

CAS SCIFINDER®

常见问题解答

2022年8月



CAS SciFinder[®]是美国化学文摘社（CAS）出品的新一代的权威科学研究工具，是化学及相关学科智能研究平台，提供全球全面、可靠的化学及相关学科研究信息和分析工具。CAS SciFinder[®] 由国际科学家团队追踪全球科技进展，每日收录汇总、标引、管理着世界上的专利、科技期刊等内容，并通过 CAS SciFinder[®] 平台提供的先进检索技术高效揭示重要的技术信息，确保研究人员及时同步全球重要的研究进展。CAS SciFinder[®] 涵盖了化学及相关领域，如化学、生物、医药、材料、食品、应用化学、化学工程、农学、高分子、物理等多学科、跨学科的科技信息；收录的文献类型包括期刊、专利、会议论文、学位论文、图书、技术报告、评论、预印本和网络资源等。

CAS SciFinder[®] 独特内容和特色：

- **提升文献检索效率：**业界最先进的检索引擎之一，将文献检索时间缩短一半，获得更精确的结果，提高检索效率。
- **高效设计合成计划：**充分利用全球最大的单步和多步反应数据库之一，全面考量反应条件、产率、催化剂和实验步骤，高效设计出合成计划（可节省一半的时间）。
- **Synthetic Methods 合成方法解决方案：**Synthetic Methods 是CAS SciFinder[®]中的模块，是世界上最大合成方法合集之一，涵盖顶级期刊及专利中的合成制备信息，提供合成方法的每步详细操作信息，以易于阅读的表格形式展示实验详情，包括实验操作步骤、实验原料、实验条件、实验量级、反应转化类型、合成产物谱图信息、合成产物形态等
- **CAS PatentPak[®]专利分析解决方案：**CAS PatentPak 是 CAS SciFinder[®]中的模块，服务于科研人员和知识产权人士。PatentPak 在定位和分析大量专利中的化学结构方面，可以为研究人员节省一半以上的时间。PatentPak 是加速化学专利分析最可靠的工具之一；迄今为止只有 PatentPak 采用人工标引——研究人员可以快速识别专利中难以发现的物质（例如，表格化合物和图形图像内的化合物）。使用 PatentPak 可以访问 CAS REGISTRYSM——世界上最全面的可公开获取的物质信息集合。
- **逆合成路线设计工具Retrosynthesis：**基于全球最大的化学反应数据合集CAS REACTIONS结合先进的算法和人工智能，综合多种因素如原子经济性、收率、绿色、成本等为已被报道分子/未被报道分子提供实验验证或预测的逆合成路线。为合成化学家节省时间并提供新的思路和见解。
- **支撑生物学研究：**生物序列检索工具Biosequences Search 提供超过12亿条可检索生物序列，可进行 FTO 检索、侵权检索。
- **可视化检索结果：**用户友好的可视化工具可以帮助用户快速做出更好的决策，这些工具可以精确定位趋势、模式和异常值，帮助将信息转化为洞察。
- **CAS REGISTRY:**全球最大的物质数据合集，收录自19世纪初至今公开披露的超过1.9亿

个独特的物质（包括合金、配合物、矿物、混合物、聚合物和盐），CAS登记号被誉为化学物质的黄金标准，是向WHO提交INN申请时必须提供的信息，被广泛地应用在科研界及商务流程中。

- **CAS Reactions:** CAS创立的全球最大化学反应合集，收录1840年以来源自专利和非专利文献的1.4亿多条单步和多步反应。CAS的科学家在标引化学反应过程中提供了独特的增值信息，包括：实验安全信息、反应类型、反应条件及详细的实验操作步骤等，节省了用户从全文中总结、归纳相关反应信息所花费的时间。
- **马库什结构:** CAS是全球唯一提供专利马库什结构的机构。从全球64家专利授权机构公开的专利中提取超过130万个可检索及浏览的马库什结构。一个马库什结构可能涵盖数千甚至数万个化合物，提升了用户进行化合物结构新颖性和创造性检索的能力。

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账号问题

Q1: 如何登录 CAS SciFinder[®]?

A1: 如果已经有 CAS SciFinder 账号, 请使用 CAS SciFinder 账号和密码登录即可。如果没有 CAS SciFinder 账号, 则请与贵单位 CAS SciFinder 管理人员联系获取账号。CAS SciFinder[®] 的登录网址为: <https://scifinder-n.cas.org>。

Q2: 我是一名学生。作为新用户, 怎样才能访问 CAS SciFinder[®]?

A2: 学校的新用户需要先通过学校的 CAS SciFinder[®] 注册链接注册账号后才能使用 CAS SciFinder[®]。账号的具体注册方法, 请访问所在学校图书馆网页或咨询所在学校图书馆的负责老师。

Q3: 我可以在智能设备上使用 CAS SciFinder[®] 吗?

A3: 请使用授权 IP 范围内的网络登录智能设备, 即可以使用。

Q4: 我在上一家单位 (学校) 曾经注册过 CAS SciFinder[®] 账号, 在目前的单位能够继续使用吗?

A4: 不可以, 到新单位后需要重新申请 (注册) 账号。

Q5: 我在校注册的 CAS SciFinder[®] 帐号可以在校外机构使用吗?

A5: 不可以。只能供自己和研究课题使用, 禁止为他人代查。

Q6: 我毕业之后可以继续使用在学校注册的 CAS SciFinder[®] 账号吗?

A6: 不可以。在学校注册的帐号仅能在学校就读期间使用, 毕业后则不能再使用。

Q7: 我可以与他人分享我的 CAS SciFinder[®] 账号吗?

A7: 不可以, 自己注册的帐号仅能自己使用, 不可与他人分享。

Q8: 忘记登录密码怎么办?

A8: 登录 SciFinder-n.cas.org, 在当前页面点击 Can't log In, 在弹出页面根据要求填写相应信息找回密码即可。如果您无法自己找回密码, 请联系 china@acs-i.org, 由相关客服人员协助您解决密码找回问题。

Q9: 为什么显示此 IP 没有授权?

A9: 用户需要在授权 IP 范围内才能使用 CAS SciFinder[®]。如果您在使用时遇到 IP 未被授权的问题, 请使用网址 <http://web.cas.org/cgi-bin/casip> 查询您的电脑 IP 地址, 并将页面截图及您的 SciFinder 登录账号及注册 SciFinder 时使用的单位域名邮箱发送至 china@acs-i.org, 便于 CAS 客服人员尽快解决您的问题。

Q10: 我在本校注册的 CAS SciFinder[®] 帐号可以在校外机构使用吗?

A10: 不可以, 只能在学校授权 IP 范围内使用, 禁止在本校外的任何机构使用。如果您正在某商业机构实习或为某商业机构工作, 也不允许在这些商业机构中使用在学校注册的 CAS SciFinder[®] 帐号。

Q11: CAS SciFinder[®] 有并发用户限制吗?

A11: 没有并发用户数限制。

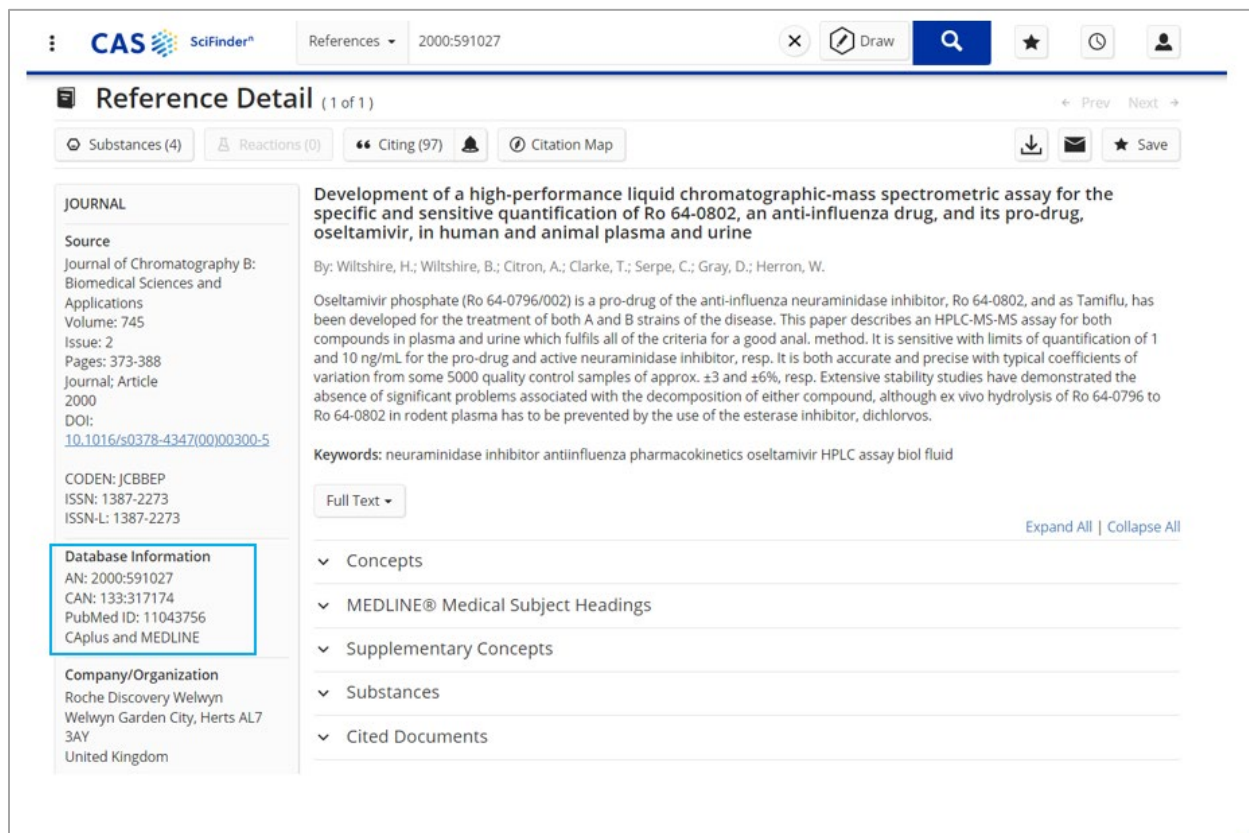
Q12: 如果 CAS SciFinder[®] 账号无法登陆, 如何联系 CAS 中国大陆地区客服?

A12: CAS SciFinder[®] 账号无法登陆或者其他有关 CAS SciFinder[®] 的问题, 可拨打电话或者发送邮件与 CAS 中国大陆区客服人员联系: 电话: 010-62508026/7, 电子邮箱: china@acs-i.org。

文献检索

Q1: CAS SciFinder® 文献结果集中会出现重复的文献吗?

A1: CAS SciFinder® 涵盖的两个文献数据库 CAplus 和 Medline 有部分重复的文献。但是在展示的结果集中，已经自动进行了去重处理。对于 CAplus 和 Medline 重复收录的文献，在其文献详情页面左侧会看到如下信息：



The screenshot displays the 'Reference Detail' page for the article: 'Development of a high-performance liquid chromatographic-mass spectrometric assay for the specific and sensitive quantification of Ro 64-0802, an anti-influenza drug, and its pro-drug, oseltamivir, in human and animal plasma and urine'. The article is from the 'Journal of Chromatography B: Biomedical Sciences and Applications', Volume 745, Issue 2, pages 373-388, published in 2000. The DOI is 10.1016/s0378-4347(00)00300-5. The article is indexed in several databases, including CAplus and MEDLINE. The 'Database Information' section is highlighted with a blue box, showing the following information:

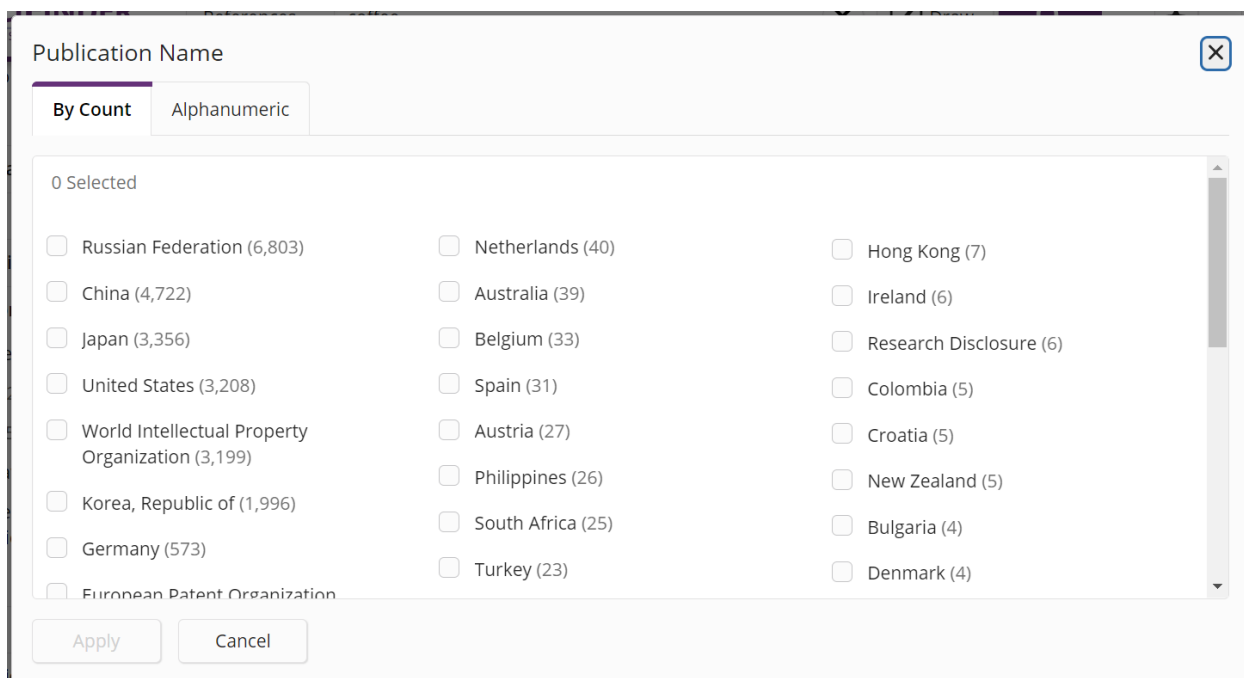
- AN: 2000:591027
- CAN: 133:317174
- PubMed ID: 11043756
- CAplus and MEDLINE

Q2: 在文献结果集中，如何使用专利号筛选文献?

A2: 点击文献结果集页面左下角的 Search Within Results, 在输入框中输入专利号，然后点击 Find, 即完成用专利号筛选文献。

Q3: 专利文献结果集中，如何通过专利国家对结果进行筛选?

A3: 在文献结果集页面左侧选择 Publication Name, 在弹出的页面即可根据国家进行筛选，如下图所示。



Q4: 如何在 CAS ScFinder[®] 中查看专利法律状态?

A4: 在 CAS SciFinder[®] 专利文献详情页面, 可以查看专利的 Kind Code。

Q5: 当我选择 References 检索时, 输入物质名称和结构检索有何差别?

A5: 输入物质名称时, 在检索时会进行同义词的扩展 (即物质的其他名称), 命中的结果中可能是名称完全匹配的结果, 也可能是匹配片段名的结果。用名称检索时, 检索的范围为标题、摘要、Concepts, Substances、Substance Role 等。

输入结构时, 匹配的是文献中 Substances 部分展示的结构, 可以通过 As Drawn 或 Substructure 来筛选文献结果。如下如所示:

The screenshot displays the CAS SciFinder[®] search results page. At the top, there is a search bar with the text "References" and "Enter a query...". Below the search bar, there are several icons for editing, searching, and saving. The main content area shows a list of references. The first reference is highlighted, showing its title, authors, and abstract. The chemical structure of the compound is displayed above the first reference, with an "Edit Drawing" button below it. The interface also includes a sidebar with filters for "Structure Match", "Filter Behavior", "Document Type", "Substance Role", and "Language".

Q6: CAS SciFinder[®] 中布尔逻辑算符运算的优先性?

A6: 在 SciFinder-n 中支持使用布尔逻辑算符 AND、OR 和 NOT。默认的运算优先顺序为 OR > AND > NOT。在使用逻辑算符时，可以使用括号 ()，括号里的算符优先运算。如：(A NOT B) AND C，则会优先运算括号中的 NOT，然后再运算 AND。

Q7: 如何筛选晶型研究相关的文献?

A7: 在 CAS SciFinder[®] 主页选择 References, 在输入框中输入关键词，比如 crystal polymorphs, crystal structure, 获取晶型研究的相关文献。可以在文献结果集左侧，通过 Concept 列表查看和晶型研究相关的概念词，对文献结果进行精炼。

如果涉及某具体物质的晶型研究，则可以采用文本与结构联用的方式进行检索。

Q8: 在物质结果集页面筛选出具有潜在生物活性物质后，如何获得它们的合成工艺专利?

A8: 点击获得具有潜在生物活性物质结果集页面顶端的 References, 获得报道这些物质的文献结果集。然后在文献结果集页面左侧的 Substance Role 选项中勾选 Preparation, Process。最后在文献结果集页面左侧 Document Type 选项中勾选 Patent, 即可得到物质的合成工艺专利。

Q9: 如何检索某个年份的 ADC 技术的专利, 尤其是寻找关于如何偶联 (conjugate) 的专利?

A9: 有 2 种方法实现, 分别按以下步骤进行。

方法一:

1. 在 CAS SciFinder[®] 主页选择 References, 在输入框中输入相关检索式, 如, “antibody drug conjugate” or ADC, 检索后得到文献结果集
2. 点击文献结果集页面左侧的 Filter by, 在 Document Type 选项下勾选 Patent, 将结果限定为专利
3. 点击专利文献结果集页面左侧 Filter by, 再点击 Concept 下的 View All, 在弹出窗口中勾选 crosslinking agents 等相关词语, 以获得更精准的检索结果。
4. 点击专利文献结果集页面左侧 Filter by, 在 Publication Year 下勾选需要的某个年份即可

方法二:

1. 如果确定使用关键词 crosslinking, 则可以按方法一所述第一步的输入框中输入检索式 (“antibody drug conjugate” or ADC) and crosslinking
2. 按照方法一所述的第 2 和第 4 步操作即可。

Q10: 如何检索某机构关于合成和工艺方面的研究文献?

A10: 按以下步骤操作:

1. 在 CAS SciFinder[®] 主页面选择 References, 再点击 Add Advanced Search Field
2. 点击 Select, 在弹出列表中选择 Organization Name, 然后在输入框中输入机构名, 检索后得到该机构的文献
3. 点击文献结果集左侧 Filter by, 在 Search Within Results 下面的输入框中输入 preparation/synthesis/process/catalysis 等类似关键词来筛选合成和工艺方面的研究文献。

如果需要查看具体的反应, 可以点击文献结果页眉下方的 Reactions 获取文献中涉及的重要反应结果。

Q11: 如何检索与 pvdF 修饰相关的文献?

A11: 点击 References, 在输入框中输入主题词进行检索, 例如 modified pvdF。如果对于修饰的方法有明确的限定, 可以利用布尔逻辑算符进一步精准构建检索式, 例如 pvdF and "hydroxyl group", 或"CF4 plasma" and PVDF 等。

Q12: 如何检索 MOF 材料的电致发光材料的研究文献?

A12: 在 CAS SciFinder® 中, 可通过布尔逻辑符, 结合恰当的关键词, 灵活构建检索式, 比如: (Electrochemiluminescence or ECL) and MOF, 获得目标结果。

Q13: 如何查某一个药物在体内的代谢产物, 次级代谢产物?

A13: 按以下步骤操作:

- (1) 通过药物名或药物结构获取药物的物质信息, 在物质结果集页面点击 References, 获得药物的文献结果集;
- (2) 在获得的文献结果集页面, 点击左侧 Filter by: Concept, 勾选 Drug metabolism 等与代谢有关的词语, 获得药物代谢研究的文献;

Q14: 如何获取研究高强、高导铜合金的文献?

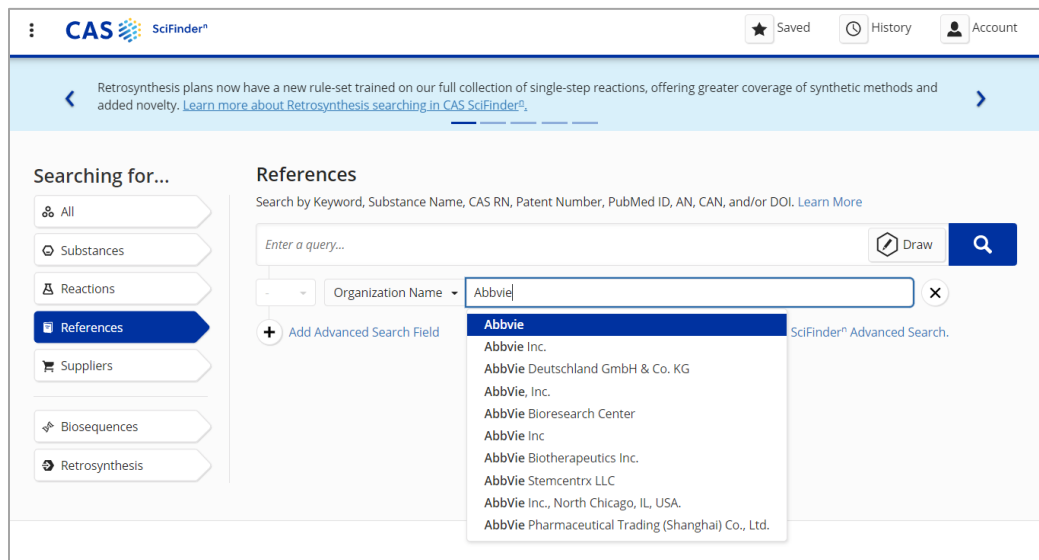
A14: 选择 References, 在输入框中输入检索式, 检索式中可考虑使用恰当的布尔逻辑运算符, 以获取预期结果。如输入: High-strength and high-conductivity and "copper alloy" 或 "High-strength" and "high-conductivity" and "copper alloy"等。

Q15: 已经知道结构修饰位点, 如何检索一个特定小分子化合物的前药研究专利?

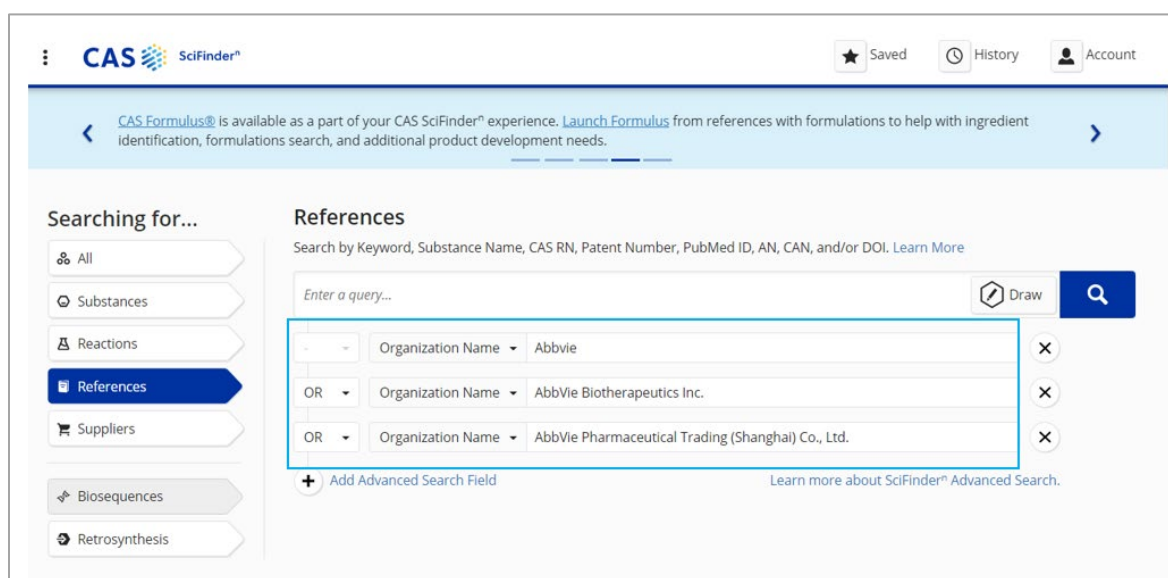
A15: 选择 References。绘制小分子结构式, 同时在输入框中输入关键词 (如, prodrug and doxorubicin), 采用文本+结构联合检索方式得到文献结果集。再在文献结果集页面左侧 Filter By: Document Type 选择 Patents, 即可获得该小分子前药研究专利。

Q16: 如何检索某个机构的研究文献?

A16: 点击 References, 再点击 Add Advance Search Field, 然后点击 Select, 在弹出列表中选择 Organization Name, 输入机构名, 例如 Abbvie。



如果需要考虑其分支机构, 则可参考输入框中提示的分支机构名, 并使用逻辑算符 OR 输入多个名称同时进行检索。



Q17: 在 CAS SciFinder[®] 中如何检索异氰酸酯环氧树脂?

A17: 在结构信息不明确时, 推荐以下两种检索方式:

(1) 在 CAS SciFinder[®] 主页面点击 Substances, 然后在输入框中输入 “Isocyanate epoxy”, 点击检索 (将在物质名称或名称的注释部分进行检索)。

注: 在用物质名称检索时, 使用双引号 “”, 那么双引号中的词会同时被检索到。

The screenshot shows the CAS SciFinder interface with the search term "Isocyanate epoxy" entered in the search bar. The results are displayed in a grid of six cards, each representing a different chemical substance. Each card includes a CAS number, a title, a note, and buttons for Reference, Reactions, and Suppliers. The filter behavior panel on the left shows the search criteria and the number of results for each filter category.

Result #	CAS Number	Notes	Reference	Reactions	Suppliers
1	144855-54-9	Notes: An epoxy-isocyanate resin (France) Unspecified Alsthom IVA 18311	1	0	0
2	1825287-34-0	Notes: An isocyanate epoxy resin (Shin-A) Unspecified SEB 500	1	0	0
3	1387584-47-5	Notes: An epoxy isocyanate curing agent (China) Unspecified JF 9001	1	0	0
4	1387584-06-6	Notes: An epoxy isocyanate curing agent (China) Unspecified JF 9000	1	0	0
5	2415225-58-8	Notes: An isocyanate-modified epoxy resin (China) Unspecified OX 10 (epoxy resin)	1	0	0
6	92229-73-7	Notes: A Russian isocyanate-modified epoxy resin adhesive Unspecified VK 19	1	0	0

(2) 在 CAS SciFinder[®] 主页面, 点击 References, 在输入框中输入文献关键词后, 点击检索。

注: 如果使用双引号, 则可以相对精准地获取检索结果, 例如 “Isocyanate epoxy”, 那么双引号中的关键词不会出现词形变化, 但可出现单数或复数; 且多个关键词会同时出现。

The screenshot shows the CAS SciFinder interface. At the top, the search bar contains the query "Isocyanate epoxy". Below the search bar, the "References" section is active. On the left, there are filter options for Substances, Reactions, and Citing. A notification banner for CAS Formulus is visible. The main results area shows 319 results, sorted by Relevance. The first result is "Isocyanate-epoxy reactions in bulk and solution" by Senger, J. S.; Yilgor, I.; McGrath, J. E.; Patsiga, R. A. The second result is "Reaction during cure of a blocked isocyanate-epoxy resin adhesive" by Hartz, Roy E. The interface includes a "Load More Results" button and a "Filter Behavior" section with options like "Filter by" and "Exclude".

Q18: 在 CAS SciFinder® 中如何检索铁中毒癌症的靶点研究?

A18: 推荐使用 References 进行关键词检索，然后通过 Concept 对结果进行精炼。操作步骤如下：

1) 首先，在 CAS SciFinder 主页面点击 References，在输入框中输入关键词，例如：ferroptosis and (cancer or tumor) and target。如果已经知道某些关联的靶点，则可以一并输入对应的关键词，例如：ferroptosis and (cancer or tumor) and target or “glutathione peroxidase” or “GPX-4” or “glutathione peroxidase 4”。

(2) 点击检索结果集页面左侧 Filter by: Concept 来精炼结果。可以通过 Top Count 或

Alphanumeric 浏览，也可以通过 Search 来检索，例如：输入 target，选中感兴趣的概念词，点击 Apply，就可以获得精炼后的文献。

References | ferropoptosis and (cancer or tumor) and target or "glutath" | Draw | Search | Notification | Clock | Profile

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](#)

1,145 Results | Sort: Relevance | View: Partial Abstract

1

DHODH-mediated ferroptosis defence is a targetable vulnerability in cancer
 By: Mao, Chao; Liu, Xiaoguang; Zhang, Yilei; Lei, Guang; Yan, Yuelong; Lee, Hyemin; Koppula, Pranavi; Wu, Shiqi; Zhuang, Li; Fang, Bingliang; et al
 Nature (London, United Kingdom) (2021), 593(7860), 586-590 | Language: English, Database: CAPlus and MEDLINE

Ferroptosis, a form of regulated cell death that is induced by excessive lipid peroxidation, is a key **tumor** suppression mechanism. **Glutathione peroxidase 4** (GPX4)5,6 and **ferroptosis** suppressor protein **1** (FSP1)7,8 constitute two major **ferroptosis** defense systems. Here we show that treatment of **cancer** cells with GPX4 inhibitors results in acute depletion of N-carbamoyl-L-aspartate, a pyrimidine biosynthesis intermediate, with concomitant accumulation of uridine. Supplementation with dihydroorotate orotate the substrate and product of dihydroorotate dehydrogenase (DHODH) attenuates or poten...
[View More](#)

Full Text | Substances (11) | Reactions (0) | Citing (94) | Citation Map

2

Cytochrome P450 oxidoreductase contributes to phospholipid peroxidation in ferroptosis
 By: Zou, Yilong; Li, Haoxin; Graham, Emily T.; Deik, Amy A.; Eaton, John K.; Wang, Wenyu; Sandoval-Gomez, Gerardo; Clish, Clary B.; Doench, John G.; Schreiber, Stuart L.
 Nature Chemical Biology (2020), 16(3), 302-309 | Language: English, Database: CAPlus and MEDLINE

Abstract: **Ferroptosis** is widely involved in degenerative diseases in various tissues including kidney, liver and brain, and is a **targetable** vulnerability in multiple primary and therapy-resistant **cancers**. Accumulation of phospholipid hydroperoxides in cellular membranes is the hallmark and rate-limiting step of **ferroptosis**; however, the enzymes contributing to lipid peroxidation remain poorly characterized. Using genome-wide, CRISPR-Cas9-mediated suppressor screens, we identify cytochrome P 450 oxidoreductase (POR) as necessary for ferroptotic cell death in **cancer** cells exhibiting inherent and...
[View More](#)

Full Text | Substances (15) | Reactions (0) | Citing (121) | Citation Map

3

MTORC1 couples cyst(e)ine availability with GPX4 protein synthesis and ferroptosis regulation
 By: Zhang, Yilei; Swanda, Robert V.; Nie, Litong; Liu, Xiaoguang; Wang, Chao; Lee, Hyemin; Lei, Guang; Mao, Chao;
[Koppula, Pranavi; Cheng, William et al](#)

Concept

Top Count | Alphanumeric | Search

Concept Name
 target [Search](#)

4 Selected

<input checked="" type="checkbox"/> Drug targets (99)	<input checked="" type="checkbox"/> Target of rapamycin complex 1 (12)
<input checked="" type="checkbox"/> Mechanistic Target of Rapamycin Complex 1 (6)	<input checked="" type="checkbox"/> Target of rapamycin complexes (1)

[Apply](#) [Cancel](#)

Q19: 如何在 CAS SciFinder[®] 中检索 EGFR 和配体分子?

A19: 推荐使用 References 进行关键词检索, 然后使用 Concept 精炼结果, 同时可以通过文献来获取关联的物质结果。操作步骤如下:

(1) 在 CAS SciFinder[®] 主页面点击 References, 在输入框中输入关键词, 例如: EGFR and ligand; 然后在文献结果集页面左侧点击 Filter by: Concept 精炼结果 (如, 筛选 ligands)。

The screenshot shows the CAS SciFinder interface with the search query 'EGFR and ligand' entered in the search bar. The page displays 11,681 results, sorted by Relevance. Two results are visible:

Result 1: A single ligand is sufficient to activate EGFR dimers
By: Liu, Ping; Cleveland, Thomas E. IV; Bouyain, Samuel; Byrne, Patrick O.; Longo, Patti A.; Leahy, Daniel J.
Proceedings of the National Academy of Sciences of the United States of America (2012), 109(27), 10861-10866, S10861/1-S10861/15 | Language: English, Database: CAplus and MEDLINE
Crystal structures of human epidermal growth factor receptor (EGFR) with bound ligand revealed sym., doubly ligated receptor dimers thought to represent physiol. active states. Such complexes fail to rationalize neg. cooperativity of epidermal growth factor (EGF) binding to EGFR and the behavior of the ligandless EGFR homolog ErbB2/HER2, however. We report cell-based assays that provide evidence for active, singly ligated dimers of human EGFR and its homolog, ErbB4/HER4. We also report crystal structures of the ErbB4/HER4 extracellular region complexed with its ligand, Neuregulin-1B that resoly...

Result 2: Differential effects of EGFR ligands on endocytic sorting of the receptor
By: Roepstorff, Kirstine; Grandal, Michael Vibo; Henriksen, Lasse; Knudsen, Stine Louise Jeppe; Lerdrup, Mads; Groevdal, Lene; Willumsen, Berthe Marie; van Deurs, Bo
Traffic (Oxford, United Kingdom) (2009), 10(8), 1115-1127 | Language: English, Database: CAplus and MEDLINE
Endocytic downregulation is a pivotal mechanism turning off signaling from the EGF receptor (EGFR). It is well established that, whereas EGF binding leads to lysosomal degradation of EGFR, transforming growth factor (TGF)- α causes receptor recycling. TGF- α therefore leads to continuous signaling and is a more potent mitogen than EGF. In addition to EGF and TGF- α , five EGFR ligands have been identified. Although many of these ligands are upregulated in cancers, very little is known about their effect on EGFR trafficking. The authors have compared the effect of six different ligands on endocytic...

The interface includes a 'Filter Behavior' sidebar on the left with options for Document Type, Language, Publication Year, Author, Organization, Publication Name, and Concept. The Concept filter is expanded, showing 'Epidermal growth factor receptors (10K)', 'Human (7,129)', and 'Homo sapiens (7,127)'. The top navigation bar shows 'References' and 'EGFR and ligand' in the search bar. The bottom navigation bar shows 'Substances (2)', 'Reactions (0)', 'Citing (85)', and 'Citation Map'.

Concept
✕

Top Count

Alphanumeric

Search

1 Selected

<input type="checkbox"/> Epidermal growth factor receptors (10K)	<input type="checkbox"/> Lung neoplasm (1,012)	<input type="checkbox"/> T cell (753)
<input type="checkbox"/> Human (7,129)	<input type="checkbox"/> CD19 antigens (1,007)	<input type="checkbox"/> Immunotherapy (747)
<input type="checkbox"/> Homo sapiens (7,127)	<input type="checkbox"/> Hepatocyte growth factor receptor c-Met (992)	<input type="checkbox"/> p53 (protein) (743)
<input type="checkbox"/> Humans (6,156)	<input type="checkbox"/> Monoclonal antibodies (990)	<input type="checkbox"/> CD3 antigens (735)
<input type="checkbox"/> ErbB Receptors (4,854)	<input type="checkbox"/> Lung Neoplasms (964)	<input type="checkbox"/> Aged (734)
<input type="checkbox"/> Signal transduction (4,557)	<input type="checkbox"/> Peptides (928)	<input type="checkbox"/> Chimeric fusion proteins (731)
<input type="checkbox"/> Animals (3,560)	<input type="checkbox"/> Cytotoxic T-lymphocyte-associated protein 4 (924)	<input type="checkbox"/> Gene Expression Regulation, Neoplastic (727)
<input type="checkbox"/> Antitumor agents (3,387)	<input type="checkbox"/> Antigen (912)	<input type="checkbox"/> Type II interferons (726)
<input type="checkbox"/> Epidermal growth factor receptor HER2 (2,777)	<input type="checkbox"/> Prognosis (910)	<input type="checkbox"/> Epidermal growth factor receptor HER4 (705)
<input checked="" type="checkbox"/> Ligands (2,641)	<input type="checkbox"/> Mucin 1 (903)	<input type="checkbox"/> CD44 antigens (700)
<input type="checkbox"/> Proteins (2,539)	<input type="checkbox"/> Protein motifs (884)	<input type="checkbox"/> Colorectal neoplasm (698)
<input type="checkbox"/> Cell proliferation (2,237)	<input type="checkbox"/> Immunoglobulin fragments	<input type="checkbox"/> Receptor, ErbB-2 (694)

Apply

Cancel

(2) 如果需要获取关联的物质，可以在文献结果集页面点击 Substances 获取物质。然后通过物质结果集页面左侧筛选项进一步筛选物质，如通过 Substance Class 筛选物质类型，通过 bioactivity identifier 筛选具有生物活性的物质等。

CAS SciFinder®

References EGFR and ligand

Draw

Return to Home

References

Substances Reactions Citing

Save and Alert

CAS Formulus®, the comprehensive formulations database and workflow solution, is now available for all SciFinder® users. Use the [CAS Solutions: Formulus filter](#) to view available content. [Learn more about Formulus.](#)

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: **Ligands** × Clear All Filters

2,642 Results Sort: Relevance View: Partial Abstract

1

A single ligand is sufficient to activate EGFR dimers
 By: Liu, Ping; Cleveland, Thomas E. IV; Bouyain, Samuel; Byrne, Patrick O.; Longo, Patti A.; Leahy, Daniel J.
 Proceedings of the National Academy of Sciences of the United States of America (2012), 109(27), 10861-10866, S10861/1-S10861/15 | Language: English, Database: CAlplus and MEDLINE

Crystal structures of human **epidermal growth factor receptor (EGFR)** with bound **ligand** revealed sym., doubly ligated receptor dimers thought to represent physiol. active states. Such complexes fail to rationalize neg. cooperativity of epidermal growth factor (EGF) binding to **EGFR** and the behavior of the ligandless **EGFR** homolog ErbB2/HER2, however. We report cell-based assays that provide evidence for active, singly ligated dimers of human **EGFR** and its homolog, ErbB4/HER4. We also report crystal structures of the ErbB4/HER4 extracellular region complexed with its **ligand**, Neuregulin-1B that resolv...

[View More](#)

Filter Behavior

Filter by Exclude

Document Type

Language

Substances

References ▾ Reactions ▾ Suppliers ▾ ↓ ✉ 🔔 Save and Alert

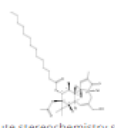
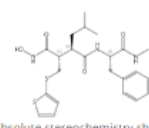
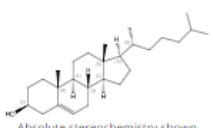
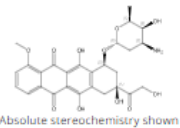
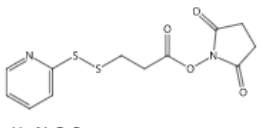
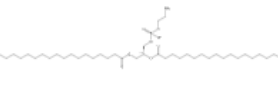
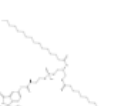
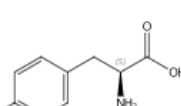
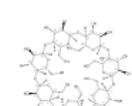
Filtering: Substance Class: Organic/Inorganic Small M... ✕ Clear All Filters

7,129 Results Sort: Relevance ▾ View: Partial ▾

Filter Behavior

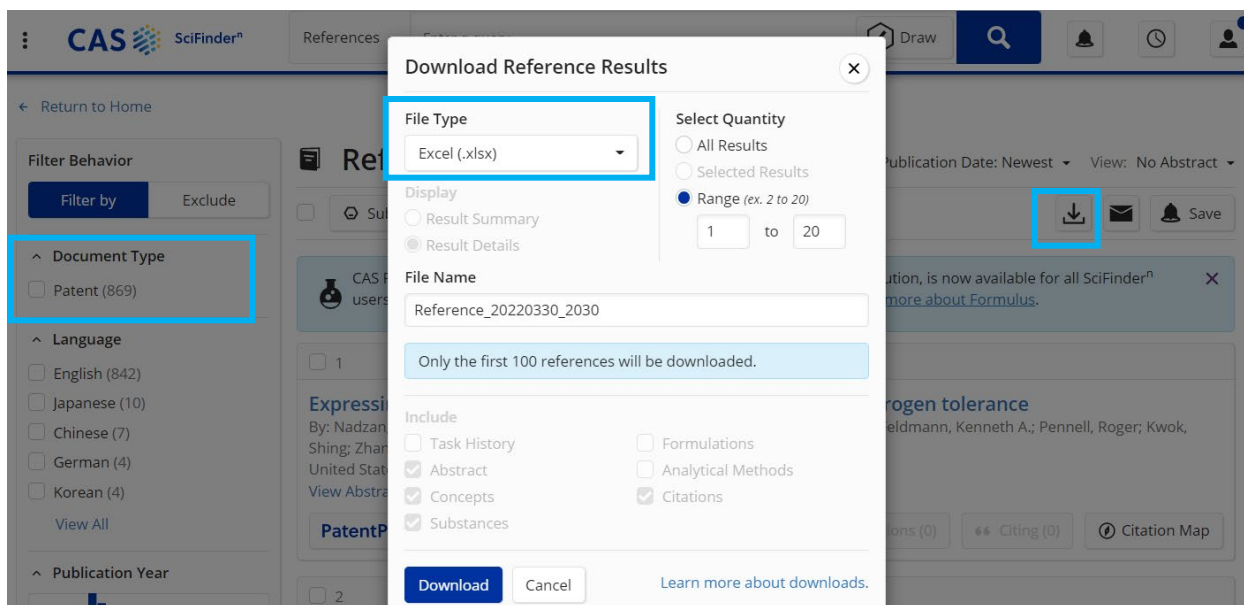
Filter by Exclude

- ▾ Reaction Role
- ▾ Reference Role
- ▾ Commercial Availability
- ▾ Number of Components
- ▾ Molecular Weight
- ▾ Stereochemistry
- ▾ Substance Class
 - Protein/Peptide Sequence (18K)
 - Manual Registration (15K)
 - Organic/Inorganic Small Molecule (7,129)
 - Nucleic Acid Sequence (5,446)
 - Polymer (467)
 - [View All](#)
- ▾ Isotopes
- ▾ Metals
- ▾ Experimental Property
- ▾ Experimental Spectrum
- ▾ Bioactivity Indicator
 - Antitumor agents (2,813)
 - Anti-infective agents (1,204)
 - Nervous system agents (990)
 - Anti-inflammatory agents (930)
 - Enzyme inhibitors (896)
 - [View All](#)

<p><input type="checkbox"/> 1</p> <p>16561-29-8 ↶ ↷</p>  <p>Absolute stereochemistry shown</p> <p>C₃₆H₅₆O₈ Phorbol 12-myristate 13-acetate</p> <p>📖 39K 🔬 51 🛒 80 References Reactions Suppliers</p>	<p><input type="checkbox"/> 2</p> <p>130370-60-4 ↶ ↷</p>  <p>Absolute stereochemistry shown</p> <p>C₂₃H₃₁N₃O₄S₂ Batimastat</p> <p>📖 835 🔬 4 🛒 57 References Reactions Suppliers</p>	<p><input type="checkbox"/> 3</p> <p>57-88-5 ↶ ↷</p>  <p>Absolute stereochemistry shown</p> <p>C₂₇H₄₆O Cholesterol</p> <p>📖 391K 🔬 4,881 🛒 156 References Reactions Suppliers</p>
<p><input type="checkbox"/> 4</p> <p>23214-92-8 ↶ ↷</p>  <p>Absolute stereochemistry shown</p> <p>C₂₇H₂₉NO₁₁ Doxorubicin</p> <p>📖 95K 🔬 1,428 🛒 54 References Reactions Suppliers</p>	<p><input type="checkbox"/> 5</p> <p>68181-17-9 ↶ ↷</p>  <p>C₁₂H₁₂N₂O₄S₂ N-Succinimidyl 3-(2-pyridyl)dithio propionate</p> <p>📖 1,913 🔬 399 🛒 86 References Reactions Suppliers</p>	<p><input type="checkbox"/> 6</p> <p>1069-79-0 ↶ ↷</p>  <p>Absolute stereochemistry shown</p> <p>C₄₁H₈₂NO₈P 1,2-Distearoyl-<i>sn</i>-glycero-3-phosphoethanolamine</p> <p>📖 1,452 🔬 168 🛒 66 References Reactions Suppliers</p>
<p><input type="checkbox"/> 7</p> <p>87706-98-7 ↶ ↷</p> 	<p><input type="checkbox"/> 8</p> <p>60-18-4 ↶ ↷</p> 	<p><input type="checkbox"/> 9</p> <p>7585-39-9 ↶ ↷</p> 

Q20: 在 CAS SciFinder[®] 中如何导出文献检索结果中的专利号?

A20: 首先通过文献结果集页面左侧 Document Type: 选择 Patent, 获得专利文献。然后, 点击文献结果集右侧下载图标 ↓, 在弹出窗口中 File Type 下选择 Excel, 将专利文献导出为 Excel 格式文件。导出文件中包含 Patent Number 专利号栏。



Patent Number	Title	Abstract
US10815494 B2	Expressing Arabidopsis thaliana genes in	Methods and materials for modulating low-
US20200255482 A1	Insecticidal combinations of cysteine-rich	New insecticidal nucleotides, peptides,
US20200207818 A1	Expression of insecticidal proteins in	New insecticidal proteins, nucleotides,
US20190167779 A1	Synthetic antigen constructs against	The invention relates to immunogenic
WO2017201347 A1	Use of mRNA encoding cystic fibrosis	The invention relates to mRNA therapy for
WO2017143076 A1	Chimeric antigen receptors comprising	Provided are chimeric antigen receptors
US20170233446 A1	Methods and compositions using Klotho-FGF	The present invention is directed to
WO2017109167 A2	Reconstitution of DNA-end repair pathway in	Suggested is a method for engineering and/or
WO2017066845 A1	Organisms with modified growth and	Disclosed are methods and constructs for
WO2017050963 A1	Activation of taste receptor genes in	Suggested is a method for enhancing the
WO2017025323 A1	Cells for immunotherapy engineered for	Methods of developing genetically engineered

Q21: 在 CAS SciFinder[®] 中如何检索酶催化综述文献?

A21: 推荐使用 References 关键词检索，并通过 Filter by: Document Type 精炼文献类型，CA Section 浏览学科领域分类，Concept 精炼具体的研究点等。操作步骤如下：

1) CAS SciFinder[®] 中进行关键词检索时，推荐关键词间使用布尔逻辑运算符。例如：enzyme and catalysis or "enzyme catalyst"，可以全面精准地获取酶催化相关的研究文献。在获得的文献结果集页面，通过 Document Type: Review 即可获取综述文献。

(2) 如果需要快速纵览或继续精炼检索结果，则可通过 CAS Section 学科领域分类和 Concept 核心概念词库进行浏览和精炼。

注：Concept 中的 Top Count 可浏览 top 100 最密集的研究点。若想快速获取某研究点，则可点击 Search，输入感兴趣的词（如，enzyme 或 catalyst*），即可查看所有涉及到的酶和催化反应。点击 Search 后，在输入词语时可使用通配符（如，*），* 代表 0 或多个字符，因而可以扩展检索词或词干。

The screenshot displays the CAS SciFinder® interface for a search query: "enzyme and catalysis or 'enzyme catalyst'". The search results are sorted by Relevance and shown as Partial Abstracts. The results are filtered by Document Type: Review (4,837) and CA Section: 2 Selected. Two reference entries are shown:

- Structure-stability relationship in proteins: fundamental tasks and strategy for the development of stabilized enzyme catalysts for biotechnology**
 By: Mozhaev, V. V.; Berezin, I. V.; Martinek, Karel
 Critical Reviews in Biochemistry (1988), 23(3), 235-81 | Language: English, Database: CPlus and MEDLINE
 A review, with 317 references, on the chem., phys., and biol. aspects of protein stability and stabilization. Topics discussed include the exptl. and theor. approaches to studies on the relationship between protein structure and stability, the mol. basis of protein stability, and exptl. methods of obtaining highly stable enzyme preparations
- An integrated model for enzyme catalysis emerges from studies of hydrogen tunneling**
 By: Klinman, Judith P.
 Chemical Physics Letters (2009), 471(4-6), 179-193 | Language: English, Database: CPlus and MEDLINE
 A review. The origins of the enormous rate accelerations brought about by enzymes are discussed. Here, the author focuses on enzymic C-H activation, which has been shown to take place via tunneling. Four enzyme systems illustrate the impact of site-specific mutagenesis, changes in temperature or changes in protein solvation on tunneling properties. A model emerges in which conformational sampling is required to access a subset of protein conformers where the H-donor and acceptor undergo a close approach. The evidence for an inverse relation between protein flexibility and active site compressi...

Concept

- Catalysis (2,370)
- Enzymes (1,763)
- Humans (988)
- Animals (981)
- Protein conformation (884)
- [View All](#)

CA Section

- Enzymes (4,579)
- Fermentation and Bioindustrial Chemistry (645)
- Biochemical Methods (539)
- General Biochemistry (526)
- Unavailable (372)
- General Organic Chemistry (276)
- Catalysis, Reaction Kinetics, and Inorganic Reaction Mechanisms (258)
- Pharmacology (255)
- Electrochemical, Radiational, and Thermal Energy

- [View All](#)

CA Section ✕

By Count Alphanumeric

2 Selected

<input checked="" type="checkbox"/> Enzymes (4,579) <input type="checkbox"/> Fermentation and Bioindustrial Chemistry (645) <input type="checkbox"/> Biochemical Methods (539) <input type="checkbox"/> General Biochemistry (526) <input type="checkbox"/> Unavailable (372) <input type="checkbox"/> General Organic Chemistry (276) <input checked="" type="checkbox"/> Catalysis, Reaction Kinetics, and Inorganic Reaction Mechanisms (258) <input type="checkbox"/> Pharmacology (255) <input type="checkbox"/> Electrochemical, Radiational, and Thermal Energy	<input type="checkbox"/> General Physical Chemistry (32) <input type="checkbox"/> Catalysis and Reaction Kinetics (31) <input type="checkbox"/> Fossil Fuels, Derivatives, and Related Products (27) <input type="checkbox"/> Organometallic and Organometalloidal Compounds (25) <input type="checkbox"/> Unit Operations and Processes (25) <input type="checkbox"/> Mammalian Hormones (22) <input type="checkbox"/> Cellulose, Lignin, Paper, and Other Wood Products (20) <input type="checkbox"/> Biomolecules and Their	<input type="checkbox"/> Ceramics (6) <input type="checkbox"/> Industrial Carbohydrates (6) <input type="checkbox"/> Nonmammalian Biochemistry (6) <input type="checkbox"/> Phase Equilibria, Chemical Equilibria, and Solutions (6) <input type="checkbox"/> Agrochemical Bioregulators (5) <input type="checkbox"/> Microbial Biochemistry (5) <input type="checkbox"/> Surface Active Agents and Detergents (5) <input type="checkbox"/> Synthetic High Polymers (5) <input type="checkbox"/> Thermodynamics, Thermochemistry, and Thermal Properties (5)
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Concept ✕

Top Count Alphanumeric Search

4 Selected

<input checked="" type="checkbox"/> Catalysis (2,370) <input checked="" type="checkbox"/> Enzymes (1,763) <input type="checkbox"/> Humans (988) <input type="checkbox"/> Animals (981) <input type="checkbox"/> Protein conformation (884) <input type="checkbox"/> Models, Molecular (817) <input type="checkbox"/> Enzyme functional sites, active (812) <input type="checkbox"/> Binding Sites (615) <input type="checkbox"/> Substrate Specificity (592) <input type="checkbox"/> Kinetics (552) <input type="checkbox"/> Amino Acid Sequence (383)	<input type="checkbox"/> Escherichia coli (164) <input type="checkbox"/> Enzyme inhibitors (162) <input type="checkbox"/> Transition state structure (152) <input type="checkbox"/> Cytochrome P-450 Enzyme System (150) <input type="checkbox"/> Catalysts (148) <input type="checkbox"/> Models, Biological (142) <input type="checkbox"/> Conformational transition (137) <input type="checkbox"/> Enzyme mimics (135) <input type="checkbox"/> Oxygen (126) <input type="checkbox"/> Biotechnology (124)	<input type="checkbox"/> Enzyme functional sites, substrate-binding (88) <input type="checkbox"/> Chemical Phenomena (87) <input type="checkbox"/> Protein motifs (86) <input type="checkbox"/> RNA, Catalytic (86) <input type="checkbox"/> Electron transport (85) <input type="checkbox"/> Stereochemistry (85) <input type="checkbox"/> Crystal structure (81) <input type="checkbox"/> Molecular recognition (81) <input checked="" type="checkbox"/> Oxidation (77) <input type="checkbox"/> Sequence Alignment (77) <input checked="" type="checkbox"/> Isoenzymes (76)
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Concept ✕

Top Count Alphanumeric **Search**

Concept Name

enzyme Search

4 Selected

<input type="checkbox"/> Antioxidant enzymes (3)	<input type="checkbox"/> Enzyme functional sites, cofactor-binding (9)	<input type="checkbox"/> Enzymes, multienzymes (7)
<input type="checkbox"/> Carbohydrate-metabolizing enzymes (1)	<input type="checkbox"/> Enzyme functional sites, inhibitor-binding (6)	<input type="checkbox"/> Enzymes, oligomeric (1)
<input type="checkbox"/> Cellulolytic enzymes (1)	<input type="checkbox"/> Enzyme functional sites, ligand-binding (1)	<input type="checkbox"/> Enzymes, oxidizing (3)
<input type="checkbox"/> Cholesterol Side-Chain Cleavage Enzyme (1)	<input type="checkbox"/> Enzyme functional sites, metal-binding (60)	<input type="checkbox"/> Enzymes, pyridoxal phosphate-dependent (5)
<input type="checkbox"/> Clinical enzyme tests (5)	<input type="checkbox"/> Enzyme functional sites, redox (4)	<input type="checkbox"/> Enzymes, redox (13)
<input type="checkbox"/> Cytochrome P450 enzyme inducers (4)	<input type="checkbox"/> Enzyme functional sites, regulatory (2)	<input type="checkbox"/> Enzymes, respiratory (2)
<input type="checkbox"/> Cytochrome P-450 Enzyme Inhibitors (6)		<input type="checkbox"/> Enzymes, ribulose diphosphate carboxylase-activating (1)

Concept ✕

Top Count Alphanumeric **Search**

Concept Name

catalyst* Search

4 Selected

<input type="checkbox"/> Abstraction reaction catalysts (1)	<input type="checkbox"/> Electrochemical reduction catalysts (2)	<input type="checkbox"/> Oxidation catalysts (37)
<input type="checkbox"/> Aldol condensation catalysts (1)	<input type="checkbox"/> Electrolysis catalysts (1)	<input type="checkbox"/> Petroleum cracking catalysts (1)
<input type="checkbox"/> Allylic substitution reaction catalysts (1)	<input type="checkbox"/> Electron transfer catalysts (1)	<input type="checkbox"/> Petroleum hydrodesulfurization catalysts (1)
<input type="checkbox"/> Amination catalysts (1)	<input type="checkbox"/> Epoxidation catalysts (4)	<input type="checkbox"/> Petroleum hydrodewaxing catalysts (1)
<input type="checkbox"/> Bond cleavage catalysts (1)	<input type="checkbox"/> Exchange reaction catalysts (1)	<input type="checkbox"/> Petroleum refining catalysts (1)
<input type="checkbox"/> Catalysts (148)	<input type="checkbox"/> Fischer-Tropsch catalysts (1)	<input type="checkbox"/> Phase transfer catalysts (2)
<input type="checkbox"/> Catalysts, surface (3)	<input type="checkbox"/> Friedel-Crafts reaction catalysts (1)	
	<input type="checkbox"/> Glycosylation catalysts (1)	

Q22: 在 CAS SciFinder[®] 中如何全面、精准地进行作者名检索?

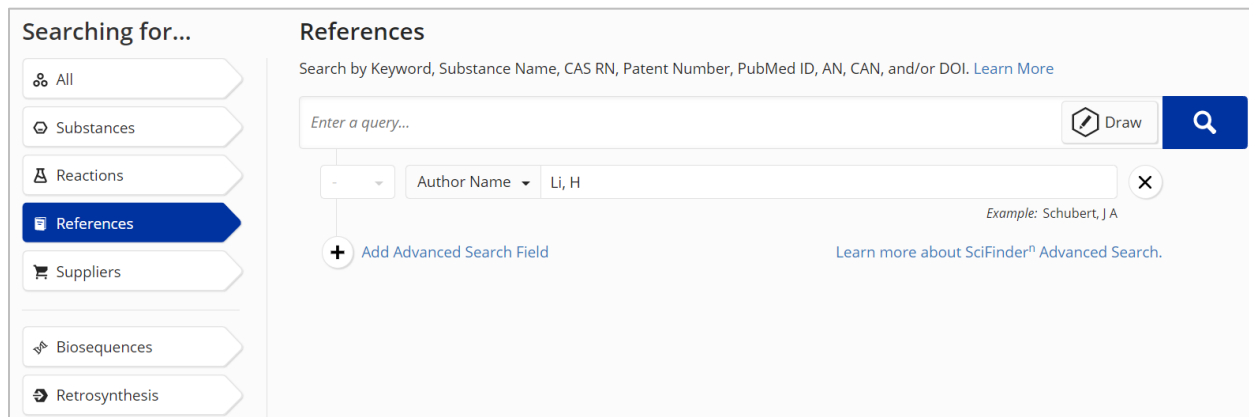
A22: 推荐检索步骤如下:

(1) 在主页面点击 References, 然后在 Advanced Search Field: Author Name, 输入作者名。第一步输入姓加名的第一个字母, 中间用英文的逗号隔开。比如, 需要检索李海滨这位作者, 可输入 Li, H。

(2) 在获得的文献结果集页面, 点击左侧 Filter by: Author, 再点击 View All, 通过 Search 搜索精准的作者名。

(3) 请注意作者名的不同书写形式: 例如输入 Li, H。选择符合要求的名字, 比如: Li, Haibing; Li, Hai Bing; Li, Hai-Bing 等。同时参考 Li, H B 和 Li, H. B., 尤其是不确定作者署名格式时, 需勾选所有书写形式, 确保获取该作者最完整的文献。

(4) 可使用机构名进一步筛选, 以获取更精准的某作者的文献: 在完成步骤 (3) 后, 再点击结果集页面左侧 Filter by: Organization, 然后点击 View All, 展开机构列表, 选中该作者的工作单位, 点击 Apply 即可精准地获得该作者的文献。



The screenshot displays the SciFinder search interface. On the left, a sidebar titled "Searching for..." lists various search categories: All, Substances, Reactions, References (highlighted in blue), Suppliers, Biosequences, and Retrosynthesis. The main area is titled "References" and includes a search bar with the placeholder "Enter a query...". Below the search bar, a dropdown menu is set to "Author Name" with the query "Li, H" entered. A "Draw" button and a search icon are also visible. Below the search bar, there is a link to "Add Advanced Search Field" and a link to "Learn more about SciFinder[®] Advanced Search." An example query "Example: Schubert, J A" is shown below the search bar.

Author ×

Top Count Alphanumeric **Search**

Author Name (Last, First Middle)

Li, H Search

Ex: Schubert, J A

5 Selected

<input type="checkbox"/> Li, H (1)	<input type="checkbox"/> li, Haibin (1)	<input type="checkbox"/> Li, Hai-chuan (12)
<input type="checkbox"/> Li, H (1,649)	<input checked="" type="checkbox"/> Li, Hai Bing (8)	<input type="checkbox"/> Li, Haichuan (41)
<input type="checkbox"/> Li, H. (6,037)	<input checked="" type="checkbox"/> Li, Hai-Bing (32)	<input type="checkbox"/> Li, Hai-chun (3)
<input type="checkbox"/> Li, H A (4)	<input checked="" type="checkbox"/> Li, Hai-bing (47)	<input type="checkbox"/> Li, Haichun (85)
<input type="checkbox"/> Li, H-A (2)	<input checked="" type="checkbox"/> Li, HaiBing (6)	<input type="checkbox"/> Li, Hai-Cong (5)
<input type="checkbox"/> Li, H. A. (3)	<input checked="" type="checkbox"/> Li, Haibing (511)	<input type="checkbox"/> Li, Hai-cong (7)
<input type="checkbox"/> Li, Ha (1)	<input type="checkbox"/> Li, Hai Bo (35)	<input type="checkbox"/> Li, Haicong (13)
<input type="checkbox"/> Li, Hae Chong (1)	<input type="checkbox"/> Li, Hai-Bo (251)	<input type="checkbox"/> Li, Haicui (7)
<input type="checkbox"/> Li, Hae Nam (1)	<input type="checkbox"/> Li, Hai-bo (245)	<input type="checkbox"/> Li, Haicun (23)

← Prev 1 2 3 4 5 ... 64 Next → | Go to Page:

Apply Cancel

Author ×

Top Count Alphanumeric **Search**

Author Name (Last, First Middle)

Li, H Search

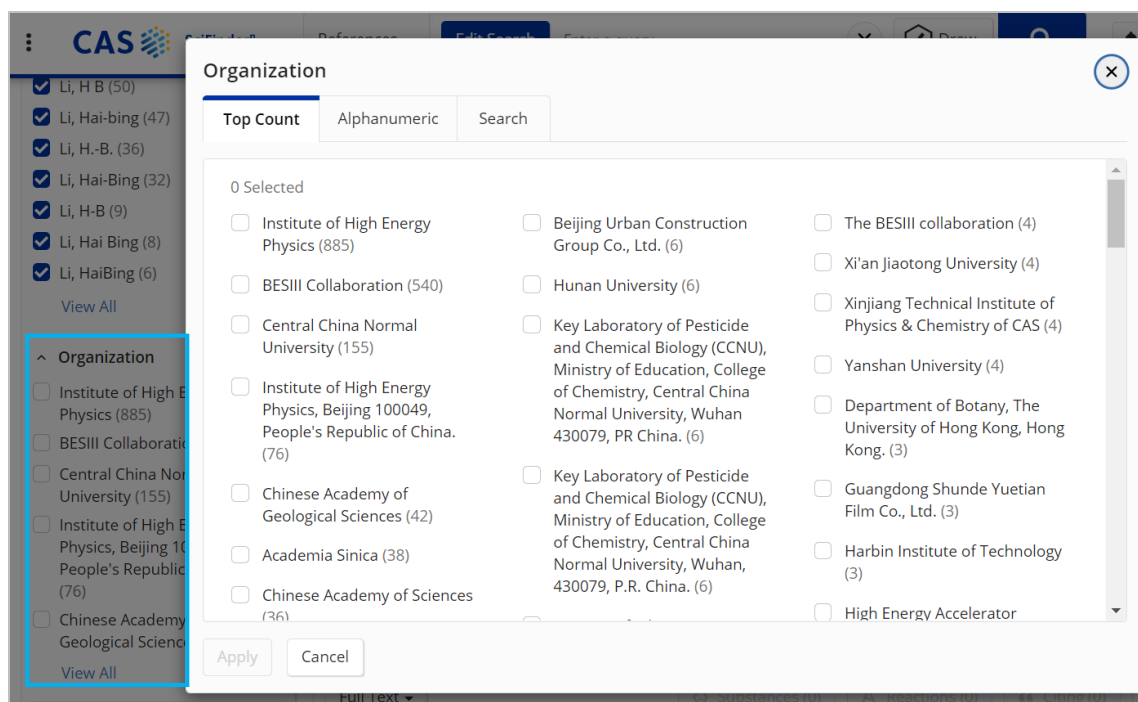
Ex: Schubert, J A

9 Selected

<input type="checkbox"/> Li, Hayashi (3)	<input type="checkbox"/> Li, He-an (1)	<input type="checkbox"/> Li, Hector (1)
<input type="checkbox"/> Li, Haying (1)	<input type="checkbox"/> Li, Hean (3)	<input type="checkbox"/> Li, Hecui (1)
<input type="checkbox"/> Li, Hayley H. (3)	<input type="checkbox"/> Li, Heao (2)	<input type="checkbox"/> Li, Hecun (17)
<input checked="" type="checkbox"/> Li, H B (50)	<input type="checkbox"/> Li, Hebai (3)	<input type="checkbox"/> Li, Heda (1)
<input checked="" type="checkbox"/> Li, H-B (9)	<input type="checkbox"/> Li, Hebao (7)	<input type="checkbox"/> Li, Hedan (12)
<input checked="" type="checkbox"/> Li, H. B. (1,184)	<input type="checkbox"/> Li, He-bei (1)	<input type="checkbox"/> Li, Hede (6)
<input checked="" type="checkbox"/> Li, H.-B. (36)	<input type="checkbox"/> Li, Hebei (2)	<input type="checkbox"/> Li, Hedi (8)
<input type="checkbox"/> Li, H. Bruce (1)	<input type="checkbox"/> Li, Hebi (10)	<input type="checkbox"/> Li, Hedian (1)
<input type="checkbox"/> Li, H. C. (11)	<input type="checkbox"/> Li, Hebiao (4)	<input type="checkbox"/> Li, He Dong (7)

← Prev 1 ... 15 16 17 18 19 ... 64 Next → | Go to Page:

Apply Cancel



Q23: 如何检索活性碳的表面含氧基团的分析方法?

A23: 推荐如下检索方法:

- (1) 使用关键词进行文献检索。例如: "activated carbon" and "oxygen-containing" group.

References search for "'activated carbon' and 'oxygen-containing' group"

Substances Reactions Citing

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](#)

751 Results Sort: Relevance View: Partial Abstract

1

Influence of oxygen plasma treatment on hydrogen chloride removal of activated carbon fibers
 By: Park, Soo-Jin; Kim, Byung-Joo
 Journal of Colloid and Interface Science (2004), 275(2), 590-595 | Language: English, Database: CAlplus and MEDLINE

The oxygen plasma treatment of activated C fibers (ACFs) was carried out to introduce oxygen-containing groups onto C surfaces. Surface properties of the ACFs were determined by XPS and SEM. N₂/77 K adsorption isotherms were studied by BET and D-R plot methods to characterize sp. surface area, pore volume, and pore size distribution. The efficiency of hydrochloride removal was confirmed by 2 kinds of methods; one is detecting tubes (range: 1-40 ppm), and the other is a gas chromatog. technique. As expt. results, the hydrochloride removal efficiency of the ACFs was increased with the number of...

View More

Full Text Substance (1) Reactions (0) Citing (61) Citation Map

2

Detection of low concentration oxygen containing functional groups on activated carbon fiber surfaces through fluorescent labeling
 By: Feng, Xue; Dementev, Nikolay; Feng, Wenguo; Vidic, Radisav; Borguet, Eric
 Carbon (2006), 44(7), 1203-1209 | Language: English, Database: CAlplus

Covalent fluorescent labeling of surface species (FLOSS) was used to detect relatively low concentrations of surface functional groups (OH, COOH and CHO) on activated carbon fiber surfaces. The chromophores were attached to the surface through a reaction specific to each type of surface functional group. FLOSS indicated the presence of 8.7×10^{11} COOH groups/cm² and 1.3×10^{12} CHO groups/cm² on the ACF 25 fiber surface. Neither the IR spectrum nor the X-ray photoelectron spectrum showed evidence

(2) 在获得的文献结果集页面，通过左侧聚类分析项 Concept，浏览文献中涉及的核心研究点。可以在 Top Count 中选择研究热点，也可以通过 Search 搜索感兴趣的研究热点，例如输入 spec* (通配符代表 0 或多个字符)，搜索分析谱学研究。选中研究热词后，点击 Concept 窗口左下角 Apply，即可获得精炼后的文献结果。

Concept ✕

Top Count Alphanumeric Search

2 Selected

<input type="checkbox"/> Adsorption (304)	<input type="checkbox"/> Water Pollutants, Chemical (30)	<input type="checkbox"/> Adsorption enthalpy (15)
<input type="checkbox"/> Surface area (245)	<input type="checkbox"/> Electric current-potential relationship (25)	<input type="checkbox"/> Heavy metals (15)
<input type="checkbox"/> Pore size (137)	<input checked="" type="checkbox"/> Raman spectra (24)	<input checked="" type="checkbox"/> Hydroxyl group (15)
<input type="checkbox"/> Pore size distribution (134)	<input type="checkbox"/> Carbon fibers (23)	<input type="checkbox"/> Mesopore (15)
<input type="checkbox"/> Functional groups, oxygen-containing group (108)	<input type="checkbox"/> Cyclic voltammetry (23)	<input type="checkbox"/> Phenols (15)
<input type="checkbox"/> Adsorbents (105)	<input type="checkbox"/> Carbon (22)	<input type="checkbox"/> Oxygen (14)
<input type="checkbox"/> Oxidation (98)	<input type="checkbox"/> Kinetics (22)	<input type="checkbox"/> Reaction kinetics (14)
<input type="checkbox"/> Surface structure (95)	<input type="checkbox"/> Lactones (22)	<input type="checkbox"/> Supercapacitor electrodes (14)
<input type="checkbox"/> Activated carbon fibers (77)	<input type="checkbox"/> Mesoporous materials (22)	<input type="checkbox"/> Thermodynamics (14)
<input type="checkbox"/> Pore structure (72)	<input type="checkbox"/> Particle size (21)	<input type="checkbox"/> Water vapor (14)
<input type="checkbox"/> pH (70)	<input type="checkbox"/> Air pollution control (20)	<input type="checkbox"/> Carbon nanotubes (13)
<input type="checkbox"/> Adsorptive wastewater treatment (66)	<input type="checkbox"/> Catalysts (20)	<input type="checkbox"/> Plasma (13)
		<input type="checkbox"/> Steam (13)

Concept ✕

Top Count Alphanumeric **Search**

Concept Name

Select All on Page

<input type="checkbox"/> Absorption spectra (1)	<input type="checkbox"/> IR reflection spectra (1)	<input type="checkbox"/> Spectroscopy, Fourier Transform Infrared (9)
<input type="checkbox"/> Attenuated-total-reflectance Fourier-transform IR spectroscopy (1)	<input type="checkbox"/> IR spectra (43)	<input type="checkbox"/> Spectrum Analysis (1)
<input type="checkbox"/> Dielectric spectroscopy (1)	<input type="checkbox"/> IR spectroscopy (2)	<input type="checkbox"/> Spectrum Analysis, Raman (1)
<input type="checkbox"/> Electron Spin Resonance Spectroscopy (1)	<input type="checkbox"/> Mass spectra (2)	<input type="checkbox"/> UV and visible spectra (1)
<input type="checkbox"/> Energy-dispersive x-ray spectra (1)	<input type="checkbox"/> Photoelectron spectra (1)	<input type="checkbox"/> UV-visible diffuse reflection spectra (1)
<input type="checkbox"/> Energy-dispersive x-ray spectroscopy (2)	<input type="checkbox"/> Photoelectron spectroscopy (4)	<input type="checkbox"/> XANES spectra (3)
<input type="checkbox"/> EXAFS spectra (1)	<input type="checkbox"/> Raman spectra (24)	<input type="checkbox"/> X-ray photoelectron spectra (47)
	<input type="checkbox"/> Raman spectroscopy (3)	<input type="checkbox"/> X-ray photoelectron spectroscopy (8)
	<input type="checkbox"/> Reactive oxygen species (1)	

References search for ""activated carbon" and "oxygen-containing" group"

Substances Reactions Citing Save and Alert

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: 32 Selected [x](#) [Clear All Filters](#)

117 Results Sort: Relevance View: Partial Abstract

1

Detection of low concentration oxygen containing functional groups on activated carbon fiber surfaces through fluorescent labeling
 By: Feng, Xue; Dementev, Nikolay; Feng, Wenguo; Vidic, Radisav; Borguet, Eric
 Carbon (2006), 44(7), 1203-1209 | Language: English, Database: CAplus

Covalent fluorescent labeling of surface species (FLOSS) was used to detect relatively low concentrations of surface functional groups (OH, COOH and CHO) on activated carbon fiber surfaces. The chromophores were attached to the surface through a reaction specific to each type of surface functional group. FLOSS indicated the presence of 8.7×10^{11} COOH groups/cm² and 1.3×10^{12} CHO groups/cm² on the ACF 25 fiber surface. Neither the IR spectrum nor the X-ray photoelectron spectrum showed evidence of the existence of those low concentration groups. The concentration of OH groups on the fiber sur...
[View More](#)

Full Text Substances (3) Reactions (0) Citing (43) Citation Map

2

Effects of surface chemical properties of activated carbon fibers modified by liquid oxidation for CO₂ adsorption
 By: Bai, Byong Chol; Kim, Eun Ae; Lee, Chul Wee; Lee, Young-Seak; Im, Ji Sun
 Applied Surface Science (2015), 353, 158-164 | Language: English, Database: CAplus

Activated carbon fibers (ACFs) with controlled pore sizes were prepared by KOH activation to efficiently capture CO₂ mols. The surfaces of the ACFs were modified by liquid oxidation using hydrofluoric acid to enhance the adsorption of CO₂ by the fibers based on the effects of the oxygen-containing functional groups introduced on the surface. Oxygen-containing functional groups were effectively introduced onto the surfaces of the ACFs based on the fluorine radical effect, and they attached themselves to the

Filter Behavior

Filter by Exclude

Document Type

Language

Publication Year

Author

Organization

Publication Name

Concept

Adsorption (304)

X-ray photoelectron spectra (47)

IR spectra (43)

Raman spectra (24)

Q24: 如何检索从某一植物中提取的化合物信息?

A24: 推荐如下检索步骤:

(1) 在 CAS SciFinder[®] 主页面, 选择 References, 输入此植物种 (属) 名。可以使用 CAS 词库 (CAS Lexicon), 扩展植物名。

Searching for...

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

References

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

"Euphorbia fischeriana" or "Genus Euphorbia" ✕ Draw 🔍

AND ▼ Author Name ▼ *Enter last name, first name middle name.* ✕

Example: Schubert, J A

+ Add Advanced Search Field Learn more about SciFinder[®] Advanced Search.

Launch CAS Lexicon CAS Lexicon enables you to browse the CAS General Thesaurus to find indexed concepts and substances to build a Reference query with up to 1,000 indexed search terms. Feedback

Search CAS Lexicon

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

Preferred Term

Euphorbia
This will search synonyms: Spurge

Broader Terms (1) Select All

Euphorbioideae

Narrower Terms (827) Select All

- Euphorbia aaron-rossii
- Euphorbia abbreviata
- Euphorbia abramsiana
- Euphorbia abyssinica
- Euphorbia acalyphoides
- Euphorbia acanthothamnos
- Euphorbia acurensis

Your Query

- Euphorbia ✕
- Euphorbioideae ✕

Select a boolean operator OR ▼ Add Term(s) Learn more about CAS Lexicon searching. 🔍

(2) 获得文献结果后，可在结果集页面左侧通过 Concept 进一步精炼文献结果，例如选择 diterpene; 也可在 Concept 里搜索，例如 extract*。

References search for ""Euphorbia fischeriana" or "Genus Euphorbia""

Substances Reactions Citing Save and Alert

Filter Behavior: Filter by Exclude

Document Type Language Publication Year Author Organization Publication Name

Concept

- Euphorbia fischeriana (729)
- Pharmaceutical natural products (446)
- Homo sapiens (143)
- Human (143)
- Sophora flavescens (139)
- [View All](#)

981 Results Sort: Times Cited View: Partial Abstract

1

Chemical and Pharmacological Research of the Plants in Genus Euphorbia
 By: Shi, Qing-Wen; Su, Xiao-Hui; Kiyota, Hiromasa
 Chemical Reviews (Washington, DC, United States) (2008), 108(10), 4295-4327 | Language: English, Database: CAPLUS and MEDLINE
 In this review article, the authors summarize the phytochem. progress and list all of the compounds isolated from the **genus Euphorbia** over the past few decades. Also included are the biol. activities of compounds isolated in recent years and structure-activity relationships.

Full Text Substances (0) Reactions (0) Citing (328) Citation Map

2

Total Synthesis of Ingenol
 By: Tanino, Keiji; Onuki, Kei; Asano, Kohei; Miyashita, Masaaki; Nakamura, Tsuyoshi; Takahashi, Yoshinori; Kuwajima, Isao
 Journal of the American Chemical Society (2003), 125(6), 1498-1500 | Language: English, Database: CAPLUS and MEDLINE
 Total synthesis of ingenol (I), a diterpene isolated from the **genus Euphorbia**, was accomplished on the basis of the novel key reactions. The highly strained ingenane skeleton was constructed through an intramol. cyclization reaction of an acetylene dicobalt complex followed by a rearrangement reaction of an epoxy alc. II. The C(3),C(4),C(5)-triol moiety was introduced by a stereoselective double dihydroxylation reaction of a diene having C(2)-C(3) and C(4)-C(5) double bonds.
[View More](#)

Full Text Substances (68) Reactions (396) Citing (119) Citation Map

Concept

Top Count Alphanumeric Search

4 Selected

<input checked="" type="checkbox"/> Euphorbia fischeriana (729)	<input type="checkbox"/> Notopterygium (45)	<input type="checkbox"/> Saposhnikovia divaricata (35)
<input type="checkbox"/> Pharmaceutical natural products (446)	<input type="checkbox"/> Topical drug delivery systems (45)	<input type="checkbox"/> Vespa (35)
<input type="checkbox"/> Homo sapiens (143)	<input type="checkbox"/> Coptis (44)	<input type="checkbox"/> Vinegar (35)
<input type="checkbox"/> Human (143)	<input type="checkbox"/> Myrrh resin (44)	<input type="checkbox"/> Corydalis (34)
<input type="checkbox"/> Sophora flavescens (139)	<input type="checkbox"/> Clematis (42)	<input type="checkbox"/> Paeonia (34)
<input type="checkbox"/> Euphorbia (123)	<input type="checkbox"/> Pharmaceutical natural products, Bombyx batryticatus (41)	<input type="checkbox"/> Stellera chamaejasme (34)
<input checked="" type="checkbox"/> Diterpenes (92)	<input type="checkbox"/> Morus (plant) (40)	<input type="checkbox"/> Zanthoxylum bungeanum (34)
<input type="checkbox"/> Angelica sinensis (85)	<input type="checkbox"/> Mulberry (40)	<input type="checkbox"/> Antibacterial agents (33)
<input type="checkbox"/> Antitumor agents (81)	<input type="checkbox"/> Pesticides (40)	<input type="checkbox"/> Apoptosis (33)
<input type="checkbox"/> Selinum monnieri (73)	<input type="checkbox"/> Pharmaceutical natural products, WuBeiZi (40)	<input type="checkbox"/> Cinnamomum (33)
<input checked="" type="checkbox"/> Euphorbia ebracteolata (70)	<input type="checkbox"/> Animals (39)	<input checked="" type="checkbox"/> Extraction (33)
<input type="checkbox"/> Angelica dahurica (68)		<input type="checkbox"/> Gleditsia sinensis (33)
		<input type="checkbox"/> Humic acids (33)

Apply Cancel

Concept ✕

Top Count Alphanumeric **Search**

Concept Name

Search

102 Selected

<input checked="" type="checkbox"/> Euphorbia (123)	<input checked="" type="checkbox"/> Euphorbia coerulescens (2)	<input checked="" type="checkbox"/> Euphorbia francoisii (1)
<input checked="" type="checkbox"/> Euphorbia abyssinica (1)	<input checked="" type="checkbox"/> Euphorbia confinalis (1)	<input checked="" type="checkbox"/> Euphorbia geniculata (3)
<input checked="" type="checkbox"/> Euphorbia acanthothamnus (1)	<input checked="" type="checkbox"/> Euphorbia confinalis rhodesiaca (1)	<input checked="" type="checkbox"/> Euphorbia geroldii (1)
<input checked="" type="checkbox"/> Euphorbia adenochlora (1)	<input checked="" type="checkbox"/> Euphorbia convolvuloides (1)	<input checked="" type="checkbox"/> Euphorbia giessii (1)
<input checked="" type="checkbox"/> Euphorbia alluaudii (1)	<input checked="" type="checkbox"/> Euphorbia cooperi (1)	<input checked="" type="checkbox"/> Euphorbia globosa (2)
<input checked="" type="checkbox"/> Euphorbia alluaudii onoclada (1)	<input checked="" type="checkbox"/> Euphorbia copiapina (1)	<input checked="" type="checkbox"/> Euphorbia glochidiata (1)
<input checked="" type="checkbox"/> Euphorbia ambarivatoensis (1)	<input checked="" type="checkbox"/> Euphorbia cornigera (1)	<input checked="" type="checkbox"/> Euphorbia glomerulans (1)
<input checked="" type="checkbox"/> Euphorbia ammak (1)	<input checked="" type="checkbox"/> Euphorbia cotinifolia (1)	<input checked="" type="checkbox"/> Euphorbia gottlebei (1)
<input checked="" type="checkbox"/> Euphorbia amygdaloides (2)	<input checked="" type="checkbox"/> Euphorbia cylindrifolia (1)	<input checked="" type="checkbox"/> Euphorbia graminea (1)
		<input checked="" type="checkbox"/> Euphorbia grandicornis (1)

← Prev 1 2 Next →

Apply Cancel

(3) 精炼文献后，点击页面左上角的 Substance，可获取文献中的物质结果。

References search for "Euphorbia fischeriana" or "Genus Euphorbia"

Substances Reactions Citing

Get Substances from References

All Results Selected Results

Document Type Language Publication Year Author Organization Publication Name Concept

Concept

- Euphorbia fischeriana (729)
- Pharmaceutical natural products (446)
- Homo sapiens (143)
- Human (143)
- Sophora flavescens (139)
- Solvent extraction (55)
- Extraction (33)
- Plant extracts (31)
- Ultrasonic extraction (7)
- Sophora flavescens extract (4)
- Supercritical extraction (3)

Filtering: Concept: 10 Selected

129 Results Sort: Relevance View: Partial Abstract

1

Four new diterpenoids from the roots of Euphorbia fischeriana
 By: Wang, Hong-Bing; Chen, Wei; Zhang, Ying-Ying; Wang, Xiao-Yang; Liu, Li-Ping; Tong, Ling-Jiang; Chen, Yi
 Fitoterapia (2013), 91, 211-216 | Language: English, Database: CPlus and MEDLINE

Four new diterpenoids (1,4,5,9), together with 7 known diterpenoids (2,3,6-8,10,11), were isolated from the roots to Euphorbia fischeriana. On the basis of 1D and 2D NMR, HR-ESI-MS spectroscopic anal., structures of the new compounds were elucidated as 11β-hydroxy-8,14-epoxy-ent-abieta-13(15)-en-16,12-olide (1), 3,20-dihydroxy-ent-1(10), 15-rosadiene (4), 3,7-dihydroxy-ent-1(10), 15-rosadiene (5), ingenol 6,7-epoxy-3- tetradecanoate (9). The compounds isolated were evaluated for their cytotoxicity against four cancer cell lines (A549, BEL7402, HCT116, and MDA-MB-231). Three ingenol diterpenoid.

View More

Full Text Substances (10) Reactions (0) Citing (29) Citation Map

2

Chemical Constituents and Biological Activities of Euphorbia fischeriana Steud.
 By: Sun, Yong-Xu; Liu, Ji-Cheng
 Chemistry & Biodiversity (2011), 8(7), 1205-1214 | Language: English, Database: CPlus and MEDLINE

A review of bioactive phytoconstituents from Euphorbia fischeriana root, including diterpenoids, triterpenes, steroids, aromatic compounds, and tannins. Their biol. activities are also discussed.

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

3

ent-Atisane diterpenoids from Euphorbia fischeriana inhibit mammosphere formation in MCF-

Concept

Top Count Alphanumeric Search

Concept Name

extract* Search

10 Selected

- Extraction (33)
- Solid phase extraction (2)
- Ultrasonic extraction (7)
- Inonotus obliquus extract (1)
- Solvent extraction (55)
- Yeast extract (2)
- Matrix solid phase dispersive extraction (2)
- Sophora flavescens extract (4)
- Supercritical extraction (3)
- Plant extracts (31)

Apply Cancel

(4) 在物质结果集页面，通过左侧 Reference role，选择 Occurrence，获取天然来源的物质；选择 natural product occurrence 精准获取来自天然产物中的物质。

Substances

References Reactions Suppliers Save and Alert

Filter Behavior: Filter by Exclude

Reaction Role: Product (484), Reactant (373), Reagent (354), Catalyst (301), Solvent (144)

Reference Role: **Biological Study (597)**, Preparation (582), Biological Study, Unclassified (576), Properties (576), Uses (566), View All, Commercial Availability, Available (517)

604 Results Sort: Relevance View: Partial

- 30220-46-3** C20H28O5 Ingenol (353 References, 454 Reactions, 63 Suppliers)
- 83036-62-8** C34H54O6 3-O-Tetradecanoylingenol (21 References, 8 Reactions, 4 Suppliers)
- 866556-16-3** C20H30O5 (4aR,6aR,7R,10aS,11R,11aR,11bR)-2,3,4,4a,5,6,6a,7,10a,11,11a,11b-Dodecahydro-6a... (16 References, 0 Reactions, 5 Suppliers)
- 1252785-68-4** (Absolute stereochemistry shown)
- 247020-79-7** (Absolute stereochemistry shown)
- 90397-85-6** (Absolute stereochemistry shown)

Reference Role

By Count Alphanumeric

2 Selected

- Biological Study (597)
- Preparation (582)
- Biological Study, Unclassified (576)
- Properties (576)
- Uses (566)
- Purification or Recovery (549)
- Therapeutic Use (548)
- Pharmacological Activity (539)
- Occurrence (536)
- Analytical Study (534)
- Analyte (526)
- Process (504)
- Synthetic Preparation (502)
- Physical, Engineering, or Chemical Process (500)
- Technical or Engineered Material Use (471)
- Adverse Effect (469)
- Agricultural Use (469)
- Modifier or Additive Use (465)
- Food or Feed Use (453)
- Other Use, Unclassified (451)
- Pollutant (446)
- Cosmetic Use (434)
- Industrial Manufacture (434)
- Formation, Non-preparative (428)
- Natural Product Occurrence (425)
- Analytical Role, Unclassified (423)
- Removal or Disposal (402)
- Nanoscale (397)
- Miscellaneous (394)
- Catalyst Use (393)
- Reagent (375)
- Biosynthetic Preparation (374)
- Diagnostic Use (371)
- Prophetic Synthesis or Use (366)
- Analytical Matrix (365)
- Bioindustrial Manufacture (334)
- Polymer in Formulation (329)
- Geological or Astronomical Occurrence (322)
- Byproduct (295)

Apply Cancel

Substances

References Reactions Suppliers Save and Alert

Filtering: Reference Role: Natural Product Occurrence X Clear All Filters

1,056 Results Sort: Relevance View: Partial

Filter Behavior

Filter by Exclude

Reaction Role

- Product (820)
- Reactant (624)
- Reagent (530)
- Catalyst (441)
- Solvent (201)

Reference Role

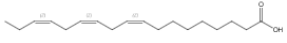
- Biological Study (1,663)
- Preparation (1,603)
- Properties (1,562)
- Uses (1,532)
- Biological Study, Unclassified (1,531)
- Natural Product Occurrence (1,056)
 - [View All](#)

Commercial Availability

- Available (891)
- Not Available (165)

1

463-40-1



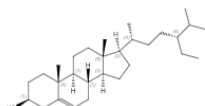
Double bond geometry shown

C₁₈H₃₀O₂
Linolenic acid

65K References 810 Reactions 107 Suppliers

2

83-46-5



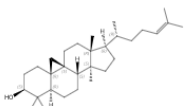
Absolute stereochemistry shown

C₂₉H₅₀O
(-)-β-Sitosterol

27K References 561 Reactions 93 Suppliers

3

469-38-5



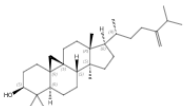
Absolute stereochemistry shown, Rotation (+)

C₃₀H₅₀O
Cycloartenol

1,825 References 42 Reactions 24 Suppliers

4

1449-09-8

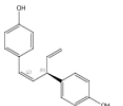


Absolute stereochemistry shown

C₃₁H₅₂O
24-Methylenecycloartenol

5

96895-25-9

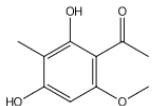


Absolute stereochemistry shown, Rotation (-)
Double bond geometry shown

C₁₇H₁₆O₂
Nvagal

6

83459-37-4



C₁₀H₁₂O₄
2,4-Dihydroxy-6-methoxy-3-methylacetophenone

如需更多 CAS SciFinder[®] 帮助, 请联系 china@acs-i.org, 010-63508026/7

31

物质检索

Q1: 在 CAS PatentPak 中如何搜索 CAS 登记号？

A1: 使用 Ctrl+F, 输入 CAS 登记号, 即可快速定位到所关注的物质。

Q2: 用结构式检索后, As Drawn、Substructure 和 Similarity 中哪个结果集可以使用 Chemscape 来进行分析？

A2: As Drawn、Substructure 或 similarity 选项中的物质都可以利用 Chemscape 来进行分析。

Q3: 如何根据碎片结构检索潜药？

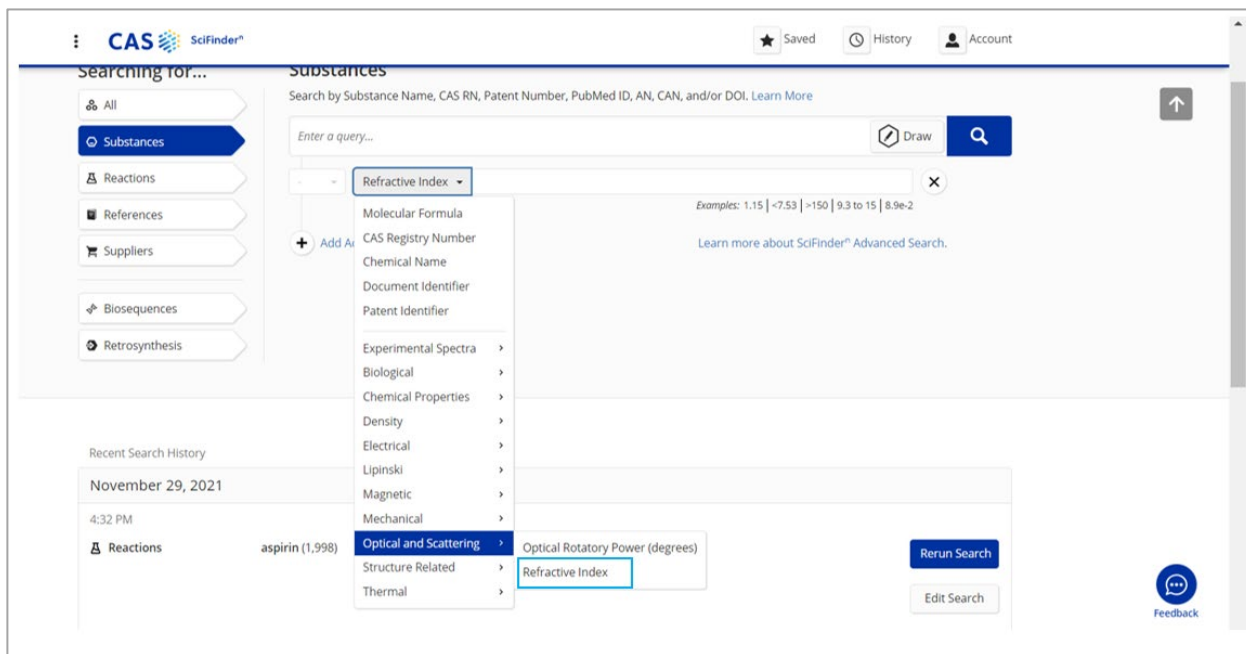
A3:

- 1) 首先在结构编辑器中绘制碎片结构 (各个碎片结构之间无需任何连接), 结构上传后进行检索。通过物质结果集页面左侧的 Number of Components, 确定这些碎片结构呈现在一个 (选数字 1) 还是多个 (除 1 以外的其他数字) 化学结构中;
- 2) 再通过物质结果集页面左侧的 Bioactivity Indicator 或 Target Indicator 筛选具有潜在生物活性的物质;
- 3) 最后, 点击物质结果集页面的 References 获取潜药的相关文献。

Q4: 如何根据折射率来获取物质？

A4: 先点击 CAS SciFinderⁿ 主页左侧的 Substances, 再点击 Add Advanced Search Field, 然后点击 Select, 在出现的列表中选择 Optical and Scattering, 再选择 Refractive Index, 在输入框中输入希望检索的定值 (比如 2) 或者区间值 (比如 >1, 2 to 3), 点击检索, 即可获得符

合要求的物质结果集。如下图所示：



Q5: 怎样绘制苯并杂环的通式结构?

A5:

- (1) 首先绘制一个苯环，然后在苯环上绘制一个并环，根据需要使用重复键重复原子或片段，获得期望的环。
- (2) 如果有特定的杂原子可选，则可以使用 R 基团，将需要的杂原子定义在 R 基团中，如果对并环是否饱和无特殊要求，则并环中的键可用… (unspecified bond) 来表示。

Q6: 在一个含有 N 杂环的物质 Substructure 检索结果集中，快速筛选出含有 2 个或者 3 个 N 原子数的物质的方法?

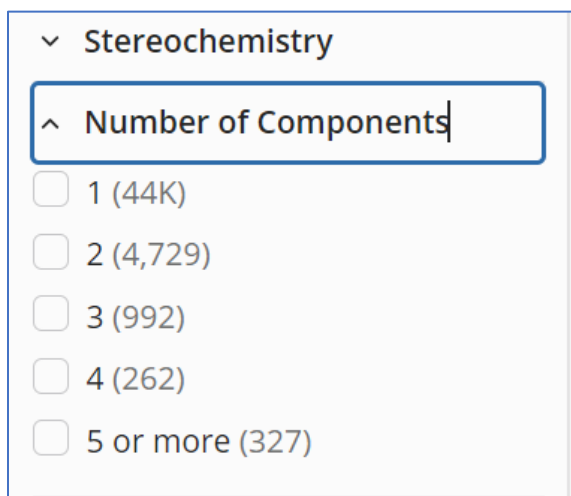
A6: 点击结果集页面左下角的 Search Within Results，打开结构编辑器，在结构编辑器中绘制指定的原子，比如要求筛选出含有 2 个 N 原子的物质，则在结构编辑器中绘制 2 个 N 原子，2 个 N 原子之间无需任何连接，单独绘制即可。检索后即可得到指定原子个数的物质。

Q7: 已知分子式及部分结构片段，如何快速得到目标物质?

A7: 通过分子式进行检索，在得到的物质结果集页面左下角选择 Search Within Results，在打开的结构编辑中输入结构片段，然后检索，即可快速获得目标物质。

Q8: 如何通过组分数筛选组合物?

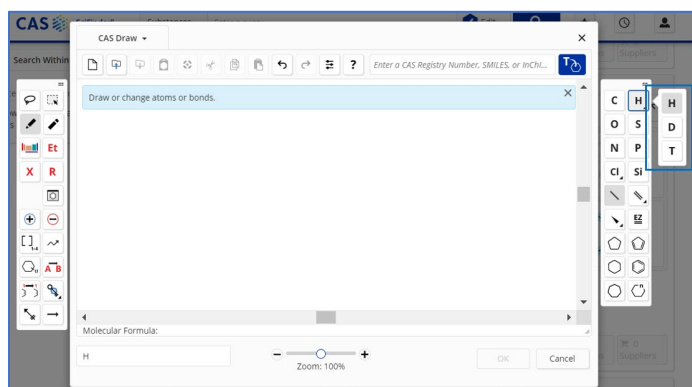
A8: 在物质结果集页面左侧选择 Number of Components，即可通过组分数筛选组合物，如下图所示:



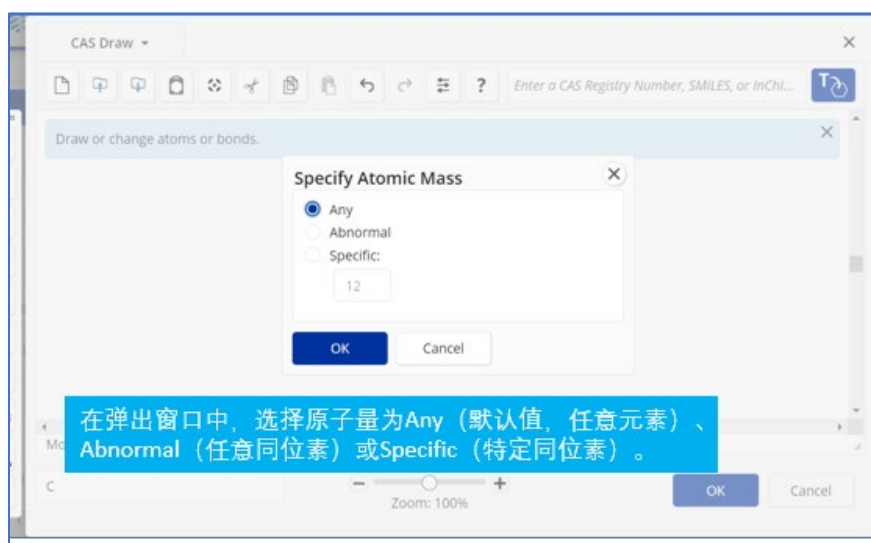
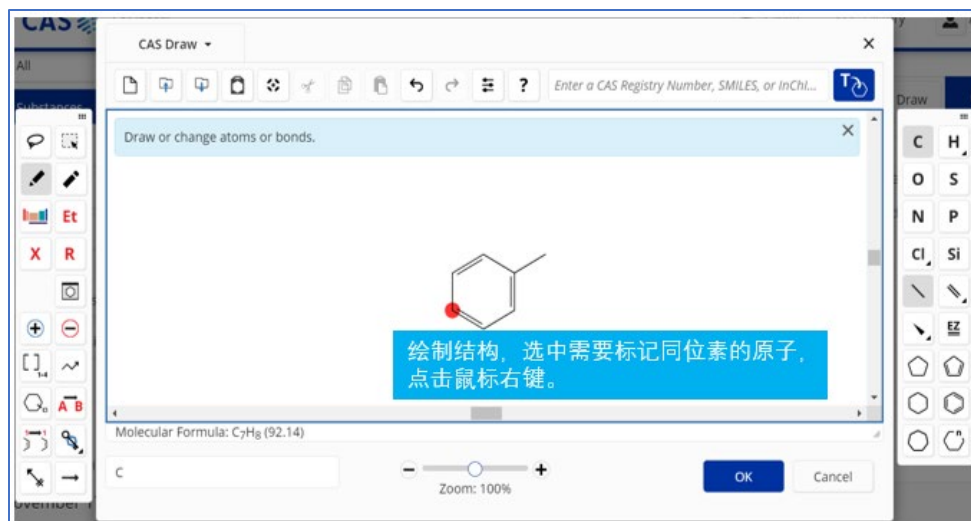
Q9: 如何检索同位素标记的化合物

A9: 以下三种方法可以获取到同位素标记的物质:

- 1) 对于含有 H 的同位素物质，可以在结构编辑器面板点击 H，在弹出框中直接选择 D, T 进行结构绘制。如下图所示



- 2) 在绘制结构时不考虑同位素，通过结构检索得到物质结果集页面后，点击物质结果集页面左侧 Filter by: Isotopes，选择 containing isotopes，即可获得各种同位素标记的物质。
- 3) 绘制任意特定原子的同位素方法如下:



Q10: 怎么找到物质的衍生物?

A10: 按照下述步骤操作:

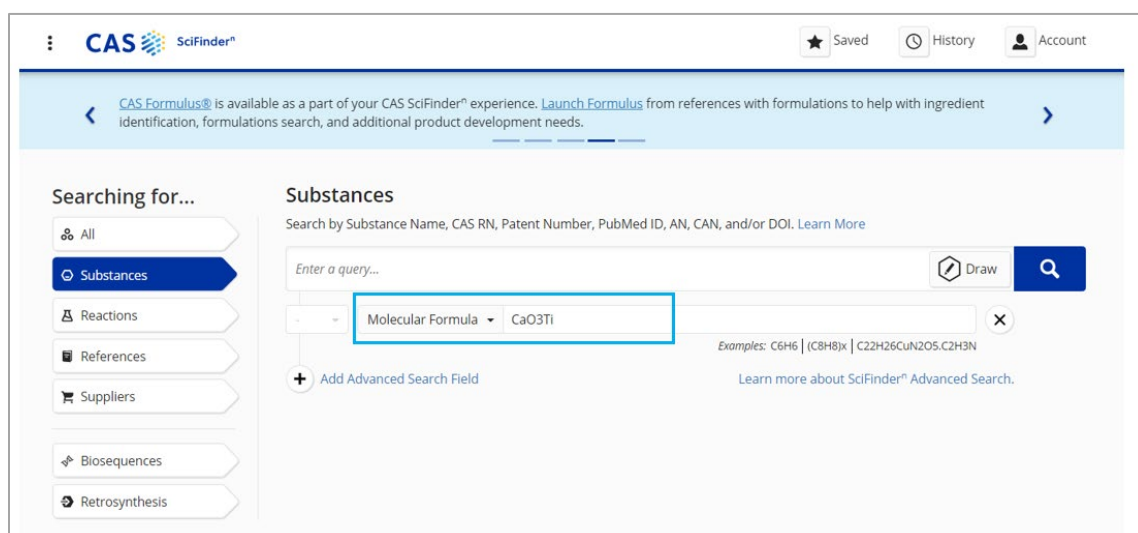
- 点击 Substances, 打开结构编辑器, 绘制结构。上传结构并检索
- 通过结构检索可同时获取 As Drawn, Substructure 和 Similarity 检索结果集, 默认展示 As Drawn 结果集。
- 点击 Substructure, 可获取绘制结构母核不变的衍生物; 点击 Similarity, 参考一定范围的相似度分值, 可以获取绘制结构母核发生一定变化的衍生物。

Q11: CAS SciFinder[®] 中的结构是否区分构象异构体?

A11: 在 CAS SciFinder[®] 结构编辑器中绘制结构时, 可使用结构面板的异构体键, 绘制旋光异构体或顺反异构体。在绘制结构和展示物质结果集时, 不区分构象异构或位阻异构等其他异构体, 这些异构可通过文献详情获取。

Q12: 如何检索无机氧化物, 比如 CaTiO₃?

A12: 点击 Substances, 再点击 Add Advanced Search, 点击 Select, 在下拉选项中选择 Molecular Formula。在输入框中输入 CaO₃Ti, 点击 Search 即可获得 CaTiO₃ 的物质信息。如下图:



The screenshot displays the CAS SciFinder[®] search interface. On the left, a sidebar titled "Searching for..." lists various search categories: All, Substances (highlighted), Reactions, References, Suppliers, Biosequences, and Retrosynthesis. The main area is titled "Substances" and includes a search bar with the placeholder "Enter a query...". Below the search bar, a dropdown menu is set to "Molecular Formula" and the input field contains "CaO₃Ti". A search button with a magnifying glass icon is visible. Below the search bar, there are examples: "Examples: C₆H₆ | (C₈H₈)_x | C₂₂H₂₆CuN₂O₅.C₂H₃N". A link "Learn more about SciFinder[®] Advanced Search." is also present.

Substance Detail (1 of 2) ← Prev Next →

References (8,211) Reactions (53) Suppliers (32) Download Email Save

CAS Registry Number
12049-50-2

Component	Ratio	CAS RN
O	3	17778-80-2
Ca	1	7440-70-2
Ti	1	7440-32-6

Ca.O.Ti
Components: 3
CaO₃Ti
Calcium titanium oxide (CaTiO₃) (8CI, 9CI, ACl)

Key Physical Properties	Value	Condition
Density (Experimental)	4.02 g/cm ³	Temp: Room temp

[Experimental Properties](#) | [Spectra](#)

在输入分子式时，需要遵循 Hill 规则：分子式中不含碳原子时，各元素排序根据字母顺序表进行排列；分子式中含碳原子时，“C”排首位，如有氢则紧随其后，其它元素符号按字母顺序排在氢的后面。

Q13: 如何检索对苯二甲酸和 Zn 组成的 MOF 材料?

A13: 按以下步骤操作:

- (1) 选择 Substances, 打开结构编辑器, 绘制对苯二甲酸和 Zn, 进行结构检索。
- (2) 在结果集页面, 可直接查看 As Drawn 结果, 如果需要查看有这类配体衍生物组成的 MOF 材料, 则可查看 Substructure 结果。

在物质结果集页面左侧选择 Filter By : Number of Components 选 1, 即获取配体和金属中心在同一个结构中的物质; 如果需要, 可进一步通过 substance class 选择 coordination compound 或 polymer。

Q14: 根据手性物质进行结构检索, 为什么结果中呈现的物质数量有时候少于 As Drawn 显示的结果数?

A14: As Drawn 涵盖的物质既包含 Absolute Stereo Match, 还包含 Stereo that doesn't Match Query 的物质。在展示结果时, CAS SciFinderⁿ 自动勾选了 Absolute Stereo Match, 这样就导致了呈现的物质数量与 As Drawn 展示数量不一致的情况。如果需要 As Drawn 包含的所有物质, 则可在结果集页面左侧勾选 Filter by: Stereochemistry 下所有选项。如下所示:

The screenshot shows the CAS SciFinder interface. On the left, under 'Structure Match', 'As Drawn (4)' is selected. Below that, 'Stereochemistry' is expanded, and 'Absolute Stereo Match (1)' is checked. The main search results area shows 'Substances (1)' with a filter for 'Stereochemistry: Absolute Stereo Match'. The first result is '2492423-29-5', which is a chemical structure of Uridine, 4-oxime, 5'-(2-methylpropanoate), (4Z)-. The structure is shown with absolute stereochemistry and double bond geometry. Below the structure, the molecular formula $C_{13}H_{19}N_3O_7$ and the name 'Uridine, 4-oxime, 5'-(2-methylpropanoate), (4Z)-' are displayed. At the bottom of the result card, there are statistics: 96 References, 96 Reactions, and 38 Suppliers.

Q15: 一个含有酰胺($O=C-NH$)的环系化合物, 如何获取其互变异构形成的-OH?

A15: 用结构式进行物质检索。在获得的结果集页面左侧, 点击 Analyze Structure Precision, 选择 Tautomers and Zwitterions 获取互变异构体和两性离子化合物。

The screenshot shows the CAS SciFinder web interface. At the top, there is a search bar with the text "Enter a query...". Below the search bar, there are navigation options: "Return to Home", "Structure Match", "Substructure (6M)", and "Similarity (43)". The "Structure Precision" section is expanded, showing "Conventional Results (449)" and "Tautomers and Zwitterions (2)". The "Filter Behavior" section has "Filter by" selected. The "Commercial Availability" section shows "Not Available (2)". The main content area displays two substance results:

- 253874-46-3**: Pyridinium, 1,2,6,7-tetrahydro-2-oxo-. Chemical structure: C1CCN(C1)=O with a positive charge on the nitrogen atom.
- 77979-51-2**: 2H-Pyrrol-2-one, 1,2-dihydro-, ion(1-). Chemical structure: C1CC(=O)N1 with a negative charge on the nitrogen atom.

Q16: 如何检索沸点是特定沸点的溶剂，且这个化合物不包含-COOH 和金属？

A16: 按如下步骤进行：

- 选择 Substances，点击 Add Advanced Search Field
- 点击 Select，在展示字段中点击 Thermal，然后点击 Boiling Point
- 在输入框中输入沸点范围或者确定的值（输入格式可为：500 to 600，> 500, 或 550 这类格式）；进行检索，得到物质结果集。
- 在物质结果集页面左侧点击 Exclude
- 点击 Metals: containing metals；排除含有金属原子的物质
- 点击 Search within Results，打开结构编辑器，在结构编辑器中输入 CO₂H，上传后进行检索，得到不含-CO₂H 的物质，如下所示：

CAS SciFinder[®] ★ Saved ⌚ History 👤 Account

← CAS Analytical Methods[®] is available as part of your CAS SciFinder[®] experience. [Identify and compare](#) the latest published analytical methods, featuring step-by-step instructions, in pharmacology, HPLC, food analysis, natural product isolation analysis, water analysis and more. →

Searching for...

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

Substances

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

Enter a query...

Boiling Point (°C) 500 to 600 Draw 🔍

Include predicted values. Examples: 1.15 | <-7.53 | >150 | 9.3 to 15 | 8.9e-2

+ Add Advanced Search Field [Learn more about SciFinder[®] Advanced Search.](#)

CAS SciFinder[®] Substances - Edit Search Enter a query... Draw 🔍 ★ ⌚ 👤

Filter by **Exclude** References Reactions Suppliers Save

Excluding: Metals: Containing Metals Search Within Results: Draw Structure Clear All Filters

Commercial Availability

Reaction Role

Reference Role

Stereochemistry

Number of Components

Substance Class

Isotopes

Metals

Containing Metals (14)

Not Containing Metals (425)

Molecular Weight

Experimental Property

Experimental Spectrum

Regulatory Data by Country

Regulatory Data by List

Bioactivity Indicator

Target Indicator

Search Within Results


Search for up to 3 structures within the result set.

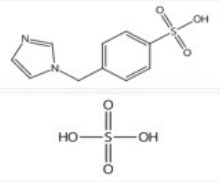
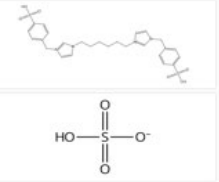
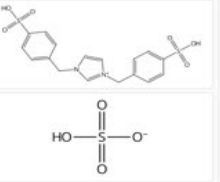
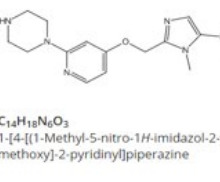
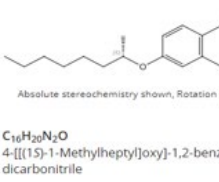
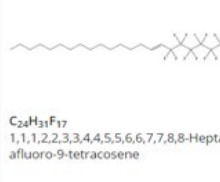
Draw

Search

Searching for... Clear All

Remove and Edit



<p>1</p> <p>1332456-96-8</p>  <p><chem>C10H10N2O3S.H2O4S</chem> Components: 2 Benzenesulfonic acid, 4-(1H-imidazol-2-ylmethyl), sulfate (1:1)</p> <p>2 References 6 Reactions 0 Suppliers</p>	<p>2</p> <p>1328886-83-4</p>  <p><chem>C26H32N4O6S2.2HO4S</chem> Components: 2 1H-Imidazolium, 1,1'-(1,6-hexanedyl)bis[3-[(4-sulfophenyl)methyl]-, sulfate (1:1)</p> <p>2 References 10 Reactions 0 Suppliers</p>	<p>3</p> <p>1328886-81-2</p>  <p><chem>C17H17N2O6S2.HO4S</chem> Components: 2 1H-Imidazolium, 1,3-bis[(4-sulfophenyl)methyl]-, sulfate (1:1)</p> <p>3 References 10 Reactions 0 Suppliers</p>
<p>4</p> <p>1270127-82-6</p>  <p><chem>C14H18N6O3</chem> 1-[4-[[1-(Methyl-5-nitro-1H-imidazol-2-yl)methoxy]-2-pyridinyl]piperazine</p> <p>1 Reference 5 Reactions 1 Supplier</p>	<p>5</p> <p>1268157-06-7</p>  <p><chem>C16H20N2O</chem> 4-[[[(1S)-1-Methylheptyl]oxy]-1,2-benzene dicarbonitrile</p> <p>1 Reference 3 Reactions 1 Supplier</p>	<p>6</p> <p>1244062-16-5</p>  <p><chem>C24H31F17</chem> 1,1,1,2,2,3,3,4,4,5,5,6,6,7,7,8,8-Heptafluoro-9-tetracosene</p> <p>1 Reference 0 Reactions 2 Suppliers</p>
7	8	9

Q17: 如何获取物质的旋光度?

A17: (1) 若已知物质名称、CAS 登记号或结构式等, 通过物质检索获取到物质信息后, 在物质详情页面 Experimental Properties: Optical and Scattering, 获取 optical rotatory power 旋光度信息。

Substance Detail (1 of 1)

References (7,730)

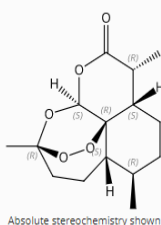
Reactions (2,949)

Suppliers (96)



CAS Registry Number

63968-64-9

C₁₅H₂₂O₅

3,12-Epoxy-12H-pyrano[4,3-j]-1,2-benzodioxepin-10(3H)-one, octahydro-3,6,9-trimethyl-, (3R,5aS,6R,8aS,9R,12S,12aR)-(9CI, AC1)

Key Physical Properties	Value	Condition
Molecular Weight	282.33	-
Melting Point (Experimental)	156-157 °C	-
Boiling Point (Predicted)	389.9±42.0 °C	Press: 760 Torr
Density (Experimental)	1.300 g/cm ³	-

Experimental Properties | Spectra

Other Names and Identifiers

Experimental Properties

Biological	Chemical	Density	Flow and Diffusion	Lipinski	Optical and Scattering	Structure Related	Thermal																																
<table border="1"> <thead> <tr> <th>Property</th> <th>Value</th> <th>Condition</th> <th>Source</th> </tr> </thead> <tbody> <tr> <td>Optical Rotatory Power</td> <td>+87.9 deg</td> <td>Solvent: 1,4-Dioxane; λ: 589.3 nm</td> <td>(1) CAS</td> </tr> <tr> <td>Optical Rotatory Power</td> <td>+75-+78 deg</td> <td>c: 1.0 g/100mL; Solvent: Ethanol; λ: 589.3 nm; Temp: 20 °C</td> <td>(2) CAS</td> </tr> <tr> <td>Optical Rotatory Power</td> <td>+68.2 deg</td> <td>c: 0.97 g/100mL; Solvent: Chloroform; Temp: 25 °C</td> <td>(3) IC</td> </tr> <tr> <td>Optical Rotatory Power</td> <td>+67.6 deg</td> <td>c: 1.75 g/100mL; Solvent: Chloroform; λ: 589.3 nm; Temp: 25 °C</td> <td>(4) CAS</td> </tr> <tr> <td>Optical Rotatory Power</td> <td>+66.6 deg</td> <td>c: 1.57 g/100mL; Solvent: Chloroform; λ: 589.3 nm; Temp: 24 °C</td> <td>(4) CAS</td> </tr> <tr> <td>Optical Rotatory Power</td> <td>+66.3 deg</td> <td>c: 1.64 g/100mL; Solvent: Chloroform; λ: 589.3 nm; Temp: 17 °C</td> <td>(5) APC</td> </tr> <tr> <td>Optical Rotatory Power</td> <td>+61 deg</td> <td>c: 0.2 g/100mL; Solvent: Chloroform; λ: 589.3 nm; Temp: 24 °C; Pathlength: 1 dm</td> <td>(6) CAS</td> </tr> </tbody> </table>								Property	Value	Condition	Source	Optical Rotatory Power	+87.9 deg	Solvent: 1,4-Dioxane; λ: 589.3 nm	(1) CAS	Optical Rotatory Power	+75-+78 deg	c: 1.0 g/100mL; Solvent: Ethanol; λ: 589.3 nm; Temp: 20 °C	(2) CAS	Optical Rotatory Power	+68.2 deg	c: 0.97 g/100mL; Solvent: Chloroform; Temp: 25 °C	(3) IC	Optical Rotatory Power	+67.6 deg	c: 1.75 g/100mL; Solvent: Chloroform; λ: 589.3 nm; Temp: 25 °C	(4) CAS	Optical Rotatory Power	+66.6 deg	c: 1.57 g/100mL; Solvent: Chloroform; λ: 589.3 nm; Temp: 24 °C	(4) CAS	Optical Rotatory Power	+66.3 deg	c: 1.64 g/100mL; Solvent: Chloroform; λ: 589.3 nm; Temp: 17 °C	(5) APC	Optical Rotatory Power	+61 deg	c: 0.2 g/100mL; Solvent: Chloroform; λ: 589.3 nm; Temp: 24 °C; Pathlength: 1 dm	(6) CAS
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Sources

(1) Yadav, J. S.; Tetrahedron Letters, (2003), 44(2), 387-389, CAplus

(2) Lapkin, Alexei A.; Journal of Natural Products, (2006), 69(11), 1653-1664, CAplus

(3) Ye, Bin; Journal of the Chemical Society, Chemical Communications, (1990)(10), 726-7, CAplus

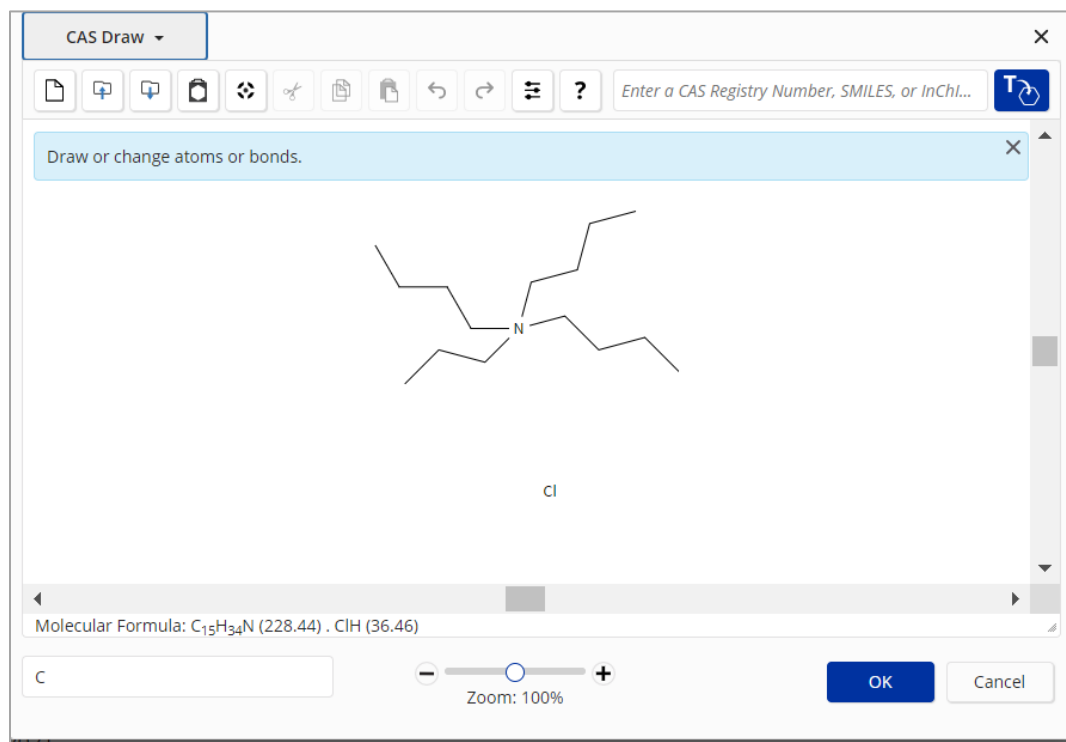
(2) 如果不知道物质结构或名称等信息，可以根据旋光度值来检索物质。点击 Substances: 再点击 Advanced Search Field，选择 Optical and Scattering: Optical Rotatory Power (degrees)，输入旋光度值（定值或者范围值都可以）。

(3) 如果物质详情中没有提供旋光度值信息，可通过输入主题词（如：optical rotatory dispersion and methyloxirane），获取特定物质的旋光度研究文献。

Q18: 如何检索有机盐?

A18: 通过以下两种方式获取:

(1) 两个组分同时画出来，不用任何键连接



获得所需结果

CAS SciFinder[®] Substances

[Return to Home](#)

Structure Match

- As Drawn (1)**
- Substructure (6,275)
- Similarity (90K)

Analyze Structure Precision

Chemscape Analysis

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

Create Chemscape Analysis

Filter Behavior

Filter by Exclude

Commercial Availability

Not Available (1)

Substances (1)

References **Reactions** **Suppliers**

1

1643849-82-4

C₁₅H₃₄N.Cl

Components: 2

Component RN: 29814-64-0

1-Butanaminium, *N,N*-dibutyl-*N*-propyl-, chloride (1:1)

7 8 0

References Reactions Suppliers

(2)绘制其中一个组分的结构

CAS Draw

Click an object to delete. Click and drag to delete multiple objects.

Molecular Formula: C₁₅H₃₄N (228.44)

Zoom: 100%

OK Cancel

获得结果集

← Return to Home

Structure Match

As Drawn (31)

Substructure (38K)

Similarity (159K)

Analyze Structure Precision

Chemscape Analysis

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

Create Chemscape Analysis

Filter Behavior

Filter by Exclude

Commercial Availability

Available (3)

Not Available (28)

Reaction Role

Substances (31) Sort: CAS RN: Descending View: Partial

References Reactions Suppliers

1 2611535-75-0

C15H34N.HO

Components: 2

Component RN: 29814-64-0

1-Butanaminium, *N,N*-dibutyl-*N*-propyl-, hydroxide (1:1)

1 Reference 0 Reactions 0 Suppliers

2 2447025-59-2

C15H34N.C6H8N3O2

Components: 2

Absolute stereochemistry shown

1 Reference 0 Reactions 0 Suppliers

3 2283341-71-7

C15H34N.F6P

Components: 2

1-Butanaminium, *N,N*-dibutyl-*N*-propyl-, hexafluorophosphate(1-)(1:1)

5 References 0 Reactions 0 Suppliers

在结果集中可以用物质类别筛选出盐

Substructure (38K)

Similarity (159K)

Analyze Structure Precision

Chemscape Analysis

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

Create Chemscape Analysis

Filter Behavior

Filter by Exclude

Commercial Availability

Reaction Role

Reference Role

Stereochemistry

Number of Components

Substance Class

Salt and Compound With (15)

Coordination Compound (14)

Organic/inorganic Small Molecule (2)

Isotopes

Metals

Molecular Weight

Filtering: Substance Class: Salt and Compound With Clear All Filters

1 2611535-75-0

C15H34N.HO

Components: 2

Component RN: 29814-64-0

1-Butanaminium, *N,N*-dibutyl-*N*-propyl-, hydroxide (1:1)

1 Reference 0 Reactions 0 Suppliers

2 2447025-59-2

C15H34N.C6H8N3O2

Components: 2

Absolute stereochemistry shown

1 Reference 0 Reactions 0 Suppliers

3 1643849-82-4

C15H34N.Cl

Components: 2

Component RN: 29814-64-0

1-Butanaminium, *N,N*-dibutyl-*N*-propyl-, chloride (1:1)

7 References 8 Reactions 0 Suppliers

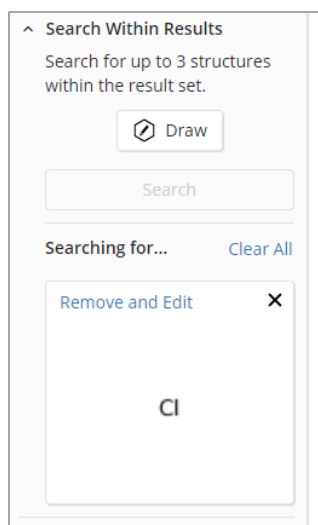
4 1425637-19-9

C15H34N.S2F6

5 1190079-34-5

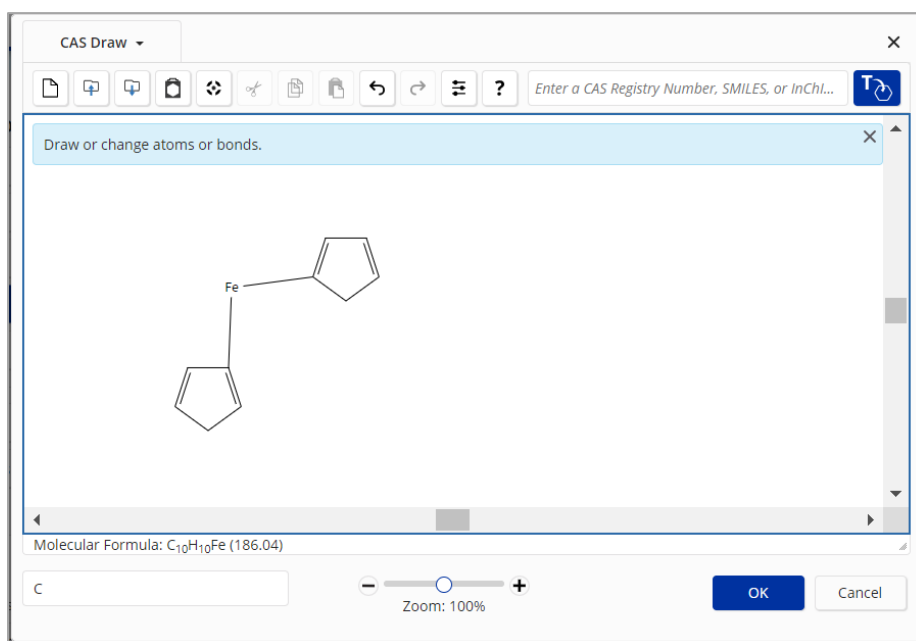
6 1092562-51-0

也可以在 search within results 中, 通过结构筛选另一组分



Q19: 如何绘制二茂铁类金属有机化合物?

A19: 使用单键, 或者不确定键, 连接金属原子和配体, 点击 OK。



根据需求选择锁环锁原子检索结果 (As Drawn) ;亚结构检索结果 (Substructure) 或者相似结构检索结果 (Similarity) 。

The screenshot shows the CAS SciFinder search results page for 'Substances' (746). The left sidebar is set to 'Structure Match' with 'As Drawn (746)' selected. The main content area displays three search results:

- 2734791-01-4**: $(C_{24}H_{18} \cdot C_{10}H_{10}Fe)_x$, Components: 2
- 2684300-23-8**: $C_{14}H_{20}O_2 \cdot Zn \cdot C_{10}H_{10}Fe$, Components: 2
- 2635404-85-0**: $C_{20}H_{14} \cdot C_{10}H_{10}Fe$, Components: 2

根据组分数，物质类别，是否包含同位素等筛选选项，获得结果。

The screenshot shows the CAS SciFinder search results page with various filters applied. The left sidebar shows the following filters:

- Reference Role**
- Number of Components**: 1 (10) [checked], 2 (516), 3 (133), 4 (36), 5 or more (6)
- Substance Class**: Coordination Compound (10) [checked], Polymer (2), Radical Ion (2), Ring Parent (1)
- Isotopes**: Containing Isotopes (15), Not Containing Isotopes (10) [checked]
- Metals**
- Molecular Weight**
- Experimental Property**
- Experimental Spectrum**
- Regulatory Data by Country**

The main content area displays nine search results:

- 119087-69-3**: $C_{10}H_{10}Fe$, Ferrocene, ion(2-)
- 86549-93-1**: $C_{10}H_{10}Fe$, Ferrocenium(2+)
- 67269-42-5**: $C_{10}H_{10}Fe$, Ferrocene, radical ion(1-)
- 51937-67-8**: $(C_{10}H_{10}Fe)_x$, Ferrocene polymer
- 12125-80-3**: $C_{10}H_{10}Fe$, Ferrocenium
- 9022-10-0**: $(C_{10}H_{10}Fe)_x$, Ferrocenium, homopolymer

Q20: 聚合物属性 dn/dc 怎么获取?

A20: 属性值的获取有以下几个操作选项供选择。

(1) 若需要通过属性值来获取物质, 则可在 CAS SciFinder[®] 主页面点击 Substances, 然后在 Advanced Search Filed 选择对应的属性值选项输入值即可进行检索, 获取相应的物质;

(2) 若需查询某个特定物质的属性值, 则可以先通过 Substances 检索获取到该物质, 再点击其 CAS 登记号打开 Substance Detail 页面, 在 Substance Detail 可查看该物质的各种属性值;

(3) 若通过方法 (1) 或 (2) 无法获取到期望的属性值, 则可通过 References 获取文献来实现。如, 获取聚合物的 dn/dc 值, 推荐在 References 输入框中输入 "refractive index increment" or dn/dc and polymer, 获取聚合物 dn/dc 研究文献。

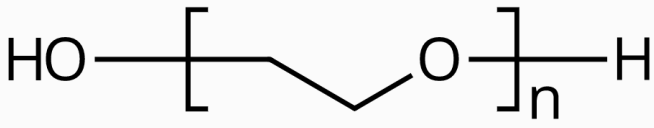
The screenshot shows the CAS SciFinder interface. At the top, the search bar contains the query "refractive index increment" or dn/dc and polymer. The page displays search results for this query, with 5,773 results found. The first result is titled "Determination of refractive index increment dn/dc of polymers in mixed solvent solutions. Relation between dn/dc and the partial specific volume of the polymers" by Hert, M.; Strazielle, C., published in the European Polymer Journal (1973), 9(6), 543-57. The second result is titled "Conformation and dn/dc determination of cellulose in N,N-dimethylacetamide containing lithium chloride" by Dupont, Anne-Laurence; Harrison, Gabrielle, published in Carbohydrate Polymers (2004), 58(3), 233-243. The interface includes a filter sidebar on the left with options for Document Type and Language, and a top navigation bar with various icons and a search button.

此外，与 dn/dc 值相关的 refractive index 值可以点击某聚合物 CAS 登记号，查看物质详情获取。

Substance Detail

References (405K) Reactions (55K) Suppliers (597) Download Email Save

CAS Registry Number
25322-68-3



$(C_2H_4O)_n \cdot H_2O$
Poly(oxy-1,2-ethanediyl), α -hydro- ω -hydroxy- (9CI, ACI)

Polymer Class Terms
Polyether

Key Physical Properties	Value	Condition
Melting Point (Experimental)	57.5 °C	-
Boiling Point (Experimental)	>325 °C	-
Density (Experimental)	1.127 g/cm ³	Temp: 20 °C

Experimental Properties | Spectra

Experimental Properties

Biological Chemical Density Electrical Flow and Diffusion Interface Magnetic Mechanical Nuclear **Optical and Scattering** Structure Related Thermal

Property	Value	Condition	Source
Refractive Index	1.47	-	(1) CAS
Refractive Index	1.4690	λ : 589.3 nm; Temp: 20.00 °C	(2) CAS
Refractive Index	1.4665	λ : 589.3 nm; Temp: 30.00 °C	(2) CAS
Refractive Index	1.4626	λ : 589.3 nm; Temp: 20.00 °C	(2) CAS
Refractive Index	1.462	-	(3) CAS
Refractive Index	1.4607	λ : 589.3 nm; Temp: 40.00 °C	(2) CAS
Refractive Index	1.4605	λ : 589.3 nm; Temp: 20 °C	(4) CAS
Refractive Index	1.46	-	(1) CAS
Refractive Index	1.4599	λ : 589.3 nm; Temp: 35.00 °C	(5) CAS
Refractive Index	1.4582	λ : 589.3 nm; Temp: 30.00 °C	(2) CAS
Refractive Index	1.4582	Temp: 25 °C	(6) CAS
Refractive Index	1.4563	-	(7) CAS
Refractive Index	1.4563	λ : 589.3 nm	(8) CAS
Refractive Index	1.4547	λ : 589.3 nm; Temp: 40.00 °C	(2) CAS
Refractive Index	1.4539	λ : 589 nm; Temp: 20 °C	(9) CAS
Refractive Index	1.4537	-	(10) CAS
Refractive Index	1.362	-	(11) CAS
Birefringence - 1 Source	See Full Text		(12) CAS

也可以在物质高级检索项中，通过 refractive index 值来检索聚合物。

CAS SciFinder®

Saved and Alerts History Account

Searching for...

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

Substances

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

Enter a query... Draw Q

Molecular Formula

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

Learn more about SciFinder® Advanced Search.

+ Add Advanced Search Field

- Molecular Formula
- CAS Registry Number
- Chemical Identifier
- Document Identifier
- Patent Identifier
- Experimental Spectra
- Biological
- Chemical Properties
- Density
- Electrical
- Lipinski
- Magnetic
- Mechanical
- Optical and Scattering
- Structure Related
- Thermal
- Optical Rotatory Power (degrees)
- Refractive Index**

View All Search History

Run Search Edit Search

Recent Search History

April 26, 2022

- References *refractive index in 4:18 PM

CAS SciFinder®

Saved and Alerts History Account

Searching for...

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

Substances

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

Enter a query... Draw Q

Refractive Index >1.5

Examples: 1.15 | <7.53 | >150 | 9.3 to 15 | 8.9e-2

Search key property values only.

Learn more about SciFinder® Advanced Search.

+ Add Advanced Search Field

The screenshot displays the CAS SciFinder® interface for searching substances. The search criteria are set to 'Substance Class: Polymer', resulting in 895 items. The results are sorted by 'Number of References: Descending' and shown in a 'Partial' view. A left-hand sidebar provides various filters such as Reaction Role, Reference Role, Commercial Availability, Molecular Weight, Stereochemistry, and Substance Class. The Substance Class filter is currently set to 'Polymer (895)'. The main area shows six result cards, each containing a chemical structure, a name, a formula, and counts for references, reactions, and suppliers.

Card #	Chemical Structure	Name	Formula	References	Reactions	Suppliers
1	<chem>=</chem>	Ethene, homopolymer	$(C_2H_4)_x$	452K	20K	95
2	<chem>C=CC</chem>	Polypropylene	$(C_3H_6)_x$	297K	7,172	28
3	<chem>C=Cc1ccccc1</chem>	Polystyrene	$(C_8H_8)_x$	267K	15K	166
4	<chem>O=C(Oc1ccc(cc1)C(=O)O)O</chem>	Poly(ethylene terephthalate)	$(C_{10}H_8O_4)_n$	-	-	-
5	<chem>C=CO</chem>	Poly(vinyl alcohol)	$(C_2H_4O)_x$	-	-	-
6	<chem>C=CCl</chem>	Poly(vinyl chloride)	$(C_2H_3Cl)_x$	-	-	-

Q21: 三氯化铁结构式怎么画?

A21: 在绘制三氯化铁结构式时, 如果不清楚其键型, 则可使用 CAS Draw 面板右侧虚线键来绘制 Fe---Cl 键。然后在物质结果中, 可通过 Substance Class 浏览相关结构的分子类型。

CAS SciFinder® Substances

Return to Home

Substances

References Reactions Suppliers

Structure Match

As Drawn (2,772)

Substructure (16K)

Similarity (2,101)

Analyze Structure Precision

Chemscape Analysis

Visually explore structure similarity with a powerful new tool.
Learn more about Chemscape.

Create Chemscape Analysis


Filter Behavior

Filter by Exclude

Reaction Role

2,772 Results


1 7705-08-0



Cl₃Fe
Iron chloride (FeCl₃)

114K References 78K Reactions 50 Suppliers

2 10025-77-1



Cl₃Fe·6H₂O
Components: 2
Component RN: 7705-08-0
Ferric chloride hexahydrate

9,619 References 5,869 Reactions 71 Suppliers

3 144920-78-5

Component	Ratio
Cl	x
HO	x
Fe	x
Al	x

Al.Cl.Fe.HO
Components: 4
Aluminum iron chloride hydroxide

857 References 1 Reaction 2 Suppliers

4 12173-26-1

5 68896-16-2

6 1303-91-9

Substance Class

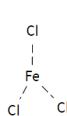
- Tabular Inorganic (1,002)
- Coordination Compound (954)
- Salt and Compound With (531)
- Alloy (177)
- Mineral (61)
- Polymer (61)
- Mixture (50)
- Radical Ion (4)
- Organic/Inorganic Small Molecule (4)
- Generic Registration (2)
- Manual Registration (2)

[View Fewer](#)

CAS Draw

Enter a CAS Registry Number, SMILES, or InChI...

Draw or change atoms or bonds.



Molecular Formula: Cl₃Fe (162.21)

Zoom: 140%

OK Cancel

结构检索可以获得三个精准度的结果（As Drawn, Substructure, Similarity）。
如果分子组成已经确定，也可以使用分子式检索三氯化铁，快速获取结果。

Searching for...

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

Substances

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

Enter a query...

Molecular Formula Cl₃Fe

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

[Add Advanced Search Field](#) [Learn more about SciFinder[®] Advanced Search.](#)

CAS SciFinder[®] Substances [Edit Search](#) Enter a query...

Substances

References Reactions Suppliers Save and Alert

Filter Behavior

Filter by Exclude

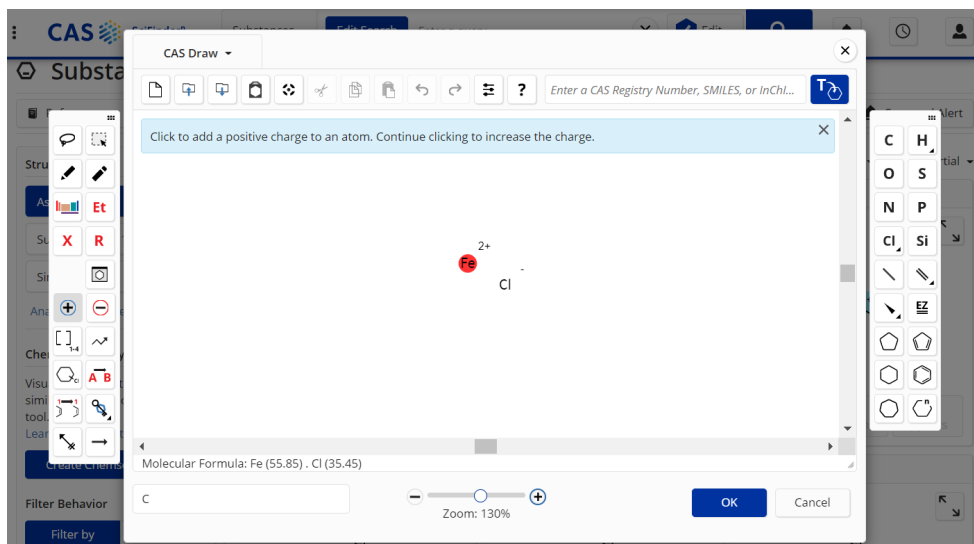
- Reaction Role
- Reference Role
- Commercial Availability
- Number of Components
- Molecular Weight
- Substance Class
 - Coordination Compound (5)
 - Organic/Inorganic Small Molecule (4)
 - Mineral (2)
 - Tabular Inorganic (1)
- Isotopes
- Metals

11 Results Sort: Number of References: Descending View: Partial

<p>1</p> <p>7705-08-0</p> <p>Cl₃Fe Iron chloride (FeCl₃)</p> <p>114K References 78K Reactions 50 Suppliers</p>	<p>2</p> <p>14639-85-1</p> <p>Cl₃Fe Molybdenum trichloride (MoCl₃)</p> <p>43 References 0 Reactions 0 Suppliers</p>	<p>3</p> <p>43562-08-9</p> <p>Cl₃Fe Ferrate(1-), trichloro-</p> <p>28 References 0 Reactions 0 Suppliers</p>
<p>4</p> <p>120028-37-7</p> <p>⁵⁷Fe</p>	<p>5</p> <p>18497-67-1</p> <p>⁵⁹Fe</p>	<p>6</p> <p>66546-71-2</p> <p>⁵⁵Fe</p>

Q22: 在绘制结构时, 如何输入电荷?

A22: 在 CAS Draw 面板中, 使用左侧正负电荷工具 , 点击对应原子进行电荷标注。点击一下, 即会在原子上标注一个正/负电荷, 多次点击则会标注多个电荷。



Q23: 如何检索一个物质的同分异构体?

A23: 在 CAS SciFinder[®] 主页面点击 Substances, 在 Advanced Search Field: Molecular Formula 输入框中输入此物质的分子式, 就可以检索到此物质的各种同分异构体。例如: $(C_2H_4O)_n C_4H_8O$ 。

Reference ID	Chemical Structure	Molecular Formula	Name	References	Reactions	Suppliers
31497-33-3		$(C_2H_4O)_n C_4H_8O$	Poly(oxy-1,2-ethanediyl), α -(2-methyl-2-propen-1-yl)- ω -hydroxy-	1,366	1,271	5
27252-80-8		$(C_2H_4O)_n C_4H_8O$	Polyethylene glycol allyl methyl ether	839	442	13
85600-94-8		$(C_2H_4O)_n C_4H_8O$	Poly(oxy-1,2-ethanediyl), α -3-buten-1-yl- ω -hydroxy-	35	15	0

Q24: 反应物已知，产物的一级质谱图和二级质谱图已知，如何猜测产物的可能结构呢？

A24: 推荐思路和检索步骤：

(1) 根据一级质谱和二级质谱信息可以分析出产物的分子量范围和部分结构碎片，再结合反应物的结构进一步确认产物可能的结构碎片。

(2) 然后基于这两部分信息在 CAS SciFinder[®] 中联合分子量和片段结构检索，获得相关的物质信息。如果还知道核磁数据，可以一并联合检索。

The screenshot shows the 'Substances' search page in CAS SciFinder. On the left, there is a 'Searching for...' sidebar with options: All, Substances (selected), Reactions, References, Suppliers, Biosequences, and Retrosynthesis. The main search area is titled 'Substances' and includes a search bar with the text 'Enter a query...'. Below the search bar, there is a filter for 'Molecular Weight' set to '400 to 500'. A note below the filter says 'Predicted values only.' and provides examples: 'Examples: 46...'. There is a '+ Add Advanced Search Field' button and a 'Learn more about Sci...' link. On the right side of the search area, there is an 'Edit' button and a search icon. Below the search area, there is a drawing tool with 'Edit Drawing' and 'Remove' buttons, and a checkbox for 'Search Patent Markush'.

The screenshot shows the 'Substances' search page in CAS SciFinder. On the left, there is a 'Searching for...' sidebar with options: All, Substances (selected), Reactions, References, Suppliers, Biosequences, and Retrosynthesis. The main search area is titled 'Substances' and includes a search bar with the text 'Enter a query...'. Below the search bar, there are three filters: 'Molecular Weight' set to '400 to 500', 'Carbon-13 NMR' set to 'Multiple entries must be delimited by a comma.', and 'Proton NMR' set to 'Multiple entries must be delimited by a comma.'. Notes below the filters include 'Predicted values only.' and 'Allowance of ± 2 ppm.' for the NMR filters. Examples are provided: 'Examples: 46...' for molecular weight, and 'Examples: 152.3, 127.6, 133.1 |' and 'Examples: 8.03, 7.2, 2...' for the NMR filters. There is a '+ Add Advanced Search Field' button and a 'Learn more about SciFinder[®] Advanced Search.' link. On the right side of the search area, there is an 'Edit' button and a search icon. Below the search area, there is a drawing tool with 'Edit Drawing' and 'Remove' buttons, and a checkbox for 'Search Patent Markush'.

(3) 获得相关的物质结果后，可根据结果集页面左侧 Reaction Role、Reference Role 限定物质在反应和文献中的角色。如果要获取反应信息，可点击物质下方 Reactions 或页眉上方的 Reactions。根据需要，在反应结果集页面，通过左侧 Search Within Results 限定原料的结构。

CAS SciFinder® Substances (216,941) Edit Search Enter a query... X Edit Q Save And Alerts

Structure Match: As Drawn (0) Substructure (216K) Similarity (0) Analyze Structure Precision

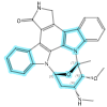
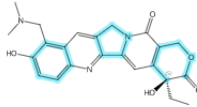
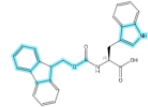
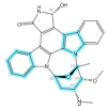
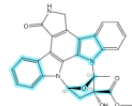
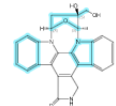
Chemscape Analysis: Visually explore structure similarity with a powerful new tool. Learn more about Chemscape. Create Chemscape Analysis

Filter Behavior: Filter by Exclude

Commercial Availability: Reaction Role: Product (75K), Reactant (18K), Reagent (30), Catalyst (47); Reference Role: Preparation (82K), Synthetic Preparation (81K), Uses (47K)

Substances (216,941) Sort: Number of References: Descending View: Partial

References Reactions Suppliers Save And Alerts

<p>1</p> <p>62996-74-1</p>  <p>Absolute stereochemistry shown, Rotation (+)</p> <p>$C_{28}H_{26}N_4O_3$ Staurosporine</p> <p>9,438 References 165 Reactions 92 Suppliers</p>	<p>2</p> <p>123948-87-8</p>  <p>Absolute stereochemistry shown</p> <p>$C_{23}H_{23}N_3O_5$ Topotecan</p> <p>7,919 References 92 Reactions 57 Suppliers</p>	<p>3</p> <p>35737-15-6</p>  <p>Absolute stereochemistry shown, Rotation (-)</p> <p>$C_{26}H_{22}N_2O_4$ Fmoc-L-tryptophan</p> <p>3,636 References 26K Reactions 84 Suppliers</p>
<p>4</p> <p>112953-11-4</p>  <p>Absolute stereochemistry shown</p> <p>$C_{28}H_{26}N_4O_4$ 7-Hydroxystaurosporine</p> <p>776 References 7 Reactions 24 Suppliers</p>	<p>5</p> <p>99533-80-9</p>  <p>Absolute stereochemistry shown, Rotation (+)</p> <p>$C_{27}H_{21}N_3O_5$ (+)-K 252a</p> <p>710 References 60 Reactions 54 Suppliers</p>	<p>6</p> <p>111358-88-4</p>  <p>Absolute stereochemistry shown</p> <p>$C_{26}H_{21}N_3O_4$ Lestaurtinib</p> <p>710 References 40 Reactions 40 Suppliers</p>

The screenshot displays the CAS SciFinder interface for a reaction search. The search criteria are '62996-74-1'. The left sidebar shows filter options, with 'Product (59)' selected. The main content area shows a single result for the reaction 'Process for the preparation of midostaurin with high purity'. The reaction scheme shows a complex polycyclic reactant with absolute stereochemistry, reacting to form a similar product with absolute stereochemistry and a rotation of (+). Below the reaction, there are buttons for 'Suppliers (14)' and 'Suppliers (92)'. The 'Reaction Summary' section provides details for two steps: 1.1 (Reagents: Trifluoroacetic acid, Triethylsilane; Solvents: Dichloromethane; 1 h, 0 - 5 °C) and 1.2 (Reagents: Sodium bicarbonate; Solvents: Methanol, Water). The summary indicates 1 step and 80% yield.

Q25: CAS RN 174362-96-0 结果详情的显示中为什么有两个 CAS RN?

A25: 如截图所示: CAS RN 174362-96-0 是均聚物的 CAS 登记号, 而 CAS RN 174362-95-9 是聚合物单体的 CAS 登记号。

CAS SciFinder[®] Substances 174362-96-0

← Return to Results

Substance Detail (1 of 1)

References (13) Reactions (0) Suppliers (0)

CAS Registry Number
174362-96-0

174362-95-9
C₁₃H₂₃NO₉

(C₁₃H₂₃NO₉)_x
Propanoic acid, 3,3'-[[2-amino-2-[(2-carboxyethoxy)methyl]-1,3-propanediyl]bis(oxy)]bis-, homopolymer (9CI, ACI)

Q26: 如何检索具有拓扑结构的可形成氢键的物质?

A26: 可以从结构和关键词两方面进行检索。

(1) 如果有具体的母核结构，在结构绘制时，可根据氢键形成的原理，加入 N-H, O-H, S-H, O=, N=等元素进行物质结构检索；得到物质结果后，再通过物质结果获取文献；在文献结果集页面，通过左侧 Filter by: Search Within Results 输入 topol 或 hydrogen bond 来精炼文献结果。

(2) 如果没有特定的结构信息，则推荐通过关键词直接检索相关的研究文献，例如：(topology or topol) and “hydrogen bond”，在文献结果集页面左侧通过 Filter by: Concept，限定感兴趣的核心研究点，例如，通过 hydrogen bond, molecular topology 等精炼相关文献。

The screenshot shows the CAS SciFinder search results page. The search query is "(topology or topol) and 'hydrogen bond'". The results are sorted by Relevance and shown as Partial Abstracts. There are 4,942 references. The left sidebar shows filter options, with 'Concept' selected and 'Hydrogen bond' and 'Molecular topology' checked. The main content area displays two search results:

1
Experimental electron density overlapping in hydrogen bonds: topology vs. energetics
 By: Espinosa, E.; Lecomte, C.; Molins, E.
 Chemical Physics Letters (1999), 300(5,6), 745-748 | Language: English, Database: CAPlus

We have investigated the relationship between the energetic properties of the hydrogen bond (HB) interaction and the topol. overlapping of the electronic clouds at the H...O critical point r_{CP} . This study involves a total of 83 X-H...O (X = C, N, O) HBs, which have been described in terms of the topol. properties of the electron d. $\rho(r)$ for a large set of compounds Kinetic $G(r_{CP})$ and potential $V(r_{CP})$ contributions to the local energy d. of electrons exhibit linear functionalities against, resp., the pos. and neg. curvatures of $\rho(r)$ at the critical point, showing an effective deconvoluti.

2
Enumeration of topology-distinct structures of hydrogen bonded water clusters
 By: Miyake, Toshiko; Aida, Misako
 Chemical Physics Letters (2002), 363(1,2), 106-110 | Language: English, Database: CAPlus

We present a graph theor. procedure to generate all the topol.-distinct structures for water clusters. The hydrogen bond matrix (H-

Q27: CAS 在标引聚合物时，会关注聚合物的哪些信息？

A27: CAS 科学家标引聚合物时，会关注聚合物的结构式、分子式、名称、制备、用途、工艺等信息。

Q28: 检索反应时，一个是催化剂结构，一个是反应物结构，怎么通过角色定义来检索这样的反应？

A28: 推荐以下操作方法：

(1) 先选择 Substances，检索催化剂。在获得的物质结果集页面，通过左侧 Filter by: Reaction Role, 将物质限定为在反应中的角色为 catalyst;

(2) 点击物质结果集页面左上方的 Reactions，获得步骤 (1) 中物质作为催化剂参与的反应结果集，在反应结果集页面左侧点击 Search within results，在结构编辑器中绘制结构，使用反应角色定义工具将其限定为原料 (reactant)。

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

- Search Bar:** "Substances" with a query input field.
- Navigation:** "References", "Reactions", and "Suppliers" tabs.
- Structure Match:**
 - As Drawn (805)
 - Substructure (6,994)
 - Similarity (6,861)
 - Analyze Structure Precision
 - Chemscape Analysis: "Visually explore structure similarity with a powerful new tool. Learn more about Chemscape. Create Chemscape Analysis"
 - Filter Behavior: "Filter by" and "Exclude" buttons.
 - Reaction Role:
 - Product (39)
 - Reactant (1)
 - Reagent (15)
 - Catalyst (29)
- Filtering:** "Reaction Role: Catalyst" with a close button.
- Results:** 29 results found, sorted by "Number of References: Descending".
 - Result 1:** 7550-45-0. Structure: Cl[Ti](Cl)(Cl)Cl. Name: Cl_4Ti Titanium tetrachloride. 56K References, 76K Reactions, 76 Suppliers.
 - Result 2:** 11130-18-0. Structure: Cl[Ti]Cl. Name: Cl_2Ti Titanium chloride. Components: 2. 1,442 References, 26 Reactions, 3 Suppliers.
 - Result 3:** 12003-13-3. Structure: Cl[Al](Cl)[Ti]Cl. Name: $AlCl_2Ti$ Aluminum titanium chloride ($AlTi_2Cl_3$). Components: 3. 377 References, 13 Reactions, 17 Suppliers.
 - Result 4:** 53195-03-2. Structure: [Cl-].[Ti+4](Cl)(Cl)Cl.
 - Result 5:** 1800582-27-7. Structure: Cl[Ti]Cl.
 - Result 6:** 67113-71-7. Structure: Cl[Ti]Cl. Component: Cl, Ratio: 11.

Reactions

References ▾

Filtering: Substance Role: Catalyst ✕ Search Within Results: Drawn Structure ▾ ✕
[Clear All Filters](#)

20 Results
Group: By Document ▾ View: Expanded ▾

Filter Behavior

Filter by Exclude

Substance Role

Reagent (100)

Catalyst (20)

Yield

Number of Steps

Non-Participating Functional Groups

Experimental Protocols

Reaction Type

Reagent

Catalyst

Solvent

Commercial Availability

Reaction Notes

Search Within Results

Search for up to 3 structures within the result set.

Draw

Searching for... [Clear All](#)

Remove and Edit ✕

Preparation of pyrrolopyridinone and pyrrolopyrimidinone derivatives as TYK2 inhibitors and uses thereof

By: Dahlgren, Markus; Greenwood, Jeremy Robert; Harriman, Geraldine C.; Kennedy-Smith, Joshua Jahmil; Masse, Craig E.; et al
World Intellectual Property Organization, WO2016138352 A1 2016-09-01 | Language: English, Database: CAplus

PatentPak ▾ Full Text ▾

Suppliers (60)

Suppliers (87)

Suppliers (5)

Reaction Summary Steps: 1 Yield: 100%

1.1 Catalysts: [Titanium tetrachloride](#)
Solvents: [Dichloromethane](#); rt; 18 h, rt

1.2 Reagents: [Water](#); cooled

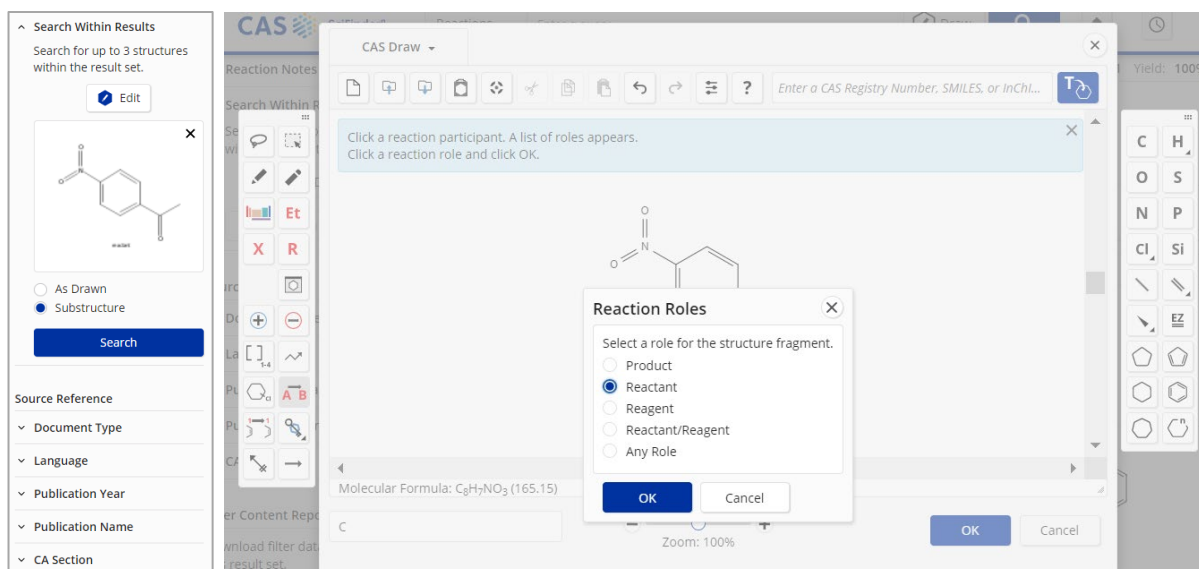
[View Reaction Detail](#)

2

One-pot three components synthesis of β-amido ketones

By: Yang, Deli; Li, Jiarong; Sun, Kening; Lu, Hongyan; Liu, Mingxing; et al
Youji Huaxue (2013), 33(11), 2341-2348 | Language: Chinese, Database: CAplus

Full Text ▾ View 3 Related Reactions



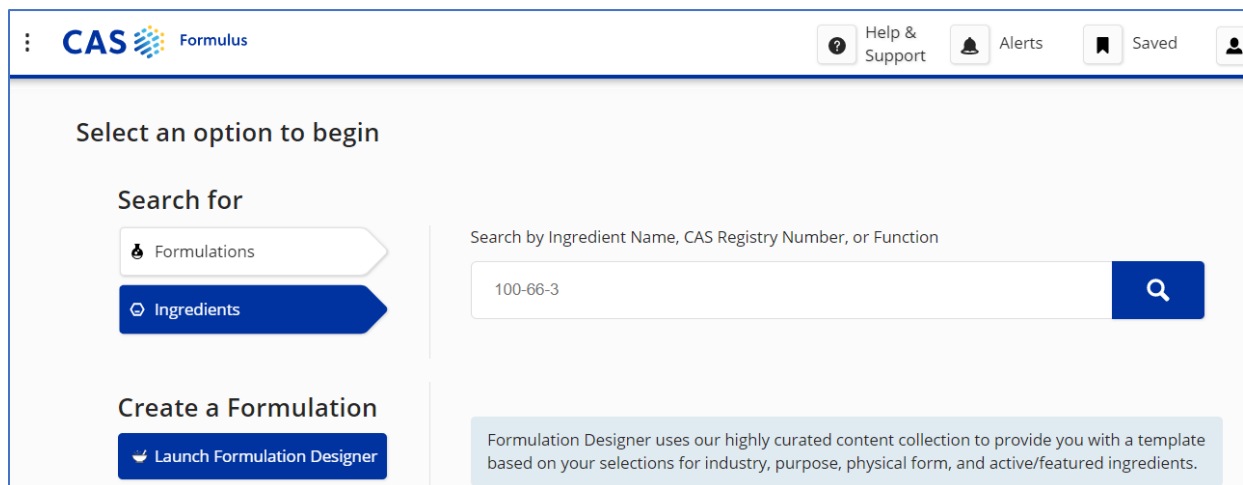
Q29: 怎样查找化合物的用途信息?

A29: 以苯甲醚 (CAS RN 100-66-3) 为例, 分别介绍其在配方中的应用、在化学反应中的应用 (作为反应物或溶剂)。

(1) 在配方中的应用。

登录 <https://formulus.cas.org/#/search>, 进入 CAS Formulus 进行检索:

a. 点击 Ingredients, 输入苯甲醚 CAS 登记号。



b. 点击 View Details 或 Commonly Formulated with 查看其在配方中的用途。

The screenshot displays the CAS SciFinder® interface for the ingredient Anisole. The search bar at the top shows 'Ingredients' and the CAS number '100-66-3'. The left sidebar contains filter options under 'Filter by', including Industry, Regulatory Information, Experimental Properties, and Commercial Availability. The main content area shows the chemical structure of Anisole (C₇H₈O) and a table of key physical properties.

Key Physical Properties	Value	Condition
Molecular Weight	108.14	-
Melting Point (Experimental)	-37.3 °C	-
Boiling Point (Experimental)	155.5 °C	Press: 760 Torr
Density (Experimental)	0.9956 g/cm ³	Temp: 18 °C

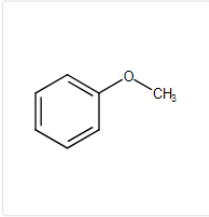
Commonly Used As: Odor and Odorous substances; Solvents; Dispersing agents; Flavor enhancers; Pharmaceutical carriers...

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

Buttons at the bottom: Formulations, Suppliers, Add to Designer.

c. 通过 Commonly Formulated with 可查看其在配方中的常见用途，点击右侧 View formulations 可查看相应配方。

CAS RN: [100-66-3](#)



C₇H₈O

Additional information available:
[View in CAS SciFinder[®]](#)

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

Anisole

Key Physical Properties	Value	Condition
Molecular Weight	108.14	-
Melting Point (Experimental)	-37.3 °C	-
Boiling Point (Experimental)	155.5 °C	Press: 760 Torr
Density (Experimental)	0.9956 g/cm ³	Temp: 18 °C

Commonly Used As: Odor and Odorous substances; Solvents; Dispersing agents; Flavor enhancers; Pharmaceutical carriers...

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

Commonly Used As

Function or Role	
Odor and Odorous substances	View Formulations
Solvents	View Formulations
Dispersing agents	View Formulations
Flavor enhancers	View Formulations
Pharmaceutical carriers	View Formulations
Polymerization inhibitors	View Formulations
Deodorants	View Formulations
Plasticizers	View Formulations
Polar solvents	View Formulations
Repellents	View Formulations

d. 获得苯甲醚用作驱虫剂的配方详情。

The screenshot shows the 'Formulations' search results page. On the left, there is a 'Filter by' sidebar with categories: Industry (Agrochemical), Purpose (Insect attractants, repellents, insecticides), Physical Form (Aerosols, Liquids), State of Matter, Information Included (Component Amount), and Document Type (Patent, Claim). The main content area displays the title 'Insect Attractant Composition: Insect Attractants' with its location in claims, purpose, and target. A table lists components and their functions: Anisole (apolar phase, repellent), alkanols, Sesquiterpenes, Alkenyl alcohols, and Rose oxide (insect attractants). A 'PATENT' section on the right provides details for a patent titled 'Method for attracting cambiohagous, xylophagous and/or mycetophagous insects' by Fluegel GmbH.

(2) 在反应中的应用。通过 CAS SciFinder[®]，可以便捷获取苯甲醚在反应中的应用。获取反应用途的具体操作如下：

a. 在 CAS SciFinder[®] 主页面，选择 Reactions，输入苯甲醚的 CAS 登记号，点击右侧放大镜，检索其参与的化学反应。在反应结果集页面，通过左侧 substance role: solvent，查看苯甲醚作为溶剂参与的反应。

The screenshot shows the 'Reactions' search results page. The search criteria are 'Reactions' and '100-66-3'. The left sidebar shows 'Filter Behavior' with 'Filter by' selected. Under 'Substance Role', 'Solvent (22K)' is checked. The main content area shows 'Filtering: Substance Role: Solvent' and '22,202 Results'. A reaction scheme is displayed for 'Scheme 1 (151 Reactions)' with 'Steps: 1' and 'Yield: 100%'. The reaction shows a benzene ring with a vinyl group. Below the reaction, there are 'Suppliers (87)' and 'Suppliers (112)' buttons. A 'Reaction Summary' section at the bottom provides details for a reaction involving Hexamethyltriethylenetetramine and 2-((1,1-Dimethylethoxy)carbonyl)aminoethyl 2-bromo-2-

b.选择 Substance role: reactant, 可获取苯甲醚作为反应物参与的反应。

The screenshot shows the CAS SciFinder interface. The search query is '100-66-3'. The results are filtered by 'Substance Role: Reactant', showing 11,747 results. A chemical reaction scheme is displayed, showing the Friedel-Crafts alkylation of anisole with benzyl bromide. The reaction is summarized as: Anisole + Benzyl bromide → Alkylated anisole. The reaction conditions are: Steps: 1, Yield: 100%. The catalyst used is MOF-5, as mentioned in the reference: 'MOF-5 as an efficient heterogeneous catalyst for Friedel-Crafts alkylation reactions' by Phan, Nam T. S., et al.

(3) 在 CAS 在 SciFinder[®] 中, 通过文献检索, 可获取全面的苯甲醚用途报道的文献。

a. 在检索主页面, 点击左侧 References, 然后通过页面中央选择高级检索字段, 点击 Substances: CAS Registry Number 输入苯甲醚的 CAS 登记号。点击右侧放大镜, 可检索获取苯甲醚相关的研究文献。

The screenshot shows the CAS SciFinder search interface. The search query is '100-66-3'. The search is performed using the 'CAS Registry Number' field. The search results are displayed under the 'References' section. The search criteria are: Search by Keyword, Substance Name, CAS RN, Patent ID, AN, CAN, and/or DOI. The search results are filtered by 'Substance Role: Uses', showing 11,747 results. The search results are displayed in a list format, showing the title, authors, and publication information for each reference. The search results are sorted by relevance. The search results are displayed in a list format, showing the title, authors, and publication information for each reference.

b.在文献检索结果集页面, 选择左侧 Substance Role: Uses, 筛选出苯甲醚用途研究的文献。

The screenshot shows the CAS SciFinder search results page. The search query is "100-66-3" CAS Registry Number. The results are filtered by "Substance Role: Uses", resulting in 4,239 results. The first result is titled "Facile approach to multifunctionalized 5-alkylidene-3-pyrrolin-2-ones via regioselective oxidative cyclization of 2,4-pentanediones with primary amines and sodium sulfonates". The second result is titled "High refractive index overcoat formulation and method of use with inkjet printing".

Filter Behavior

Filter by Exclude

Document Type

- Journal (1,444)
- Patent (2,746)
- Review (11)
- Conference (22)
- Dissertation (3)
- [View All](#)

Substance Role

- Reactant or Reagent (10K)
- Uses (4,239)
- Properties (3,306)
- Preparation (2,110)
- Process (1,728)
- [View All](#)

Language

Filtering: Substance Role: Uses X Clear All Filters

4,239 Results Sort: Relevance View: Partial Abstract

1

Facile approach to multifunctionalized 5-alkylidene-3-pyrrolin-2-ones via regioselective oxidative cyclization of 2,4-pentanediones with primary amines and sodium sulfonates
 By: Liu, Donghan; Lu, Xihang; Zhang, Qiaohu; Zhao, Yuxuan; Zhang, Biao; Sun, Yulin; Dai, Weifeng; Xu, Yu; Yu, Fuchao
 Organic Chemistry Frontiers | Language: English, Database: CAplus

A multi-component cascade cyclization reaction of readily available 2,4-alkanediones, primary amines and sodium sulfonates was reported. Highly functionalized 5-alkylidene-3-pyrrolin-2-ones were efficiently synthesized in moderate to excellent yields under mild conditions. This cascade cyclization was achieved by direct regioselective transformation of C(sp³)-H bonds at two weakly nucleophilic sites in the enaminone intermediate while two strongly nucleophilic sites of the structure were not involved.

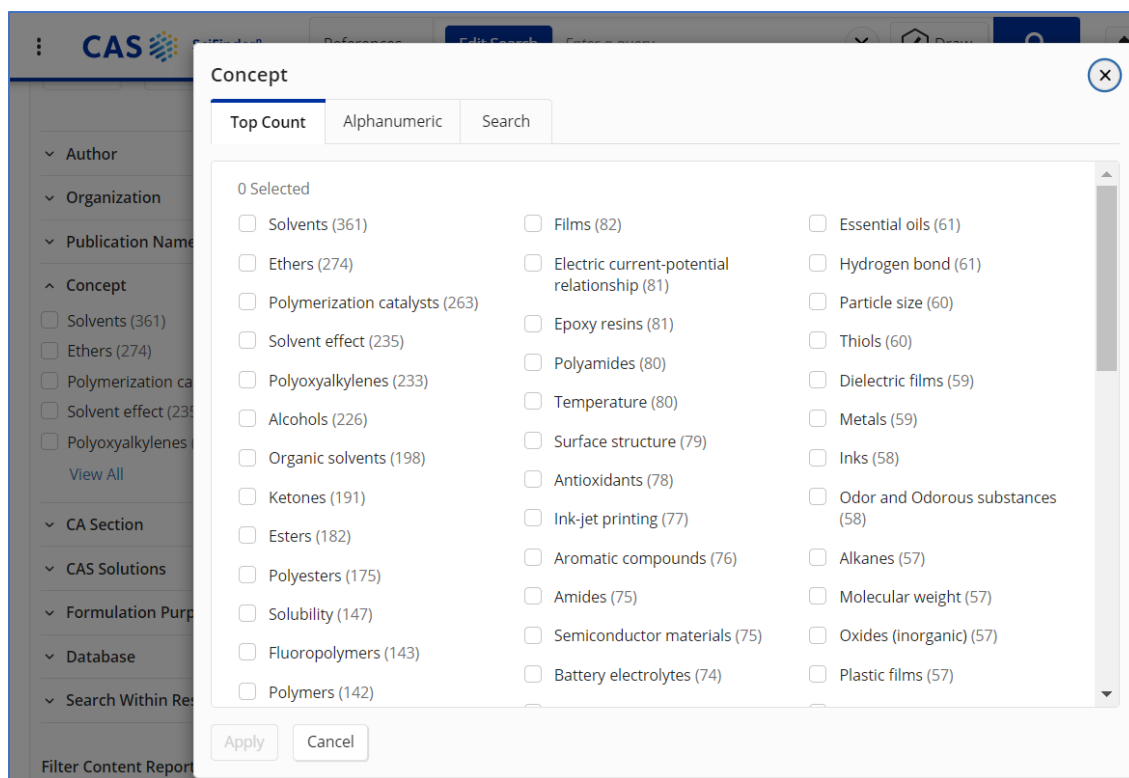
Full Text Substances (53) Reactions (0) Citing (0) Citation Map

2

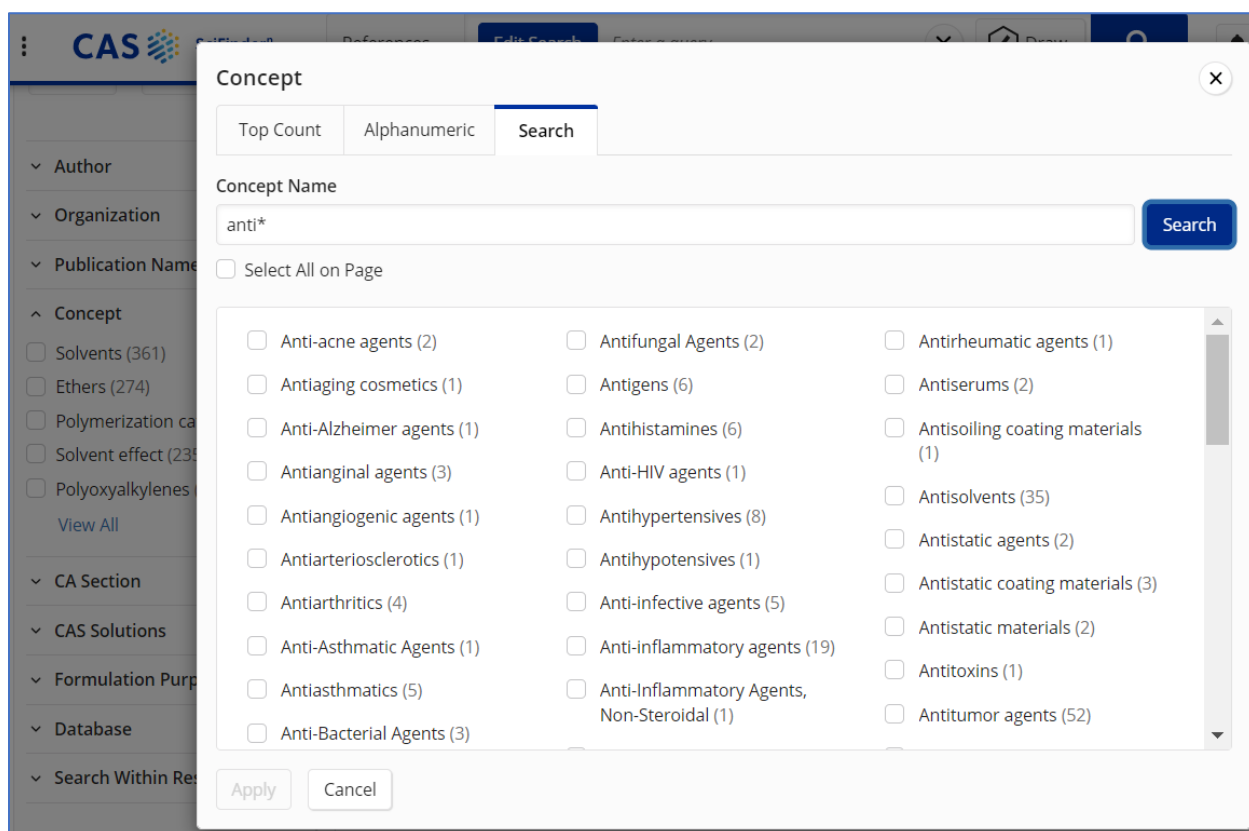
High refractive index overcoat formulation and method of use with inkjet printing
 By: Abramson, Igor; Vora, Ankit; Azari, Sara; Zhang, Keren
 World Intellectual Property Organization, WO2022147180 A1 2022-07-07 | Language: English, Database: CAplus

A formulation for inkjet printing includes one or more solvents and a plurality of nanoparticles mixed with the one or more solvents. The plurality of nanoparticles has a first refractive index greater than 1.9. A method includes depositing a layer of the formulation by

c.在筛选后的文献结果集中，通过 concept 查看与用途相关的词



d. 也可以选择 search 输入感兴趣的词，查看相关结果。星号 (*) 代表 0 或者多个字符。



Q29: 如何检索不含有噻唑的苯的并环结构?

A29: 检索思路如下:

- (1) 通过 Substance 进行物质结构检索, 检索苯;
- (2) 在物质检索结果页面中, 通过左侧 Filter Behavior: Exclude 排除苯的非并环结构 (使用锁定工具);
- (3) 在 (2) 的结果中, 继续使用 Exclude, 排除噻唑结构。

根据需要, 还可以根据结果左侧 Number of Components 精炼单组份物质, 根据 Substance class 精炼小分子物质等。

The screenshot displays the CAS SciFinder search results for a drawn structure of benzene. The interface includes a search bar at the top with the text "Substances" and "Enter a query...". Below the search bar, there are navigation options like "References", "Reactions", and "Suppliers". The main search results are displayed in a grid format, showing three results with their respective chemical structures and identifiers:

- Result 1: 1059174-58-1, C_6H_4 , Bicyclo[3.1.0]hexa-1,3,5-triene, radical ion(1+)
- Result 2: 139196-38-6, $(C_8H_6)_x$, Bicyclo[4.2.0]octa-1,3,5,7-tetraene, homopolymer
- Result 3: 72881-24-4, C_8H_6 , Bicyclo[4.2.0]octa-1,3,5,7-tetraene, radical ion(1+)

On the left side, there is a "Filter Behavior" section with two buttons: "Filter by" and "Exclude". The "Exclude" button is highlighted in blue. Above the results, there are filtering options: "Number of Components: 1" and "Substance Class: Organic/Inorganic Small M...".

在物质结果页面左侧, 点击 Filter Behavior 下面的 Filter by 则可对左侧列表中的聚类分析项进行精炼, 点击 Exclude 则可对聚类分析项进行排除。

例如, 点击 Exclude, 然后在结果页面使用左下角 Search Within results, 先后输入被锁定的苯和噻唑, 那么这两类结果即便排除。

The image shows a close-up of the "Filter Behavior" section. It contains two buttons: "Filter by" and "Exclude". The "Exclude" button is highlighted in blue, indicating it is the active filter.

点击 Filter by, 通过左侧 Number of Components 选择 1, 即可查看单组份的物质。

Q30: 如何检索 pKa 在 7-8 之间的化合物?

推荐如下检索步骤:

(1) 通过 Substances 的高级检索项, 选择 Chemical Properties 中的 pKa。

The screenshot shows the CAS SciFinder search interface. On the left, there is a 'Searching for...' sidebar with options: All, Substances (selected), Reactions, References, Suppliers, Biosequences, and Retrosynthesis. The main area is titled 'Substances' and includes a search bar with the text 'Enter a query...'. Below the search bar, a dropdown menu is open, showing 'Molecular Formula' selected. A secondary dropdown menu is open under 'Chemical Properties', with 'pKa' highlighted. To the right of the search bar, there are 'Draw' and 'Search' buttons. Below the search bar, there are examples: 'Examples: C6H6 | (C8H8)x | C22H26CuN2O5.C2H3N'. At the bottom right, there are 'Rerun Search' and 'Edit Search' buttons. On the left, there is a 'Recent Search History' section showing a search for 'activated carbon' on August 1, 2022.

(2) 根据输入框右下角提供的 examples 格式输入属性值或范围, 例如: 7 to 8 (从小到大输入范围值)。点击右侧放大镜, 进行物质检索。

The screenshot shows the CAS SciFinder search interface after the search. The search bar now contains 'pKa 7 to 8'. Below the search bar, there is a note: 'Predicted values only.' and examples: 'Examples: -1.77 | <9.25 | >2.4 | 5.25 to 8.25'. The 'Recent Search History' section is still visible on the left.

(3) 获得符合属性要求的物质结果。点击物质 CAS RN, 可查看物质详情。

CAS SciFinder® Substances Enter a query...

← Return to Home

Substances search for "7 to 8" pKa

References Reactions Suppliers Save and Alert

21,709,873 Results Sort: Relevance View: Partial

Filter Behavior

Filter by Exclude

Reaction Role

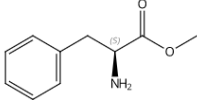
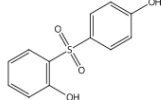
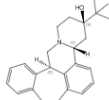
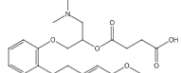
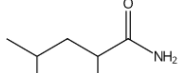
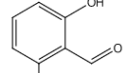
- Product (2.7M)
- Reactant (673K)
- Reagent (2,691)
- Catalyst (7,181)
- Solvent (202)

Reference Role

- Preparation (4M)
- Synthetic Preparation (3.8M)
- Biological Study (3.3M)
- Uses (3.2M)
- Prophetic Synthesis or Use (2.2M)

[View All](#)

Commercial Availability

<p><input type="checkbox"/> 1</p> <p>2577-90-4</p>  <p>Absolute stereochemistry shown, Rotation (+)</p> <p>$C_{10}H_{13}NO_2$ L-Phenylalanine, methyl ester</p> <p>3,573 References 4,024 Reactions 55 Suppliers</p>	<p><input type="checkbox"/> 2</p> <p>5397-34-2</p>  <p>$C_{12}H_{10}O_4S$ 2-[(4-Hydroxyphenyl)sulfonyl]phenol</p> <p>541 References 63 Reactions 54 Suppliers</p>	<p><input type="checkbox"/> 3</p> <p>51152-91-1</p>  <p>Absolute stereochemistry shown, Rotation (-)</p> <p>$C_{25}H_{31}NO$ (-)-Butaclamol</p> <p>353 References 0 Reactions 5 Suppliers</p>
<p><input type="checkbox"/> 4</p> <p>125926-17-2</p> 	<p><input type="checkbox"/> 5</p> <p>13079-20-4</p> 	<p><input type="checkbox"/> 6</p> <p>387-46-2</p> 

CAS SciFinder® Substances [Edit Search](#) Enter a query...

← Return to Results ← Prev (1 of 21,709,873) Next →

CAS Registry Number: 2577-90-4

References (3,573) Reactions (4,024) Suppliers (55) Download Email Save

Absolute stereochemistry shown, Rotation (+)

C₁₀H₁₃NO₂
L-Phenylalanine, methyl ester (9CI, AC1)

Key Physical Properties	Value	Condition
Molecular Weight	179.22	-
Melting Point (Experimental)	131-133 °C	-
Boiling Point (Experimental)	84 °C	Press: 0.25 Torr
Density (Predicted)	1.100±0.06 g/cm ³	Temp: 20 °C; Press: 760 Torr
pKa (Predicted)	7.13±0.33	Most Basic Temp: 25 °C

[Experimental Properties](#) | [Spectra](#)

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

- Other Names and Identifiers
- Experimental Properties
- Experimental Spectra
- ^ Predicted Properties

Biological	Chemical	Density	Lipinski	Structure Related	Thermal																																								
<table border="1"> <thead> <tr> <th>Property</th> <th>Value</th> <th>Condition</th> <th>Source</th> </tr> </thead> <tbody> <tr> <td>Koc</td> <td>1.0</td> <td>pH 1; Temp: 25 °C</td> <td>(1) ACD</td> </tr> <tr> <td>Koc</td> <td>1.0</td> <td>pH 2; Temp: 25 °C</td> <td>(1) ACD</td> </tr> <tr> <td>Koc</td> <td>1.0</td> <td>pH 3; Temp: 25 °C</td> <td>(1) ACD</td> </tr> <tr> <td>Koc</td> <td>1.0</td> <td>pH 4; Temp: 25 °C</td> <td>(1) ACD</td> </tr> <tr> <td>Koc</td> <td>1.0</td> <td>pH 5; Temp: 25 °C</td> <td>(1) ACD</td> </tr> <tr> <td>Koc</td> <td>7.73</td> <td>pH 6; Temp: 25 °C</td> <td>(1) ACD</td> </tr> <tr> <td>Koc</td> <td>47.2</td> <td>pH 7; Temp: 25 °C</td> <td>(1) ACD</td> </tr> <tr> <td>Koc</td> <td>97.6</td> <td>pH 8; Temp: 25 °C</td> <td>(1) ACD</td> </tr> <tr> <td>Koc</td> <td>109</td> <td>pH 9; Temp: 25 °C</td> <td>(1) ACD</td> </tr> </tbody> </table>						Property	Value	Condition	Source	Koc	1.0	pH 1; Temp: 25 °C	(1) ACD	Koc	1.0	pH 2; Temp: 25 °C	(1) ACD	Koc	1.0	pH 3; Temp: 25 °C	(1) ACD	Koc	1.0	pH 4; Temp: 25 °C	(1) ACD	Koc	1.0	pH 5; Temp: 25 °C	(1) ACD	Koc	7.73	pH 6; Temp: 25 °C	(1) ACD	Koc	47.2	pH 7; Temp: 25 °C	(1) ACD	Koc	97.6	pH 8; Temp: 25 °C	(1) ACD	Koc	109	pH 9; Temp: 25 °C	(1) ACD
Property	Value	Condition	Source																																										
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Koc	97.6	pH 8; Temp: 25 °C	(1) ACD																																										
Koc	109	pH 9; Temp: 25 °C	(1) ACD																																										

Molar Solubility	0.12 mol/L	pH 7; Temp: 25 °C	(1) ACD
Molar Solubility	0.057 mol/L	pH 8; Temp: 25 °C	(1) ACD
Molar Solubility	0.051 mol/L	pH 9; Temp: 25 °C	(1) ACD
Molar Solubility	0.050 mol/L	pH 10; Temp: 25 °C	(1) ACD
Molar Solubility	0.050 mol/L	Unbuffered Water pH 9.92; Temp: 25 °C	(1) ACD
Molecular Weight	179.22	-	
pKa	7.13±0.33	Most Basic Temp: 25 °C	(1) ACD
Vapor Pressure	9.86 x 10 ⁻³ Torr	Temp: 25 °C	(1) ACD

Sources

(1) Calculated using Advanced Chemistry Development (ACD/Labs) Software V11.02 (© 1994-2022 ACD/Labs)

▼ Predicted Spectra

▼ Regulatory Information

▼ Additional Details

反应检索

Q1: 如何获取无机盐的反应信息?

A1: 无机盐的反应信息获取策略如下:

- 1) 选择 substances, 是在检索框中输入无机盐的化学名、分子式或通过结构编辑器绘制无机盐的化学结构式 (然后上传结构式), 检索得到无机盐的物质结果集;
- 2) 在无机盐的物质结果集页面点击 Reactions, 即可得到无机盐的反应信息。可以利用反应结果集页面左侧的 Filter 对反应结果集进行筛选。

Q2: 如何获取含有羧基的离子型或配位型化合物的反应信息?

A2:

(1) 离子型化合物的反应信息获取策略: 先点击 Substances, 通过物质检索获得离子型化合物的物质信息 (可以在结构编辑器中绘制离子型化合物的结构式, 如羧基离子型化合物的结构式可绘制为 $O=C-O\cdots M$), 在获得物质信息后。通过物质结果集页面左侧的 Substance Class 筛选项将结果限定为 salt and compound with (注意区分是否需要带水合物的盐)。如果离子化合物的分子组成明确, 也可直接使用分子式检索, 比如 $CH_2O_2.H_2O.K$)。获得离子型化合物的物质信息后, 在物质结果集页面点击 Reactions, 即可获得其反应信息。

(2) 配位型化合物的反应信息获取策略: 可以直接将此配合物绘制在反应式中, 使用 \cdots (unspecified bond) 来绘制羧基配合物, 比如 $O=C-O\cdots Pd$ 。

Q3: 如何合并来自同一篇文献的反应?

A3: 通过反应结果集页面右侧 Group: by Document 合并来自同一篇文献的反应。如下图

Q4: 在反应结果集筛选项中的 Non-Participating Functional Groups 是什么意思?

A4: Non-Participating Functional Groups 表示该官能团不参与化学反应。

Q5: CAS 会收录权利要求书中用化学通式表示的化学反应吗?

A5: 如果专利中披露的反应其起始物和 (或) 产物的信息很明确, CAS 就会收录该反应。

另, 还可以直接通过 CAS PatentPak 下载专利全文, 直接在专利原文中获取相关反应。

Q6: 在 CAS SciFinder[®] 结果集页面点击物质结构时, 在弹出窗口会显示 Reactions, Synthesize 和 Start Retrosynthetic Analysis, 请问这三者的区别是什么?

A6: Reactions 表示该物质参与的所有反应; Synthesize 表示该物质作为产物的反应; Start Retrosynthetic Analysis 表示生成该物质作为终产物的逆合成路线。

Q7: 在一个硝基苯还原为苯胺的还原反应中, 如果原料和产物中都含有 Boc 取代基, 但在反应前后不发生变化。如何检索这样的反应?

A7: 这属于片段结构的化学选择性反应检索, 可分为分子间和分子内两种情况:

- (1) 如果 Boc 取代基和硝基苯/苯胺可以存在不同的结构中, 即分子间选择性反应, 那么可以绘制片段结构直接进行反应检索, 比如反应物绘制硝基苯和 Boc 两个片段, 产物也绘制为苯胺和 Boc 两个片段。
- (2) 如果 Boc 取代基和硝基苯在同一个原料中以及 BOC 和苯胺在同一个产物中 (Boc 与硝基苯及苯胺间有其他连接片段), 即分子内选择性反应, 那么可以通过如下三步实现精准检索:

第一步: 绘制硝基苯和 Boc 片段, 进行物质检索。查看 Substructure 结果集, 并在页面左侧 number of components 筛选项下选择 1, 这样即可将硝基苯和 Boc 限定在同一个结构中。

第二步: 在第一步物质结果集页面点击 Reactions, 得到第一步获得的物质结果集的反应信息, 并在页面左侧 Substance Role 筛选项下选择 Reactant。

第三步: 点击第二步获得的反应结果集页面左下角的 Search within Results, 在弹出的结构编辑器中绘制反应式, 原料为硝基苯和 Boc 片段, 产物为苯胺和 Boc 片段, 同时使用结构编辑器左下角原子标记工具来标注原料中与硝基相连的碳原子, 以及产物中与氨基相连的碳原子, 同时标记原料和产物中 Boc 的羰基碳原子, 从而限定原料和产物中对应的是同一个原子。选择 Substructure, 点击 Find 即可获得精准的反应结果。

Q8: 如何检索酶催化羰基还原反应? 比如苯乙酰还原为苯乙醇反应

A8: 有两种方法:

- 1) 直接进行反应检索。在 CAS SciFinder[®] 主页选择 Reactions, 打开结构编辑器, 绘制苯乙酰还原为苯乙醇的反应式, 进行反应检索。在得到的反应结果集页面左侧 Catalyst 筛选项中查看有哪些催化剂, 选择酶, 将反应结果集限定为酶作为催化剂的反应。
- 2) 采用文本与反应式联用进行文献检索。在 CAS SciFinder[®] 主页选择 References, 在输入框中输入主题词, 如, “carbonyl reductase” or SSCR。再打开结构编辑器, 绘制

苯乙酰还原为苯乙醇的反应式，上传反应式后，进行检索。在得到的文献结果集中，可选择左侧 As Drawn 查看锁环锁原子反应对应的文献结果集。

Q9: 已知起始物料和 API 的 CAS RN，怎么检索合成路线？

A9: 在 CAS SciFinder[®] 主页选择 Reactions，进行反应检索。打开结构编辑器，分别通过 CAS RN 将起始原料和 API 的结构导入到结构编辑器后，再添加反应箭头，进行反应检索即可获得对应的合成路线。

Q10: 如何全面准确检索合成丙烯酸的反应，同时排除由丙烯酸衍生物制备丙烯酸的合成方法？

A10: 按下述步骤进行：

- 1) 在 CAS SciFinder[®] 主页面选择 Reactions，在输入框中输入丙烯酸的 CAS 登记号 79-10-7，检索后得到丙烯酸参与的化学反应
- 2) 在反应结果集页面左侧 Filter By 筛选项 Substance Role 下勾选 Product，将结果限定为丙烯酸为产物的反应
- 3) 点击反应结果集页面左侧的 Exclude，点击 Search Within Results 下的结构编辑器，绘制丙烯酸的结构并将其限定为 Reactant，上传结构后，选择 Substructure 进行检索，即可排除丙烯酸衍生物作为底物参与的反应。

Q11: CAS SciFinder[®] 中，对于反应结果集而言，默认的排序规则是什么？

A11: 通过反应式检索得到的反应结果集，其默认的排序规则是综合考量相似分 (Tanimoto Score)、反应步数、产物结构、产率等多个参数。在 Scheme 下的 Reaction Summary 中，反应按照步数、产率、公开日期和文献标题来排序。

Q12: 如何检索某一类催化剂涉及的某类型反应的机理？

A12: 用以下两种方法来进行检索：

- (1) 如果没有具体的反应式，仅知道反应类型或催化剂的类型，则建议选择 References，输入主题词进行检索。可根据需要灵活构建检索式，如：reaction mechanism and "carbon-carbon" coupling and (trivalent manganese or manganese catalyst)。在得到的

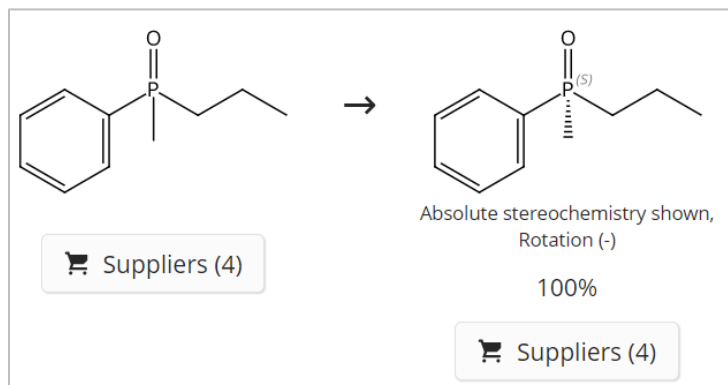
文献结果集页面，点击左侧 Filter by Concept，选择 Reaction mechanism，获取锰催化剂或三价锰催化的 C-C 偶联反应的机理研究文献。

The screenshot displays the CAS SciFinder® interface. At the top, the search bar contains the query "reaction mechanism and 'carbon-carbon' coupling and". The left sidebar shows the "Filter Behavior" section with "Filter by" selected, and the "Concept" filter is set to "Reaction mechanism (328)". The main content area shows a list of references. The first reference is "Mechanism and Selectivity in Nickel-Catalyzed Cross-Electrophile Coupling of Aryl Halides with Alkyl Halides" by Biswas, Soumik; Weix, Daniel J. The abstract discusses the direct cross-coupling of two different electrophiles, such as an aryl halide with an alkyl halide, and its advantages over conventional cross-coupling methods. A chemical reaction scheme is shown, illustrating the mechanism involving a nickel catalyst, a polar step, and a radical chain. The second reference is "Electrochemical, Manganese-Assisted Carbon-Carbon Bond Formation between β -Keto Esters and Silyl Enol Ethers" by Strehl, Julia; Hilt, Gerhard. The abstract mentions the formation of C-C bonds between β -keto esters and silyl enol ethers.

(2) 如果有具体的反应式，则推荐选择主题词和结构式/反应式联用的方法进行检索。如下图所示：

Q13: 含有手性结构的化合物拆分的反应怎么检索?

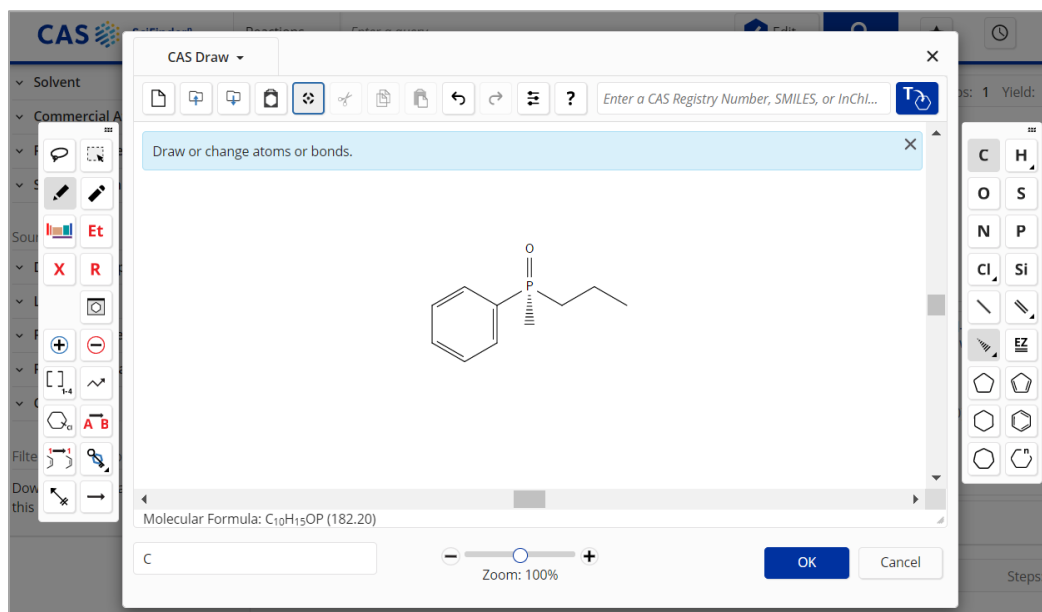
A13: 手性化合物的拆分反应可以直接绘制反应式进行快速检索，也可以从物质检索出发，在获取到手性结构后，再获取其反应信息。以下面的反应为例：



(a) 直接绘制上述反应式进行检索，可以快速获取各类手性拆分反应。

(b) 如果希望获取拆分后的产物为特定手性的反应，可先检索精准手性的物质，然后再获取反应。

例如，先使用结构编辑器下方的手性键，绘制 S 构型的拆分产物，并进行物质检索；通过物质结果左侧 Stereochemistry 获取 absolute stereo match 立体构型完全匹配的物质。



CAS RN 1515-99-7 为立体构型完全匹配的物质，点击其下方的 Reactions，获取其参与的反应。在反应结果集页面左侧 Filter by 限定 Reaction Role 为 Product, 并在 Search Within Results 中输入原料的结构，且使用反应角色标记工具标注其角色为 reactant, 进行二次反应结构检索。即可获得手性精准的拆分反应。

Q14: 如何获取金属络合物的制备方法?

A14: 通过以下两种方式可获取金属络合物的制备方法:

1) 直接绘制反应式, 进行反应检索。如下图:

2) 也可以通过绘制结构进行物质检索，再从物质获取其反应信息。金属络合物的绘制，可通过配体、中心原子及连接键（虚线键）来绘制即可。结构检索结果有 3 个选项 (As Drawn, Substructure, Similarity) , 可根据需要查看感兴趣的物质，并根据物质获取其反应信息。如下所示：

Q15: 如何查找 MOFs 催化的二氧化碳加氢反应?

A15: 点击 References, 输入关键词

在文献结果集页面点击 Substances

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](#)

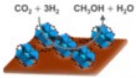
Return to Home

References (6,649) Sort: Relevance View: Full Abstract

Substances Reactions Citing

1

Copper Nanocrystals Encapsulated in Zr-based Metal-Organic Frameworks for Highly Selective CO₂ Hydrogenation to Methanol
By: Rungtaweeworant, Bunyarat; Baek, Jayeon; Araujo, Joyce R.; Archanjo, Braulio S.; Chol, Kyung Min; Yaghi, Omar M.; Somorjai, Gabor A.
Nano Letters (2016), 16(12), 7645-7649 | Language: English, Database: CAplus and MEDLINE

 The activity and selectivity of Cu catalyst can be promoted by a Zr-based metal-organic framework (MOF), Zr₆O₄(OH)₄(BDC)₃ (BDC = 1,4-benzenedicarboxylate), UiO-66, to have a strong interaction with Zr oxide [Zr₆O₄(OH)₄(-CO₂)₁₂] secondary building units (SBUs) of the MOF for CO₂ hydrogenation to methanol. These interesting features are achieved by a catalyst composed of 18 nm single Cu nanocrystal (NC) encapsulated within single crystal UiO-66 (Cu@UiO-66). The performance of this catalyst construct exceeds the benchmark Cu/ZnO/Al₂O₃ catalyst and gives a steady 8-fold enhanced yield and 100% selectivity for methanol. The XPS data obtained on the surface of the catalyst show that Zr 3d binding energy is shifted toward lower oxidation state in the presence of Cu NC, suggesting that there is a strong interaction between Cu NC and Zr oxide SBUs of the MOF to make a highly active Cu catalyst.

Full Text Substances (25) Reactions (4) Citing (211) Citation Map

2

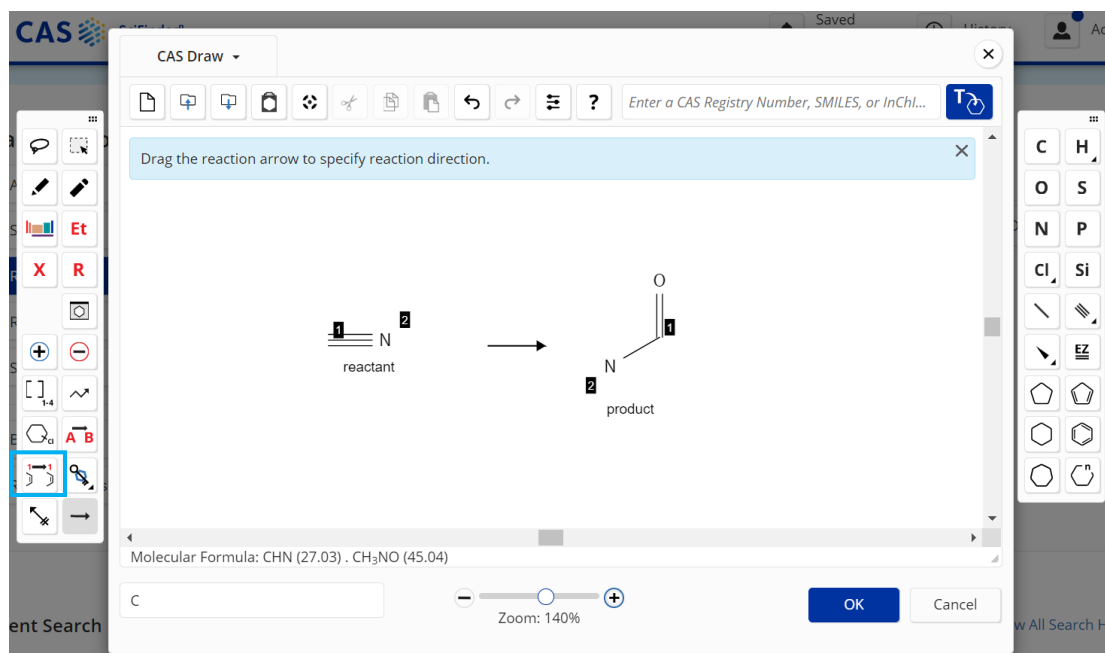
Ultrasmall Ni nanoparticles embedded in Zr-based MOFs provide high selectivity for CO₂ hydrogenation to methane at low temperatures
By: Zhao, Zhi-Wei; Zhou, Xiao; Liu, Ya-Nan; Shen, Cong-Cong; Yuan, Cheng-Zong; Jiang, Yi-Fan; Zhao, Sheng-Jie; Ma, Liu-Bo; Cheang, Tuck-Yun; Xu, An-Wu
Catalysis Science & Technology (2018), 8(12), 3160-3165 | Language: English, Database: CAplus

Of great significance from an energy-saving viewpoint is the direct use of CO₂ as a C1 source to mitigate the anthropogenic CO₂ emission into the earth's atm. and to produce methane that can be turned into chems. and fuels. Herein, we report the use of UiO-66 metal-organic frameworks to anchor ultrasmall Ni nanoparticles (NPs), thus avoiding the sintering of Ni NPs protected by the frameworks. Transmission electron microscope images and EDX mappings show that Ni NPs with an average size of 2 nm are highly

Q16: 如何获取报道羧基还原为酰胺的文献?

A16: 获取报道相关反应的文献, 推荐以下两种方式:

(1) 直接检索反应: 绘制反应式。在绘制反应式时, 可以使用原子标记工具, 标记反应前后未发生变化的同一原子。例如:



CAS SciFinder®

Reactions Enter a query...

Return to Home

Structure Match

- As Drawn (2)
- Substructure (156K)
- Similarity (23K)

Filter Behavior

Filter by Exclude

Yield

- 90-100% (14K)
- 80-89% (17K)
- 70-79% (15K)
- 50-69% (22K)
- 30-49% (13K)

View All

Number of Steps

Non-Participating Functional Groups

- Halide (40K)
- Alkene (30K)
- Ether (30K)
- Phenyl halide (24K)
- Cyclic alkene (23K)

View All

Reactions (156,010)

References

1

Formamide

By: Magill, P. L.
Industrial and Engineering Chemistry (1934), 26, 611-14 | Language: Undetermined, Database: CAPLUS

Full Text

Suppliers (4)

Suppliers (113)

Reaction Summary

Steps: 1

1.1 Reagents: [Sulfuric acid](#)

View Reaction Detail

2

Tandem Acceptorless Dehydrogenative Coupling-Decyanation under Nickel Catalysis

(2) References 检索：构建文献检索关键词，例如：reduction and (nitrile or cyano)。然后在文献结果集页面左侧 Filter by: Substance Role 精炼主题词中的 nitrile 和 cyano 在文献中的研究角色；或通过 Concept 精炼文献研究核心点。

The screenshot shows the CAS SciFinder interface. At the top, the search query is "cyano or nitrile and reduction". The left sidebar contains filter options under "Filter Behavior" (Filter by, Exclude) and "Document Type". The "Substance Role" filter is expanded, showing options like Properties (78), Occurrence (67), Process (62), Formation, Non-preparative (27), and Uses (27). The "Concept" filter is also expanded, showing options like Nitriles (5,168), Melting point (2,650), Reduction (2,068), Esters (1,866), and Humans (1,834). The main results area shows four search results, each with a title, authors, journal information, and options for full text, substances, reactions, and citations.

References (18,880) Sort: Relevance View: No Abstract

Substances Reactions Citing Save And Alerts

CAS Formulus®, the comprehensive formulations database and workflow solution, is now available for all SciFinder® users. Use the CAS Solutions: Formulus filter to view available content. Learn more about Formulus.

1
Reaction of InCl_3 with Various Reducing Agents: InCl_3 - NaBH_4 -Mediated Reduction of Aromatic and Aliphatic Nitriles to Primary Amines
By: Saavedra, Jaime Z.; Resendez, Angel; Rovira, Alexander; Eagon, Scott; Haddenham, Dustin; Singaram, Bakthan
Journal of Organic Chemistry (2012), 77(1), 221-228 | Language: English, Database: CPlus and MEDLINE
View Abstract
Full Text Substances (38) Reactions (19) Citing (51) Citation Map

2
Ultrathin graphitic carbon nitride nanosheets: a low-cost, green, and highly efficient electrocatalyst toward the reduction of hydrogen peroxide and its glucose biosensing application
By: Tian, Jingqi; Liu, Qian; Ge, Chenjiao; Xing, Zhicai; Asiri, Abdullah M.; Al-Youbi, Abdulrahman O.; Sun, Xuping
Nanoscale (2013), 5(19), 8921-8924 | Language: English, Database: CPlus and MEDLINE
View Abstract
Full Text Substances (5) Reactions (0) Citing (254) Citation Map

3
Folarographische and electrolytic reduction of the cyano group in substituted benzo nitriles
By: Manoek, O.; Zuman, P.
Chemisches Zentralblatt (1967), 138(1), 90-90 | Language: German, Database: CHEMZENT
View Abstract
ChemZent Full Text Substances (4) Reactions (0) Citing (0) Citation Map

4
Structural Basis of Biological Nitrile Reduction
By: Chikwana, Vimbai M.; Stec, Boguslaw; Lee, Bobby W. K.; de Crecy-Lagard, Valerie; Iwata-Reuyl, Dirk; Swairjo, Manal A.
Journal of Biological Chemistry (2012), 287(36), 30560-30570 | Language: English, Database: CPlus and MEDLINE
View Abstract
Full Text Substances (3) Reactions (0) Citing (24) Citation Map

Q17: Retrosynthesis tool 在满足什么条件时即终止运算？

A17: 在使用逆合成反应路线工具 Retrosynthesis 时，首先输入一个单一的，具体的结构；然后需要预设参数；最后获得结果。在自动运算结果时，系统会根据预设参数选项

(Retrosynthesis Plan Options) 中的 Synthetic Depth, Rules 和 Starting Materials Cost Limit 来决定何时停止运算, 最后的结果中包括最优路线和所有的替代路线 (Alternative Steps)。

Retrosynthesis Plan Options Powered by ChemPlanner[®]

Select Synthetic Depth [Learn more.](#)

1 2 3 4

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

Common
 Uncommon (includes Common Rules)
 Rare (includes Common and Uncommon Rules)

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

10 USD/mol
 Email me when my plan is complete USD/mol
 USD/g

[Create Retrosynthesis Plan](#)

Break and Protect Bonds [Learn more.](#)

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

Retrosynthesis Powered by ChemPlanner[®]

Overview **Steps** Predicted Results

View step specific evidence and alternate steps below or select the node between steps on the plan.

A ⇒ B + C
 Average Yield: 74%
 Evidence (6,831)
 Alternative Steps (13)

B ⇒ D
 Maximum Yield: 100%
 Evidence (1)
 Alternative Steps (4)

C ⇒ E + F
 Maximum Yield: 99%
 Evidence (35)
 Alternative Steps (23)

D ⇒ G Stereoselective
 Maximum Yield: 49%
 Evidence (120,797)
 Alternative Steps (9)

Retrosynthesis Step Key
 Hover on the options below to highlight experimental and predicted steps within this plan. View Steps Menu.

Experimental Steps
 Predicted Steps

Reset

Q18: 在获取到多步反应后，如何查看其实验详情？

A18: 通过反应结果集页面左侧 Filter by 对反应步数和实验详情等进行筛选。

(1) 通过 Filter by: Number of steps 选中反应步数，例如 3；

(2) 通过 Filter by: Experimental Protocols 可获取具有反应详情的反应：选择 Synthetic Methods，可在反应结果中查看 CAS 科学家标引的实验详情；选择 Experimental Procedures 可查看来自原文的实验详情。

然后根据感兴趣的反应，点击 Reaction Summary 下面的 Experimental protocols, 即可查看多步反应的详情，包括多步反应路线、反应中的物质信息、反应步骤、产物表征数据和物质物理形态等信息。

The screenshot displays the CAS SciFinder web interface. On the left, the 'Filtering' section is active, with 'Number of Steps: 3' selected. Below this, the 'Number of Steps' filter is expanded, showing a list of options: 1 (542), 2 (424), 3 (260) (which is checked), 4 (182), 5 (108), and 6-10 (170). The 'Experimental Protocols' section is also visible, with 'Synthetic Methods (169)' and 'Experimental Procedure (131)' selected. The main content area shows a search result for 'A Doxorubicin Prodrug Activated by the Staudinger Reaction'. The reaction scheme shows the conversion of a complex starting material to a prodrug. Below the reaction, the 'Reaction Summary' section lists the reagents and solvents for three steps: 1.1 (Oxygen, Benzenesulfonic acid, 3,3',3"-phosphinidynetris-, sodium salt (1:3) in Water, 20 h, 37 °C), 2.1 (Sodium nitrite, Hydrochloric acid, Sodium azide in Water, rt to 4 °C, 30 min, 4 °C; 30 min, < 5 °C; 1.5 h, 4 °C), and 2.2 (Water, cooled).

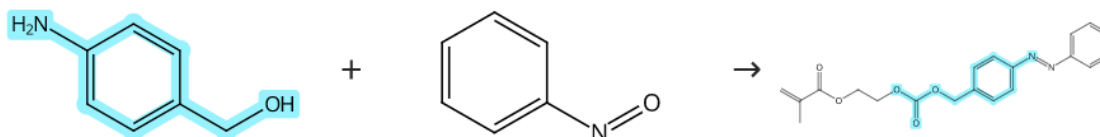
Enzyme-Triggered Cascade Reactions and Assembly of Abiotic Block Copolymers into Micellar Nanostructures

By: Rao, Jingyi; Hottinger, Christine; Khan, Anzar

Journal of the American Chemical Society (2014), 136(16), 5872-5875 | Language: English, Database: CAplus and MEDLINE

Full Text ▾

[View 2 Related Reactions](#)



[Suppliers \(101\)](#)

[Suppliers \(57\)](#)

Reaction Summary

Steps: 3

1.1 Solvents: [Acetic acid](#); 15 min, rt; 3 h, rt; 30 min, cooled

2.1 Reagents: [Triethylamine](#)
Solvents: [Tetrahydrofuran](#); 2 h, rt

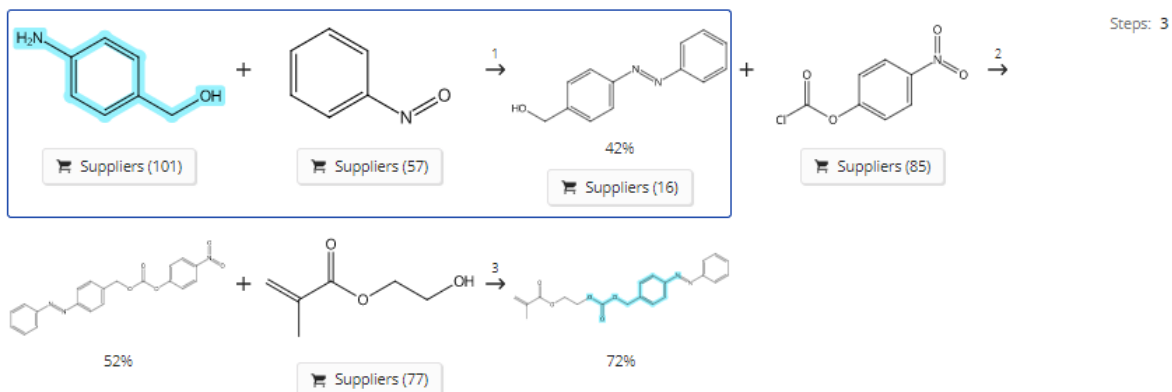
3.1 Reagents: [4-\(Dimethylamino\)pyridine](#)
Solvents: [Dichloromethane](#); 16 h, rt

[View Reaction Detail](#)

[Experimental Protocols](#)

Reaction Detail

[Download](#) [Email](#) [Save](#)



Step 1
Step 2
Step 3

[Alternative Steps \(4\)](#)

Stage	Reagents	Catalysts	Solvents	Conditions
1	-	-	Acetic acid	15 min, rt; 3 h, rt; 30 min, cooled

CAS Reaction Number: [31-191-CAS-1436663](#)

Experimental Protocols

Synthetic Methods

Experimental Procedure

Products	4-(2-Phenyldiazenyl)benzenemethanol, Yield: 42%
Reactants	Nitrosobenzene 4-Aminobenzyl alcohol
Solvents	Acetic acid
Procedure	<ol style="list-style-type: none"> 1. Add a solution of 4-aminobenzyl alcohol (2.0 g) in acetic acid (10 mL) to a solution of nitrosobenzene (1.91 g) in acetic acid (10 mL) via a dropping funnel over a period of 15 minutes at ambient temperature. 2. After 3 hours, cool the reaction mixture by placing it in a fridge for a period of 30 minutes. 3. Filter the orange precipitate. 4. Wash the filtrate with water. 5. Repeat the cooling and filtering process once more. 6. Purify the resulting solid by silica gel column chromatography (EtOAc/hexane, 30:70).
Transformation	Conversion of Aromatic Amines to Azo Compounds/ Mills Reaction
Scale	gram

Characterization Data

^ 4-(2-Phenyldiazenyl)benzenemethanol

Proton NMR Spectrum	δ, ppm, 300 MHz, CDCl ₃ : 7.91 (m, 4H), 7.50 (m, 5H), 4.78 (d, <i>J</i> = 5.93 Hz, 2H), 1.81 (t, <i>J</i> = 5.93 Hz, 1H).
Carbon-13 NMR	δ, ppm, 75 MHz, CDCl ₃ : 152.83, 152.32, 143.97, 131.15, 129.24, 127.57, 123.23, 122.99, 65.05.
Mass Spectrum	ESI (observed: 213.10 M+H, calc. 213.10 for C ₁₃ H ₁₃ N ₂ O).
State	orange solid.

JOURNAL

Enzyme-Triggered Cascade Reactions and Assembly of Abiotic Block Copolymers into Micellar Nanostructures

By: Rao, Jingyi; et al
[View All](#) ▾

Journal of the American Chemical Society (2014), 136(16), 5872-5875

[View PDF](#) [Full Text](#) ▾

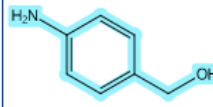
Company/Organization

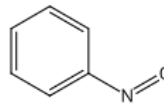
ETH-Zurich
 Department of Materials
 Zurich CH-8093
 Switzerland

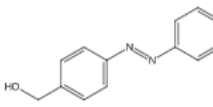
Reaction Detail

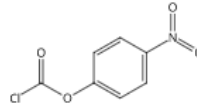
[Download](#) [Email](#) [Save](#)

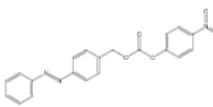
Steps: 3

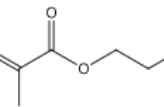

 Suppliers (101)

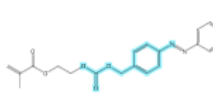

 Suppliers (57)


 Suppliers (16)


 Suppliers (85)


 52%


 Suppliers (77)


 72%

Step 1
Step 2
Step 3

[Alternative Steps \(4\)](#)


Stage	Reagents	Catalysts	Solvents	Conditions
1	-	-	Acetic acid	15 min, rt; 3 h, rt; 30 min, cooled

CAS Reaction Number: 31-191-CAS-1436663

Experimental Protocols

Synthetic Methods

Experimental Procedure



Hydroxy-azobenzene: To a solution of nitrosobenzene (1.91 g, 17.86 mmol) in acetic acid (10 mL) was added a solution of 4-aminobenzyl alcohol (2.0 g, 16.24 mmol) in acetic acid (10 mL) via a dropping funnel over a period of 15 minutes at ambient temperature. After 3 hours, the reaction mixture was cooled by placing it in a fridge for a period of 30 minutes. This treatment resulted in formation of an orange precipitate that was filtered and washed with water. The cooling and filtering process was repeated once more and the resulting solid was purified by silica gel column chromatography (EtOAc/Hexane, 30:70) to give 1.472 g of product. Yield = 42 %, orange solid. ¹H-NMR (δ, ppm, 300 MHz, CDCl₃): 7.91 (m, 4H), 7.50 (m, 5H), 4.78 (d, J = 5.93 Hz, 2H), 1.81 (t, J = 5.93 Hz, 1H); ¹³CNMR (δ, ppm, 75 MHz, CDCl₃): 152.83, 152.32, 143.97, 131.15, 129.24, 127.57, 123.23, 122.99, 65.05; ESI (observed: 213.10 M+H, calc. 213.10 for C₁₃H₁₃N₂O).

JOURNAL

Enzyme-Triggered Cascade Reactions and Assembly of Abiotic Block Copolymers into Micellar Nanostructures

By: Rao, Jingyi; et al
[View All](#)

Journal of the American Chemical Society (2014), 136(16), 5872-5875

[View PDF](#)
[Full Text](#)

Company/Organization

ETH-Zurich
 Department of Materials
 Zurich CH-8093
 Switzerland

序列检索

Q1: Biosequences 检索时，如何获取来自 CAS SciFinder[®] 的相关文献？

A1: 点击序列展示页面右边的 References，即可获得来自 SciFinder[®] 的相关文献，如下图所示。

1 Alignment Identity: 100%

Query 1 7

Subject 1 111

Matches: 7
Mismatches: 0

View Less ▾

Alignment Subject References

Alignment Data
BLAST Score: 47
E-Value: 98.5942

Q	1	AASNLES	7
S	54	AASNLES	60

Q2: CAS SciFinder[®] 中 Biosequences Search 数据的来源？

A2: CAS SciFinder[®] 中 Biosequences Search 数据来自专利、期刊、NCBI 等。

Q3: 如何优先展示生物序列检索结果中 Subject Coverage%高的结果？

A3: 点击 Biosequences 结果集页面右上侧 Sort 下拉菜单，选择 Subject Coverage，序列结果将按照 Subject Coverage%从高到低排列。如下图：

Sequence Type: Nucleotide
NCBI Included: No
Query Coverage: 90%
E-Value: 10^6

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

Filter by
E-Value
0 to 10^6
Query Coverage %
0 to 100
Subject Coverage %
0 to 100

Biosequences (18,208)
Sort: Alignment Identity View: Expanded

Query Details > Seq 1: 1 UAUUGUGAGGAAUUUUUGUCAA 21 View More

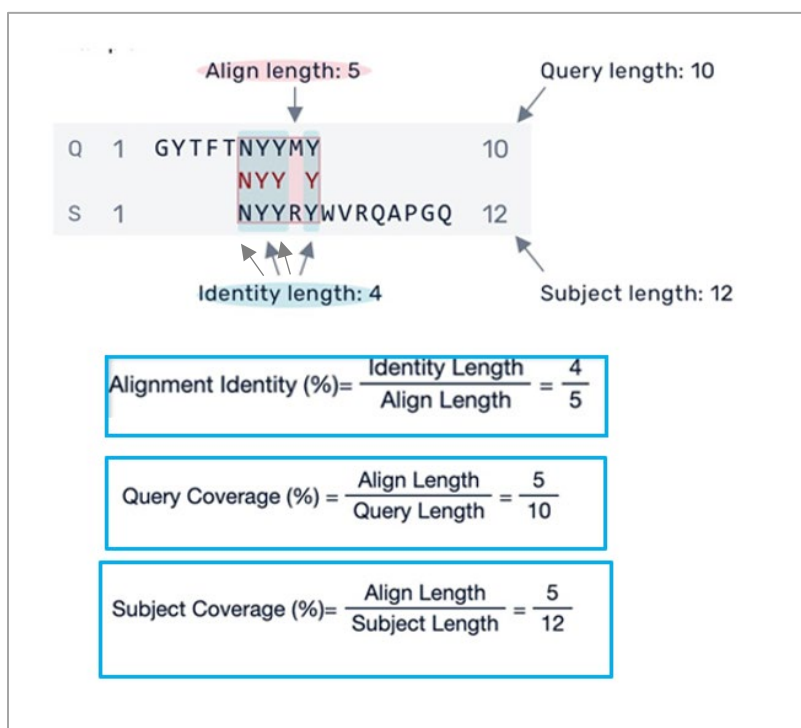
Alignment Identity: 100%
Matches: 21
Mismatches: 0

Alignment Data
BLAST Score: 21
E-Value: 0.00319188

```
Q 1 TATTGTGAGG ATTTTGTCA A 21
      |||
S 1 TATTGTGAGG ATTTTGTCA A 21
```

Q4: Biosequences Search 中 Query Coverage%, Subject Coverage%和 Alignment identity%是如何计算的?

A4: 请参见如下示意图



Q5: 如何输入序列获取其相关信息?

A5: 点击 Biosequences, 根据检索需要, 可选择 BLAST、CDR、Motif 输入序列, 然后进行检索。

Help shape the future of scientific discovery. [Sign up to share your insights](#) on upcoming CAS SciFinder[®] enhancements.

Searching for...

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

Biosequences

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

BLAST CDR Motif Clear Search

UAAUUGUGAGGAAUUUUUGUCA

Sequence Type:
 Nucleotide Protein

Include NCBI Sequences

Limit Total Sequence Results to:
20000

Advanced Biosequence Search Reset All

Query Coverage % E-Value

如果需要检索的序列长度和输入的序列一致, 可在结果左侧将 Subject Coverage 设置为 100%, 或者通过右上角 Sort: Subject Coverage 按照 Subject Coverage% 从高至低重新排序。点击结果中的 Subject 查看目标序列 (包括修饰和非修饰序列) 及对应的 CAS RN。

The screenshot shows the CAS SciFinder interface. On the left, there are filter options for E-Value (0 to 10⁶), Query Coverage % (100 to 100), Subject Coverage % (100 to 100), and Alignment Identity % (0 to 100). The main area displays 'Biosequences (31)' with a 'Sort: Subject Coverage' dropdown menu. The results show a sequence alignment with 100% identity and 21 matches. The alignment data is as follows:

```

Alignment Data
BLAST Score: 21
E-Value: 0.00319188
Q   1  TATTGTGAGG  ATTTTGTCA  A  21
      |||
S   21 TATTGTGAGG  ATTTTGTCA  A  41
  
```

将下面的 CAS RN 拷贝至 Substances 检索输入框，进行物质检索，可获得修饰序列的物质结果。

The screenshot shows the CAS SciFinder interface with a search for 'CAS Registry Numbers'. The results show a sequence alignment with 100% identity and 21 matches. The alignment data is as follows:

```

CAS Registry Numbers: 1929626-77-6, 1931967-48-4, 1931160-43-8, 1932562-64-5, 1931155-94-0, 2248790-61-4, 2249775-78-6
Length: 21 nt
Sequence
1  UUGACAAAAA  UCCUCACAAU  A
  
```

CAS SciFinder® Substances 1929626-77-6, 1931967-48-4, 1931160-43-8, 1932562-6-6 Draw Search

Return to Home

Substances (7) Sort: Relevance View: Partial

Filter Behavior: Filter by Exclude

- Commercial Availability
 - Not Available (7)
- Reference Role
 - Biological Study (7)
 - Properties (7)
 - Biological Study, Unclassified (5)
 - Therapeutic Use (5)
 - Uses (5)
 - Pharmacological Activity (2)
- Substance Class
- Isotopes
- Metals
- Bioactivity Indicator
- Target Indicator
- Search Within Results

Filter Content Report

1	2	3
<p>2249775-78-6</p> <p>Image Not Available</p> <p>Unspecified</p> <p>Nucleic Acid Sequence</p> <p>Sequence Length: 21</p> <p>1 Reference 0 Reactions 0 Suppliers</p>	<p>2248790-61-4</p> <p>Image Not Available</p> <p>Unspecified</p> <p>RNA, (U-U-G-A-C-A-A-A-A-U-C-C-U-C-A-C-A-U-A)</p> <p>Nucleic Acid Sequence</p> <p>Sequence Length: 21</p> <p>1 Reference 0 Reactions 0 Suppliers</p>	<p>1932562-64-5</p> <p>Image Not Available</p> <p>Unspecified</p> <p>RNA, ((2'-deoxy-2'-fluoro)U-sP-Um-sP-(2'-deoxy-2'-fluoro)G-Am-(2'-deoxy-2'-fluor...</p> <p>Nucleic Acid Sequence</p> <p>Sequence Length: 21</p> <p>1 Reference 0 Reactions 0 Suppliers</p>
4	5	6
<p>1931967-48-4</p> <p>Image Not Available</p> <p>Unspecified</p> <p>RNA, ((2'-deoxy-2'-fluoro)U-sP-Um-sP-(2'-deoxy-2'-fluoro)G-Am-(2'-deoxy-2'-fluor...</p> <p>Nucleic Acid Sequence</p> <p>Sequence Length: 21</p> <p>1 Reference 0 Reactions 0 Suppliers</p>	<p>1931160-43-8</p> <p>Image Not Available</p> <p>Unspecified</p> <p>RNA, (U-U-G-A-C-A-A-A-A-U-C-C-U-C-A-C-A-U-A)</p> <p>Nucleic Acid Sequence</p> <p>Sequence Length: 21</p> <p>1 Reference 0 Reactions 0 Suppliers</p>	<p>1931155-94-0</p> <p>Image Not Available</p> <p>Unspecified</p> <p>RNA, ((2'-deoxy-2'-fluoro)U-sP-Um-sP-(2'-deoxy-2'-fluoro)G-Am-(2'-deoxy-2'-fluor...</p> <p>Nucleic Acid Sequence</p> <p>Sequence Length: 21</p> <p>1 Reference 0 Reactions 0 Suppliers</p>

点击 CAS RN 查看序列详情。

Substance Detail (1 of 13) Prev Next

References (93) Reactions (0) Suppliers (0) Save

CAS Registry Number
1420706-45-1

Image Not Available

Unspecified

RNA, (A-U-G-G-A-A-Um-A-C-U-C-U-U-G-G-U-Um-A-C-dT-dT), complex with RNA (G-Um-A-A-Cm-Cm-A-A-G-A-G-Um-A-Um-Um-Cm-Cm-A-Um-dT-dT) (1:1) (ACI)

Nucleic Acid Sequence
Sequence Length: 42 (21, 21)
12 a, 7 c, 7 g, 4 t, 12 u
multistranded (2); modified

Related Sequences (5)

Expand All | Collapse All

Other Names and Identifiers

^ Sequence Details

Sequence 1: Length 21; RNA; linear

1 auggaaucu cuugguuact t - -

Sequence 2: Length 21; RNA; linear

1 guaccaaga guauccaut t - -

Sequence Modifications

Type	Location	Description
modified base	strand 1 uridine-7	um
modified base	strand 1 uridine-17	um
modified base	strand 2 uridine-2	um
modified base	strand 2 cytidine-5	cm
modified base	strand 2 cytidine-6	cm
modified base	strand 2 uridine-12	um
modified base	strand 2 uridine-14	um
modified base	strand 2 uridine-15	um
modified base	strand 2 cytidine-16	cm
modified base	strand 2 cytidine-17	cm
modified base	strand 2 uridine-19	um

v Target Indicators

v Regulatory Information

v Additional Details

Q6: 如何将.txt 文件中的多条序列导入 Biosequences 进行序列检索?

A6: 利用 CAS SciFinder[®] 中的 Biosequences 检索序列时, 可直接输入待检索序列或以.txt/.fasta 文件上传待检索序列(注: 通过.txt 文件可上传单条序列; .fasta 文件可上传多条序列)。在 Biosequences 中最多可同时检索 100 条序列。

通过.txt 或.fasta 格式上传待检索序列操作方法如下所示:

Searching for...

All

Substances

Reactions

References

Suppliers

Biosequences

Retrosynthesis

Biosequences

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

BLAST CDR Motif Upload Sequence Clear Search

Enter a query or upload a file...

Sequence Type:

Nucleotide Protein

Search Within:

Nucleotides Proteins

Include NCBI Sequences

Limit Total Sequence Results to:

1000

Start Biosequence Search

Find Biosequences - BLAST

Find biosequences that match your query, which can be a protein/nucleotide string or a .txt/.fasta file.

1. Enter or copy and paste a protein/nucleotide string, or upload a sequence file:

- **Single sequence:** .txt file
- **Multiple sequences:** .fasta file

Note: The **maximum number** of sequences is **100**.

如果.txt 文件中含有多条序列, 可以先为序列添加格式和序号(下图示例), 然后将文件后缀改为.fasta, 就可以转化为含有多条序列的.fasta 文件。点击 upload sequence 上传.fasta 文件, 完成多条序列的上传。上传后, 点击 Start Biosequence Search 即开始序列检索。


```

>NM_001
GGAGTTTATTATAACGCGCTCTCCAAGTATACGTGGCAATGCGTTGCTGGGTATT
TTAATCATTCTAG

GCATCGTTTTCCTCCTTATGCCTCTATCATTCTCCCTATCTACACTAACATCCCACG
CTCTGAACGCGC

GCCATTAATACCTTCTTCTCCACTCTCCCTGGGACTCTTGATCAAAGCGCGGCC
CTTCCCCAGCC

>NM_002
TTAGCGAGGCGCCCTGCAGCCTGGTACGCGCGTGGCGTGGCGGTGGGCGCGCAGTG
CGTTCTCGGTGTGG

AGGGCAGCTGTTCCGCTGCGATGATTTATACTCACAGGACAAGGATGCGGTTTGTC
AAACAGTACTGCT

```

Q7: 在 Biosequences 中使用 .fasta 文件上传多条序列后，在检索时，这些序列间的运算逻辑是 OR 还是 AND?

A7: 在 Biosequences 中通过 .fasta 上传多条序列后，在检索时这些序列间的运算逻辑为 OR。

Q8: 通过 Biosequences 的 BLAST 对核酸序列进行检索时，为什么查询序列是 TACTTGGAGAGCATCACTG，而检索结果 Subject 中会出现和查询序列不一样的目标序列 CAGUGAUGCUCUCCAAGUA 呢?

A8: 通过 Biosequences 的 BLAST 进行核酸序列检索时，会同时检索 DNA, RNA 及其（反向）互补链。另外，CAS 科学家在标引序列时，也会标引 DNA 和 RNA 的混体，T 和 U 等同，所以在检索结果中会出现 DNA、RNA 的（反向）互补链。

在本例中，BLAST 检索时查询的核苷酸序列是：TACTTGGAGAGCATCACTG，其反向链是 GTCACTACGA GAGGTTTCAT，T 和 U 互换后，即为 GUCACUACGA GAGGUUCAU。BLAST 比对时，其互补链（complimentary strands）为：CAGUGAUGCUCUCCAAGUA，所以在 Subject 目标序列中会出现这条序列结果。

5' CAGUGAUGCUCUCCAAGUA 3'

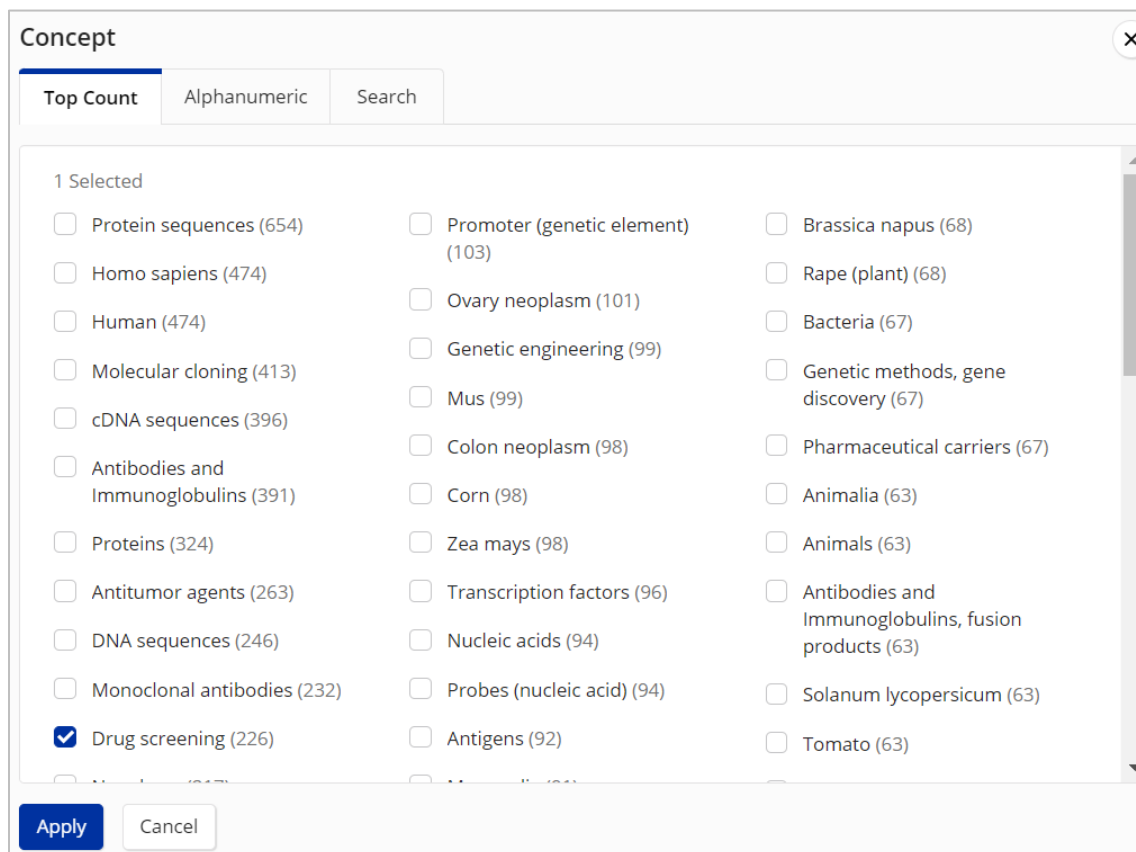
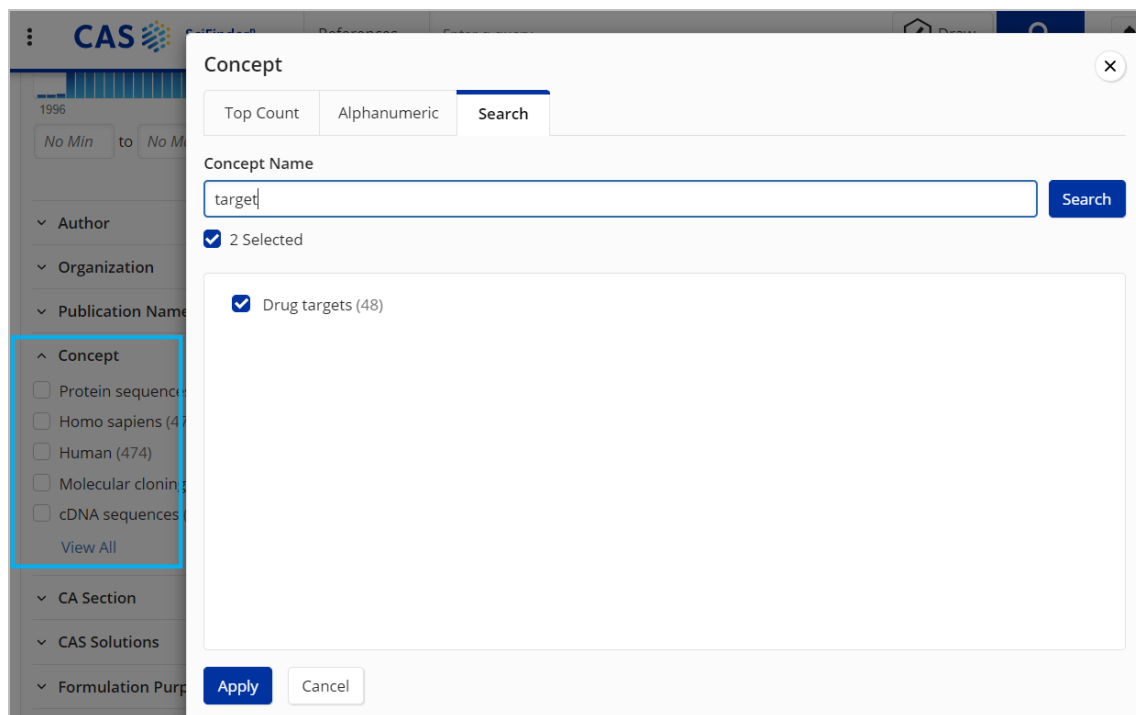
|||||

3' GUCACUACGA GAGGUUCAU 5'

Q9: 如何在 Biosequences 检索结果中获取对应的靶点研究信息？

A9: 在 Biosequences 结果中，点击目标序列对应的 References 获取报道该序列的文献。然后在文献结果集页面左侧点击 Filter by: Concept 下面的 View All，打开 Concept 列表，浏览或筛选与靶点相关的研究点。如需快速筛选，则可点击 Search，在输入 drug target, drug screening 等关键词后，点击 Apply，即可获得和靶点相关的研究文献。

The screenshot shows the CAS SciFinder Biosequences interface. At the top, there is a search bar with the text "Enter a query..." and a "Draw" button. Below the search bar, the "Biosequences" logo is visible. A "References" tab is highlighted with a blue box. The main content area shows search results for "NM_001". The results are sorted by "Subject Coverage" and are in "Expanded" view. The first result shows an alignment with 100% identity. The query sequence is 210 bp long, and the subject sequence is 330 bp long. The alignment shows a purple box for the query and a green box for the subject, with a 100% alignment identity. The interface also displays search details like BLAST algorithm, alignment identity, and query coverage.



Q10: CAS Biosequences 中是否包含专利全文中表格里的序列、专利列表中的序列？

A10: CAS Biosequences 包含来自期刊、专利和 NCBI 中的序列。其中，专利中的序列涵盖权利要求书、说明书、全文表格，以及专利申请人向专利授权机构提交的列表中的序列等。

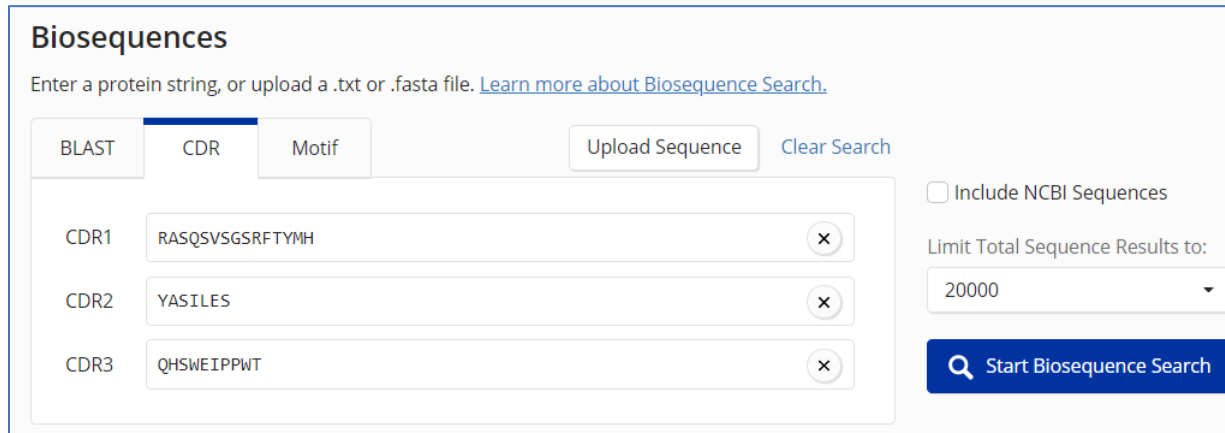
Q11: 同时用 3 个 CDR 检索抗体序列，获得的包含 2 个或 3 个 CDR 的序列结果是在同一条链上吗？

A11: 是的。

Q12: 如何获取跟抗体轻链和重链中 6 个 CDR 序列均相关的专利？

A12: 分四步完成，以下为详细的操作过程：

第一步：输入抗体其中一条链中的 3 个 CDR，获取 3 个 CDR 均被包含的序列结果集，再点击序列结果集页面左上角 References 按钮，获取报道这些序列的专利文献，点击文献结果集右上角 Save 按钮，保存结果集并命名，如：此例命名为“CDR to combine 1”。



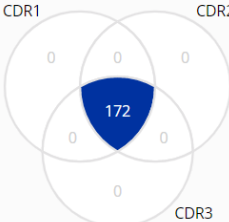
The screenshot shows the Biosequences search interface. At the top, there are tabs for BLAST, CDR (selected), and Motif. Below the tabs, there are three input fields for CDR1, CDR2, and CDR3. CDR1 contains the sequence RASQSVSGSRFTYMH, CDR2 contains YASILES, and CDR3 contains QHSWEIPPWT. To the right of the input fields, there is a checkbox for 'Include NCBI Sequences' which is unchecked, and a dropdown menu for 'Limit Total Sequence Results to:' set to 20000. At the bottom right, there is a blue button with a magnifying glass icon and the text 'Start Biosequence Search'.

Biosequences search for your query

References

CDR Segments

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



CDR1 CDR2 CDR3

Apply Reset Segments

Bioscape Analysis

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

Create Bioscape Analysis

Filter by

^ E-Value

Query Details [View Less](#)

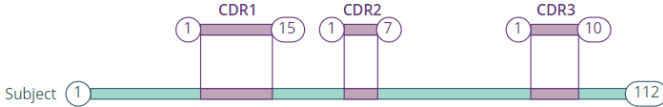
> CDR1
RASQSVSGSRFTYMH

> CDR2
YASILES

> CDR3
QHSWEIPPW

172 Results Sort: Alignment Identity View: Expanded

1 Alignment Identity: 100%



Subject 1 112

Matches: 32
Mismatches: 0

[View Less](#)

Alignment Subject References

Alignment Data

References from your sequence

Substances Reactions Citing

Save

Filter Behavior

Filter by Exclude

Document Type

Patent (295)

Language

English (264)

Korean (15)

Japanese (11)

Chinese (3)

French (1)

Turkish (1)

295 Results Sort: Times Cited View: Partial Abstract

1

Methods and compositions for generating bioactive assemblies of increased complexity and their therapeutic and diagnostic uses

By: Chang, Chien Hsing; Goldenberg, David M.; McBride, William J.; Rossi, Edmund A.
United States, US20070086942 A1 2007-04-19 | Language: English, Database: CAplus

The present invention concerns methods and compositions for making and using bioactive assemblies of defined compositions, which may have multiple functionalities and/or binding specificities. In particular embodiments, the bioactive assembly is formed using dock-and-lock (DNL) methodol., which takes advantage of the specific binding interaction between dimerization and docking domains (DDD) and anchoring domains (AD) to form the assembly. In various embodiments, one or more effectors may be attached to a DDD or AD sequence. Complementary AD or DDD sequences may be attached to an adaptor modul...

[View More](#)

PatentPak Full Text Substances (427) Reactions (0) Citing (21) Citation Map

Save Results ✕

Name

Save Options

Selected Answers

All Answers (Up to 20,000)

Add Existing Tags (Optional)

Asymmetric Organocataly
 Asymmetric Organocataly
 5HT
 aa sequ
 aa sequence

New Tag (Optional) **Tag Color**

▼

Save
Cancel

第二步：输入抗体另一条链中 3 个 CDR，同第一步的操作，获取 3 个 CDR 均被包含的序列结果集，再点击序列结果集页面左上角的 References 按钮，获取报道这些序列的专利文献。

Biosequences

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

BLAST
CDR
Motif

Upload Sequence
Clear Search

CDR1

✕

CDR2

✕

CDR3

✕


Include NCBI Sequences

Limit Total Sequence Results to:

20000
▼

🔍 Start Biosequence Search

106

第三步：在第二步的文献结果集页面，点击右上角  combine 按钮，选择合并方式，如：此例选取交集 Intersect；在弹出对话框中选勾选想要合并取交集的已保存文献结果集，如：此例选“CDR to combine 1”。

Item	Count	Date
<input type="checkbox"/> CDR to combine 2	21 Saved Results	July 1, 2022
<input checked="" type="checkbox"/> CDR to combine 1	295 Saved Results	July 1, 2022
<input type="checkbox"/> jak1	2,341 Saved Results	June 17, 2022

第四步： 点击 View Results 按钮， 查看跟抗体轻链和重链中 6 个 CDR 序列均相关的专利文献结果。

References from Combined Results

Substances Reactions Citing

Filter Behavior

Filter by Exclude

Document Type

Patent (21)

Language

English (21)

Publication Year

21 Results

Sort: Publication Date: Newest View: Partial Abstract

1

Preparation of 6a,7,8,9,10,12-hexahydro-12-oxobenzo[e]pyrido[1,2-a][1,4]diazepine and related compounds as sequence-selective DNA mono-alkylating cytotoxic agents and their antibody conjugates containing peptidyl linkers

By: Andriollo, Paolo; Jackson, Paul; Thurston, David

World Intellectual Property Organization, WO2022023735 A1 2022-02-03 | Language: English, Database: Cplus

The invention is related to 6a,7,8,9,10,12-hexahydro-12-oxobenzo[e]pyrido[1,2-a][1,4]diazepine derivatives, analogs and their linker conjugates containing a sigma hole group, e.g., I, II and III [X = S, Se, Te, P, As, Sb, Bi, Si, Ge, Sn or Pb; Y = N, C-NH₂, C-OH; Z = O, N-Me], their pharmaceutically acceptable salts, tautomers, stereoisomers or their mixtures as DNA-binding compounds, especially DNA-alkylating agents that are useful as medicaments, such as anti-proliferative agents. The pyridinobenzodiazepines derivatives and analogs of the invention linked, either directly or indirectly, to a...

View More

Q13: Bioscape 中可以展示指定目标公司的序列吗？

A13: 可以。具体操作如下示例。

示例序列：

EALSFVSLVDGYFRLTADAHHYLCTDVAPPLIVHNIQNGCHGPICTEYAINKLRQEGSEEGM

(1) 在 CAS Biosequences 中获得的序列结果集页面， 点击页面左侧 Create Bioscape Analysis。

Biosequences search for your query

References

BLAST Search Details

Sequence Type: Protein
 Search Within: Proteins
 BLAST Algorithm: BLASTp
 NCBI Included: Yes
 Alignment Identity: -
 Query Coverage: 50%
 E-Value: 10
 Match with Gaps?: Yes
 Gap Costs: Existence 11
 Extension 1
 Word Size: 3

Bioscape Analysis

Visually explore sequence similarity with a new tool. Learn more about Bioscape.

Create Bioscape Analysis

Filter by

Query Details EALSFVSLVDGYFRLTADAHHYLCTDVAPPLIVHNIQNGCHGPICTEYAINKLRQEGSEEGM View Less

EALSFVSLVDGYFRLTADAHHYLCTDVAPPLIVHNIQNGCHGPICTEYAINKLRQEGSEEGM

7,113 Results Sort: Alignment Identity View: Expanded

1 Alignment Identity: 100%

Query 1 62

Subject 1 863

Matches: 62
 Mismatches: 0

View Less

Alignment Subject References

Alignment Data
 BLAST Score: 357
 E-Value: 1.65185e-39

(2) 在 Bioscape 可视化分析页面，点击左侧放大镜图标，在 All 中输入指定公司名，如“Compugen”，点击绿色 search 按钮，获得该页面上的指

All COMPUGEN

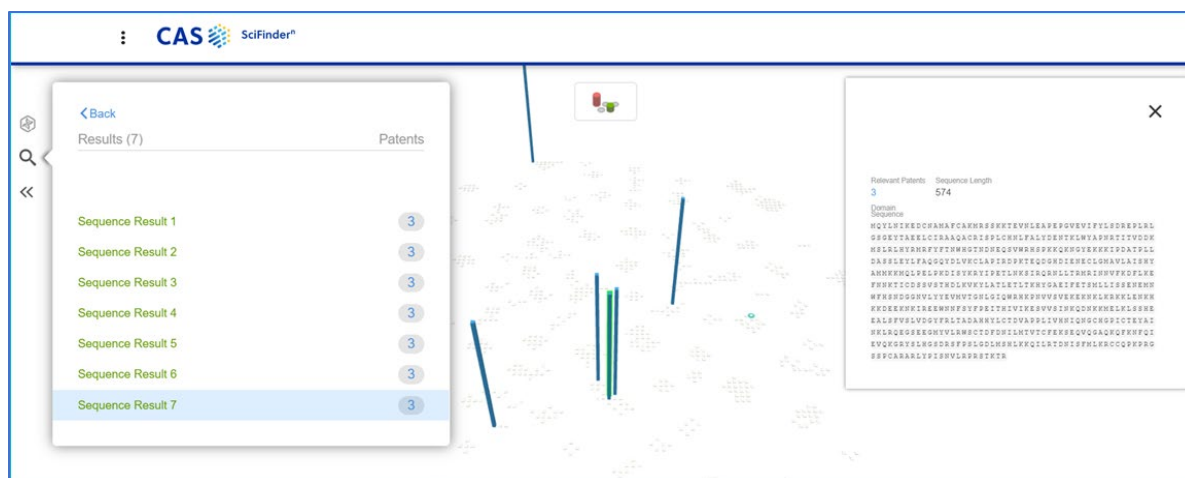
Tit./Abs./Cla.

Simple legal status None

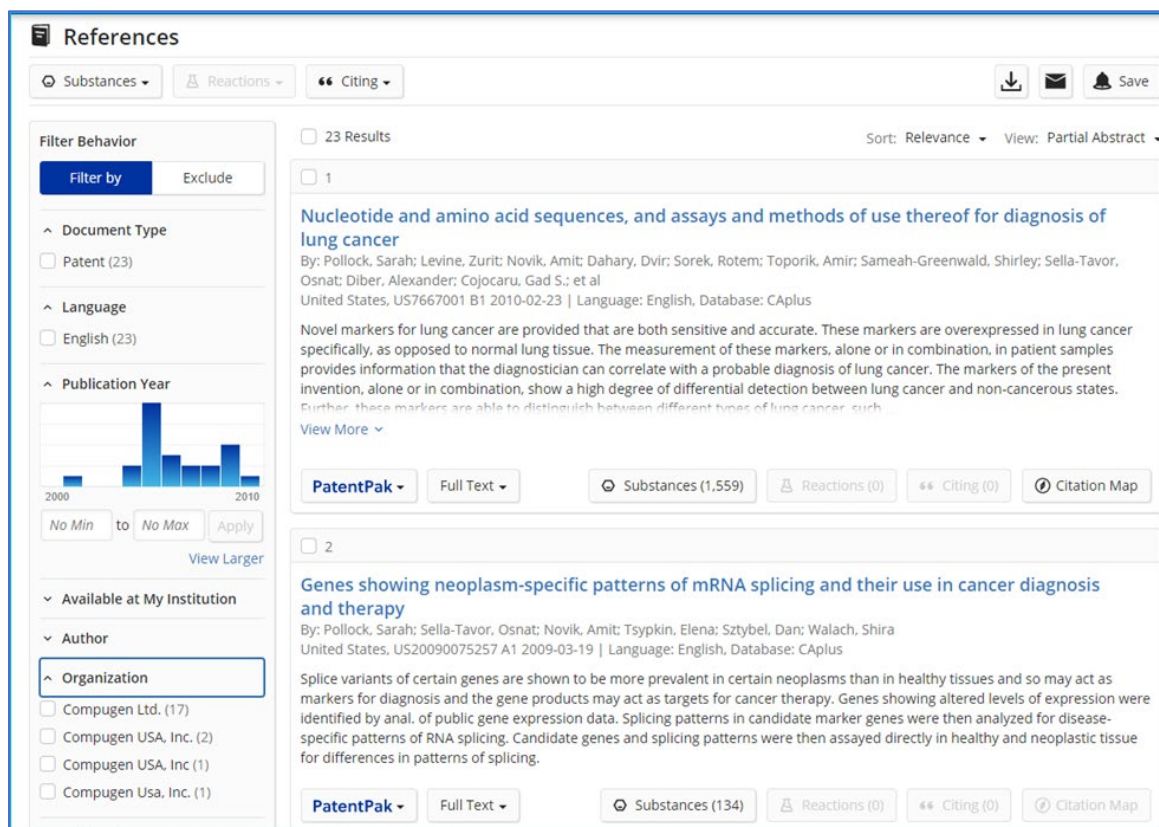
Search

Reset

(3) 点击柱体代表的序列，会在右侧弹出框中呈现该序列、序列长度、相关专利数量，点击代表专利数量的蓝色数字，可获取该选中序列（绿框框柱的柱体）的相关专利合集。



(4) 在专利结果集页面左侧 Organization 筛选选项下，可见该专利结果集专利权人包含指定的“Compugen”。



CAS Formulus

Q1: CAS Formulus 中, Formulation Designer, Formulation, Ingredient 的区别?

A1:

- Formulation Designer 根据用户选择的应用领域、用途、物理形态和活性/主要成分, 提供配方设计模板。模板中包括建议的成分(活性成分、辅料、润滑剂、分散剂等)、功能、替代的成分, 对应的管控信息链接、组分含量, 以及配方工艺等。用户可以使用模板中建议的成分, 或者手动添加其他感兴趣的成分, 最终可以导出为 Excel 格式的文件, 无缝对接配方设计工作流程。
- Formulation 是根据成分、功能、形态、用途、递送途径等来检索 Formulus 中的制剂/配方信息。
- Ingredient 是根据配方成分的化学名、CAS 号等来检索配方中的物质信息。获得的物质信息包括该物质的 CAS 号、化学名、结构式、理化性质、其常见的配伍成分、管控信息(FDA、ANMAT、DMF、EMA 等)、常见用途、配方详情和供应商信息等。

Q2: 如何通过技术手段检索制剂信息?

A2: 在 CAS SciFinder® 主页面选择 References, 在检索框中输入有关技术手段的关键词, 检索得到文献结果集。在文献结果集页面左侧 CAS Solutions 选项中勾选 CAS Formulus, 获得制剂研究的文献结果集。在文献详情页面点解 View CAS Formulus Detail, 链接至 CAS Formulus 获得制剂实验操作详情。

Formulations

Analgesic Composition: Pharmaceutical, Antiheadache Agent

[View CAS Formulus® Detail](#)

Location: Claim 9
Purpose: pharmaceutical, antiheadache agent
Target: humans

Component	Function	Amount Reported
Group: Nonnarcotic analgesics	active agent	-
Group: Antiemetics	-	-
Group: Central nervous system stimulants	-	-
Pharmaceutical carriers	carrier	-

Additional Components Reported in Full Text

Analgesic Composition: Pharmaceutical, Antiheadache Agent

[View CAS Formulus® Detail](#)

Location: Example 16
Purpose: pharmaceutical, antiheadache agent
Target: humans, animals

CAS Formulus

Formulations

Dimethyl sulfoxide	solvent (<i>preferred</i>)	-	Mandatory
Polyoxyethylene sorbitan monooleate	auxiliary agents, diluents	10 %	Mandatory

Process

the powder of the analgesic activity extract of *Bidens pilosa* was dissolved in dimethyl sulfoxide, and then Tween-80 was used as a pharmaceutical auxiliary to prepare an analgesic pharmaceutical composition.

Effective Dose

Descriptor	Solvent	Details
-	-	20 mg/kg
Experimental Activity		
Descriptor	Notes	Details
analgesic rate	analgesic rate of the composition was determined using aspirin group	79.7 %
View More		
-	-	4 mg/kg
Experimental Activity		
Descriptor	Notes	Details
analgesic rate	analgesic rate of the composition was determined using chloroform low dose group	62.1 %

Q3: 如何通过结构式检索制剂信息?

A3: 按下述步骤进行:

- 1) 在 CAS SciFinder[®] 主页面选择 References
- 2) 打开结构编辑器、绘制结构, 检索后得到文献结果集。
- 3) 在文献结果集页面左侧 Filter by 筛选项 CAS Solutions 下勾选 Formulus, 即可获得绘制结构制剂研究的文献。
- 4) 在文献结果集页面, 点击 View CAS Formulus Detail 链接至 CAS Formulus 获取制剂研究其他更多详细信息。

CAS Analytical Methods

Q1: 如何通过已知结构, 检索相似结构的分析检测方法?

A1: 操作步骤如下:

- 1) 在 CAS SciFinder[®] 主页选择 Substances, 然后 打开结构编辑器绘制结构, 再进行物质检索。
- 2) 在物质结果集页面左侧选择 Similarity, 获得绘制结构的相似结构结果集。点击该结果集页面顶端的 References, 获得报道这些结构的文献结果集。
- 3) 勾选文献结果集页面左侧 Substance Role 选项中的 Analytical Study, 或者 Analyte 获得与分析研究相关的文献结果集。
- 4) 或者勾选 CAS Solutions 选项下的 Analytical Methods。在文献详情页面点击 CAS Method Number 链接至 CAS Analytical Methods 获取分析方法实验操作详情。

The screenshot displays the CAS SciFinder interface. At the top, there is a search bar with the text '2010:635115' and a search icon. Below the search bar, there are several icons: a close button, a 'Draw' button, a search icon, a star, a clock, and a user profile icon. The main content area is divided into two columns. The left column contains metadata for the document, including the source (Analele Universitatii 'Ovidius' Constanta, Seria: Chimie), volume (20), issue (1), pages (5-10), journal (2009), CODEN (AUOCCG), database information (AN: 2010:635115, CAN: 154:438752, CAplus), company/organization (Department of Chemical Engineering and Technology, Ovidius University of Constanta), publisher (Ovidius University Press), and language (English). The right column contains the abstract, keywords (petroleum cracking coking fraction thermocatalysis GC MS HPLC), and a list of related CAS Analytical Methods. The first method, 'Analysis of Decyl butyrate in Gasoline by Gas chromatography-mass spectrometry', is highlighted with a blue box and its CAS Method Number, 1-135-CAS-32545, is also highlighted. Other methods listed include 'Analysis of Decyl butyrate in Petroleum fractions by HPLC' (1-135-CAS-38904) and 'Analysis of Decyl butyrate in Gasoline by Gas chromatography' (1-135-CAS-66100). The interface also includes a 'Full Text' button and an 'Expand All | Collapse All' link.

CAS Analytical Methods

Gas chromatographic system, GC 6890, Agilent
Mass spectrometer, MS 5973, Agilent

Conditions

Instrument

Column: Agilent HP-5MS, 30 m long, with the inner diameter of 0.25 mm column packed with a non-polar substance, 5%-(phenyl)-methylpolysiloxane; injection volume: 1 - 2 μ L/100 mL; split less mode: splitless mode from 20 °C to 300 °C; splitting rate: 10/1; flow rate: 1 mL/min; velocity: 36 cm/sec

Instructions

Preparation of gasoline samples

1. Collect petroleum fractions containing whole fluid catalytic cracking (FCC) gasoline (cut in narrower fractions (cut at 100 °C)) and the middle distillate fractions (boiling points up to 300 °C) from the thermocatalytic cracking processes in an oil refinery the coke unit and the fluid catalytic cracking (FCC).
2. Obtain the petroleum products by processing a naphthenic crude oil (crude oil C).

Gas chromatography - mass spectrometry procedure

1. Perform the analysis using a gas chromatographic system and mass spectrometer with GC 6890 and MS 5973 Agilent.
2. Perform the separation using Agilent HP-5MS, 30 m long, with the inner diameter of 0.25 mm column packed with a non-polar substance, 5%-(phenyl)-methylpolysiloxane.
3. Inject 1 - 2 μ L/100 mL of sample concentration prepared in water or in methanol/water solvent (15% vol. methanol).
4. Perform the analysis in splitless mode from 20 °C to 300 °C.
5. Set the heating rate at 20 °C/min (10 minutes).
6. Set CIS mode at 45 °C (1.5 minutes), up to 300 °C, heating by 12 °C/sec (10 minutes).
7. Set the splitting rate of the column at 10/1.
8. Apply initial pressure of 7.04 psi.
9. Set the flow rate at 1 mL/min (constant) and velocity at 36 cm/sec.
10. Program the oven conditions as follows: 40 °C (2 minutes) up to 150 °C, heating rate: 10 °C/min; 6 °C/min up to 300 °C (1 minute).

其他

Q1: 我最近将 KMP alerts 从 CAS SciFinder 转移到了 CAS SciFinderⁿ。但是为什么我在 CAS SciFinderⁿ 中得到的结果比 CAS SciFinder 少呢?

A1: 在 CAS SciFinder 中用于 KMP alerts 的筛选项不会自动全部转移到 CAS SciFinderⁿ。因此您需要在 CAS SciFinderⁿ 中更改 Alert 检索策略。

Q2: 在哪里可以获得筛选检索结果的选项?

A2: 可在 CAS SciFinderⁿ 结果集页面获取所有的筛选选项。

The screenshot displays the CAS SciFinderⁿ search results page. On the left, there is a 'Filter Behavior' sidebar with a 'Filter by' button and several expandable filter categories: Commercial Availability, Reaction Role, Reference Role, Stereochemistry, Number of Components, Substance Class, Isotopes, Metals, Molecular Weight, Experimental Property, Experimental Spectrum, Regulatory Data by Country, Regulatory Data by List, Bioactivity Indicator, and Search Within Results. The main content area shows a grid of search results. Each result card includes a chemical structure, a molecular formula (e.g., $(C_{24}H_{18}.C_{10}H_{10}Fe)_x$), the number of components (2), and buttons for 'Reference', 'Reactions', and 'Suppliers'. The results are numbered 4, 5, and 6. The first result (2624129-66-2) shows a chemical structure of a ferrocene derivative. The second result (2620391-49-1) shows a biphenyl derivative. The third result (2620391-48-0) shows a ferrocene derivative with a benzene ring.

Q3: 选择 All 进行检索，将得到什么信息？在检索框中需要输入什么类型的信息？

A3: 当选择 All 选项时，可以在检索框中输入关键词、CAS 登记号、专利号或文献收录号 (Accession Number) 等，将获得与输入信息相关的物质、文献、反应和供应商等信息。

Return to Home

Show only

- Substances (1)
- Reactions (16,738)
- References (243,265)
- Suppliers (155)

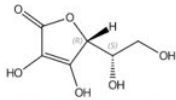
All Answer Types

Top two answers by relevance from each answer type.

Substances (1)

1

50-81-7



Absolute stereochemistry shown

C₆H₈O₆
L-Ascorbic acid

243K References 16K Reactions 155 Suppliers

[View All Substances](#)

Q4: CAS SciFinder[®] 支持哪些操作系统和浏览器?

A4: 请参考如下建议, 同时不建议使用 360、Sogo 等浏览器。

- Windows 10: 谷歌 60 或更高版本、火狐 55 或更高版本、火狐 52 (ESR)、IE11、Edge 15 或更高版本
- Windows 8.1: 谷歌 60 或更高版本、火狐 55 或更高版本、火狐 52 (ESR)、IE11
- Windows 7: 谷歌 60 或更高版本、火狐 55 或更高版本、火狐 52 (ESR)、IE11
- Mac OS X 10.13: Safari 11.x、谷歌 60 或更高版本、火狐 55 或更高版本、火狐 52 (ESR)
- Mac OS X 10.12: Safari 10.x、谷歌 60 或更高版本、火狐 55 或更高版本、火狐 52 (ESR)
- Mac OS X 10.11: Safari 9.3 或更高版本、谷歌 60 或更高版本、火狐 55 或更高版本、火狐 52 (ESR)
- iOS 11: Safari 11.x、谷歌 60 或更高版本、火狐 8.0 或更高版本
- iOS 10: Safari 10.x、谷歌 60 或更高版本、火狐 8.0 或更高版本
- iOS 9: Safari 9.3、谷歌 60 或更高版本、火狐 8.0 或更高版本

- Android 7.x: 谷歌 60 或更高版本、火狐 55 或更高
- Android 6.x: 谷歌 60 或更高版本、火狐 55 或更高
- Android 5.x: 谷歌 60 或更高版本、火狐 55 或更高
- Android 4.x: 谷歌 60 或更高版本、火狐 55 或更高

网络连接要求

- SSL (https)通过端口 443 连接 scifinder-n.cas.org;
- https 通过端口 80 连接 chemport.cas.org 用于获取全文链接。

其他建议和要求

- 必须启用 JavaScript 和 cookie;
- 将 https://scifinder-n.cas.org 添加为浏览器信任站点 (Trusted Site) 及非弹出阻止程序 (Pop-up blocker Exceptions lists) ;
- PDF Reader 用于导出和打印 CAS SciFinderⁿ 检索结果及其他信息。Adobe Reader 可用于 Mac 或 Windows 计算机。Mac OS X 提供免费浏览器 Preview。