

CAS SciFinder Discovery Platform™ (Academic)

驱动科研创新与学科发展



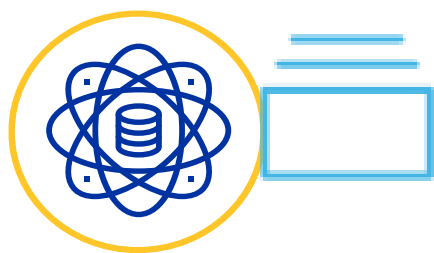
刘子露
ZLiu@acs-i.org
美国化学文摘社(CAS)北京代表处

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®
- 分析方法解决方案CAS Analytical Methods™
- 配方/制剂解决方案CAS Formulus®

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

—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

—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

—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

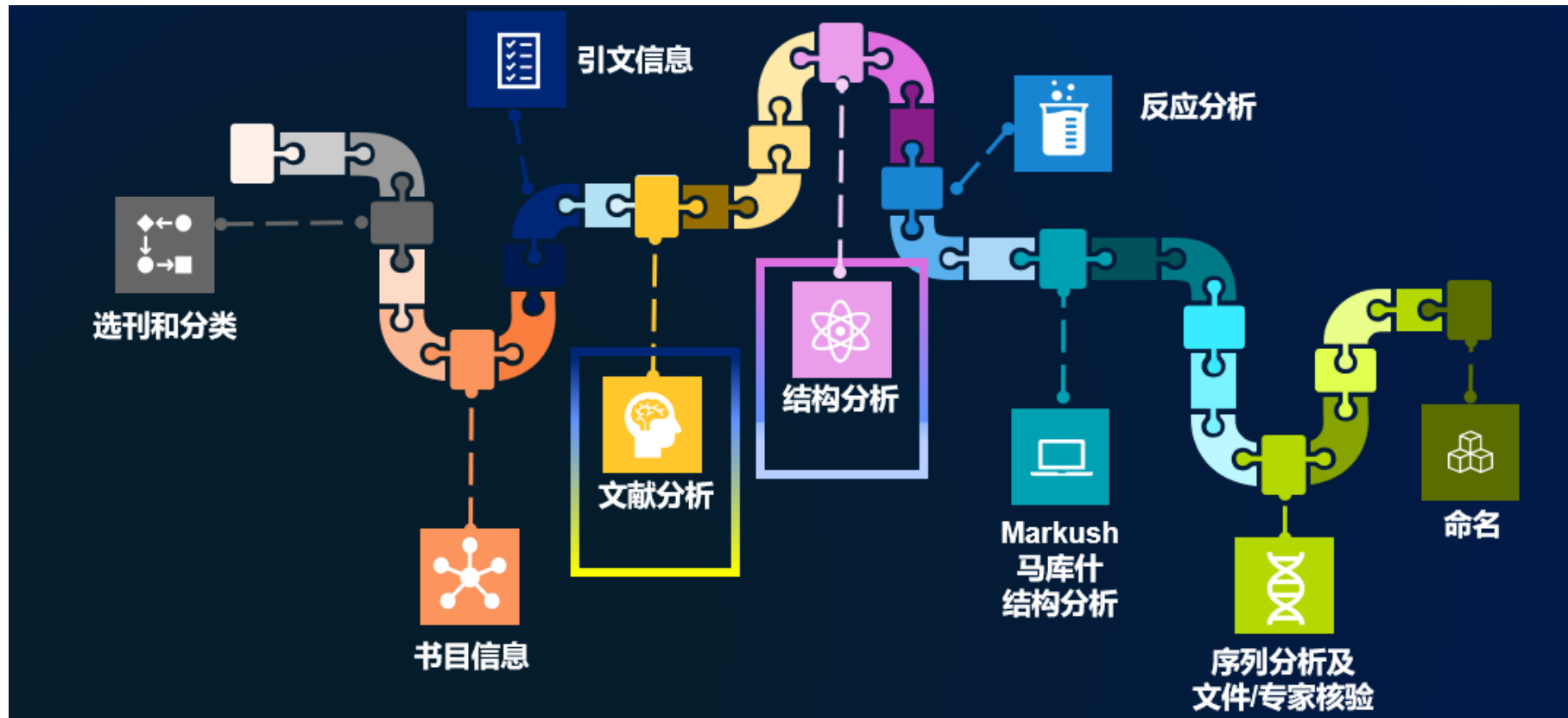
—应用化学各领域：

大气污染、陶瓷、精油、化妆品、化石燃料、黑色金属、合金

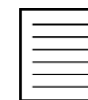
—物理、无机、分析化学各领域：

表面化学、催化剂、相平衡、核现象、电化学

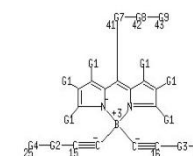
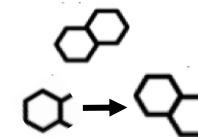
CAS科学家的智力标引



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



1990
Smith, M.
anthracene



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

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



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STN IP Protection Suite™

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Custom Solutions

CAS Custom ServicesSM

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 SciFinderⁿ——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——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——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 SciFinderⁿ
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- 配方/制剂解决方案CAS Formulus

CAS SciFinderⁿ——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

CAS独特的内容合集



来源:

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

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

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



Log in to SciFinder®

Username or Email Address

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Log in to SciFinder®

Welcome, ZLiu@acs-i.org [Not You?](#)

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账号与CAS SciFinder相同

CAS SciFinderⁿ主界面

The screenshot displays the CAS SciFinderⁿ main interface. On the left is a sidebar menu with categories: CAS SCIFINDER DISCOVERY PLATFORM, CAS SciFinder, CAS Analytical Methods, CAS Formula, STN IP PROTECTION SUITE, CAS 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 CAS SciFinder logo and user icons. Below this is a 'Good Afternoon' greeting and a '灵活检索选项' (Flexible Search Options) section. The search bar contains the text 'Antitumor'. Below the search bar are filters for 'AND', 'Author Name', and a text input field with the placeholder 'Enter last name, first name middle name.' and an example 'Schubert, J A'. A blue arrow points from the search bar to a chemical structure of a bicyclic amide. Below the search bar are three search options: 'Retrosynthetic Analysis', 'Search CAS Lexicon', and 'Search CAS Sequences'. At the bottom is a 'Recent Search History' section showing a search for 'Semaglutide' on April 15, 2025, with buttons for 'Rerun Search' and 'Edit Search'.

CAS SciFinderⁿ主界面

Good Afternoon

灵活检索选项

Antitumor

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

+ Add Advanced Search Field

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

Search CAS Lexicon Build powerful searches using CAS concepts, chemical classes, and taxonomy.

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

Recent Search History

April 15, 2025

Search Reactions Semaglutide

4:42 PM

Rerun Search

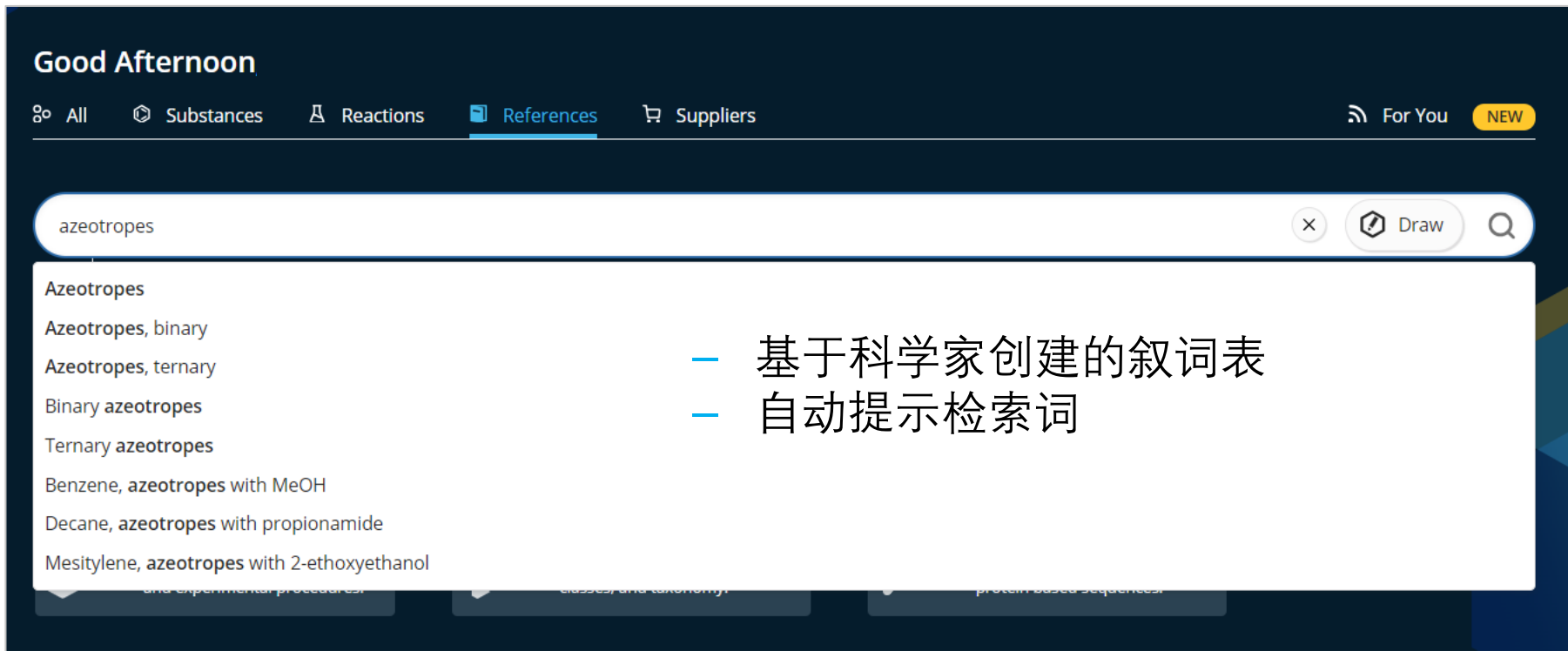
Edit Search

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

- 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)



The screenshot shows the CAS database interface. At the top, there's a navigation bar with tabs: All, Substances, Reactions, References (selected), and Suppliers. A 'For You' button with a 'NEW' tag is also present. Below the navigation bar is a search bar containing the text 'azeotropes'. To the right of the search bar are icons for 'x', 'Draw', and a search icon. A dropdown menu is open below the search bar, displaying a list of suggestions:

- Azeotropes
- Azeotropes, binary
- Azeotropes, ternary
- Binary azeotropes
- Ternary azeotropes
- Benzene, azeotropes with MeOH
- Decane, azeotropes with propionamide
- Mesitylene, azeotropes with 2-ethoxyethanol

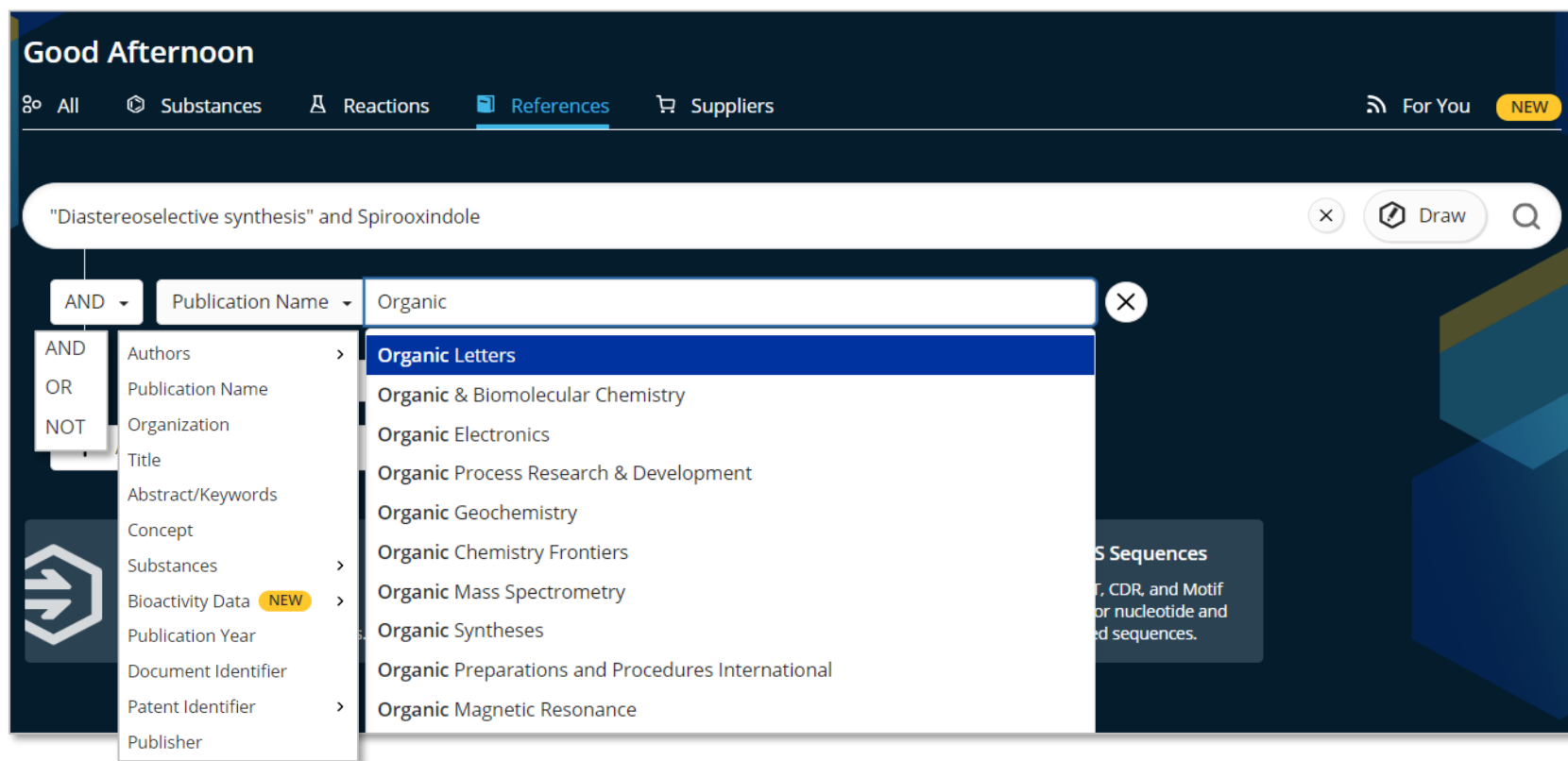
Below the search bar, there are two blue lines of text:

- 基于科学家创建的叙词表
- 自动提示检索词

高级检索： 高效实现多项自定义组合检索

可单独使用，或联用以下检索方法：

- 关键词、物质名称、CAS Registry Number®、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

Search CAS Lexicon [Learn more about CAS Lexicon searching.](#)

Coupling reaction

^ Preferred Concept

☒ Coupling reaction
This will search synonyms: 2-Component **coupling reaction**; **Coupling**; ...
[View more synonyms](#)

^ Broader Concepts (1) [Select All](#)

☐ Reaction

^ Narrower Concepts (30) [Select All](#)

☒ Azo coupling reaction
☒ Castro-Stephens coupling reaction
☒ Catellani reaction
☒ Chan-Lam coupling reaction
☐ Corey-Posner reaction
[View All](#)

^ Related Concepts (5) [Select All](#)

☐ 1,4-Diphenyl-1,3-butadiyne
☐ 4,4'-Dimethylbiphenyl
☒ Coupling reaction catalysts
☐ Coupling reaction enthalpy
☐ Coupling reaction kinetics

Coupling reaction - Preferred Concept

^ Coupling reaction - Narrower Concepts (4)

Azo coupling reaction
Castro-Stephens coupling reaction
Catellani reaction
Chan-Lam coupling reaction

^ Coupling reaction - Related Concept (1)

Coupling reaction catalysts

快速浏览CAS科学家标引的:

- 概念词 (Concepts)
- 物质

在CAS Lexicon词库层级中选择
适合的主题词:

- Preferred Concept
- Broader Concepts
- Narrower Concepts
- Related Concepts

文献检索： 主题词+结构联合检索

The screenshot displays the CAS SciFinder web interface. At the top, the search bar contains 'References' and 'Antitumor'. A blue arrow points from the 'Antitumor' text to a chemical structure of 2-azaspiro[4.4]nonan-1-one, which is shown in a pop-up window with 'Edit Drawing' and 'Remove' buttons. Below the search bar, the text 'References search for "Antitumor" + drawn structure' is visible. The left sidebar shows filter options under 'Filter Behavior' and 'Search Within Results'. The main content area displays search results, including the title 'Synthesis of 2-azaspiro[4.4]nonan-1-ones via phosphine-catalyzed [3+2]-cycloadditions' and the title 'Notoamides A-D: prenylated indole alkaloids isolated from a marine-derived fungus, Aspergillus sp.'.

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

Filter Behavior

Filter by Exclude

Search Within Results

Concept

CA Section

Life Science Data

CAS Content

Publication Year

Language

Publication Name

Organization

Author

Document Type

Substance Role

Database

Filter Content Report

Download filter data from this result set.

Filtering: Publication Year: 2010 to No Max X Substance Role: Pollutant X Clear All Filters

5,248 Results

Sort: Relevance View: Partial Abstract

1

Relevance

Times Cited

Accession Number: Ascending

Accession Number: Descending

Publication Date: Newest

Publication Date: Oldest

Life in the "Plastisphere": Microbial Communities on Plastic Debris

By: Zettler, Erik R.; Mincer, Tracy J.; Amaral-Zettler, Linda A. Environmental Science & Technology (2013), 47(13), 7137-7146 | Language: English, Database: CAPLUS and MEDLINE

Plastics are the most abundant and persistent pollutants in the environment. Documented impacts in some ocean ecosystems is poorly understood. Marine debris (PMD) collection and analysis is analyzed with SEM and next-generation sequencing to characterize the attached microbial communities. A diverse microbial community of heterotrophs, autotrophs, predators, and symbionts was unveiled, a community referred to as the Plastisphere. Pits visualized in...

View More

Full Text

Substances (2) Reactions (0) Citing (1,743) Citation Map

2

Microplastics Can Change Soil Properties and Affect Plant Performance

By: de Souza Machado, Anderson Abel; Lau, Chung W.; Kloas, Werner; Bergmann, Joana; Bachelier, Julien B.; Faltin, Erik; Becker, Roland; Goerlich, Anna S.; Rillig, Matthias C. Environmental Science & Technology (2019), 53(10), 6044-6052 | Language: English, Database: CAPLUS and MEDLINE

Screening of the impacts of microplastics across ecological levels

Plant performance

Soil microbiome

Biomass allocation, leaf & root traits

Microbial activity & plant-microbe symbiosis

Microplastics can affect biophys. properties of the soil. However, little is known about the cascade of events in fundamental levels of terrestrial ecosystems, i.e., starting with the changes in soil abiotic properties and propagating across the various components of soil-plant interactions, including soil microbial communities and plant traits. We investigated here the effects of six different microplastics (polyester fibers, polyamide beads, and four

- 聚类筛选项一目了然
- 高效定位所需信息
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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

.....

文献结果集的处理、下载、保存及定题追踪

References for 9003-07-0

Substances Reactions Citing Knowledge Graph

Filter Behavior: Filter by Exclude

Filtering: Concept: Surface area X Publication Year: 2022 to No Max X Document Type: Journal X Substance Role: Pollutant X

199 Results Sort: Relevance View: Partial Abstract

1

Short-term effects of polyethene and polypropylene microplastics on soil phosphorus and nitrogen availability
By: Li, Haixiao; Liu, Le
Chemosphere (2022), 291(Part_2), 132984 | Language: English, Database: Cplus and MEDLINE

Microplastics are an emerging threat to soils, but little is known about their effects on soil nitrogen (N) and phosphorus (P) cycling. In this study, a three-month soil incubation experiment has been conducted to analyze the effects of polyethene (PE) and polypropylene (PP) microplastics in sizes of 0-1 mm and 1-5 mm on soil available phosphate, nitrate, and ammonium contents under different fertilization regimes. Soil phosphorus and nitrogen availability were continuously determined in-situ by ion-exchange membrane method during the incubation. Microplastic surface chem. composition and the ...

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Full Text Substances (7) Reactions (0) Citing (44) Citation Map

支持结果集的:

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文献详情

Synthesis and Cellular Profiling of Diverse Organosilicon Small Molecules

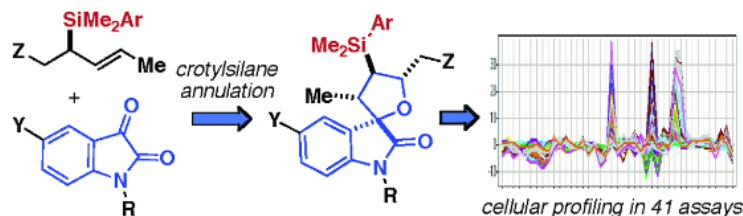
82 133 178 Citation Map

In this Reference

- Concepts
- Substances
- Cited Documents

By: Franz, Annaliese K.; Dreyfuss, Philip D.; Schreiber, Stuart L.
DOI: 10.1021/ja067552n

Small-mol. synthesis coupled with cellular profiling using multidimensional screening can be used to assess the impact of varying stereochem. and appendage contexts on biol. activity. The synthesis and cellular profiling of chiral organosilicon small mols. derived from a crotylsilane annulation pathway. Incorporating a main-group element, such as Si, within the chiral environment of a more complex product could provide new structures where the distinctive chem. properties of Si may contribute to new biol. activity. The annulation of various indole-2,3-dione (isatin) reagents with functionalized crotylsilanes provides efficient access to spiro-oxindole structures for biol. evaluation. The modular placement of aryl iodide functional groups in the isatin component can be used in appending processes for further substitution, such as conversion of the aryl iodide to various amido functionalities using the Buchwald amidation. The high-feature biol. signatures revealed from multidimensional screening provide a 1st quant. glimpse of the rich activities of Si-containing small mols. within varying stereochem. and appendage contexts. Also, these signatures demonstrate the validity of implementing functional group and stereochem. diversity (cf. differential performance of enantiomeric pairs of products).



Keywords: growth inhibition hepatocellular carcinoma cell chiral organosilicon crotylsilane annulation; crotylsilane annulation cellular profiling; mol crystal structure spirocyclic silane preparation

View Source Full Text

Publication Information Journal View More

Expand All | Collapse All

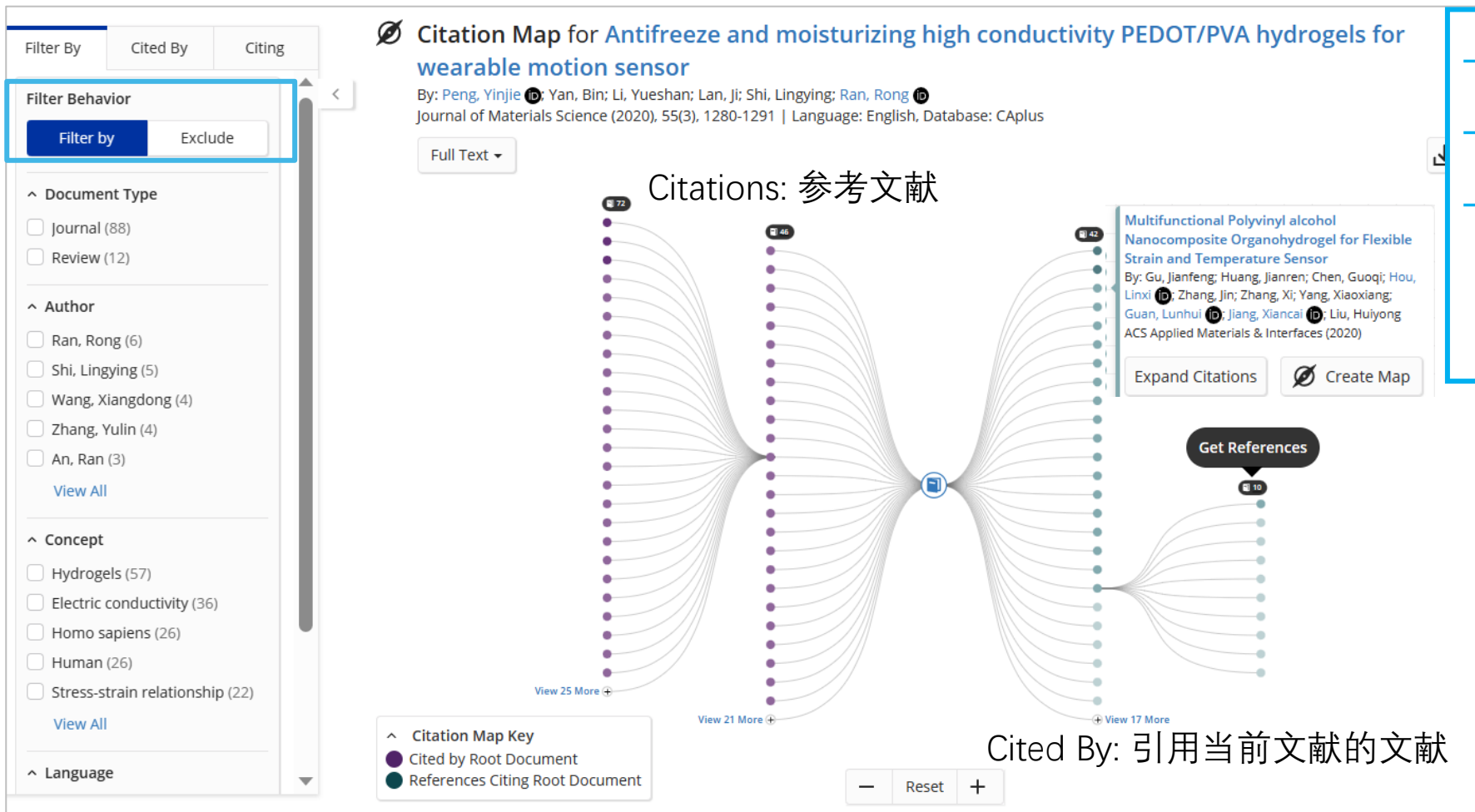
- CAS Concepts
- MEDLINE® Medical Subject Headings
- Supplementary Concepts
- Substances
- Cited Documents

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 CPlus、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

引文地图：便捷地获取关联文献



- 通过聚类选项筛选引文
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- 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 and sulfite"

Substances Reactions Citing Knowledge Graph

We are displaying the most relevant results.
[Learn about result relevance.](#)
[Load All Results](#)

Filtering: Database: CHEMZENT × Clear All Filters

47 Results Sort: Relevance View: Partial Abstract

1

The reduction of sulfite by yeast enzymes
By: Wainwright, T.
Chemisches Zentralblatt (1963), 134(31), 13233-13233 | Language: German, Database: CHEMZENT

Machine Translated: Yeast extracts containing **sulfite** (I) to sulphide reducing in 6 protein fractions fragmenting. The complete Syst required out last still I, phosphate buffer and NADPH. It is neither H₂S from SH-Verbb. such as cysteine, more oxidizing it NADPH; it is of cyanide and arsenite inhibited. 4 Prot a, A, O, β and δ, with waters dialysierbar, a and y are without phosphate unstable. Cn.y are against heat and at low pH relatively stable.

ChemZent Full Text Substances (3) Reactions (0) Citing (0) Citation Map

2

Sulfite reduction by yeast enzymes
By: Wainwright, T.
Chemisches Zentralblatt (1963), 134(24), 10127-10127 | Language: German, Database: CHEMZENT

Machine Translated: Authors describes 2 **enzymes** (I and II) in extracts from brauerei yeast in common, but not solely, in presence of Triphosphopyridinnucleotid in phosphate buffer **sulfite** to sulphide slightly **reduce**. Product I is stable to heating to 55 °,

Database
☐ CAplus (1,117)
☐ MEDLINE (893)
☒ CHEMZENT (47)

1963 E. Enzymologie. Gärung 13233

Biosynthese von Purinen. 28. Mitt. Der Wirkungsmechanismus von Adenylsuccinase. Richard W. Miller und John M. Buchanan. (J. biol. Chemistry 237, 491–96, Febr. 1962; engl.) — 27. vgl. vorst. Referat. — Durch Inkubation von Di-Na-Fumarat (I), 5-Amino-1-ribosylimidazolyl-(4)-carbonsäureamid-5'-phosphat (II) u. Adenylsuccinase (III) in Ggw. von Cysteinhydrochlorid u. H₂O werden ³H-N-[5-Amino-1-ribosylimidazolyl-(4)-carbonyl]-L-asparaginsäure-5'-phosphat (³H-IV) u. analog aus AMP ³H-6-[L-1,2-Dicarboxyethylamino]-9-β-D-riboseylpurin-5'-phosphat (³H-V) sowie aus I, NH₃ u. H₂O in Ggw. von Aspartase (VI) aus *Bacterium cadaveris* ³H-L-Asparaginsäure (³H-VII) dargestellt. Durch enzymat. Spaltung von ³H-IV bzw. ³H-V mit N-[5-Amino-1-ribosylimidazolyl-(4)-carbonyl]-L-asparaginsäure-5'-phosphatkinosynthetase bzw. III erhaltene ³H-VII wird durch VI zu inakt. I gespalten, wodurch die Stereospezifität der enzymat. Addition von II u. Adenosinmonophosphat an I, der Spaltung von VII in I sowie der Einbau von jeweils 1 Atom ³H in die β-Stellung von ³H-VII bzw. des VII-Teiles von ³H-IV u. ³H-V bewiesen wird. Analog der Darst. von ³H-V wird in D₂O ³H-V erhalten u. durch Vgl. mit der Spaltungs-Geschw. von V u. ³H-V das Fehlen eines Isotopeneffektes festgestellt. Dieses Ergebnis beweist, daß das β-Proton der Aspartateinheit in einer von der geschwindigkeitsbegrenzenden Rk. verschiedenen Stufe eingebaut bzw. abgespalten wird. F. Heller. 4210 □

Thermische Denaturierung von Kaltblüter-Enzymproteinen. G. Siebert, A. Schmitt, R. v. Malortie und E. Adloff. (Experientia [Basel] 16, 491–92, 1960; Mainz, Univ., Physiolog.-chem. Inst.; dt.) — Die therm. Denaturierung von Enzymen (I) von in fangfrischem Zustand (auf See) tiefgefrorenem Dorschfilet erfolgte so, daß die gewünschte Temp. in einer wassergefüllten Durchströmungs-App. während 60 Min. einwirkte. Durch Extrapolation wurde die Temp. ermittelt, bei der 50% der Anfangsaktivität zerstört sind. Untersucht wurden für glykolyt. I ein mit 1% ig. KCl-Lsg. erhaltener Extrakt, für proteolyt. Enzyme ein mit 1% ig. LiBr-Lsg. hergestelltes Homogenisat. Die Meßtemp. bzw. die Temp. der 50% ig. Zerstörung sind: *Kathepsin* (II) im Rohextrakt: 37 bzw. 44°; II teilweise gereinigt: 37, 52°; *Glycylglycylindipeptidase* (III): 40, 42°; *Milchsäuredehydrogenase*: 25, 52°; *Aldolase*: 25, 41°; *Triosephosphatdehydrogenase*: 25, 51°; *Enolase*: 25, 45°; *Brenztraubensäurekinase*: 25, 51°; *Isocitronensäuredehydrogenase*: 25, 30°. — III aus Rindermuskel: 40, 46°. — Die Ermittlung der Q₁₀-Werte im Bereich von +37° bis –13° für II u. III führte ebenfalls zu dem Schluß, daß es keinen allg. Unterschied in der Hitzebeständigkeit der I von Warmblütern u. Kaltblütern gibt. A. Hesse. 4210 ◇

Enzymkonservierung in frostsubstituierten Gewebeschnitten. Jeffrey P. Chang und Samuel H. Hori. (J. Histochem. Cytochem. [Baltimore] 10, 592–95, 1962; Houston, Tex., Univ. of Texas, M. D. Anderson Hosp. and Tumor Inst., Dep. of Path., Sect. of Exp. Path.; engl.) — Von den Aktivitäten alkal. u. saurer Phosphatase, Adenosintriphosphatase, 5'-Nucleotidase, Glucose-6-phosphatase (I), Succinatdehydrogenase, Di- u. Triphosphopyridinnucleotiddiaphorase konnten im Falle I noch 22% u. im Falle der übrigen Enzyme mehr als 70% in frostsubstituierten Gewebeschnitten der Rattenleber nachgewiesen werden. In mit Formol-Ca-Aceton fixierten oder gefriergetrockneten Geweben waren die Enzymaktivitäten niedriger. L. Macher. 4210 ◇

CAS PatentPak[®]: 专利流程解决方案

- 唯一提供在专利中快速定位物质相关化学信息的工具
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 - 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
- 通过CAS PatentPak浏览器，快速定位专利PDF文件中的重要物质页码信息，迅速找到难以查找的化学信息，可为研究人员节省一半以上的时间
- 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

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

208

0

3

Citation Map

Save

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In this Reference

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

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, polymyxins, and lipopeptides.

Keywords: antibacterial toll like receptor agonist; TLR agonist antibacterial combination therapy bacterial infection

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Publication Information • Patent

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专利族信息

Patent Family

Patent	Language	Kind Code	PatentPak Options	Publication Date	Application Number	Application Date
WO2015011254	English	A1	PDF PDF+ Viewer	2015-01-29	WO2014-EP66007	2014-07-25
EP3024476	English	A1		2016-06-01	EP2014-749736	2014-07-25
EP3632458	English	A1	PDF	2020-04-08	EP2019-207885	2014-07-25
US20160151453	English	A1	PDF	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

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优先权信息

Publication Information • Patent

Patent Number WO2015011254	Publication Date 2015-01-29	Application Number WO2014-EP66007	Application Date 2014-07-25	Kind Code A1
Assignee INSERM (Institut National de la Sante et de la Recherche Medicale), France Universite de Droit et de la Sante de Lille 2, France Centre National de la Recherche Scientifique (CNRS), France Institut Pasteur de Lille, France Universite de Lille 1 Sciences et Technologies, France ETH Zurich, France Universidad de la Republica, France	Source World Intellectual Property Organization CODEN: PIXXD2	Database Information AN: 2015:167126 CAN: 162:266207 CAplus	Language English	

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, CAS RN 1003-68-5, and CAS RN 1229705-85-4. The main area shows a patent document (CN 109535200 A) with chemical structures and text in Chinese. A blue arrow points from a chemical structure in the patent to a detailed view of the same structure on the right.

CAS PatentPak:

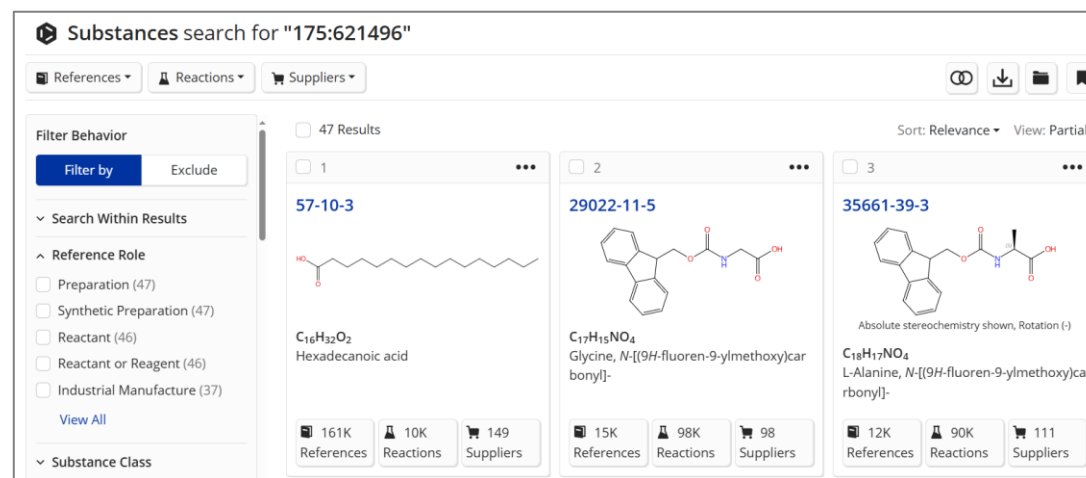
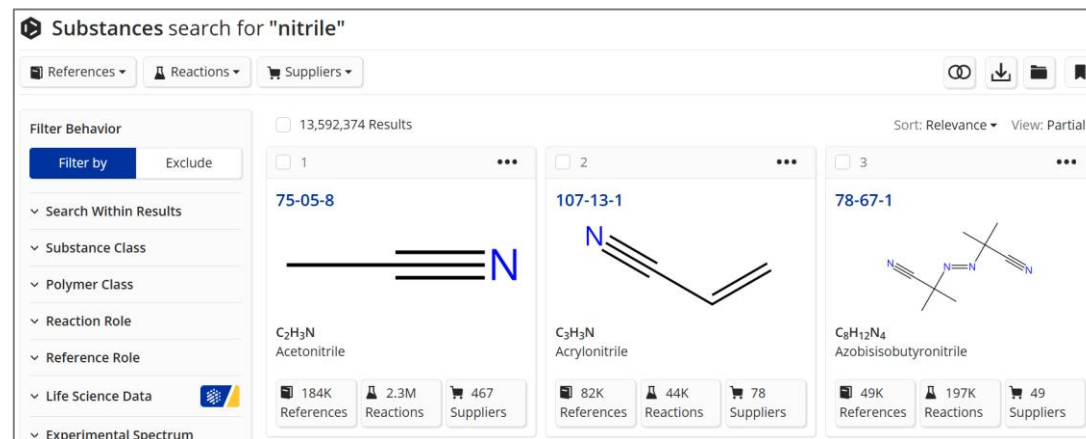
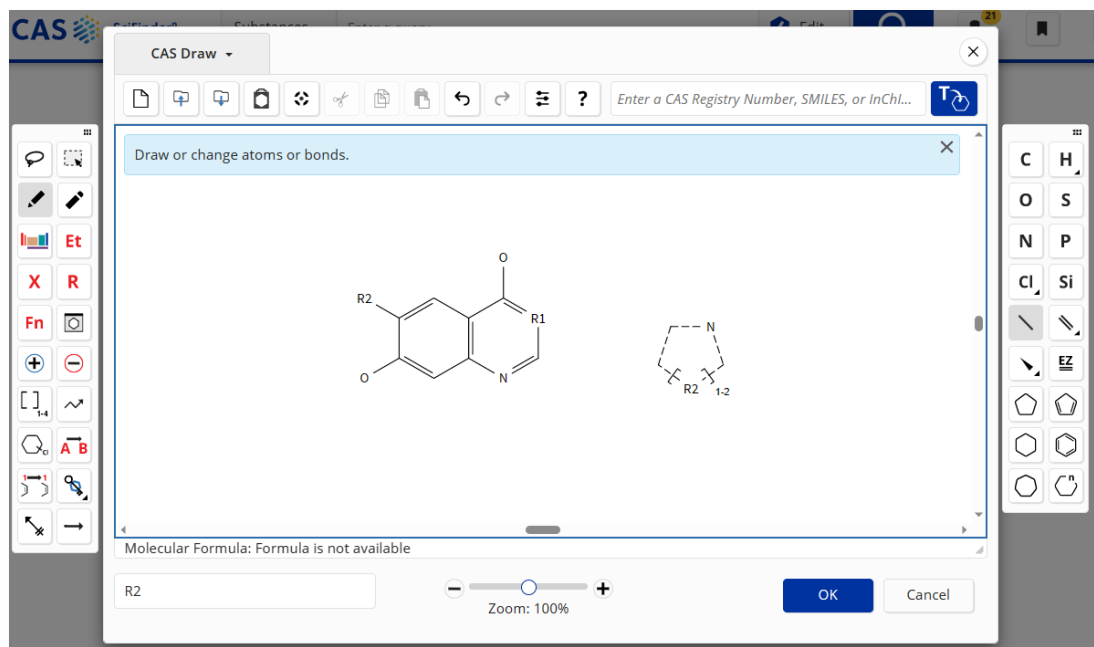
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- 阅读熟悉语言撰写的等同专利
- 快速理解专利

This panel provides a detailed view of the chemical structure 2H-Pyran, 2-[4-bromo-2-(trifluoromethyl)phenoxy]tetrahydro-. It includes the CAS RN (2306115-70-6) and a list of actions: Substance Detail, Reactions (2), Synthesize (1), Create Retrosynthesis Plan, References (1), and Suppliers (0). At the bottom, there are buttons for 'Edit Structure', 'Reset', and a download icon.

CAS Substances: 物质检索

物质检索方法

- 物质或文献标识符
- 结构式
- 高级检索：分子式、属性值、谱图数值检索
- 官能团和物质类别



属性值、谱图数值联用检索物质

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

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

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

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

+ Add Advanced Search Field

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

Substances search for 3 Advanced Fields

References Reactions Suppliers

Filtering: Bioactivity Data: 3 Selected X Clear All Filters

15 Results Sort: Molecular Formula: Ascending View: Partial

1	2	3
296262-16-3 <chem>Cc1nc(C)c2c(n1)sc(CS(=O)(=O)CC(=O)O)c2</chem> $C_{10}H_{10}N_2O_2S_2$ 2-[(5,6-Dimethylthieno[2,3-d]pyrimidin-4-yl)thio]acetic acid 5 References 42 Reactions 44 Suppliers	723-46-6 <chem>Cc1cc2nc(S(=O)(=O)Nc3ccc(N)cc3)no2</chem> $C_{10}H_{11}N_3O_3S$ Sulfamethoxazole 24K References 961 Reactions 120 Suppliers	1631737-39-7 <chem>C[C@H]1O[C@@H]2C[C@H](O)[C@H](O)[C@H]2O[C@H]1</chem> $C_{10}H_{15}N_3O_5$ (2R,3R,4S,5R)-4,5-Dihydro-5-(hydroxymethyl)-3'-methylspiro[furan-2(3H),7'(6'H)]-... Absolute stereochemistry shown, Rotation (-) 2 References 22 Reactions 0 Suppliers
4	5	6
442571-27-9 <chem>Cc1nc(C)c2c(n1)sc(CS(=O)(=O)CC(=O)O)c2</chem> $C_{10}H_{10}N_2O_2S_2$ 2-[(5,6-Dimethylthieno[2,3-d]pyrimidin-4-yl)thio]acetic acid 5 References 42 Reactions 44 Suppliers	1927010-88-5 <chem>CC[C@H]1C(=O)OC(=O)C1</chem> $C_5H_8O_3$ 1927010-88-5 24K References 961 Reactions 120 Suppliers	697787-29-4 <chem>Cc1cc2nc(NC(=O)Nc3ccc(N)cc3)no2</chem> $C_{10}H_{11}N_3O_3$ 697787-29-4 24K References 961 Reactions 120 Suppliers

Filter Behavior: Filter by Exclude

Reaction Role: Product (15), Reactant (11), Reagent (1), Catalyst (1)

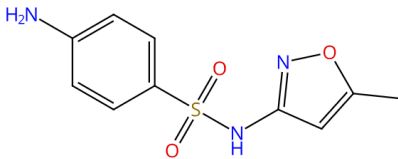
Reference Role: Preparation (15), Synthetic Preparation (15), Biological Study (14), Pharmacological Activity (14), Uses (14)

Bioactivity Data: Structure Activity Relationships (15), Toxicity (2), Absorption, Distribution, Metabolism, Excretion (1)

物质详情

CAS Registry Number: [723-46-6](#)

30K 1,050 110 View in [CAS BioFinder](#)



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

Key Physical Properties

Key Physical Properties	Value	Condition
Molecular Weight	253.28	-
Melting Point (Experimental)	167 °C	-
Boiling Point (Predicted)	482.145±55.00 °C	Press: 760.00 Torr
Density (Experimental)	1.08 g/cm ³	-
pKa (Predicted)	5.811±0.50	Most Acidic Temp: 25 °C

Experimental Properties | Spectra

Expand All | Collapse All

- Other Names and Identifiers
- Experimental Properties
- Experimental Spectra
- Structure Activity Relationships [CAS LIFE SCIENCES](#)
- Absorption, Distribution, Metabolism, and Excretion Data [CAS LIFE SCIENCES](#)
- Toxicity [CAS LIFE SCIENCES](#)
- Predicted Properties
- Predicted Spectra
- Bioactivity Indicators
- Target Indicators
- Regulatory Information
- GHS Hazard Statements
- Additional Details

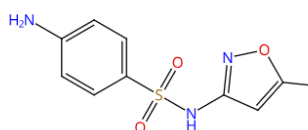
Structure Activity Relationships [CAS LIFE SCIENCES](#)

Clear All Filters Knowledge Graph

Target	Function	Parameter	Value	Disease	Organism	Assay	Source
Cytochrome P450 2C9	Inhibitor	Activity	-17.1 %	-	HOMO SAPIENS	View Detail	(1) CAS
Cytochrome P450 3A4	Inhibitor	Activity	40 %	-	HOMO SAPIENS	View Detail	(2) CAS
Cytochrome P450 2A6	Inhibitor	Activity	45 %	-	HOMO SAPIENS	View Detail	(2) CAS
Cytochrome P450 2C9	Inhibitor	Activity	95 %	-	HOMO SAPIENS	View Detail	(3) CAS
Cytochrome P450 2C9	Inhibitor	Activity	69 %	-	HOMO SAPIENS	View Detail	(3) CAS
Cytochrome P450 3A4	Inactivator	Enzymatic activity (CYP)	Percentage of P450 enzyme inactivation < threshold at 10 %	-	HOMO SAPIENS	View Detail	(4) CAS

Assay Data [CAS LIFE SCIENCES](#)

← Prev (6 of 27) Next →

Ligand 723-46-6  C₁₀H₁₁N₃O₃S Benzenesulfonamide, 4-amino-N-(5-methyl-3-isoxazolyl)-	Target Cytochrome P450 3A4 Assay Name - Procedure Percent inactivation of Cytochrome P450 3A4 in human liver microsomes upon incubation for 30 min in 0.1 M sodium phosphate buffer in presence of 250 mM G6P, 20 units/ml G6PDH and 25 mM beta-NADP+ at 100 uM compound concentration using 2.5 uM midazolam as substrate Assay Comment - Condition - Parameter Enzymatic activity (CYP) Value Percentage of P450 enzyme inactivation < threshold at 10 % Measurement Remarks Percentage of P450 enzyme inactivation < threshold at 10 % Ligand Dose - Biological System HOMO SAPIENS; liver microsomes; HUMAN Source Combination of GSH trapping and time-dependent inhibition assays as a predictive method of drugs generating highly reactive metabolites By: Nakayama, Shintaro; Takakusa, Hideo; Watanabe,
---	---

CAS Markush检索

CAS SciFinder

Substances Enter a query...

Patent Markush search for drawn structure

References

Patent Markush Match

As Drawn (2)

Substructure (5)

Filter Behavior

Filter by Exclude

Patent Office

United States (1)

World Intellectual Property Organization (1)

CA Section

Pharmacology (1)

Steroids (1)

Filter Content Report

Download filter data from this result set.

2 Results

1

US20060025393

Steroid derivatives, including cholesterol derivatives, for the treatment of prostate cancer

Assignee: The University of Chicago
United States, US20060025393 A1 2006-02-02 | Language: English, Database: CAplus

Patent claim 1

PatentPak Full Text

171: alkyl <containing 1-12 C> (opt. substd.)
577: alkyl <containing 1-20 C> (substd. by G22)
623: alkyl <containing 1-12 C> (opt. substd.)

2

WO2000066611

Preparation of steroid derivatives

Assignee: Arch Development Corporation
World Intellectual Property Organization, WO2000066611 A1 2000-11-09 | Language: English, Database: CAplus

Patent claim 1

PatentPak Full Text

437: alkyl <containing 1-8 C> (opt. substd. by 1 or more G3)

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CAS SciFinder

Substances Enter a query...

Substances search for drawn structure

References Reactions Suppliers

Structure Match

As Drawn (0)

Substructure (0)

Similarity (239K)

Chemscape Analysis

Visually explore structure similarity with a powerful new tool.
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Create Chemscape Analysis

Filter Behavior

Filtering: Similarity: 85-89 X Number of Compounds

56 Results

1 90 ...

126209-83-4

Absolute stereochemistry shown

C₃₀H₄₉ClO₂
Olean-13(18)-ene-3,23-diol, 22-

3 References 4 Reactions 0 Suppliers

2 89 ...

58545-27-0

Absolute stereochemistry shown

C₃₀H₄₉ClO₂
Olean-12-ene-3,28-diol, 12-chloro-

1 Reference 1 Reaction 0 Suppliers

3

25697

Absolute stereochemistry shown

C₂₅H₄₂ClO
1-Chloro-2-methyl-19-nor-10,13-epoxy-5α-androstane-3β,17β-diol

1 Reference

CAS Sequences: 分子生物学解决方案

- 超过13亿条序列
- 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

BLAST: 检索DNA、RNA、蛋白质、肽

 **Search CAS Sequences**  CAS LIFE SCIENCES

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

BLAST

CDR

Motif

Clear Search

MHAAITSMKREHPSHLLAVVPASAPRYEEGYNTENEKTHQKENLLDLSLP

Advanced Sequence Search ▼

高级检索参数设置

Upload Sequence (.fasta or .txt)

Sequence Type:

Nucleotide

Protein

Search Within:

☐ Nucleotides

☒ Proteins

☒ Include NCBI Sequences

 Search Sequences

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

选择是否包含NCBI中的序列

CAS Sequences: CDR和Motif检索

CDR: 抗体或细胞中的互补决定区

 Search CAS Sequences 

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

BLAST CDR Motif Clear Search

CDR1 RASQSVSGSRFTYMH

CDR2 YASILES

CDR3 QHSWEIPPWT

支持单个或多个CDR序列检索并用

Upload Sequence (.fasta or .txt)

☐ Include NCBI Sequences

 Search Sequences

Motif: 检索未指定的氨基酸和核苷酸，且更适合检索短序列。

 Search CAS Sequences 

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

BLAST CDR Motif Clear Search

[SG]x{4}GK[DT]

- []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

Advanced Sequence Search 

Sequence Type: Nucleotide Protein

☒ Include NCBI Sequences

 Search Sequences

CAS Reactions: 反应检索

- 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
 - 自然语言

Reactions search for "175:621496"

References

Filter Behavior

Filter by Exclude

Search Within Results

Yield

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

133 Results

Group: By Scheme Sort: Relevance View: Collapsed

Scheme 1 (1 Reaction)

Steps: 1 Yield: 92%

Suppliers (104)

Suppliers (41)

Suppliers (60)

Expand Scheme

Reactions search for "Semaglutide"

References

Filter Behavior

Filter by Exclude

Search Within Results

Yield

- ☐ 90-100% (5)
- ☐ 80-89% (8)
- ☐ 70-79% (3)
- ☐ 50-69% (3)
- ☐ 30-49% (3)

366 Results

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

Scheme 1 (3 Reactions)

Steps: 11-12

910463-68-2
Image Not Available

Suppliers (112)

Suppliers (429)

Suppliers (45)

Expand Scheme

Reactions References Suppliers

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

Draw

Reactions search for drawn structure

References

Structure Match

As Drawn (74)

Substructure (46K)

Similarity (18K)

Filter Behavior

Filter by Exclude

Search Within Results

74 Results

Group: By Scheme Sort: Relevance View: Collapsed

Scheme 1 (5 Reactions)

By Scheme

By Document

By Transformation

Relevance

Publication Date: Newest

Publication Date: Oldest

Yield

Number of Steps: Ascending

Number of Steps: Descending

Suppliers (69)

Suppliers (45)

Expand Scheme

利用自然语言检索反应，降低检索难度

AI识别检索意向，智能识别反应的底物、产物、溶剂、试剂、催化剂、物质类别等信息

Reactions search for "synthesis of aldehyde catalyzed by Palladium diacetate"

References

Filter Behavior

Filter by Exclude

Search Within Results

Non-Participating Functional Groups

Experimental Protocols

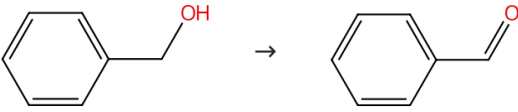
Catalyst

- Palladium diacetate (111K)
- Grubbs second generation catalyst (56K)
- Grubbs' catalyst (53K)
- Monopotassium monosodium tartrate tetrahydrate (53K)
- Water (27K)

111,878 Results

Group: By Scheme Sort: Relevance View: Collapsed

Scheme 1 (63 Reactions) Steps: 1 Yield: 100%



Suppliers (168) Suppliers (81)

31-480-CAS-15515097 Steps: 1 Yield: 100%

1.1 Reagents: Oxygen

Catalysts: Pyridine, Palladium diacetate

Solvents: Acetic acid; 2 h, 1 atm, 60 °C

Highly selective monodisperse molecular

By: Choi, K

New Journal

Full Text

Reactions search for "synthesis of paclitaxel catalyzed by triphenylphosphine"

References

Filter Behavior

Filter by Exclude

Search Within Results

Non-Participating Functional Groups

- Alcohol (1)
- Alkene (1)
- Carboxylic ester (1)
- Cyclic alcohol (1)
- Cyclic alkene (1)

View All

Experimental Protocols

- Synthetic Methods (6,976)

7,007 Results

Group: By Document Sort: Relevance View: Collapsed

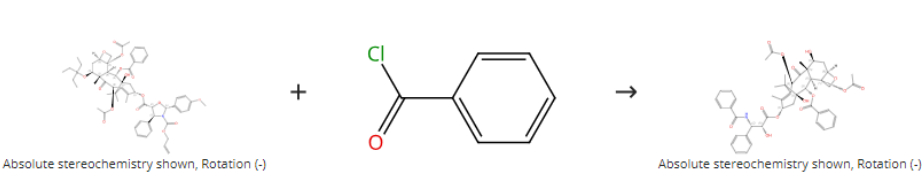
1

Method for producing side chain precursor of paclitaxel and docetaxel

Assignee: Ensulko Sugar Refining Co., Ltd.

World Intellectual Property Organization, WO2017006573 A1 2017-01-12 | Language: Japanese, Database: CAPLUS

PatentPak Full Text View 27 Related Reactions



Absolute stereochemistry shown, Rotation (-) Suppliers (84) Suppliers (126)

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

Filter Behavior

Filter by Exclude

Search Within Results

Yield

Reaction Scale

Reaction Notes

Number of Steps

Reagent

Solvent

Experimental Protocols

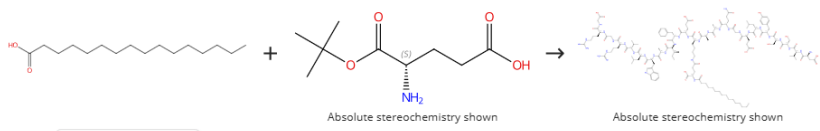
Synthetic Methods (132)

Non-Participating Functional Groups

Reaction Mapping

Stereochemistry

Scheme 4 (2 Reactions) Steps: 6-7



Suppliers (149)

Suppliers (86)

View Reaction Detail Steps: 7

1.1 Reagents: [Diisopropylcarbodiimide](#), [N-Hydroxysuccinimide](#)
Solvents: [Acetonitrile](#), [Dichloromethane](#); overnight, rt

1.2 Reagents: [Diisopropylethylamine](#); overnight, rt

2.1 Reagents: [Diisopropylcarbodiimide](#), [N-Hydroxysuccinimide](#)
Solvents: [Acetone](#); overnight, rt

2.2 2 d, rt

3.1 Reagents: [Ethylenediaminetetraacetic acid](#)
Solvents: [Water](#); overnight, rt

[View All](#)

[Experimental Protocols](#)

Copper(II) lysinate and pseudoproline assistance in the convergent synthesis of the GLP-1 receptor agonists [Liraglutide](#) and [Semaglutide](#)

By: [Guryanov, Ivan](#) et al

Organic Process Research & Development (2021), 25(7), 1598-1611

Full Text

Procedure

1. Add a solution of HOSu (9.0 g, 0.0780 mol) in 100 mL of acetonitrile and DIC (12.2 mL, 0.0780 mol) to a solution of palmitic acid (20.0 g, 0.0780 mol) in 100 mL of dichloromethane.
2. Stir the reaction mixture overnight.
3. Filter the precipitate.
4. Add H-Glu-OtBu (17.4 g, 0.0858 mol) and DIPEA (27.2 mL, 0.0156 mol).
5. Stir the reaction mixture overnight.
6. Evaporate the solvent and dissolve the oil in 200 mL of ethyl acetate.
7. Wash the product with 10% KHSO₄ (3 × 300 mL) and 300 mL of water.
8. Dry the solution over MgSO₄, and evaporate the solvent.
9. Recrystallize the product twice from hot petroleum ether.

Transformation	Acylation of Nitrogen Nucleophiles by Carboxylic Acids
Scale	gram

Characterization Data

1-(1,1-Dimethylethyl) hydrogen *N*-(1-oxohexadecyl)-L-glutamate

Proton NMR Spectrum

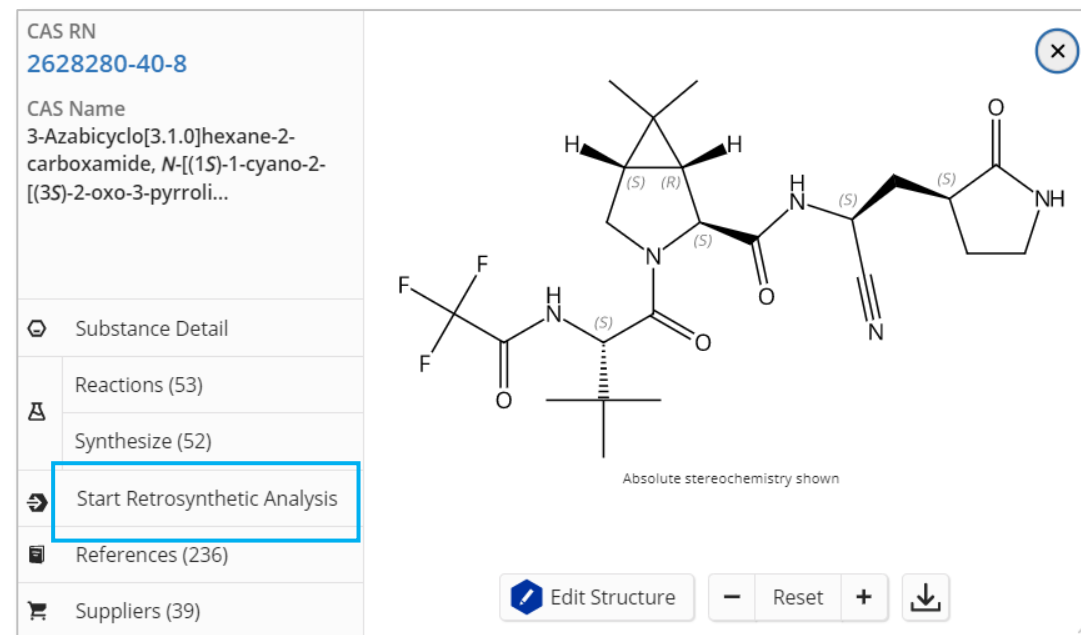
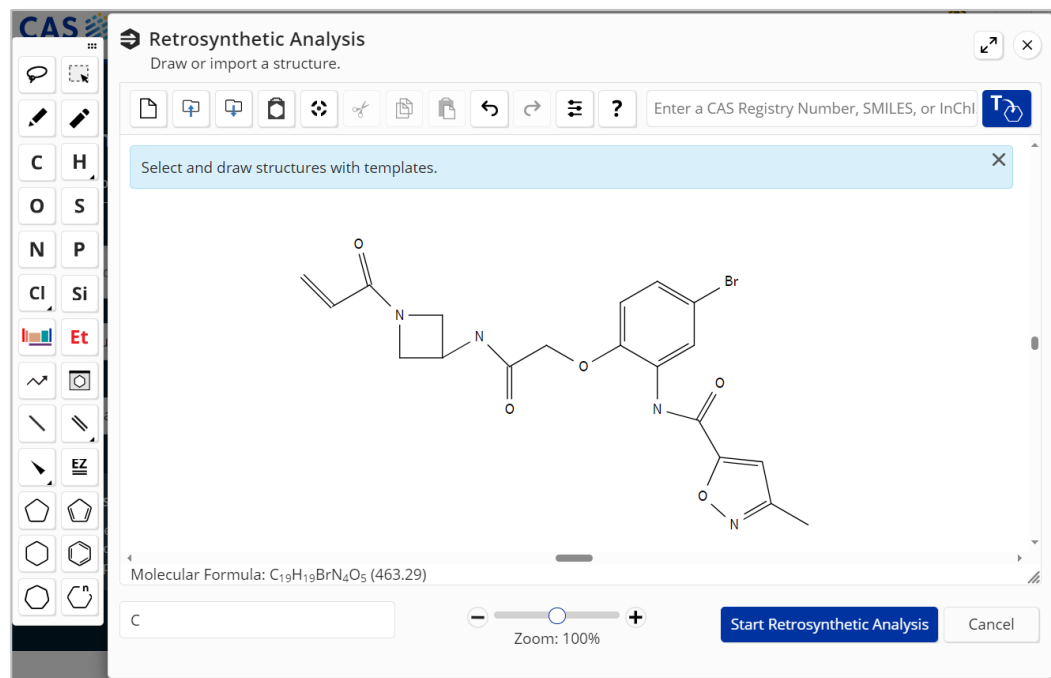
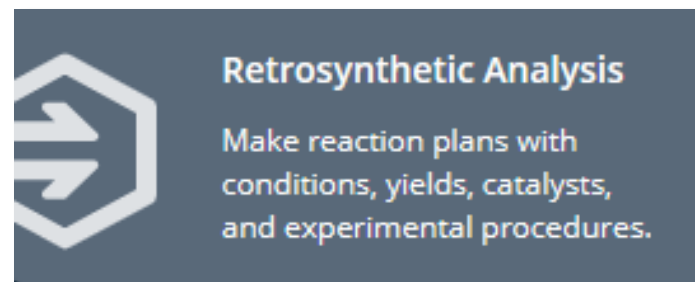
(200 MHz, CDCl₃): δ = 0.87 (m, 3H, CH₃), 1.25 (s, 24H, 12CH₂), 1.47 (s, 9H, tBu), 1.62 (m, 2H, CH₂), 2.05–1.70 (m, 2H, CH₂), 2.30–2.15 (m, 2H, CH₂), 2.50–2.35 (m, 2H, CH₂), 4.65–4.45 (m, 1H, CH), 6.25 (d, J = 8 Hz, 1H, NH).

IR Absorption Spectrum

(KBr): ν_{max} 3376, 2909, 2842, 1722, 1707, 1649, 1522 cm⁻¹.

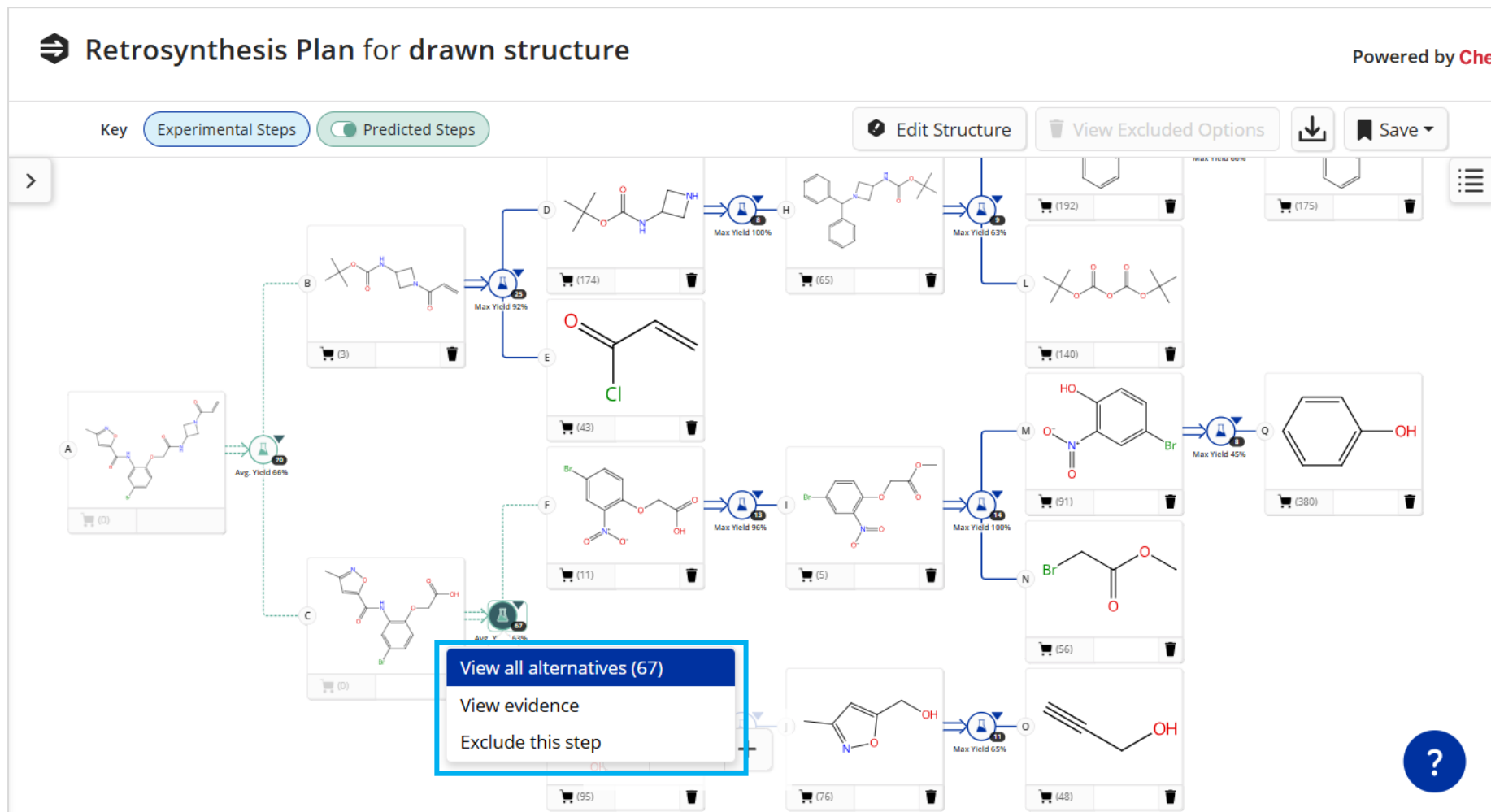
CAS Retrosynthesis Tool: 逆合成工具

- 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: 逆合成工具

获得逆合成路线后，可以查看每一步反应的依据和备选路线



Project项目管理：支持多人协作

可管理文献、物质，并分享项目给其他用户

The screenshot shows the 'Project Collaborators' dialog box. It has a search bar at the top with the placeholder text 'Add project collaborators using an email address...'. Below this, there is a table of collaborators. The first collaborator is 'Dex' with the email 'dxdu@mail.ustc.edu.cn' and the role 'Administrator'. The role is currently set to 'Viewer'. There is a dropdown menu for the role, showing 'Editor', 'Viewer' (selected), and 'Remove Access'. A blue arrow points from the 'Add' button in the 'Collaborators' section of the main interface to the '+Add' button in the dialog.

Name	Email	Role
Dex	dxdu@mail.ustc.edu.cn (Pending)	Viewer

设置项目成员权限

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 SciFinderⁿ
- 分析方法解决方案CAS Analytical Methods
- 配方/制剂解决方案CAS Formulus

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CAS SciFinderⁿ登录账号相同)

The screenshot displays the CAS Methods website interface. At the top, it says "Good Morning" and features a search bar with the placeholder text "Search for keywords, matrices or analyte." Below the search bar, there are two main sections: "Advanced Search" and "Explore Methods". The "Advanced Search" section includes a magnifying glass icon and the text "Search methods using criteria like keywords, analytes, matrices and more." The "Explore Methods" section includes a binoculars icon and the text "Search methods using criteria like method categories and subcategories." To the right of these sections, there is a detailed view of the "Explore Methods" interface. This view includes a "Method Category" list with options like "Agricultural Applications / Bioassays", "Biomolecule Isolation", "Environmental Analysis", "Food Analysis", "Fuels / Geology / Biofuels", "Historical Analysis / Dating", "Miscellaneous", "Organic Compound Analysis" (highlighted), "Organometallics / Inorganics", "Pharmacology / Toxicology", "Polymer Analysis", and "Water Analysis". The "Method Subcategory" list includes "Active Pharmaceutical", "Chiral Separation" (highlighted), "Natural Product Isolation", and "Organic Compound Analysis". There is also an "Include Keywords" section with a text input field and a "+ Add Another Keyword" button. A "Search Methods" button is located at the bottom right of the "Explore Methods" section.

Good Morning

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.

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

- 主题检索或分类浏览;
- 筛选分析物、介质、方法类别、分析技术等

方法分类共13大类，45小类：包括农业应用、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

分析方法详情

Filter By

^ Analyte

^ Matrix

☐ Gasoline (2)

☒ Kerosene (2)

☐ Diesel fuel (1)

☐ Natural gas condensates (1)

☐ Petroleum (1)

^ Method Category

^ Technique

^ Validation

☐ Concentration (2)

☒ Limit of Detection (2)

☐ Accuracy (1)

☐ Limit of Quantitation (1)

☐ Linearity Range (1)

View All

^ Year

Analysis of Titanium in Kerosene by Inductively coupled plasma mass spectrometry

实验原料

CAS Method Number
1-135-CAS-84928

Method Category
Petroleum Product Analysis

Technique
Inductively coupled plasma mass spectrometry

Analyte

Tin
Cadmium
Silver
Mercury
Iron
View All ^

Matrix

Natural gas condensates
Kerosene
Gasoline

Material

Fused silica capillary of 180 µm i.d. (375 µm o.d.)
Heated spray chamber
Low port-to-port dead volume micro-injection valve
View All ^

Reagent

Biological Reagent

Validation

数据有效性

Linearity Range
0.250 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
3 µg/kg (gas condensate), Titanium
1 µg/kg (gas condensate), Vanadium
10 µg/kg (gas condensate), Chromium
20 µg/kg (gas condensate), Iron
0.4 µg/kg (gas condensate), Silver
1 µg/kg (gas condensate), Cadmium
0.5 µg/kg (gas condensate), Tin
2 µg/kg (gas condensate), Mercury
0.2 µg/kg (gas condensate), Lead

实验仪器 操作步骤

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 O₂ 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 thermostating at a desired temperature).
3. Use a dual syringe pump (Model 140C, Applied Biosystems, Foster City, CA, USA) to assure a stable delivery of xylene into the ICP at a flow rate of 20 µL/min without the use of a splitter to limit the solvent consumption.
4. Use another pump (Smartline Pump 1000, Knauer, Berlin, Germany) to introduce xylene containing 50 µg/kg indium and cerium (internal standards) at a flow of 10 µL/min.
5. Add molybdenum at 50 µg/kg in each matrix analyzed to monitor the ionization efficiency.
6. Measure ⁴⁵Ti, ⁵¹V, ⁵⁷Fe, ¹⁰⁷Ag, ¹¹²Cd, ¹¹⁴Cd, ²⁰²Hg, ²⁰⁸Pb and ⁵³Cr isotopes in light petroleum matrices, ⁹⁸Mo as a spiked analyte, ¹¹⁴In as the internal standard and ⁵⁸Ni in the CRM 1634c.
7. Set the ICP-MS operating parameters as follows: RF power: 1300 W; Ar nebulizer gas: 0.8 L/min and auxiliary O₂ flow: 45 mL/min.
8. Inject 5 µL of sample using a low port-to-port dead volume micro-injection valve (8125i, Rheodyne, Rohnert Park, CA, USA) fitted with a 5 µm sample loop into the carrier xylene at a flow rate of 20 µL/min.
9. Circulate the heating liquid (glycol/water) through a Neslab RTE-111 (Thermo Fisher Scientific, Waltham, MA) thermostat.
10. Control oxygen gas flow by a mass flow controller, mixed with the carrier argon nebulizer gas via a T-connection prior to nebulization to prevent carbon deposition on the sampler and skimmer cones of the instrument.
11. Set the integration time per isotope to 20 ms, record three readings per analysis and perform each injection in triplicate.
12. Perform quantitation by standard addition method using the multielement S21 standard at concentrations of 10, 25, 50, 100, 150 and 200 µg/kg.

Source 文献来源

JOURNAL

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; Merdrignac, 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 Abstract ^ Full Text ^

直观的分析方法对比

Compare Methods		
Expand All Collapse All		
	1	2
Title	Analysis of Chromium in Barium sulfate by Electrothermal atomic absorption spectroscopy	Analysis of Chromium 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	Chromium	Chromium
Matrix	Barium sulfate	Barium sulfate
Other Materials	Nitric acid; Pyrolytic coated graphite tubes	Nitric acid
Equipment Used	Atomic absorption spectrometer, AAS ZEEnit 60, Analytik Jena, Jena, Germany; Solid sampling system, SSA-5, Analytik Jena, Jena, Germany; Microbalance, M2P, Sartorius, View All	Atomic absorption spectrometer, AAS ZEEnit 60, Analytik Jena, Jena, Germany; Microbalance, M2P, Sartorius, Gottingen, 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	Chromium determination in pharmaceutical grade barium sulfate by solid sampling electrothermal atomic absorption spectrometry with Zeeman-effect background View All	Chromium determination in pharmaceutical grade barium sulfate by solid sampling electrothermal atomic absorption spectrometry with Zeeman-effect background View All
Preparation	Collection and preparation of samples - Obtain the powdered pharmaceutical grade BaSO₄ samples from pharmaceutical industries and dry them in a conventional oven at 105 °C × 2 h. - Spike the samples by addition of chromium reference solutions of 0.48 µg/g. Preparation of standard solutions - Prepare the reference solutions daily by serial dilutions of stock chromium (Cr) solutions (1 g/L Cr in 2% HNO₃). View Less	Preparation of nitric acid solution - 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. Collection and preparation of samples - Obtain the powdered pharmaceutical grade BaSO₄ samples from pharmaceutical industries and dry them in a conventional oven at 105 °C × 2 h. Preparation of standard solutions - Prepare the reference solutions daily by serial dilutions of stock chromium (Cr) solutions (1 g/L Cr in 2% HNO₃). View Less
Method	Direct solid sampling (DSS) - electrothermal-atomic absorption spectrometric (ETAAS) analysis Carry out the chromium determinations using a model View All	Acid digestion procedure using nitric acid Perform sample acid digestion (extraction) in closed quartz vessels using a high pressure model Multiwave View All
Linearity Range	100 - 1800 µg	
Limit of Detection	2.4 µg	
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

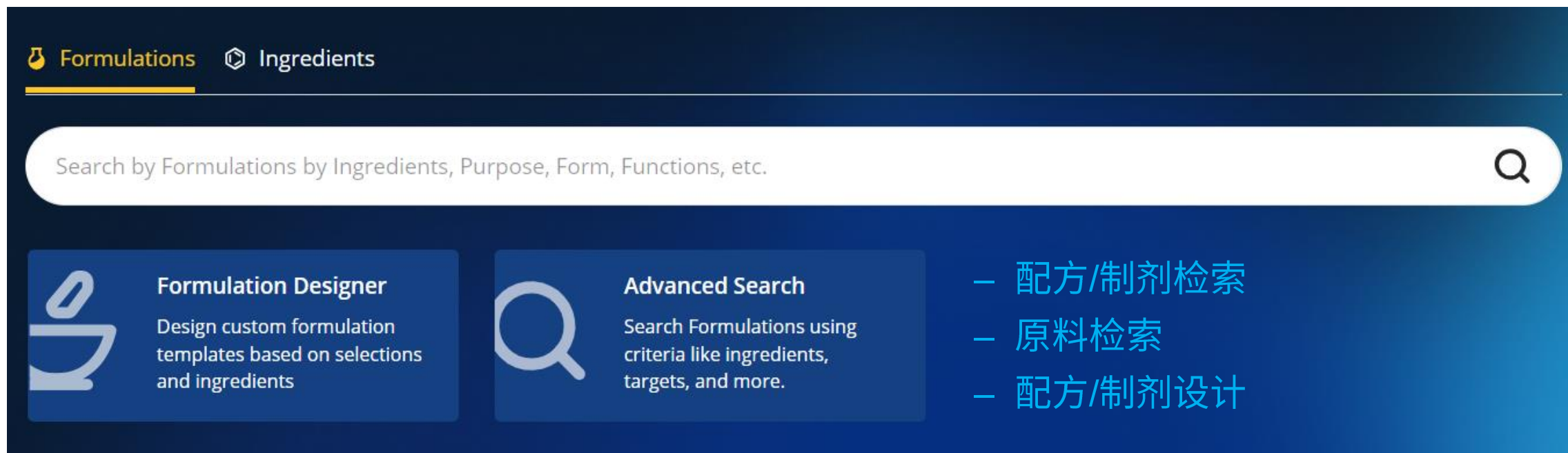
- CAS（美国化学文摘社）及CAS SciFinder Discovery Platform简介
- 新一代科研创新信息工具CAS SciFinderⁿ
- 分析方法解决方案CAS Analytical Methods
- 配方/制剂解决方案CAS Formulus

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、产品说明书中标引的配方信息
- 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 SciFinderⁿ登录账号相同)



Formulations Ingredients

Search by Formulations by Ingredients, Purpose, Form, Functions, etc.

Formulation Designer
Design custom formulation templates based on selections and ingredients

Advanced Search
Search Formulations using criteria like ingredients, targets, and more.

- 配方/制剂检索
- 原料检索
- 配方/制剂设计

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

- 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

Paclitaxel-Piperine Pharmaceutical Nanoparticles: Drug Delivery Systems or Antitumor Agents

Download Save

Purpose	Target	Delivery Route	Physical Form	Source
Antitumor agents, Drug delivery systems	paclitaxel, Homo sapiens, Mammary gland neoplasm, Ovary neoplasm, lungs cancer	Oral drug delivery systems	Particles	View

U.S. Pharmacopeia

Formulation Ingredients [Expand All Groups](#) [Collapse All Groups](#) [Feedback](#)

Component	Function	Amount Reported	Optionality
Group: paclitaxel nanoparticles	-	-	Mandatory
Piperine	bioenhancers	-	Mandatory

More Formulations like this...

Pharmaceutical Composition

Purpose: Pharmaceutical formulations

Target: Homo sapiens

Delivery Route: Oral drug delivery syst...

Physical Form: Capsules

Pharmaceutical Composition

Purpose: Pharmaceutical formulations

Target: Homo sapiens

Delivery Route: Oral drug delivery syst...

Physical Form: Capsules

Pharmaceutical Composition:

Purpose: Pharmaceutical component

Target: Homo sapiens

Delivery Route: -

Physical Form: -

Pharmaceutical Composition:

Anticancer

Purpose: Antitumor agents

Target: Homo sapiens

Delivery Route: -

Physical Form: -

Process

the paclitaxel-piperine pharmaceutical nanoparticles is prepared by: adding the Eudragit and drug which contain paclitaxel is dissolved in acetone to obtain the organic phase; pouring it into the aqueous phase having surfactant which is composed of polyvinyl alcohol and distilled water to produce the oil in water type emulsion; crushing it into the nanoparticles using sonicator-driven external energy; the organic solvent is evaporated during magnetic stirrer for 2 hours at 300 rpm under the atmospheric conditions to the obtain paclitaxel nanoparticles is prepared; the obtained paclitaxel nanoparticles are combined with piperine.

Experimental Activity		
Descriptor	Notes	Details
area under curve(0-infinite)	the plasma concentration of paclitaxel after oral administration of nanoparticle to 10 rats, was evaluated in terms of area under curve(0-infinite).	12315.2 ± 916.3
area under curve(0-t)	the plasma concentration of paclitaxel after oral administration of nanoparticle to 10 rats, was evaluated in terms of area under curve(0-t).	10335.3 ng. h/mL ± 983.2 ng. h/mL
clearance rate of drug	the plasma concentration of paclitaxel after oral administration of nanoparticle to 10 rats, was evaluated in terms of clearance rate of drug (CL).	6.9 L/h ± 1.8 L/h
cytotoxicity test	the cytotoxic action of cell lines was determined by high throughput MTT assay and the cell growth was measured by calorimetric assay.	cell apoptosis and better anticancer activity.
drug diffusion	the drug diffusion of the composition was evaluated at 0.5 hours.	9.15 %
drug diffusion	the drug diffusion of the composition was evaluated at 1 hours.	9.55 %
drug diffusion	the drug diffusion of the composition was evaluated at 5 hours.	22.2 %
drug diffusion	the drug diffusion of the composition was evaluated at 9 hours.	29.02 %
drug diffusion	the drug diffusion of the composition was evaluated at 24 hours.	38.15 %
drug diffusion	the drug diffusion of the composition was evaluated at 48 hours.	46.02 %
drug diffusion	the drug diffusion of the composition was evaluated at 72 hours.	58.18 %
drug entrapment efficiency	-	56.12 %
drug loading	-	55.71 %
half-life	the plasma concentration of paclitaxel after oral administration of nanoparticle to 10 rats, was evaluated in terms of half life.	11.5 h ± 2.2 h
mean residence time	the plasma concentration of paclitaxel after oral administration of nanoparticle to 10 rats, was evaluated in terms of mean residence time.	15.3 h ± 2.6 h
particle size	the particle size of the nanoparticle was evaluated by transmission electron microscopy.	130.29 nm
Source Journal		
Synthesis and characterization of paclitaxel nanoparticles for drug delivery		
Materials Today: Proceedings		
Language: English		
Location: Article page 2, 3, 4, 5, Table 1, 2, 3		
Full Text View in CAS SciFinder		

不同制剂或配方信息的直观对比

Comparing your Formulations			P 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	Group: Ti-TNTs wire implants Function: implant Amount Reported: Optionality: Mandatory Ti wires Function: additives Amount Reported: - Optionality: - Acetone Function: Solvents Amount Reported: - Optionality: - Ethanol Function: Solvents Amount Reported: - Optionality: -	Group: surgical implant Function: Amount Reported: Optionality: Mandatory Dental implants Function: - Amount Reported: - Optionality: - Plates Function: - Amount Reported: - Optionality: - pin Function: - Amount Reported: - Optionality: -	

- 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

原料检索及配方设计

- 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

Ingredients search for "PEG"

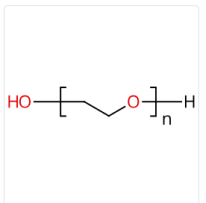
Filter by

- Industry
 - Agrochemical
 - Cleaning & Surfactant Products
 - Cosmetics & Personal Care
 - Food & Related
 - Inks, Paints, & Coatings
- Regulatory Information
 - ANMAT (1)
 - Cosing: Cosmetic Ingredient Inventory (1)
 - Drug Master File List (1)
 - EPA Pesticide Inactive Ingredients (1)
 - EPA Safer Chemical

2 Results

1

CAS RN: 25322-68-3
[View Details](#)



(C₂H₄O)_nH₂O

Polyethylene glycol 
[PEG](#)

Key Physical Properties	Value	Condition
Melting Point (Experimental)	50-58 °C	-
Boiling Point (Experimental)	227 °C	-
Density (Experimental)	1.128 g/cm ³	Temp: 25 °C

Commonly Used As: Plasticizers; Solvents; Coating materials; Binders; Lubricants...

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

[Get Formulations](#) [Get Suppliers](#) [Add to Formulation Designer](#)

- 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

Base Selections				
Industry	Purpose	Physical Form	Active or Featured Ingredient	
Cosmetics & Personal Care	Skin care products	Gels	Vitamin A polyethylene glycol	
Edit	Edit	Edit	Edit	

Template				
Function	Ingredient	Regulatory 	Top Alternatives	Amounts
Active or Featured Ingredient:	Vitamin A	ANMAT	-	Amount not available ×
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 ×
Function: Carriers	Polyethylene glycol View More Alternatives	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% ×
Function: Skin conditioners	Glycerol View More Alternatives	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% ×

- 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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