

CAS SciFinder Discovery Platform™ (Academic)

全面高效获取科技信息



刘子露

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美国化学文摘社(CAS)北京代表处

CAS

A Division of the  
American Chemical Society

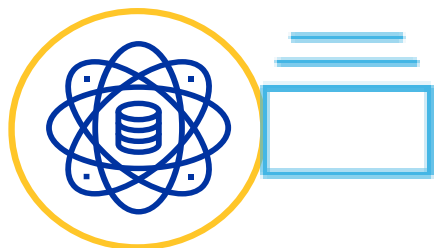


# 大纲

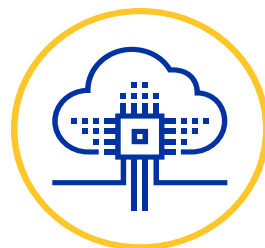
- CAS（美国化学文摘社）及CAS SciFinder Discovery Platform简介
- 新一代科研创新信息工具CAS SciFinder<sup>n</sup>
- 分析方法解决方案CAS Analytical Methods<sup>TM</sup>
- 配方/制剂解决方案CAS Formulus<sup>®</sup>

# 美国化学文摘社 (CAS) 隶属美国化学会(ACS)

- 拥有超过110年的经验；创立权威化学索引《化学文摘》（CA）
- 密切追踪、标引和提炼全球化学相关的文献（包括专利）
- 提供各种科学信息和相关技术产品与服务
- 协助创新和保护创新，助力于解决科研方面的难题与挑战



**UNPARALLELED**  
SCIENTIFIC CONTENT



**SPECIALIZED**  
TECHNOLOGY



**UNMATCHED**  
HUMAN EXPERTISE



# CAS数据覆盖学科

## 五大类80小类

### 一生物化学：

农化产品管控信息、生化遗传学、发酵、免疫化学、药理学

### 一有机化学各领域：

氨基酸、生物分子、碳水化合物、有机金属化合物、类固醇

### 一大分子化学各领域：

纤维素、木质素、造纸；涂料、墨水

染料、有机颜料；合成橡胶；纺织品、纤维

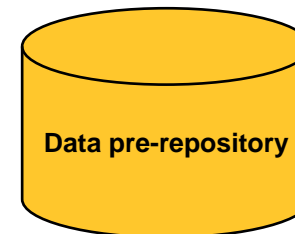
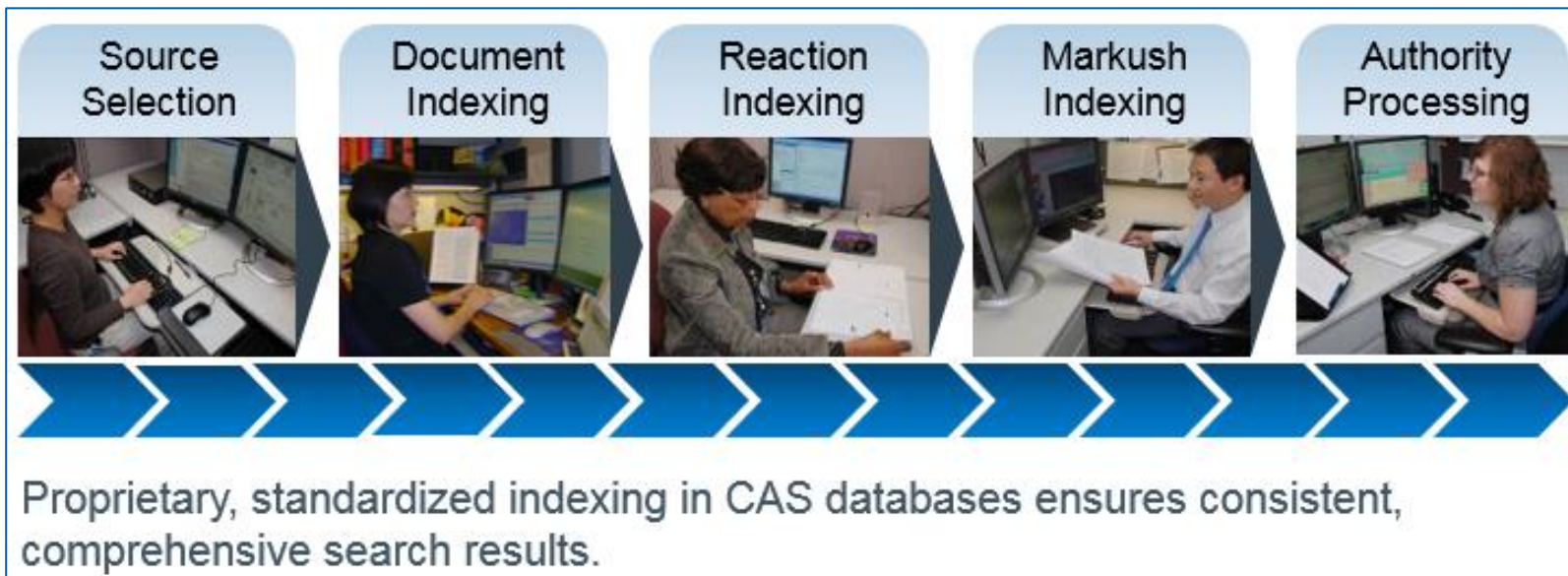
### 一应用化学各领域：

大气污染、陶瓷、精油、化妆品、化石燃料、黑色金属、合金

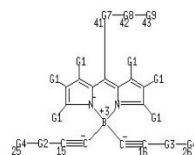
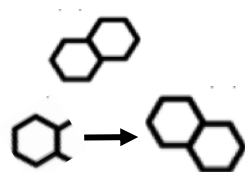
### 一物理、无机、分析化学各领域：

表面化学、催化剂、相平衡、核现象、电化学

# CAS科学家的智力标引



1990  
Smith, M.  
anthracene



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

CAS科学家利用人类智慧对公开内容进行揭示，使相关信息更容易被挖掘

# Data frame process at CAS

Expert scientists combined with a wide range of ML optimize connections

Published content

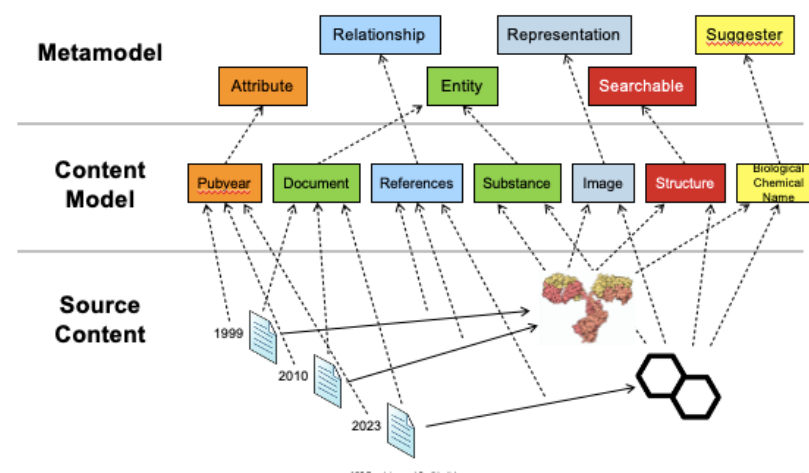
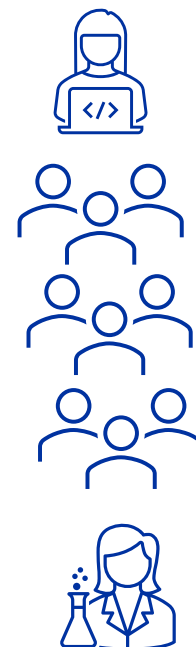
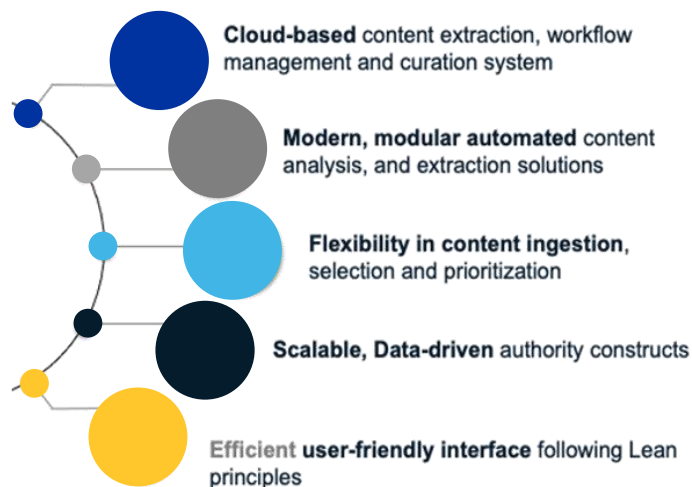
Curated, modeled data

Continually acquire scientific content

Classify and align to workflows

Human driven, supervised science value collection

Data modeling and data lake creation



# 经过CAS科学家的揭示，相关信息更易被挖掘

- 人工标引——精准揭示关键技术信息
- 科学家组成的编辑团队深刻理解客户的实际需求
- 审阅、筛选、摘要、标引以覆盖并揭示全球所有已公开的化学及相关信息
- CAS登记号——物质的黄金标准
- CAS Roles (CAS物质角色)——生物研究、性能用途、分析检测、合成制备
- CAS Index Terms (CAS技术词语标准)——揭示技术词语相互间的关联
- CA Sections (CAS学科分类, 80个类别)——精准定位具体研究领域

# CAS解决方案与服务



Discovery

## CAS SciFinder Discovery Platform™

Get discoveries to market faster and optimize margins by giving researchers the information they need



Intellectual Property

## STN IP Protection Suite™

Ensure that your intellectual property is protected and find opportunities to extend into new markets



Custom Solutions

## CAS Custom Services<sup>SM</sup>

Customized data, analytics and insights to maximize the value of information assets and fuel digitalization success



# CAS SciFinder Discovery Platform 平台解决方案

## CAS SciFinder<sup>n</sup> ——加速科学发现的业界领先的科学工具

业界最领先的相关性搜索引擎，提供和化学相关的各学科文献、物质、反应和生物序列等检索内容，检索智能、高效、简单。可用于基金申请的文献准备、为新课题制定实验计划、寻求学术合作者、进行逆合成分析以及更多其他的教学和科研活动。

## CAS Analytical Methods<sup>TM</sup> ——借助CAS科学家深度加工的科学方法，提升研究效率

分析方法解决方案涵盖来自期刊中的化学分析方法，提供检索和对比功能，可快速获得能直接在实验室操作的分析方法。可为法医学、食品科学、农学、制药、环境等学科的教学和实验提供帮助。

## CAS Formulus<sup>®</sup> ——助力开发安全、有效的产品

集成配方（制剂）数据与工作流程的解决方案，提供来自期刊、专利和产品说明中的配方详情。可检索制药、化妆品、食品、农化、油墨、涂料等众多领域中的配方，及其工艺、成分、目标成分的常见配伍成分、设计配方、和探索合规要求等。

# 大纲

- CAS（美国化学文摘社）及CAS SciFinder Discovery Platform简介
- 新一代科研创新信息工具CAS SciFinder<sup>n</sup>
- 分析方法解决方案CAS Analytical Methods<sup>TM</sup>
- 配方/制剂解决方案CAS Formulus<sup>®</sup>

# CAS SciFinder<sup>n</sup> ——加速科学发现的业界领先的科学工具

- 基于用户习惯、需求、检索策略和革新技术，采用新方法将CAS内容传递给研究人员
- 先进的平台不仅需要实现信息的获取，还要帮助用户发现最佳起点
- CAS的化学信息历史积累、系统知识和人工智力能够加速您的工作

用户需求的演进、内容的增长和广度的扩展推动  
新的技术解决方案的出现！

# CAS独特的内容合集




来源：

<https://www.cas.org/cas-data>

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

# CAS SciFinder<sup>n</sup> 登录网址: <https://SciFinder-n.cas.org>




Log In to SciFinder<sup>n</sup>

Username or Email Address

Next

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



Log In to SciFinder<sup>n</sup>

Welcome, Zilu Liu [Not You?](#)

Password

Log In

Keep me signed in

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

账号与CAS SciFinder相同

# CAS SciFinder<sup>®</sup>主界面

The screenshot displays the CAS SciFinder<sup>®</sup> main interface. On the left is a navigation sidebar with the CAS logo and a list of services including SCIFINDER DISCOVERY PLATFORM, CAS SciFinder<sup>®</sup>, CAS Analytical Methods, CAS Formulus, STN IP PROTECTION SUITE, STNext, CAS Scientific Patent Explorer, REGULATORY, CAS Chemical Compliance Index, ACCOUNT MANAGEMENT, and CAS Profile. The main content area features a top navigation bar with the SciFinder<sup>®</sup> logo, Alerts (13), Saved, and a user profile for Zilu Liu. Below this is a 'Searching for...' section with a list of search categories: All, Substances, Reactions, References (highlighted), Suppliers, Sequences, and Retrosynthesis. The 'References' section is active, showing a search box with 'Antitumor' and a search button. Below the search box are options for 'AND' and 'Author Name' with a placeholder 'Enter last name, first name middle name.' and an 'Add Advanced Search Field' button. A 'Launch CAS Lexicon' button is also present, with a tooltip explaining its function. A chemical structure drawing of a benzene ring with a fused five-membered ring containing a carbonyl group and a hydroxyl group is shown with 'Edit Drawing' and 'Remove' options. The 'Recent Search History' section shows a search from February 8, 2023, for 'CSF-1R inhibitor (371K Results)' at 10:25 AM, with 'Rerun Search' and 'Edit Search' buttons. Annotations in Chinese point to the search box, the chemical structure, and the recent search history.

灵活检索选项

文本与结构检索便捷联用

快速运行之前的检索项目

# 文献检索——主题词

The screenshot shows a search interface with a left sidebar and a main search area. The sidebar, titled 'Searching for...', contains buttons for 'All', 'Substances', 'Reactions', 'References' (highlighted in blue), 'Suppliers', 'Sequences', and 'Retrosynthesis'. The main search area is titled 'References' and includes a search bar with the text 'Seebeck'. Below the search bar is a dropdown menu with the following suggestions: 'Seebeck effect', 'Seebeck coefficient', 'Seebeck thermoelec. effect', 'Seebeck thermoelectric effect', 'Thermoelectric Seebeck effect', and 'Thermoelectric Seebeck coefficient'. To the right of the dropdown menu, there are three bullet points: '— 基于科学家创建的叙词表', '— 自动提示检索词', and '— 自动纠错功能'. The search bar also features a 'Draw' button and a search icon.

- 支持布尔逻辑运算符(and, or, not), 默认运算顺序or > and > not;
- ( ) 优先运算;
- “ ” 不允许词形变化, 但可出现单数或复数;
- 支持通配符\*或? (\*代表0或多个字符; ? 代表0或1个字符)

# 高级检索—高效实现多项自定义组合检索

## References

Search by Keyword, Substance Name, CAS RN, Patent Number, PubMed ID, AN, CAN, and/or DOI. [Learn More](#)

(PVDF or PEDOT) and "wearable device"



Draw



AND

Publication Name

ACS Applied



AND

OR

NOT

Authors

Publication Name

Organization

Title

Abstract/Keywords

Concept

Substances

Publication Year

Document Identifier

Patent Identifier

Publisher

ACS Applied Materials & Interfaces

ACS Applied Energy Materials

ACS Applied Nano Materials

ACS Applied Bio Materials

ACS Applied Polymer Materials

ACS Applied Electronic Materials

ACS Applied Engineering Materials



ACS Applied Optical Materials

- 可单独使用，或可联用以下检索方法：
- 关键词、物质名称、CAS RN<sup>®</sup>、文献号；
- 高级检索：刊物名、Concepts、物质等
- 结构检索



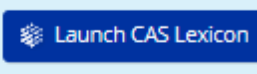
# CAS Lexicon—利用词库选词启发检索

**References**  
Search by Keyword, Substance Name, CAS RN, Patent Number, PubMed ID, AN, CAN, and/or DOI. [Learn More](#)

Enter a query...  Draw 

- Author Name Enter last name, first name middle name

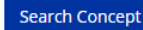
+ Add Advanced Search Field

 Launch CAS Lexicon CAS Lexicon enables you to browse the CAS substances to build a Reference query with

在CAS Lexicon词库层级中选择适合的主题词：

- Preferred Term
- Broader Terms
- Narrower Terms
- Related Terms

**Search CAS Lexicon**

Seebeck effect  Your Query: Seebeck effect. You may include up to 1,000 terms in a search. [Clear All](#)

**Preferred Term**

Seebeck effect  
This will search synonyms: Seebeck coefficient; Seebeck thermoelectric effect; Seebeck thermoelectric effect; Thermoelectric Seebeck coefficient; Thermoelectric Seebeck effect  
[View fewer synonyms](#)

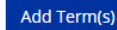

**Broader Terms (1)** [Deselect All](#)

Thermoelectricity

**Related Terms (3)** [Deselect All](#)

Joule effect  
 Peltier effect  
 Thermocouples

Seebeck effect   
Seebeck effect - Related Terms (3 Concepts)   
Thermoelectricity

Select a boolean operator [OR](#)  [Learn more about CAS Lexicon searching.](#) 

快速浏览CAS科学家标引的：

- 概念词 (Concepts)
- 物质

# 文献检索—主题词+结构联合检索

The screenshot displays the CAS SciFinder search interface. At the top, the search bar contains the query "bacterium and (mutton or beef)". A chemical structure is overlaid on the search results, with a pop-up menu offering "Edit Drawing" and "Remove" options. The left sidebar includes filters for "Structure Match" (As Drawn (3), Substructure (3)), "Filter Behavior" (Filter by, Exclude), and "Document Type", "Substance Role", and "Language". The main results area shows 3 results, with the first result titled "Bacterial endotoxin-induced gene expression in the choroid plexus and paraventricular and supraoptic hypothalamic nuclei of the sheep". The abstract text describes the study's findings on endotoxin-induced gene expression in sheep. At the bottom, there are buttons for "Full Text", "Substances (4)", "Reactions (0)", "Citing (27)", and "Citation Map".

主题词+结构联合检索，大大提高检索的效率

# 直观的结果页面，丰富的聚类分析

- 聚类筛选项一目了然
- 高效定位所需信息
- 无需逐步二次检索和限定

文献类型  
文献语言  
出版年份  
作者  
机构名  
刊物名  
Concept  
CA Section  
二次检索  
.....

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  
Substance Role  
Language  
Publication Year  
Available at My Institution  
Author  
Organization  
Publication Name  
Concept  
CA Section  
CAS Solutions  
Database  
Search Within Results

Filter Content Report  
Download filter data from this result set. [Download](#)

687 Results  
Sort: Relevance View: Partial Abstract

1  
**High-Performance Flexible All-Solid-State Supercapacitor from Layered PEDOT/PSS Films**  
By: Liu, Yuqing; Weng, Bo; Razal, Joselito M.; Xu, Qun; Zhao, Chen; Hou, Yuyang; Seyedin, 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<sup>-2</sup> was achieved at a scan rate of 10 mV s<sup>-1</sup> 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  
Stretchable electronic circuits are critical for soft robots, **wearable technologies** and biomedical applications. Development of sophisticated stretchable circuits requires new materials with stable conductivity over large strains, and low-resistance interfaces between soft and conventional (rigid) electronic components. To address this need, we introduce biphasic Ga-In, a printable conductor with high conductivity (2.06 x 10<sup>6</sup> S m<sup>-1</sup>), extreme stretchability (>1,000%), negligible resistance change when strained, cyclic stability (consistent performance over 1,500 cycles) and a reliable interf...  
[View More](#)

Full Text Substances (17) Reactions (0) Citing (91) Citation Map

3  
**A self-powered skin-patch electrochromic biosensor**  
By: Santiago-Malagon, Sara; Rio-Colin, Diego; Azizkhani, Haniyeh; Aller-Pellitero, Miguel; Guirado, Gonzalo; del Campo, F. Javier  
Biosensors & Bioelectronics (2021), 175, 112879 | Language: English, Database: CPlus and MEDLINE  
[Analytical Methods](#)  
One of the limitations of many skin-patch wearable sensors today is their dependence on silicon-based electronics, increasing their complexity and unit cost. Self-powered sensors in combination with electrochromic materials allow simplifying the construction of

- 排序:
- 更快锁定目标信息

# 文献结果集的处理、下载、保存及定题追踪

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

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: Concept: Hydrogels X Clear All Filters  
Excluding: Search Within Results: dop\* X

41 Results Sort: Relevance View: Partial Abstract

1

**Enhancing Strain-Sensing Properties of the Conductive Hydrogel by Introducing PVDF-TrFE**  
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 and MEDLINE

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

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Full Text

Substances (7) Reaction (1) Citing (1) Citation Map

支持结果集的:

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# 文献详情

**EGFR-Targeted Nanobody Functionalized Polymeric Micelles Loaded with mTHPC for Selective Photodynamic Therapy**

Substances (16) Reactions (11) Citing (28) Citation Map

**JOURNAL**  
Source  
Molecular Pharmaceutics  
Volume: 17  
Issue: 4  
Pages: 1276-1292  
Journal: Article; Research Support, Non-U.S. Gov't  
2020  
DOI: [10.1021/acs.molpharmaceut.9b01280](https://doi.org/10.1021/acs.molpharmaceut.9b01280)  
CODEN: MPOHBP  
E-ISSN: 1543-8392  
ISSN-L: 1543-8384

**Database Information**  
AN: 2020:437343  
CAN: 176:347527  
PubMed ID: 32142290  
Cplus and MEDLINE

**Company/Organization**  
Department of Pharmaceutics,  
Utrecht Institute for  
Pharmaceutical Sciences  
Utrecht University  
Utrecht 3584 CS  
Netherlands

**Publisher**  
American Chemical Society

**Language**  
English

By: Liu, Yanna; Scrivano, Luca; Peterson, Julia Denise; Fens, Marcel H. A. M.; Hernandez, Irati Beltran; Mesquita, Barbara; Torano, Javier Sastre; Hennink, Wim E.; van Nostrum, Cornelius F.; Oliveira, Sabrina

Meta-Tetra(hydroxyphenyl)chlorin (mTHPC) is one of the most potent second-generation photosensitizers, clin. used for photodynamic therapy (PDT) of head and neck squamous cell carcinomas. However, improvements are still required concerning its present formulation (i.e., Foscan, a solution of mTHPC in ethanol/propylene glycol (40:60 weight/weight)), as mTHPC has the tendency to aggregate in aqueous media, e.g., biol. fluids, and it has limited tumor specificity. In the present study, polymeric micelles with three different diameters (17, 24, and 45 nm) based on benzyl-poly(ε-caprolactone)-b-poly(ethylene glycol) (PCL<sub>n</sub>-PEG; n = 9, 15, or 23) were prepared with mTHPC loadings ranging from 0.5 to 10 weight % using a film-hydration method as advanced nanoformulations for this photosensitizer. To favor the uptake of the micelles by cancer cells that overexpress the epidermal growth factor receptor (EGFR), the micelles were decorated with an EGFR-targeted nanobody (named EGa1) through maleimide-thiol chem. The enhanced binding of the EGFR-targeted micelles at 4°C to EGFR-overexpressing A431 cells, compared to low-EGFR-expressing HeLa cells, confirmed the specificity of the micelles. In addition, an enhanced uptake of mTHPC-loaded micelles by A431 cells was observed when these were decorated with the EGa1 nanobody, compared to nontargeted micelles. Both binding and uptake of targeted micelles were blocked by an excess of free EGa1 nanobody, demonstrating that these processes occur through EGFR. In line with this, mTHPC loaded in EGa1-conjugated PCL<sub>23</sub>-PEG (EGa1-P<sub>23</sub>) micelles demonstrated 4 times higher photocytotoxicity on A431 cells, compared to micelles lacking the nanobody. Importantly, EGa1-P<sub>23</sub> micelles also showed selective PDT against A431 cells compared to the low-EGFR-expressing HeLa cells. Finally, an in vivo pharmacokinetic study shows that after i.v. injection, mTHPC incorporated in the P<sub>23</sub> micelles displayed prolonged blood circulation kinetics, compared to free mTHPC, independently of the presence of EGa1. Thus, these results make these micelles a promising nanomedicine formulation for selective therapy.

Keywords: EGFR targeted nanobody polymer micelle mTHPC photodynamic therapy; EGFR; nanobody; photodynamic therapy; polymeric micelles; selectivity; targeting

Open Access Full Text

Expand All | Collapse All

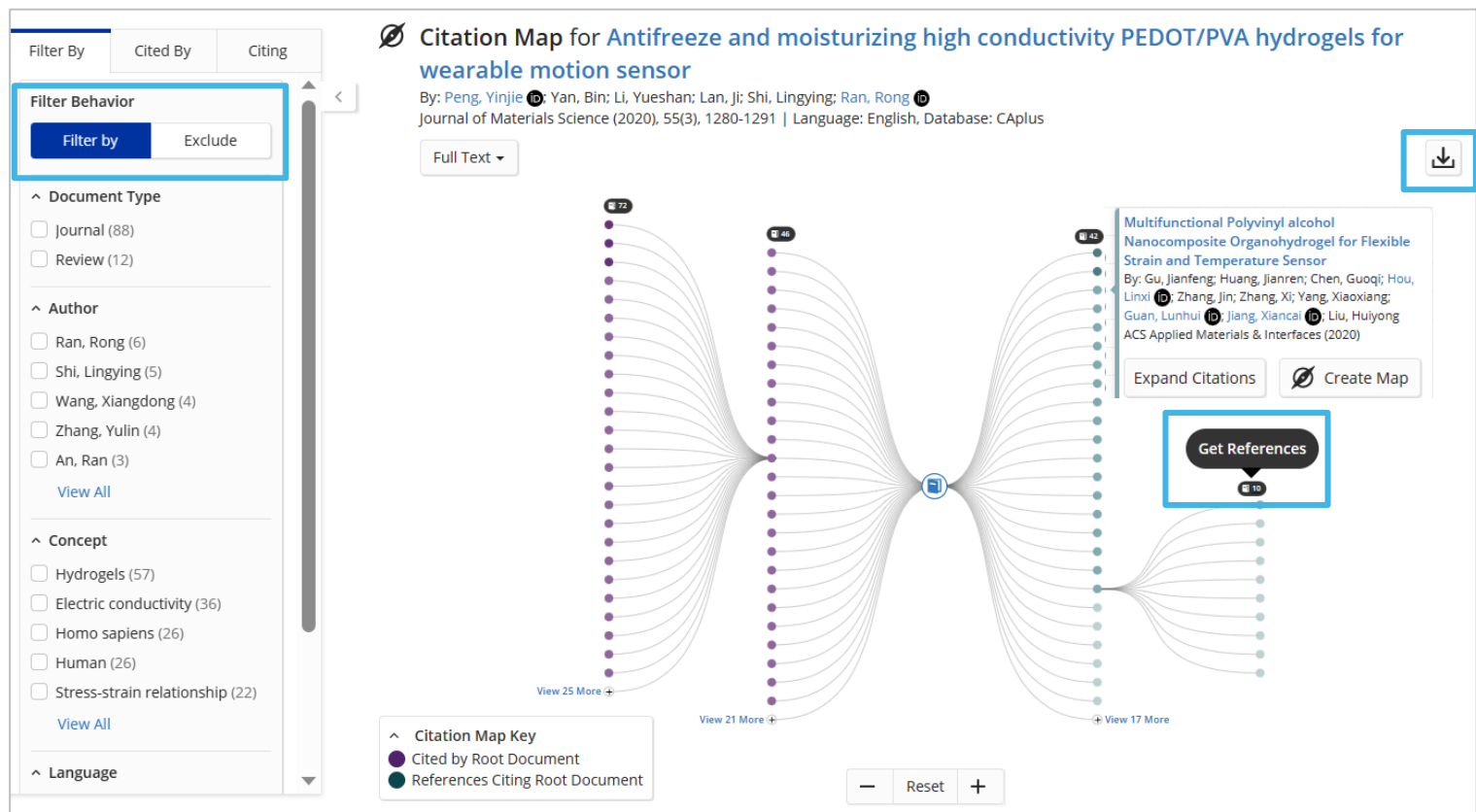
- Concepts
- MEDLINE® Medical Subject Headings
- Supplementary Concepts
- Substances
- Cited Documents

## 文献详情界面包括:

- 标题
- 摘要
- 原文关键词
- 文献中重要的技术术语 (含Caplus、Medline的关键词)
- 文献中重要的物质
- 书目信息
- 获得文献中的物质、反应
- 参考文献
- 链接原文
- 引文地图

CAS科学家增值标引的信息

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Cited By: 引用当前文献的文献

# ChemZent<sup>®</sup>: 追溯学科早期的研究

- ChemZent<sup>®</sup>是最古老的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
- 化学研究相关文献可回溯至1830年，可用于追溯化学科学起源时期的研究，丰富化学历史知识

References search for "enzyme and reduction" + drawn structure

Substances Reactions Citing Knowledge Graph Save and Alert

Structure Match: As Drawn (0), Substructure (8,881)

Filter Behavior: Filter by Exclude

Filtering: Database: CHEMZENT 31 Results Sort: Relevance View: Partial Abstract

**Fabric change of CARB azole in rats and rabbit**  
By: Johns, S. R.; Wright, S. E.  
Chemisches Zentralblatt (1966), 137(5), 01578-01578 | Language: German, Database: CHEMZENT

Machine Translated: After administration of carbazoles is 3-hydroxy carbazole, conjugate with glucuronic acid in the urine separated Hauptstoffwechselprod. in rats and rabbits. The hydroxylation in 3-position is in accordance with the etching oxidizing enzymes at the position of greatest electron density. For the investigation of werden carbazole-14 C is used. Experiments: 14C-carbazole (I), Melting Point 242-244 ° (from benzene) by diazotization and reduction of 14C-aniline to 14C-phenylhydrazine (240-245 ° F) with cyclohexanone in 14C-tetrahydrocarbazole is converted. Dehydrogenation to Pd-C gives I. Respect m...

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ChemZent Full Text Substances (14) Reactions (0) Citing (0) Citation Map

**Cobamide and ribo nucleotide reduction. 3. Part The content of the Cobamid-abhängigen Ribonucleosid-triphosphatreduktase in Lactobacillus leichmanii influencing factors**  
By: Ghambeer, R. K.; Blakley, R. L.  
Chemisches Zentralblatt (1968), 139(28), 160-160 | Language: German, Database: CHEMZENT

Machine Translated: Hysic. Res. common. 20 (1965) 20. — the content of ribo nucleoside triphosphate reductase (I) in extracts of L. leichmanii depends on the age of the culture. During the linear growth if I-Geh. with increasing age up to the end of the linear phase on and falls then. Extracts from stationary cells exhibit no significant I-Aktivität. The rapid I-Synth. during the linear growth by chloramphenicol and ActinomycinD inhibited. The decrease of I-Geh. after completion of the linear growth is based not on the presence one increased amount proteolit. Enzymes, nor on incomplete release of said enzyme. The

Nr. 5-1559 E-6. Pharmakologie, Therapie, Toxikologie, Hygiene 1966

68-74, 1963; Washington, D.C. George Washington Univ., School of Med., Dep. of Pharmacol.; engl.) — Die i.p. Injektion von 1 mg des adeninanalogen Purin-antimetaboliten 4-Aminoglyoxyuridin (I) verursachte bei Mäusen einen Anstieg der Gesamtleberlipide innerhalb 24 Std. auf das 3-4fache. Hieran waren an erster Stelle die Neutrallipide, in geringerem Ausmaß auch das Cholesterin (II) beteiligt, während der Phospholipid-(III)-Geh. unverändert blieb. I-Gabe hemmte den in vitro-Einbau von <sup>14</sup>C<sub>11</sub>-Acetat (IV) in die Lipide von Leberschnitten, hatte aber wenig Einfl. auf die Ox. von IV u. <sup>14</sup>C<sub>11</sub>-Palmitat (V) in vitro. Die Plasmalipidkonz. sank nach I-Applikation u. war durch einen Abfall der Triglyceride u. des II hervorgerufen. III u. freie Fettsäuren waren nicht beteiligt. V wurde von den Lebern der mit I behandelten Tiere schlechter aufgenommen als von den Lebern der Kontrolltiere. Obgleich der Einbau von <sup>14</sup>C<sub>11</sub>-Orotsäure in RNS durch I gehemmt wurde, konnte kein verminderter Einbau von <sup>14</sup>C<sub>11</sub>-Glycin in Leber-u. Plasmaproteine festgestellt werden. Die normalerweise massive Hyperlipidämie nach Gabe von Triton WR-1339 wurde durch I verhindert. VI schließt aus den Unters., daß I wahrscheinlich die Sekretion von Triglyceriden aus der Leber hemmt. H. Zöllner 4607

1559 Stoffwechsel des Carbazols in Ratten und Kaninchen. S. R. Johns und S. E. Wright. (J. med. Chem. 7, 158-161, 1964; Sydney, Univ. of Sydney, Dep. of Pharmacy; engl.) — Nach Gabe von Carbazol ist 3-Hydroxycarbazol, konjugiert mit Glucuronsäure, das im Harn ausgeschiedene Hauptstoffwechselprod. bei Ratten u. Kaninchen. Die Hydroxylierung in 3-Stellung ist in Übereinstimmung mit dem Angriff oxydierender Enzyme an der Stellung mit der größten Elektronendichte. Für die Unters. wurde Carbazol-<sup>14</sup>C verwendet.

Versuche: <sup>14</sup>C-Carbazol (I), F. 242-244° (aus Bzl.) durch Diazotierung u. Red. von <sup>14</sup>C-Anilin zu <sup>14</sup>C-Phenylhydrazinhydrochlorid (F. 240-245°), das mit Cyclohexanon in <sup>14</sup>C-Tetrahydrocarbazol übergeführt wird. Dehydrierung an Pd-C ergibt I. Hergestellte Bezugs-substanzen: 1-Hydroxycarbazol, F. 160-162° durch Cyclisierung von Cyclohexan-1,2-diaminophenylhydrazin (F. 183-185°) in äthanol. Essigsäure über 1,2,3,4-Tetrahydro-1-oxocarbazol (F. 169°), das an Pd-C dehydriert wird. 3-Hydroxycarbazol (II), F. 260-261° über folgende Stufen: p-Methoxyphenylhydrazinhydrochlorid (III), F. 198-200° (aus A.) durch Diazotierung u. Red. von p-Anilidin — 3-Methoxy-1,2,3,4-tetrahydrocarbazol (IV), C<sub>12</sub>H<sub>14</sub>NO, F. 94-95° (aus A.), durch Rk. von III mit Cyclohexanon in wss. Essigsäure (50%ig) bei Ggw. von Natriumacetat. 3-Methoxycarbazol (V) C<sub>12</sub>H<sub>11</sub>NO,

N-Butyl-, Äthobromid, DL<sub>50</sub> 38,4. Curarisierungswirkg., 30,7, cholinolyt. Aktivität, 0,04; N-Cyclohexyl-, Äthobromid, 33,5/28/0,02; N-Phenyl-, Äthobromid, 17,5/20/0,09; N-Phenyl-, Benzylbromid, 11/13/0,14; N-β-Phen-äthyl-, Äthobromid, 21/22/0,1; N-Octyl-, Äthobromid, 6,8/8,7/1,5; Lauryl-, Äthobromid, 21,5/12,6/18; N-Butyl-Hydrochlorid, 115/-/0,02; N-Cyclohexyl-, HCl, 75/-/0,02; N-Phenyl-, HCl, 47,5/-/cholinerg.; N-β-Phenäthyl-, HCl, 60/-/0,03; N-Octyl-, HCl, 47/-/0,5; N-Lauryl-, HCl, 37,5/-/1,5; N,N-dialkylcarbaminsäure-β-di-äthylaminoäthylester, Äthobromide: diäthyl-, DL<sub>50</sub> 26, Curarisierungswirkg., 26, spasmolyt. Aktivität, 50 (Papaverin = 100), 0,05 (I = 100), Anticholinerg. aktivität, — (Promethazin = 100); dibutyl-, 8/11/2100/6/4,3; dicyclohexyl-, 2,2/4,8/2300/2,4/0,05; Diphenyl-, 9,5/11,6/310/0,13/0,03; Di-β-phenäthyl-, 6,5/6,5/570/0,38/0,07; Dibutyl-, Benzylbromid, 7,5/5,5/200/0,11/-; Carbazol(II), Äthobromid, 3,3/4,6/730/0,20/0,20; Acridan (III), Äthobromid, 5,4/4,5/770/0,6/0,20; Phenozasin (IV), Äthobromid, 4,0/5,3/1400/1,3/0,5; Phenothiazin (V), Äthobromid, 3,0/4,6/800/0,8/0,5/0; Hydrochloride: Dibutyl-, 38/-/1000/3,0/3,0; Dicyclohexyl-, 22/-/1130/2,4/0,1; Di-phenyl-, 42,5/-/770/4,5/0,1; Di-β-phenäthyl-, 10,3/-/400/0,14/0,2; II, 20/-/280/0,1/0,3; III, 35/-/1800/1/1; IV, 24,5/-/770/0,8/1; V, 25/-/12000/18/20.

K. Maier 4607

1561 Wirkung von Chlorcyclizin und anderen Stoffen auf die Toxizität verschiedener Organophosphat-Anticholinesterasen. Richard M. Welch und J. M. Coon. (J. Pharmacol. exp. Therapeut. 143, 192-98, 1964; Philadelphia, Pa., Jefferson Med. Coll., Dep. of Pharmacol.; engl.) — Vt. untersuchten verschiedene Substanzen mit bekannter Wirkg. auf die Lebermikrosomen-Enzym-Systeme, auf deren Wirkg. auf die Toxizität einiger Organophosphatsektizide an Mäusen. Eine Vorbehandlung der Tiere täglich über 4 Tage mit Chlorcyclizin (I), Phenobarbital (II), SKF-525A (s.s. Diphenyl-α-propyl-essigsäure-β-diäthylaminoäthylester - HCl; III) oder Cyclizin zeigte einen deutlichen Schutz gegen die Toxizität von Malathion, Parathion (IV) u. EPN (p-Nitrophenyl-thionbenzylphosphoräthylether). Eine I-Vorbehandlung erhöhte außerdem wesentlich die orale DL<sub>50</sub> von Paraoxon (V), TEPP (Tetraäthylpyrophosphat) u. Physostigmin. Eine s.e. Dosis von I, II oder III schützte gegen IV. Die Umwandlung von IV in V durch Mäuseleber erfolgte etwa 2mal so schnell, wenn das Tier 4 Tage vorher mit I vorbehandelt wurde. Eine I-Dosis senkte deutlich die Serum-Paraoxonase (VI; A-Esterase), erhöhte aber dagegen gering die Leber-VI I erhöhte innerhalb von 24 Std. das Verhältnis Lebergew. zu Körpergew. um

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- 唯一提供在专利中快速定位物质相关化学信息的工具
- 安全、快捷地获得来自全球46个专利授权机构的PDF格式专利文件
  - 无需在多个不同专利局网站上耗费时间
  - 可获得的专利数量是其他科学信息检索工具的7倍
  - 新的专利文件每日上传更新
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- 在CAS专利族文献中找到您所熟悉语言的专利



# 专利文献详情

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## Methods using toll-like receptor (TLR) agonists in combination with antibiotics for the treatment of bacterial infections

By: Hardt, Wolf-Dietrich; Kaiser, Patrick; Sirard, Jean-Claude; Carnoy, Christophe; Fougeron, Delphine; Chabalgoity, Jose Alejandro; Munoz, Natalia

The invention relates to methods and pharmaceutical compositions for the treatment of bacterial infections. In particular, the invention relates to a toll-like receptor (TLR) agonist (e.g. flagellin polypeptide, biomols., peptides, antibodies, nucleic acids) for use in a method for the treatment of a bacterial infection in a subject in need thereof wherein the TLR agonist is administered to the subject in combination with at least one antibiotic. In another aspect of the invention the antibiotic is selected from the group consisting of aminoglycosides, beta-lactams, quinolones or fluoroquinolones, macrolides, sulfonamides, sulfamethoxazoles, tetracyclines, streptogramins, oxazolidinones, rifamycins, glycopeptides, polymixins, and lipopeptides.

Keywords: antibacterial toll like receptor agonist, antibiotic, toll like receptor agonist, antibiotic combination therapy bacterial infection

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### Patent Family

Patent	Language	Kind Code	PatentPak Options	Publication Date	Application Number	Application Date
<a href="#">WO2015011254</a>	English	A1	<a href="#">PDF</a>   <a href="#">PDF+</a>   <a href="#">Viewer</a>	2015-01-29	WO2014-EP66007	2014-07-25
EP3024476	English	A1		2016-06-01	EP2014-749736	2014-07-25
EP3632458	English	A1	<a href="#">PDF</a>	2020-04-08	EP2019-207885	2014-07-25
US20160151453	English	A1	<a href="#">PDF</a>	2016-06-02	US2016-14906747	2016-01-21
US9919029	English	B2		2018-03-20	US2016-14906747	2016-01-21

### Priority Application

Priority Application Number	Application Date
EP2013-306086	2013-07-26
EP2014-749736	2014-07-25
WO2014-EP66007	2014-07-25

Expand All | Collapse All

IPC Data

CAS PatentPak

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### Key Substances in Patent

- CAS RN 723-46-60  
Nc1ccc(cc1)C(=O)Nc2ccoc2  
derivs.
- CAS RN 11006-76-1D  
Virginiamycin derivs.
- CAS RN 1406-11-7  
Polymyxin
- CAS RN 57-62-5  
Cc1c(O)c(O)c(O)c(O)c1

WO 2015/011254

PCT/EP2014/066007

sulfonamides, sulfamethoxazoles, tetracyclines, streptogramins, oxazolidinones, rifamycins, glycopeptides, polymixins, and lipo-peptide antibiotics.

18. The method of claim 1 wherein the antibiotic is a tetracycline selected from the group consisting of chlortetracycline, demeclocycline, doxycycline, minocycline, oxytetracycline, chlortetracycline, methacycline, meccocycline, tigecycline, limecycline, and tetracycline.

19. The method of claim 1 wherein the antibiotic is an aminoglycoside selected from the group consisting of amikacin (Amikin®), gentamicin (Garamycin®), kanamycin (Kantrex®), neomycin (Mycifradin®), netilmicin (Netromycin®), paromomycin (Humatin®), streptomycin, and tobramycin (TOBI Solution®, TobraDex®).

20. The method of claim 1 wherein the antibiotic is a macrolide selected from the group consisting of azithromycin (Zithromax®), clarithromycin (Biaxin®), dirithromycin (Dynabac®), erythromycin, clindamycin, josamycin, roxithromycin and lincomycin.

21. The method of claim 1 wherein the antibiotic is a fluoroquinolone selected from the group consisting of nalidixic acid, cinoxacin, oxolinic acid, flumequine, piperidic acid, rosoxacin, norfloxacin, lomefloxacin, ofloxacin, enrofloxacin, ciprofloxacin, enoxacin, amifloxacin, feroxacin, gatifloxacin, gemifloxacin, clinafloxacin,

## CAS PatentPak:

- 直接下载专利原文
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- 阅读熟悉语言撰写的等同专利
- 快速理解专利

# CAS PatentPak™—专利流程解决方案

在CAS PatentPak浏览器中单击结构，打开物质菜单检索具体信息

The screenshot displays the CAS PatentPak interface. On the left, a sidebar lists 'Key Substances in Patent' with three entries: CAS RN 2306115-70-6 (highlighted), CAS RN 1003-68-5, and CAS RN 1229705-85-4. The main area shows a patent document (CN 109535200 A) with Chinese text and chemical reaction schemes. A blue arrow points from a chemical structure in the patent to a detailed substance information panel on the right. This panel includes the CAS RN (2306115-70-6), CAS Name (2H-Pyran, 2-[4-bromo-2-(trifluoromethyl)phenoxy]tetrahydro-), and a list of actions: Substance Detail, Reactions (2), Synthesize (1), Create Retrosynthesis Plan, References (1), and Suppliers (0). Below the list is a large chemical structure of the substance, with buttons for 'Edit Structure', 'Reset', and a download icon.

# CAS Sequences™—分子生物学解决方案

- 超过14亿条序列
- 涵盖专利、非专利文献披露的序列
- 专有的CAS人工标引的化学修饰序列
- NCBI中的序列
- 可实现新颖性、创造性检索
- 简洁直观的检索界面 & 便捷的筛选、可视化分析、相关信息获取和下载功能
- 三种检索方式：BLAST、CDR、Motif

# CAS Sequences™ — Blast检索

**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

AACAACAACATATCAAATCCTACTGGTGGCACAACCTGA

Sequence Type:  
 Nucleotide  Protein

Search Within:  
 Nucleotides  Proteins  
 Include NCBI Sequences

Start Sequence Search

**高级检索参数设置**

Advanced Sequence Search Adjust Parameters for Short Sequences | Reset All

Alignment Identity % 80	Match with Gaps? <input type="radio"/> Yes <input checked="" type="radio"/> No	Gap Costs Existence 5 Extension 2
Query Coverage % 90	Word Size 11	Reward for Match Penalty for Mismatch 2, -3
BLAST Algorithm BLASTn	E-Value 10	Exclude Low Complexity Regions <input type="radio"/> Yes <input checked="" type="radio"/> No

BLAST: 检索核酸或蛋白

选择是否包含NCBI中的序列

四种检索选择:

Protein-Protein

Protein-Nucleotides

Nucleotide-Nucleotides

Nucleotide-Proteins

# CAS Sequences™—CDR检索

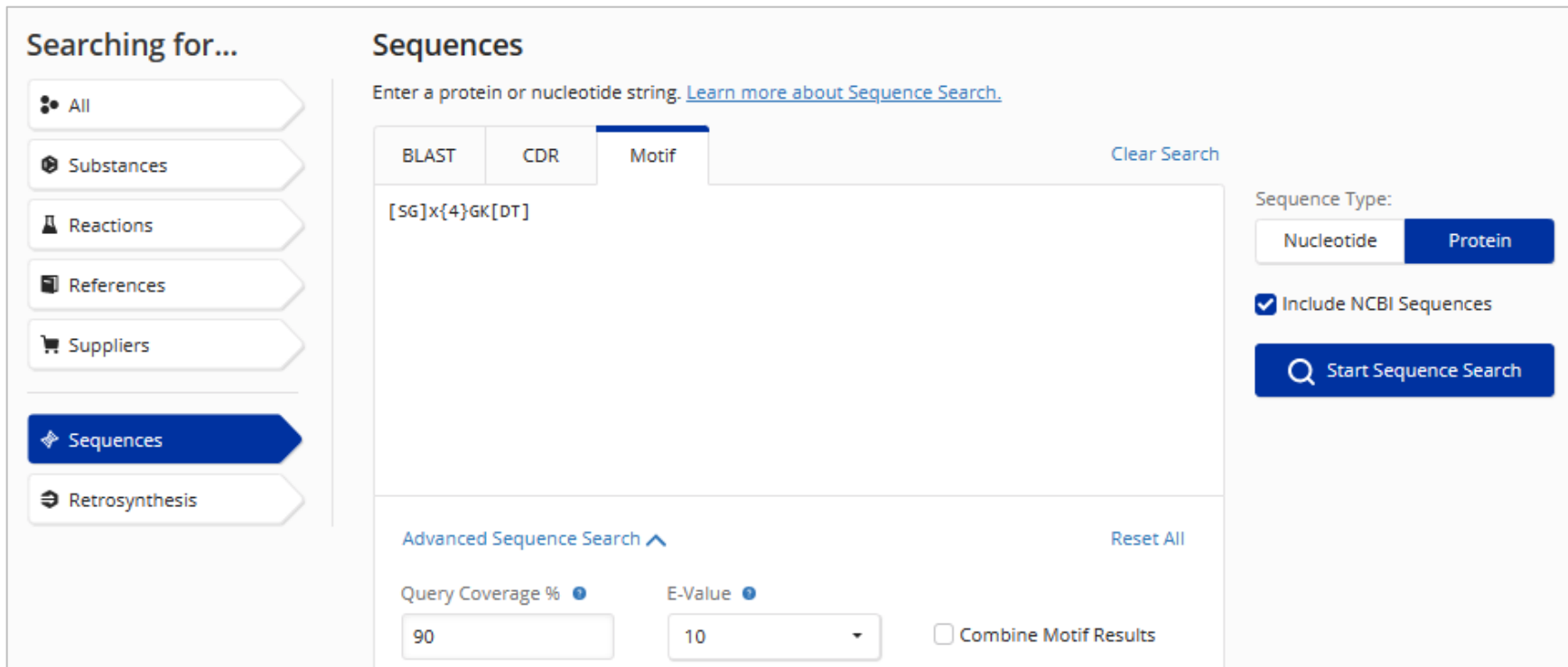
CDR: 抗体或细胞中的互补决定区

The screenshot displays the CAS Sequences search interface. On the left, a sidebar titled "Searching for..." contains navigation buttons for "All", "Substances", "Reactions", "References", "Suppliers", "Sequences" (highlighted in blue), and "Retrosynthesis". The main area is titled "Sequences" and includes a text input field with the instruction "Enter a protein string, or upload a .txt or .fasta file. [Learn more about Sequence Search.](#)". Below this are three tabs: "BLAST", "CDR" (selected), and "Motif". To the right of the tabs are buttons for "Upload Sequence" and "Clear Search". A checkbox labeled "Include NCBI Sequences" is also present. A large blue button labeled "Start Sequence Search" is located on the right side. The CDR search area contains three input fields: "CDR1" with the sequence "RASQSVSGSRFTYMH", "CDR2" with "YASILES", and "CDR3" with "QHSWEIPPWT". Each field has a small "x" icon for clearing the text.

支持单个或多个CDR序列检索并用

# CAS Sequences™—Motif检索

Motif: 可用于检索序列中有不确定位点的DNA、RNA或蛋白; 推荐检索短序列。



Searching for...

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

### Sequences

Enter a protein or nucleotide string. [Learn more about Sequence Search.](#)

BLAST CDR **Motif** Clear Search

[SG]x{4}GK[DT]

Sequence Type:  
Nucleotide **Protein**

Include NCBI Sequences

**Start Sequence Search**

Advanced Sequence Search [^](#) Reset All

Query Coverage %  E-Value   Combine Motif Results

- []中括号: 或者, 该位置的氨基酸或核苷酸是括号中的任意一个
- {}大括号: 重复次数
- X代表未指定氨基酸; N代表未指定核苷酸

# CAS Retrosynthesis Tool—逆合成工具

- 依据一个确定的结构进行设计
- 有报道且结构明确的物质，无论是否有反应信息报道
- 未报道且结构明确的物质
- 节省设计、实施合成新方法所花费的时间

# CAS Retrosynthesis Tool—由物质获得

获得已知化合物的逆合成路线：

点击物质结构，弹出的物质菜单中点击 Start Retrosynthetic Analysis

The screenshot displays the CAS Retrosynthesis Tool interface. On the left, a search result for CAS RN 2628280-40-8 is shown, including the chemical structure and the name: 3-Azabicyclo[3.1.0]hexane-2-carboxamide, N-[(1S)-1-cyano-2-[(3S)-2-oxo-3-pyrroli...]. Below the structure, it indicates 'Absolute stereochemistry shown' and provides the molecular formula C<sub>23</sub>H<sub>32</sub>F<sub>3</sub>N<sub>5</sub>O<sub>4</sub>. At the bottom, there are buttons for 'References (236)', 'Reactions (53)', and 'Suppliers (39)'. On the right, a detailed view of the same compound is shown, with a menu that includes 'Substance Detail', 'Reactions (53)', 'Synthesize (52)', 'Start Retrosynthetic Analysis' (highlighted with a blue box), 'References (236)', and 'Suppliers (39)'. The chemical structure in the detailed view is annotated with stereochemistry labels (S, R) and has a button for 'Edit Structure' and 'Reset'.

- 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



# CAS Retrosynthesis Tool—直接绘制结构

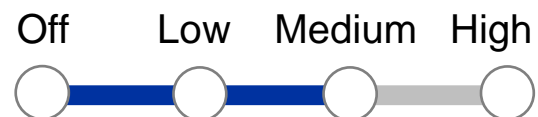
绘制目标化合物：

从Retrosynthesis检索项打开绘图板，绘制目标化合物，获得实验路线

The screenshot displays the CAS Retrosynthesis Tool interface. On the left, a sidebar titled "Searching for..." lists various search categories: All, Substances, Reactions, References, Suppliers, Biosequences, and Retrosynthesis (which is highlighted in blue). The main area is titled "Retrosynthesis" and contains a text input field for "Enter a CAS Registry Numbers, SMILES..." and a drawing toolbar. The drawing toolbar includes icons for drawing atoms (C, H, O, S, N, P, Cl, Si, Et, EZ) and bonds, as well as a "Start Retrosynthetic Analysis" button. The central canvas shows a chemical structure of a bicyclic amine with a carboxylic acid group. Below the canvas, the molecular formula is displayed as  $C_8H_{13}NO_2$  (155.20). At the bottom, there is a zoom control set to 100% and a search input field containing the letter "C".

# CAS Retrosynthesis Tool—已知化合物

获得逆合成路线后，可继续通过Scoring灵活调整预测参数



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

Retrosynthesis Plan for drawn structure

Powered by ChemPlanner®

Overview Steps Predicted Results ON

View Excluded Options Save

**Plan Information 路线概览**

Estimated Yield: 49%  
Overall Price: \$96.82  
(USD per 100 grams)

Commercially Available: A, B, C

**Plan Options**

Synthetic Depth: 3  
Predicted Rules: Common  
Break & Protect Bonds: No  
Starting Material Cost Limit: \$100.00/mol  
Edit Plan Options

**Scoring Profiles**

Complexity Reduction ●  
Convergence ●  
Evidence ●  
Cost ●  
Yield ●

Retrosynthesis Step Key

Reset

Feedback

# CAS Retrosynthesis Tool—已知化合物

- 快速获取最优的逆合成路线
- 可获取预测逆合成路线
- 可查看每步路线的详细条件
- 可自定义选择可替代路线

The screenshot displays the CAS Retrosynthesis Tool interface. The main window shows a retrosynthetic plan for a target molecule (A) with predicted results. The plan includes several steps (B, C, D, E, F, G) with associated chemical structures and yields. A sidebar on the left provides an overview of the steps, including evidence and alternative steps. A pop-up window titled "A ⇒ B + C + D Alternative Steps (93)" is open, showing a list of alternative steps with filters for Alternative Step Type and Stereochemistry. The first alternative step (1 of 34) is highlighted, showing a predicted step with a 41% average yield. The second alternative step (2 of 34) is also highlighted, showing a predicted step with a 59% average yield. The main window also includes a "Retrosynthesis Step Key" and a "Reset" button.

# Synthetic Methods™: 合成方法详情解决方案

- 迄今为止全球最大的为合成科学家提供的实验方法详情解决方案
- CAS科学家通过分析大量的顶级科技期刊及专利原文，收集、整理、筛选出来的实验方法
- 无需下载阅读全文，即可获得合成实验所需的所有信息
- 极大节省在期刊全文中查找信息的时间

# Synthetic Methods™: 合成方法详情解决方案

- 分类显示详尽信息，方便操作
- 不仅包含原文中描述的实验内容，还包括supporting information中涉及的实验内容

Structure Match

As Drawn (32)

Substructure (8,521)

Similarity (0)

Filter Behavior

Filter by Exclude

Yield

Number of Steps

Non-Participating Functional Groups

Reaction Mapping

Experimental Protocols

Synthetic Methods (40)

Experimental Procedure (83)

Filtering: Non-Participating Functional Groups: Halide X

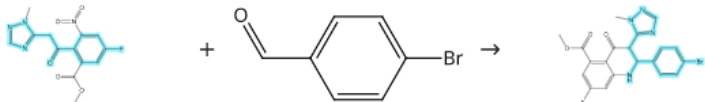
Experimental Protocols: Synthetic Methods X

Clear All Filters

40 Results

Group: By Scheme Sort: Relevance View: Collapsed

Scheme 1 (1 Reaction) Steps: 1 Yield: 98%



Suppliers (15) Suppliers (89)

31-614-CAS-24450288 Steps: 1 Yield: 98%

DoE Optimization Empowers the Automated Preparation of Enantiomerically Pure [<sup>18</sup>F]Talazoparib and its In Vivo Evaluation as a PARP Radiotracer

By: Bowden, Gregory D. et al  
Journal of Medicinal Chemistry (2021), 64(21), 15690-15701

1.1 Reagents: Hydrochloric acid, Titanium chloride (TiCl<sub>3</sub>)  
Solvents: Methanol, Tetrahydrofuran, Water; rt; 30 min, rt; 2 h, 30 - 50 °C

1.2 Reagents: Water

Experimental Protocols Full Text

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 NaHCO<sub>3</sub> (3 x 60 mL) and NaHSO<sub>3</sub> (3 x 100 mL).
9. Dry the organic fractions with sodium sulfate (Na<sub>2</sub>SO<sub>4</sub>).
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

CAS Method Number 3-315-CAS-33168860

# 大纲

- CAS（美国化学文摘社）及CAS SciFinder Discovery Platform简介
- 新一代科研创新信息工具CAS SciFinder<sup>n</sup>
- 分析方法解决方案CAS Analytical Methods<sup>TM</sup>
- 配方/制剂解决方案CAS Formulus<sup>®</sup>

# CAS Analytical Methods™—分析实验方法解决方案

分析方法的类别：13大类45小类；某些子类属多个大类

Organic Compound Analysis: 天然产物分离分析，手性分离，活性药物成分及代谢产物分析...

Organometallics / Inorganics: 地质分析，无机物分析，金属有机化合物分析

Pharmacology / Toxicology: 成瘾药物检测，有毒物检测...

Bioassays: 生物探针，生物标定细胞实验，生物标定药物实验，生物医学材料分析，生物分子/生物组织分离测定...

Water Analysis: 阴阳离子分析，元素测定，痕量元素分析，废水分析，生物标记公共卫生分析...

Historical Analysis / Dating: 考古分析，同位素分析

Environmental Analysis: 土壤/空气/水分析，农药残留分析...

Agricultural Applications / Analysis: 除草剂分析...

Food Analysis: 脂肪酸分析，脂肪酸酯分析，蛋白质分析...

Fuels / Geology / Biofuels: 生物燃料分析，油气分析，石油产品分析，煤炭加工...

Miscellaneous: 化妆品分析，爆炸物分析，纳米材料分析...

Water: 阴阳离子分析、环境分析、废水分析、微量元素分析...

Polymer: 聚合物分析...

# 分析实验方法的获取

<https://methods.cas.org> (与SciFinder-~~n~~登录账号相同)

- 主题检索或分类浏览;
- 筛选分析目标物、介质、方法类别、分析技术等

The screenshot shows the CAS Analytical Methods website. At the top, there is a navigation bar with "CAS Solutions" on the left and "Saved" and "Account" on the right. Below the navigation bar is the "CAS Analytical Methods" logo. The main content area is titled "Search" and contains a search input field with the placeholder text "Enter keyword, matrix, analyte, etc." and a search button. Below the search field is a link for "Advanced Search". Underneath, there is a section titled "Browse Method Categories" which lists various analytical method categories in a grid format:

<a href="#">Agricultural Applications / Analysis</a>	<a href="#">Fuels / Geology / Biofuels</a>	<a href="#">Pharmacology / Toxicology</a>
<a href="#">Bioassays</a>	<a href="#">Historical Analysis / Dating</a>	<a href="#">Polymer Analysis</a>
<a href="#">Biomolecule Isolation</a>	<a href="#">Miscellaneous</a>	<a href="#">Water Analysis</a>
<a href="#">Environmental Analysis</a>	<a href="#">Organic Compound Analysis</a>	
<a href="#">Food Analysis</a>	<a href="#">Organometallics / Inorganics</a>	



# 分析方法详情

## Analysis of Titanium in Kerosene by Inductively coupled plasma mass spectrometry

CAS MN: 1-135-CAS-84928

Method Category: Petroleum Product Analysis

Technique: Inductively coupled plasma mass spectrometry

### 实验原料

Materials	Role	Image	CAS RN
Cadmium	analyte	<a href="#">View Structure</a>	7440-43-9
Mercury	analyte	<a href="#">View Structure</a>	7439-97-6
Lead	analyte	<a href="#">View Structure</a>	7439-92-1
Silver	analyte	<a href="#">View Structure</a>	7440-22-4
Iron	analyte	<a href="#">View Structure</a>	7439-89-6
Vanadium	analyte	<a href="#">View Structure</a>	7440-62-2
Tin	analyte	<a href="#">View Structure</a>	7440-31-5
Titanium	analyte	<a href="#">View Structure</a>	7440-32-6
Chromium	analyte	<a href="#">View Structure</a>	7440-47-3

### Source

Sensitivity improvement in ICP MS analysis of fuels and light petroleum matrices using a microflow nebulizer and heated spray chamber sample introduction

Caumette, Guilhem; Lienemann, Charles-Philippe; Merdignac, Isabelle; Paucot, Hugues; Bouyssiere, Brice; Lobinski, Ryszard

Talanta (2009), 80 (2), 1039 - 1043. Elsevier B.V.

CODEN: TLNTA2 | ISSN: 00399140 | DOI: 10.1016/j.talanta.2009.08.017 | [View in SciFinder<sup>®</sup>](#)

Full Text ▾

Abstract ^

Reasons for signal suppression during the anal. of light petroleum matrixes by inductively coupled plasma mass spectrometry (ICP MS) were examined. A decrease of the ionization efficiency of the plasma was the principal factor responsible for this loss of sensitivity. Consequently, an interface based on a total consumption micronebulizer and a heated spray chamber was constructed to alleviate this problem. A method based on flow-injection ICP MS using this interface was developed for the direct multielement anal. of undiluted fuels (gasoline, kerosene) and gas condensates offering an increase in sensitivity by at least a factor of 3-4 in comparison with the existing setups.

### 文献来源

### Equipment Used

ICP-MS system, Elan 6000, PE-SCIEX1, PerkinElmer, ON, Canada

Microflow nebulizer

Syringe pump, 140C, Applied Biosystems, Foster City, CA, USA

Pump, Smartline Pump 1000, Knauer, Berlin, Germany

Thermostat, Neslab RTE-111, Thermo Fisher Scientific, Waltham, MA

### Conditions

#### Instrument

RF power: 1300 W; Ar nebulizer gas: 0.8 L/min and auxiliary O<sub>2</sub> flow: 45 mL/min; integration time per isotope: 20 ms

Flow rate: 20 µL/min

### Instructions

#### Sample Preparation

1. Collect petroleum samples (kerosene, gasoline and full range gas condensate).

#### Standards Preparation

1. Use conostans monoelemental standards in oil (1000 mg/kg) and multielemental S-21 oil (100 mg/kg) as standards.

#### ICP-MS analysis

1. Analyze the sample using a PerkinElmer Elan 6000 (PE-SCIEX1, ON, Canada).

2. Introduce the sample using microflow nebulizer consisting of a fused silica capillary of 180 µm i.d. (375 µm o.d.) and heated spray chamber (jacketed to allow the

### 实验仪器

### 分析条件

### 操作步骤

### Validation

Linearity Range	1 - 250 µg/kg
Limit of Detection	0.8 µg/kg (gasoline), Titanium 0.1 µg/kg (gasoline), Vanadium 5 µg/kg (gasoline), Chromium 7 µg/kg (gasoline), Iron 0.04 µg/kg (gasoline), Silver 0.3 µg/kg (gasoline), Cadmium 0.2 µg/kg (gasoline), Tin 1 µg/kg (gasoline), Mercury 0.1 µg/kg (gasoline), Lead

### 数据有效性

# 直观的分析方法对比

Compare Methods		
	1	2
Title	Analysis of <b>Chromium</b> in Barium sulfate by Electrothermal atomic absorption spectroscopy	Analysis of <b>Chromium</b> in Barium sulfate by Electrothermal atomic absorption spectroscopy
CAS Method Number	1-142-CAS-3223998	1-142-CAS-3186641
Method Category	Trace Element Analysis; Active Pharmaceutical Ingredient and Metabolite Analysis	Trace Element Analysis; Active Pharmaceutical Ingredient and Metabolite Analysis
Technique	Electrothermal atomic absorption spectroscopy	Acid digestion; Electrothermal atomic absorption spectroscopy
Analyte	<b>Chromium</b>	<b>Chromium</b>
Matrix	Barium sulfate	Barium sulfate
Other Materials	Nitric acid; Pyrolytic coated graphite tubes	Nitric acid
Equipment Used	Atomic absorption spectrometer, AAS ZEE nit 60, Analytik Jena, Jena, Germany; Solid sampling system, SSA-5, Analytik Jena, Jena, Germany; Microbalance, M2P, Sartorius, Göttingen, Germany; Sub-boiling system, duoPUR 2.01 E, View All	Atomic absorption spectrometer, AAS ZEE nit 60, Analytik Jena, Jena, Germany; Microbalance, M2P, Sartorius, Göttingen, Germany; Sub-boiling system, duoPUR 2.01 E, View All
Conditions	Instrument: hollow cathode lamp power: 4 mA; wavelength: 357.9 nm; spectral bandpass: 0.8 nm; integration time: 12 s; atomization temperature: 2400 °C; pyrolysis temperature: View All	Instrument: hollow cathode lamp power: 4 mA; wavelength: 357.9 nm; spectral bandpass: 0.8 nm

Source	<b>Chromium</b> determination in pharmaceutical grade barium sulfate by solid sampling electrothermal atomic absorption spectrometry with Zeeman-effect background View All	<b>Chromium</b> determination in pharmaceutical grade barium sulfate by solid sampling electrothermal atomic absorption spectrometry with Zeeman-effect background View All
Preparation	<p>Collection and preparation of samples</p> <ol style="list-style-type: none"> <li>Obtain the powdered pharmaceutical grade BaSO<sub>4</sub> samples from pharmaceutical industries and dry them in a conventional oven at 105 °C × 2 h.</li> <li>Spike the samples by addition of <b>chromium</b> reference solutions of 0.48 µg/g.</li> </ol> <p>Preparation of standard solutions</p> <ol style="list-style-type: none"> <li>Prepare the reference solutions daily by serial dilutions of stock <b>chromium</b> (Cr) solutions (1 g/L Cr in 2% HNO<sub>3</sub>).</li> </ol> <p>View Less</p>	<p>Preparation of nitric acid solution</p> <ol style="list-style-type: none"> <li>Doubly distill the concentrated nitric acid in a Milestone sub-boiling system (model duoPUR 2.01 E, Bergamo, Italy) and use this for sample digestion/extraction.</li> </ol> <p>Collection and preparation of samples</p> <ol style="list-style-type: none"> <li>Obtain the powdered pharmaceutical grade BaSO<sub>4</sub> samples from pharmaceutical industries and dry them in a conventional oven at 105 °C × 2 h.</li> </ol> <p>Preparation of standard solutions</p> <ol style="list-style-type: none"> <li>Prepare the reference solutions daily by serial dilutions of stock <b>chromium</b> (Cr) solutions (1 g/L Cr in 2% HNO<sub>3</sub>).</li> </ol> <p>View Less</p>
Method	Direct solid sampling (DSS) - electrothermal-atomic absorption spectrometric (ETAAS) analysis View All	Acid digestion procedure using nitric acid View All
Linearity Range	100 - 1800 pg	
Limit of Detection	2.4 pg	
Recovery	98% - 103% in 0.48 µg/g spiked concentration	
Concentration	0.45 ± 0.04 µg/g (sample data)	0.32 ± 0.04 µg/g (sample data)

# 大纲

- CAS（美国化学文摘社）及CAS SciFinder Discovery Platform简介
- 新一代科研创新信息工具CAS SciFinder<sup>n</sup>
- 分析方法解决方案CAS Analytical Methods<sup>TM</sup>
- 配方/制剂解决方案CAS Formulus<sup>®</sup>

# CAS Formulus®——助力开发安全、有效的产品

- 一个集成配方（制剂）数据与工作流程的解决方案
- 由CAS科学家从期刊、专利中标引的配方信息
- 涵盖制药、化妆品、食品、农化、化妆品、油墨、涂料等众多领域
- 可检索配方及其工艺、成分、目标成分的常见配伍成分、设计配方，探索合规要求等
- 支持自主设计配方/制剂

# 检索配方或制剂

https://formulus.cas.org (与CAS SciFinder-n登录账号相同)

配方/制剂检索

原料检索

配方/制剂设计

The screenshot displays the Formulus search interface. On the left, under 'Searching for...', there are three options: 'Formulations' (selected), 'Ingredients', and 'Formulation Designer'. Below 'Formulation Designer' is a light blue box with the text: 'Design custom formulations templates based on selections and ingredients.' On the right, under 'Formulations', there is a search bar containing the text 'orthopedic and implant' and a search button. Below the search bar, it says 'Try [Advanced Search](#) for a more precise search experience'.

在检索框输入检索式，如制剂或配方的原料、用途、物理形态、功能或文献识别符进行检索

# 制剂或配方详情

**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			
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 (otic).  
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.

**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®

- 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

# 不同制剂或配方信息的直观对比

Comparing your Formulations

Predicted value

	Formulation 1	Formulation 2
Title	Implants: Antitumor Agents	Composition for Promoting Bone Formation
Purpose	Antitumor agents	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	implant	pharmaceutical implants
Experimental Activity	Available	Not Available
Components	<p>Group: Ti-TNTs wire implants Function: implant Amount Reported: Optionality: Mandatory</p> <p><b>Ti wires</b> Function: additives Amount Reported: - Optionality: -</p> <p><b>Acetone</b> Function: Solvents Amount Reported: - Optionality: -</p> <p><b>Ethanol</b> Function: Solvents Amount Reported: - Optionality: -</p>	<p>Group: surgical implant Function: Amount Reported: Optionality: Mandatory</p> <p><b>Dental implants</b> Function: - Amount Reported: - Optionality: -</p> <p><b>Plates</b> Function: - Amount Reported: - Optionality: -</p> <p><b>pin</b> Function: - Amount Reported: - Optionality: -</p>

- 选择感兴趣的制剂或配方进行对比
- 一次最多可以比较三种不同制剂或配方的信息详情

# 检索原料

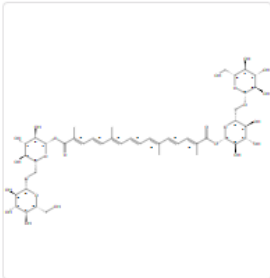
- 制剂或配方中，与该原料同时使用的其它配伍成分
- 管控信息及清单
- 实验属性
- 使用该原料的制剂或配方
- 原料供应商信息
- 可将原料添加至Formulation Designer

Ingredients search for "crocin"

5 Results

1

**CAS RN: 42553-65-1**  
[View Details](#)



$C_{44}H_{64}O_{24}$

**Crocin**

Key Physical Properties	Value	Condition
Molecular Weight	976.96	-
Melting Point (Experimental)	186 °C	-

Commonly Used As: Coloring materials; Antioxidants; Antitumor agents; Hair preparations

[Commonly Formulated With](#) | [Regulatory Information](#) | [Experimental Properties](#)

[Formulations](#) | [Suppliers](#) | [Add to Designer](#)



# 制剂或配方的设计

Base Selections				
Industry	Purpose	Physical Form	Active or Featured Ingredient	
Cosmetics & Personal Care	Skin care products	Gels	Vitamin A	
<a href="#">Edit</a>	<a href="#">Edit</a>	<a href="#">Edit</a>	<a href="#">Edit</a>	
polyethylene glycol				
Template				
Function	Ingredient	Regulatory	Top Alternatives	Amounts
Active or Featured Ingredient:	Vitamin A	ANMAT	-	Amount not available <span>✕</span>
Active or Featured Ingredient:	polyethylene glycol	ANMAT; CosIng; Cosmetic Ingredient Inventory; Drug Master File List; EPA Pesticide Inactive Ingredients; FDA GRAS (Part 181, Subpart B); FDA Inactive Ingredients Database	-	Amount not available <span>✕</span>
Function: Carriers	Polyethylene glycol  <a href="#">View More Alternatives</a>	ANMAT; CosIng; Cosmetic Ingredient Inventory; Drug Master File List; EPA Pesticide Inactive Ingredients; FDA GRAS (Part 181, Subpart B); FDA Inactive Ingredients Database	Water; Ethylene glycol	Approximate Range: 3 - 4% <span>✕</span>
Function: Skin conditioners	Glycerol  <a href="#">View More Alternatives</a>	ANMAT; CosIng; Cosmetic Ingredient Inventory; Drug Master File List; EMA Excipients List; EPA Pesticide Inactive Ingredients; FDA GRAS (Part 182,	Allantoin; Ethylene glycol; 1,2-Octanediol; Tricaprin; Palm-oil glycerides, monoglycerides, diglycerides and triglycerides, hydrogenated	Approximate Range: 3 - 11% <span>✕</span>

- 原料详情
- 原料管制信息
- 可替代的原料选项

# 使用注意事项

- 一人注册一个帐号
- 实名注册， 请提供真实姓名信息（中文名用汉语拼音全拼）
- 不得过量下载（<https://www.cas.org/legal/infopolicy>）
- 不得账号分享
- 不得将账号用于非学术研究

# THANK YOU!



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