲

- CAS 与 CAS SciFinder 简介
- 科研信息的高效查阅
 - **如何拓展文献调研?**
 - 如何调研某类物质?
 - 如何调研反应信息?
 - 怎么查、怎么选具体的实验方案?
- 常见问题



如何拓展文献检索？

- 主题词怎么选择？如何构建？
- 研究某结构相关的文献？
- 如何筛选文献？追踪最新进展？
- 关注某篇文献的被引文献和引文——引文地图

检索目标课题研究文献

主题词、物质名称、CAS 登记号、专利号、PubMed ID、文献号、DOI 号

The screenshot shows a search interface with a dark header. The navigation bar includes 'All', 'Substances', 'Reactions', 'References' (highlighted), and 'Suppliers'. The search bar contains the text 'Vinblasti'. To the right of the search bar are icons for 'Draw' and a search magnifying glass. Below the search bar, a list of suggestions is displayed:

- Vinblastin
- Vinblastine
- Vinblastine III
- Vinblastine DIBO
- Vinblastinoic acid
- Vinblastine sulfate
- Vinblastine tartrate
- Vinblastine chloride

The text '自动提示' (Automatic suggestions) is centered over the list.

利用布尔逻辑运算符 & 通配符精准检索相关文献

- 支持布尔逻辑运算符 (or/and/not), 默认运算顺序 or > and > not
- “ ” 不允许词形变化, 但可出现单数或复数; () 优先运算, 括号中表达式还可以和其他术语交互
- 支持通配符 * 或 ?, * 代表 0 或多个字符, ? 代表 0 或 1 个字符

The screenshot displays the CAS search interface with the following elements:

- Navigation Bar:** All, Substances, Reactions, **References**, Suppliers.
- Search Bar:** Contains the query "Vinblastine or vincristine and "acute lymphoblastic leukemia" 长春碱或长春新碱治疗急淋性白血病的研究文献". It includes a "Draw" button and a search icon.
- Advanced Search Section:**
 - Operator: AND
 - Field: Author Name
 - Input: Enter last name, first name middle name. (Example: Schubert, J A)
 - Button: + Add Advanced Search Field
- Search Options:**
 - Retrosynthetic Analysis:** Make reaction plans with conditions, yields, catalysts, and experimental procedures.
 - Search CAS Lexicon:** Build powerful searches using CAS concepts, chemical classes, and taxonomy. (This option is highlighted with a yellow border in the image.)
 - Search CAS Sequences:** Query BLAST, CDR, and Motif algorithms for nucleotide and protein based sequences.

CAS Lexicon 词库检索近义词和相关技术术语

Search CAS Lexicon Learn more about CAS Lexicon searching.

Natural product drugs Search Concept

Preferred Concept **首选词**

Pharmaceutical natural products

This will search synonyms: Ayurvedic **drugs**; Ayurvedic herbal medicine; Ayurvedic herbs; Ayurvedic medicine; Botanical; Botanical ext.; Botanical extract; Botanical extracts; Botanical exts.; Botanicals; Botanicals agents; Chinese **drugs**; Chinese herbal medicine; Chinese materia medica; Chinese medicines; Chinese traditional medicines; **Drugs**, Oriental; Galenic pharmaceuticals; Herbal agent; Herbal agents; Herbal **drugs**; Herbal medicine; Herbal medicines; Kampo; Kanpo; Kanpo pharmaceutical **natural products**; MeSH ID: D001688; **Natural drugs**; **Natural** pharmaceutical; **Natural** pharmaceuticals; **Natural product** pharmaceuticals; Oriental **drugs**; Oriental medicine; Oriental pharmaceuticals; Pharmaceutical **natural product**; Pharmaceuticals **natural products**; Traditional Chinese medicines; Traditional medicines [View fewer synonyms](#)

Broader Concepts (2) **上位词** [Select All](#)

Drugs ⓘ

Natural products

Narrower Concepts (291) **下位词** [Select All](#)

(S)-[6]Gingerol

Aloin ⓘ

Artemisinin

Pharmaceutical natural products - Preferred Concept ×

Pharmaceutical natural products - Narrower Concepts (3)

(S)-[6]Gingerol ×

Aloin ⓘ ×

Artemisinin ×

Pharmaceutical natural products - Related Concepts (2)

Natural antioxidants ⓘ

Traditional and alternative medicine ⓘ

- Pharmaceutical natural products, Colla Corii Asini
- Pharmaceutical natural products, DaChengQi decoction
- Pharmaceutical natural products, Dahuang
- Pharmaceutical natural products, Dahuang GanCao decoction
- Pharmaceutical natural products, DaHuang ZheChong Wan
- Pharmaceutical natural products, Daisaikoto
- Pharmaceutical natural products, DangGui
- Pharmaceutical natural products, DangGui LongHui Pian
- Pharmaceutical natural products, DangGuiShaoYao San
- Pharmaceutical natural products, DangShen
- Pharmaceutical natural products, Danhong injection

AND OR NOT Add to Query Clear Query Search

Related Concepts (6) **相关词**

Botanical pesticides

Bryostatin ⓘ

Dietary supplements ⓘ

Natural antioxidants ⓘ

Traditional and alternative medicine ⓘ

[View All](#)

根据作者/出版物/研究机构/物质结构检索相关文献

Supports structure search

Rotigotine or Pramipexole and "Parkinson disease" not "Restless legs syndrome"

AND Abstract/Keywords Parkinson

+ Add Advanced Search Field

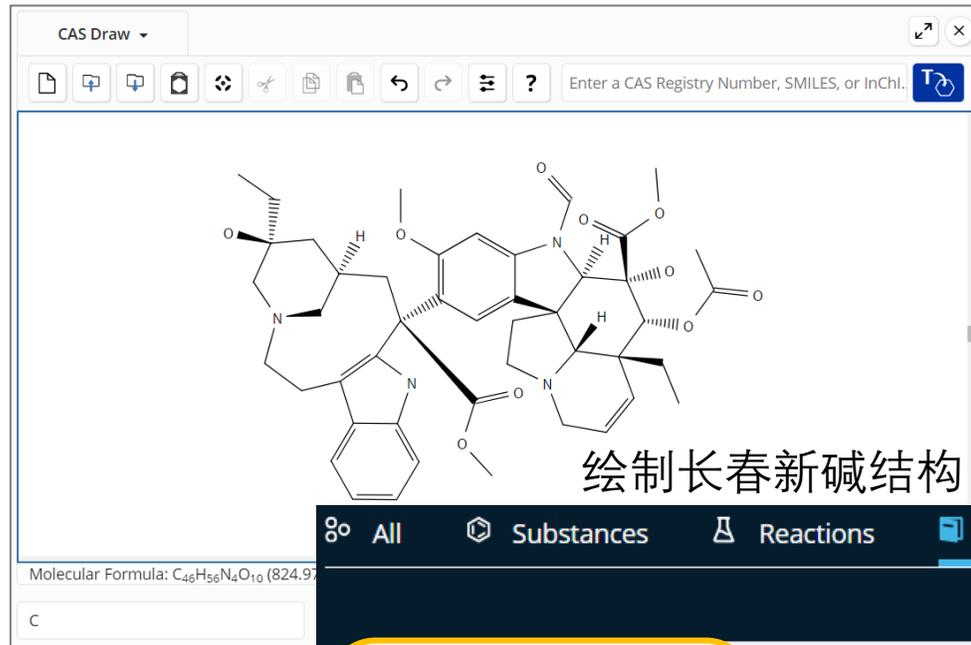
- Authors
- Publication Name
- Organization
- Title
- Abstract/Keywords
- Concept
- Substances
- Bioactivity Data **NEW**
- Publication Year
- Document Identifier
- Patent Identifier
- Publisher

Retrosynthetic Analysis
Make reaction plans with conditions, yields, catalysts, and experimental procedures.

Search CAS Sequences
Query BLAST, CDR, and Motif algorithms for nucleotide and protein based sequences.

自定义高级检索项

物质结构与关键词联合检索文献



文本与物质结构检索符合“and”关系

All Substances Reactions References Suppliers

"Acute lymphoblastic leukemia"

AND Author Name Enter last name, first name middle name. Example: Schubert, J A

+ Add Advanced Search Field

Edit Drawing Remove

检索结果分析与筛选

References search for ""Acute lymphoblastic leukemia"" + drawn structure

Sort: Relevance

Substances Reactions Citing Knowledge Graph

Structure Match

As Drawn (2,152)

Substructure (2,152)

Filter Behavior

Filter by Exclude

Search Within Results

Concept

CA Section

Publication Year

Organization

Substance Role

2,152 Results

Sort: Relevance View: Partial Abs

1

Effects of inhibitors of the chemokine receptor CXCR4 on acute lymphoblastic leukemia cells in vitro

By: Juarez, J.; Bradstock, K. F.; Gottlieb, D. J.; Bendall, L. J.
Leukemia (2003), 17(7), 1294-1300 | Language: English, Database: CPlus and MEDLINE

Stromal cell-derived factor-1 (SDF-1) is a key regulator of the behavior of normal and leukemic precursor-B (pre-B) cells. It is possible that inhibiting SDF-1-driven processes in pre-B acute lymphoblastic leukemia (ALL) may have therapeutic implications. In this study, the authors examined the ability of SDF-1 inhibitors to modulate pre-B ALL cell responses to SDF-1, including chemotaxis, migration into bone marrow stroma, and stroma-supported survival and proliferation on human bone marrow stromal layers. The polyphemusin II-derived inhibitors, T140, TC140012, and T134, and the bicyclam AMD3...

View More

Full Text

Substances (8) Reactions (0) Citing (159) Citation Map

2

Long-term results of the pediatric oncology group studies for childhood acute lymphoblastic leukemia 1984-2001: a report from the children's oncology group

结果集二次检索研究内容: Search Within Results

References search for "Acute lymphoblastic leukemia" + drawn structure

Substances Reactions Citing Knowledge Graph

Structure Match

- As Drawn (3,436)
- Substructure (3,437)

Filter Behavior

Filter by Exclude

Search Within Results

Search for up to 3 text strings within the result set.

Enter a query...

Search

Searching for... Clear All

dexamethasone X

Concept

CA Section

Filtering: Search Within Results: dexamethasone X Clear All Filters

1,048 Results Sort: Relevance View: Partial Abstract

1

Effects of inhibitors of the chemokine receptor CXCR4 on acute lymphoblastic leukemia cells in vitro

By: Juarez, J.; Bradstock, K. F.; Gottlieb, D. J.; Bendall, L. J.
Leukemia (2003), 17(7), 1294-1300 | Language: English, Database: CAPLUS and MEDLINE

Stromal cell-derived factor-1 (SDF-1) is a key regulator of the behavior of normal and leukemic precursor-B (pre-B) cells. It is possible that inhibiting SDF-1-driven processes in pre-B acute lymphoblastic leukemia (ALL) may have therapeutic implications. In this study, the authors examined the ability of SDF-1 inhibitors to modulate pre-B ALL cell responses to SDF-1, including chemotaxis, migration into bone marrow stroma, and stroma-supported survival and proliferation on human bone marrow stromal layers. The polyphemusin II-derived inhibitors, T140, TC140012, and T134, and the bicyclam AMD3100, effectively inhibited binding of the anti-CXCR4 monoclonal antibody 12G5 on the pre-B ALL cell line NALM6, with IC₅₀ values of 0.9, 0.9, 0.9, and 1.9 nM, resp. Similar results were obtained with ALL samples. T140 (0.1 μM) and AMD3100 (1 μM) completely blocked SDF-1-induced chemotaxis and attenuated the migration of pre-B ALL cells into bone marrow stromal layers. AMD3100 and TC140012 at a concentration of 50 μM significantly inhibited stroma-dependent proliferation of 6 and 4 of the 8 cases tested, resp., without reducing the cell viability. In addition, AMD3100 and TC140012 enhanced the cytotoxic and antiproliferative effects of the cytotoxic agents vincristine and dexamethasone. The ability of SDF-1 inhibitors to modulate these biol. important functions of leukemic cells warrants further investigation.

View Less

Full Text

Substances (8) Reactions (0) Citing (159) Citation Map

Search Within Results

Search for up to 3 text strings within the result set.

dexamethasone

Search

地塞米松联合治疗

物质角色筛选文献: Substance Role

^ Substance Role

- Biological Study (526)
- Uses (510)
- Analytical Study (2)
- Miscellaneous (1)
- Process (1)

[View All](#)

Substance Role

By Count Alphanumeric

3 Selected

<input checked="" type="checkbox"/> Biological Study (526)	<input type="checkbox"/> Adverse Effect (80)	<input type="checkbox"/> Analytical Study (2)
<input checked="" type="checkbox"/> Therapeutic Use (510)	<input type="checkbox"/> Biological Study, Unclassified (57)	<input type="checkbox"/> Miscellaneous (1)
<input type="checkbox"/> Uses (510)	<input type="checkbox"/> Pharmacokinetics (5)	<input type="checkbox"/> Physical, Engineering, or Chemical Process (1)
<input checked="" type="checkbox"/> Pharmacological Activity (388)	<input type="checkbox"/> Analyte (2)	<input type="checkbox"/> Process (1)

排序:
文献数量
字母顺序

确定文献核心研究内容: Concept

Concept

Top Count | Alphanumeric | Search

3 Selected

<input type="checkbox"/> Humans (644)	<input type="checkbox"/> Acute B-cell leukemia (92)
<input type="checkbox"/> Homo sapiens (517)	<input type="checkbox"/> Stem cell transplantation (90)
<input type="checkbox"/> Human (517)	<input type="checkbox"/> Prednisone (87)
<input type="checkbox"/> Precursor cell lymphoblastic leukemia-lymphoma (507)	<input type="checkbox"/> Retrospective Studies (86)
<input type="checkbox"/> Female (422)	<input type="checkbox"/> Daunorubicin (84)
<input type="checkbox"/> Male (419)	<input type="checkbox"/> Survival Rate (81)
<input checked="" type="checkbox"/> Acute lymphocytic leukemia (398)	<input type="checkbox"/> Mercaptopurine (80)
<input type="checkbox"/> Antineoplastic Combined Chemotherapy Protocols (394)	<input type="checkbox"/> Recurrence (80)
<input checked="" type="checkbox"/> Antitumor agents (352)	<input type="checkbox"/> Chemotherapy (76)
<input checked="" type="checkbox"/> Child (332)	<input type="checkbox"/> CVAD protocol (75)
<input type="checkbox"/> Vincristine (308)	<input type="checkbox"/> Acute T-cell leukemia (70)
	<input type="checkbox"/> Apoptosis (70)

Apply | Cancel

Concept

Top Count | Alphanumeric | Search

Concept Name

tumor 自定义检索

3 Selected

<input type="checkbox"/> Animal gene, tumor suppressor (1)	<input type="checkbox"/> Tumor Cells, Cultured (30)
<input type="checkbox"/> Biomarkers, Tumor (16)	<input type="checkbox"/> Tumor hypoxia (1)
<input type="checkbox"/> Cell Line, Tumor (52)	<input type="checkbox"/> Tumor lysis syndrome (8)
<input type="checkbox"/> Circulating tumor cell (1)	<input type="checkbox"/> Tumor markers (12)
<input type="checkbox"/> Genes, Wilms Tumor (1)	<input type="checkbox"/> Tumor microenvironment (5)
<input type="checkbox"/> Proteins, TRADD (tumor necrosis factor receptor 1-associated death domain) (1)	<input type="checkbox"/> Tumor Necrosis Factor-alpha (3)
<input type="checkbox"/> Receptors, Tumor Necrosis Factor (1)	<input type="checkbox"/> Tumor necrosis factor receptor 1 (1)
	<input type="checkbox"/> Tumor necrosis factor receptors (1)

Apply | Cancel

^ Concept

- Humans (644)
- Homo sapiens (517)
- Human (517)
- Precursor cell lymphoblastic leukemia-lymphoma (507)
- Female (422)

[View All](#)

筛选不同研究领域文献：CA Section

- ^ CA Section
- Pharmacology (940)
 - Unavailable (801)
 - Mammalian Pathological Biochemistry (199)
 - Immunochemistry (75)
 - Mammalian Hormones (23)
- [View All](#)

CA Section

By Count | Alphanumeric

1 Selected

<input checked="" type="checkbox"/> Pharmacology (940)	<input type="checkbox"/> Heterocyclic Compounds (More Than One Hetero Atom) (11)	<input type="checkbox"/> Animal Nutrition (2)
<input type="checkbox"/> Unavailable (801)	<input type="checkbox"/> Pharmacodynamics (11)	<input type="checkbox"/> Amino Acids, Peptides, and Proteins (1)
<input type="checkbox"/> Mammalian Pathological Biochemistry (199)	<input type="checkbox"/> Biochemical Genetics (5)	<input type="checkbox"/> Biomolecules and Their Synthetic Analogs (1)
<input type="checkbox"/> Immunochemistry (75)	<input type="checkbox"/> Radiation Biochemistry (5)	<input type="checkbox"/> Carbohydrates (1)
<input type="checkbox"/> Mammalian Hormones (23)	<input type="checkbox"/> Biochemical Methods (4)	<input type="checkbox"/> Enzymes (1)
<input type="checkbox"/> Pharmaceuticals (17)	<input type="checkbox"/> Microbial, Algal, and Fungal Biochemistry (3)	<input type="checkbox"/> Hormone Pharmacology (1)

文献结果集管理

References search for "Acute lymphoblastic leukemia" + drawn structure

Substances ▾ Reactions ▾ Citing ▾ Knowledge Graph

Structure Match

As Drawn (3,436)

Substructure (3,437)

Filter Behavior

Filter by Exclude

Search Within Results

Search for up to 3 text strings within the result set.

Enter a query...

Search

Searching for... Clear All

dexamethasone X

Concept

Homo sapiens (801)

Filtering: Search Within Results: dexamethasone X Clear All Filters

1,048 Results Sort: Relevance ▾ View: Partial Abstract ▾

1

Effects of inhibitors of the chemokine receptor CXCR4 on acute lymphoblastic leukemia cells in vitro

By: Juarez, J.; Bradstock, K. F.; Gottlieb, D. J.; Bendall, L. J.
Leukemia (2003), 17(7), 1294-1300 | Language: English, Database: CPlus and MEDLINE

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View Less ^

Full Text ▾

Substances (8) Reactions (0) Citing (159) Citation Map

Save and Alert

Share Results

Copy Search to Clipboard

保存、提醒和下载

Save Results

Name
vincristine and acute lymphoblastic leukemia

Search Options
 Query Only Selected Answers All Answers (Up to 20,000)

Add Existing Tags (Optional)

- 乐可为修饰序列文献
- GMU
- Haisco
- indole and palladium ref
- Innocare

New Tag (Optional) Tag Color
Add tag name Light Blue

Alerts

Frequency
As Available

Add Email(s)
Add Recipient(s)

- As Available
- Weekly
- Monthly

Save Cancel

Download Reference Results

File Type
PDF

Select Quantity
 All Results
 Selected Results
 Range (ex. 2 to 20)

Display
 Result Summary
 Result Details

File Name
Reference_20230628_1301

File Type
PDF

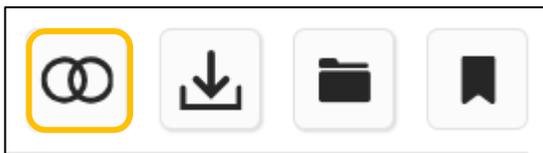
- Citation (.ris)
- Excel (.xlsx)
- PDF
- Quoted (.txt)
- Rich Text (.rtf)
- Tagged (.txt)

Include
 Task History
 Abstract
 Concepts
 Substances

Download Cancel [Learn more about downloads.](#)

多种下载格式，.ris 文件
可导入文献管理软件

合并



Combine Reference Results

Select a Combine Option:

Add
Select

Intersect
Select

Subtract
Select

[Learn More About Combine](#)

- 并集
- 交集
- 差集

Combine Reference Results: Subtract

Select 1 Saved Item: [Return to Combine Option](#)

<input checked="" type="radio"/>	"Acute lymphoblastic leukemia"	Query	October 8, 2024
----------------------------------	--------------------------------	-------	-----------------

Select 1 Saved Item to Subtract:

Subtract the selected saved item from the current answer set.

Subtract the current answer set from the selected saved item.

[View Results](#) [Cancel](#) [Learn More About Combine](#)

绘制知识谱图: Knowledge Graph

References search for "Acute lymphoblastic leukemia" + drawn structure

Substances

Reactions

Citing

Knowledge Graph



Save and Alert

Knowledge Graph from "Acute lymphoblastic leukemia" + drawn structure References Search

Key

References

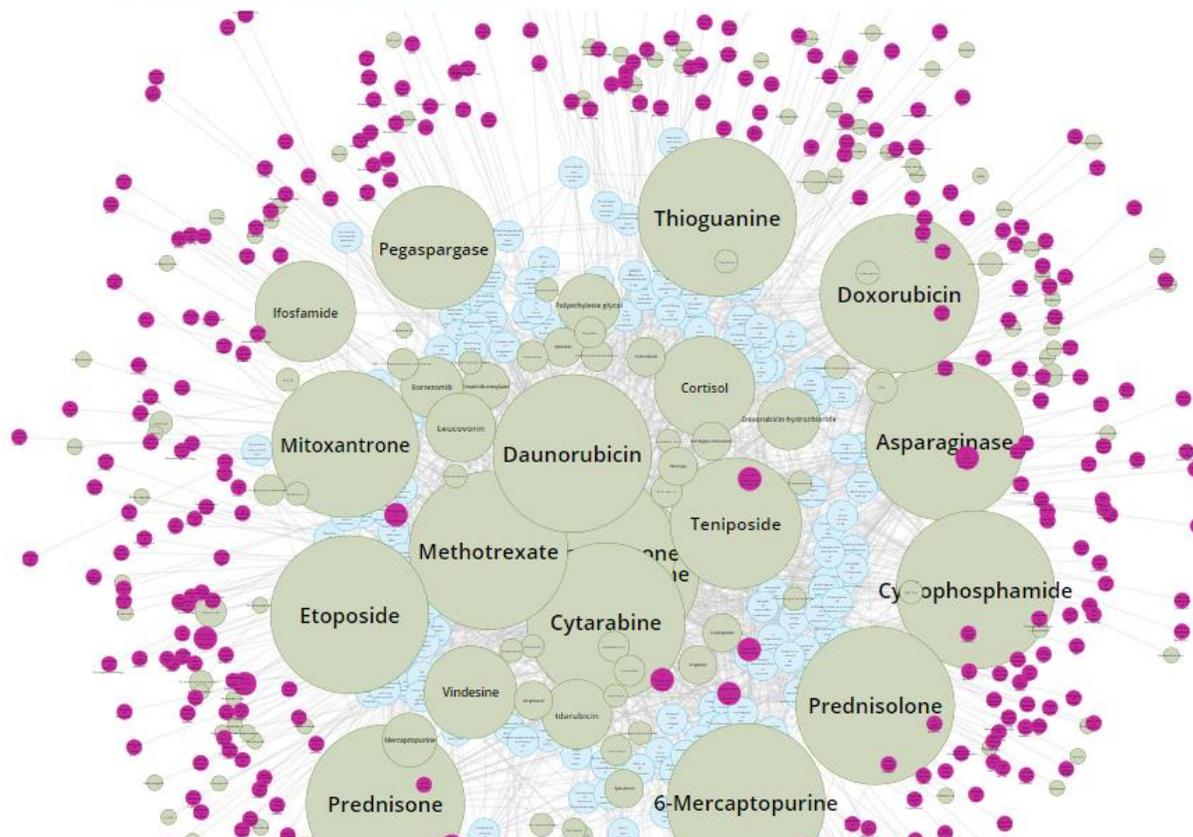
Authors

Concepts

Substances

Organizations

Search the graph...



Reset

查看目标文献详情

Prospective study of hemostatic alterations in children with acute lymphoblastic leukemia

11

0

49



Citation Map

In this Reference

- Concepts
- Substances
- Cited Documents

By: Giordano, Paola; Molinari, Angelo Claudio; Del Vecchio, Giovanni Carlo; Saracco, Paola; Russo, Giovanna; Altomare, Paolo; Crescenzo, Nicoletta; Santoro, Nicola; Marchetti, Marina; et al
[View All](#)

DOI: [10.1002/ajh.21665](https://doi.org/10.1002/ajh.21665)

In a group of newly diagnosed acute lymphocytic leukemia (ALL) children we evaluated a number of hemostatic and inflammatory markers at diagnosis and at different time points during chemotherapy for the remission induction to identify alterations in the levels of prothrombotic markers before and during the course of chemotherapy. The following plasma markers were evaluated: thrombin-antithrombin complex (TAT), D-Dimer, plasminogen activator inhibitor 1 (PAI-1), antithrombin, fibrinogen, von Willebrand factor antigen and high mol. weight VWF (HMW-VWF) multimers, P-selectin, tumor necrosis factor alpha (TNF- α), and interleukin 6 (IL-6). Blood samples were collected at the following time points: at TO (baseline) and T1 (+24 days of therapy), T2 (+36 days of therapy). The results show that, at diagnosis, ALL children presented with laboratory signs of increased thrombin formation (i.e. high TAT and D-dimer levels), fibrinolysis inhibition (i.e. high PAI-1 level), endothelial activation (i.e. high soluble P-selectin levels) and inflammation (i.e. high TNF-alpha and IL-6 levels). After starting induction therapy, thrombin formation and inflammatory cytokines significantly decreased. To the opposite, PAI-1 and P-selectin significantly increased. In addition, venous thromboembolism (VTE) episodes developed in two cases during induction therapy, which did not allow to determine the predictive value for VTE of laboratory markers.

Keywords: hemostatic alteration child acute lymphoblastic leukemia

[View PDF](#)

[Full Text](#)

Publication Information • Journal

Source	Database Information	Company/Organization	Publisher	Language
American Journal of Hematology	AN: 2010:674136	Pediatric Department	Wiley-Liss, Inc.	English

CAS Concepts

CAS 科学家提供的核心研究点

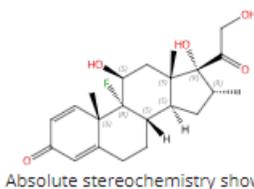
Acute lymphocytic leukemia	Fibrinogens Role: Biological Study, Unclassified
Biomarkers	Homo sapiens
Blood plasma	Human
Blood platelet	Inflammation
Child development	Interleukin 6 Role: Biological Study, Unclassified

Substances

重点研究物质

Substances (11)

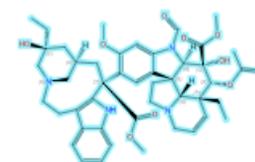
50-02-2



C₂₂H₂₉FO₅
Dexamethasone

Role: Pharmacological Activity, Therapeutic Use, Biological Study, Uses

57-22-7



Absolute stereochemistry shown, Rotation (+)

C₄₆H₅₆N₄O₁₀
Vincalukoblastine, 22-oxo-

Role: Pharmacological Activity, Therapeutic Use, Biological Study, Uses

物质角色

绘制引文地图: Citation Map

Citation Map for **Prospective study of hemostatic alterations in children with acute lymphoblastic leukemia**

By: Giordano, Paola; Molinari, Angelo Claudio; Del Vecchio, Giovanni Carlo; Saracco, Paola; Russo, Giovanna; Altomare, Maria; Perutelli, Paolo; Crescenzo, Nicoletta; Santoro, Nicola; Marchetti, Marina; et al

American Journal of Hematology (2010), 85(5), 325-330 | Language: English, Database: CAPLUS and MEDLINE

Full Text ▾



Thrombotic complications in childhood acute lymphoblastic leukemia: a meta-analysis of 17 prospective studies comprising 1752 pediatric patients

By: Caruso, Vanesa; Iacoviello, Licia; Di Castelnuovo, Augusto; Storti, Sergio; Mariani, Guglielmo; de Gaetano, Giovanni; Donati, Maria Benedetta
Blood (2006)

Expand Citations

Create Map

39

48

17



Reset



^ Citation Map Key

Cited by Root Document

References Citing Root Document

查看专利详情

Rotigotine ionic liquid and compositions for use as dopamine D2 receptor agonists or antiparkinson agent

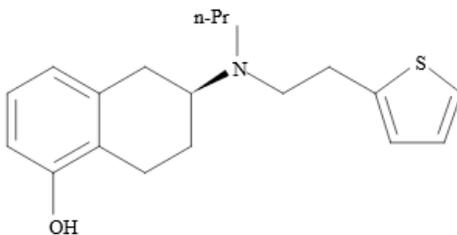
34 2 1 Citation Map

In this Reference

By: Janssen, Christian

The present invention provides ionic liquids of rotigotine, pharmaceutical compositions comprising said ionic transdermal compositions and methods of preparing such ionic liquids An ionic liquid comprising at least one and at least one counter ion derived from an organic compound is used in the treatment, prevention, amelioration of a disease susceptible to a dopamine D2 receptor agonist or an antiparkinson agent. The invention further provides compositions described herein to overcome problems arising from polymorphism, solubility and delivery, to improve functionality, to enhance efficacy, and to improve ease of use and manufacture For example, an ionic liquid comprising rotigotine and an octanoic anion was obtained in quant. yield using rotigotine and octanoic acid.

- [IPC Data](#)
- [CAS Concepts](#)
- [Substances](#)
- [Reactions](#)
- [Formulations](#)
- [Cited Documents](#)



Keywords: rotigotine ionic liquid preparation antiparkinson dopamine D2 receptor agonist

PatentPak Viewer

Get Prior Art Analysis

Full Text

Priority Application

Priority Application Number	Application Date
EP2010-15079	2010-11-29
US2010-61419070P	2010-12-02
WO2011-EP71321	2011-11-29
WO2011-US62364	2011-11-29

IPC Data

CAS Concepts

Substances

Reactions

Formulations

Cited Documents

View Less

Publication Information • Patent

Patent Number	Publication Date	Application Number	Application Date	Kind Code
WO2012074988	2012-06-07	WO2011-US62364	2011-11-29	A1

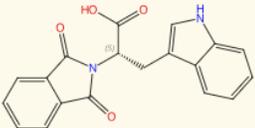
PatentPak Viewer 高效阅读专利

CAS PatentPak

PAGE 14 / 30 ZOOM - + DOWNLOAD PDF PDF+

Key Substances in Patent

CAS RN 48208-26-0



Analyst Markup Locations (2)

- Page 14
- Page 14

CAS RN 9037-42-7

DNA methyltransferase

Analyst Markup Locations (1)

- Page 16

CAS RN 320-67-2



Analyst Markup Locations (2)

- Page 16
- Page 21

EP 1 574 499 A1

Fig. 3

[0060] The effect of RG108 on human cell lines. (a) Growth of HCT116 (left panel) and NALM-6 cells (right panel) in medium supplemented with 10 μM RG 108 (filled circles) or 10 μM 5-azacytidine (grey diamonds). Controls are shown as open squares. (b) Viability of HCT116 and NALM-6 cells under the same conditions as described in (a). (c) Genomic cytosine methylation levels of HCT116 (left panel) and NALM-6 cells (right panel) in medium supplemented with 10 μM RG 108 (black bars) or 10 μM 5-azacytidine (grey bars). Controls are shown as white bars. DNA methylation levels were determined after 5 and 15 days, as indicated. DNA from NALM-6 cells incubated with 5-azacytidine for 15 days could not be analyzed due to degradation. All results were obtained from multiple experiments. Standard deviations for panels (a) and (b) were negligible.

Fig. 4

[0061] The carboxyl-group of RG108 is important for its interaction with DNA methyltransferases. (a) Structure of ΔC -RG108, a control compound that lacks the carboxyl-group of RG-108. (b) Calculated binding energies of ΔC -RG108 (grey bar) docked into the DNMT1 active site are compared to cytidine (white bar) and RG108 (black bar). (c) Genomic cytosine methylation levels of HCT116 cells incubated with ΔC -RG108 (black bar) are compared to methylation levels of corresponding cells incubated with no inhibitor (white bar) or RG108 (grey bar).

Fig. 5

[0062] RG108 causes complete demethylation of the human hMLH1 gene in cells treated with 10 micromolar RG108, while no demethylation was observed in control experiments without inhibitor or with 10 micromolar 5-azacytidine (Sigma), respectively (Fig. 5). M indicates amplification products from methylated templates, U indicates amplification

精准定位

小结

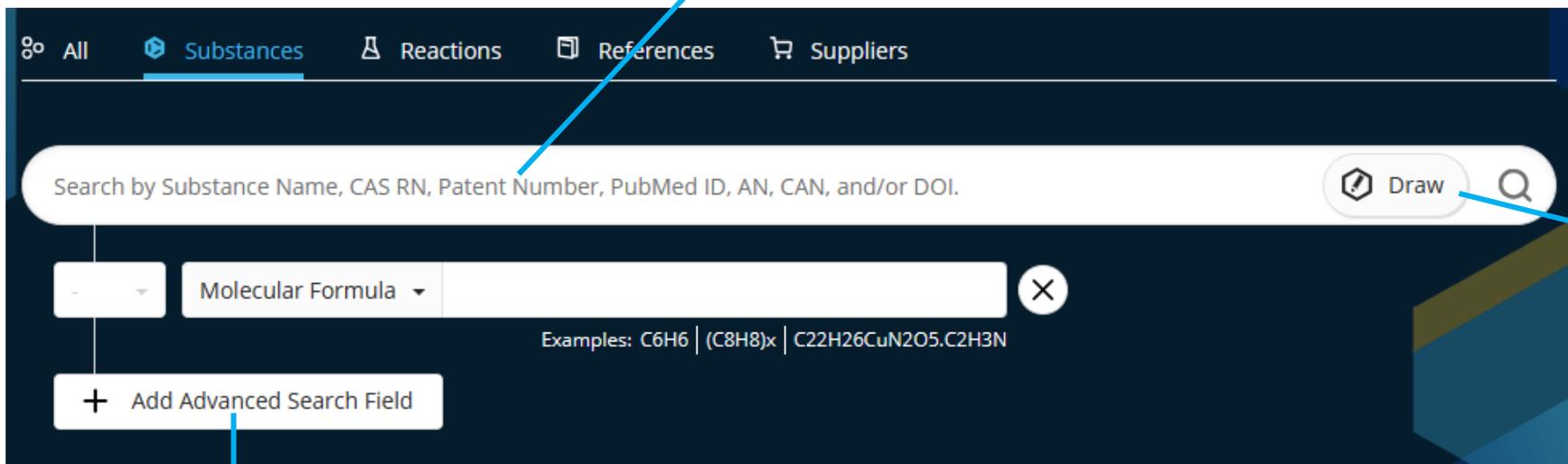
1. 检索词的构建：使用布尔逻辑算符及通配符连接主题词，CAS Lexicon 丰富选词
2. 利用高级检索选项以及文本与结构联合进行自定义组合检索
3. 通过聚类筛选工具快速获得目标文献
4. 利用引文地图拓展检索
5. 使用 PatentPak 高效阅读专利

如何调研某类物质？

- 快速检索聚合物或无机化合物？
- 利用谱图数值确认产物或杂质？从属性值出发，调研某类材料？
- 检索完整分子结构？通式结构？或含有某些片段的物质？
- 如何确认结构新颖性？

研究某种/某类物质？

- 通过物质标识符、文献标识符检索物质



使用结构绘制面板
进行结构检索

- 高级检索

- 检索策略推荐
 - 有机化合物，金属配合物，天然产物：结构检索
 - 无机物，合金：分子式检索
 - 高分子化合物：分子式检索和结构检索

物质检索—物质/文献标识符

- 可同时检索多个物质识别符（物质名称或CAS 登记号）
- 不同物质使用空格隔开（2000个字符）

- 迅速获得关注文献中的物质信息

Substances search for "Paxlovid 2628280-40-8"

Filter Behavior: Filter by, Exclude

Reaction Role: Product (1), Reactant (1)

Reference Role: Adverse Effect (2), Analyte (2), Analytical Study (2), Biological Study (2), Biological Study, Unclassified (2)

Commercial Availability, Number of Components, Molecular Weight

2 Results

1: 2628280-40-8
C₂₃H₃₂F₃N₅O₄
3-Azabicyclo[3.1.0]hexane-2-carboxamide, N-[[1(S)-1-cyano-2-[[3(S)-2-oxo-3-pyrroli...
319 References, 106 Reactions, 39 Suppliers

2: 2803933-60-8
C₃₇H₄₈N₆O₅S₂ · C₂₃H₃₂F₃N₅O₄
Components: 2
Paxlovid
39 References, 0 Reactions, 0 Suppliers

CAS SciFinder® Substances 10.1126/science.abl4784

Substances search for "10.1126/science.abl4784"

References, Reactions, Suppliers

Filter Behavior: Filter by, Exclude

Reaction Role: Product (9), Reactant (7), Reagent (4), Catalyst (2), Solvent (2)

Reference Role: Biological Study (10), Biological Study, Unclassified (10)

10 Results

1: 147-85-3
C₅H₉NO₂
L-Proline
117K References, 48K Reactions, 164 Suppliers

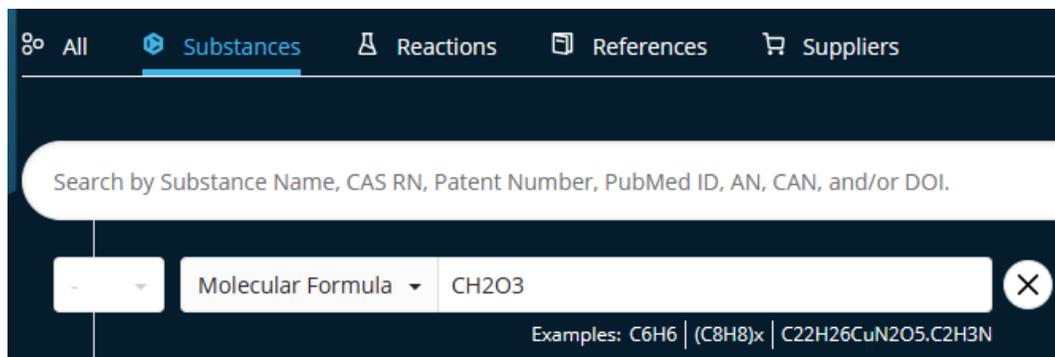
2: 61-90-5
C₆H₁₃NO₂
L-Leucine
125K References, 6,092 Reactions, 164 Suppliers

Relevance
CAS RN: Ascending
CAS RN: Descending
Molecular Formula: Ascending
Molecular Formula: Descending
Molecular Weight: Ascending
Molecular Weight: Descending
Number of References: Ascending
Number of References: Descending
Number of Suppliers

物质排序：相关度、CAS RN、分子式、分子量、文献量、供应商数量

分子式检索：高效检索聚合物或无机化合物

- 含碳化合物，C排第一位，H排第二位，其他元素符号按照首字母顺序进行排列
- 不含碳化合物，按照元素符号的首字母顺序进行排列
- 不同组分之间用“.”隔开，如：铁钴镍合金 Co.Fe.Ni
- 无机含氧盐：阳离子和阴离子用点（.）分开；阴离子以氢补齐至电中性



适用于分子式检索的物质类型包括：

- 无机化合物：合金，无机表格化合物，多氧簇金属化合物等
- 聚合物

属性值、谱图数值联用检索物质

Search by Substance Name, CAS RN, Patent Number, PubMed ID, AN, CAN, and/or DOI.

Molecular Weight 220 to 280
Predicted values only. Examples: 46.07 | 125 to 350 | >300

AND pKa 1.3 to 1.8
Predicted values only. Examples: -1.77 | <9.25 | >2.4 | 5.25 to 8.25

AND Carbon-13 NMR 114 to 171, 96, 11.5
Allowance of ± 2 ppm. Examples: 152.3, 127.6, 133.1 | 155.02 to 207.59 | 187

+ Add Advanced Search Field

- 分子量：220至280之间
- pKa：1.3至1.8之间
- C谱特征峰：114至171之间，96，11.5

Substances search for 3 Advanced Fields

References Reactions Suppliers

Filtering: Bioactivity Data: 3 Selected X

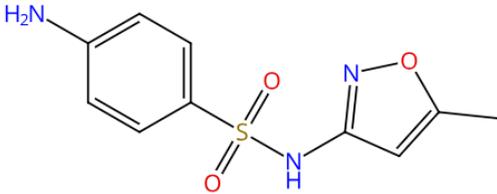
15 Results Sort: Molecular Formula: Ascending View: Partial

Result ID	Chemical Name	Chemical Formula	References	Reactions	Suppliers
296262-16-3	2-[[[5,6-Dimethylthieno[2,3-d]pyrimidin-4-yl]thio]acetic acid	C ₁₀ H ₁₀ N ₂ O ₂ S ₂	5	42	44
723-46-6	Sulfamethoxazole	C ₁₀ H ₁₁ N ₃ O ₃ S	24K	961	120
1631737-39-7	(2R,3R,4S,5R)-4,5-Dihydro-5-(hydroxy methyl)-3'-methylspiro[furan-2(3H),7(6'H)]-...	C ₁₀ H ₁₅ N ₃ O ₅	2	22	0
442571-27-9	2-[[[5,6-Dimethylthieno[2,3-d]pyrimidin-4-yl]thio]acetic acid	C ₁₀ H ₁₀ N ₂ O ₂ S ₂	5	42	44
1927010-88-5	2-[[[5,6-Dimethylthieno[2,3-d]pyrimidin-4-yl]thio]acetic acid	C ₁₀ H ₁₀ N ₂ O ₂ S ₂	5	42	44
697787-29-4	2-[[[5,6-Dimethylthieno[2,3-d]pyrimidin-4-yl]thio]acetic acid	C ₁₀ H ₁₀ N ₂ O ₂ S ₂	5	42	44

物质详情

CAS Registry Number: **723-46-6**

References (26K) Reactions (995) Suppliers (127)   



C10H11N3O3S
Benzenesulfonamide, 4-amino-N-(5-methyl-3-isoxazolyl)- (9CI, ACI)



Key Physical Properties

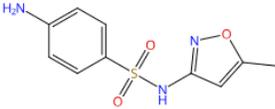
- Molecular Weight
- Melting Point (Experimental)
- Boiling Point (Predicted)
- Density (Experimental)
- pKa (Predicted)

Experimental Properties | Spectra

- Other Names and Identifiers
- Experimental Properties
- Experimental Spectra
- Structure Activity Relationships
- Absorption, Distribution, Metabolism, and Excretion Data
- Toxicity
- Predicted Properties
- Predicted Spectra
- Bioactivity Indicators
- Target Indicators
- Regulatory Information
- GHS Hazard Statements
- Additional Details

- 折叠菜单显示物质各类信息

723-46-6



C10H11N3O3S

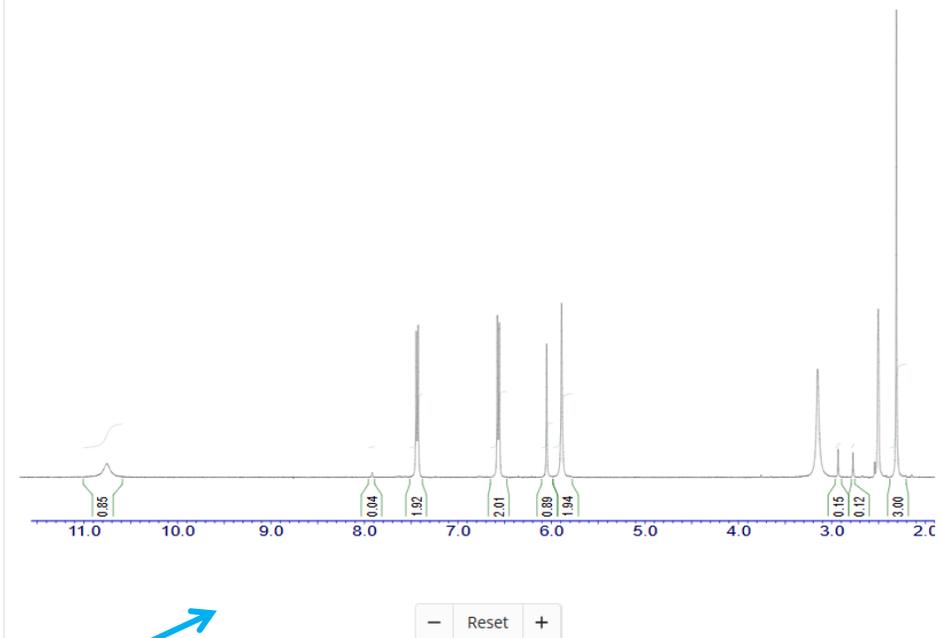
CAS Name
Sulfamethoxazole

Conditions

- Working Frequency
400 MHz
- Solvent
[Dimethyl sulfoxide \(67-68-5\)](#)
[Carbon tetrachloride \(56-23-5\)](#)
- Temperature
20 °C

Spectrum Summary

- Spectrum ID
F0175-0013
- Source
Spectral data were obtained from Life Chemicals



Experimental Spectra

- ¹H NMR**
- ¹³C NMR
- Hetero NMR
- IR
- Mass
- Raman
- UV and Visible

[View Proton NMR Spectrum](#) Source
(1) LC

[View Proton NMR Spectrum](#) (2) ENAMINE

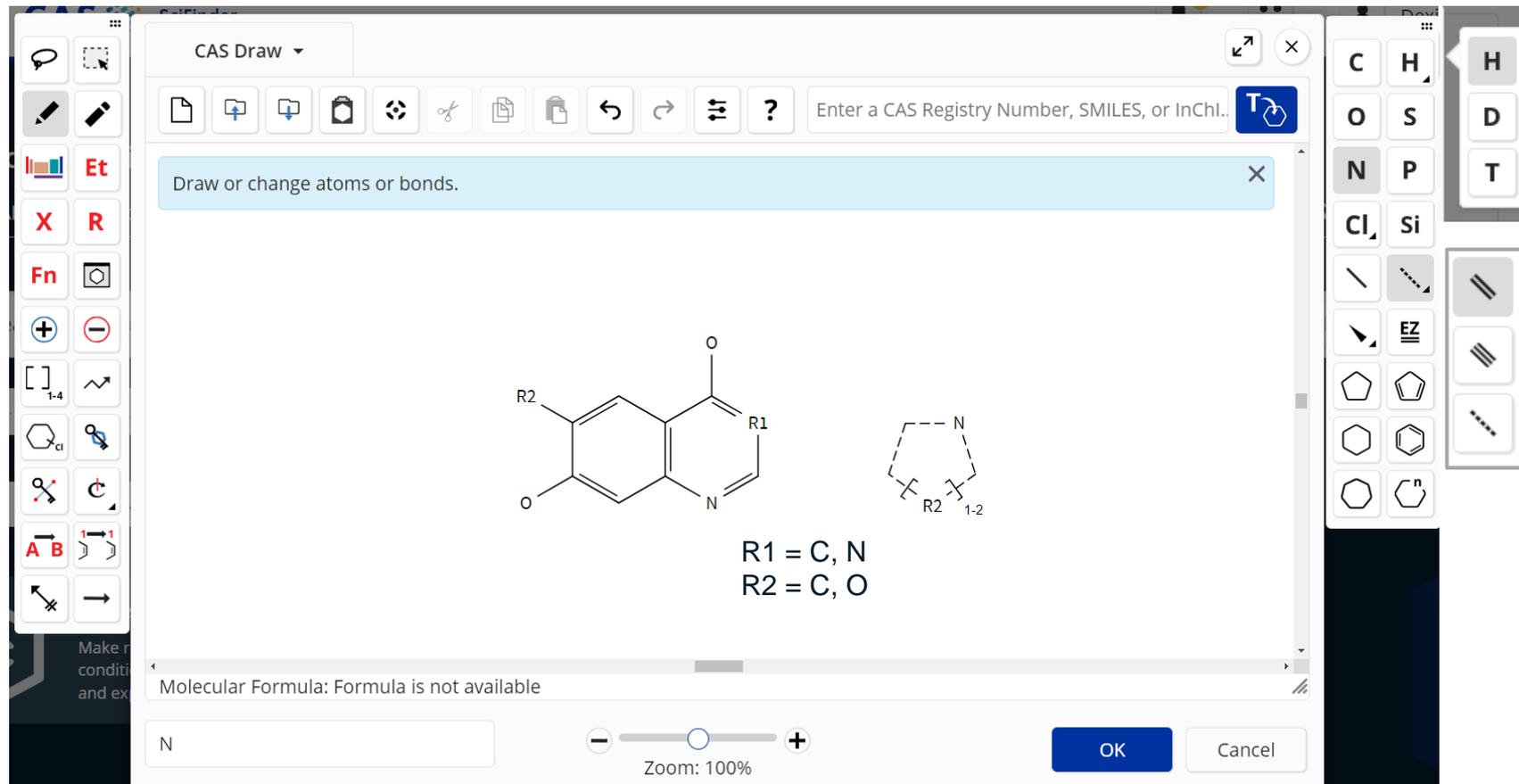
结构检索

灵活构建通式结构，提高物质/反应信息的检索效率

-  选择可变基团
-  自定义R基团
-  片段结构
-  重复工具
-  取代位置可变
-  环锁定工具
-  原子锁定工具

利用绘图工具自定义相似结构:

1. 化学键型键级不确定 
2. 骨架结构上指定出现的原子 
3. 环系范围的定义 



结构检索

例：已知结构片段的物质检索

结构检索时，无需分步进行，一次检索即可得到As Drawn, Substructure和Similarity结果

Substances search for drawn structure

References Reactions Suppliers

Structure Match

As Drawn (81)

Substructure (148)

Similarity (38K)

Analyze Structure Precision

Chemscape Analysis

Visually explore structure similarity with a powerful new tool. [Learn more about Chemscape.](#)

Create Chemscape Analysis

Filter Behavior

Filter by Exclude

81 Results

Sort: Relevance View: Partial

1 2447-54-3

C20H14NO4
Sanguinarine

2 777808-75-0

C20H11NO4T3
[1,3]Benzodioxolo[5,6-c]-1,3-dioxolo[4,5-i]phenanthridinium, 13-(methyl-t3)-

3 117-00-0

C20H14NO4.HO
Components: 2
Component RN: 2447-54-3
[1,3]Benzodioxolo[5,6-c]-1,3-dioxolo[4,5-i]phenanthridinium, 13-methyl-, hydroxi...

2,605 References 113 Reactions 44 Suppliers

0 References 0 Reactions 0 Suppliers

37 References 0 Reactions 0 Suppliers

Filter Behavior

Filter by Exclude

Search Within Results

Substance Class

Reaction Role

Reference Role

Number of Components

Experimental Property

Experimental Spectrum

Bioactivity Data

Bioactivity Indicator

Target Indicator

Regulatory Data by Country/Region

GHS Hazard Statements

物质筛选类别

:

二次检索

物质类别

反应角色

文献角色

组分数

实验物性数据

实验谱图

.....

物质检索结果的筛选

Search Within Results

Substance Class **物质类别**

- Salt and Compound With (50)
- Mixture (20)
- Organic/Inorganic Small Molecule (7)
- Polymer (4)

Reaction Role **物质在反应中的角色**

- Product (33)
- Reactant (2)

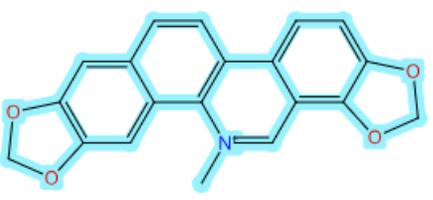
Reference Role **物质在文献中的研究角色**

- Biological Study (53)
- Uses (46)
- Preparation (45)
- Synthetic Preparation (40)
- Therapeutic Use (36)

[View All](#)

4

693824-79-2



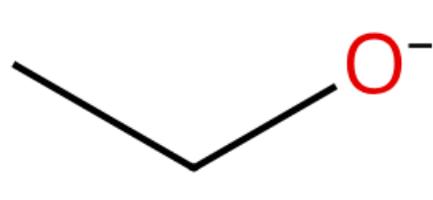
C#N

$C_{20}H_{14}NO_4 \cdot CN$
Components: 2
[1,3]Benzodioxolo[5,6-c]-1,3-dioxolo[4,5-i]phenanthridinium, 13-methyl-, cyanide

5 References 0 Reactions 0 Suppliers

5

117235-09-3



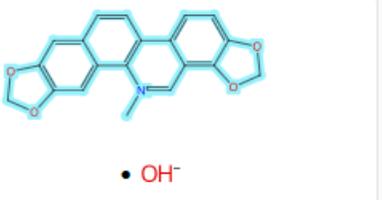
C2H5O-

$C_{20}H_{14}NO_4 \cdot C_2H_5O$
Components: 2
[1,3]Benzodioxolo[5,6-c]-1,3-dioxolo[4,5-i]phenanthridinium, 13-methyl-, salt wi...

1 Reference 0 Reactions 0 Suppliers

6

6533-66-0



[OH-]

$C_{20}H_{14}NO_4 \cdot C_2H_6O \cdot HO$
Components: 3
[1,3]Benzodioxolo[5,6-c]-1,3-dioxolo[4,5-i]phenanthridinium, 13-methyl-, hydroxi...

0 References 0 Reactions 0 Suppliers

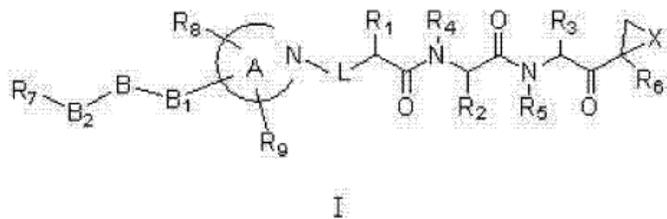
CAS Markush检索，助力结构查新

CN 104945470 A

权利要求书

1/3 页

1. 一种杂环构建的三肽环氧化物类化合物，具有下述结构通式 I：



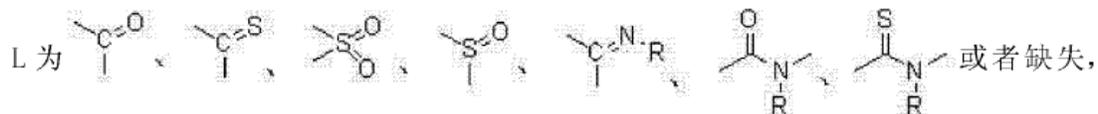
其中：

R_1, R_2, R_3 各自独立选自 H、 C_{1-6} 烷基 -D、卤代的 C_{1-6} 烷基 -D、 C_{1-6} 羟基烷基、 C_{1-6} 巯基烷基、 C_{1-6} 烷氧基烷基、芳基、芳烷基、杂芳基或杂芳烷基；其中：D 为 N(R_a) (R_b) 或缺失， R_a, R_b 各自独立选自 H、OH、 C_{1-6} 烷基、卤代的 C_{1-6} 烷基或 N 末端保护基；

R_4, R_5 各自独立选自 H、OH、 C_{1-6} 烷基、卤代的 C_{1-6} 烷基或芳烷基；

R_6 选自 H、 C_{1-6} 烷基、卤代的 C_{1-6} 烷基、 C_{1-6} 羟基烷基、 C_{1-6} 烷氧基、卤代的 C_{1-6} 烷氧基、C(O)O- C_{1-6} 烷基、C(O)NH- C_{1-6} 烷基、芳烷基；

X 为 O、S、NH、N- C_{1-6} 烷基或 N- 卤代的 C_{1-6} 烷基；



其中 R 选自 H、 C_{1-6} 烷基或卤代的 C_{1-6} 烷基；

环 A 选自 5 ~ 7 元的饱和脂肪杂环、不饱和杂环、或者有取代的 5 ~ 7 元的饱和脂肪杂环、不饱和杂环，所述的杂环包含 0 ~ 3 个选自 O、N 和 S 的杂原子并任选地被 R_8, R_9 和 B_1 基团取代；

R_8, R_9 分别独立选自 H、OH、 C_{1-6} 烷基、 C_{1-6} 烷氧基、 C_{1-6} 羟基烷基、 C_{1-6} 巯基烷基、 C_{1-6} 烷

具体物质[Specific Substance]：以具体化学结构陈述的特定物质，会被分配CAS RN

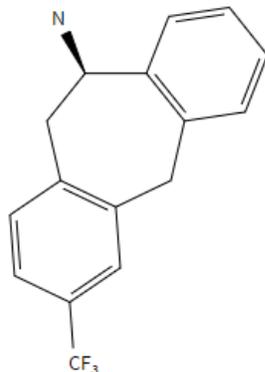
预测性物质[Prophetic Substance]：

- 使用Markush结构陈述的预测物质，一个Markush可以陈述成百上千，甚至更多的结构
- 被Markush结构包含，但未被实施或呈现在表格、权利要求书或说明书中的结构，不会被CAS分配CAS Registry Number
- Markush检索，能检索到通过Substance可能检索不到的结构

CAS Markush检索

第一步：物质结构检索

- As drawn结果为0
- Substructure结果为2
- Similarity相似度最高85-89%



Structure Match: 2 Results

As Drawn (0)

Substructure (2)

Similarity (5,664)

Analyze Structure Precision

Chemscape Analysis

Visually explore structure similarity with a powerful new tool.

Learn more about Chemscape.

Create Chemscape Analysis

146364-17-2

C₁₇H₁₄F₃N

10,5-(Iminomethano)-5H-dibenzo[a,d]cycloheptene, 10,11-dihydro-3-(trifluoromethyl)-

146364-18-3

C₁₈H₁₆F₃N

10,5-(Iminomethano)-5H-dibenzo[a,d]cycloheptene, 10,11-dihydro-12-methyl-3-(trifluoromethyl)-

Structure Match

As Drawn (0)

Substructure (2)

Similarity (5,664)

Chemscape Analysis

Visually explore structure similarity with a powerful new tool.

Learn more about Chemscape.

Create Chemscape Analysis

Filter Behavior

Filter by Exclude

Similarity

- 85-89 (1)
- 80-84 (2)
- 75-79 (20)
- 70-74 (140)
- 65-69 (958)
- 60-64 (4,211)

Reaction Role

Reference Role

Filtering: Number of Components: 1

5,332 Results

Sort: Number of References: Descending

View: Partial

1 61

1210-33-9

C₁₅H₁₃Cl

5-Chlorodibenzosuberane

143 References 130 Reactions 61 Suppliers

2 64

1057277-76-5

C₁₆H₁₄F₃N

1,2,3,4-Tetrahydro-2-[4-(trifluoromethyl)phenyl]isoquinoline

90 References 121 Reactions 2 Suppliers

3 68

7005-53-0

C₁₅H₁₅N

IEM 2115

58 References 78 Reactions 14 Suppliers

4 60

3436-04-2

C₁₈H₁₇Br

5-(3-Bromopropylidene)-10,11-dihydro-5H-dibenzo[a,d]cycloheptene

5 62

1729-63-1

C₁₆H₁₃N

10,11-Dihydro-5H-dibenzo[a,d]cycloheptene-5-carbonitrile

6 64

35764-73-9

C₂₁H₂₄F₃N

Fluotracen

Relative stereochemistry shown

Feedback

为了尽可能完整地获得公开的结构信息，需要同时进行Substance和Markush结构检索

CAS Markush检索

第二步：Markush结构检索
获得四项专利文献

- 直观呈现检索结构与专利原文中Markush匹配部分的结构；
- 标引其在专利中出现的位置；
- 详细的结构取代信息描述

CAS SciFinder® Substances Enter a query... Edit Search

Return to Home

Patent Markush search for drawn structure

References

Patent Markush Match

As Drawn (4)

Substructure (33)

Filter Behavior

Filter by Exclude

Patent Office

- World Intellectual Property Organization (3)
- European Patent Organization (1)

CA Section

- Agrochemical Bioregulators (1)
- Electric Phenomena (1)
- Heterocyclic Compounds (More Than One Hetero Atom) (1)
- Pharmacology (1)

Filter Content Report

4 Results

1

WO2011025969

Compounds that treat malaria and prevent malaria transmission

By: Su, Xin-Zhuan; Yuan, Jing; Raj, Dipak; Pattaradilokrat, Sittiporn; Johnson, Ron; Huang, Ruili
World Intellectual Property Organization, WO2011025969 A1 2011-03-03 | Language: English, Database: CAplus
Assignee: United States Dept. of Health and Human Services

Patent claim 1

PatentPak Full Text

Patent	Language	Kind Code	PatentPak Options
WO2011025969	English	A1	PDF PDF+ Viewer
CN102595894	Chinese	A	PDF
US20120196882	English	A1	PDF PDF+ Viewer
US9375424	English	B2	PDF
US20160303103	English	A1	PDF

2

EP502788

Antitumor and...

By: Regnier, Gilbert; Dhambaut, Alain; Alessi, Gianmario; Pierre, Alain; Leonce, Stephane
European Patent Organization, EP502788 A1 1992-09-09 | Language: French, Database: CAplus
Assignee: Adir et Cie.

Patent claim 11

Full Text

物质检索小结

1. 物质检索方法：物质、文献标识符检索；分子式、物性参数、谱图数据检索；及结构式检索，充分利用结构绘制工具，合理扩大或限定结构检索范围
2. 正确理解As Drawn、Substructure、Similarity检索结果集的意义和范围
3. 充分利用物质筛选项准确定位目标物质：Reaction Role、Reference Role等
4. 利用CAS Markush检索尽可能全面的获得结构的公开信息

如何进行反应调研?

- 如何从我感兴趣的底物、产物或催化剂出发，找到关联的反应？
- 如何查找相似反应？
- 如何关注特定转化类型的反应？
- 如何在大量反应结果中，快速找到最想要的反应？
- 如何查找涉及机理研究的反应？或人名反应？
- 如何设计新化合物的逆合成路线？

研究某种/某类反应?

- 反应检索方法
 - 物质或文献标识符
 - 结构式
 - 关键词与结构联用



1

910463-68-2

Image Not Available

Unspecified
Semaglutide

Protein/Peptide Sequence
Sequence Length: 34

1,527 References **259 Reactions** 32 Suppliers

Reactions search for "Semaglutide"

References -

Filter Behavior

Filter by Exclude

Substance Role

- Product (222)
- Reactant (10)

Yield

- 90-100% (3)

228 Results

Group: By Scheme Sort: Number of Steps: Descending View: Collapsed

Scheme 1 (1 Reaction) Steps: 7

Absolute stereochemistry shown, Rotation (+)

Suppliers (98)

Suppliers (64)

910463-68-2
Image Not Available

Suppliers (28)

Reactions search for "175:621496"

References -

Filter Behavior

Filter by Exclude

Yield

- 90-100% (3)
- 80-89% (5)
- 70-79% (2)
- 50-69% (3)
- No Yield Available (120)

133 Results

Group: By Scheme Sort: Number of Steps: Descending View: Collapsed

Scheme 1 (2 Reactions) Steps: 7-8

Absolute stereochemistry shown

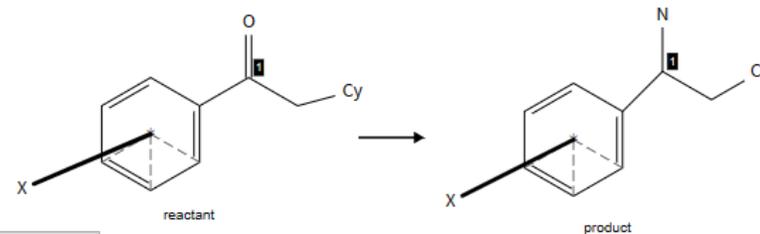
Suppliers (145)

Suppliers (77)

204656-20-2
Image Not Available

Suppliers (37)

查找亚结构反应或相似反应



As Drawn
亚结构反应
相似反应

Reactions search for drawn structure

References

Structure Match

- As Drawn (34)
- Substructure (8,044)
- Similarity (0)

Filter Behavior

Filter by Exclude

Search Within Results

Yield

- 80-89% (4)
- 70-79% (2)
- 50-69% (1)
- No Yield Available (9)

Reaction Scale

- Milligram (2)
- Gram (1)
- No Scale Provided (13)

Non-Participating Functional Groups

Filtering: Reaction Mapping: Mapping Data Available

16 Results

Group: By Scheme

- By Scheme
- By Document
- By Transformation

Sort: Relevance

- Relevance
- Publication Date: Newest
- Publication Date: Oldest
- Yield
- Number of Steps: Ascending
- Number of Steps: Descending

View: Collapsed

Scheme 1 (5 Reactions)

Suppliers (93) Suppliers (15)

Expand Scheme

Scheme 2 (1 Reaction) Steps: 1 Yield: 76%

Suppliers (53) Suppliers (3)

31-614-CAS-28968228 Steps: 1 Yield: 76% Preparation of heterocyclic compounds as selective subtype alpha 2 adrenergic agents

1.1 Reagents: [O-Methylhydroxylamine hydrochloride](#)
Solvents: [Pyridine](#); rt; 1 h, 50 °C

By: Heidelberg, Todd M.; et al

反应排序:
相关度
公布时间
产率
步数

反应分组:
按反应式
按文献
按转化类型

高效筛选目标反应

反应筛选类别:

产率、规模、步数
不参与反应的官能团
实验步骤
反应类型、立体化学
试剂、催化剂、溶剂
商品信息……

文献筛选类别:

文献类型、语言
出版年份、刊物名

折叠菜单: 相同反应类型的反应在同一菜单里, 方便阅读和筛选

The screenshot displays a search interface for chemical reactions. On the left, there are two filter panels. The top panel, 'Structure Match', includes 'As Drawn (34)', 'Substructure (8,044)', and 'Similarity (0)'. The bottom panel, 'Filter Behavior', has 'Filter by' and 'Exclude' buttons. Below these are two vertical filter menus. The first menu includes 'Commercial Availability', 'Reaction Notes', 'Source Reference', 'Document Type', 'Language', 'Publication Year', 'Organization', 'Publication Name', and 'CA Section'. The second menu, 'Search Within Results', includes 'Yield', 'Reaction Scale' (with options for Milligram, Gram, and No Scale Provided), 'Non-Participating Functional Groups', 'Number of Steps', 'Reaction Mapping', 'Experimental Protocols', 'Reaction Type', 'Stereochemistry', 'Reagent', 'Catalyst', and 'Solvent'. At the bottom of the filter menus is a 'Filter Content Report' section with a download icon. The main results area shows 8,044 results, grouped by transformation. The first result is 'Reductive Alkylation of Ammonia or Amines' with 108 related reactions, showing a chemical reaction between a carbonyl compound and an amine. The second result is 'Formation of N/O/S Heterocycles' with 47 related reactions, showing the cyclization of a 1,2-dicarbonyl compound. The third result is '1,3-Dipolar Addition' with 37 related reactions. The interface also shows options for 'Group: By Transformation', 'Sort: Reaction Count: Descending', and 'View: Collapsed'.

筛选工具：不参与反应官能团

不参与反应官能团：出现在反应前后，但未发生变化的官能团

Structure Match

As Drawn (34)

Substructure (8,044)

Similarity (0)

Filter Behavior

Filter by Exclude

Search Within Results

Yield

Reaction Scale

Non-Participating Functional Groups

Halide (205)

Phenyl halide (203)

Amide (66)

Alkene (62)

Cyclic alkene (58)

View All

Number of Steps

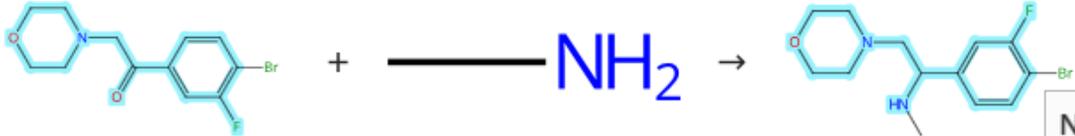
Reaction Mapping

Experimental Protocols

Filtering: Non-Participating Functional Groups: Halide X Clear All Filters

205 Results Group: By Scheme Sort: Relevance View: Collapsed

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



Suppliers (122)

31-313-CAS-11425767 Steps: 1 Yield: 100%

1.1 Solvents: [Tetrahydrofuran](#); 15 min, rt

1.2 Reagents: [Acetic acid](#), [Sodium cyanoborohydride](#); rt → 40 °C; 24 h, 40 °C

1.3 Reagents: [Sodium carbonate](#) Solvents: [Water](#)

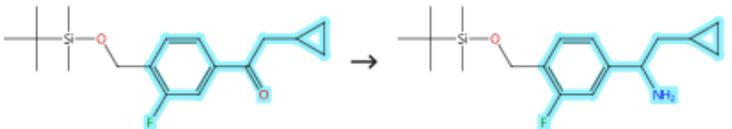
Preparation of N-[1-biphenyl(morpholinyl-aryl)ethyl]glycinamide derivatives as antagonists of urotensin II

By: Neeb, Michael J.; et al
World Intellectual Property Organization, WO2008-01-24

PatentPak Full Text

Collapse Scheme

Scheme 2 (1 Reaction) Steps: 1 Yield:



Non-Participating Functional Groups

By Count Alphanumeric

1 Selected

Halide (205)

Phenyl halide (203)

Amide (66)

Alkene (62)

Cyclic alkene (58)

Diene (45)

Ether (37)

Amine (15)

Tertiary amine (15)

Carboxamide (14)

Urea (12)

Carboxylic ester (9)

Carbamate (8)

Imine (8)

Acyclic ketone (7)

Ketone (7)

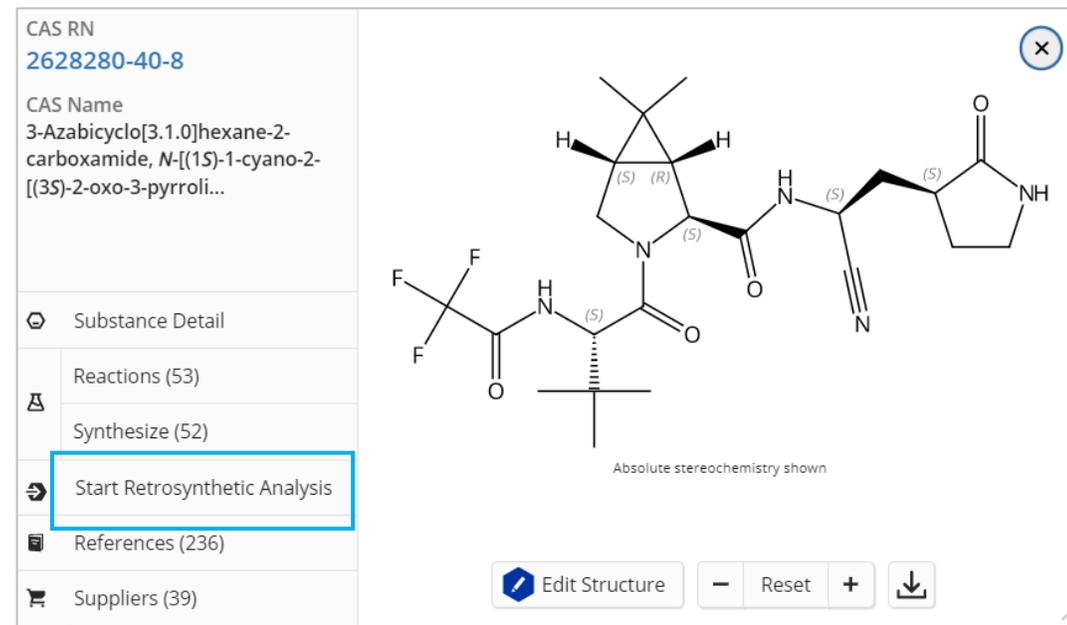
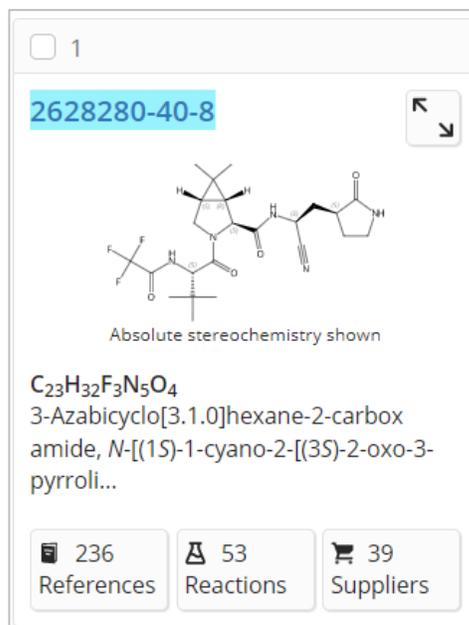
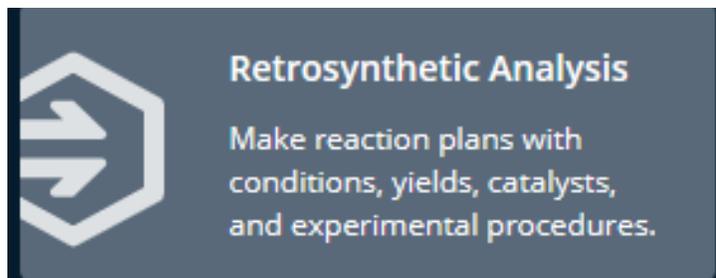
OK Cancel

如何获得逆合成路线?

(1) 已知/未知化合物: 点击Retrosynthesis检索项, 打开绘图板, 绘制目标化合物, 获得实验路线

CAS Retrosynthesis Tool:

- 逆合成反应路线设计功能
- 启发合成实验设计思路
- 高效获取逆合成反应路线



(2) 已知化合物: 点击物质结构, 弹出的物质菜单中点击 Start Retrosynthetic Analysis

预设和调节参数

Retrosynthesis Plan Options for drawn structure P

Select Synthetic Depth **合成深度** [Learn more.](#)

1
 2
 3
 4



Break and Protect Bonds

[Clear All Bond Selections](#)

断裂键或保护键

Set Rules Supporting Predicted Reactions [Learn more.](#)

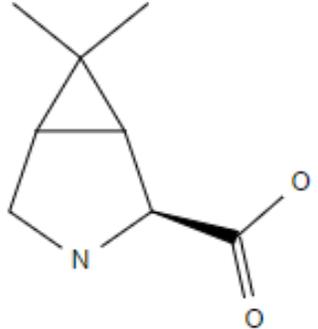
Common **反应规则常见性**
 Uncommon (includes Common Rules)
 Rare (includes Common and Uncommon Rules)

Set Starting Materials Cost Limit [Learn more.](#)

100 **起始原料费用** USD/mol

Email me when my plan is complete

[Create Retrosynthesis Plan](#)



反应路线概览

Retrosynthesis Plan for drawn structure

Powered by ChemPlanner®

Key Experimental Steps Predicted Steps Edit Plan Options

View Excluded Options



Save

Plan Information

Estimated Yield: 81%
Overall Price: \$20,446.59
(USD per 100 grams)

Scoring Profiles

Complexity Reduction

Convergence 原料结构相对复杂性

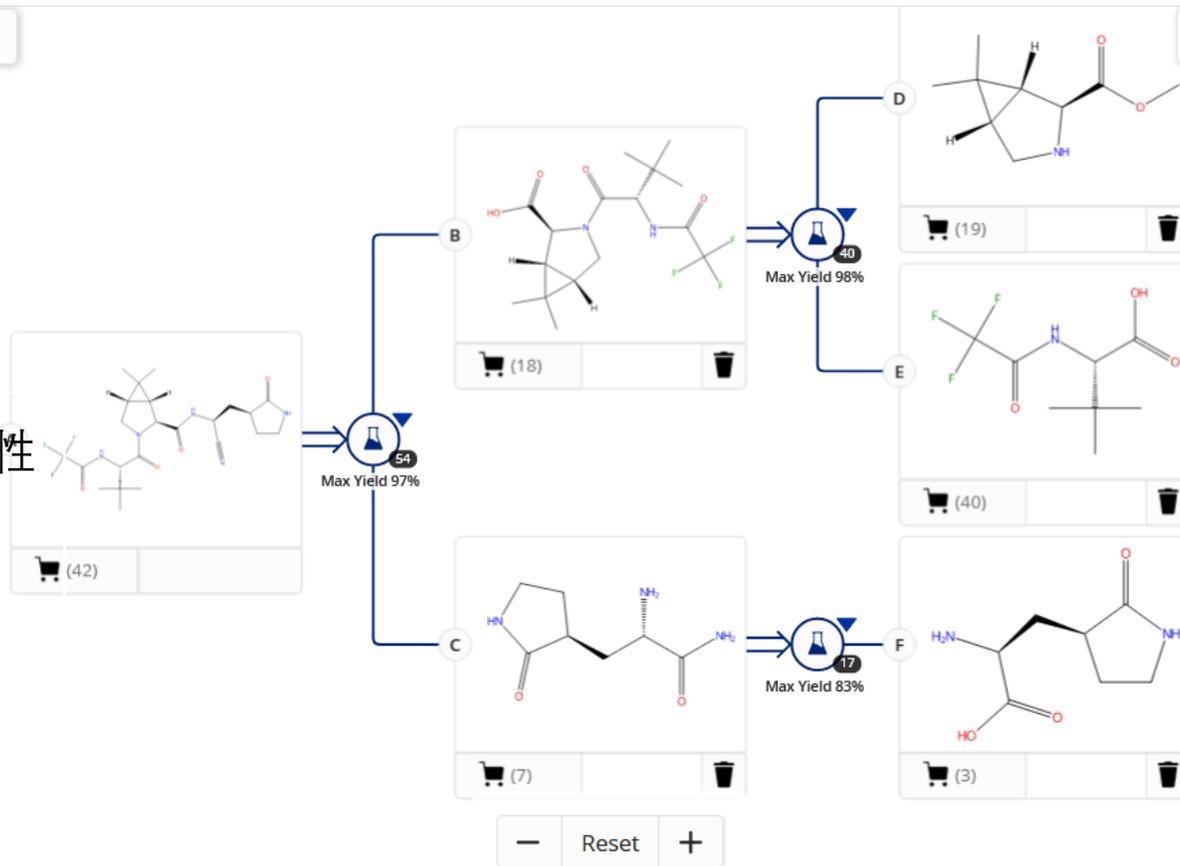
Evidence 路线收敛程度

Cost 文献数量

Yield 成本

Atom Efficiency 产率

原子转化效率



Step

Evidence

A ⇒ B + C

Maximum Yield: 97%
Evidence (2)
Alternative Steps (54)

1.1 Reagents: 4-Methylmorpholine
Catalysts: Isobutyl chloroformate
Solvents: Ethyl acetate; 0 °C; 12 - 18 h, 25 °C
View All ▾

B ⇒ D + E

Maximum Yield: 98%
Evidence (2)
Alternative Steps (40)

1.1 Reagents:
O-(7-Azabenzotriazol-1-yl)-N,N,N',N'-tetramethyluronium hexafluoro phosphate
; 4 h, 20 - 25 °C

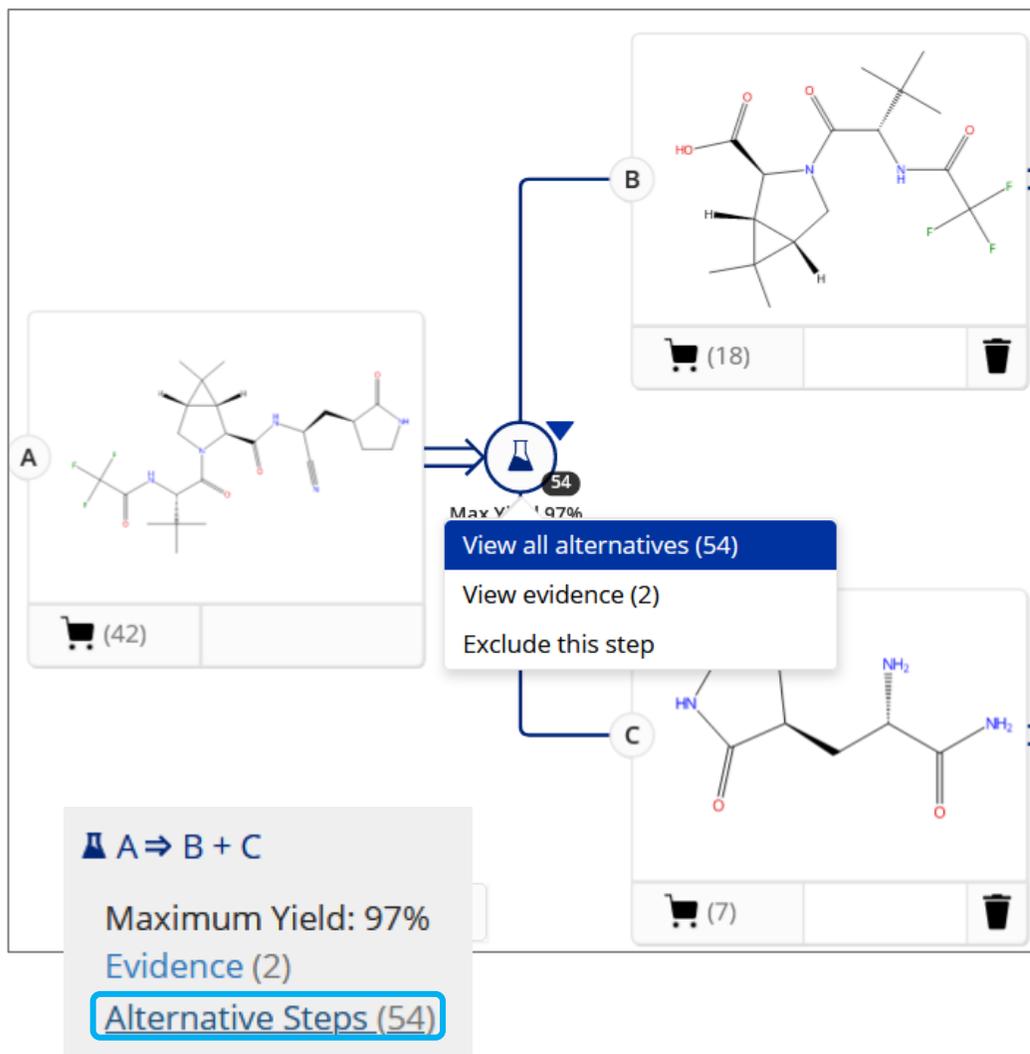
C ⇒ F

Maximum Yield: 83%
Evidence (45,398)
Alternative Steps (17)

1.1 Reagents: Thionyl chloride
Solvents: Methanol; 10 °C; 20 h, rt; rt → 0 °C
View All ▾

分步浏览反应

路线优化，考虑替换路线？



报道反应



反应检索小结

1. 通过物质标识符、文献标识符、结构式进行反应信息检索
2. 反应结果集的浏览与筛选
3. 关键词与反应式的联合检索
4. 获取已知化合物或新化合物的逆合成路线，查看文献支持，自定义选择替代路线

具体的实验方案怎么查、怎么选？

- 如何获取获得具体的实验操作和表征数据等信息？
- 能一键获取从原文中提取的分析操作和数据详情吗？
- 如何对多种分析方法进行充分评估？
- 我研究的物质有什么具体的配方应用？
- 专利配方的组成和制备工艺是什么？如何进行实验评估？



直观的合成实验详情 Synthetic Methods

- CAS科学家标引的合成详情
- 节省阅读全文的时间，高效获得所需的合成实验信息

CAS Reaction Number: 31-614-CAS-24450288

Filter Behavior

Filter by Exclude

Yield

Number of Steps

Non-Participating Functional Groups

Reaction Mapping

Experimental Protocols

Synthetic Methods (40)

Experimental Procedure (83)

Suppliers (15)

Suppliers (89)

98%

Step 1

Stage	Reagents	Catalysts	Solvents	Conditions
1	Hydrochloric acid Titanium chloride (TiCl₃)	-	Methanol Tetrahydrofuran Water	rt; 30 min, rt; 2 h, 30 - 50 °C
2	Water	-	-	-

Alternative Steps (2)

Experimental Protocols

Synthetic Methods

Products [Methyl 2-\(4-bromophenyl\)-7-fluoro-1,2,3,4-tetrahydro-3-\(1-methyl-1H-1,2,4-triazol-5-yl\)-4-oxo-5-quinolinecarboxylate](#), Yield: 98%

Reactants [4-Bromobenzaldehyde](#)
[Benzoic acid, 5-fluoro-2-\(2-\(1-methyl-1H-1,2,4-triazol-5-yl\)acetyl\)-3-nitro-... methyl ester](#)

Reagents [Hydrochloric acid](#)
[Titanium chloride \(TiCl₃\)](#)
[Water](#)

Journal of Medicinal Chemistry (2021), 64(21), 15690-15701

View PDF Full Text

Company/Organization
Werner Siemens Imaging Center,
Department of Preclinical Imaging and Radiopharmacy
Eberhard Karls University
Tuebingen 72076
Germany

- Procedure
1. Suspend methyl 5-Fluoro-2-(2-(1-methyl-1H-1,2,4-triazol-5-yl)acetyl)-3-nitrobenzoate (8.1 g, 25.2 mmol) and 4-bromobenzaldehyde (8.9 g, 50.5 mmol) in THF (50 mL) and MeOH (10 mL).
 2. Add titanium(III) chloride solution [20% wt solution in HCl (2 M), 130 mL, 6 equiv] to the resulting mixture in dropwise fashion over 30 minutes at room temperature.
 3. Maintain the reaction temperature between 30 and 50°C for 2 hours.
 4. Quench the mixture by the slow addition of water (260 mL).
 5. Pour the reaction mixture into a separating funnel.
 6. Extract the mixture with ethyl acetate (4 x 140 mL).
 7. Pool the organic fractions.
 8. Wash the organic fractions with NaHCO₃ (3 x 60 mL) and NaHSO₃ (3 x 100 mL).
 9. Dry the organic fractions with sodium sulfate (Na₂SO₄).
 10. Concentrate the solvent under reduced pressure to obtain a thick yellow syrup.
 11. Wash the residue with aliquots of diethyl ether (3 x 10 mL), carefully.
 12. Dry the resulting yellow syrup under high vacuum to obtain product.

Transformation Mannich Reaction/ Mannich-Type Reactions/ Biginelli Condensation
Condensation Reaction between Compounds with Active Hydrogen and Aldehydes or Ketones/
Knoevenagel Reaction
Reduction of Nitro Compounds to Amines

Scale gram

Characterization Data

5-Quinolinecarboxylic acid, 2-(4-bromophenyl)-7-fluoro-1,2,3,4-tetrahydro-3-(1-methyl-1H-1,2,4-triazol-5-yl)-4-oxo-, methyl ester

State yellow amorphous solid

Transformations

1. Mannich Reaction/ Mannich-Type Reactions/ Biginelli Condensation
2. Condensation Reaction between Compounds with Active Hydrogen and Aldehydes or Ketones/ Knoevenagel Reaction
3. Reduction of Nitro Compounds to Amines

CAS Method Number 3-315-CAS-33168860

关注文献关联的分析方法？

方法一：点击CAS Content中的 Analytical Methods获得有具体分析实验方法的文献，从文献详情页中链接至分析方法

The image shows a screenshot of the CAS database search interface. On the left is a 'Filter Behavior' sidebar with 'Filter by' and 'Exclude' buttons. Under 'Search Within Results', 'CAS Content' is expanded, and 'Analytical Methods (126)' is selected. The main search results area shows 'Filtering: CAS Content: Analytical Methods' and '126 Results'. A single result is displayed with the title 'An optimised electrochemical biosensor for the label-free detection of C-reactive protein in blood'. A callout box highlights the 'Analytical Methods' section in the sidebar. A second callout box shows a detailed view of the selected paper, where the 'Analytical Methods' link in the 'In this Reference' section is highlighted. At the bottom of the detailed view, a button labeled 'View in CAS Analytical Methods' is also highlighted.

Filter Behavior

Filter by Exclude

Search Within Results

Concept

CA Section

Publication Year

Organization

CAS Content

Analytical Methods (126)

Formulations (63)

Author

Document Type

Publication Name

Filtering: CAS Content: Analytical Methods X Clear All Filters

126 Results Sort: Relevance View: Full Abstract

1

An optimised electrochemical biosensor for the label-free detection of C-reactive protein in blood

By: Bryan, Thomas; Luo, Xiliang; Bueno, Paulo R.; Davis, Jason J.
Biosensors & Bioelectronics (2013), 39(1), 94-98 | Language: English, Database: CPlus and MEDLINE

C-reactive protein (CRP) is an acute phase protein whose levels are increased in many disorders. There exists, in particular, a great deal of interest in the correlation between blood serum levels and the severity of risk for cardiovascular disease. A sensitive, label-free, non-amplified and reusable electrochem. impedimetric biosensor for the detection of CRP in blood serum was developed herein based on controlled and coverage optimized antibody immobilization on standard polycrystalline gold electrodes. Charge transfer resistance changes were highly target specific, linear with log CRP concentration across a 0.5-50 nM range and associated with a limit of detection of 176 pM. Significantly, the detection limits are better than those of current CRP clin. methods and the assays are potentially cheap, relatively automated, reusable, multiplexed and highly portable. The generated interfaces were capable not only of comfortably quantifying CRP across a clin. relevant range of concentrations but also of doing this in whole blood serum with interfaces that were, subsequently, reusable. The importance of optimizing receptor layer resistance in maximising assay sensitivity is also detailed.

An optimised electrochemical biosensor for the label-free detection of C-reactive protein in blood

5 0 172 Citation Map

In this Reference

- Concepts
- Substances
- Analytical Methods
- Cited Documents

By: Bryan, Thomas; Luo, Xiliang; Bueno, Paulo R.; Davis, Jason J.
DOI: 10.1016/j.bios.2012.06.051

C-reactive protein (CRP) is an acute phase protein whose levels are increased in many disorders. There exists, in particular, a great deal of interest in the correlation between blood serum levels and the severity of risk for cardiovascular disease. A sensitive, label-free, non-amplified and reusable electrochem. impedimetric biosensor for the detection of CRP in blood serum was developed herein based on controlled and coverage optimized antibody immobilization on standard polycrystalline gold electrodes. Charge transfer resistance changes were highly target specific, linear with log CRP concentration across a 0.5-50 nM range and associated with a limit of detection of 176 pM. Significantly, the detection limits are better than those of current CRP clin. methods and the assays are potentially cheap, relatively automated, reusable, multiplexed and highly portable. The generated interfaces were capable not only of comfortably quantifying CRP across a clin. relevant range of concentrations but also of doing this in whole blood serum with interfaces that were, subsequently, reusable. The importance of optimizing receptor layer resistance in maximising assay sensitivity is also detailed.

Keywords: electrochem biosensor C reactive protein blood

View Source Full Text View in CAS Analytical Methods

Analytical Methods

Method Title

Analysis of C-reactive protein in Blood serum by Amperometric immunoassay

CAS 分析实验方法详情

Analysis of C-reactive protein in Blood serum by Amperometric immunoassay

CAS Method Number

2-111-CAS-49948

Method Category

Biomarker Medicine Assay;
Biomolecule Isolation Assay

Analyte

C-reactive protein

Matrix

Blood serum

实验原料

Material

Gold
Immuno
Self-ass
3.0, 1.0
spray
View All

Equipment Used

Potentiostat, Autolab 12, Metrohm Autolab B.V.

分析仪器

Conditions

Instrument

supporting electrolyte: phosphate buffered saline (PBS) with Tween-20 (PBST, 10 mM, pH 7.4) with 1.0 mM $[\text{Fe}(\text{CN})_6]^{3-/4-}$; detection potential: 0.25 V

分析条件

Source

JOURNAL

[An optimised electrochemical biosensor for the label-free detection of C-reactive protein in blood](#)

Bryan, Thomas; Luo, Xiliang; Bueno, Paulo R.; Davis, Jason J.

Biosensors & Bioelectronics (2013), 39 (1), 94 - 98. Elsevier B.V.

CODEN : BBIOE4 | ISSN : 09565663 | DOI : 10.1016/j.bios.2012.06.051

View Abstract

Full Text

来源文献

Instructions

Reagent Preparation

1. Prepare phosphate buffered saline (PBS) with Tween-20 (PBST, 10 mM, pH 7.4) by dissolving PBS tablets (Sigma Aldrich) in water.
2. Add 0.2% v/v Tween-20 and filter using a 0.22 μm membrane filter.

Sample Preparation

1. Collect human blood serum samples.

Preparation of electrochemical biosensor

1. Polish gold electrodes with 3.0, 1.0 and 0.1 μm diamond spray (Kemet International Ltd) in sequence and ultrasonically wash in water for about 5 min prior to immersion in freshly prepared piranha solution (concentrated $\text{H}_2\text{SO}_4:\text{H}_2\text{O}_2$, v/v 3:1) for 15 min.
2. Polish electrodes electrochemically by potential cycling (CV) between 0.1 and 1.25 V to obtain a stable reduction peak.
3. Dry the pre-treated gold electrodes in a flow of nitrogen gas and immediately immerse in a 10 mM solution of HS-C₁₁-(EG)₃-OCH₂-COOH in ethanol for 16 h at room temperature.
4. Rinse gold surfaces with ethanol and water.
5. Dry in a flow of nitrogen gas prior to incubation in a solution containing 0.4 M 1-ethyl-3-(3-dimethylaminopropyl) carbodiimide (EDC) and 0.1 M N-hydroxysuccinimide (NHS) for 15 min (terminal carboxyl group activation) and 10 mM C-reactive protein (CRP) antibody solution (PBST, pH 7.4) for 1 h.

Amperometric immunoassay

1. Perform electrochemical experiments on an Autolab potentiostat 12 equipped with a FRA2 module (Metrohm Autolab B.V.).
2. Use conventional three-electrode system with a gold disk working electrode (1.6 mm diameter, BASi), platinum wire counter electrode and a silver/silver chloride (Ag/AgCl) reference electrode (CH Instruments).
3. Use phosphate buffered saline (PBS) with Tween-20 (PBST, 10 mM, pH 7.4) with 1.0 mM $[\text{Fe}(\text{CN})_6]^{3-/4-}$ as supporting electrolyte.
4. Set detection potential to 0.25 V.

Validation

Linearity Range 0.5 - 50 nM
Limit of Detection 176 \pm 18 pM (buffer)
262 \pm 28 pM (serum at concentrations up to 20% v/v)

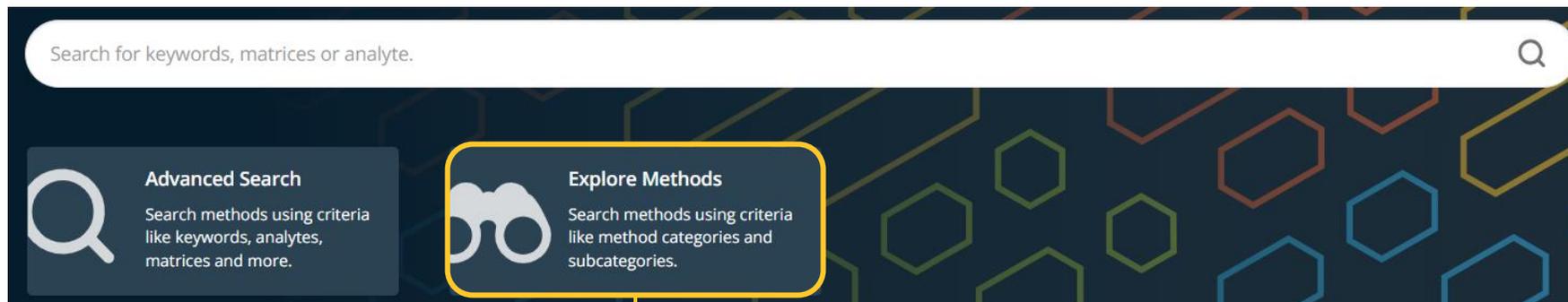
操作步骤

数据有效性

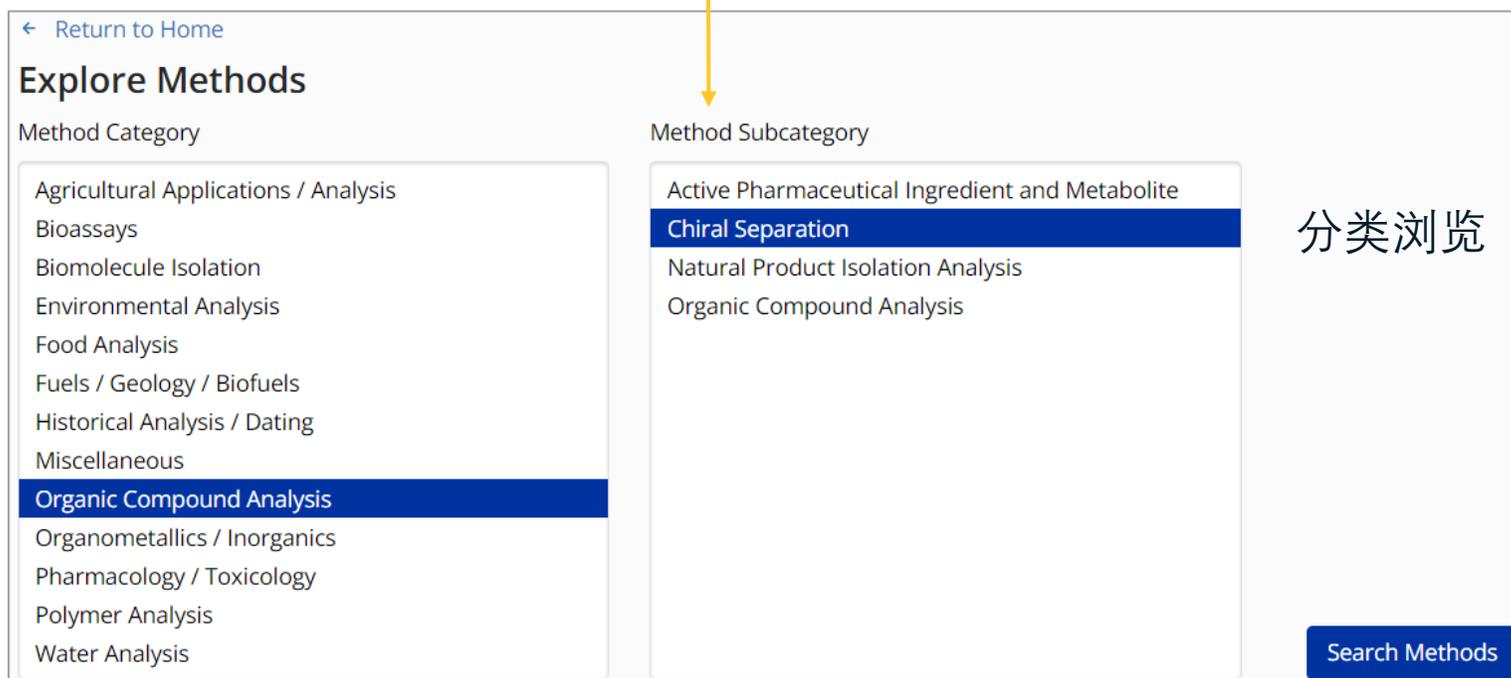
- CAS科学家标引的分析实验详情
- 无需下载全文，高效获得所需的分析实验信息

直接检索感兴趣的分析实验方法

方法二：登录 <https://methods.cas.org> 进行主题检索或分类浏览



直接输入主题检索



分类浏览

方法分类: 13大类, 45小类

农业应用、生物鉴定、生物分子分离、环境、食品、考古、有机物、药学、毒理学分析等

如何选择合适的分析方法?

Results for α -Pinene

Compare (2/3) Save

Sort: Relevance Group: By Method

14103 Results

1

Analysis of (\pm)- α -Pinene by Microplate spectroscopy

By: Turkez, Hasan; Aydin, Elanur
In vitro assessment of cytogenetic and oxidative effects of α -pinene
Toxicology and Industrial Health (2016), 32 (1), 168-176. Sage Publications

Analyte (\pm)- α -Pinene
Other Materials Reagent: Dimethyl sulfoxide; [3-(4,5-Dimethylthiazol-2-yl)-2,5-diphenyltetrazolium bromide]
Material: Blood cell; 48-well plates
Method Category Bioassay
Technique Microplate spectroscopy
Equipment Used Microplate reader

View Abstract Full Text View in CAS SciFinder

2

Analysis of (\pm)- α -Pinene in Eucalyptus by Gas chromatography JOURNAL

By: Cerceau, Cristiane I.; Barbosa, Luiz C. A.; Filomeno, Claudinei A.; Alvarenga, Elson S.; Demuner, Antonio J.; Fidencio, Paulo H.
An optimized and validated ^1H NMR method for the quantification of α -pinene in essential oils
Talanta (2016), 150, 97-103. Elsevier B.V.

Analyte (\pm)- α -Pinene; Essential oils
Matrix Dianthus; Eucalyptus
Other Materials Reagent: Octadecane; Dichloromethane
Material: Fused silica capillary column (SBP5, 30 m x 0.25 mm ID, 0.25 μm film thickness)
Method Category Natural Product Isolation Analysis
Technique Gas chromatography; Flame ionization detectors

Filter By

Analyte

- (\pm)- α -Pinene (12560)
- β -Pinene (8972)
- Myrcene (7925)
- Limonene (7239)
- (\pm)-Camphene (6883)

View All

Matrix

- Leaf (3984)
- Essential oils (3062)
- Plant organ (1804)
- Flower (1187)
- Fruits (683)

View All

Method Category

Technique

- Distillation (7925)
- Gas chromatography-mass spectrometry (3060)
- Gas chromatography (2885)
- Spectrophotometry (2577)
- Microbial cell culture (2389)

View All

Year

- 分析目标物
- 介质
- 方法类别
- 分析技术
- 发表年份

如何选择合适的分析实验方法？

便捷对比实验方法和数据

	Method 1 ×	Method 2 ×	Method 3 ×
	Analysis of (±)-α-Pinene by Microplate spectroscopy	Analysis of (±)-α-Pinene in Eucalyptus by Gas chromatography	Analysis of (±)-α-Pinene in Eucalyptus by
CAS Method Number	2-107-CAS-144805	1-131-CAS-295750	
Method Category	Bioassay	Natural Product Isolation Analysis	
Technique	Microplate spectroscopy	Gas chromatography; Flame ionization det	
Analyte	(±)- α -Pinene	(±)- α -Pinene; Essential oils	
Matrix	-	Dianthus; Eucalyptus	
Other Materials	Dimethyl sulfoxide; [3-(4,5-Dimethylthiazol-2-yl)-2,5-diphenyltetrazolium bromide]; Blood cell; 48-well plates	Octadecane; Dichloromethane; Fused silica capillary column (SBP5, 30 m x 0.25 mm ID, 0.25 μ m film thickness)	
Equipment Used	Microplate reader, Microquant	GC system, 17A, Shimadzu; Flame ionization detector (FID), Shimadzu	
Conditions	Instrument: Absorbance wavelength: 570 nm	Instrument: Column: fused silica capillary (SBP5, 30 m x 0.25 mm ID, 0.25 μ m film	

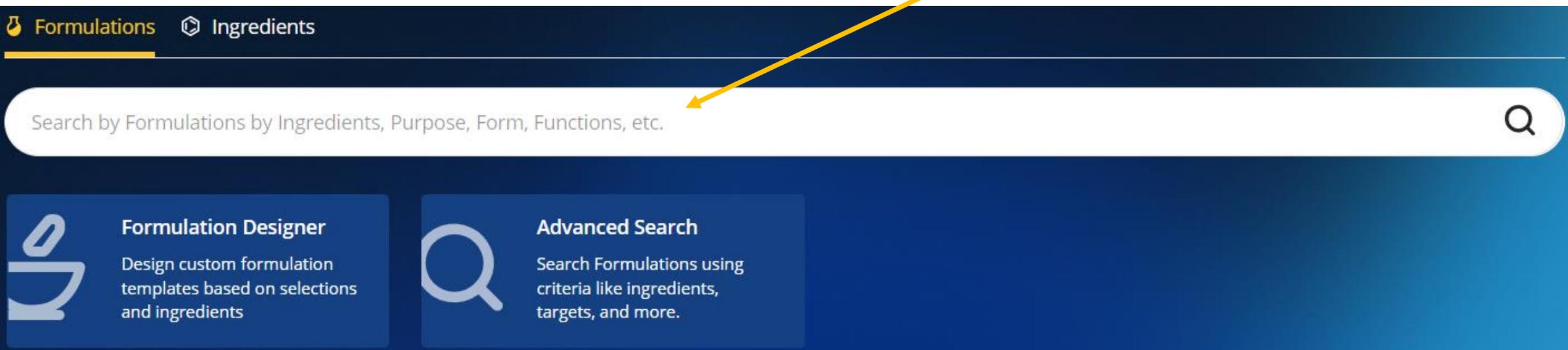
Method	Method 2	Method 3	
Cell viability assay	Gas chromatography analysis with flame ionization detection using external standardization (GC-ES) method	Gas chromatography analysis with flame ionization detection using internal standardization (GC-IS) method	
<ol style="list-style-type: none"> Seed human blood cells in 48-well plates. Incubate the cells at 37 °C in a humidified 5% carbon dioxide and 95% air mixture. Treat with α-pinene at different concentrations (0, 10, 25, 50, 75, 100, 150 and 200 mg/L) for 24 h. Use the 3-(4,5-dimethyl-2-thiazolyl)-2,5-diphenyl tetrazolium bromide (MTT) substrate solution according to the manufacturer's instructions (Cayman Chemical Company, USA). Add MTT to the cell cultures for 3 h. Dissolve the formed formazan crystals in dimethyl sulfoxide. Analyze the plates using Microquant reader at 570 nm wavelength. <p>View Less ^</p>	<ol style="list-style-type: none"> Analyze the samples using a Shimadzu equipment, model 17A, connected to a flame ionization detector (GC-FID), equipped with a fused silica capillary column (SBP5-Supelco, 30 m x 0.25 mm ID, 0.25 μm film thickness). Perform separation with a fused silica capillary column (SBP5-Supelco, 30 m x 0.25 mm ID, 0.25 μm film thickness). Program the column temperature as follows: from 40 °C (4 min) to 200 °C at a rate of 3 °C/min. Use nitrogen as carrier gas. Set the flow rate at 1.80 mL/min. Set the injector temperature to 200 °C. Inject 10 μL (1.0% w/v solution of the oil in dichloromethane) of the sample with a split ratio of 1:10. Set the detector temperature to 240 °C. <p>View Less ^</p>	<ol style="list-style-type: none"> Analyze the samples using a Shimadzu equipment, model 17A, connected to a flame ionization detector (GC-FID), equipped with a fused silica capillary column (SBP5-Supelco, 30 m x 0.25 mm ID, 0.25 μm film thickness). Perform separation with a fused silica capillary column (SBP5-Supelco, 30 m x 0.25 mm ID, 0.25 μm film thickness). Program the column temperature as follows: from 40 °C (4 min) to 200 °C at a rate of 3 °C/min. Use nitrogen as carrier gas. Set the flow rate at 1.80 mL/min. Set the injector temperature to 200 °C. Inject 10 μL (1.0% w/v solution of the oil in dichloromethane) of the sample with a split ratio of 1:10. Set the detector temperature to 240 °C. <p>View Less ^</p>	
Helpful Hints	interferent: safetyInfo: troubleshooting: View All v	interferent: safetyInfo: troubleshooting: View All v	interferent: safetyInfo: troubleshooting: View All v
Bioactivity	90, 91, 91, 90, 92, 91 and 90% (Read from figure, cell viability) at 0, 10, 25, 50, 75, 100 and 150 mg/L added concentrations, respectively	-	-
Concentration	-	34% (read from figure, <i>E. saligna</i>), 15% (read from figure, pink pepper essential oils, <i>Schinus terebinthifolius</i>), 37% (read from figure, hybrid <i>E. urophylla</i> x <i>E. grandis</i>), 13% (read from figure, <i>E.</i>	34% (read from figure, <i>E. saligna</i>), 10.3% (read from figure, pink pepper essential oils, <i>Schinus terebinthifolius</i>), 33% (read from figure, hybrid <i>E. urophylla</i> x <i>E. grandis</i>), 10.3% (read from figure, <i>E.</i>

详细的分析实验方法对比

研究课题在产品中的应用？配方的检索与设计

方法一：登 <https://formulus.cas.org> 输入检索式

原料、用途、物理形态、功能或文献标识符



The screenshot shows the top navigation bar with 'Formulations' and 'Ingredients' tabs. Below is a search bar with the placeholder text 'Search by Formulations by Ingredients, Purpose, Form, Functions, etc.' and a magnifying glass icon. A yellow arrow points from the text '原料、用途、物理形态、功能或文献标识符' to the search bar. Below the search bar are two main sections: 'Formulation Designer' with a mortar and pestle icon and the description 'Design custom formulation templates based on selections and ingredients', and 'Advanced Search' with a magnifying glass icon and the description 'Search Formulations using criteria like ingredients, targets, and more.'

- 制药、化妆品、食品、农化、油墨、涂料等多领域中的配方
- 工艺、成分、目标成分的常见配伍成分、设计配方、探索合规要求等

配方结果集

Formulations search for "orthopedic and implant"

Get Additional References

Compare (0/3)



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Filter by

Industry

- Cleaning & Surfactant Products
- Cosmetics & Personal Care
- Pharmaceutical
- Unclassified

Purpose

- Pharmaceutical formulations (256)
- Drug delivery systems (128)
- Analgesics (106)
- Pharmaceutical implants (87)
- Stabilizing agents (87)

[View All](#)

Physical Form

- Tablets (256)
- Capsules (230)
- Pharmaceutical implants (171)
- Powders (163)
- Solutions (124)

[View All](#)

256 Results

Sort: Relevance

1

Oral Solid Composition: Pharmaceutical Formulations

Location: Table 1, Comparative Example 1

Purpose: Pharmaceutical formulations

Target: Homo sapiens

Delivery Route: Oral drug delivery systems

Physical Form: Tablets

一次最多可以比较三种不同制剂或配方的信息详情

Add to Compare

Component	Function	Amount Reported
Levonorgestrel	-	1.5 mg
D-Glucose, 4-O-β-D-galactopyranosyl-, hydrate (1:?)	-	125.2 mg
Starch	additives	7 mg
Poly(vinylpyrrolidone)	additives	4.2 mg

Additional components reported

[View Formulation Detail](#)

[76 Similar Formulations - View All](#) (opens in a new window)

PATENT

Oral solid composition comprising progestin and levonorgestrel, its manufacturing method, and method for manufacturing oral tablet

Assignee : Fuji Pharma Co., Ltd.
JP2020132640
Language: Japanese

Patent PDF

View in [CAS SciFinder](#)

Delivery Route

- Oral drug delivery systems (166)
- Intramuscular injections (95)
- Intraperitoneal injections (93)
- Subcutaneous drug delivery systems (88)
- Buccal drug delivery systems (83)

[View All](#)

Information Included

- Component Amount (159)
- Process (120)
- Experimental Activity (91)
- Effective Dose (8)

Document Type

- Patent (256)
 - Claim (94)
 - Comparative Example (2)
 - Example (160)

Organization

- SSP Co., Ltd. (42)
- Coeruleus Ltd. (40)
- Biogen Idec, Inc. (27)
- Skyepharma, Inc. (27)
- Fuji Pharma Co., Ltd. (12)

[View All](#)

Publication Year

配方的制备？ 实验评估？

Oral Solid Composition: Pharmaceutical Formulations

Save

Purpose	Target	Delivery Route	Physical Form	Source
Pharmaceutical formulations	Homo sapiens	Oral drug delivery systems	Tablets	View

Formulation Ingredients

Component	Function	Amount Reported	Optionality
Levonorgestrel	-	1.5 mg	Mandatory
D-Glucose, 4-O-β-D-galactopyranosyl-, hydrate (1:?)	-	125.2 mg	Mandatory
Starch	additives	7 mg	Mandatory
Poly(vinylpyrrolidone)	additives	4.2 mg	Mandatory
Silica	fluidizing agents	0.7 mg	Mandatory
Magnesium stearate	pharmaceutical lubricants	1.4 mg	Mandatory

More Formulations like this... NEW

[Pharmaceutical Tablet Containing Entecavir: Antiviral Agents](#)

Purpose: Antiviral agents
Target: Hepatitis B, Homo sapiens
Delivery Route: Oral drug delivery syst...
Physical Form: Tablets

[Oral Pharmaceutical Composition: Pharmaceutical Formulations](#)

Purpose: Pharmaceutical formulations
Target: Homo sapiens
Delivery Route: Oral drug delivery syst...
Physical Form: Capsules, Compression...

[Fluconazole Tablet Composition: Drug Delivery Systems](#)

Purpose: Drug delivery systems
Target: fluconazole
Delivery Route: -
Physical Form: Tablets

[Pharmaceutical Formulation for Treating Tumor: Antitumor Agents](#)

Purpose: Antitumor agents
Target: Homo sapiens, Neoplasm
Delivery Route: -
Physical Form: Capsules, Granular mat...

Process

production of tablets: (1) pre-mixing lactose hydrate (200 M), corn starch and povidone K-30 are mixed in a V-type mixer (5L, mixed at Tokuju Kosakusho Co., Ltd.). (2) granulation/drying the powder mixed by the premixing of (1) is put into a fluidized bed granulator (FD-MP-01 D, manufactured by Paulec Co., Ltd.), and 95% with levonorgestrel. An ethanol suspension composed of ethanol was sprayed at an air volume of 0.3 m/min, an air supply temperature of 60 °C., a spray volume of 14 g / min, and a spray air volume of 55 L/min, granulated, and then dried. levonorgestrel having a cumulative 10% particle diameter of 1 μm, a cumulative 50% particle diameter of 4 μm, and a cumulative 90% particle diameter of 7 μm was used. It was confirmed that the amount of residual ethanol in the dried powder was less than the concentration limit value described in the 17 th Revised Japanese Pharmacopoeia "residual solvent". (3) primary mixing the powder dried in (2), light anhydrous silicic acid were mixed with a locking mixer (RM-10-2, manufactured by Aichi electric Co., Ltd.). secondary mixing powder mixed in the primary mixing of (3) and Magnesium stearate were mixed with a locking mixer (RM-10-2, manufactured by Aichi electric Co., Ltd.). (5) locking the powder mixed by the secondary mixing of (4) is subjected to a locking machine (VIRGO 0512552AY, manufactured by Kikusuisaisakusho co. . Ltd.) at a locking pressure of 7 kN, a lock diameter of 7.0 mm, and a mass of 140 mg.

Experimental Activity

Descriptor	Notes	Details
dissolution rate	dissolution rate of the tablet was evaluated for 0 month at 15 minutes	45.2
dissolution rate	dissolution rate of the tablet was evaluated for 0 month at 30 minutes	56.4
dissolution rate	dissolution rate of the tablet was evaluated for 0 month at 45 minutes	62.3
dissolution rate	dissolution rate of the tablet was evaluated for 0 month at 60 minutes	66.2
dissolution rate	dissolution rate of the tablet was evaluated for 0 month at 90 minutes	70.6

Source Patent

[Oral solid composition comprising progesterin and levonorgestrel, its manufacturing method, and method for manufacturing oral tablet](#)

Assignee : Fuji Pharma Co., Ltd.
JP2020132640
Language: Japanese
Location: Table 1, Comparative Example 1

[Patent PDF](#) [View in CAS SciFinder®](#)

设计配方



Formulation Designer

Design custom formulation templates based on selections and ingredients

Formulation Designer ?

[Clear All Selections](#)

Industry

Pharmaceutical
Cosmetics & Personal Care
Agrochemical
Cleaning & Surfactant Products
Food & Related
Inks, Paints, & Coatings

Purpose

Cosmetics and Personal care products
Skin conditioners
Sunscreens
Hair dyes
Hair preparations
Antiperspirants
Cleaning compositions
Skin-lightening cosmetics
Skin cleansers
Oral hygiene products
Skin care products
[- View More Purposes -](#)

Physical Form

Emulsions
Cream preparations
Cosmetic lotions
Cosmetic packs
Gels
Liquids
Solutions
Nanospheres
Pastes
Capsules
[- View More Physical Forms -](#)

Add up to 5 Ingredients

Vitamin A



Polyethylene glycol



[+ Add Another Ingredient](#)

[Create Template](#)

设计配方

Formulation Designer Clear All Selections

Industry	Purpose	Physical Form	Active or Featured Ingredient
Cosmetics & Personal Care	Skin care products	Gels	Vitamin A Polyethylene glycol

[Edit Selections](#) ↓

Your Template

Function	Ingredient	Regulatory	Top Alternatives	Amounts
Active or Featured Ingredient:	Vitamin A	ANMAT; NMPA	-	Amount not available
Active or Featured Ingredient:	Polyethylene glycol	ANMAT; Cosing: Cosmetic Ingredient Inventory; Drug Master File List; EPA Pesticide Inactive Ingredients; EPA Safer Chemical Ingredients; FDA GRAS (Part 181, Subpart B); FDA Inactive Ingredients Database	-	Amount not available
Function: Carriers	Ethylene glycol View More Alternatives	Cosing: Cosmetic Ingredient Inventory; EPA Pesticide Inactive Ingredients; FDA Inactive Ingredients Database	Water; Polyethylene glycol	
Function: Skin conditioners	Ethylene glycol View More Alternative	Cosing: Cosmetic Ingredient Inventory; EPA Pesticide Inactive Ingredients; FDA Inactive Ingredients Database	Glycerol; Allantoin; 1,2-Octanediol; Tricaprin; Palm-oil glycerides, monoglycerides, diglycerides and triglycerides, hydrogenated	Approximate Range: 2 - 14%

- 原料详情
- 原料管制信息
- 可替代的原料选项

Alternative Ingredients (Showing all 7)

Select the ingredient you would like to use:

Allantoin	Tricaprin	hydrogenated
Ethylene glycol	Palm-oil glycerides, monoglycerides,	Glyceryl polyacrylate
1,2-Octanediol	diglycerides and triglycerides,	N-(2-Hydroxyethyl)acetamide

文献关联的配方

方法二：在文献结果集页面，点击CAS Content中的 Formulations 获得有具体配方或制剂信息的文献，从文献详情页中链接获取

References search for ""wound healing" and hydrogel"

Substances Reactions Citing Knowledge Graph

Filter Behavior

Filter by Exclude

Search Within Results

Concept

CA Section

Publication Year

Organization

CAS Content

Formulations (1,093)

Analytical Methods (133)

Author

Document Type

Publication Name

Formulation Purpose

Language

Filtering: CAS Content: Formulations X Clear All Filters

1,093 Results Sort: Relevance View: Partial Abstract

1

Engineering a sprayable and elastic hydrogel adhesive with antimicrobial properties for wound healing

By: Annabi, Nasim; Rana, Devyesh; Shirzaei Sani, Ehsan; Portillo-Lara, Roberto; Gifford, Jessie L.; Fares, Mohammad M.; Mithieux, Suzanne M.; Weiss, Anthony S.

Biomaterials (2017), 139, 229-243 | Language: English, Database: CPlus and MEDLINE

Hydrogel-based bioadhesives have emerged as alternatives for sutureless wound closure, since they can mimic the composition and physicochem. properties of the extracellular matrix. However, they are often associated with poor mech. properties, low adhesion to native tissues, and lack of antimicrobial properties. Herein, a new sprayable, elastic, and biocompatible composite hydrogel, with broad-spectrum antimicrobial activity, for the treatment of chronic wounds is reported. The composite hydrogels were engineered using two ECM-derived biopolymers, gelatin methacryloyl (GelMA) and methacryloyl-...

View More

Full Text

Substances (5) Reactions (0) Citing (407) Citation Map

2

An injectable self-healing hydrogel with adhesive and antibacterial properties effectively promotes wound healing

By: Chen, Honglei; Cheng, Junwen; Ran, Luoxiao; Yu, Kun; Lu, Bitao; Lan, Guangqian; Dai, Fangying; Lu, Fei

文献关联的配方

 Engineering a sprayable and elastic **hydrogel** adhesive with antimicrobial properties for **wound healing**

5 0 407 Citation Map

In this Reference

- Concepts
- Substances
- Formulations**
- Cited Documents

By: Annabi, Nasim; Rana, Devyesh; Shirzaei Sani, Ehsan; Portillo-Lara, Roberto; Gifford, Jessie L.; Fares, Mohammad M.; Mithieux, Suzanne M.; Weiss, Anthony S.

DOI: 10.1016/j.biomaterials.2017.05.011

Hydrogel-based bioadhesives have emerged as alternatives for sutureless **wound closure**, since they can mimic the composition and physicochem. properties of the extracellular matrix. However, they are often associated with poor mech. properties, low adhesion to native tissues, and lack of antimicrobial properties. Herein, a new sprayable, elastic, and biocompatible composite **hydrogel**, with broad-spectrum antimicrobial activity, for the treatment of chronic **wounds** is reported. The composite **hydrogels** were engineered using two ECM-derived biopolymers, gelatin methacryloyl (GelMA) and methacryloyl-substituted recombinant human tropoelastin (MeTro). MeTro/GelMA composite **hydrogel** adhesives were formed via visible light-induced crosslinking. Addnl., the antimicrobial peptide Tet213 was conjugated to the **hydrogels**, instilling antimicrobial activity against Gram (+) and (-) bacteria. The phys. properties (e.g. porosity, degradability, swellability, mech., and adhesive properties) of the engineered **hydrogel** could be fine-tuned by varying the ratio of MeTro/GelMA and the final polymer concentration. The **hydrogels** supported in vitro mammalian cellular growth in both two-dimensional and three dimensional culture **in vivo**. The engineered MeTro/G promote **healing** of chronic w

Keywords: **hydrogel** adhesive

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Formulations View All Formulations

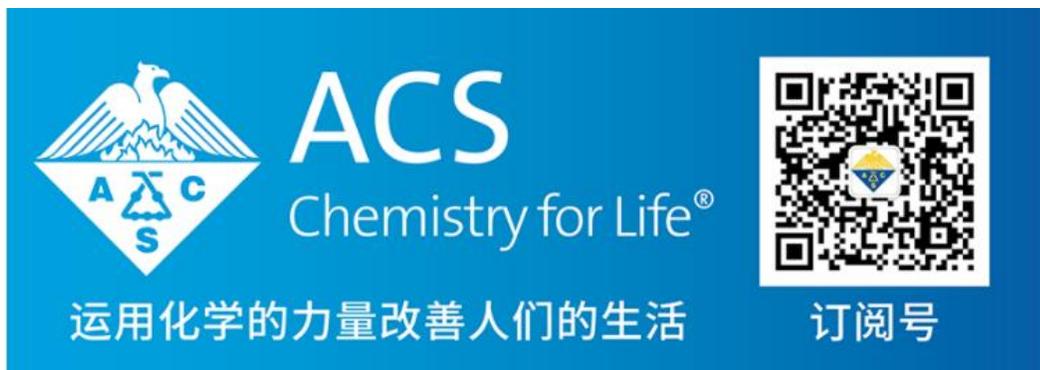
Formulation Title
Gelatin Methacryloyl and Methacryloyl-Substituted Recombinant Human Tropoelastin Antimicrobial Peptides Hydrogel: Wound Healing Promoters
Gelatin Methacryloyl and Methacryloyl-Substituted Recombinant Human Tropoelastin Composite Hydrogel: Antimicrobial or Wound Healing Promoters
Composite Hydrogel: Antimicrobial or Wound Healing Promoters
Gelatin Methacryloyl and Methacryloyl-Substituted Recombinant Human Tropoelastin-Zinc Oxide Hydrogel: Antimicrobial or Wound Healing Promoters
Gelatin Methacryloyl and Methacryloyl-Substituted Recombinant Human Tropoelastin Composite Hydrogel: Antimicrobial or Wound Healing Promoters
Gelatin Methacryloyl and Methacryloyl-Substituted Recombinant Human Tropoelastin Composite Hydrogel: Antimicrobial or Wound Healing Promoters
Gelatin Methacryloyl and Methacryloyl-Substituted Recombinant Human Tropoelastin Composite Hydrogel: Antimicrobial or Wound Healing Promoters
Gelatin Methacryloyl and Methacryloyl-Substituted Recombinant Human Tropoelastin Antimicrobial Peptides Hydrogel: Wound Healing Promoters

实验方案检索小结

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Reference Id: GU75LMF9iZnhTq6mymUog

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CAS SCIFINDER DISCOVERY PLATFORM™

2024专题论坛直播时间表

结合CAS信息科学家精心撰写的相关洞察报告，了解不同领域的研究进展、趋势与创新、挑战与机会，同时进行安全的专利布局和侵权风险管理，助力自信应对立项布局、研发流程和专利调研相关的信息挑战。

9月26日 | 药物立项调研策略



11月14日 | 电池及电化学能源材料



10月24日 | 聚合物的研发与应用



12月19日 | 专利查新与规避专利侵权风险



CAS SciFinder Discovery Platform

9月至12月的四场专题论坛

直播时间为**周四15:00 - 16:00**。扫描二维码注册，观看直播有机会获得**CAS定制纪念品**，欢迎在直播中提问互动。