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在线学习检索技能，并参加线上考试。

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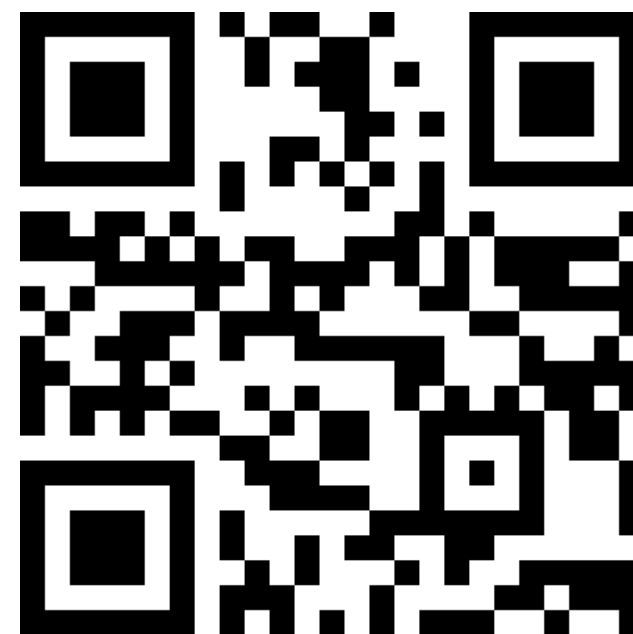
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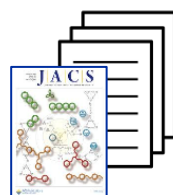
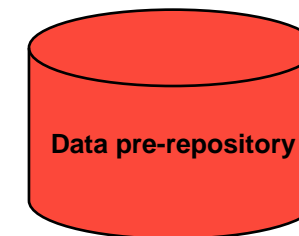
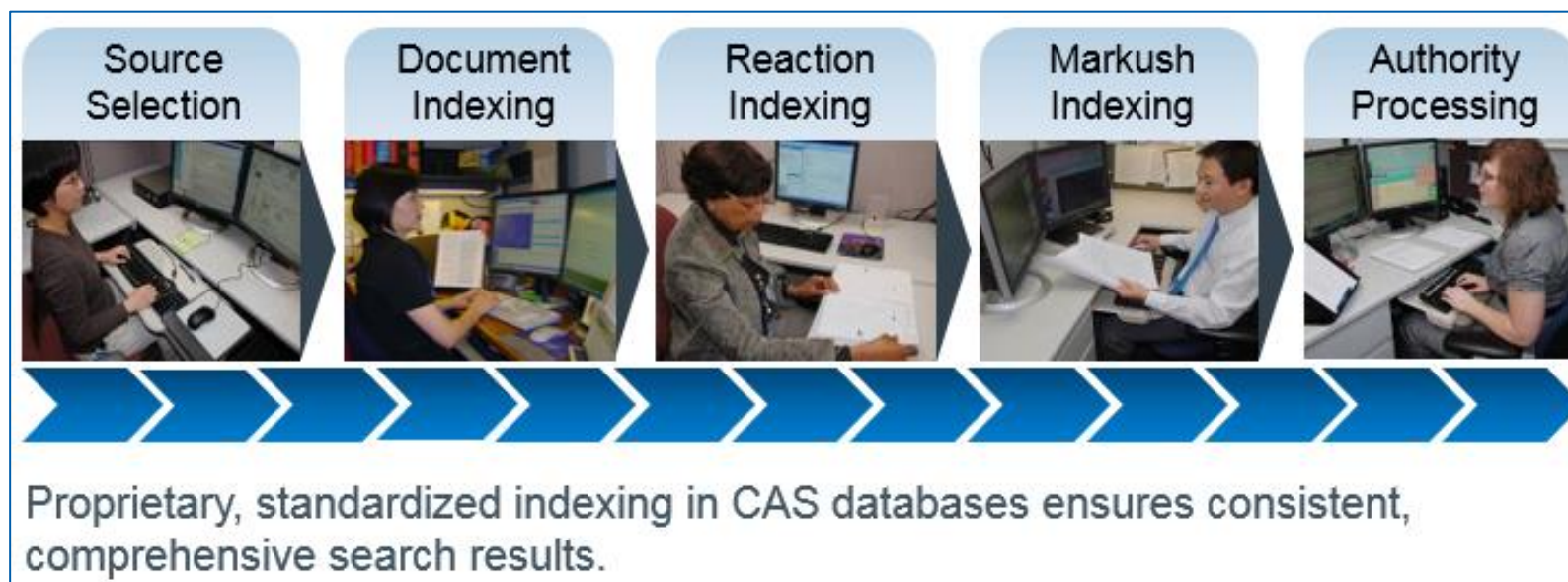
现在即可开始学习，第一阶段线上考核将于4月8日正式开始。

大纲

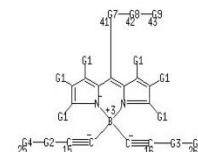
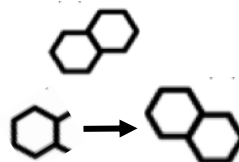
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- 常见问题Q&A



CAS科学家的智力标引



1990
Smith, M.
anthracene



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

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CAS科学家增值的文献研究

J. Med. Chem. 2012, 55, 5, 1868–1897

<https://doi.org/10.1021/jm201331s>

Journal of
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Article
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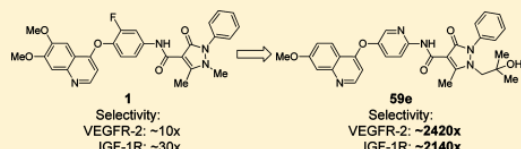
Structure-Based Design of Novel Class II c-Met Inhibitors: 2. SAR and Kinase Selectivity Profiles of the Pyrazolone Series

Longbin Liu,^{*,†} Mark H. Norman,[†] Matthew Lee,[§] Ning Xi,[†] Aaron Siegmund,[†] Alessandro A. Boezio,^{||} Shon Booker,[†] Debbie Choquette,^{||} Noel D. D'Angelo,[†] Julie Germain,^{||} Kevin Yang,[†] Yajing Yang,[†] Yihong Zhang,[‡] Steven F. Bellon,[†] Douglas A. Whittington,[†] Jean-Christophe Harmange,^{||} Celia Dominguez,[†] Tae-Seong Kim,[†] and Isabelle Dussault[†]

[†]Departments of Medicinal Chemistry, [‡]Oncology Research, and [§]Molecular Structure, Amgen Inc., One Amgen Center Drive, Thousand Oaks, California 91320, United States

^{||}Departments of Medicinal Chemistry and ^{||}Molecular Structure, Amgen Inc., 360 Binney Street, Cambridge, Massachusetts 02142, United States

Supporting Information



ABSTRACT: As part of our effort toward developing an effective therapeutic agent for c-Met-dependent tumors, a pyrazolone-based class II c-Met inhibitor, N-(4-((6,7-dimethoxyquinolin-4-yl)oxy)-3-fluorophenyl)-1,5-dimethyl-3-oxo-2-phenyl-2,3-dihydro-1H-pyrazole-4-carboxamide (**1**), was identified. Knowledge of the binding mode of this molecule in both c-Met and VEGFR-2 proteins led to a novel strategy for designing more selective analogues of **1**. Along with detailed SAR information, we demonstrate that the low kinase selectivity associated with class II c-Met inhibitors can be improved significantly. This work resulted in the discovery of potent c-Met inhibitors with improved selectivity profiles over VEGFR-2 and IGF-1R that could serve as useful tools to probe the relationship between kinase selectivity and in vivo efficacy in tumor xenograft models. Compound **59e** (AMG 458) was ultimately advanced into preclinical safety studies.

INTRODUCTION

The receptor tyrosine kinase (RTK) c-Met is mainly expressed by epithelial cells. Activation of c-Met is regulated by its ligand, hepatocyte growth factor (HGF), also known as scatter factor (SF).¹ Upon binding of HGF at the extracellular domain, c-Met receptor undergoes dimerization that results in transphosphorylation of the intracellular tyrosine residues (Y1234, Y1235) within the catalytic site.² Further phosphorylation of residues Y1349 and Y1356 mobilizes the intracellular C-terminal docking domain that recruits and subsequently activates a wide range of downstream signaling molecules (e.g., Grb2, Gab1, PI3K, Akt, Ras, Erk, and STAT3) that modulate the survival, proliferation, migration, and invasion of cells. As such, normal HGF/c-Met signaling plays an important role during embryogenesis and tissue injury repair.³ On the other hand, dysregulation of this pathway (through, e.g., either overexpression of HGF/c-Met or activating mutation of *MET* gene) can render many cellular processes unchecked and promote tumorigenesis. It has been established that aberrant signaling of the HGF/c-Met pathway correlates with aggressive tumor growth and poor prognosis in cancer patients.⁴ Different

approaches to inhibition of the HGF/c-Met pathway in cancer cells have been documented.⁵ These include antagonistic ligands to c-Met, antibodies against either HGF or c-Met, and small molecule kinase inhibitors targeting the intracellular kinase domain. Numerous c-Met kinase inhibitors have been reported in the literature.⁶ These inhibitors can be categorized into either class I or class II based on their binding mode in the c-Met kinase domain (vide infra). While class I molecules tend to be very selective for c-Met, thus far, a majority of the class II molecules are multikinase inhibitors. Improving the selectivity of class II c-Met inhibitors has been a significant challenge. In fact, until recently, no selective class II c-Met inhibitors have been reported and little is known as to whether the kinase selectivity profiles of class II c-Met inhibitors can be improved. Schroeder et al. reported the design of a pyridone-based c-Met inhibitor that was selective over a number of kinases, including IGF-1R.⁷ The selectivity over VEGFR-2 was modest (46-fold). We postulated that knowledge from kinase structural analysis

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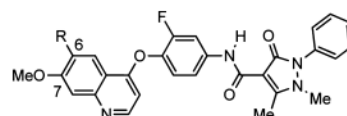
1868

dx.doi.org/10.1021/jm201331s | J. Med. Chem. 2012, 55, 1868–1897

Journal of Medicinal Chemistry

Article

Table 1. Modification of the Quinoline Ring^a

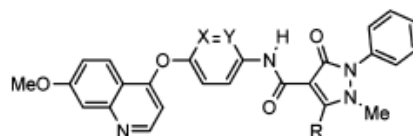


compd	R	c-Met		VEGFR-2		IGF-1R		PC3 IC ₅₀
		K _i	Fold	K _i	Fold	K _i	Fold	
1	OMe	1	7.8	8	32.1	32	20.2	
11a	Br	5.1	78.9	16	149	29	652	
11b	Me	3.4	–	–	146	43	461	
11c	Et	2.4	38	16	70.2	29	534	
11d	H	1.1	23.7	22	178	162	37.1	

^aK_i (nM): inhibitory constant for the phosphorylation of gastrin by c-Met, VEGFR-2, or IGF-1R. Fold: ratio of K_i(kinase)/K_i(c-Met). PC3 IC₅₀ (nM): inhibitory concentration for HGF-mediated c-Met phosphorylation in PC3 cells. Both K_i and IC₅₀ values are reported as an average for n > 2. See Supporting Information for standard deviations.

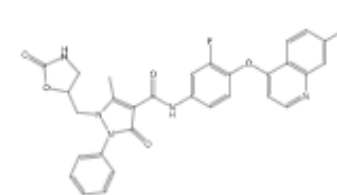
Journal of Medicinal Chemistry

Table 3. Effects of C5-Substituents on Selectivity Profiles^a



compd	R	X	Y	c-Met		VEGFR-2		IGF-1R		PC3 IC ₅₀
				K _i	Fold	K _i	Fold	K _i	Fold	
11d	CH ₃ -	CF	CH	1.1	23.7	22	178	162	37.1	
22a	CH ₃ -	CH	N	1.2	42	35	618	515	83	
26b	NH ₂ CH ₂ -	CF	CH	1.4	541	378	928	649	42	
26a	BocNHCH ₂ -	CF	CH	29	1240	43	>6600	>230	–	
26c	Et(Me)NCH ₂ -	CF	CH	2.3	903	386	744	317	76.7	
26d		CF	CH	1.5	1310	879	1800	1206	83.9	

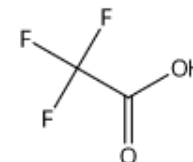
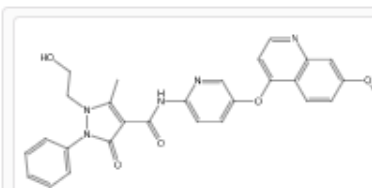
1361236-60-3



C₃₁H₂₆FN₅O₆
N-[3-Fluoro-4-[(7-methoxy-4-quinolinyl)oxy]phenyl]-2,3-dihydro-5-methyl-3-oxo-1-...

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

1374343-52-8



C₂₈H₂₅N₅O₅·xC₂HF₃O₂
1H-Pyrazole-4-carboxamide, 2,3-dihydro-1-(2-hydroxyethyl)-N-[(7-methoxy-4-qui...

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

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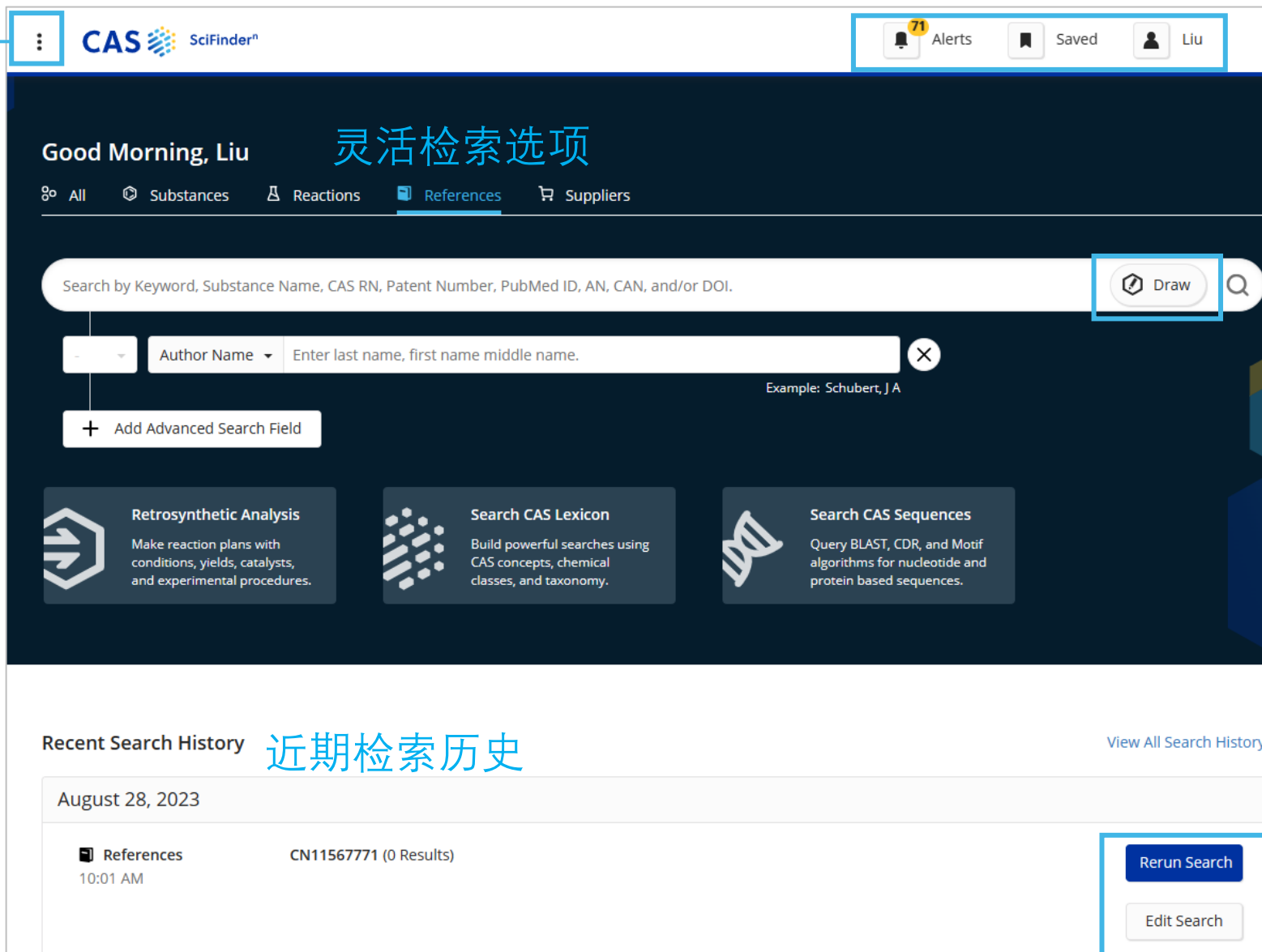
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Good Morning, Liu

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Author Name Enter last name, first name middle name. ✕
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Retrosynthetic Analysis
Make reaction plans with conditions, yields, catalysts, and experimental procedures.

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August 28, 2023

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The screenshot displays the CAS SciFinder web interface. At the top, there is a navigation bar with tabs for 'All', 'Substances', 'Reactions', 'References', and 'Suppliers'. Below this is a search bar with the text 'Search by Keyword, Substance Name, CAS RN, Patent Number, PubMed ID, AN, CAN, and/or DOI.' and a 'Draw' button. A secondary search bar contains the query 'Elasticity-dependent fast underwater adhesion demonstra...'. The main content area shows a 'References search for "Elasticity-dependent fast underwater adhesion demonstrated by macroscopic s..."' with a '1 Result' indicator. The search results are filtered to show '1' result. The first result is highlighted with a blue box and is titled 'Elasticity-Dependent Fast Underwater Adhesion Demonstrated by Macroscopic Supramolecular Assembly'. The authors listed are Ju, Guannan; Cheng, Mengjiao; Guo, Fengli; Zhang, Qian; Shi, Feng. The journal is 'Angewandte Chemie, International Edition (2018), 57(29), 8963-8967'. The abstract text begins with 'Macroscopic supramol. assembly (MSA) is a recent development in supramol. chem. to associate visible building blocks through non-covalent interactions in a multivalent manner. Although various substrates (e.g. hydrogels, rigid materials) have been used, a general design rule of building blocks in MSA systems and interpretation of the assembly mechanism are lacking and are required. Herein we design three model systems with varied elastic modulus and correlated the MSA probability with the elasticity. Based on the effects of substrate deformability on multivalency, we have proposed an elastic-m...'. Below the abstract is a 'View More' link. At the bottom of the result card, there are buttons for 'Full Text', 'Substances (14)', 'Reactions (2)', 'Citing (66)', and 'Citation Map'. A 'Filter Behavior' sidebar is visible on the left, with 'Filter by' selected. The page footer includes the text '© 2024 American Chemical Society. All rights reserved.' and the American Chemical Society logo.

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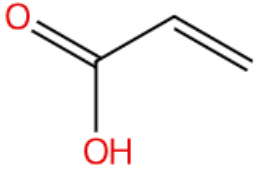
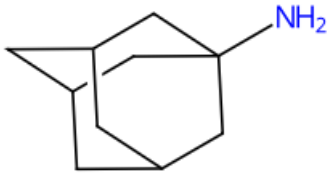
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Substances

Substances (14)

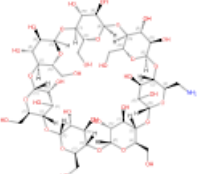
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1200829-09-9

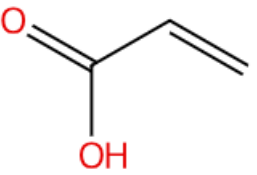


$C_{10}H_{17}N \cdot C_3H_4O_2$
2-Propenoic acid, compd. with tricyclo[3.3.1.1.3,7]decan-1-amine (1:1)
Role: Properties

1122464-65-6



Absolute stereochemistry shown

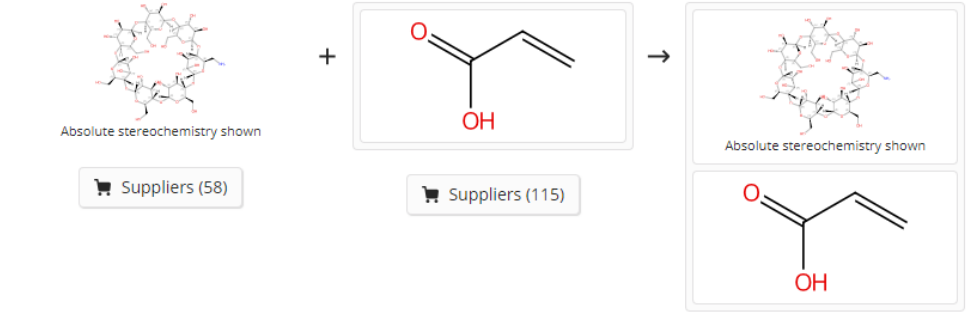


$C_{42}H_{71}NO_{34} \cdot x(C_3H_4O_2)_x$
 β -Cyclodextrin, 6^A-amino-6^A-deoxy-, compd. with 2-propenoic acid homopolymer
Role: Reactant, Reactant or Reagent

物质角色

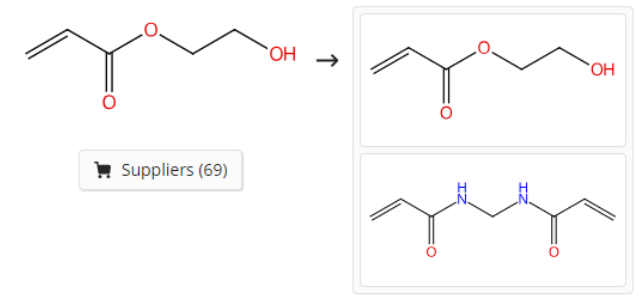
2 Results Group: By Scheme Sort: Yield View: Collapsed

Scheme 1 (1 Reaction) Steps: 1



Expand Scheme

Scheme 2 (1 Reaction) Steps: 1



Concepts

CAS科学家提供的标准技术术语

Adhesion, physical Modifier: underwater	Hydrogels
Elasticity	Multilayers
Gelatins Modifier: copolymer with dimethylacrylamide	Polyelectrolytes
Role: Properties	Stress-strain relationship
	Young's modulus

American Chemical Society

专利文献详情

1

Process for manufacturing high purity 2-chloro-1,1,1,2-tetrafluoropropane

By: Jungong, Christian; Merkel, Daniel C.
United States, US10125066 B1 2018-11-13 | Language: English, Database: CAplus

A **method** for producing 2-chloro-1,1,1,2-tetrafluoropropane (HCFC-244bb) from a reaction of HCFC-244bb and 2-chloro-3,3,3-trifluoropropene (HCFO-1233xf) by selectively hydrogenating the mixture in a vapor phase in the presence of hydrogen gas and a catalyst to generate a product HCFC-244bb and hydrogenation products of HCFO-1233xf, such as 2-chloro-1,1,1-trifluoropropane, separated from the HCFC-244bb by distillation. The separated HCFC-244bb may then be purified.

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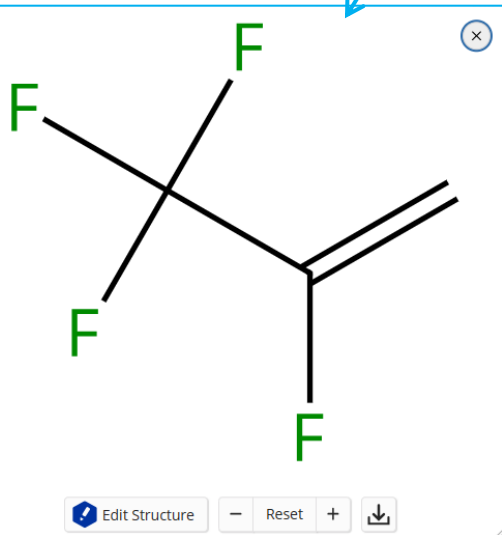
PatentPak Full Text Substances (11) Reactions (2)

Patent	Language	Kind Code	PatentPak Options
US10125066	English	B1	PDF PDF+ Viewer
WO2019108574	English	A1	PDF PDF+ Viewer
CN111479792	Chinese	A	PDF
JP2021504365	Japanese	T	PDF

CAS RN
754-12-1

CAS Name
2,3,3,3-Tetrafluoropropene

- Get Substance Details
- Get Bioactivity Data
- Get Reactions (1,467)
- Synthesize (1,150)
- Start Retrosynthetic Analysis
- Get References (3,783)
- Get Suppliers (23)



CAS PatentPak

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Key Substances in Patent

CAS RN 754-12-1

Analyst Markup Locations (1)
Page 7

CAS RN 421-73-8

Analyst Markup Locations (1)
Page 8

Example 4

Batch Acid Neutralization with 10 pH Solution of Soda Ash in Water, Followed by Drying

The acid neutralization step was conducted using a 10 gallon (3.9 L) vessel equipped with an agitator. All distilled HCFC-244bb, at 99.94% purity and <10 ppm acidity, was washed using a 10 pH solution of soda ash in water (Na₂CO₃/H₂O). The wash procedure entailed charging 15 lb (6.8 kg) of the 10 pH soda ash solution into the 10 gallon (3.9 L) vessel, followed by 50 lb (22.7 kg) of HCFC-244bb. This addition sequence allows HCFC-244bb to sieve

US 10,125,066 B1

13 palladium catalyst diluted in an alpha aluminum support to a palladium loading between 0.3 wt. % and 0.5 wt. %, based on the total weight of the palladium catalyst and the alpha aluminum support, to generate a product composition including unreacted HCFC-244bb and 2-chloro-1,1,1-trifluoropropane (HCFC-253db).

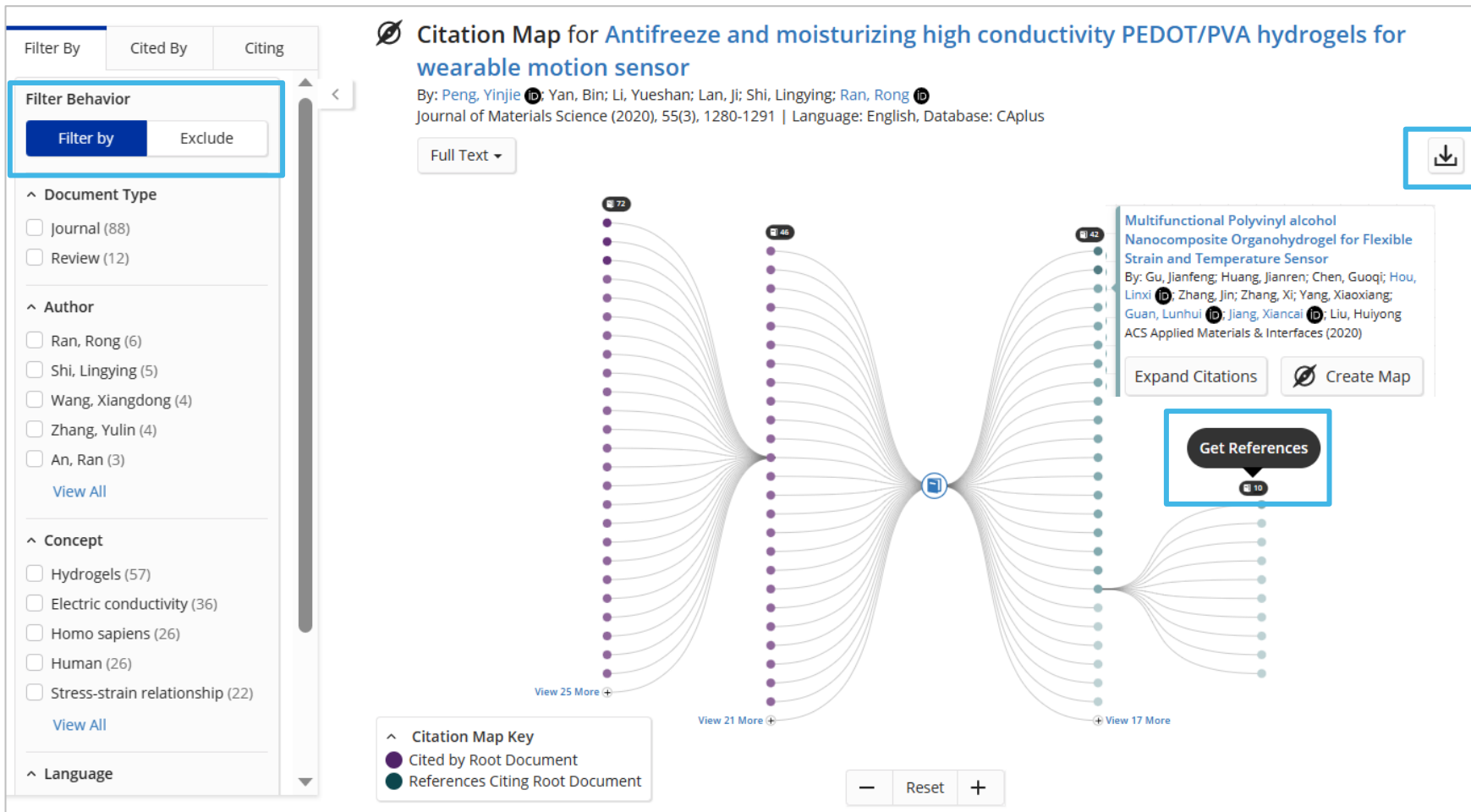
14 catalyst and the alpha aluminum support, at a temperature between 100° C. and 250° C. to generate a product composition including unreacted HCFC-244bb and 2-chloro-1,1,1-trifluoropropane (HCFC-253db); and separating the HCFC-244bb and the HCFC-253db.

11. The method of claim 10, further comprising the

CAS PatentPak®:

- 快速理解专利
- 一键下载原文
- 快速定位专利中的物质
- 阅读其他语言撰写的等同专利

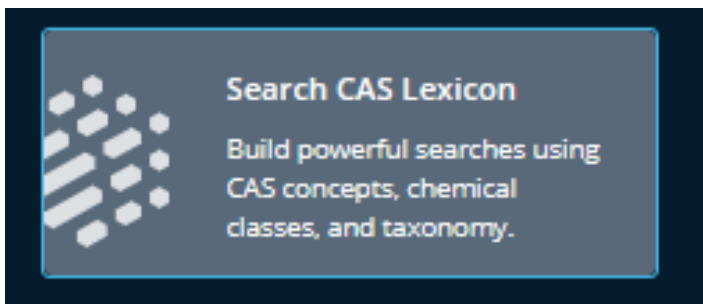
1.1 引文地图: 便捷地获取关联文献



- Citations: 参考文献
- Cited By: 引用当前文献的文献
- 通过聚类选项筛选引文
- 可下载引文地图
- 显示引文和被引文献的数量, 点击可链接至对应的文献结果页面

1.2 如何选择概念词？借助CAS Lexicon词库

- 在CAS词库层级中浏览CAS标引的概念词（Concepts）和物质
- 建立用于检索文献的检索式（最多可用1000个词）



Search CAS Lexicon

Carbon fiber-reinforced plastics Search Concept

Your Query
You may include up to 1,000 terms in a search. Clear All

碳纤维复合材料

^ Preferred Term

Carbon fiber-reinforced plastics

This will search synonyms: Carbon fiber-reinforced plastic; Reinforced plastic, carbon fiber-; Reinforced plastics, carbon fiber-
[View fewer synonyms](#)

^ Broader Terms (1) Select All

Fiber-reinforced plastics

^ Narrower Terms (4) Select All

Carbon fiber-reinforced plastics, prepregs

Carbon fiber-reinforced plastics, thermosetting

Carbon fiber-reinforced plastics, unidirectional

Graphite fiber-reinforced plastics

Select a boolean operator AND Add Term(s) [Learn more about CAS Lexicon searching.](#) Q

Lubricants X

AND

Carbon fiber-reinforced plastics X

Search CAS Lexicon

Phase change materials **相变材料** Search Concept

^ Preferred Term

Phase change materials

This will search synonyms: Materials, phase-change; Phase change ag...
[View more synonyms](#)

^ Broader Terms (1) Select All

Materials

^ Narrower Terms (1) Deselect All

Phase change materials, heat-storage phase-change materials

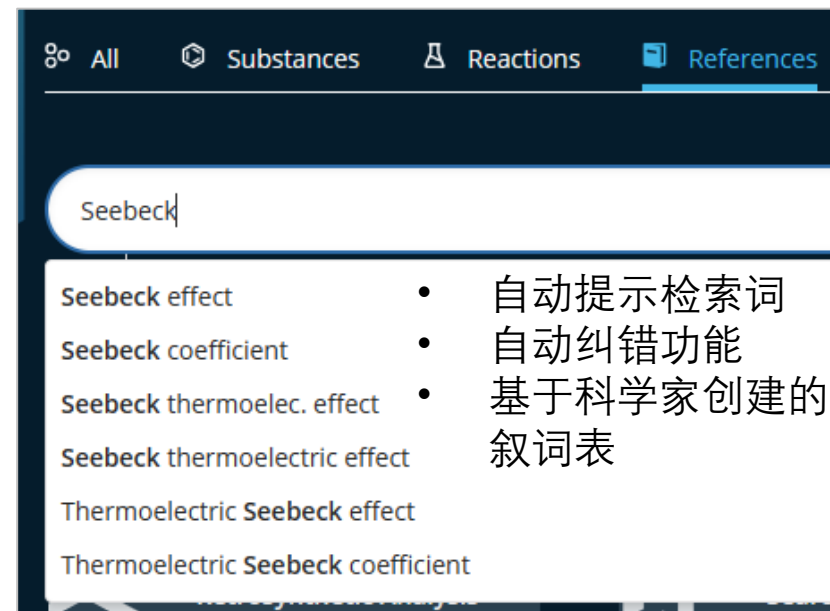
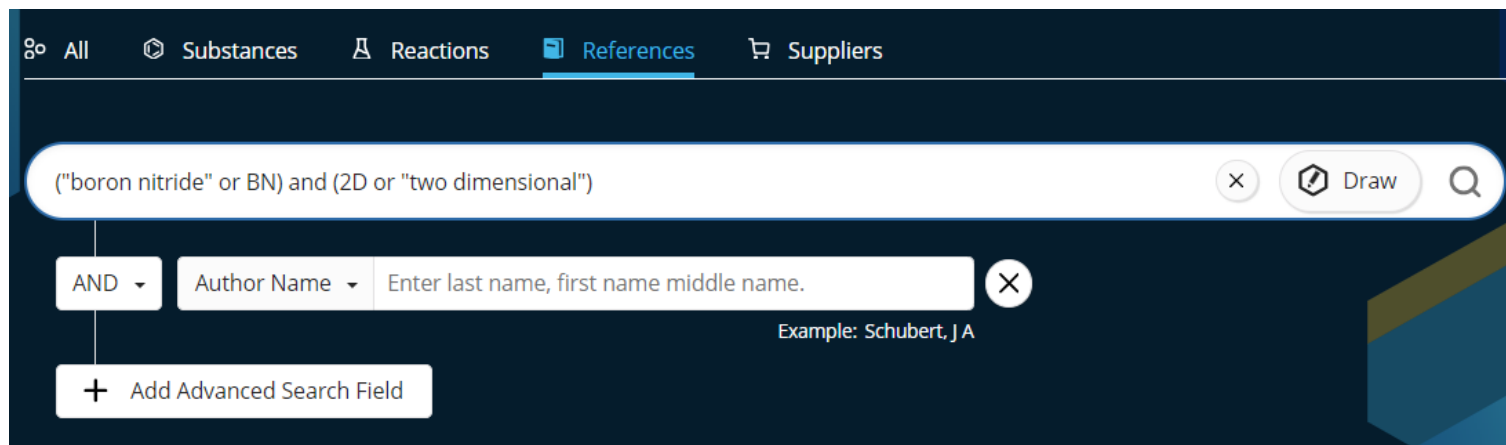
^ Related Terms (1) Select All

Phase transition

- 在CAS Lexicon词库层级中选择适合的主题词：
 - Preferred Term
 - Broader Terms
 - Narrower Terms
 - Related Terms

如何精准构建检索主题？

- 布尔逻辑运算符(and, or, 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?, 如 poly*可代表polymer, polymerization, polyethylene等 (*代表0或多个字符; ? 代表0或1个字符)



精准构建检索主题

poly* not polyethylene

检索：聚合物，排除聚乙烯

References search for "poly* not polyethylene"

Substances Reactions Citing Knowledge Graph

Filter Behavior: Filter by Exclude

Document Type: Journal (12.5M), Patent (5.9M), Review (1M), Biography (1,536), Book (22K)

Substance Role: Uses (5.5M), Biological Study (2.4M), Properties (2.1M)

19,203,161 Results

Sort: Relevance View: Full Abstract

1

Electrophoretic transfer of proteins from polyacrylamide gels to nitrocellulose sheets: Procedure and some applications

By: Towbin, Harry; Staehelin, Theophil; Gordon, Julian
Proceedings of the National Academy of Sciences of the United States of America (1971), 68(12), 1569-1572 | Database: CAlplus and MEDLINE

A method was devised for the electrophoretic transfer of proteins from polyacrylamide gels onto nitrocellulose sheets. This procedure is simple and efficient, and it is applicable to a wide variety of proteins. The transfer is obtained with no loss of resolution, but the transfer was not as simple as conventional procedures. The immobilized protein capacity on the nitrocellulose was blocked with excess protein. The specific protein was then detected by either autoradiography or immunodiffusion. In the latter case, as little as 100 pg of protein was clearly detectable.

Full Text Substance

(poly* not polyethylene) and "conductive device"
检索：聚乙烯以外的聚合物，作导电器件

References search for "(poly* not polyethylene) and "conductive device"

Substances Reactions Citing Knowledge Graph

Filter Behavior: Filter by Exclude

Document Type: Journal (53), Patent (134), Review (6)

Substance Role: Uses (104)

187 Results

Sort: Relevance View: Partial Abstract

1

Liquid Metal Droplets Wrapped with Polysaccharide Microgel as Biocompatible Aqueous Ink for Flexible Conductive Devices

By: Li, Xiankai; Li, Mingjie; Zong, Lu; Wu, Xiaochen; You, Jun; Du, Peikang; Li, Chaoxu
Advanced Functional Materials (2018), 28(39), n/a | Language: English, Database: CAlplus

Nanometerization of liquid metal in organic systems can facilitate deposition of liquid metals onto substrates and then recover its conductivity through sintering. Although having broader potential applications, producing stable aqueous inks of liquid metals keeps challenging because of rapid oxidation of liquid metal when exposing to water and oxygen. Here, a biocompatible aqueous ink is produced by encapsulating alloy nanodroplets of gallium and indium (EGaln) into microgels of marine polysaccharides. During sonicating bulk EGaln in aqueous alginate solution, alginate not only facilitates the...

View More

Full Text Substances (4) Reactions (0) Citing (36) Citation Map

2

Conductive polymers and devices

By: Vannikov, A. V.

自定义组合检索

检索方法可单独使用，也可联用：

- 关键词、物质名称、CAS RN、文献号；
- 高级检索（刊物名、机构名、Concepts、标题等）；
- 结构检索（包括物质结构和反应式）

The screenshot displays the CAS search interface. At the top, there are navigation tabs: All, Substances, Reactions, References (selected), and Suppliers. A search bar contains the query "Carbon dioxide and 'catalytic hydrogenation'". Below the search bar, a dropdown menu is open, showing search criteria options: AND, OR, NOT, and a list of fields including Publication Name, Authors, Organization, Title, Abstract/Keywords, Concept, Substances, Publication Year, Document Identifier, Patent Identifier, and Publisher. The "Publication Name" field is selected, and a list of journals is displayed, including Chem, Chemisches Zentralblatt, Chemical Physics Letters, Chemical Communications (Cambridge, United Kingdom), Chemosphere, Chemical Engineering Journal (Amsterdam, Netherlands), Chemistry - A European Journal, Chemistry Letters, Chemical & Pharmaceutical Bulletin, and Chemical Engineering Science.

1.3 文献结果：最新 & 引用最多 & 早期科学研究

References search for "(PVDF or PEDOT) and "wearable device""

Substances Reactions Citing Knowledge Graph

Sort: Publication Date: Newest View: Partial Abstract

818 Results

1

Ultra-stretchable and biodegradable elastomers for soft, transient electronics
By: Han, Won Bae; Ko, Gwan-Jin; Lee, Kang-Gon; Kim, Donghak; Lee, Joong Hoon; Yang, Seung Min; Kim, Dong-Je; Shin, Jeong-Woong; Jang, Tae-Min; Han, Sungkeun; et al
Nature Communications (2023), 14(1), 2263 | Language: English, Database: CPlus and MEDLINE

As rubber-like elastomers have led to scientific breakthroughs in soft, stretchable characteristics-based **wearable**, implantable electronic **devices** or relevant research fields, developments of degradable elastomers with comparable mech. properties could bring similar technol. innovations in transient, bioresorbable electronics or expansion into unexplored areas. Here, we introduce ultra-stretchable, biodegradable elastomers capable of stretching up to 1600% with outstanding properties in toughness, tear-tolerance, and storage stability, all of which are validated by

View More

Full Text

Filter Behavior: Filter by Exclude

Search Within Results

CAS Solutions

Substance Role

- Relevance
- Times Cited
- Accession Number: Ascending
- Accession Number: Descending
- Publication Date: Newest**
- Publication Date: Oldest

排序方式：
相关性
引用次数
收录号
发表时间

- ChemZent®：最早期的化学文摘——德国化学文摘的英文版，唯一提供可用英文获取德国化学文摘的解决方案，将化学研究相关文献回溯至十九世纪初。

References search for "solar cell"

Substances Reactions Citing Knowledge Graph

Filtering: Database: CHEMZENT

2,382 Results

Sort: Publication Date: Oldest View: Partial Abstract

1

Experiments over the photoelectric fatigue of alkali metals
By: Bergwitz, K.
Chemisches Zentralblatt (1907), 78 Book 2(6), 439-439 | Language: German, Database: CHEMZENT

Machine Translated: Periodically ELSTER and GEITEL produced Na-, K- und Rb-Zellen (cathode solid alkali metal anode Al in a water fabric vacuum of 0.33) can be in exposure to visible light no fatigue determining nor to one cell with liquid K-Na-Legierung, the surface of which in the vacuum renew it. In one **photoelectric cell** by exposure induced current by a sensitive telephone are detected.

ChemZent Full Text

Filter Behavior: Filter by Exclude

Document Type

Language

Filter Behavior

Filter by Exclude

Document Type

Language

▼ Concept

▲ Database

- CPlus (416K)
- MEDLINE (33K)
- CHEMZENT (2,382)


筛选目标文献

文献类型、语言、作者
发表机构、发表年份
CAS标引的技术术语
CAS标引的学科研究方向
二次检索
下载数据分析报告





...

- Organization
- Publication Name
- Concept
- CA Section
- CAS Solutions
- Database
- Search Within Results

Filter Content Report

Download filter data from this result set. 

References search for "(PVDF or PEDOT) and "wearable device""

Substances Reactions Citing Knowledge Graph     Save and Alert

687 Results Sort: Relevance View: Partial Abstract

1

High-Performance Flexible All-Solid-State Supercapacitor from Large Free-Standing Graphene-PEDOT/PSS Films

By: Liu, Yuqing; Weng, Bo; Razal, Joselito M.; Xu, Qun; Zhao, Chen; Hou, Yuyang; Seyedin, Shayan; Jalili, Rouhollah; Wallace, Gordon G.; Chen, Jun
Scientific Reports (2015), 5, 17045 | Language: English, Database: CPlus and MEDLINE




Although great attention has been paid to **wearable electronic devices** in recent years, flexible lightweight batteries or supercapacitors with high performance are still not readily available due to the limitations of the flexible electrode inventory. In this work, highly flexible, bendable and conductive rGO-**PEDOT**/PSS films were prepared using a simple bar-coating method. The assembled device using rGO-**PEDOT**/PSS electrode could be bent and rolled up without any decrease in electrochem. performance. A relatively high areal capacitance of 448 mF cm⁻² was achieved at a scan rate of 10 mV s⁻¹ usin...

[View More](#)

Full Text Substances (13) Reactions (0) Citing (173) Citation Map

2

Highly stretchable multilayer electronic circuits using biphasic gallium-indium

By: Liu, Shanliangzi ; Shah, Dylan S. ; Kramer-Bottiglio, Rebecca 
Nature Materials (2021), 20(6), 851-858 | Language: English, Database: CPlus and MEDLINE

筛选工具 CAS Section & Concept

CA Section

By Count | Alphanumeric | **学科研究方向**

6 Selected

- Electrochemical, Radiational, and Thermal Energy Technology (210)
- Electric Phenomena (169)
- Biochemical Methods (83)
- Textiles and Fibers (55)
- Plastics Fabrication and Uses (52)
- Pharmaceuticals (22)
- Plastics Manufacture and Processing (20)
- Optical, Electron, and Mass Spectroscopy and Other Related Properties (18)
- Unavailable (8)
- Electrochemistry (7)
- Inorganic Analytical Chemistry (5)
- Radiation Chemistry, Photochemistry, and Photographic and Other Reprographic Processes (5)
- Surface Chemistry and Colloids (5)
- Synthetic Elastomers and Natural Rubber (4)
- Air Pollution and Industrial Hygiene (3)
- Chemistry of Synthetic High Polymers (3)
- Magnetic Phenomena (3)
- Coatings, Inks, and Related Products (2)

Apply **Cancel**

Concept

Top Count | Alphanumeric | Search | **纵览并精准定位核心研究点**

7 Selected

- Wearable devices (501)
- Fluoropolymers (343)
- Electric conductivity (155)
- Electrodes (128)
- Surface structure (124)
- Homo sapiens (117)
- Human (117)
- Nanofibers (101)
- Electric current-potential relationship (100)
- Polyesters (92)
- Carbon nanotubes (8)
- Flexibility (84)
- Stress-strain relationships (82)
- Electrospinning (82)
- Current density (50)
- Hydrogels (50)
- Humans (48)
- Polymers (48)
- Carbon black (47)
- Electronics (47)
- Coating materials (30)
- Electrolytes (29)
- Sheet resistance (29)
- Surface area (29)
- Skin (28)
- Supercapacitor electrodes (28)

Apply **Cancel**

Concept

Top Count | Alphanumeric | **Search** | **精准定位感兴趣的核心研究点**

Concept Name: nano*

17 Selected

- Carbon nanofibers (14)
- Carbon nanotube fibers (4)
- Carbon nanotubes (86)
- Cellulosic nanofibers (1)
- Core-shell nanoparticles (1)
- Electric nanogenerators (24)
- Metal Nanoparticles (3)
- Nanofibril (2)
- Nanofilms (6)
- Nanofilters (1)
- Nanoflakes (2)
- Nanoflowers (2)
- Nanohorns (1)
- Nanoimprint lithography (1)
- Nanosheets (23)
- Nanospheres (1)
- Nanostructured materials (9)
- Nanostructures (18)
- Nanotechnology (4)
- Nanotubes (12)
- Nanotubes, Carbon (11)

筛选工具 Search within results

合并、交集和去重

References search for "(PVDF or PEDOT) and "wearable device""

Substances Reactions Citing Knowledge Graph

Filtering: Concept: Hydrogels X

Excluding: Search Within Results: dop* X

41 Results Sort: Relevan

1

Enhancing Strain-Sensing Properties of the Conductive Hydrogel by Introduc
By: Hu, Zhirui; Li, Jie; Wei, Xiaotong; Wang, Chen; Cao, Yang; Gao, Zhiqiang; Han, Jing; Li, Yingchun
ACS Applied Materials & Interfaces (2022), 14(40), 45853-45868 | Language: English, Database: CAPlus

Conductive hydrogels have attracted attention because of their wide application. However, it is still a challenge to achieve conductive hydrogels with high sensitivity and response for smart wearable strain sensors. Here, we report a composite hydrogel with piezoelec. sensing for flexible strain sensors. The composite hydrogel consists of quaternary ammonium salt (CHACC) as the hydrogel matrix, poly(3,4-ethylenedioxythiophene):poly(styrenesulfonate) (PEDOT: PSS) as the conductive fluori...

Full Text

Substances (7) Reaction (1)



Save and Alert

Clear All Filters

Based on your query, we've returned the most relevant results. Would you like to load the entire result set?
Learn about result relevance.
Load More Results

Filter Behavior
Filter by Exclude

Document Type

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

Enter a query...

Search

Searching for... **dop*** Clear All

Save Results and Create Alert 定题追踪

Name: Wearable Device

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

Alert Frequency:
 No Alerts
 As Available
 Weekly
 Monthly

Add Existing Tags (Optional):
 Biotech
 catalyst
 Chem Engineering
 Formulus
 High Entropy

New Tag (Optional): Polymer Tag Color: Light Green

Save Cancel

1.4 如何获得结构相关的文献?

策略: 从Reference出发, 主题词+结构联合检索

CAS SciFinder[®] References Organic photovoltaic

← Return to Home

References search for "Organic photovoltaic" + drawn structure

Substances Reactions Citing Knowledge Graph

Structure Match: As Drawn (0) Substructure (505)

Filter Behavior: Filter by Exclude

Search Within Results: Substance Role

- Uses (456)
- Properties (280)
- Preparation (124)
- Reactant or Reagent (118)
- Process (86)
- Polymer in Formulation (7)
- Nanoscale (4)

View All

Filtering: Substance Role: 4 Selected

298 Results Sort: Publication Date: Newest View: Partial Abstract

1

Hexanary blends: a strategy towards thermally stable organic photovoltaics
By: Paleti, Sri Harish Kumar; Hultmark, Sandra; Han, Jianhua; Wen, Yuanfan; Xu, Han; Chen, Si; Jarsvall, Emmy; Jalan, Ishita; Villalva, Diego Rosas; Sharma, Anirudh; et al
Nature Communications (2023), 14(1), 4608 | Language: English, Database: CAPLUS and MEDLINE

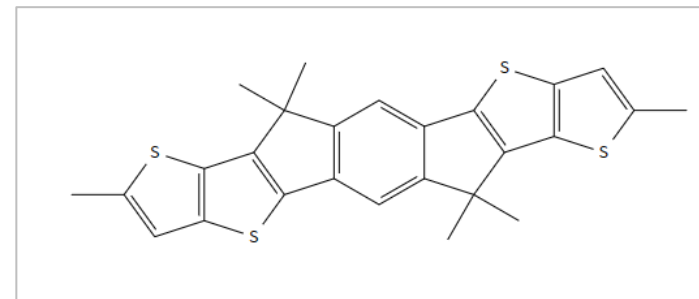
Non-fullerene based organic solar cells display a high initial power conversion efficiency but continue to suffer from poor thermal stability, especially in case of devices with thick active layers. Mixing of five structurally similar acceptors with similar electron affinities, and blending with a donor polymer is explored, yielding devices with a power conversion efficiency of up to 17.6%. The hexanary device performance is unaffected by thermal annealing of the bulk-heterojunction active layer for at least 23 days at 130 °C in the dark and an inert atm. Moreover, hexanary blends offer a high...

Full Text Substances (16) Reactions (0) Citing (0) Citation Map

2

High-performance vertical field-effect organic photovoltaics
By: Wu, Xiaomin; Gao, Changsong; Chen, Qizhen; Yan, Yujie; Zhang, Guocheng; Guo, Tailiang; Chen, Huipeng
Nature Communications (2023), 14(1), 1579 | Language: English, Database: CAPLUS and MEDLINE

定位物质在文献中的研究角色



16 Results

1

126213-51-2

(C₆H₆O₂S)_x
Poly(3,4-ethylenedioxythiophene)

47K References 1,489 Reactions 7 Suppliers

2

50851-57-5

(C₈H₈O₃S)_x
Poly(styrenesulfonic acid)

39K References 879 Reactions 2 Suppliers

4

2304444-49-1

C₈₂H₈₆F₄N₈O₂S₅
2,2'-[[12,13-bis(2-ethylhexyl)-12,13-dihydro-3,9-diundecylbisthieno[2'',3'':4',5...]]

905 References 42 Reactions 30 Suppliers

5

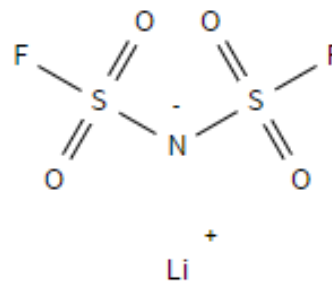
2097998-59-7

C₉₄H₇₈F₄N₄O₂S₄
2,2'-[[6,6,12,12-tetrakis(4-hexylphenyl)-6,12-dihydrodithieno[2,3-d':2',3'-d']-s...]]

524 References 5 Reactions 27 Suppliers

1.4 如何获得结构相关的文献?

关注锂电池技术中特定的热点材料



The screenshot shows the CAS SciFinder search interface. The search query is "lithium battery" or "lithium-ion battery" or "Li-ion batt". The search results are displayed in a list format. The first result is "Pyrrolinium-based Ionic Liquid as a Flame Retardant for Binary Electrolytes of Lithium-ion Batteries" by Kim, Hyung-Tae; Kang, Jaesik; Mun, Junyoung; Oh, Seung M.; Yim, Taeun; Kim, Young Gyu. The second result is "Anionic Effect on Enhancing the Stability of a Solid Electrolyte Interphase Film for Lithium Deposition on Graphite" by Yang, Gaojing; Zhang, Simeng; Weng, Suting; Li, Xiaoyun; Wang, Xuefeng; Wang, Zhaoxiang; Chen, Liquan. The interface includes filters for Structure Match, Filter Behavior, Document Type, Substance Role, and Language. A blue box highlights the Substance Role filter, which is currently set to "Uses (1,368)".

The Substance Role filter panel is shown, with the "By Count" tab selected. The "Uses (1,368)" option is checked. Other options include "Reactant or Reagent (56)", "Technical or Engineered Material Use (1,237)", "Properties (255)", "Industrial Manufacture (20)", "Physical, Engineering, or Chemical Process (178)", "Synthetic Preparation (19)", "Process (178)", "Reagent (6)", "Modifier or Additive Use (83)", "Nanoscale (5)", "Other Use, Unclassified (72)", "Purification or Recovery (4)", and "Analyte (2)". The "Apply" button is highlighted in blue.

文献检索小结

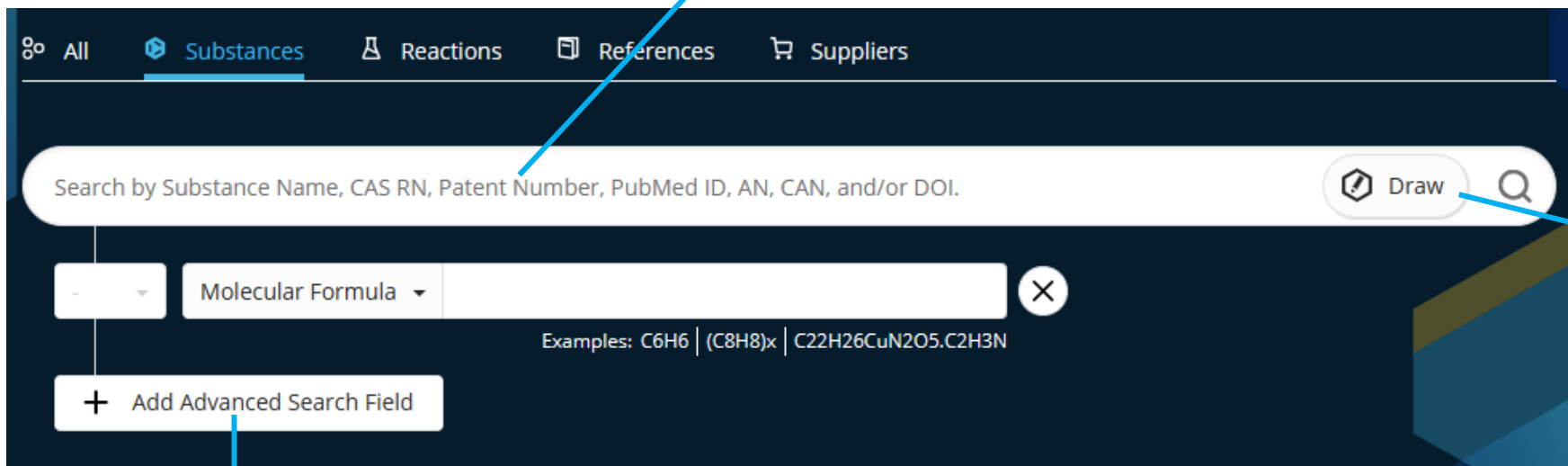
1. 利用引文地图拓展文献检索
2. 检索词的构建：利用CAS Lexicon精准选词，使用布尔逻辑算符及通配符连接主题词，利用高级检索选项进行自定义组合检索
3. 利用丰富的筛选工具，快速获得目标文献
4. 主题词+结构联合检索快速获得文献

2.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？
- 如何查找相似的序列？

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 RN）
- 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 "polyformaldehyde"

References Reactions Suppliers

Get References for Substances

All Results Selected Results

Search Within Results

Substance Class

Reference Role

Reaction Role

Aromatic Rings

Functional Group

Element

2 Selected 2 Results

1 9002-81-7

[*]COC[*]

$(\text{CH}_2\text{O})_n$

Polyformaldehyde

8,683 References 287 Reactions 10 Suppliers

2 30525-89-4

[*]COC[*]

$(\text{CH}_2\text{O})_x$

Polyformaldehyde

22K References 205 Reactions 94 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 (1)

10 Results

Sort: Molecular Formula: Ascending View: Partial

1 147-85-3

OC(=O)C1CCCN1

Absolute stereochemistry shown, Rotation (-)

$\text{C}_5\text{H}_9\text{NO}_2$

L-Proline

117K References 48K Reactions 164 Suppliers

2 61-90-5

CC(C)C[C@@H](C(=O)O)N

Absolute stereochemistry shown, Rotation (-)

$\text{C}_6\text{H}_{13}\text{NO}_2$

L-Leucine

125K References 6,092 Reactions

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

2.1 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： 高熵碳化物 C.Hf.Nb.Ta.Ti.Zr
- 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 Na_2SO_4 : $\text{H}_2\text{O}_4\text{S}.2\text{Na}$

The screenshot shows the CAS search interface for the molecular formula "(CH2O)n". The search results are displayed in a grid format, showing 5 results. The first three results are highlighted:

- Result 1: 9002-81-7, Polyformaldehyde, $(\text{CH}_2\text{O})_n$. 8,683 References, 287 Reactions, 10 Suppliers.
- Result 2: 32107-82-7, Poly(hydroxymethylene), $(\text{CH}_2\text{O})_n$. 37 References, 3 Reactions, 0 Suppliers.
- Result 3: 32008-59-6, Poly(oxymethylene- d_2), $(\text{CD}_2\text{O})_n$. 32 References, 23 Reactions, 27 Suppliers.

The interface also includes a search bar, filters for References, Reactions, and Suppliers, and a "Filter Behavior" section with options for "Filter by" and "Exclude".

$(\text{C}_2\text{H}_4\text{O})_n\text{H}_2\text{O}$: 括号中是重复结构单元， 括号外为n
 $(\text{C}_2\text{H}_6\text{O}_2)_x$: 括号中是单体， 括号外为x

2.2 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 Formula

Examples: C6H6 | (C8H8)_x | C22H26CuN2O5.C2H3N

Experimental Spectra

- Proton NMR
- Carbon-13 NMR
- Nitrogen-15 NMR
- Fluorine-19 NMR
- Phosphorus-31 NMR

实验核磁谱图数值助力结构解析

Recent Searches

August 15, 2024

Substance

10:44 AM

As Drawn (2)
Substructure (6,704)
Similarity (242K)

高级检索字段:

- CAS RN (物质、组份)、物质标识符、分子式、文献号、专利号
- 实验谱图: ^1H , ^{13}C , ^{15}N , ^{19}F , ^{31}P NMR
- 化学标识符: 化学名称、InChI key
- 生物: 生物富集因子、LD50
- 化学: Koc, LogD, LogP、溶解度、分子量、pKa、蒸汽压
- 密度属性: 密度、摩尔体积
- 电学: 电导/电导率、电阻/电阻率
- Lipinski: 自由旋转键、H受体/供体
- 磁: 磁力矩
- 机械属性: 拉伸强度
- 光散射: 旋光性、折射率
- 结构: 极性表面积
- 热学: 熔点、沸点、闪电、玻璃转化温度、蒸发焓

Chemical Properties

- Koc
- logD
- logP
- Mass Intrinsic Solubility (g/L)
- Mass Solubility (g/L)
- Molar Intrinsic Solubility (mol/L)
- Molar Solubility (mol/L)
- Molecular Weight
- pKa
- Vapor Pressure (Torr)

属性值联用检索物质

例如检索满足多属性值要求的聚合物：密度 $1-2\text{g/cm}^3$ 、拉伸强度 $>1000\text{MPa}$ 、熔点 $>150^\circ\text{C}$

The screenshot displays a chemical search interface with the following components:

- Navigation:** All, Substances, Reactions, References, Suppliers.
- Search Bar:** Search by Substance Name, CAS RN, Patent Number, PubMed ID, A...
- Advanced Search Fields:**
 - Tensile Strength (Mpa) >1000
 - Density (g/cm³) 1.0 to 2.0
 - Melting Point (°C) >150
- Filter Behavior:** Filter by (selected), Exclude.
- Search Within Results:** Substance Class (checked), Element (10), Alloy (3), Manual Registration (3), Mineral (1).
- Reference Role, Reaction Role, Aromatic Rings, Functional Group, Element, Number of Components, Commercial Availability, Molecular Weight:** Available (21).
- Substances search for 3 Advanced Fields:**
 - Filtering: Substance Class: Polymer
 - 21 Results
 - Sort: Relevance, View: Partial
 - Results grid showing chemical structures and statistics for various polymers:

Substance ID	Chemical Structure	Formula	Name	References	Reactions	Suppliers
31694-16-3		(C ₁₉ H ₁₂ O ₃) _n	Poly(oxy-1,4-phenyleneoxy-1,4-phenylenecarbonyl-1,4-phenylene)	16K	357	2
25014-41-9		(C ₃ H ₃ N) _x	Polyacrylonitrile	58K	1,953	35
9002-89-5		(C ₂ H ₄ O) _x	Poly(vinyl alcohol)	271K	13K	246
26100-51-6		(C ₃ H ₆ O ₃) _x	(±)-Poly(lactic acid)			
9002-81-7		(CH ₂ O) _n	Polyformaldehyde			
88995-51-1						

在物质类别 Substance Class 中，锁定polymer

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 Save and Alert

Filter Behavior: Filter by Exclude




Filtering: Bioactivity Data: 3 Selected X Clear All Filters

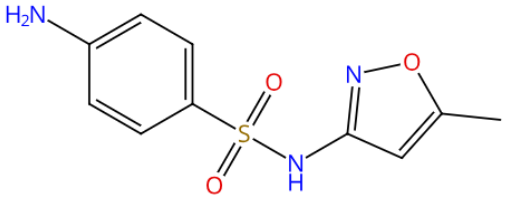
15 Results Sort: Molecular Formula: Ascending View: Partial

Result	Chemical Name	Molecular Formula	References	Reactions	Suppliers
1	296262-16-3	<chem>C10H10N2O2S2</chem> 2-[[[5,6-Dimethylthieno[2,3-d]pyrimidin-4-yl]thio]acetic acid	5	42	44
2	723-46-6	<chem>C10H11N3O3S</chem> Sulfamethoxazole	24K	961	120
3	1631737-39-7	<chem>C10H15N3O5</chem> (2R,3R,4S,5R)-4,5-Dihydro-5-(hydroxy methyl)-3'-methylspiro[furan-2(3H),7(6'H)]-...	2	22	0
4	442571-27-9	<chem>C10H10N2O2S2</chem> 2-[[[5,6-Dimethylthieno[2,3-d]pyrimidin-4-yl]thio]acetic acid	5	42	44
5	1927010-88-5	<chem>C10H11N3O3S</chem> Sulfamethoxazole	24K	961	120
6	697787-29-4	<chem>C10H15N3O5</chem> (2R,3R,4S,5R)-4,5-Dihydro-5-(hydroxy methyl)-3'-methylspiro[furan-2(3H),7(6'H)]-...	2	22	0


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

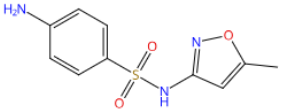
- Molecular Weight
- Melting Point (Experimental)
- Boiling Point (Predicted)
- Density (Experimental)
- pKa (Predicted)

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

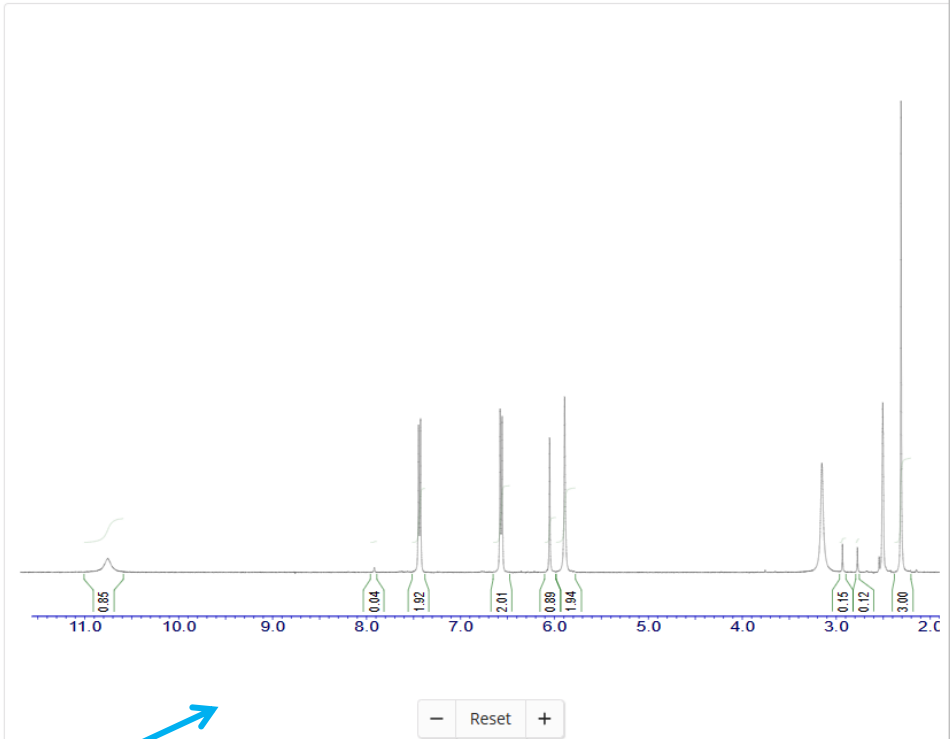
CAS Name
Sulfamethoxazole

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 (1) LC

View Proton NMR Spectrum (2) ENAMINE

Source

2.4 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

X 选择可变基团

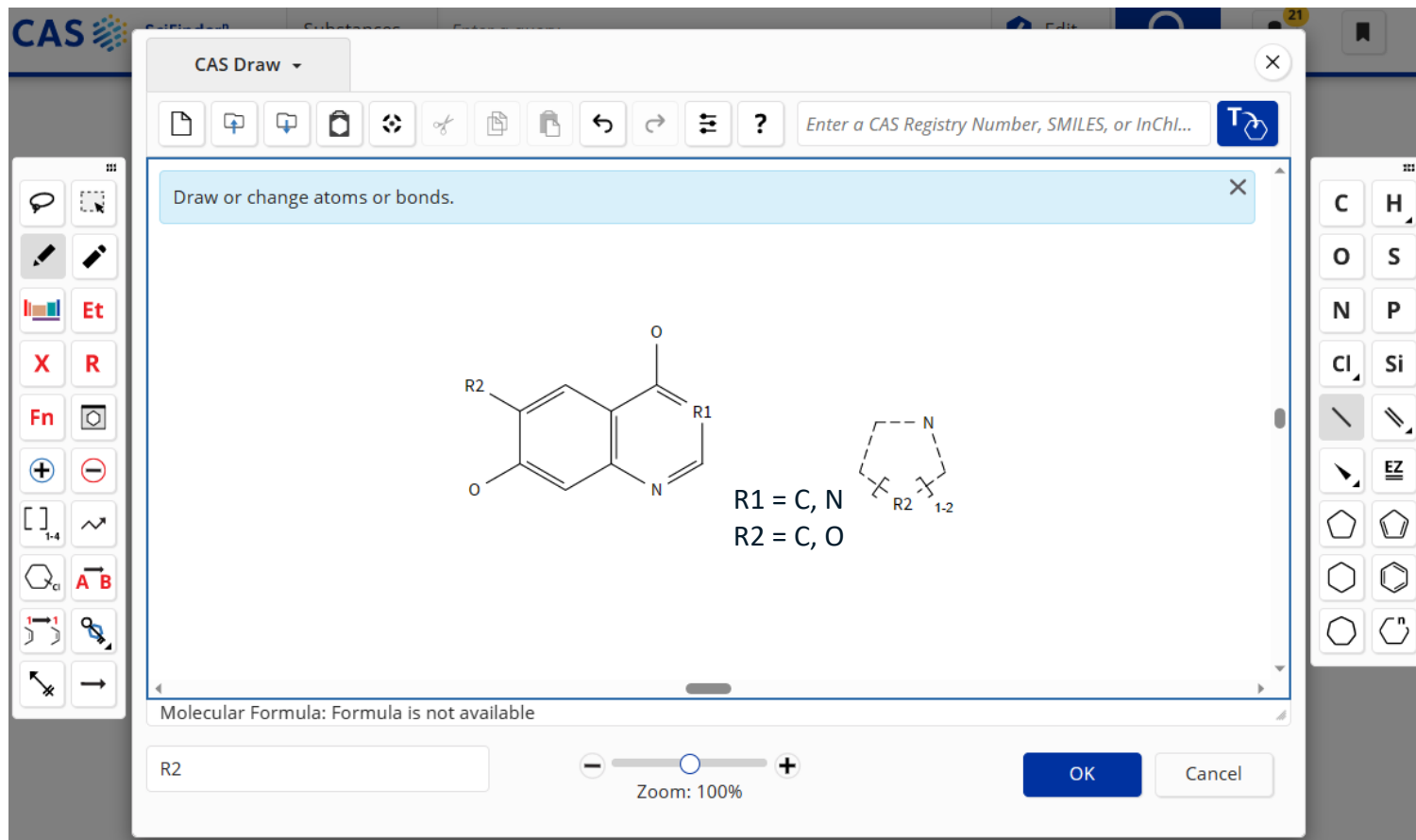
R 自定义R基团

Fn 片段结构


[]₁₋₄ 重复工具

 取代位置可变

 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 **R**
3. 环系范围的定义 **[]**₁₋₄

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

The screenshot displays the CAS Substances search interface for a drawn structure. The search bar shows "Substances search for drawn structure" with tabs for References, Reactions, and Suppliers. The search results are displayed in a grid, with the first three results highlighted. The first result is 685504-28-3, the second is 807307-30-8, and the third is 635299-07-9. The interface also includes a "Filter Behavior" section on the right, which is currently set to "Filter by".

Structure Match:

- As Drawn (0)
- Substructure (732)
- Similarity (9)

Filter Behavior:

- Filter by
- Exclude

Reaction Role

Reference Role

Commercial Availability

Number of Components

Molecular Weight

Stereochemistry

Element

Substance Class

Isotopes

Metals

Experimental Property

Bioactivity Indicator

Search Within Results

物质筛选类别:

反应角色

文献角色

立体化学

物质类别

同位素

金属包含

实验物性数据

二次检索……

物质检索结果的筛选

Filter by Exclude

Reaction Role

- Product (216)
- Reactant (53)
- Reagent (3)
- Catalyst (36)

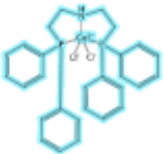
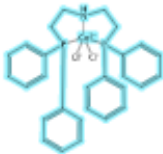
Reference Role

Commercial Availability

Number of Components

Molecular Weight

Reaction Role: 物质在反应中的角色

1087216-22-5	2170923-58-5
	
$C_{28}H_{29}Cl_2CoNP_2$ Dichloro[2-(diphenylphosphino-κP)-N-[2-(diphenylphosphino-κP)ethyl]ethanamine-κN...	$C_{28}H_{29}Cl_2CoNP_2$ (TB-5-13)-Dichloro[2-(diphenylphosphino-κP)-N-[2-(diphenylphosphino-κP)ethyl]eth...
8 References, 105 Reactions, 0 Suppliers	1 Reference, 32 Reactions, 0 Suppliers

Substance Class: 物质类别

Number of Components

- 1 (23)
- 2 (285)
- 3 (92)
- 4 (12)
- 5 or more (11)

Molecular Weight


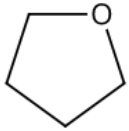

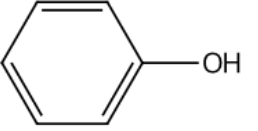
Stereochemistry

Element

Substance Class

- Polymer (92)
- Coordination Compound (42)
- Salt and Compound With (9)
- General Derivative (3)

Isotopes

849402-50-2	62306-29-0
 	 
$(C_4H_8O.C_4H_4S)_x.xCH_4O$ Components: 3 Furan, tetrahydro-, polymer with thiophene, methyl ether, graft	$(C_6H_6O.C_4H_4S.CH_2O)_x$ Components: 3 Formaldehyde, polymer with phenol and thiophene
1 Reference, 0 Reactions, 0 Suppliers	2 References, 0 Reactions, 0 Suppliers

Reference Role: 物质在文献中的研究角色

Filter by

Reaction Role

Reference Role

- Preparation (489)
- Synthetic Preparation (488)
- Properties (245)
- Reactant (98)
- Reactant or Reagent (98)
- Industrial Manufacture (9)

View All

Commercial Availability

- Not Available (9)

579490-58-7	579490-62-3
	
$C_{37}H_{31}NNiP_2$ (SP-4-1)-[2-(Diphenylphosphino-κP)-N-[2-(diphenylphosphino-κP)phenyl]benzenamina...	$C_{38}H_{33}NNiP_2$ (SP-4-1)-[2-(Diphenylphosphino-κP)-N-[2-(diphenylphosphino-κP)phenyl]benzenamina...
7 References, 22 Reactions, 0 Suppliers	6 References, 21 Reactions, 0 Suppliers

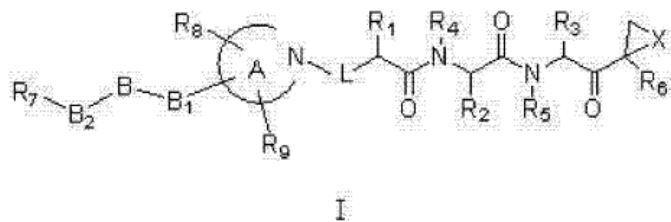
2.5 CAS Markush检索，助力结构查新

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：



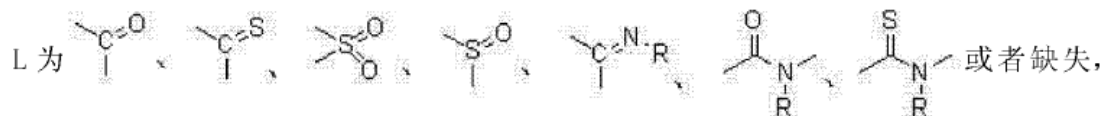
其中：

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

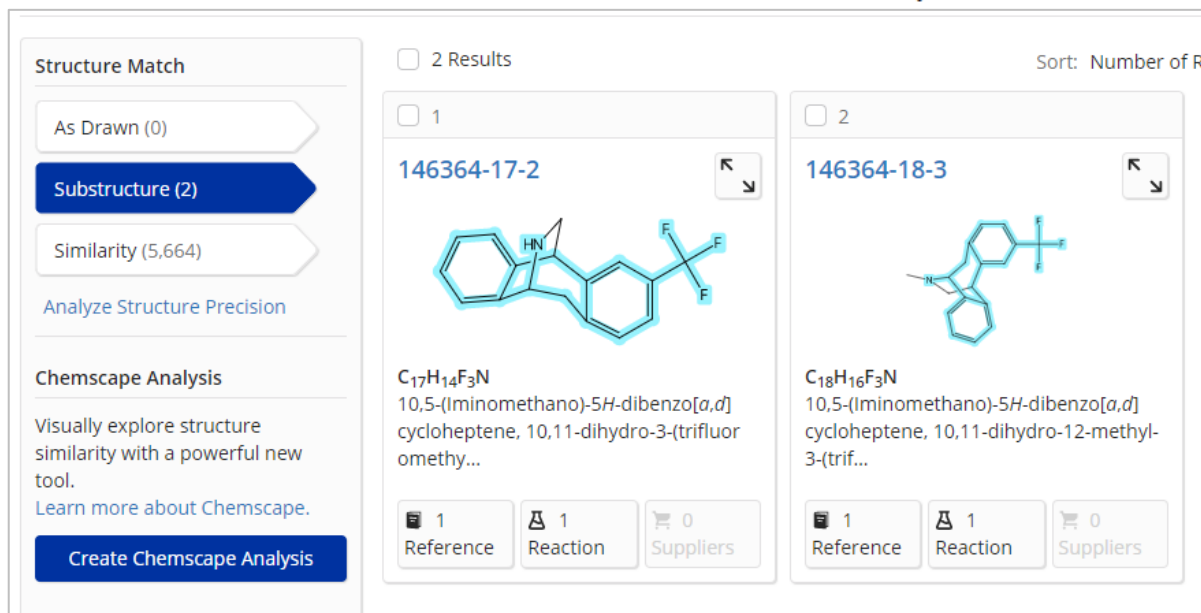
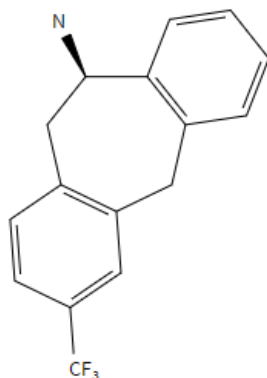
预测性物质[Prophetic Substance]：

- 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

As Drawn (0)

Substructure (2)

Similarity (5,664)

Analyze Structure Precision

Chemscrape Analysis

Visually explore structure similarity with a powerful new tool.

Learn more about Chemscrape.

Create Chemscrape Analysis

2 Results

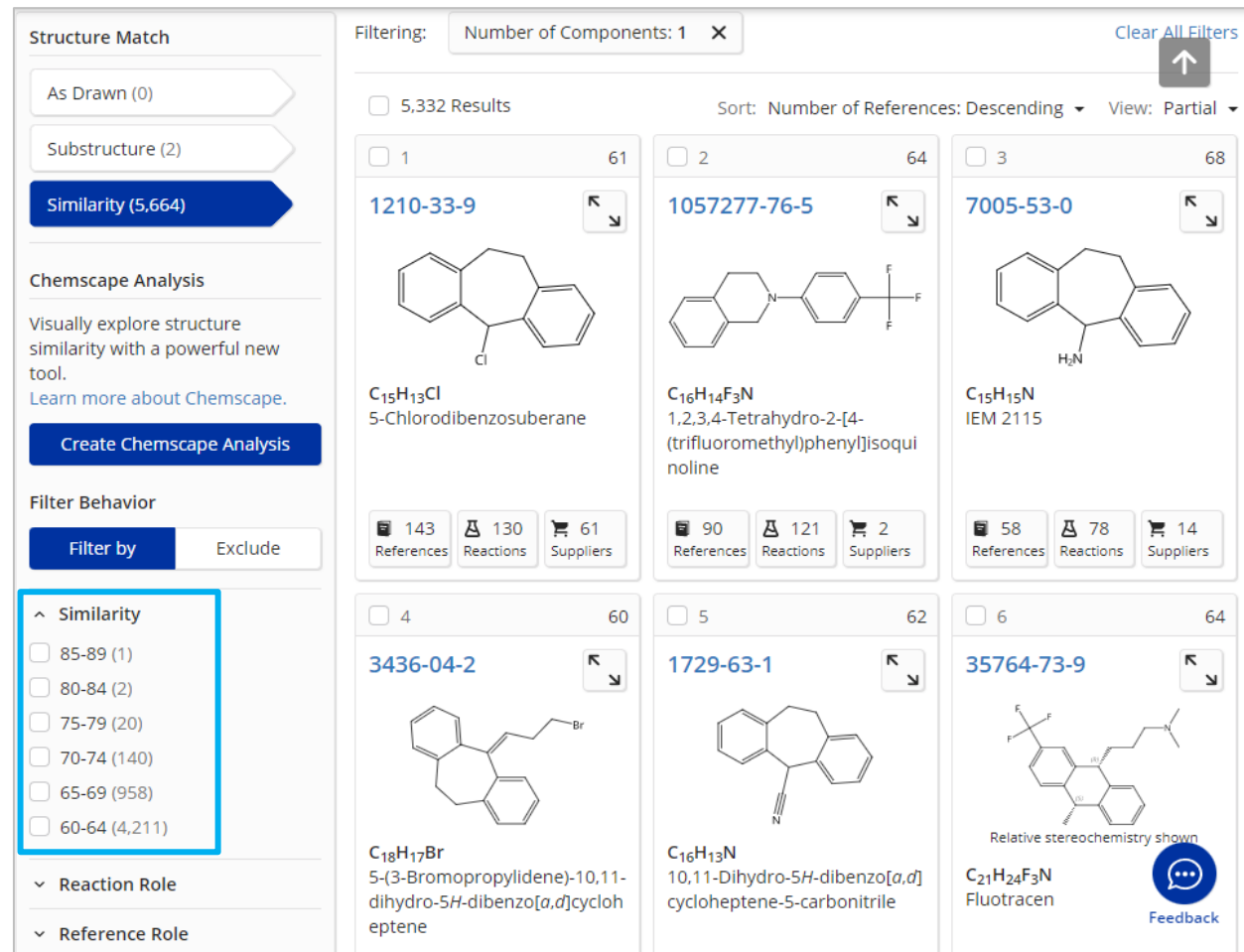
Sort: Number of R

146364-17-2

$C_{17}H_{14}F_3N$
10,5-(Iminomethano)-5H-dibenzo[a,d]cycloheptene, 10,11-dihydro-3-(trifluoromethyl)-

146364-18-3

$C_{18}H_{16}F_3N$
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)

Chemscrape Analysis

Visually explore structure similarity with a powerful new tool.

Learn more about Chemscrape.

Create Chemscrape 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 X

Clear All Filters

5,332 Results

Sort: Number of References: Descending View: Partial

1 61

1210-33-9

$C_{15}H_{13}Cl$
5-Chlorodibenzosuberene

143 References 130 Reactions 61 Suppliers

2 64

1057277-76-5

$C_{16}H_{14}F_3N$
1,2,3,4-Tetrahydro-2-[4-(trifluoromethyl)phenyl]isoquinoline

90 References 121 Reactions 2 Suppliers

3 68

7005-53-0

$C_{15}H_{15}N$
IEM 2115

58 References 78 Reactions 14 Suppliers

4 60

3436-04-2

$C_{18}H_{17}Br$
5-(3-Bromopropylidene)-10,11-dihydro-5H-dibenzo[a,d]cycloheptene

5 62

1729-63-1

$C_{16}H_{13}N$
10,11-Dihydro-5H-dibenzo[a,d]cycloheptene-5-carbonitrile

6 64

35764-73-9

$C_{21}H_{24}F_3N$
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
获得四件专利文献

- 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

Patent claim 11


Full Text

2.6 CAS SciFinderⁿ中的序列检索



- BLAST
- CDR
- Motif



CAS Sequences Search™ — Blast检索



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

 **Search CAS Sequences** 

Enter a protein or nucleotide string, or upload a .txt or .fasta file. [Learn more about CAS Sequences.](#)

BLAST | CDR | Motif Clear Search


Enter a query or upload a file...

Upload Sequence (.fasta or .txt)

Sequence Type:
 Nucleotide Protein

Search Within:
 Nucleotides Proteins

Include NCBI Sequences

Advanced Sequence Search 

可选择是否包含NCBI中的序列

支持四种检索选择：
Protein-Protein
Protein-Nucleotides
Nucleotide-Nucleotides
Nucleotide-Proteins

高级检索——设置相关参数

Sequences

Enter a protein or nucleotide string, or upload a .txt or .fasta file. [Learn more about Sequence Search.](#)

BLAST CDR Motif Upload Sequence Clear Search

AACAACAACATATCAAATCCTACTGGTGGCACAACCTTGA

Sequence Type:
 Nucleotide Protein

Search Within:
 Nucleotides Proteins
 Include NCBI Sequences

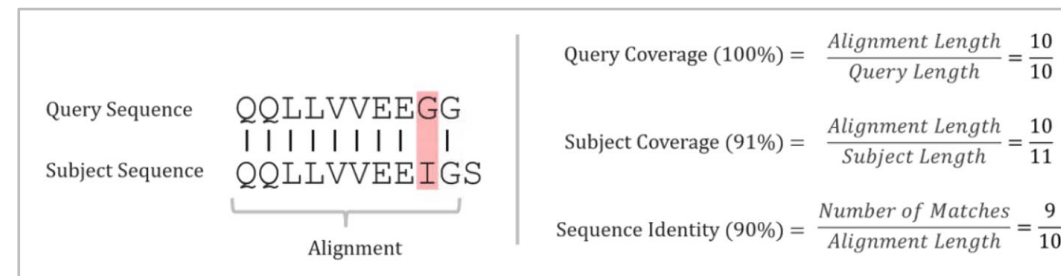
[Start Sequence Search](#)

Advanced Sequence Search Adjust Parameters for Short Sequences | Reset All

Alignment Identity % Match with Gaps? Yes No Gap Costs

Query Coverage % Word Size Reward for Match Penalty for Mismatch

BLAST Algorithm E-Value Exclude Low Complexity Regions Yes No



Recent Search History

[View All Search History](#)

February 13, 2023

Sequences 11:26 AM	Sequence Type: Nucleotide Search Within: Nucleotides NCBI Included: Yes BLAST Algorithm: BLASTn Alignment Identity: 80% Query Coverage: 90%	AACAACAACATATCAAATCCTACTGGTGGCACAACCTTGA	View Results Edit Options Searching...
-----------------------	--	--	--

Results will expire on Mar 15, 2023.

Recent Search History

[View All Search History](#)

February 13, 2023

Sequences 11:26 AM	Sequence Type: Nucleotide Search Within: Nucleotides NCBI Included: Yes BLAST Algorithm: BLASTn Alignment Identity: 80% Query Coverage: 90%	AACAACAACATATCAAATCCTACTGGTGGCACAACCTTGA	View Results Edit Search Complete
-----------------------	--	--	---

Results will expire on Mar 15, 2023.

BLAST检索结果

6 Alignment Identity: 100%

Query 1 39

Subject 1 1,060

Matches: 39
Mismatches: 0

View Less ▾

Alignment Subject References

CAS Registry Number: [785872-37-9](#)
Length: 1,060 nt

Sequence

```

1  CATTGGGTAC CTCGAGGCCG GCCGGGAGCT CGCACTCACT CACTCACAAG TCACACAGCC ACACTTGAAC CGTGCCCGC
81  AGCGGAGGGA GCTTGACGGG GCCAACGCAC ACATAACACA AGTCGTCGT CGATGGCGCG GTGGGCTGCG GTGCTGGCGC
161 TGGCCGCGGC CACGGCCATC GCCGTGGCGT CCGTGGCGGG CGGCGACATG AACGCGGACA AGACGGAGTG CGCGGACCAG
241 CTGGTGGGCC TGGCGCCGTG CCTGCAGTAC GTGCAGGGG AGGCCCGCGC GCCCGCGCCC GACTGCTGCG GCGGCTTGGC
321 CCAAGTGCTG GGAAGAGCC CCAAGTGCTG GTGCGTGCTC GTC AAGGACA AGGACGACCC CAACCTGGGC ATCAAGATCA
  
```

Alignment Subject References

Nucleic acid molecules and other molecules associated with plants
Assignees: LA ROSA, THOMAS J.; ZHOU, YIHUA; KOVALIC, DAVID K.; CAO, YONGWEI; LIU, JINGDONG; CHEIKH, NORDINE; SHUKLA, HRIDAYABHIRANJAN; RUFF, THOMAS G.; HARDEMAN, KRISTINE J.; EDGERTON, MICHAEL D.; VARAGONA, MARGUERITE; WU, WEI; CONNER, TIMOTHY W.
US20120216318 A1 | Seq ID No: 16999

Nucleic acid molecules and other molecules associated with plants
Assignees: LA ROSA, THOMAS; ZHOU, YIHUA; KOVALIC, DAVID; CAO, YONGWEI; LIU, JINGDONG; CHEIKH, NORDINE; SHUKLA, HRIDAYABHIRANJAN; RUFF, THOMAS; HARDEMAN, KRISTINE; EDGERTON, MICHAEL; VARAGONA, MARGUERITE; WU, WEI; CONNER, TIMOTHY
US20040214272 A1 | Seq ID No: 16999

Nucleic acid molecules and other molecules associated with plants

Substance Detail

Reference (1) Reactions (0) Suppliers (0)

CAS Registry Number
785872-37-9

Image Not Available

Unspecified
DNA (Zea mays clone MRT4577_11549C.1 protein fragment-specifying cDNA) (9CI)

Nucleic Acid Sequence
Sequence Length: 1060
204 a, 336 c, 311 g, 209 t

Sequence Details

Sequence: DNA: linear

1	cattgggtac	ctcgaggccg	gccgggagct	cgcaactcact	cactcacaag
51	tcacacagcc	acacttgaac	cgctgccgc	agcggaggga	gcttgacagg
101	gccaacgcac	acataacaca	agctcgtcgt	cgatggcgcg	gtggcctgcg
151	gtgtggcgc	tggcccgccg	cacggccatc	gccgtggcgt	ccgtggcggg
201	cgccgacatg	aacgaggaca	agacggagtg	cgcgaccag	ctggtggccc
251	tggcccgctg	cctgcagtac	gtcagggggc	aggcccgcgc	gcccgcgcc
301	gactgctgcg	gcccctgctg	ccaggtgctg	gggaagagcc	ccaagtgcct
351	gtgctgtctc	gtcaaggaca	aggacgaccc	caactgggc	atcaagatca
401	acgccacct	cgcgctcgcg	ctcccaacg	cctcgggcgc	caccgcgcc
451	aacgtctccc	actgcgtca	gctcctgcat	attccccggg	gctccaaaga
501	cgccgcgtc	ttcagtcctg	gcagcagaaa	gggtccact	gccgtccag
551	ccaaggacaa	ctcgacggcg	acgaccgact	cccgcgcct	cgaggcgacc
601	accggacgcg	gcgtgtcctc	ctcggcggcg	accgccggtg	ctgcactcac



Other Name for 1999: PN: US20040214272

Patent Annotations

Source: Zea mays
Reference: US20040214272. SEQID 16999: claimed

Feature	Location	Description
misc_feature		Clone ID: MRT4577_1154C.1

Sequences Search™——Motif检索


 Search CAS Sequences 

Enter a protein or nucleotide string. [Learn more about CAS Sequences.](#)

BLAST CDR **Motif** Clear Search

[SG]x{4}GK[DT]

- X代表未指定氨基酸，可以是常见或不常见氨基酸
- 对于核苷酸序列：N代表未指定核苷酸

[Advanced Sequence Search](#) 

Motif中有可变部分，可借助符号来表示：

“[]”中括号：代表或者，表示出现在该位置的氨基酸或核苷酸是括号中的任意一个

“{}”大括号：代表氨基酸或核苷酸的重复次数。其中字段可用逗号开，{2,6}表示在大括号左边紧密相连的氨基酸可重复2-6次

Motif Search Details

Sequence Type: Protein
NCBI Included: Yes
Query Coverage: 90%
E-Value: 10

Bioscope Analysis

Visually explore sequence similarity with a new tool. [Learn more about Bioscope.](#)

[Create Bioscope Analysis](#)

Filter by

▼ E-Value

▼ Query Coverage %

▲ Subject Coverage %

0 to 100

▲ Alignment Identity %

0 to 100

▲ Sequence Length


8 to


Query Details [View More](#)

> Seq 1: 1 SXXXXGKD 8

248 Results Sort: Alignment Identity View: Expanded


1 Alignment Identity: 75%

Query ①  ⑧

Subject ①  ⑪④

Matches: 6
Mismatches: 2


[View Less](#)


Alignment Subject References 

Alignment Data
BLAST Score: 77
E-Value: 0.00104148

```
Q 1 SXXXXGKD 8
  |||||++|
S 94 SXXXXXKD 101
```

2 Alignment Identity: 75%

Query ①  ⑧

Subject ①  ⑥④③

Matches: 6
Mismatches: 2

Sequences Search™——CDR检索

CDR (complementarity—determining regions): 抗体或细胞中的互补决定区

Searching for...

- All
- Substances
- Reactions
- References
- Suppliers
- Sequences**
- Retrosynthesis

Sequences

Enter a protein string, or upload a .txt or .fasta file. [Learn more about Sequence Search.](#)

BLAST **CDR** Motif Upload Sequence Clear Search

CDR1	<input type="text" value="RASQSVSGSRFTYMH"/>	X
CDR2	<input type="text" value="YASILES"/>	X
CDR3	<input type="text" value="QHSWEIPPWT"/>	X

Include NCBI Sequences

Start Sequence Search

支持单个或多个CDR序列检索并用

CDR检索结果

Sequences search for your query

References

CDR Segments

Select a segment below to view individual or intersecting CDR results.

Apply

Reset Segments

Bioscape Analysis

Visually explore sequence similarity with a new tool. [Learn more about Bioscape.](#)

Create Bioscape Analysis

Filter by

E-Value

0 to 10⁶

Query Coverage %

0 to 100

Subject Coverage %

0 to 100

Query Details [View Less](#)

> CDR1
RASQSVSGSRFTYMH

> CDR2
YASILES

> CDR3
QHSWEIPPWT

21,934 Results Sort: Alignment Identity View: Expanded

Alignment Identity: 100%

Matches: 32
Mismatches: 0

[References](#)

Alignment Data
BLAST Score: 84
E-Value: 7.45568461509489

CDR1	1	RASQSVSGSR	FTYMH	15
S	24	RASQSVSGSR	FTYMH	38
CDR2	1	YASILES		7
S	54	YASILES		60
CDR3	1	QHSWEIPPWT		10
S	93	QHSWEIPPWT		102

获取披露该序列的文献

CDR Segments

Select a segment below to view individual or intersecting CDR results.

Apply

Reset Segments

CDR Segments:

- 匹配到一个或者多个CDR的subject序列的序列数量
- 可根据已知信息和需求查看1-3个CDR被包含的序列结果

Reset segments:

- 重新选择查看匹配的序列结果

物质检索小结

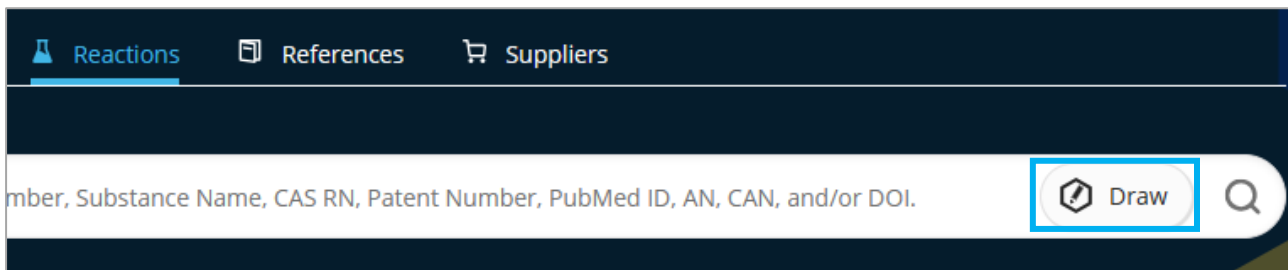
1. 物质检索方法：物质、文献标识符检索；分子式、物性参数、谱图数据检索；及结构式检索，充分利用结构绘制工具，合理扩大或限定结构检索范围
2. 正确理解As Drawn、Substructure、Similarity检索结果集的意义和范围
3. 充分利用物质筛选项准确定位目标物质：Reaction Role、Reference Role等
4. 利用CAS Markush检索尽可能全面的获得结构的公开信息

3.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

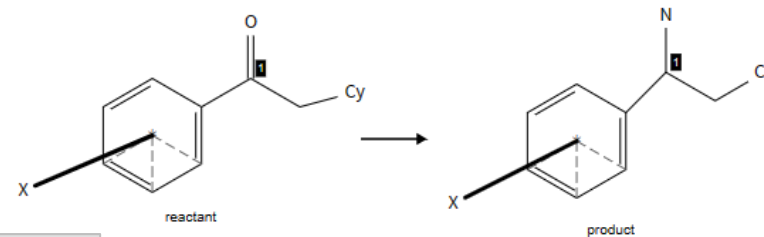
Suppliers (145)

Suppliers (77)

204656-20-2
Image Not Available

Suppliers (37)

3.2 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 × Clear All Filters

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

反应分组：
按反应式
按文献
按转化类型

反应排序：
相关度
公布时间
产率
步数

3.3 高效筛选目标反应

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

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

The screenshot displays a search interface for chemical reactions. On the left, there are two filter panels. The top panel, 'Structure Match', has 'Substructure (8,044)' selected. The bottom panel, 'Filter Behavior', has 'Filter by' selected. A third panel on the left contains various filters such as 'Commercial Availability', 'Reaction Notes', 'Source Reference', 'Document Type', 'Language', 'Publication Year', 'Organization', 'Publication Name', 'CA Section', 'Filter Content Report', and a download button. 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 two examples of ring closure reactions. The third result is '1,3-Dipolar Addition' with 37 related reactions. The interface includes 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

3.4 联用检索——结构与关键词

关注反应的机理研究或人名反应？

联用检索提高检索效率

Friedel-crafts acylation

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

+ Add Advanced Search Field

Edit Drawing Remove

Reactions search for "2011:601374"

References

Filter Behavior Filter by Exclude

Search Within Results Yield Reaction Scale Non-Participating Functional Groups Number of Steps Reaction Mapping Experimental Protocols Reaction Type Reagent Catalyst Solvent Commercial Availability

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

Scheme 1 (1 Reaction) Steps: 1 Yield: 82%

Scheme 2 (1 Reaction) Steps: 1 Yield: 78%

References search for "Friedel-crafts acylation" + drawn structure

Substances Reactions Citing Knowledge Graph

Structure Match As Drawn (1,100) Substructure (2,270)

Filter Behavior Filter by Exclude

Document Type Journal (996) Patent (68) Review (31) Conference (27)

1,100 Results Sort: Relevance View: P

1

ZrCl₄-Mediated Regio- and Chemoselective Friedel-Crafts Acylation of Indole

By: Guchhait, Sankar K.; Kashyap, Maneesh; Kamble, Harshad

Journal of Organic Chemistry (2011), 76(11), 4753-4758 | Language: English, Database: CPlus and MEDLINE

An efficient method for regio- and chemoselective Friedel-Crafts acylation of acyl chlorides in the presence of ZrCl₄ has been discovered. It minimizes/eliminates common competing reactions that occur due to high and multiatom-nucleophilicity of indole. In this method, a wide range of aroyl, heteroaroyl, alkenoyl, and alkanoyl chlorides undergo smooth acylation of indoles without NH protection and afford 3-acylindoles in good to high yields.

Full Text Substances (40) Reactions (21) Citing (99) Citation Map

2

Hexafluoro-2-propanol-Promoted Intermolecular Friedel-Crafts Acylation Reaction

3.5 如何获得逆合成路线?

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

1

2628280-40-8

Absolute stereochemistry shown

$C_{23}H_{32}F_3N_5O_4$
3-Azabicyclo[3.1.0]hexane-2-carboxamide, N-[(1S)-1-cyano-2-[(3S)-2-oxo-3-pyrroli...]

236 References 53 Reactions 39 Suppliers

CAS RN
2628280-40-8

CAS Name
3-Azabicyclo[3.1.0]hexane-2-carboxamide, N-[(1S)-1-cyano-2-[(3S)-2-oxo-3-pyrroli...

Substance Detail

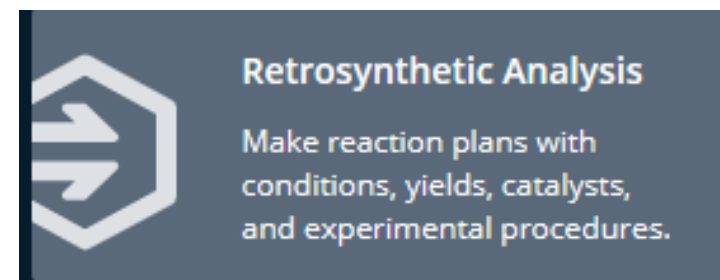
- Reactions (53)
- Synthesize (52)
- Start Retrosynthetic Analysis**
- References (236)
- Suppliers (39)

Absolute stereochemistry shown

Edit Structure Reset + Download

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



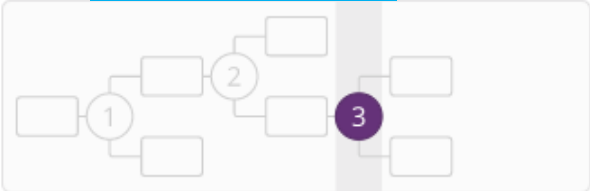
(2) 已知/未知化合物: 点击Retrosynthesis检索项, 打开绘图板, 绘制目标化合物, 获得实验路线

预设参数

Retrosynthesis Plan Options for drawn structure

Select Synthetic Depth **反应深度** [Learn more.](#)

1
 2
 3
 4



Break and Protect Bonds

Break Bond Protect Bond [Clear All Bond Selections](#)

断裂键或保护键

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

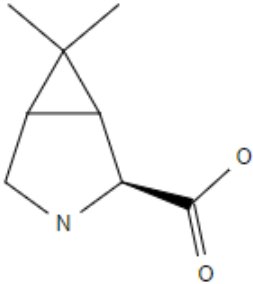
Common **反应规则常见性**
 Uncommon (includes Common Rules)
 Rare (includes Common and Uncommon Rules)

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](#)



调节参数

Retrosynthesis Plan for drawn structure Powered by ChemPlanner®

Key Experimental Steps Predicted Steps [Edit Plan Options](#)

Plan Information

Estimated Yield: 51%
Overall Price: \$29.90
(USD per 100 grams)

Scoring Profiles

Complexity Reduction

Convergence

Evidence

Cost

Yield

Atom Efficiency

路线概览

调节参数

Scoring Profiles:

- 降低每步原料结构的复杂性
- 逆合成路线中前体的数量
- 支持预测路线的文献数量多少
- 预测路线大概成本
- 每步的产率
- 每步的原子转化效率

Off Low Medium High



逆合成路线详情

Retrosynthesis Plan for drawn structure Powered by ChemPlanner®

Key Experimental Steps Predicted Steps [Edit Plan Options](#)

已知反应

预测型反应

View Excluded Options

Step	Evidence
$A \Rightarrow B + C$ Average Yield: 69% Evidence (4,925) Alternative Steps (91)	1.1 Reagents: Triethylamine Hydrogen sulfide Solvents: Dichloromethane View All
$B \Rightarrow D + E$ Average Yield: 65% Evidence (15,146) Alternative Steps (20)	1.1 Reagents: Triethylamine Solvents: Dichloromethane; 24 h, rt

View all alternatives (20)
View evidence (15,146)
Exclude this step

Reactions from Retrosynthesis Plan Evidence

References

Filter Behavior Filter by Exclude

Search Within Results

Yield

- 90-100% (1,257)
- 80-89% (1,436)
- 70-79% (1,521)
- 50-69% (2,138)
- 30-49% (1,296)

View All

Reaction Scale

- Milligram (1,578)
- Gram (391)
- Kilogram (5)
- No Scale Provided (13K)

Non-Participating Functional Groups

- Amide (6,565)

15,146 Results Group: By Scheme Sort: Relevance View: Collapsed

Scheme 1 (1 Reaction) Steps: 1 Yield: 88%

CC(=O)O + CC(=O)N1CCCN1 → CC(=O)N1CCCN1

Suppliers (18) Suppliers (92) Suppliers (9)

Expand Scheme

Scheme 2 (1 Reaction) Steps: 1

CC(=O)Cl + CC(=O)N1CCCN1 → CC(=O)N1CCCN1

Suppliers (136) Suppliers (66) Suppliers (51)

Expand Scheme

- 可查看每步反应的文献支持与详细条件

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路线优化，考虑替换路线？

The screenshot displays a chemical synthesis software interface. On the left, a reaction network is shown with nodes B, D, H, and I. Node B is highlighted with a blue box, and a context menu is open over it, showing options: "View all alternatives (20)", "View evidence (15,146)", and "Exclude this step". A blue arrow points from the "View all alternatives (20)" option to a detailed view window on the right.

The detailed view window, titled "B ⇒ D + E Alternative Steps (20)", shows a list of alternative steps. The first step is selected and highlighted with a blue box. It shows the reaction of B to D and E, with a predicted step icon, a "View Evidence (15,146)" link, and an "Average Yield: 65%" label. The second step is also highlighted with a blue box, showing a different reaction scheme, a "View Evidence (11,911)" link, and an "Average Yield: 74%" label. The third step is partially visible, showing a reaction scheme and a "View Evidence" link.

On the right side of the main interface, a table lists evidence for various steps:

Step	Evidence
A ⇒ B + C	1.1 Reagents: Triethylamine Hydrogen sulfide Solvents: Dichloromethane View All ▾ Average Yield: 69% Evidence (4,925) Alternative Steps (91)
B ⇒ D + E	1.1 Reagents: Triethylamine Solvents: Dichloromethane; 24 h, rt Average Yield: 65% Evidence (15,146) Alternative Steps (20)
C ⇒ E + G	1.1 Reagents: Ammonium chloride Average Yield: 65% Evidence (15,146) Alternative Steps (20)

点击Alternative Steps查看并选择替换路线，
得到自定义的合成路线

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

4. 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？

4.1 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

4.2 CAS分析实验方法详情

- 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

Analysis of Vanadium in Stainless steel by Electrochemical extraction

CAS MN: 1-119-CAS-286328

Method Category: Element Detection

Technique: Electrothermal atomic absorption spectroscopy; Decomposition; Electrochemical extraction

Materials	Role	Image	CAS RN
Vanadium	analyte	View Structure	7440-62-2
Stainless steel	matrix		12597-68-1
Al ₂ O ₃ cutting wheel	material		
SiC grinding paper	material		
0.05 μm pore size polycarbonate filter	material		
Standard calomel reference electrode	material		
Platinum ring counter electrode	material		
Hollow cathode lamps	material		
Electrodeless discharge lamp	material		
THGA graphite tubes	material		
Nitric acid	reagent	View Structure	7697-37-2
Hydrofluoric acid	reagent	View Structure	7664-39-3
Acetylacetone	reagent	View Structure	123-54-6
Chromium	reagent	View Structure	7440-47-3
Methanol	reagent	View Structure	67-56-1
Tetramethylammonium chloride	reagent	View Structure	75-57-0

实验原料

Source

Determination of alloying and impurity elements from matrix and inclusions from a process sample of a double stabilized stainless steel

Sipola, Teija; Alatarvas, Tuomas; Fabritius, Timo; Peramaki, Paavo

ISIJ International (2016), 56 (8), 1445 - 1451. Iron and Steel Institute of Japan

CODEN: IINTEY | ISSN: 09151559 | DOI: 10.2355/isijinternational.isijint-2016-071

文献来源

[Full Text](#)

[View in CAS SciFinder](#)

[Abstract](#)

Equipment Used

Cutting machine, Secotom-10, Struers

Ultrasonic cleaning unit, P 30 H, Elmasonic

Grinding machine, Labopol-6, Struers

Potentiostat, SP-150, BioLogic

Vacuum pump, BUSCHI

Graphite furnace atomic absorption spectrometer, AAnalyst 600, PerkinElmer

Autosampler, AS-800, PerkinElmer

Conditions

Instrument

internal gas flow rate: 250 mL/min (non-atomization), 0 mL/min (atomization); current: 15 mA; wavelength: 318.4 nm; slit width: 0.7 nm; injection volume: 10 μL

分析仪器

分析条件

Instructions

Preparation of stainless steel process samples

1. Cut stainless steel pieces from a corner piece of different slabs using a Struers Secotom-10 cutting machine with an Al₂O₃ cutting wheel.
2. Grind and polish the steel samples using a Struers Labopol-6 grinding machine with SiC grinding paper to a size of approximately 15 x 10 x 5 mm.
3. Clean the sample from grinding paper traces using an Elmasonic P 30 H ultrasonic cleaning unit (frequency 37 kHz, room temperature).
4. Clean all glassware in an acid bath, rinse with ultrapure water and methanol sequentially.

Electrolytic extraction of stainless steel using 10% acetylacetone

1. Perform electrolytic extraction on a BioLogic SP-150 potentiostat.
2. Use 10% acetylacetone (10 v/v% acetylacetone, 1 w/v% tetramethylammonium chloride and methanol) as the electrolyte.
3. Use the sample as the working electrode and set the potential to 0.150 V vs. the standard calomel electrode (SCE).
4. Suspend the sample in the electrolyte in a platinum basket and use a platinum ring as a counter electrode.
5. Filter the electrolyte through a 0.05 μm pore size polycarbonate filter with the help of a BUSCHI vacuum pump.
6. Expose the sample to ultrasound in methanol and filter the methanol with the electrolyte.

Decomposition of inclusions

1. Dry the polycarbonate filter containing the extracted inclusions overnight in a desiccator.
2. Place the dry filter in a PTFE container with 5 mL concentrated nitric acid and 2 mL HF and close gently.
3. Perform decomposition for 30 minutes at 120 °C (393.15 K).
4. Cool the containers to room temperature, remove the filter and dilute to the volume with water.
5. Prepare a blank sample similarly by filtering a fresh electrolyte through a polycarbonate filter.

Quantification of inclusions using graphite furnace atomic absorption spectrometry (GFAAS) with Cr as a matrix modifier

1. Perform GFAAS on a PerkinElmer AAnalyst 600 graphite furnace atomic absorption spectrometer equipped with an AS-800 autosampler and PerkinElmer THGA graphite tubes (standard platform B0504033).
2. Use a hollow cathode lamp (HCL) as the radiation source.
3. Use the following furnace program: ramp for 10 s to 110 °C, hold for 30 s; ramp for 10 s to 140 °C, hold for 30 s; ramp for 10 s to 1300 °C, hold for 20 s; perform atomization at 2400 °C for 6 s; ramp for 1 s to 2500 °C and hold for 5 s.
4. Set the instrument parameters as follows: internal gas flow rate: 250 mL/min (non-atomization), 0 mL/min (atomization); current: 15 mA; wavelength: 318.4 nm; slit width: 0.7 nm.
5. Add 0.05 μg Cr as a matrix modifier.
6. Inject 10 μL of the sample and perform measurements.

Validation

Linearity Range 0-400 μg/L

Concentration < 1 μg

操作步骤

数据有效性

关注文献关联的分析方法?

方法 (1): 在CAS SciFinder[®]的文献结果集页面, 点击CAS solutions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实验方法

References search for "steel and impurity"

Substances Reactions Citing Knowledge Graph

Based on your query, we've returned the most relevant results. Would you like to load the entire result set? [Learn about result relevance.](#) [Load More Results](#)

Filtering: CAS Solutions: Analytical Methods [Clear All Filters](#)

23 Results Sort: Relevance View: Partial Abstract

1

Validation of an HPLC method for analysis of nifedipine residues on stainless-steel surfaces in the manufacture of pharmaceuticals
By: Milenovic, D. M.; Lazic, M. L.; Veljkovic, V. B.; Todorovic, Z. B. *Acta Chromatographica* (2008), 20(2), 183-194 | Language: English, Database: CPlus
[Analytical Methods](#)

A simple, sensitive, and convenient HPLC method has been developed, validated, and applied to anal. of stainless-steel surfaces of equipment used in drug manufacture Cotton swabs moistened with methanol residues of the drug from the surfaces; recoveries were 82.26, 86.88, and 88.95% for 25, 125, and 250 µg the results, as relative standard deviation (RSD), was <5%. The method was validated over the concentration Small quantities of residues of the drug and its main impurities were determined by HPLC...

View More

electrolyte and arsenic in 10% acetylacetonone electrolyte were in good agreement with industrial data. Titanium and aluminum were measured from the dissolved steel matrix but titanium was also detected in the inclusions. It was concluded that the anal. results for titanium and aluminum measured using an optical emission spectrometer is affected by the inclusions within the stainless steel.

Keywords: double stabilized stainless steel alloying impurity element inclusion

[Open Access](#) [Full Text](#)

[Expand All](#) | [Collapse All](#)

Document Type
Substance Role
Language
Publication
Availability

Substances (2) Reactions (0) Citing

CAS Solutions

- Analytical Methods (23)
- Formulus (9)

Title	CAS Method Number
Analysis of Aluminum in Stainless steel by Electrochemical extraction	1-119-CAS-285768
Analysis of Aluminum in Stainless steel by Electrochemical extraction	1-119-CAS-286264
Analysis of Vanadium in Stainless steel by Electrochemical extraction	1-119-CAS-286328
Analysis of Vanadium in Stainless steel by Electrochemical extraction	1-119-CAS-286333
Analysis of Arsenic in Stainless steel by Electrochemical extraction	1-119-CAS-286759
Analysis of Copper in Stainless steel by Electrochemical extraction	1-119-CAS-286842
Analysis of Arsenic in Stainless steel by Electrochemical extraction	1-119-CAS-287300

直接检索感兴趣的分析实验方法

方法(1): 登录<https://methods.cas.org>, 主题检索或分类浏览

Good Morning, Liu

Search for keywords, matrices or analyte.

Advanced Search
Search methods using criteria like keywords, analytes, matrices and more.

Explore Methods
Search methods using criteria like method categories and subcategories.

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、毒理学等

Explore Methods

Method Category

- Agricultural Applications / Bioassays
- Biomolecule Isolation
- Environmental Analysis
- Food Analysis
- Fuels / Geology / Biofuels
- Historical Analysis / Dating
- Miscellaneous
- Organic Compound Analysis**
- Organometallics / Inorganics
- Pharmacology / Toxicology
- Polymer Analysis
- Water Analysis

Method Subcategory

- Active Pharmaceutical
- Chiral Separation**
- Natural Product Isolation
- Organic Compound Analysis

Include Keywords

+ Add Another Keyword

Search Methods

如何选择合适的分析方法？

CAS Solutions Analytical Methods steel and sulfur

Results (13) Sort Relevance

Return to Home

^ Analyte

- Sulfur (13)
- Carbon (9)
- Manganese (4)
- Aluminum (3)
- Chromium (3)

View All

^ Matrix

- Steel (13)
- Reinforced concrete (1)

^ Method Category

- Element Detection (13)

^ Technique

- Laser induced breakdown spectroscopy (10)
- Liquid scintillation counting (3)
- Neutron activation analysis (3)
- Time-of-flight mass spectrometry (2)
- Atomic emission spectrometry (1)

View All

^ Year

Analysis of Carbon in **Steel** by Laser induced breakdown spectroscopy
CAS MN: 1-119-CAS-267238

View Details & Instructions Remove from Compare

Analyte	Sulfur; Carbon
Matrix	Steel
Other Materials	Material: Continuum Surelite laser
Method Category	Element Detection
Technique	Laser induced breakdown spectroscopy
Equipment Used	Laser-induced breakdown spectrometer; Laser pulse generation system (two synchronized lasers); optical system; Ablation chamber; Spectrometer; CCD camera; Gas environment controls
Source	Double-pulse laser induced breakdown spectroscopy with ambient gas in the vacuum ultraviolet: Optimization of parameters for detection of carbon and sulfur in steel Jiang, X.; Hayden, P.; Costello, J. T.; Kennedy, E. T. Spectrochimica Acta, Part B: Atomic Spectroscopy (2014), 101, 106-113. Elsevier B.V.

Full Text View in CAS SciFinder

Abstract

Analysis of Carbon in **Steel** by Laser induced breakdown spectroscopy

关注特定的：

- ✓ 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方法?

Compare Methods

	1	2
Title	Analysis of Carbon in Steel by Laser induced breakdown spectroscopy	Analysis of Silver in Steel by Glow discharge mass spectrometry
CAS Method Number	1-119-CAS-267238	1-119-CAS-101987
Method Category	Element Detection	Element Detection
Technique	Laser induced breakdown spectroscopy	Time-of-flight mass spectrometry; Glow discharge mass spectrometry
Analyte	Sulfur ; Carbon	Titanium; Chromium; Antimony; Magnesium; Lead; Silicon; Cobalt; Sulfur ; Niobium; Tin; Nickel; Manganese; Vanadium; Boron; Molybdenum; Phosphorus; Silver; Tungsten; Copper; View All
Matrix	Steel	Steel
Other Materials	Continuum Surelite laser	Grimm-type chamber (with a 4 mm diameter anode and a 2.5 mm inner diameter flow tube)
Equipment Used	Laser-induced breakdown spectrometer; Laser pulse generation system (two synchronized lasers); optical system; Ablation chamber; Spectrometer, VM-521, Acton View All	Orthogonal time-of-flight mass spectrometer, Tofwerk, Thun, Switzerland; Dry pump, Triscroll 300, Varian Inc., Palo Alto, USA; Radio frequency glow discharge orthogonal time View All

Source	Double-pulse laser induced breakdown spectroscopy with ambient gas in the vacuum ultraviolet: Optimization of parameters for detection of carbon and sulfur in steel View All	A comparison of non-pulsed radiofrequency and pulsed radiofrequency glow discharge orthogonal time-of-flight mass spectrometry for analytical purposes View All
Method	Laser-induced breakdown spectroscopic analysis using nitrogen as ambient gas in double pulse mode View All	Glow discharge orthogonal time-of-flight mass spectrometry in pulsed mode 1. Collect the NIST 1262b certified reference steel . View All
Limit of Detection	2.9 ppm, Carbon, 1.5 ppm, Sulfur	0.3 µg/g, Boron, 0.2 µg/g, Magnesium, 0.3 µg/g, Aluminum, 1.9 µg/g, Silicon, 1.6 µg/g, Phosphorus, 1.0 µg/g, Sulfur , 2.3 µg/g, Titanium, 1.1 µg/g, Vanadium, 1.0 µg/g, Chromium, 5.5 View All
Precision		12% (RSD, reproducibility), Boron, 28% (RSD, reproducibility), Magnesium, 2% (RSD, reproducibility), Aluminum, 6% (RSD, reproducibility), Silicon, 5% (RSD, View All
Sensitivity		6 - 165 cps/(µg/g)

Method	<p>Laser-induced breakdown spectroscopic analysis using nitrogen as ambient gas in double pulse mode</p> <ol style="list-style-type: none"> 1. Perform the analysis using LIBS setup containing the laser pulse generation system (two synchronized lasers), the optical system (lenses, mirrors, polarizer and half-wave plate), an ablation chamber, spectrometer, detection system (CCD camera and computer) and finally the gas environment controls (needle valve, gauge, pressure meters). 2. Use the Q-switched Nd:YAG lasers to create the plasmas in double-pulse mode by Continuum Surelite (model III-10), operating at the fundamental wavelength of 1.06 µm with a pulse width of 6 ± 1 ns and maximum output energy of 800 mJ. 3. Operate the laser at a repetition rate of 10 Hz.. 4. Insert the optical combination of a half-wave plate and a polarizer into the Surelite laser beam to vary the pulse energy incident on the sample. 5. Focus the approximately 10-mm-diameter beams produced by Surelite laser onto the steel samples by plano-convex lenses of 125 mm and 150 mm focal 	<p>Glow discharge orthogonal time-of-flight mass spectrometry in pulsed mode</p> <ol style="list-style-type: none"> 1. Collect the NIST 1262b certified reference steel. 2. Determine the performance of the pulsed RFGD-TOFMS. 3. The radiofrequency glow discharge orthogonal time-of-flight mass spectrometer (RFGD-TOFMS) includes a RFGD bay unit (RF generator, matching box, RF connector, refrigerator disc and sample mounting system with a pneumatic piston to press the sample against the source) (GD Profiler HR instrument (Horiba Jobin Yvon, Longjumeau, France)). 4. Use the GD source of a copper-based modified Grimm-type chamber with a 4 mm diameter anode and a 2.5 mm inner diameter flow tube (EMPA, Switzerland). 5. Extract the ions originating from the source at pressure of 800 Pa through a sampler of 500 µm diameter and a 1 mm diameter skimmer. 6. The following interface region includes electrostatic focusing and deflecting components and couples the
--------	---	--

4.3 研究课题在产品中的应用？ 配方/制剂的检索与设计

方法（1）：登录CAS Formulus主页 (<https://formulus.cas.org>) 输入检索式

The screenshot displays the CAS Formulus website interface. At the top, there are two navigation tabs: "Formulations" (highlighted with a yellow underline) and "Ingredients". To the right of these tabs is a search bar containing the text "原料、用途、物理形态、功能或文献识别符". Below the navigation tabs is a large white search input field with the placeholder text "Search by Formulations by Ingredients, Purpose, Form, Functions, etc." and a magnifying glass icon on the right. Below the search field are two main navigation buttons: "Formulation Designer" (with a mortar and pestle icon) and "Advanced Search" (with a magnifying glass icon). The "Formulation Designer" button includes the text "Design custom formulation templates based on selections and ingredients". The "Advanced Search" button includes the text "Search Formulations using criteria like ingredients, targets, and more." To the right of the "Advanced Search" button is a blue button with the text "高级检索". At the bottom of the interface, there is a blue button with the text "配方、制剂设计".

配方、制剂设计

- 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/制剂结果集

- 利用聚类项精简结果：
行业、配方/制剂用途、物理形式、物质状态、递送方式、涵盖信息、文献类型、发表机构、发表年份
- 可查看制剂或配方成分，功能及用量
- 可查看原料详情
- 支持对比选中的制剂或配方
- 支持查看或下载专利全文
- 可查看制剂或配方详情

Formulations search for "orthopedic and implant"

Get Additional References Compare (0/3)

1,064 Results Sort: Relevance

Filter by

- Industry
 - Cosmetics & Personal Care
 - Pharmaceutical
 - Unclassified
- Purpose
 - Drug delivery systems (296)
 - Antitumor agents (107)
 - Pharmaceutical formulations (81)
 - Ophthalmic agents (73)
 - Antipsychotics (65)
- Physical Form
 - Pharmaceutical implants (1,064)
 - Tablets (315)
 - Capsules (226)
 - Powders (207)
 - Suspensions (154)
- State of Matter
- Delivery Route
 - Ophthalmic drug delivery systems (177)
 - Subcutaneous drug delivery systems (138)
 - Intramuscular injections (81)
 - Pharmaceutical injections (74)
 - Pharmaceutical implants (61)
- Information Included
 - Component Amount (1,393)
 - Process (1,064)
 - Experimental Activity (721)

View All

1

Implants: Antitumor Agents

Location: Article page 3, 6, 7, 8, 9
Purpose: Antitumor agents
Physical Form: **implant**

Add to Compare

Component	Function	Amount Reported
Group: TI-TNTs wire implants	implant	-
Ti wires	additives	-
Acetone	Solvents	-
Ethanol	Solvents	-
Perchloric acid	additives	1
Additional group components reported		
Trail aqueous solution	-	2 mg/mL

[View Formulation Detail](#)

2

Composition for Promoting Bone Formation

Location: Claim 23, 24, 25, 26, 27, 28, 29, 30, 31, 32, 33, 34, 35, 36, 37, 38, 39, 40, 41
Purpose: promoting bone formation
Target: Amphibia, Ape, Aves, Bos taurus, Canis familiaris, Capra, Cavia porcellus, Equus caballus, Felis catus, Fish, Gerbil, Hamster, Homo sapiens, Monkey, Mus musculus, Oryctolagus cuniculus, Ovis aries, Rattus, Reptilia, Swine
Delivery Route: Intraosseous prosthetic implants, intramedullary application
Physical Form: **pharmaceutical implants**

Add to Compare

Component	Function	Amount Reported
Group: surgical implant	-	-
Dental implants	-	-

JOURNAL

Titanium wire implants with nanotube arrays: A study model for localized cancer treatment
Biomaterials
Language: English

[Full Text](#) [View in CAS SciFinder®](#)

PATENT

Use of pro-inflammatory compounds for promoting bone formation
Assignee: Imperial Innovations Limited

- 一次最多可以比较三种不同制剂或配方的信息详情

配方/制剂的制备? 实验评估?

Implants: Antitumor Agents

Download Save

Purpose	Target	Delivery Route	Physical Form	Source
Antitumor agents	-	-	implant	View

Formulation Ingredients Expand All Groups | Collapse All Groups

Component	Function	Amount Reported	Optionality
Group: Ti-TNTs wire implants	implant	-	Mandatory
Ti wires	additives	-	Mandatory
Acetone	Solvents	-	Mandatory
Ethanol	Solvents	-	Mandatory
Perchloric acid	additives	1	Mandatory
butanol	Solvents	6	Mandatory
ethylene glycol electrolyte	solid support material	9	Mandatory
Water	Solvents	-	Mandatory
Trail aqueous solution	-	2 mg/mL	Mandatory

More Formulations like this... NEW

Ha-NP with HASE: Antitumor Agents
Purpose: Antitumor agents
Target: -
Delivery Route: -
Physical Form: Particles

CIPRODEX: Antibacterial
Purpose: Antibacterial agents
Target: Haemophilus influenzae, Hom...
Delivery Route: AURICULAR (otic)
Physical Form: Liquids, Suspensions

CIPRODEX Ciprofloxacin and Dexamethasone Suspension/Drops: Antibacterial Agents or...
Purpose: Antibacterial agents, corticos...
Target: Haemophilus influenzae, Hom...
Delivery Route: AURICULAR (optic).
Physical Form: Liquids, Suspensions

Ha-NP-Loaded Microneedle Patch: Antitumor Agents
Purpose: Antitumor agents
Target: Neoplasm
Delivery Route: skin absorption
Physical Form: Pharmaceutical patches

Process

stage 1: Ti-TNTs wire implants were loaded overnight with 2 mg/mL Trail aqueous solution for in-vitro, ex-vivo and in-vivo studies. prior to loading, implants were cleaned with ethanol, dried under sterile conditions and placed in a 30 mL drops of Trail solutions placed on a parafilm strip. after overnight drug loading, implants were dabbed with a soft tissue and dried and placed in PBS solution to monitor drug release profile at 37 °C, over a range of selected time points.

- 制剂或配方原料
- 相似的制剂或配方
- 制备工艺
- 制剂或配方实验评估
- 专利来源

Experimental Activity

Descriptor	Notes	Details
Ex-vivo study	-	no caspase-3 activity was observed for PBS-TNTs samples
cell death	-	highest cell death was observed in Trail-TNTs
drug release	-	45 %
in-vitro cytotoxicity	-	luciferase activity confirmed 100% cell death in Trail-TNTs
loading amount	-	12.63 µg

Source Journal

Titanium wire implants with nanotube arrays: A study model for localized cancer treatment

Biomaterials
Language: English
Location: Article page 3, 6, 7, 8, 9

Full Text View in CAS SciFinder®

高级检索

[← Return to Home](#)

Advanced Formulations Search

Searches the following content fields: Ingredient, Function, Purpose, Physical Form, Delivery Route, and Target.

At least two search terms are required.

Search For Operator Enter one term

Function Optional Anticorrosion

Ex: binder, surfactant, carrier

Search For Operator Enter one term

All Fields Optional coating

General search of all fields

Add Another Term

 Search

- All Fields
- All Fields
- Form
- Function
- Ingredient
- Purpose
- Route
- Target

- Optional
- Required
- Optional
- Excluded

Clear All

检索原料



Ingredients search for "propylene glycol"

2 Selected 3 Results

Filter by

- Industry
 - Agrochemical
 - Cleaning & Surfactant Products
 - Cosmetics & Personal Care
 - Food & Related
 - Inks, Paints, & Coatings
 - Pharmaceutical
- Regulatory Information
 - REACH (5)
 - Cosing: Cosmetic Ingredient Inventory (3)
 - EPA Pesticide Inactive Ingredients (3)
 - FDA Inactive Ingredients Database (3)
 - ANMAT (1)
- Experimental Properties
 - Boiling Point (3)

View All

View All

View All

View Details

CAS RN: 57-55-6

CC(O)CO

C₃H₈O₂

(±)-Propylene glycol
[Propylene glycol](#)

Key Physical Properties	Value	Condition
Molecular Weight	76.09	-
Melting Point (Experimental)	-59 °C	-
Boiling Point (Experimental)	188.2 °C	-
Density (Experimental)	1.036 g/cm ³	Temp: 25 °C

Commonly Used As: Solvents; Carriers; Plasticizers; Humectants; Antifreeze...

Similar Ingredients with Regulatory Information

- 27194-74-7 Propylene glycol monolaurate
- 29387-86-8 Propylene glycol butyl ether
- 30136-13-1 Propylene glycol monopropyl ether

View 14 More

Commonly Formulated With | Regulatory Information | Experimental Properties

Formulations Suppliers Add to Designer

- 制剂或配方中，与该原料同时使用的其它配伍成分
- 管控信息及清单
- 实验属性

- 使用该原料的制剂或配方
- 原料供应商信息
- 可将原料添加至设计工具
Formulation Designer

设计配方/制剂

👉 Formulation Designer ?

[Clear All Selections](#)

Industry	Purpose	Physical Form	Add up to 5 Ingredients
Pharmaceutical	Cosmetics and Personal care products	Emulsions	<input type="text" value="Vitamin A"/> ×
Cosmetics & Personal Care	Skin conditioners	Cream preparations	<input type="text" value="Polyethylene glycol"/> ×
Agrochemical	Sunscreens	Cosmetic lotions	+ Add Another Ingredient
Cleaning & Surfactant Products	Hair dyes	Cosmetic packs	
Inks, Paints, & Coatings	Hair preparations	Gels	
Food & Related	Antiperspirants	Liquids	
	Cleaning compositions	Powders	
	Skin cleansers	Solutions	
	Skin-lightening cosmetics	Nanospheres	
	Oral hygiene products	Pastes	
	Skin care products	- View More Physical Forms -	
	- View More Purposes -		<input type="button" value="Create Template"/>

设计配方/制剂

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

Save



Your Template

Unit Size

mg

Go

Clear

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

Carriers	Ethylene glycol	Cosing: Cosmetic Ingredient Inventory; EPA Pesticide Inactive Ingredients; FDA Inactive Ingredients Database	Water; Polyethylene glycol	Approximate Range: 2 - 14%
	View More Alternatives			

Skin conditioners	Ethylene glycol	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%
	View More Alternatives			

- 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:

Glycerol

Allantoin

1,2-Octanediol

Tricaprin

Palm-oil glycerides,

monoglycerides,

diglycerides and

triglycerides,

hydrogenated

Glyceryl polyacrylate

N-(2-

Hydroxyethyl)acetamide

文献关联的配方/制剂

方法 (2) : 在CAS SciFinder[®]的文献结果集页面, 点击CAS solutions中的 Formulus 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 "encapsulat* and resistant starch"

Substances - Reactions - Citing - Knowledge Graph

857 Results Sort: Relevance - View: Partial Abstract -

Based on your query, we've returned the most relevant results. Would you like to load the entire result set?
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Filter Behavior
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- Language
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- Organ
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1
Resistant starch from high-amylose maize increases insulin sensitivity in overweight and obese men
By: Maki, Kevin C.; Pelkman, Christine L.; Finocchiaro, E. Terry; Kelley, Kathleen M.; Lawless, Andrea L.; Schild, Arianne L.; Ra
Journal of Nutrition (2012), 142(4), 717-723 | Language: English, Database: CAlplus and MEDLINE

This study evaluated the effects of 2 levels of intake of high-amylose maize type 2 **resistant starch** (HAM-RS2) on insulin s (S_i) in participants with waist circumference ≥89 (women) or ≥102 cm (men). Participants received 0 (control starch), 15, or 3 (double-blind) of HAM-RS2 in random order for 4-wk periods separated by 3-wk washouts. Minimal model S_i was assessed end of each period using the insulin-modified i.v. glucose tolerance test. The efficacy evaluable sample included 11 men and women (mean ± SEM) age 49.5 ± 1.6 y, with a BMI of 30.6 ± 0.5 kg/m² and waist circ...

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Full Text - Substances (9) Reactions (0) Citing (131) Citat

2
Conserved and variable responses of the gut microbiome to resistant starch type 2
By: Bendiks, Zachary A.; Knudsen, Knud E. B.; Keenan, Michael J.; Marco, Maria L.
Microbiome (United States) (2020), 77, 12-28 | Language: English, Database: CAlplus and MEDLINE

2), a dietary fiber comprised solely of glucose, has been extensively studied in clin. tri
ove metabolic and systemic health. Because the health modulatory effects of RS2 and
ough modification of the gut microbiome, those studies frequently include assessme
icrobial composition and function. In this review, we identify the conserved respo

Formulation Purpose

By Count Alphanumeric

4 Selected

- Food (7)
- Antidiabetic agents (6)
- Dietary supplements (5)
- Diet (3)
- Drug delivery systems (3)
- Antimicrobial agents (2)
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- Antihypertensives (1)
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- Beverages (1)

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- Analytical Methods (4)

文献关联的配方/制剂

- ∨ Concepts
- ∨ MEDLINE® Medical Subject Headings
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- ∧ Formulations

Resistant Starch Film-Coated Microparticles for an Oral Colon-Specific Polypeptide Delivery System and Its Release Behaviors

Substances (3) Reactions (0) Citing (42) Citation Map Save

JOURNAL

Source

Journal of Agricultural and Food Chemistry
Volume: 62
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Pages: 3599-3609
Journal: Evaluation Study; Article; Research Support, Non-U.S. Gov't
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China

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American Chemical Society

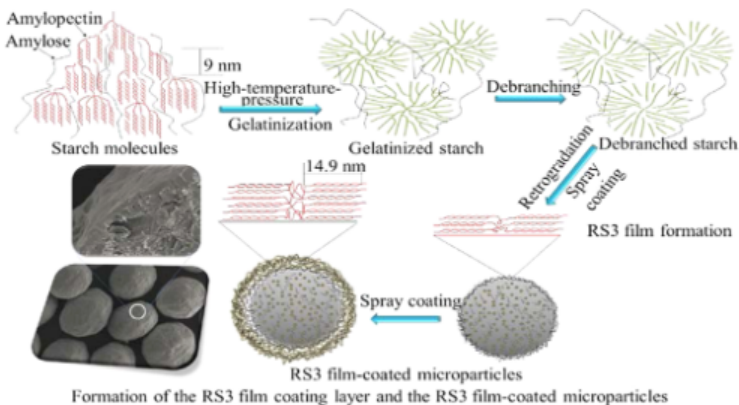
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By: Situ, Wenbei; Chen, Ling; Wang, Xueyu; Li, Xiaoxi

For the delivery of bioactive components to the colon, an oral colon-specific controlled release system coated with a resistant starch-based film through aqueous dispersion coating process was developed. Starch was modified by a high-temperature-pressure reaction, enzymic debranching, and retrogradation, resulting in a dramatic increase in the resistibility against enzymic digestion (meaning the formation of resistant starch, specifically RS3). This increase could be associated with an increase in the relative crystallinity, a greater amount of starch mol. aggregation structure, and the formation of a compact mass fractal structure, resulting from the treatment. The microparticles coated with this RS3 film showed an excellent controlled release property. In streptozotocin (STZ)-induced type II diabetic rats, the RS3 film-coated insulin-loaded microparticles exhibited the ability to steadily decrease the plasma glucose level initially and then maintain the plasma glucose level within the normal range for total 14-22 h with different insulin dosages after oral administration; no hypoglycemia or glycemic fluctuation was observed. Therefore, the potential of this new RS3 film-coated microparticle system has been demonstrated for the accurate delivery of bioactive polypeptides or protein to the colon.



Keywords: starch film coated microparticle colon polypeptide delivery insulin

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∨ Concepts

Resistant Starch (RS 3)Film-Coated Microparticles: Drug Delivery Systems--Controlled Release Drug Delivery Systems

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Location: SI Page 3 Article Page 2 Figure 15

Purpose: Drug delivery systems

Target: 5-aminosalicylic acid

Component	成分	Function	功能	Amount Reported	用量
∧ Group: bioactive component-loaded microparticle core		model active agent		-	
5-Aminosalicylic acid		-		20 %	
Cellulose		additives		Ratio: 3	
Starch		excipients		Ratio: 1	
∨ Group: RS3-based aqueous coating dispersion		coating materials		-	

Resistant Starch (RS 3)Film-Coated Microparticles: Drug Delivery Systems--Controlled Release Drug Delivery Systems

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Location: SI Page 3 Article Page 2 Figure 15

Purpose: Drug delivery systems

Target: 5-aminosalicylic acid

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- 科研信息的高效查阅
- 常见问题Q&A



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- Mac OS X (10.11, 10.12, 10.13): Safari 9.3及更高版本, Chrome 60及更高版本, Firefox 55及更高版本, Firefox 52 (ESR)
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- 分析方法检索及筛选

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