

CAS SCIFINDER®

常见问题解答

2022 年 12 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 authors listed are Wiltshire, H.; Wiltshire, B.; Citron, A.; Clarke, T.; Serpe, C.; Gray, D.; Herron, W. The article is indexed in several databases, including CAplus and MEDLINE. The 'Database Information' section is highlighted with a blue box, showing the following details:

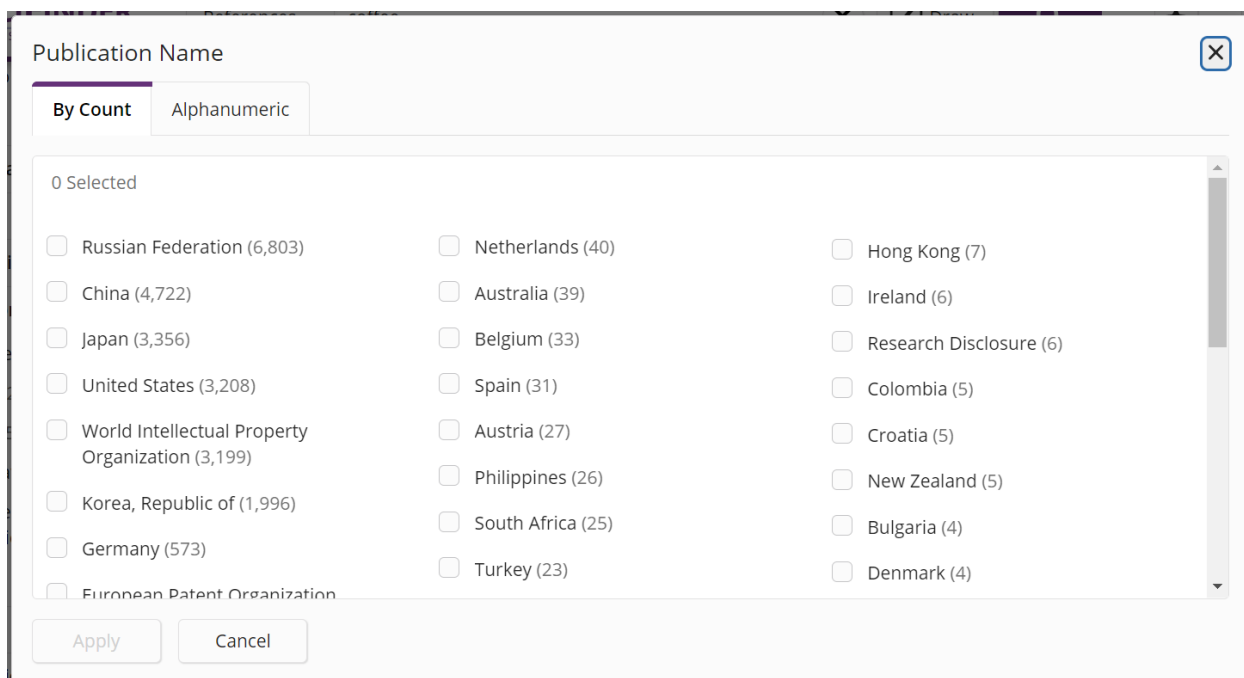
- AN: 2000:591027
- CAN: 133:317174
- PubMed ID: 11043756
- CAplus and MEDLINE

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 shows the CAS SciFinder[®] interface. At the top, there is a search bar with the text "References" and "Enter a query...". Below the search bar, there is a navigation menu with "Return to Home" and "Structure Match". The "Structure Match" section is highlighted with a red box, showing "As Drawn (14)" and "Substructure (639)". Below this, there is a "Filter Behavior" section with "Filter by" and "Exclude" buttons. The "Document Type" section is expanded, showing "Journal (12)", "Patent (2)", "Analytical Study (1)", and "Biological Study (1)". The "Substance Role" section is also expanded, showing "Reactant or Reagent (7)", "Preparation (5)", "Properties (2)", "Analytical Study (1)", and "Biological Study (1)". The "Language" section is expanded, showing "English (13)" and "German (1)".

The main content area displays a list of references. The first reference is highlighted with a red box and shows a chemical structure of a ruthenium(II) complex. The reference title is "NanoSIMS analysis of an isotopically labeled organometallic ruthenium(II) drug to probe its distribution and state in vitro [Erratum to document cited in CA163:660515]". The authors are Lee, Ronald F. S.; Escrig, Stephane; Croisier, Marie; Clerc-Rosset, Stephanie; Knott, Graham W.; Meibom, Anders; Davey, Curt A.; Johnsson, Kai; Dyson, Paul J. The reference is from Chemical Communications (Cambridge, United Kingdom) (2015), 51(92), 16577. The language is English, and the database is CAPlus and MEDLINE. The funding details were omitted from the published article; the omitted details are given. Below the reference, there are buttons for "Full Text", "Substances (9)", "Reactions (5)", "Citing (2)", and "Citation Map".

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?

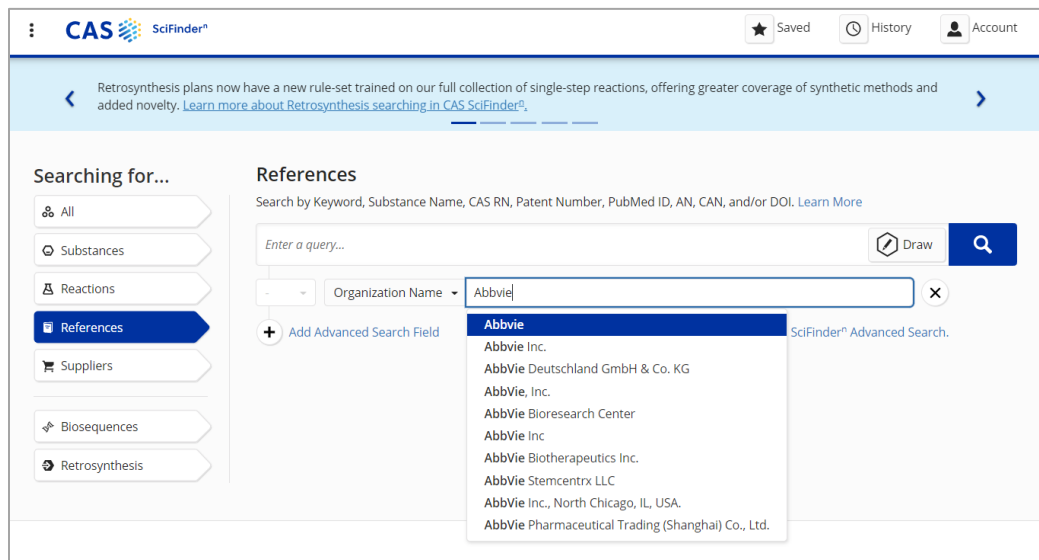
A14: 选择 References, 在输入框中输入检索式, 检索式中可考虑使用恰当的布尔逻辑运算符, 以获取预期结果。如输入: High-strength and high-conductivity and "copper alloy" 或 "High-strength" and "high-conductivity" and "copper alloy"等。

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?

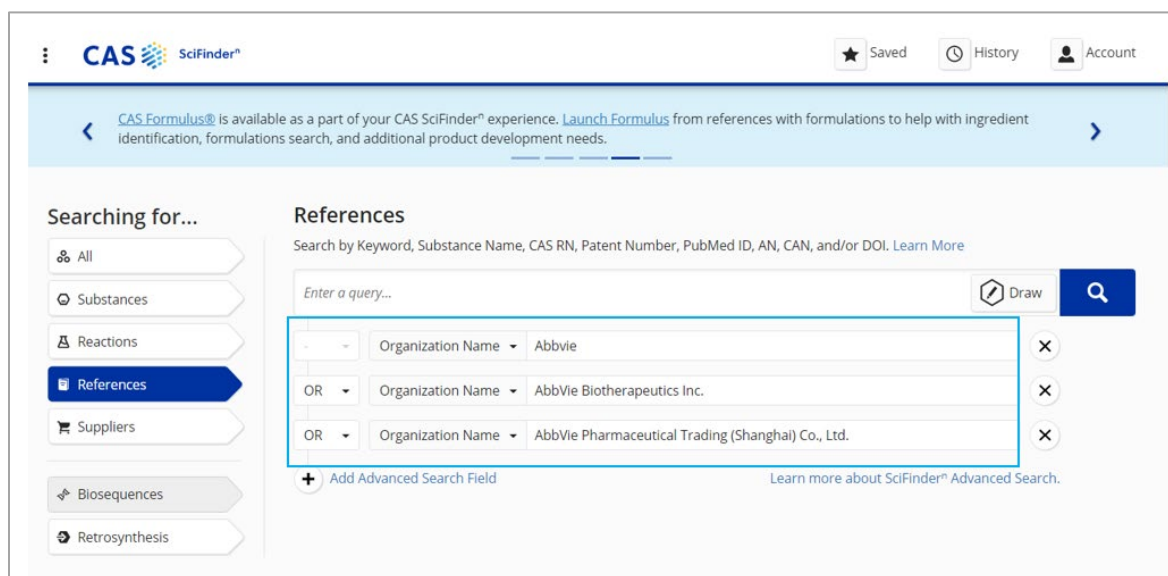
A15: 选择 References。绘制小分子结构式, 同时在输入框中输入关键词 (如, prodrug and doxorubicin), 采用文本+结构联合检索方式得到文献结果集。再在文献结果集页面左侧 Filter By: Document Type 选择 Patents, 即可获得该小分子前药研究专利。

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: 新的农药成分, 如何查询其慢性毒性?

A17: 推荐检索步骤如下:

- (1) 通过物质检索, 获得农药分子后, 再由物质获取其研究文献;

(2) 在文献结果中通过左侧 substance role:选择 adverse effect 可获得涉及副作用方面的研究文献, 通过 biological study 可获得全面的生物学相关研究;

(3) 同时可通过 concept 搜索毒性相关的词, 比如 toxi* (通配符可对其做扩展, 会同时获得 toxin, toxicity, toxicology 等概念词) 最后点击 Apply 查看相关文献结果;

如果是新农药, 研究文献有限, 建议使用新农药的母核结构, 或者文献量较大的相似结构农药, 重复上述过程, 进行检索。

Q18: CAS Lexicon 只包括 concept 的扩展联想么?

A18: CAS 词库包括 CAS 科学家标引的概念词 (Concept) 和物质。在 CAS Lexicon 中可获得检索词的相关词、同义词/近义词、上位词、下位词和相关词。

Q19: 如何查询农药的工业制备方法?

A19: 通过物质检索获得农药分子后, 可以选择获取物质结果集的文献, 或者单个物质的研究文献。

The screenshot shows the CAS SciFinder search results page. At the top, there are tabs for 'References', 'Reactions', and 'Suppliers'. The 'References' tab is selected and highlighted with a blue box. Below the tabs, there is a 'Filter Behavior' section with 'Filter by' and 'Exclude' buttons. A sidebar on the left lists various 'Reference Role' categories, including 'Agricultural Use (2)', 'Biological Study (2)', 'Uses (2)', 'Adverse Effect (1)', and 'Analyte (1)'. The main results area shows two entries. The first entry is for '272451-65-7' (Flubendiamide), which has a chemical structure image, the formula $C_{23}H_{22}F_7IN_2O_4S$, and is highlighted with a blue box. Below the name, there are buttons for 'References' (1,767), 'Reactions' (33), and 'Suppliers' (33). The second entry is for '1288524-37-7', which has 'Image Not Available' and notes: 'Notes: A flubendiamide-based insecticide (Nichino America Inc., Wilmington, DE, USA) Unspecified NNI 0771'. Below this entry, there are buttons for 'Reference' (1), 'Reactions' (0), and 'Suppliers' (0).

在文献结果集左侧 substance role 中选择 Industrial Manufacture 即可直接获得经过 CAS 科学家人工标引的农药工业制备文献。

如果以上方法未获得丰富的结果，也可以在获得文献结果集后，在页面左侧 search within results 中输入 Industrial Manufacture 等关键词进行限定，尝试检索。

Q20: 如何查看最新发布（公开）的文献？

A20: 在 CAS SciFinder[®] 文献检索结果中，可以根据排序功能查看最新发布（公开）的研究文献。

比如，在文献检索结果集页面，通过 Sort: Publication Date: Newest 优先查看最新的文献。可以通过左侧聚类分析项中的 Document Type 进行浏览，期刊、专利、综述、会议论文、预印本等。通过 Publication Year 查看逐年的文献数量趋势，并可以自定义查看特定年份范围的文献结果。

CAS SciFinder®

References rare earth

Return to Home

References search for "rare earth"

Substances Reactions Citing Knowledge Graph Save and Alert

333,558 Results Sort: Publication Date: Newest View: Partial Abstract

1

Design of single-phased magnesium alloys with typical rare earth elements for biomedical applications: Concept and proof

By: Bian, Dong; Chu, Xiao; Xiao, Jin; Tong, Zhipei; Huang, He; Jiang, Yuhang; Yu, Hui; He, Yue et al
Bioactive Materials (2023), 22, 180-200 | Language: English, Database: CAPLUS and MEDLINE

Rare earth elements (REEs) have been long applied in magnesium alloys, among which magnesium alloys containing WE43 alloy has already got the CE mark approval for clin. application. A considerable amount of REEs (7 wt%) is needed in that multi-phased alloy to achieve a good combination of mech. strength and corrosion resistance. However, the high complex RE addition accompanied with multiple second phases may bring the concern of biol. hazards. Single-phased Mg-RE alloys with simpler compositions were proposed to improve the overall performance. I.e. "Simpler alloy, better performance". The sin...

View More

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

2

Linking the effect of localised pitting corrosion with mechanical integrity of a rare earth magnesium alloy for implant use

By: van Gaalen, Kerstin; Quinn, Conall; Benn, Felix; McHugh, Peter E.; Kopp, Alexander; Vaughan, Ted J.
Bioactive Materials (2023), 21, 32-43 | Language: English, Database: CAPLUS and MEDLINE

This study presents a computational framework that investigates the effect of localised surface-based corrosion on the mech...

Publication Year

1841 2023

No Min to No Max Apply

View Larger

Author

Organization

Publication Name

Concept

CA Section

Publication Year

1841 2023

1841 - 2023 (333K)

Apply Cancel

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？

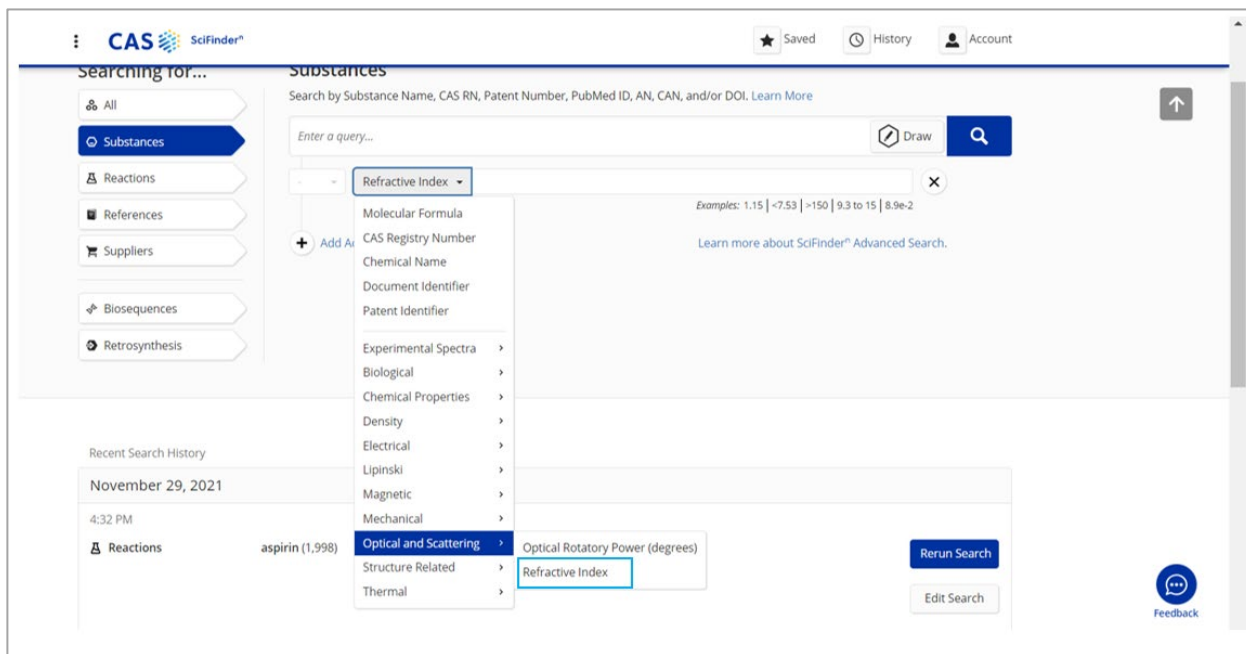
A3:

- 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?

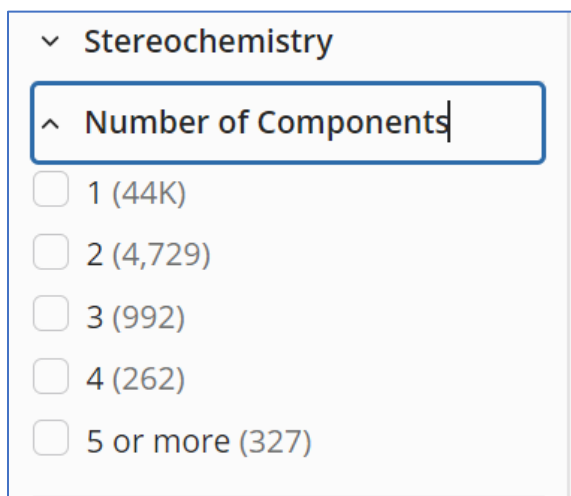
A6: 点击结果集页面左下角的 Search Within Results，打开结构编辑器，在结构编辑器中绘制指定的原子，比如要求筛选出含有 2 个 N 原子的物质，则在结构编辑器中绘制 2 个 N 原子，2 个 N 原子之间无需任何连接，单独绘制即可。检索后即可得到指定原子个数的物质。

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?

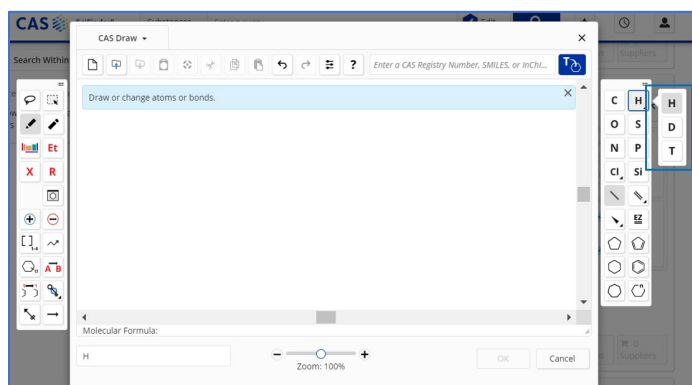
A8: 在物质结果集页面左侧选择 Number of Components，即可通过组分数筛选组合物，如下图所示:



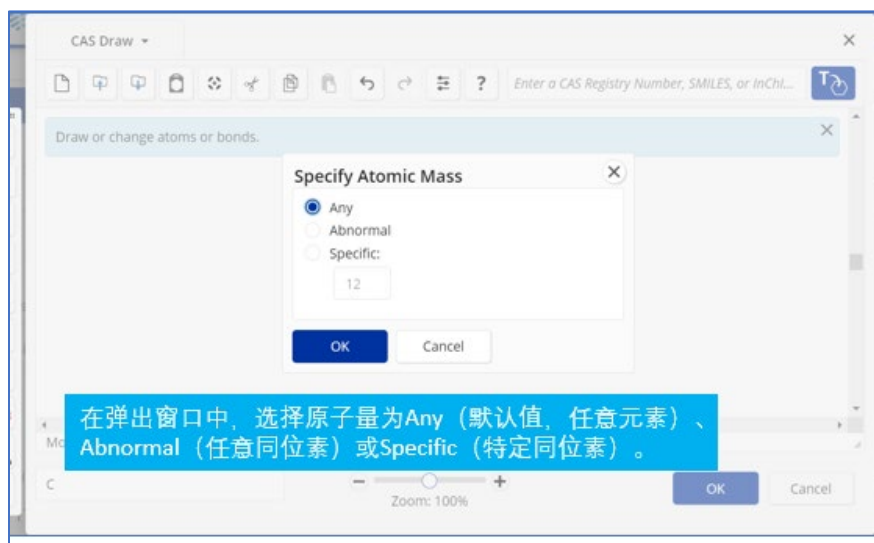
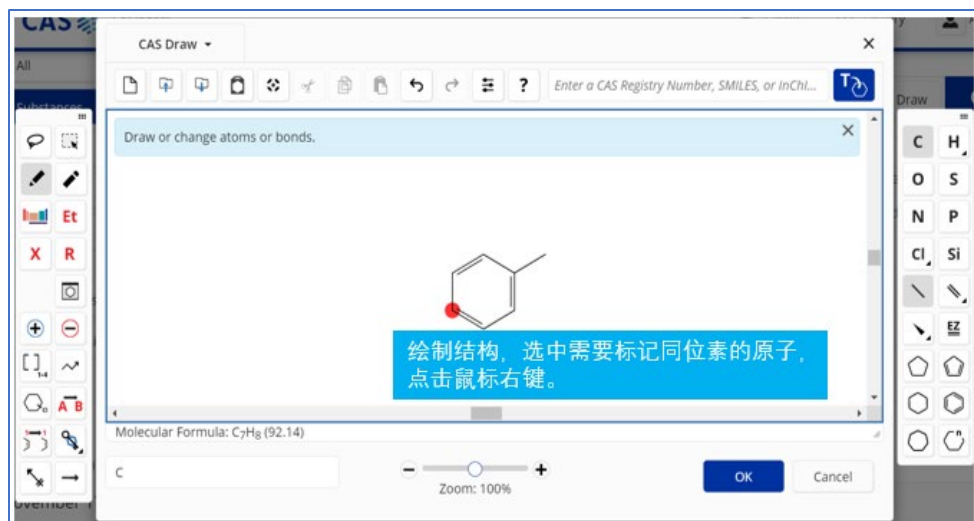
Q9: 如何检索同位素标记的化合物

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:

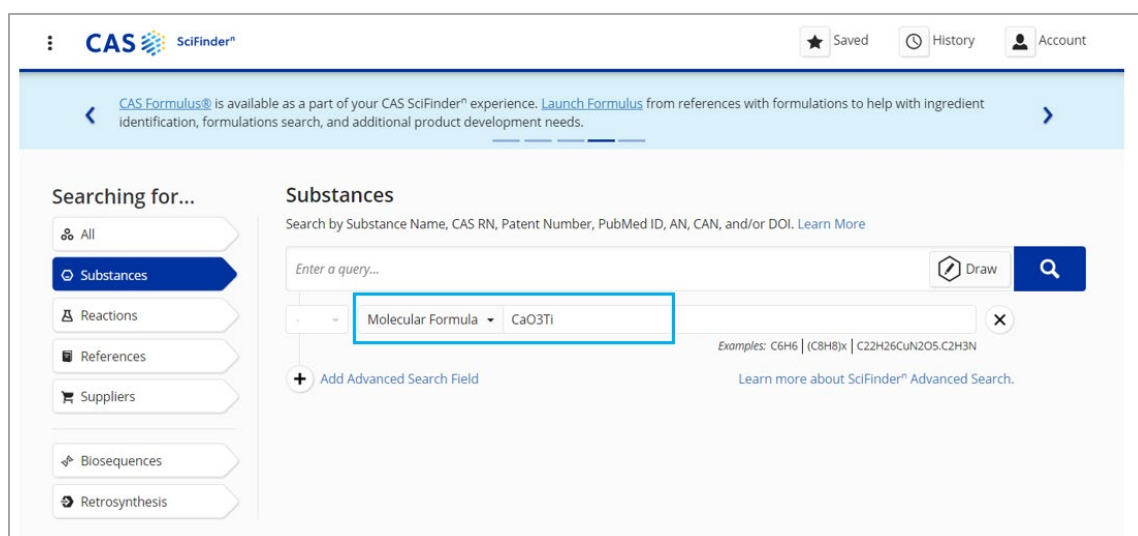
- 点击 Substances, 打开结构编辑器, 绘制结构。上传结构并检索
- 通过结构检索可同时获取 As Drawn, Substructure 和 Similarity 检索结果集, 默认展示 As Drawn 结果集。
- 点击 Substructure, 可获取绘制结构母核不变的衍生物; 点击 Similarity, 参考一定范围的相似度分值, 可以获取绘制结构母核发生一定变化的衍生物。

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. At the top, there is a search bar with 'Enter a query...' and a search button. Below the search bar, the page title is 'Substances (1)'. On the left side, there is a sidebar with various filters. Under the 'Stereochemistry' section, 'Absolute Stereo Match (1)' is selected. The main content area displays a search result for '2492423-29-5' with a chemical structure of Uridine, 4-oxime, 5'-(2-methylpropanoate), (4Z)-. The structure is shown with absolute stereochemistry. Below the structure, the chemical formula $C_{13}H_{19}N_3O_7$ and the name 'Uridine, 4-oxime, 5'-(2-methylpropanoate), (4Z)-' are displayed. There are also buttons for 'References', 'Reactions', and '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 displays the CAS SciFinder search results page. At the top, there is a search bar with the text "Enter a query...". Below the search bar, the "Substances" tab is selected, showing two results. The first result is "253874-46-3" with the chemical structure of a pyridinium ion. The second result is "77979-51-2" with the chemical structure of a pyrrolone ion. The left sidebar contains various filters and tools, including "Structure Match" (As Drawn, Substructure, Similarity), "Structure Precision" (Conventional Results, Tautomers and Zwitterions), "Chemscape Analysis", "Filter Behavior" (Filter by, Exclude), and "Commercial Availability" (Not Available).

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... 🎨 Draw 🔍

Boiling Point (°C) 500 to 600 ✕

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.

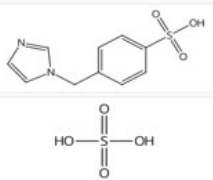
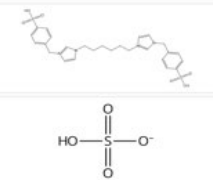
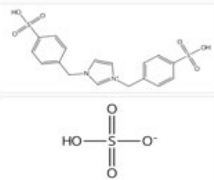
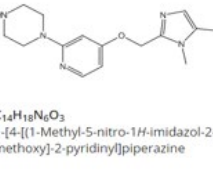
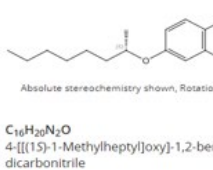
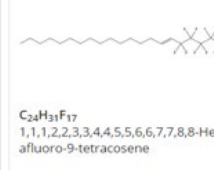
🎨 Draw

Search

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

Remove and Edit ✕



<p>1 1332456-96-8</p>  <p><chem>C10H10N2O3S.H2O.S</chem> Components: 2 Benzenesulfonic acid, 4-(1H-imidazol-2-ylmethyl), sulfate (1:1)</p> <p>2 References 6 Reactions 0 Suppliers</p>	<p>2 1328886-83-4</p>  <p><chem>C26H32N4O6S2.2HO.S</chem> Components: 2 1H-Imidazolium, 1,1'-(1,6-hexanedyl)bis[3-[(4-sulfohenyl)methyl]-, sulfate (1:1:1)</p> <p>2 References 10 Reactions 0 Suppliers</p>	<p>3 1328886-81-2</p>  <p><chem>C17H17N2O6S2.HO.S</chem> Components: 2 1H-Imidazolium, 1,3-bis[(4-sulfohenyl)methyl]-, sulfate (1:1)</p> <p>3 References 10 Reactions 0 Suppliers</p>
<p>4 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 1268157-06-7</p>  <p><chem>C16H20N2O</chem> 4-[[1(15)-1-Methylheptyl]oxy]-1,2-benzene dicyanitrile</p> <p>1 Reference 3 Reactions 1 Supplier</p>	<p>6 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)

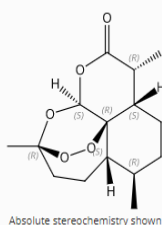
Reactions (2,949)

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, ACI)

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
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

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

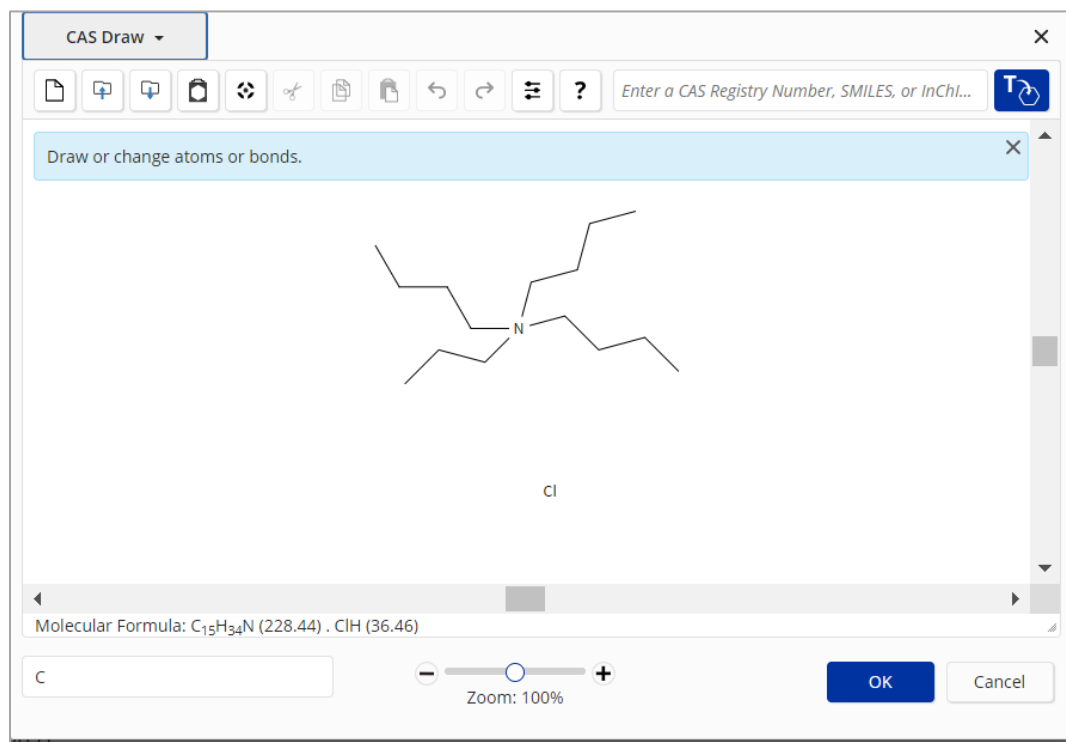
(2) 如果不知道物质结构或名称等信息，可以根据旋光度值来检索物质。点击 Substances: 再点击 Advanced Search Field，选择 Optical and Scattering: Optical Rotatory Power (degrees)，输入旋光度值（定值或者范围值都可以）。

(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 References **8** Reactions **0** 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

CCCC[NH2+].[OH-]

$C_{15}H_{34}N.HO$

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

CCCC[NH2+].CC[C@@H](C)C(=O)O

$C_{15}H_{34}N.C_6H_8N_3O_2$

Components: 2

Absolute stereochemistry shown

1 Reference 0 Reactions 0 Suppliers

3 2283341-71-7

CCCC[NH2+].F(F)(F)(F)P(F)(F)F

$C_{15}H_{34}N.F_6P$

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

CCCC[NH2+].[OH-]

$C_{15}H_{34}N.HO$

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

CCCC[NH2+].CC[C@@H](C)C(=O)O

$C_{15}H_{34}N.C_6H_8N_3O_2$

Components: 2

Absolute stereochemistry shown

1 Reference 0 Reactions 0 Suppliers

3 1643849-82-4

CCCC[NH2+].[Cl-]

$C_{15}H_{34}N.Cl$

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

CCCC[NH2+].OS(=O)(=O)N(S(=O)(=O)F)F

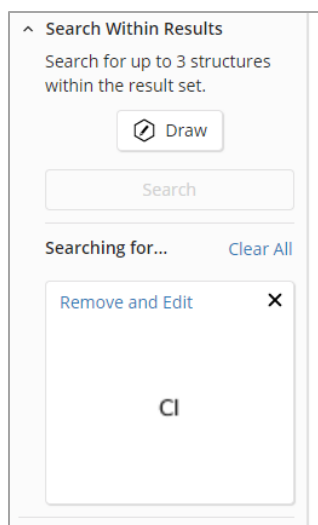
5 1190079-34-5

CCCC[NH2+].CCCCCCCCC=O

6 1092562-51-0

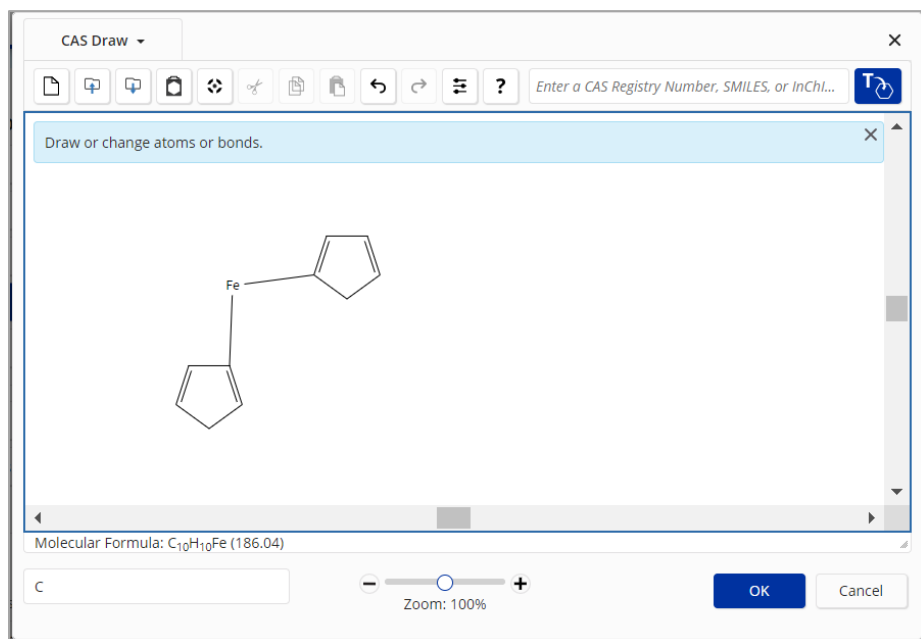
CCCC[NH2+].CC(=O)O

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 displays the CAS SciFinder search results for 'Substances' (746). The interface includes a search bar at the top, a sidebar on the left for filtering, and a main grid of results. The 'Structure Match' filter is active, with 'As Drawn (746)' selected. The results grid shows three entries:

- 2734791-01-4**: $(C_{24}H_{18} \cdot C_{10}H_{10}Fe)_x$, Components: 2. Includes 1 Reference, 0 Reactions, and 0 Suppliers.
- 2684300-23-8**: $C_{14}H_{20}O_2 \cdot Zn \cdot C_{10}H_{10}Fe$, Components: 2. Includes 1 Reference, 2 Reactions, and 0 Suppliers.
- 2635404-85-0**: $C_{20}H_{14} \cdot C_{10}H_{10}Fe$, Components: 2. Includes 1 Reference, 0 Reactions, and 0 Suppliers.

A 'Chemscape Analysis' tool is also visible in the sidebar, allowing for structure similarity analysis.

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 displays the CAS SciFinder search results for 'Substances' (746) with various filters applied. The left sidebar shows filters for 'Reference Role', 'Number of Components', 'Substance Class', 'Isotopes', 'Metals', 'Molecular Weight', 'Experimental Property', 'Experimental Spectrum', and 'Regulatory Data by Country'. The main area shows results for ferrocene and ferrocenium compounds:

- 119087-69-3**: $C_{10}H_{10}Fe$, Ferrocene, Ion(2-). Includes 1 Reference, 0 Reactions, and 0 Suppliers.
- 86549-93-1**: $C_{10}H_{10}Fe$, Ferrocenium(2+). Includes 5 References, 0 Reactions, and 0 Suppliers.
- 67269-42-5**: $C_{10}H_{10}Fe$, Ferrocene, radical ion(1-). Includes 8 References, 0 Reactions, and 0 Suppliers.
- 51937-67-8**: $(C_{10}H_{10}Fe)_x$, Ferrocene polymer. Includes 70 References, 0 Reactions, and 0 Suppliers.
- 12125-80-3**: $C_{10}H_{10}Fe$, Ferrocenium. Includes 1,235 References, 50 Reactions, and 2 Suppliers.
- 9022-10-0**: $(C_{10}H_{10}Fe)_x$, Ferrocenium, homopolymer. Includes 2 References, 0 Reactions, and 0 Suppliers.

Q20: 已知商品化农药，能否查出其靶标？已知靶标，能否查出靶向该靶标的农药？

A20:

(1) 如果已知商品化农药：通过物质检索获得农药分子后，由物质获取其研究文献，然后用已知关键词限定（如 target, receptor, channel 等），获取农药相关靶标研究文献；

(2) 如果已知靶标：通过关键词检索文献后，根据需要对文献结果进行精炼，再由文献获得物质，最后使用 substance role 筛选具有 Agricultural use 的物质。

Q21: 在农药工艺研发过程中，杂质不可避免。如何查出农药生产过程中的杂质？

A21: 推荐检索 步骤如下：

(1) 检索到农药分子后，通过物质获取其研究文献；

(2) 在结果左侧 substance role 选择 preparation 和 process，

(3) 然后用 search within results 中输入 impurities，可以获取农药生产过程中的杂质文献。

如果以上方式没有获得丰富的结果，可以尝试在获得研究文献后直接在左侧 search within results 中输入 impurities，获取该农药关于杂质的文献信息。

Q22: Substance role 的 preparation 和 process 有何不同？

A22: Preparation 包括生物工业制造、生物合成制备、副产物、（化学）工业制备、纯化回收和（化学）合成。Process 包括生化过程、地质或者天体过程、物理、工程或者化学工艺；移除或者分解等。

Q23: 如何检索特定形貌的纳米材料？例如：MoS₂ 纳米线 nanowire

A23: 方法一：直接通过关键词检索

The screenshot shows the CAS SciFinder interface for a search query "MoS2 and nanowire". The search results are displayed under the "References" tab. The top navigation bar includes the CAS SciFinder logo, a search bar with the query "MoS2 and nanowire", and icons for Draw, Search, Notifications, and User. Below the search bar, there are options for "Substances", "Reactions", "Citing", and "Knowledge Graph". The search results are sorted by "Relevance" and viewed as "Full Abstract". The first result is titled "Hydrothermal synthesis of MoS₂ nanowires" by Li, Wen-Jun; Shi, Er-Wei; Ko, Jung-Min; Chen, Zhi-zhan; Ogino, H.; Fukuda, Tsuguo, published in the Journal of Crystal Growth (2003), 250(3-4), 418-422. The abstract describes the synthesis of MoS₂ nanowires with diameters of 4 nm and lengths of 50 nm. The interface also includes a "Filter Behavior" section with "Filter by" and "Exclude" options, and a "Document Type" section with "Full Text" selected. A "Feedback" button is visible in the bottom right corner.

方法二：结构式检索，并获取文献

The screenshot shows the CAS SciFinder interface for a search query based on a drawn structure. The search results are displayed under the "Substances" tab. The top navigation bar includes the CAS SciFinder logo, a search bar with the query "Enter a query...", and icons for Edit, Search, Notifications, and User. Below the search bar, there are options for "References", "Reactions", and "Suppliers". The search results are filtered by "Number of Components: 1" and sorted by "Relevance". The first three results are displayed, each with a chemical structure diagram and a CAS number: 1317-33-5, 1309-56-4, and 12068-92-7. The chemical structure diagram shows a central Mo atom bonded to two S atoms, representing MoS₂. The interface also includes a "Structure Match" section with "As Drawn (13K)", "Substructure (36K)", and "Similarity (3,568)" options, and a "Chemscape Analysis" section. A "Feedback" button is visible in the bottom right corner.

在文献结果集中，选择 substance role: nanoscale; Concept 包含 nanowire 的结果。

← Return to Home

References from Substances

Substances ▾ Reactions ▾ Citing ▾ Knowledge Graph

Filter Behavior: Filter by Exclude

Document Type

Substance Role

- Uses (551)
- Properties (325)
- Nanoscale (316)
- Process (187)
- Preparation (164)

View All

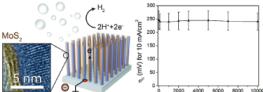
Filtering: Substance Role: Nanoscale X Concept: Nanowires X [Clear All Filters](#)

316 Results Sort: Relevance View: Full Abstract ▾

1

Core-shell MoO₃-MoS₂ Nanowires for Hydrogen Evolution: A Functional Design for Electrocatalytic Materials

By: Chen, Zhebo; Cummins, Dustin; Reinecke, Benjamin N.; Clark, Ezra; Sunkara, Mahendra K.; Jaramillo, Thomas F.
Nano Letters (2011), 11(10), 4168-4175 | Language: English, Database: CAplus and MEDLINE



The authors synthesize vertically oriented core-shell nanowires with substoichiometric MoO₃ cores of ~20-50 nm and conformal MoS₂ shells of ~2-5 nm. The core-shell architecture, produced by low-temperature sulfidization, is designed to use the best properties of each component material while mitigating their deficiencies. The substoichiometric MoO₃ core provides a high aspect ratio foundation and enables facile

Feedback

Q24: 如何画出一个化合物 A 的盐酸盐的不同比例 (1:1.5, 1:1.2, 2:3 等等) ? 就 1:1.5 和 2:3 而言, 看成相同还是不同?

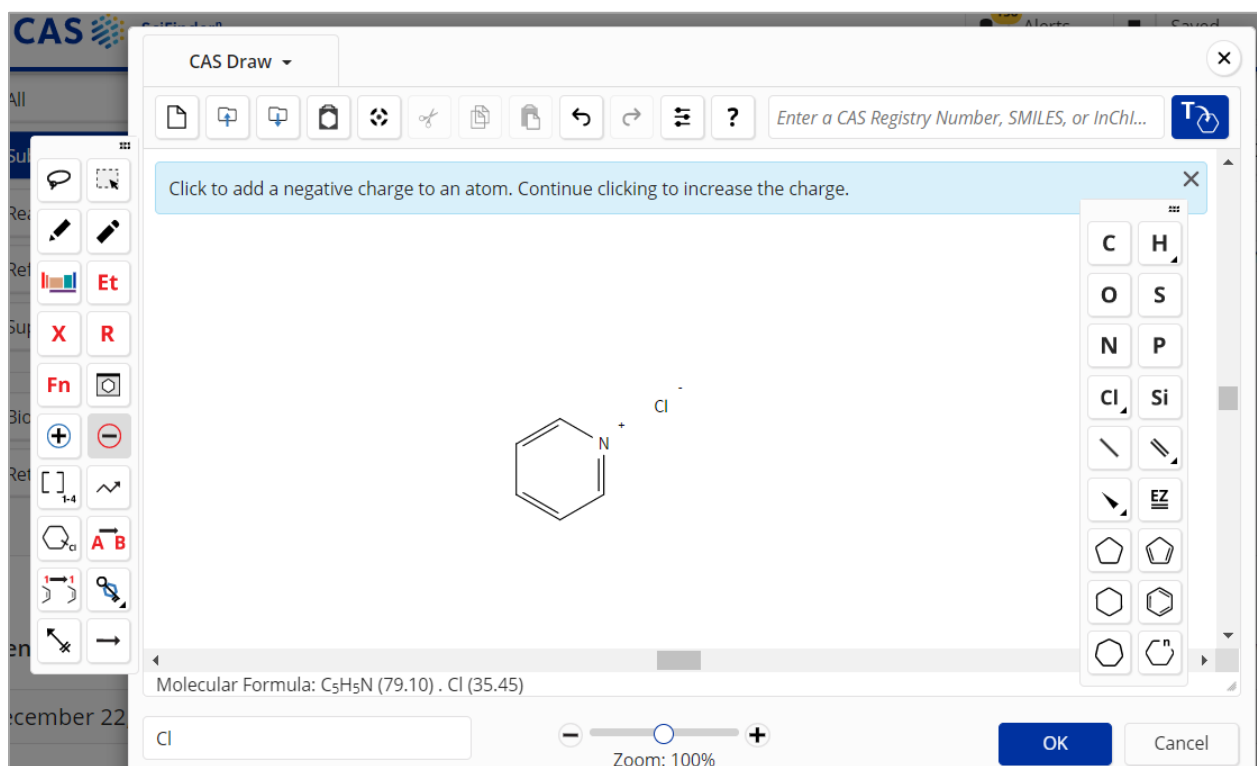
A24: 在以吡啶的盐酸盐为例。

(1) 可以通过如下结构进行物质检索

CAS Draw

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

Click to add a negative charge to an atom. Continue clicking to increase the charge.



Molecular Formula: C₅H₅N (79.10) . Cl (35.45)

Cl






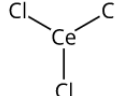

Zoom: 100%

OK Cancel

(2) 在物质结果集中，通过左侧 Substance Class，选择 Salt and compound with，限定结果为盐和组合物类。在物质结果集中可以根据结构式和名称，清楚地看到组成比例。比如，对于吡啶：盐酸比例在结构中呈现 1: 3/2 和名称中呈现的 2: 3 代表同一个物质。

The screenshot displays the CAS SciFinder search results for a drawn structure of pyridine. The search is filtered by 'Substance Class: Salt and Compound With' and 'Isotopes: Not Containing Isotopes'. The results are sorted by Relevance and shown in a grid view. Three results are visible, each with a chemical structure and associated data:

Result ID	Chemical Formula	Components	Component RN	Name	References	Reactions	Suppliers
628-13-7	$C_5H_5N.ClH$	2	110-86-1	Pyridinium chloride	2,408	10K	83
149835-57-4	$C_5H_5N.Cl$	2	110-86-1	Pyridine, compd. with at. chlorine (1:1)	8	0	0
58888-58-7	$C_5H_5N.2ClH$	2	110-86-1	Pyridine, hydrochloride (1:2)	8	0	0

<ul style="list-style-type: none"> Reference Role Commercial Availability <ul style="list-style-type: none"> <input type="checkbox"/> Available (3) <input type="checkbox"/> Not Available (97) Number of Components Molecular Weight Stereochemistry Element Substance Class <ul style="list-style-type: none"> <input checked="" type="checkbox"/> Salt and Compound With (100) <input type="checkbox"/> Coordination Compound (92) <input type="checkbox"/> Polymer (30) <input type="checkbox"/> General Derivative (1) Isotopes <ul style="list-style-type: none"> <input type="checkbox"/> Containing Isotopes (10) <input checked="" type="checkbox"/> Not Containing Isotopes (100) Metals Experimental Property Experimental Spectrum Bioactivity Indicator Target Indicator Regulatory Data by Country/Region Regulatory Data by List 	<div style="border: 1px solid #ccc; padding: 5px;"> <div style="text-align: right; margin-bottom: 5px;">4</div> <p>1210056-77-1</p>  <p>• Cl⁻</p> <p>$C_5H_5N.Cl$ Components: 2 Component RN: 110-86-1 Chloride, compd. with pyridine (1:1)</p> <p>2 References 0 Reactions 0 Suppliers</p> </div>	<div style="border: 1px solid #ccc; padding: 5px;"> <div style="text-align: right; margin-bottom: 5px;">5</div> <p>125507-59-7</p>  <p>• 6 HCl</p> <p>$C_5H_5N.6ClH$ Components: 2 Component RN: 110-86-1 Pyridine, hydrochloride (1:6)</p> <p>1 Reference 0 Reactions 0 Suppliers</p> </div>	<div style="border: 1px solid #ccc; padding: 5px;"> <div style="text-align: right; margin-bottom: 5px;">6</div> <p>125507-58-6</p>  <p>• 4 HCl</p> <p>$C_5H_5N.4ClH$ Components: 2 Component RN: 110-86-1 Pyridine, hydrochloride (1:4)</p> <p>1 Reference 0 Reactions 0 Suppliers</p> </div>
	<div style="border: 1px solid #ccc; padding: 5px;"> <div style="text-align: right; margin-bottom: 5px;">7</div> <p>45410-26-2</p>  <p>• 3/2 HCl</p> <p>$C_5H_5N.3/2ClH$ Components: 2 Component RN: 110-86-1 Pyridine, hydrochloride (2:3)</p> </div>	<div style="border: 1px solid #ccc; padding: 5px;"> <div style="text-align: right; margin-bottom: 5px;">8</div> <p>560069-18-3</p>  <p>• HCl</p> <p>$C_5H_5N.1/2ClH.1/2HI_3$ Components: 3 Hydrogen triiodide, compd. with pyridine hydrochloride (1:2:1)</p> </div>	<div style="border: 1px solid #ccc; padding: 5px;"> <div style="text-align: right; margin-bottom: 5px;">9</div> <p>227612-89-7</p>   <p>• HCl</p> <p>$C_5H_5N.1/2CeCl_3.ClH$ Components: 3 Pyridine, hydrochloride, compd. with cerium chloride (CeCl₃) (2:1)</p> </div>

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 $CH_2O_2\cdot H_2O\cdot K$)。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 search results for the query "reaction mechanism and carbon-carbon coupling". The interface includes a search bar at the top with the query and a "Draw" button. On the left, there is a "Filter Behavior" sidebar with a "Filter by" button and a list of filters. The "Concept" filter is selected, showing "Reaction mechanism (328)". The main content area shows a list of references. The first result is "Mechanism and Selectivity in Nickel-Catalyzed Cross-Electrophile Coupling of Aryl Halides with Alkyl Halides" by Biswas, Soumik; Weix, Daniel J. The abstract snippet discusses the direct cross-coupling of two different electrophiles, such as an aryl halide with an alkyl halide, and mentions the mechanism and origin of cross selectivity. The second result is "Electrochemical, Manganese-Assisted Carbon-Carbon Bond Formation between β -Keto Esters and Silyl Enol Ethers" by Strehl, Julia; Hilt, Gerhard. The abstract snippet mentions the electrochemical, manganese-assisted carbon-carbon bond formation.

(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：

CAS SciFinder[®] | References | Reaction mechanism and manganese catalyst

← Return to Home

Structure Match

As Drawn (1)

Substructure (4)

Filter Behavior

Filter by Exclude

Document Type

Journal (3)

Review (1)

Conference (1)

References (4)

Substances Reactions Citing

Edit Drawing Remove

1

Manganese-catalyzed synthesis of cis-β-amino acid esters through organometallic C-H activation of ketimines

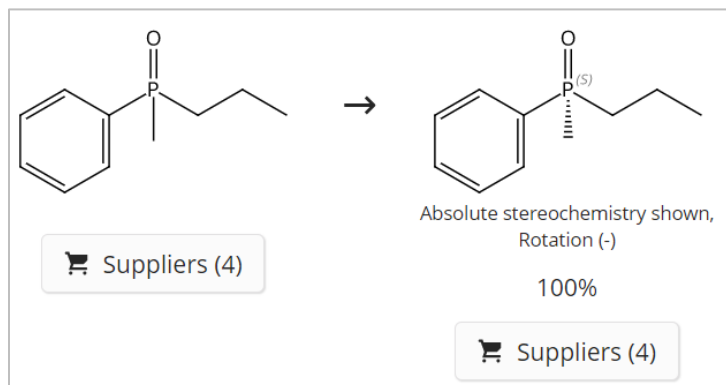
By: Liu, Weiping; Zell, Daniel; John, Michael; Ackermann, Lutz
 Angewandte Chemie, International Edition (2015), 54(13), 4092-4096 | Language: English, Database: CAplus and MEDLINE

Synthesis of cis-β-amino acid esters through manganese-catalyzed C-H site- and regioselective alkene annulations of ketimines was reported. The organometallic C-H activation occurred efficiently with high functional group tolerance, delivering densely functionalized β-amino acid derivatives with ample scope.

Full Text Substances (82) Reactions (106) Citing (118) Citation Map

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。

Return to Home

Structure Match

- As Drawn (6)
- Substructure (17K)
- Similarity (0)

Filter Behavior

Filter by Exclude

Yield

- 90-100% (1)
- 70-79% (2)
- 50-69% (1)
- No Yield Available (2)

Number of Steps

- 1 (6)

Reactions (6)

References

Scheme 1 (2 Reactions) Steps: 1 Yield: 100%

Absolute stereochemistry shown, Rotation (-)

Suppliers (3) Suppliers (4)

Reaction Summary Steps: 1 Yield: 100%

1.1 Reagents: (-)-*trans*-2,3-Bis(hydroxydiphenylmethyl)-1,4-dioxaspiro[5.4]decane
Solvents: Water; 168 h, 50 °C

Scalable Enantiomeric Separation of Dialkyl-Arylphosphine Oxides Based on Host-Guest Complexation with TADDOL-Derivatives, and their Recovery

By: Varga, Bence; et al
European Journal of Organic Chemistry (2020), 2020(12), 1840-1852

Stereochemistry

Reagent

Solvent

Commercial Availability

Reaction Notes

Search Within Results

Source Reference

Document Type

Language

Publication Year

Publication Name

CA Section

Filter Content Report

Download filter data from this result set.

Reactions (6)

Enter a query...

Scheme 2 (1 Reaction) Steps: 1 Yield: 72%

Absolute stereochemistry shown, Rotation (+)

Suppliers (3) Suppliers (6)

Reaction Summary Steps: 1 Yield: 72%

1.1 Reagents: (-)-*trans*-2,3-Bis(hydroxydiphenylmethyl)-1,4-dioxaspiro[5.4]decane
Solvents: Water; 168 h, 50 °C

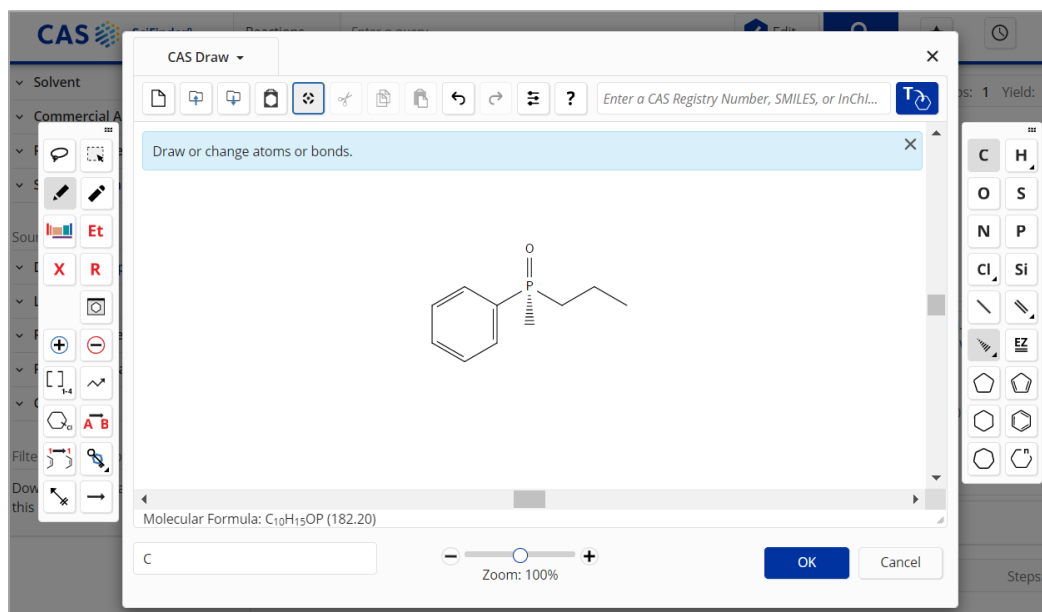
Scalable Enantiomeric Separation of Dialkyl-Arylphosphine Oxides Based on Host-Guest Complexation with TADDOL-Derivatives, and their Recovery

By: Varga, Bence; et al
European Journal of Organic Chemistry (2020), 2020(12), 1840-1852

Full Text

(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。

Reactions - 1515-99-7

Reactant (1)

Yield

Number of Steps

Reaction Type

Stereochemistry

Reagent

Solvent

Commercial Availability

Reaction Notes

Search Within Results

Search for up to 3 structures within the result set.

Draw

Search

Searching for... Clear All

Remove and Edit

Reaction 1

Scalable Enantiomeric Separation of Dialkyl-Arylphosphine Oxides Based on Host-Guest Complexation with TADDOL-Derivatives, and their Recovery

By: Varga, Bence; Herbay, Reka; Szekeley, Gyoergy; Holczbauer, Tamas; Madarasz, Janos; et al
European Journal of Organic Chemistry (2020), 2020(12), 1840-1852 | Language: English, Database: CPlus

Full Text - View 2 Related Reactions

Chemical reaction diagram showing the conversion of a phosphine oxide derivative to its enantiomer.

Absolute stereochemistry shown, Rotation (°)

Suppliers (3)

Suppliers (4)

Reaction Summary

Steps: 1 Yield: 100%

1.1 Reagents: (-)-trans-2,3-Bis(hydroxydiphenylmethyl)-1,4-dioxaspiro[5.4]decane
Solvents: Water; 168 h, 50 °C

View Reaction Detail

Reaction 2

Resolution of acyclic phosphine oxides with TADDOL- and tartaric acid derivatives

By: Varga, Bence; Csiszovszky, Anna; Bagi, Peter; Fogassy, Elemer; Keglevich, Gyorgy
Phosphorus, Sulfur and Silicon and the Related Elements (2019), 194(4-6), 556-557 | Language: English, Database: CPlus

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:

CAS Draw

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

Draw or change atoms or bonds.

Chemical structure diagram showing a palladium complex.

Molecular Formula: C₁₅H₂₁Br₂N₃Pd (509.58)

Zoom: 100%

OK Cancel

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：

The screenshot shows the CAS SciFinder search results page. The search criteria are set to "Substance Class: Coordination Compound". The results are displayed in a grid of six cards:

- Card 1:** CAS 2378047-37-9, Molecular Formula $C_{18}H_{23}Br_2N_3OPd \cdot CHCl_3$, Components: 2.
- Card 2:** CAS 2378047-32-4, Molecular Formula $C_{19}H_{22}Br_2N_4Pd \cdot CH_2Cl_2$, Components: 2.
- Card 3:** CAS 2378047-31-3, Molecular Formula $C_{18}H_{23}Br_2N_3OPd$.
- Card 4:** CAS 2378047-04-0.
- Card 5:** CAS 2378046-92-3.
- Card 6:** CAS 1350615-34-7.

Each card includes a chemical structure, a molecular formula, and a component count. The interface also features a left sidebar with filters and a top navigation bar.

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

The screenshot shows the CAS SciFinder search process. The search bar contains the text "MOFs and CO2 hydrogenation". The interface includes a search bar, a "References" section, and a "Searching for..." section with various search options.

The "References" section shows the search criteria: "MOFs and CO2 hydrogenation". The search results are displayed in a grid of six cards, each with a chemical structure, a CAS number, a molecular formula, and a component count.

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.; Choi, Kyung Min; Yaghi, Omar M.; Somorjai, Gabor A.
Nano Letters (2016), 16(12), 7645-7649 | Language: English, Database: Cplus and MEDLINE

CO2 + 3H2 >> CH3OH + H2O

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)₂] 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

Ultrascale 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: Cplus

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 ultrascale 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: 在绘制锁定的金原子以后，能不能再去添加别的结构？例如：含有金的催化剂催化降解叠氮键？

A16: 金原子锁定后不能再添加非氢结构。

如果要检索含有金催化剂降解叠氮，则推荐先检索金化合物，然后选择其作为催化剂的反应，再用叠氮结构限定结果。

CAS SciFinder® Substances

Substances search for drawn structure

References Reactions Suppliers

Structure Match: As Drawn (32K) **Substructure (98K)** Similarity (72K) Analyze Structure Precision

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

Filtering: Reaction Role: Catalyst 2,879 Results Sort: Relevance View: Partial

1 7440-57-5 **Au** Au Gold 584K 18K 959

2 16065-91-1 **Au³⁺** Au Au³⁺ 1,853 22 2

3 20681-14-5 **Au⁺** Au Gold(1+) 1,288 6 2

Reactions from Substances

References Save and Alert

Filter Behavior: Filter by Exclude

Substance Role: Product (10K) Reactant (8,719) Reagent (12K) Catalyst (106K) Solvent (1)

Yield: 0% - 100% (20K)

Filtering: Substance Role: Catalyst 106,355 Results Group: By Scheme Sort: Publication Date: Newest View: Expanded

Scheme 1 (620 Reactions) Steps: 1

Oc1ccc(cc1)N(=O)=O → Oc1ccc(cc1)N

Suppliers (124) Suppliers (97)

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

As Drawn Substructure

CAS Draw

Click a reaction participant. A list of roles appears. Click a reaction role and click OK.

N#N#N
reactant/reagent

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

References

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

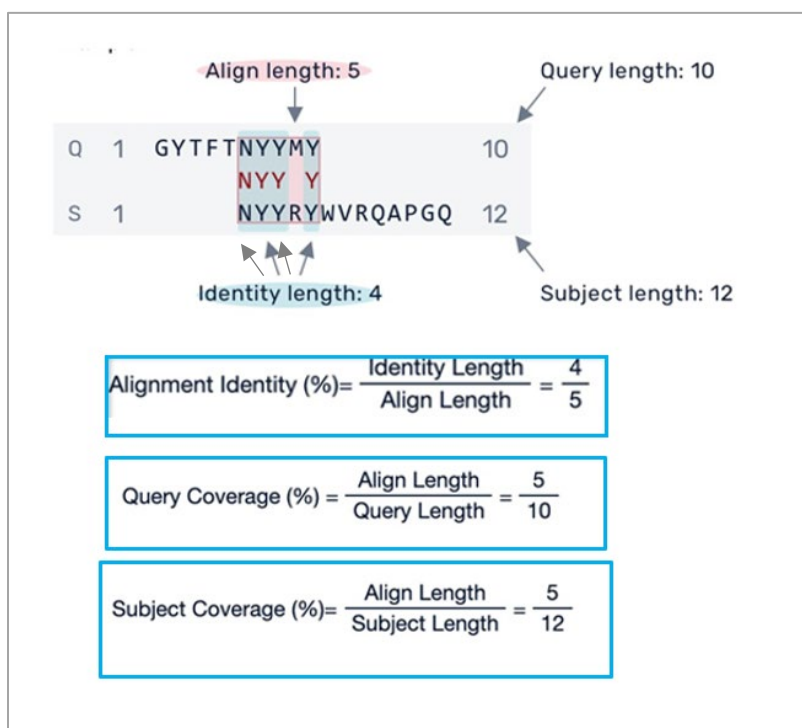
Bioscape Analysis
Visually explore sequence similarity with a new tool. Learn more about Bioscape.
[Create Bioscape Analysis](#)

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
References
Query Details > Seq 1: 1 UAUUGUGAGGAAUUUUUGUCAA 21 View More
Alignment Identity: 100%
Matches: 21
Mismatches: 0
View Less
Alignment Subject References
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。

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	auggauacu	cuugguact	t	-	-
---	-----------	-----------	---	---	---

Sequence 2: Length 21; RNA; linear

1	guaaccaaga	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

Target Indicators
 Regulatory Information
 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: CAS SciFinder® 中的 Biosequences 检索支持上传.txt 和.fasta 文件进行序列检索。其中上传的.txt 文件仅支持单条序列上传检索; 而.fasta 文件支持多条序列上传检索。最多支持同时上传 100 条序列进行检索。

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 fasta 格式，即在序列上一行添加>和序号（如下图），然后保存并关闭文件，之后，将文件后缀改为.fasta，就可以转化为含有多条序列的.fasta 文件。可以通过 upload sequence 上传.fasta 文件进行多条序列检索。

```
>NM_001
GGAGTTTATTCATAACGCGCTCTCCAAGTATACGTGGCAATGCGTTGCTGGGTATT
TTAATCATTCTAG

GCATCGTTTTCTCCTTATGCCTCTATCATTCCTCCCTATCTACACTAACATCCCAG
CTCTGAACGCGC

GCCATTAATACCTTCTTCTCCACTCTCCCTGGGACTCTTGATCAAAGCGCGGCC
CTTCCCCAGCC

>NM_002

TTAGCGAGGCGCCCTGCAGCCTGGTACGCGCGTGGCGTGGCGGTGGGCGCGCAGTG
CGTTCTCGGTGTGG

AGGGCAGCTGTTCCGCTGCGATGATTTATACTCACAGGACAAGGATGCGGTTTGTC
AAACAGTACTGCT
```

Q7: 多条 fasta 格式序列的检索，呈现的结果是与多条序列均匹配的序列，还是分别与其中一条匹配的结果？

A7: Biosequences 中支持的多条序列检索，呈现的结果是逐条分别匹配的结果。

Q8: Biosequences 检索核酸序列时，为什么查询序列和 Subject 中的目标序列不一致？比如查询序列是 TACTTGGAGAGCATCACTG，检索结果 Subject 中会出现 CAGUGAUGCUCUCCAAGUA。

A8: Biosequences 的核酸序列检索结果，会包括与检索序列匹配的序列、T 和 U 互换后匹配的序列、及其反向互补序列。

在这个例子中，BLAST nucleotide 的查询序列：TACTTGGAGAGCATCACTG (5' -3')，其反向序列 (3' -5') 为 GTCACTACGA GAGGTTTCAT；T 和 U 互换后，为 3' -GUCACUACGA GAGGUUCAU-5'，其互补序列为：5' -CAGUGAUGCUCUCCAAGUA-3'，所以这个结果会出现在 Subject 目标序列中。

```
5' CAGUGAUGCUCUCCAAGUA 3'
   |||||
3' GUCACUACGA GAGGUUCAU 5'
```

Q9: Biosequences 序列数据库中是否会包含专利全文表格里的序列、专利列表中的序列？

A9: CAS 生物序列合集中包含来自期刊、专利和 NCBI 中的序列。其中，专利中的序列会包括来自权利要求项、说明书、全文表格，以及专利申请人向专利授权机构提交的序列列表中的序列等。

例：下面截图是来自专利全文中表格里的序列。

Table 1

	A A 1	A A 2	LysR	A A 3	A A 4	A A 5	A A 6	A A 7	A A 8	A A 9	A A 10	A A 11	A A 12	A A 13	A A 14	A A 15	A A 16	A A 17	A A 18	A A 19
Exam ple 1	ASP	LE U D-PHE	LYS	G L N	G L N	G G A V	A R L P H E	G T L L A S	L R E Y S	G L Y N H										
Exam ple 2	ASP	LE U D-HomoPH E	LYS	G L N	G L N	G G A V	A R L P H E	G T L L A S	L R E Y S	G L Y N H										
Exam ple 3	ASP	LE U D-PHE	LYS	G L N	G L N	G G A V	A R L P H E	G T L L A S	L R E Y S	G L Y N H										
Exam ple 4	BH-ASP	LE U D-PHE	LYS	G L N	G L N	G G A V	A R L P H E	G T L L A S	L R E Y S	G L Y N H										
Exam ple 5	succinate	LE U D-HomoPH E	LYS	G L N	G L N	G G A V	A R L P H E	G T L L A S	L R E Y S	G L Y N H										
Exam ple 6	succinate	LE U D-HomoPH E	allosLYS	G L N	G L N	G G A V	A R L P H E	G T L L A S	L R E Y S	G L Y N H										
Exam ple 7	succinate	LE U D-HomoPH E	LYS	G L N	G L N	G G A V	A R L P H E	G T L L A S	L R E Y S	G L Y N H										
Exam ple 8	succinate	LE U D-HomoPH E	LYS	G L N	G L N	G G A V	A R L P H E	G T L L A S	L R E Y S	G L Y N H										
Exam ple 9	BH-ASP	LE U D-HomoPH E	LYS	G L N	G L N	G G A V	A R L P H E	G T L L A S	L R E Y S	G L Y N H										
Exam ple 10	succinate	LE U D-HomoPH E	allosLYS	G L N	G L N	G G A V	A R L P H E	G T L L A S	L R E Y S	G L Y N H										
Exam ple 11	succinate	LE U D-HomoPH E	LYS	G L N	G L N	G G A V	A R L P H E	G T L L A S	L R E Y S	G L Y N H										
Exam ple 12	succinate	LE U D-HomoPH E	LYS	G L N	G L N	G G A V	A R L P H E	G T L L A S	L R E Y S	G L Y N H										
Exam ple 13	succinate	LE U D-HomoPH E	LYS	G L N	G L N	G G A V	A R L P H E	G T L L A S	L R E Y S	G L Y N H										
Exam ple 14	succinate	LE U D-HomoPH E	LYS	G L N	G L N	G G A V	A R L P H E	G T L L A S	L R E Y S	G L Y N H										
Exam ple 15	succinate	LE U D-PHE	LYS	G L N	G L N	G G A V	A R L P H E	G T L L A S	L R E Y S	G L Y N H										

例：下面截图是专利申请人向专利授权机构提交的序列表中的序列。

专利 WO2004045543 中的序列 (CAS RN: 766070-31-9)

https://patentscope.wipo.int/search/en/detail.jsf?docId=WO2004045543&_cid=P11-L1XUM6-13035-1

1. WO2004045543 - FUNCTIONAL AND HYPERFUNCTIONAL SIRNA

PCT Biblio. Data Description Claims Drawings National Phase Patent Family Notices Documents

Date	Title	View	Download
30.01.2022	International Application Status Report	HTML PDF XML	PDF XML
21.03.2007	Sequence Listing	TXT	TXT ZIP XSL + TFFs
21.04.2005	Later publication of international search report (A3.16/2005)	PDF 4 p.	PDF 4 p. ZIP XSL + TFFs
03.06.2004	Initial Publication without ISR (A2.23/2004)	PDF 199 p.	PDF 199 p. ZIP XSL + TFFs

Q10: 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?

A10: 是的。下图中显示包含 2 个 CDR 和 3 个 CDR 的序列结果, 它们都出现在同一条链上。点击 Subject 即可查看目标序列信息。

CDR1
QVQLVQSGGGVWQP

CDR2
LVKDYFPEP

CDR3
TQKSLSLSPGK

427 Results

Sort: E-Value View: Expanded

Alignment Identity: 73.53%

Matches: 25
Mismatches: 9

View Less

Alignment Subject References

Alignment Data
BLAST Score: 58
E-Value: 0.000365585974

CDR1	1	QVQLVQSGGG	VWQP	14
S	1	QVQLVQSGGG	VWQP	14
CDR3	1	TQKSLSLSPG	K	11
S	440	TQKSLSLSPG	K	450

individual or intersecting CDR results.

CDR1 CDR2 CDR3

570

Apply Reset Segments

Bioscape Analysis

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

Create Bioscape Analysis

Filter by

E-Value

0 to 10⁶

Query Coverage %

0 to 100

Subject Coverage %

0 to 100

> CDR1
QVQLVQSGGGVVQP

> CDR2
LVKDYFPEP

> CDR3
TQKSLSLSPGK

570 Results Sort: E-Value View: Expanded

1 Alignment Identity: 100%

Subject 1 527

Matches: 34
Mismatches: 0

View Less

Alignment Subject References References

Alignment Data

BLAST Score: 82

E-Value: 0.006453719308

CDR1	1	QVQLVQSGGG VVQP	14
S	1	QVQLVQSGGG VVQP	14
CDR2	1	LVKDYFPEP	9
S	147	LVKDYFPEP	155
CDR3	1	TQKSLSLSPG K	11
S	439	TQKSLSLSPG K	449

individual or intersecting CDR results.

CDR1 CDR2 CDR3

570

Apply Reset Segments

Bioscape Analysis

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

Create Bioscape Analysis

Filter by

E-Value

0 to 10⁶

Query Coverage %

0 to 100

Subject Coverage %

> CDR1
QVQLVQSGGGVVQP

> CDR2
LVKDYFPEP

> CDR3
TQKSLSLSPGK

570 Results Sort: E-Value View: Expanded

Alignment Identity: 100%

CDR1 (1-14) CDR2 (1-9) CDR3 (1-11)

Subject (1-527)

Matches: 34 Mismatches: 0

View Less

Alignment Subject References

References

CAS Registry Number: -
Length: 527 aa

Sequence

```

1 QVQLVQSGGG VVQGRSLRL SCKASGYTFT RYTHHWVRQA PGKLEWIGY INPSRGYTNV NQKVKDRFTI SRDMSKNTAF
81 LQMDSLRLPED TGVYFCARYY DDHYCLDYNG QGTPVTVSSA STKGPSVFPL APSSKSTSGG TAALGCLVKD YFPEPVTVSW
161 NSGALTSGVH TFPVAVLQSSG LYSLSVVTV PSSSLGTQTY ICNVNHKPSN TKVDKKEPK SCDKTHTCP CPAPAAAGGP
241 SVFLFPPKPK DTLMISRTPE VTCVVVDVSH EDPEVKFNMY VDGVEVHNAK TKPREEQYNS TYRVSVLTV LHQDMLNGKE
321 YKCKVSNKAL PAPIEKTISK AKGQPREPQV YTLPPSREEM TKNQVSLTCL VKGFYPSDIA VEWESNGQPE NNYKTTTPVL
401 DSDGSFFLYS KLTVDKSRWQ QGNVFSCSVM HEALHNIHTQ KSLSLSPGKG GGGSGGGGSG GGGSGVTLFV ALYDYTSYNT
481 RDLSFHKGEK FQILRMEDGV WMEARSLTTG ETGYIPSNVY APVDSIQ

```

Q11: 如何获取跟抗体轻链和重链中 6 个 CDR 序列均相关的专利?

A11: 通过两次检索, 分别检索轻链和重链中的 3 个 CDR 序列; 得到两组序列结果后, 分别获取报道这些序列的专利文献; 最后使用 Combine 功能, 将同时包含这两组序列的专利文献结果取交集, 即可获得同时包含 6 个 CDR 序列的相关专利。具体操作方式如下:

方式一:

(1) 先输入抗体一条链中 3 个 CDR, 获取 3 个 CDR 均包含的序列结果集, 再点击序列结果集页面左上角 References 按钮, 获取相关专利文献结果集, 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”。

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 RASQSVSGSRFTYMH

CDR2 YASILES

CDR3 QHSWEIPPWT

Include NCBI Sequences

Limit Total Sequence Results to:

20000

Start Biosequence Search

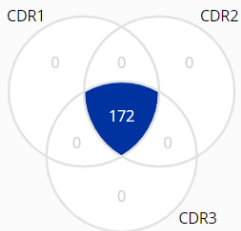


Biosequences search for your query

References

CDR Segments

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



Apply

Reset Segments

Bioscape Analysis

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

Create Bioscape Analysis

Filter by

E-Value

Query Details [View Less](#)

> CDR1
RASQSVSGSRFTYMH

> CDR2
YASILES

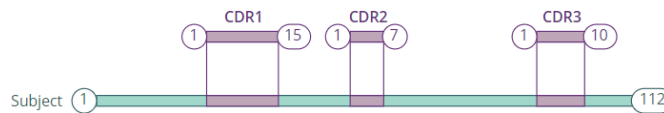
> CDR3
QHSWEIPPWT

172 Results

Sort: Alignment Identity View: Expanded

1

Alignment Identity: 100%



Matches: 32
Mismatches: 0

[View Less](#)

Alignment

Subject

References

References

Alignment Data

References from your sequence

Substances Reactions Citing

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
CDR to combine 1

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

(2) 输入抗体另一条链中 3 个 CDR，同上面操作，获取 3 个 CDR 均包含的序列结果集，再点击序列结果集页面左上角的 References 按钮，获取相关专利文献结果集。

Biosequences

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

BLAST **CDR** Motif

CDR1

CDR2

CDR3

Include NCBI Sequences

Limit Total Sequence Results to:

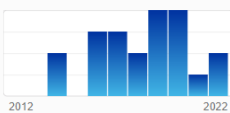
References from your sequence

Substances Reactions Citing

Filter Behavior:

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...

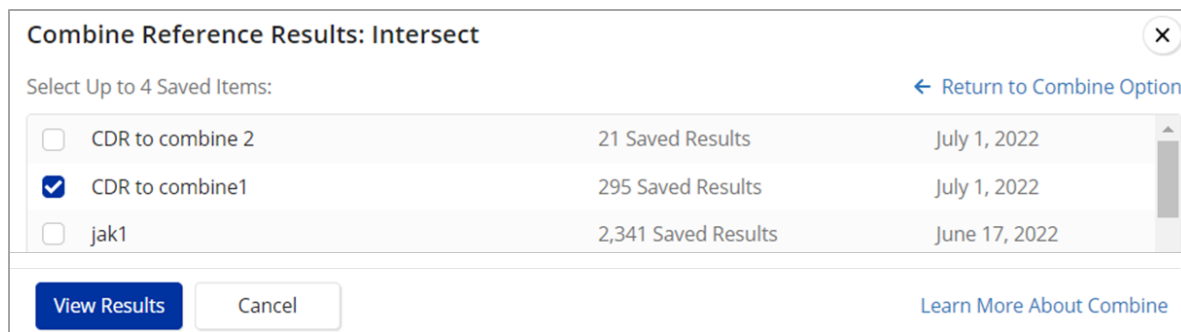
[View More](#)

(3) 在当前文献结果集页面，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”。

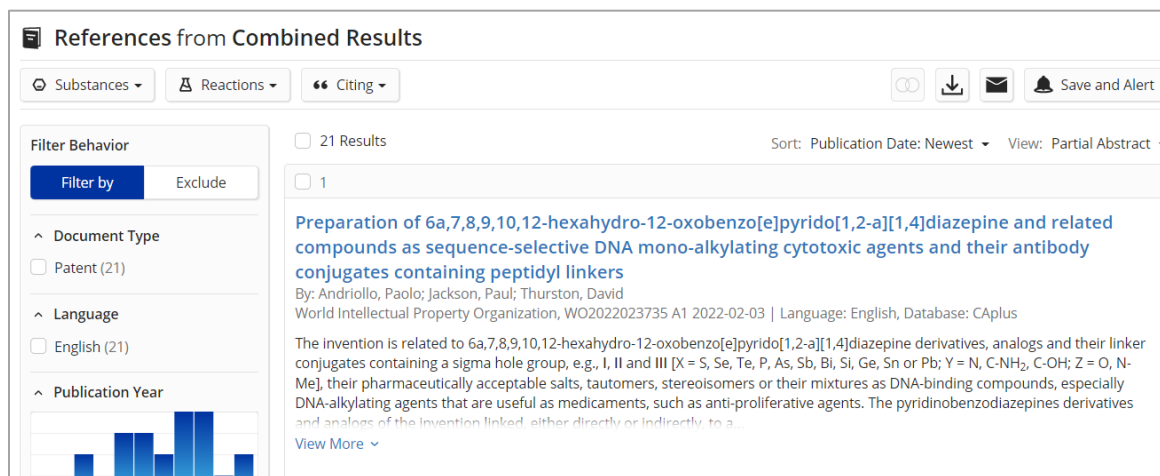
Combine Reference Results

Select a Combine Option:

[Learn More About Combine](#)



(4) 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。



方式二：利用 Biosequences 中的 CDR 检索分别检索轻链和重链中的 3 个 CDR, 分别获取 3 个 CDR 均被包含的序列结果集，再分别获取序列结果集的相关专利文献结果集，保存这 2 个专利文献结果集并命名。点击检索起始页面上方 Saved and Alerts, 在已保存结果 Saved 页面，点击 Combine Saved Results 下的 Combine, 选择 Reference, 选择 Intersect, 在弹出对话框中勾选之前保存的 2 个文献结果集，点击 View Results, 获取 2 个文献结果集的交集，即可获取到跟抗体中 6 个 CDR 序列均相关的专利文献。

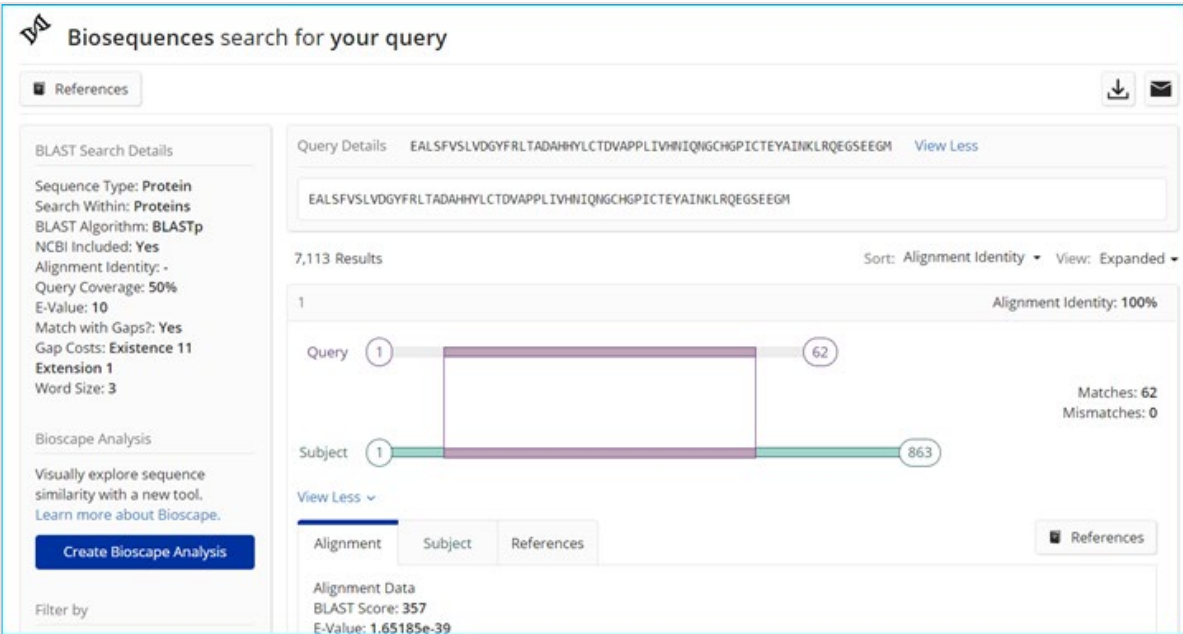
Q12: Bioscape 中可以展示指定目标公司的序列吗?

A12: 可以。具体操作如下示例。

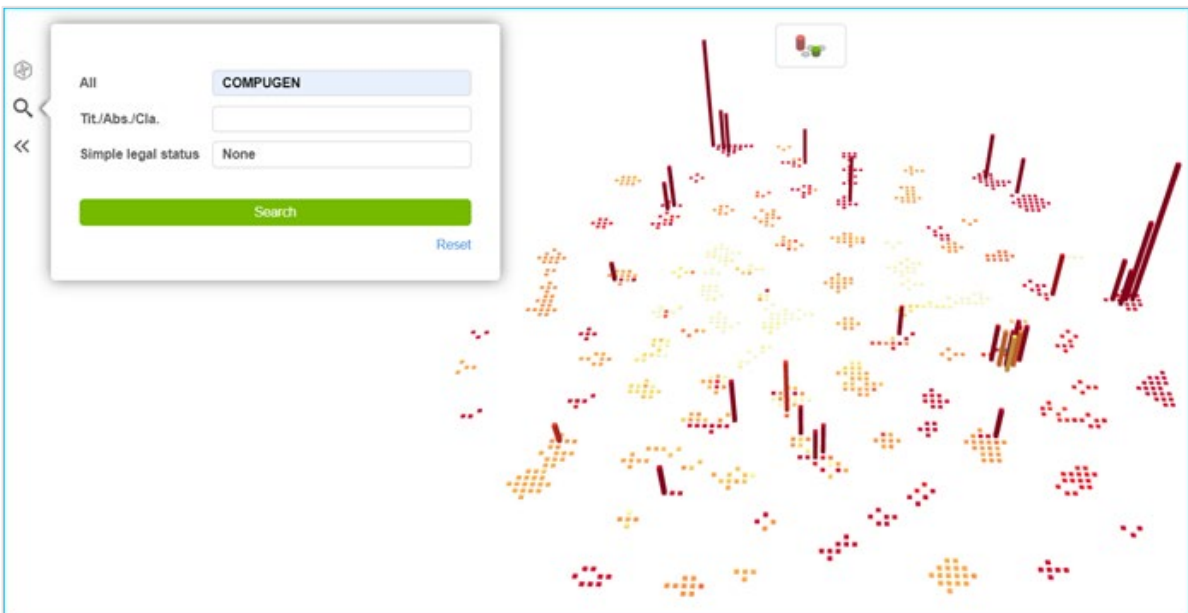
示例序列:

EALSFVSLVDGYFRLTADAHHYLCTDVAPPLIVHNIQNGCHGPICTEYAINKLRQEGSEEGM

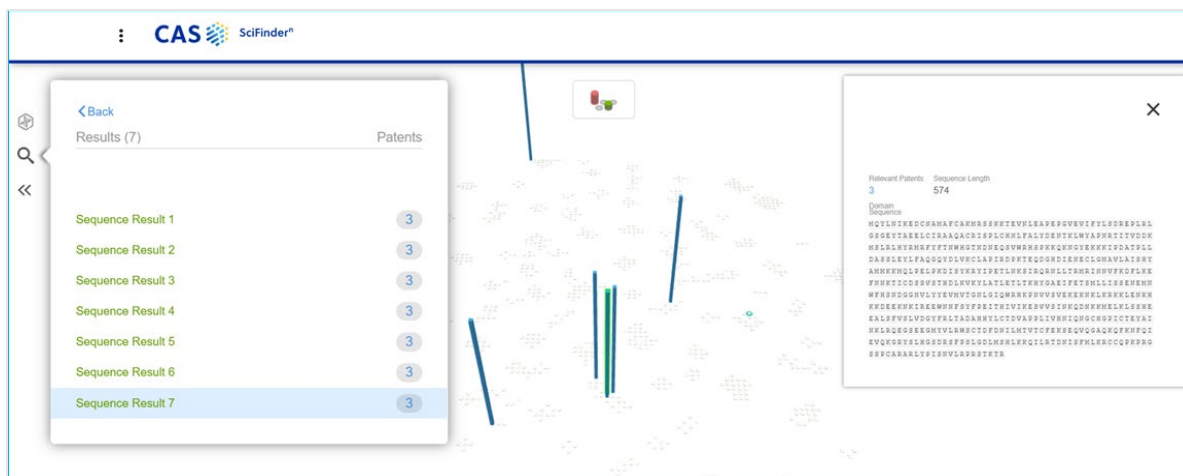
(1) 在 Biosequences 获得的序列结果集页面，点击页面左侧 Create Bioscape Analysis。



(2) 在 Bioscope 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，获得该页面上的指定公司相关结果。



(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均为指定的“Compugen”。

Q13: 如何检索非常见氨基酸?

A13: 可以使用 X 代表非天然氨基酸或非常见氨基酸。

Q14: 如何检索获取某个核苷酸药物（如 Inclisiran）被甲基化或氟代修饰的序列和文献信息？

A14: 推荐检索步骤如下：

- (1) 在 References 检索界面，主输入区输入检索式：如 (fluor* or methyl*) and Inclisiran（根据检索需求，关键词和检索式可进一步优化），进行文献检索，获取相关文献。

Searching for...

References

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

(fluor* or methyl*) and Inclisiran

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.

CAS SciFinder[®] References (fluor* or methyl*) and Inclisiran

References search for "(fluor* or methyl*) and Inclisiran"

Substances Reactions Citing

Filter Behavior Filter by Exclude

Document Type

- Journal (94)
- Patent (37)
- Review (69)
- Clinical Trial (7)
- Commentary (3)

View All

Substance Role

- Biological Study (118)
- Uses (109)
- Properties (6)
- Reactant or Reagent (6)

131 Results Sort: Relevance View: Partial Abstract

1

Inclisiran in patients at high cardiovascular risk with elevated LDL cholesterol

By: Ray, Kausik K.; Landmesser, Ulf; Leiter, Lawrence A.; Kallend, David; Dufour, Robert; Karakas, Mahir; Hall, Tim; Troquay, Roland P. T.; Turner, Tracy; Visseren, Frank L. J.; et al
New England Journal of Medicine (2017), 376(15), 1430-1440 | Language: English, Database: CAlus and MEDLINE

BACKGROUND: In a previous study, a single injection of **inclisiran**, a chem. synthesized small interfering RNA designed to target PCSK9 mRNA, was found to produce sustained reductions in low-d. lipoprotein (LDL) cholesterol levels over the course of 84 days in healthy volunteers. METHODS: We conducted a phase 2, multicenter, double-blind, placebo-controlled, multiple ascending-dose trial of **inclisiran** administered as a s.c. injection in patients at high risk for cardiovascular disease who had elevated LDL cholesterol levels. Patients were randomly assigned to receive a single dose of placebo or...

View More

Full Text Substances (3) Reactions (0) Citing (393) Citation Map

2

Inclisiran for the treatment of heterozygous familial hypercholesterolemia

- (2) 点击 Substances，获取文献结果集中报道的物质。获取物质结果集后，在物质结果集页面左侧选项 Substance class 下，选择 Nucleic acid sequence，获取核苷酸序列结果。

References search for "(fluor* or methyl*) and Inclisiran"

Substances | Reactions | Citing

Get Substances from References | 131 Results

All Results | Selected Results

Substance Class

- Organic/Inorganic Small Molecule (1,101)
- Manual Registration (378)
- Protein/Peptide Sequence (208)
- Nucleic Acid Sequence (136)
- Salt and Compound With (88)

[View All](#)

CAS SciFinder® Substances | Enter a query... | Draw | Search | Save and Alert

Substances from References

References | Reactions | Suppliers

Filter Behavior: Filter by | Exclude

Filtering: Substance Class: Nucleic Acid Sequence | Clear All Filters

136 Results | Sort: Relevance | View: Partial

Item	CAS RN	Substance Class	Sequence Length	References	Reactions	Supplier
1	1639324-58-5	Unspecified Nucleic Acid Sequence	44	111	0	1
2	1000120-98-8	Unspecified Nucleic Acid Sequence	20	226	0	1
3	915430-78-3	Unspecified Nucleic Acid Sequence	20	58	1	1
4	929881-05-0	Image Not Available				
5	1258984-36-9	Image Not Available				
6	1173755-55-9	Image Not Available				

(3) 点击 CAS RN 获取每个序列的物质详情来查看其具体修饰信息；也可利用 ctrl+F 输入 fluoro 或 methyl 等，在科学家提供的物质索引名中先做筛选。在物质详情页面，Sequence Details 下的 Sequence Modifications 中查看具体序列修饰信息，包括修饰的类型、位点及详情。

CAS SciFinder® Substances 1/19

Substances from References

References Reactions Suppliers Save and Alert

Filter Behavior: Filter by Exclude

Filtering: Substance Class: Nucleic Acid Sequence Clear All Filters

136 Results Sort: Relevance View: Partial

<input type="checkbox"/> 1 1639324-58-5 Image Not Available Unspecified RNA, (Am-s ^p -(2'-deoxy-2'-fluoro)C-s ^p -Am-(2'-deoxy-2'-fluoro)A-(2'-deoxy-2'-fluor... Nucleic Acid Sequence Sequence Length: 44 111 References 0 Reactions 1 Supplier	<input type="checkbox"/> 2 1000120-98-8 Image Not Available Unspecified DNA d(P-thio)([2'-O-(2-methoxyethyl)]rG-[2'-O-(2-methoxyethyl)]m ³ rC-[2'-O-(2-met... Nucleic Acid Sequence Sequence Length: 20 226 References 0 Reactions 1 Supplier	<input type="checkbox"/> 3 915430-78-3 Image Not Available Unspecified DNA d(P-thio)([2'-O-(2-methoxyethyl)]A-[2'-O-(2-methoxyethyl)]rG-[2'-O-(2-metho... Nucleic Acid Sequence Sequence Length: 20 58 References 1 Reaction 1 Supplier
<input type="checkbox"/> 4 929881-05-0 Image Not Available Unspecified DNA (synthetic adeno-associated virus 1... Nucleic Acid Sequence Sequence Length: 44 111 References 0 Reactions 1 Supplier	<input type="checkbox"/> 5 1258984-36-9 Image Not Available Unspecified DNA [2'-O-(2-methoxyethyl)P-thioYm ⁵ L... Nucleic Acid Sequence Sequence Length: 20 226 References 0 Reactions 1 Supplier	<input type="checkbox"/> 6 1173755-55-9 Image Not Available Unspecified RNA [P-deoxy-P-(dimethylamino)(2'-3'-... Nucleic Acid Sequence Sequence Length: 20 58 References 1 Reaction 1 Supplier

136 Results

1

1639324-58-5

Image Not Available

Unspecified
 RNA, (Am-s^p-(2'-deoxy-2'-fluoro)C-s^p-Am-(2'-deoxy-2'-fluoro)A-(2'-deoxy-2'-fluor...
 Nucleic Acid Sequence
 Sequence Length: 44

111 References 0 Reactions 1 Supplier

CAS SciFinder®		
Substances ▾ Enter a query...		Draw 🔍 🔔 ⌚ 👤
modified base	strand 2 cytidine-15	cm
modified base	strand 2 uridine-16	um
modified base	strand 2 uridine-17	um
modified base	strand 2 uridine-18	um
modified base	strand 2 uridine-19	um
modified base	strand 2 guanosine-20	gm
modified base	strand 2 uridine-21	um
modified base	strand 2 uridine-21	3'-ester
modified base	strand 2 uridine-21	3'-glycosylated
modified link	strand 1 adenosine-1 to strand 1 cytidine-2	P-thio
modified link	strand 1 cytidine-2 to strand 1 adenosine-3	P-thio
modified link	strand 1 guanosine-21 to strand 1 adenosine-22	P-thio
modified link	strand 1 adenosine-22 to strand 1 adenosine-23	P-thio
modified link	strand 2 cytidine-1 to strand 2 uridine-2	P-thio
modified link	strand 2 uridine-2 to strand 2 adenosine-3	P-thio
DNA-containing	strand 2 thymidine-11	dt
▼ Target Indicators		
▼ Regulatory Information		
▼ Additional Details		

Q15: 已知 ADC 的抗体序列，如何检索获取针对某个靶点的含有该抗体的 ADC 相关专利？

A15: 推荐检索步骤如下：

(1) Biosequences 的 BLAST 标签页下，输入抗体序列，进行 BLAST 检索，获取序列结果集。

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

```
EVQLVESGGGLVQPGGSLRLSCAASGFNIKDTYIHWVRQAPGKGLEWVARIYPTNGYTRYADSVKGRFTISADTSKNTAY
LQMNLSRAEDTAVYYCSRWGGDFYAMDYWGQGLTVTVSSASTKGPVFPPLAPS5KSTSGGTAALGCLVKDYFPEPVTVS
WNSGALTSVHTFPAVLQSSGLYSLSSVITVPSSSLGTQTYICNVIHHPKSNITKVDKVEPKSCDKTHTCPPAPPELLGG
PSVFLFPPKPKDTLHISRTPEVTCVVVDVSHEDPEVKFNHYVDGVEVHNAKTKPREEQYNSTYRVVSVLTVLHQDWLNGK
EYKCKVSNKALPAPIEKTISKAKGQPREPQVYTLPPSREEMTKNQVSLTCLVKGFYPSDIAVEHESNGQPENNYKTTTPV
LDSGDGFFLYSKLTVDKSRWQQGNVFNFSVSNMHEALHNHYTQKLSLSLSPGK
```

抗体序列

Sequence Type: Nucleotide Protein

Search Within: Nucleotides Proteins

Include NCBI Sequences

Limit Total Sequence Results to: 1000

Start Biosequence Search

[Advanced Biosequence Search](#)

BLAST Search Details

Sequence Type: Protein
Search Within: Proteins
BLAST Algorithm: BLASTp-fast
NCBI Included: No
Alignment Identity: -
Query Coverage: 100%
E-Value: 10^6
Match with Gaps?: No
Gap Costs: Existence 11
Extension 1
Word Size: 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

Query Details EVQLVESGGGLVQPGGSLRLSCAASGFNIKDTYIHWVRQAPGKGLEWVARIYPTNGYTRYADSVKGRFTISADTSKNTAYLQMN... [View More](#)

50 Results Sort: Alignment Identity View: Collapsed

1 Alignment Identity: 100%

Query 1 450

Subject 1 643

Matches: 450
Mismatches: 0

View More

2 Alignment Identity: 100%

Query 1 450

Subject 1 729

Matches: 450
Mismatches: 0

View More

3 Alignment Identity: 100%

Query 1 450

Subject 1 711

Matches: 450
Mismatches: 0

(2) 调整筛选选项：Query coverage、Subject coverage、Alignment identity 设置为 100 to 100，获取与查询序列长度相同且序列一致性为 100%的序列结果。

Filter by

^ E-Value
 to

^ Query Coverage %
 to

^ Subject Coverage %
 to

^ Alignment Identity %
 to

^ Sequence Length
 to

1 Alignment Identity: 100%

Query 1 450

Subject 1 450

Matches: 450
Mismatches: 0

[View Less](#) ▾

Alignment Subject References

References

Alignment Data
 BLAST Score: 2412
 E-Value: 0

Q	1	EVQLVESGGG	LVQPGGSLRL	SCAASGFNIK	DTYIHWRQA	PGKGLEWVAR	IYPTNGYTRY	ADSVKGRFTI	70
S	1	EVQLVESGGG	LVQPGGSLRL	SCAASGFNIK	DTYIHWRQA	PGKGLEWVAR	IYPTNGYTRY	ADSVKGRFTI	70
Q	71	SADTSKNTAY	LQMNSLRAED	TAVYYCSRWG	GDGFYAMDYW	GQGLLTVSS	ASTKGPSVFP	LAPSSKSTSG	140
S	71	SADTSKNTAY	LQMNSLRAED	TAVYYCSRWG	GDGFYAMDYW	GQGLLTVSS	ASTKGPSVFP	LAPSSKSTSG	140
Q	141	GTAALGCLVK	DYFPEPVTVS	WNSGALTSKV	HTFPAVLQSS	GLYSLSSVVT	VPSSSLGTQT	YICNVNHKPS	210
S	141	GTAALGCLVK	DYFPEPVTVS	WNSGALTSKV	HTFPAVLQSS	GLYSLSSVVT	VPSSSLGTQT	YICNVNHKPS	210

(3) 点击该条序列结果的 References 按钮，获取披露该条序列结果的相关文献结果集。

References from your sequence

Substances Reactions Citing

Filter Behavior: Filter by Exclude

Document Type: Journal (8,699), Patent (6,911), Review (2,065), Book (1), Clinical Trial (914)

Language

Publication Year: 1992 to 2022

15,775 Results | Sort: Publication Date: Newest | View: Partial Abstract

1

Variable-heavy (VH) families influencing IgA1&2 engagement to the antigen, FcαRI and superantigen proteins G, A, and L

By: Ling, Wei-Li; Su, Chinh Tran-To; Lua, Wai-Heng; Yeo, Joshua Yi; Poh, Jun-Jie; Ng, Yuen-Ling; Wipat, Anil; Gan, Samuel Ken-En
Scientific Reports (2022), 12(1), 6510 | Language: English, Database: CAplus and MEDLINE

Interest in IgA as an alternative antibody format has increased over the years with much remaining to be investigated in relation to interactions with immune cells. Considering the recent whole antibody investigations showing significant distal effects between the variable (V) and constant (C)- regions that can be mitigated by the hinge regions of both human IgA subtypes A1 and A2, we performed an in-depth mechanistic investigation using a panel of 28 IgA1s and A2s of both Trastuzumab and Pertuzumab models. FcαRI binding were found to be mitigated by the differing glycosylation patterns in IgA...

View More

Full Text

Substances (2) Reactions (0) Citing (0) Citation Map

2

Surfaceome analyses uncover CD98hc as an antibody drug-conjugate target in triple negative breast cancer

By: Montero, Juan Carlos; Calvo-Jimenez, Elisa; del Carmen, Sofia; Abad, Mar; Ocana, Alberto; Pandiella, Atanasio

(4) 利用文献的二次检索功能 Search within results, 输入 conjugate, 获取 ADC 相关文献。

Search Within Results

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

conjugate

Search

References from your sequence

Substances Reactions Citing

Filter Behavior: Filter by Exclude

Document Type: Journal (960), Patent (1,573), Review (194), Clinical Trial (48), Commentary (10)

Language

Publication Year: 1999 to 2022

Filtering: Search Within Results: conjugate X | Clear All Filters

2,561 Results | Sort: Times Cited | View: Partial Abstract

1

Trastuzumab emtansine for HER2-positive advanced breast cancer

By: Verma, Sunil; Miles, David; Gianni, Luca; Krop, Ian E.; Welslau, Manfred; Baselga, Jose; Pegram, Mark; Oh, Do-Youn; Dieras, Veronique; Guardino, Ellie; et al
New England Journal of Medicine (2012), 367(19), 1783-1791 | Language: English, Database: CAplus and MEDLINE

BACKGROUND: Trastuzumab emtansine (T-DM1) is an antibody-drug conjugate incorporating the human epidermal growth factor receptor 2 (HER2)-targeted antitumor properties of trastuzumab with the cytotoxic activity of the microtubule-inhibitory agent DM1. The antibody and the cytotoxic agent are conjugated by means of a stable linker. METHODS: We randomly assigned patients with HER2-pos. advanced breast cancer, who had previously been treated with trastuzumab and a taxane, to T-DM1 or lapatinib plus capecitabine. The primary end points were progression-free survival (as assessed by independent rev...

View More

Full Text

Substances (8) Reactions (0) Citing (1,840) Citation Map

2

Site-specific conjugation of a cytotoxic drug to an antibody improves the therapeutic index

(5) 利用 Concept 聚焦目标靶点相关文献，也可用 Concept 对话框中的 search 功能，输入目标靶点，获取相关文献。

Concept

Top Count Alphanumeric Search

2 Selected

<input type="checkbox"/> Homo sapiens (2,162)	<input type="checkbox"/> Single-chain antibodies (298)	<input type="checkbox"/> Autoimmune disease (218)
<input type="checkbox"/> Human (2,162)	<input type="checkbox"/> Colorectal neoplasm (287)	<input type="checkbox"/> Passive immunotherapy (218)
<input type="checkbox"/> Antitumor agents (1,608)	<input type="checkbox"/> Tumor antigens (285)	<input type="checkbox"/> ERBB2 protein, human (217)
<input checked="" type="checkbox"/> Epidermal growth factor receptor HER2 (1,214)	<input type="checkbox"/> Kidney neoplasm (283)	<input type="checkbox"/> Immunoglobulin Fab fragments (216)
<input type="checkbox"/> Immunoconjugates (1,070)	<input type="checkbox"/> Colon neoplasm (281)	<input checked="" type="checkbox"/> Epidermal growth factor receptor HER3 (214)
<input type="checkbox"/> Mammary gland neoplasm (1,055)	<input type="checkbox"/> Radionuclides (278)	<input type="checkbox"/> Uterine cervical neoplasm (213)
<input type="checkbox"/> Neoplasm (1,020)	<input type="checkbox"/> Drugs (273)	<input type="checkbox"/> Sialic acid-binding Ig-like lectin 2 (210)
<input type="checkbox"/> Antibodies and Immunoglobulins (1,000)	<input type="checkbox"/> Immunotoxins (272)	<input type="checkbox"/> Carcinoembryonic antigen (208)
<input type="checkbox"/> Monoclonal antibodies (719)	<input type="checkbox"/> Linking agents (272)	
	<input type="checkbox"/> Breast Neoplasms (264)	
	<input type="checkbox"/> Cytotoxic agents (263)	

Apply Cancel

Concept

Top Count Alphanumeric Search

Concept Name

HER2 Search

1 Selected

<input checked="" type="checkbox"/> Epidermal growth factor receptor HER2 (1,214)	<input type="checkbox"/> Tyrosine kinase HER2 inhibitors (20)
---	---

Apply Cancel

(6) 或者在 Search within results 中输入目标靶点，获取相关文献。

The screenshot displays the CAS SciFinder interface. At the top, there is a navigation bar with the CAS SciFinder logo, a search bar, and various utility icons. Below this, a 'Search Within Results' panel is shown, containing a text input field with 'HER2', a 'Search' button, and a 'Searching for...' section with 'conjugate' and a clear button. The main search results area shows a filter for 'Search Within Results: 2 Selected' with 'conjugate' and 'HER2' selected. The first result is titled 'Combination radioimmunotherapy and CD47 blockade in the treatment of cancer' by Ludwig, Dale L.; Seth, Sandesh; Diamond, Paul. The second result is titled 'N-Arylpropanamides and their pharmaceutical compositions for treating breast cancers and methods for preparation'.

Q16: Biosequences BLAST 支持的生物序列输入格式包括哪些?

A16: Biosequences BLAST 支持的生物序列输入格式包括: Plain、FASTA、EMBL、GCG 和 Genbank 格式。

Q17: . Biosequences 输入的查询序列和结果序列都是按 5' 到 3' 方向吗?

A17: 是。Biosequences 输入的查询序列需按 5' 至 3' 方向, 且序列结果也是按 5' 至 3' 方向呈现。如序列 5' -GUGUGCACUUCGCUUCACA-3' , 以 GUGUGCACUUCGCUUCACA 输入。

Q18: Biosequences 支持检索反向互补序列吗?

A18: Biosequences 检索结果中会包括匹配的反向互补序列结果。需点击检索结果的 Subject 标签呈现。如序列 GUGUGCACUUCGCUUCACA

4

Query ① 19

Subject ① 19

View Less ▾

Alignment Subject References

CAS Registry Number: [2752485-88-2](#)

Length: 19 nt

Organisms: **synthetic construct**

Sequence

1 UGUGAAGCGA AGUGCACAC

Q19: 如何检索化学修饰序列?

A19: 修饰的核苷酸用未修饰的核苷酸代表字母进行检索即可, 如: Af (2'-fluoro A) 用 A 或 a 替代即可。

如序列 5'-guguGfcAfCfUfucgcuucaca-3'用 GUGUGCACUUCGCUUCACA 输入检索框进行检索。点击检索结果的 CAS RN 在物质详情页面 Sequence Details 中的 Sequence Modifications 下查看序列修饰详细信息。

Biosequences

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

BLAST

CDR

Motif

Clear Search

GUGUGCACUUCGCUUCACA

1

Alignment Identity: 100%



Matches: 19
Mismatches: 0

View Less ▾

Alignment

Subject

References

References

CAS Registry Numbers: [2248790-18-1](#), [2446948-23-6](#), [1931161-35-1](#), [1931161-37-3](#), [2757128-70-2](#), [2544429-61-8](#), [1932520-84-7](#), [1931970-41-0](#), [1929628-34-1](#), [2752485-87-1](#), [2084173-08-8](#), [2083702-86-5](#), [2411359-79-8](#), [2084173-10-2](#), [2249831-07-8](#), [2649494-20-0](#), [2349433-86-7](#), [2755744-11-5](#), [2648009-64-5](#), [2648009-53-2](#)

Length: 19 nt

Organisms: synthetic construct

Sequence

1 GUGUGCACUU CGCUUCACA

Sequence Details

Sequence: RNA; linear

1 gugugcacuu cgcuucaca - - -

Sequence Modifications

Type	Location	Description
modified base	guanosine-1	gm
modified base	uridine-2	um
modified base	guanosine-3	gm
modified base	uridine-4	um
modified base	guanosine-5	2'-fl
modified base	guanosine-5	2'-deoxy
modified base	cytidine-6	cm
modified base	adenosine-7	2'-deoxy
modified base	adenosine-7	2'-fl

Q20: 检索 siRNA 序列，如何获取短序列，排除长序列（如基因组序列等）？

A20: 利用 Sequence Length 筛选目标长度的短序列。

如下图获得的 17857 个序列结果，长度范围分布在 18nt-236303nt，除了短序列还包含基因组序列等。可利用 Sequence Length 设置目标序列长度区间，来获取目标长度的序列。

如 Sequence Length 设置为 18-30，获取到 166 个短目标序列。

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

- Query Details:** Seq 1: 1 GUGUGACAUUCGCUUCACA 19. 17,857 Results. Sort: Alignment Identity. View: Expanded.
- Sequence Length Filter:** A slider set from 18 to 236303, with input boxes for 18 and 236303.
- Alignment 1:** Shows a query sequence (1-19) aligned to a subject sequence (1-23). Matched regions are highlighted in purple. Statistics: Matches: 19, Mismatches: 0.
- Alignment 2:** Shows a query sequence (1-19) aligned to a subject sequence (1-23). Matched regions are highlighted in purple.
- Alignment Data for Alignment 1:**

```
Alignment Data
BLAST Score: 19
E-Value: 0.0246955
Q      1  GTGTGCACTT  CGCTTCACA  19
      |||
S      19 GTGTGCACTT  CGCTTCACA  37
```
- Filters (left sidebar):**
 - Sequence Type: Nucleotide
 - NCBI Included: Yes
 - Query Coverage: 90%
 - E-Value: 10
 - Filter by:
 - E-Value: 0 to 10⁶
 - Query Coverage %: 0 to 100
 - Subject Coverage %: 0 to 100
 - Alignment Identity %: 0 to 100
 - Sequence Length: 18 to 30

Q21: 如何根据酶催化反应的底物或产物，快速获取作为反应催化剂的生物酶序列?

A21: 可利用反应检索及科学家标引的反应信息快捷获取

(1) 在结构编辑器中，绘制（上传结构文件、或利用 CAS RN、SMILES 或 InChI 编码输入结构）酶催化反应的产物或底物结构，并设定该结构的反应角色，执行反应检索，获取相关反应。以下图产物结构为例：

(如已知底物或产物名称、CAS RN 等信息，亦可用文本检索，获取相关反应；之后在反应结果集中限定 substance role 为 product 或 reactant。)

The image shows two screenshots from the CAS SciFinder interface. The top screenshot is the 'CAS Draw' window, which is used for drawing chemical structures. It features a toolbar with various drawing tools, a search bar for CAS Registry Number, SMILES, or InChI, and a central canvas where the chemical structure of N-methylbenzylamine is drawn. The structure consists of a benzene ring attached to a CH2 group, which is further attached to a CH group bonded to a nitrogen atom (N). The molecular formula is shown as C₈H₁₁N (121.18). The bottom screenshot shows the search results interface. On the left, there is a 'Searching for...' sidebar with options like All, Substances, Reactions (selected), References, Suppliers, Biosequences, and Retrosynthesis. The main area is titled 'Reactions' and includes a search bar with the text 'Enter a query...'. Below the search bar, there is a preview of the chemical structure drawn in the top screenshot, with 'Edit Drawing' and 'Remove' buttons.

(2) 在反应结果集筛选项 Reaction Notes 下选择 Biotransformation 和 Enzyme 选项，来获取生物转化或酶参与的反应。

Structure Match

As Drawn (11K)

Substructure (7.7M)

Filter Behavior

Filter by Exclude

- Yield
- Number of Steps
- Non-Participating Functional Groups
- Reaction Mapping
- Experimental Protocols
- Reaction Type
- Stereochemistry
- Reagent
- Catalyst
- Solvent
- Commercial Availability
- Reaction Notes
 - Stereoselective (4,771)
 - Biotransformation (2,383)
 - Enzymic (2,342)
 - Regioselective (433)

Filtering: Stereochemistry: 2 Selected X Reaction Notes: 2 Selected X Clear All Filter

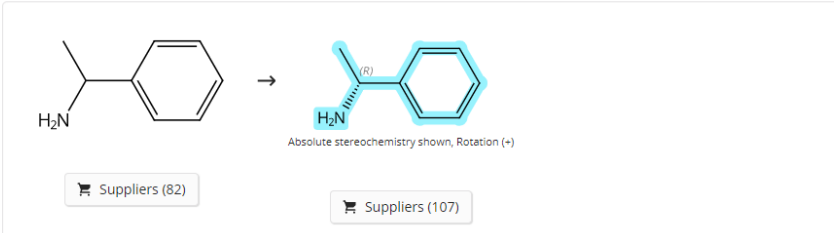
2,383 Results Group: By Document Sort: Publication Date: Oldest View: Expanded

1

Manufacture of optically active α -methylbenzylamine with bacteria

By: Mochida, Kenichi; Uejima, Takayuki
Japan, JP01174398 A 1989-07-10 | Language: Japanese, Database: CAplus

Full Text View 14 Related Reactions



31-614-CAS-27920956 Steps: 1

No Data Available

2

Enantiomeric enrichment and stereoselective synthesis of chiral amines using co-amino acid transaminase

By: Stirling, David I.; Zeitlin, Andrew L.; Matcham, George W.
United States, US4950606 A 1990-08-21 | Language: English, Database: CAplus

PatentPak Full Text View 3 Related Reactions

或者，亦可在反应结果集筛选项 Catalyst 下选择目标酶类相关选项，来获取特定酶类作为催化剂的反应。（本示例执行步骤 3-7 之前未勾选 Catalyst 下选项）

^ Catalyst

- Omega transaminase (2,074)
- Palladium (382)
- p*-Toluenesulfonic acid (347)
- 4-(Dimethylamino)pyridine (153)
- (OC-6-22)-Bis(acetato- κ O, κ O') [1,1'-[(3S)-2,2',5,5'-tetramethyl [3,3'-bithiophene]-4,4'-diyl]bis [1,1-diphenylphosphine- κ P]] ruthenium (112)
- Triacylglycerol lipase (84)
- Aminotransferase (14)
- Diamine aminotransferase (14)

View All

点击 View All，查看更多作为反应催化剂的酶类。

Catalyst

Top Count | Alphanumeric | Search

4 Selected

<input checked="" type="checkbox"/> Omega transaminase (2,074)	<input type="checkbox"/> Platinum (20)	<input type="checkbox"/> Isopropanol (9)
<input type="checkbox"/> Palladium (382)	<input type="checkbox"/> Triruthenium dodecacarbonyl (20)	<input type="checkbox"/> NAD (9)
<input type="checkbox"/> <i>p</i> -Toluenesulfonic acid (347)	<input type="checkbox"/> Nickel (18)	<input type="checkbox"/> Potassium hydroxide (9)
<input type="checkbox"/> 4-(Dimethylamino)pyridine (153)	<input type="checkbox"/> Potassium <i>tert</i> -butoxide (17)	<input type="checkbox"/> Sodium tungsten oxide (Na ₂ WO ₄) (9)
<input type="checkbox"/> (OC-6-22)-Bis(acetato-κO,κO') [1,1'-[(3S)-2,2',5,5'-tetramethyl [3,3'-bithiophene]-4,4'-diyl]bis [1,1-diphenylphosphine-κP]] ruthenium (112)	<input type="checkbox"/> Tetrabutylammonium bromide (16)	<input type="checkbox"/> Trifluoroacetic acid (9)
<input type="checkbox"/> Tetrakis(triphenylphosphine) palladium (111)	<input type="checkbox"/> Titanium tetrachloride (16)	<input type="checkbox"/> 1,1'-[(4S)-2,2,2',2'-Tetramethyl [4,4'-bi-1,3-benzodioxole]-5,5'-diyl]bis[1,1-diphenylphosphine] (8)
<input type="checkbox"/> Cuprous chloride (87)	<input type="checkbox"/> 1,1'-(4S)-[4,4'-Bi-1,3-benzodioxole]-5,5'-diylbis[1,1-bis[3,5-bis(1,1-dimethylethyl)-4-methoxyphenyl]phosphine] (15)	<input type="checkbox"/> 1,1'-Bis[(11bS)-3,5-dihydro-4 <i>H</i> -dinaphtho[2,1-c:1',2'-e]phosphinepin-4-yl]ferrocene (8)
<input checked="" type="checkbox"/> Triacylglycerol lipase (84)	<input type="checkbox"/> (+)-BINOL (15)	<input type="checkbox"/> (4S)-4-(1-Methylethyl)-5,5-diphenyl-1,3,2-oxazaborolidine (8)
<input type="checkbox"/> Palladium dihydroxide (54)	<input checked="" type="checkbox"/> Aminotransferase (14)	<input type="checkbox"/> Acetic acid (8)
<input type="checkbox"/> (SP-4-2)-Chlorotris(triphenyl phosphine)rhodium (47)	<input type="checkbox"/> Borane (14)	<input type="checkbox"/> Bis(η ⁶ -benzene)di-μ-chlorodiclororuthenium (8)
<input type="checkbox"/> Lipase CalB (Candida antarctica) (44)	<input checked="" type="checkbox"/> Diamine aminotransferase (14)	

Apply | Cancel

(3) 获取反应结果集关联的文献

Reactions search for drawn structure

References

Get References for Reactions

All Results | Selected Results

Substructure (7.7M)

Filter Behavior

Filter by | Exclude

Yield

Number of Steps

Non-Participating Functional Groups

Reaction Mapping

Experimental Protocols

Filtering: Stereochemistry: 2 Selected | Reaction Notes: 2 Selected | Clear All Filters

2,383 Results

Group: By Document | Sort: Publication Date: Oldest | View: Expanded

1

Manufacture of optically active α-methylbenzylamine with bacteria

By: Mochida, Kenichi; Uejima, Takayuki
Japan, JP01174398 A 1989-07-10 | Language: Japanese, Database: CPlus

Full Text | View 14 Related Reactions

Absolute stereochemistry shown, Rotation (+)

(4) 获取文献结果集关联的物质

(5) 在物质结果筛选项 Substance class 下，选择 Protein/Peptide Sequence 或 Nucleic Acid Sequence，获取特定产物的生物转化或酶催化反应相关的生物序列结果。

(6) 亦可进一步在 Reaction Role 筛选项下勾选 Catalyst，查看由科学家明确标引作为反应催化剂的序列。

Substances from References

References Reactions Suppliers

Filter Behavior: Filter by Exclude

Filtering: Reaction Role: Catalyst Substance Class: 2 Selected Clear All Filters

3 Results Sort: Relevance View: Partial

1 607413-25-2
Image Not Available
Unspecified
Oxidase, monoamine [336-serine] (Aspergillus niger strain MAO-N gene MAO)
Protein/Peptide Sequence
Sequence Length: 602
1 Reference 2 Reactions 0 Suppliers

2 1118219-91-2
Image Not Available
Unspecified
Pseudomonas lipase
Protein/Peptide Sequence
Sequence Length: 309
30 References 13 Reactions 0 Suppliers

3 1687851-42-8
Image Not Available
Unspecified
DNA (synthetic Fusarium oxysporum strain Fo5176 codon optimized for expression i...
Nucleic Acid Sequence
Sequence Length: 987
1 Reference 7 Reactions 0 Suppliers

Filter Behavior

Reaction Role

Catalyst (3)

Reference Role

Biological Study (3)

Biological Study, Unclassified (3)

Properties (3)

Biochemical Process (1)

Biological Use, Unclassified (1)

View All

Commercial Availability

Substance Class

Organic/Inorganic Small Molecule (570)

Manual Registration (98)

Salt and Compound With (48)

Coordination Compound (31)

Polymer (23)

Protein/Peptide Sequence (2)

Nucleic Acid Sequence (1)

还可以在 Reference Role 下，查看由科学家明确标引了文献中研究角色为 Catalyst Use 的序列。

Substances from References

References Reactions Suppliers

Filter Behavior: Filter by Exclude

Filtering: Reference Role: Catalyst Use Substance Class: 2 Selected Clear All Filters

15 Results Sort: Relevance View: Partial

1 607413-28-5
Image Not Available
Unspecified
Oxidase, monoamine [259-leucine, 260-leucine] (Aspergillus niger strain MAO-N ge...
Protein/Peptide Sequence
Sequence Length: 602
1 Reference 0 Reactions 0 Suppliers

2 1118219-91-2
Image Not Available
Unspecified
Pseudomonas lipase
Protein/Peptide Sequence
Sequence Length: 309
30 References 13 Reactions 0 Suppliers

3 2271066-38-5
Image Not Available
Unspecified
ω-Transaminase (Mycobacterium sp.NR RL B-3805)
Protein/Peptide Sequence
Sequence Length: 335
1 Reference 0 Reactions 0 Suppliers

4 2267360-21-2
Image Not Available
Unspecified
Aminotransferase (Mycobacterium strain NRRL B-3805)
Protein/Peptide Sequence
Sequence Length: 335
1 Reference 0 Reactions 0 Suppliers

5 1657044-54-6
Image Not Available
Unspecified
ω-Transaminase (synthetic clone AH-TAC M33)
Protein/Peptide Sequence
Sequence Length: 325
1 Reference 0 Reactions 0 Suppliers

6 1657044-53-5
Image Not Available
Unspecified
ω-Transaminase (synthetic clone AH-TAC M32)
Protein/Peptide Sequence
Sequence Length: 325
1 Reference 0 Reactions 0 Suppliers

Filter Behavior

Reaction Role

Catalyst (1)

Reference Role

Properties (460)

Biological Study (440)

Biological Study, Unclassified (431)

Uses (23)

Catalyst Use (15)

Biological Use, Unclassified (9)

Biosynthetic Preparation (9)

Preparation (9)

Biochemical Process (5)

Process (5)

Purification or Recovery (4)

Cosmetic Use (1)

Food or Feed Use (1)

Other Use, Unclassified (1)

Physical, Engineering, or Chemical Process (1)

View All

(7) 点击序列的 CAS RN，在物质详情中查看详细的序列结果

CAS Registry Number: 1118219-91-2





References (30) Reactions (13) Suppliers (0)   

Image Not Available

Unspecified
Pseudomonas lipase (ACI)

Protein/Peptide Sequence
Sequence Length: 309
 Related Sequences (2)

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

Other Names and Identifiers

Sequence Details

Sequence: linear

1	MNKNKTFLAA	ALVALAASFP	VHAATDYTRT	RYPVLVLSHGL	FGFKSVGPPVD
51	YMHAIVPAL	KDGAKVFATS	QSPVINSNEVR	GEQLLAQVEE	VLALTGAKEV
101	NLIGHSQGGM	TVRYVAGVAP	QLVASVTTMG	TPHKGTPVAD	AVTGFSEFLG
151	PIGTEVIASA	VEALFSVVDI	VDGGEWKGD	ALAALNSLNT	PGTARFNQRF
201	PQATPASACG	QGAETVAGVR	YYSMSGTGS	TNALDPSSAG	LAVTGLLFGE
251	ANDGLVGQCS	SHLGSVVKDN	YRMDHLDEVN	QLLGLVSLFE	SDPTQVVRQH
301	ANRLRNVGL	-	-	-	-

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 (preferred)	-	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 for a search result. The search ID is 2010:635115. The left sidebar provides metadata for the source: 'Analele Universitatii "Ovidius" Constanta, Seria: Chimie', Volume 20, Issue 1, 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, Romania), Publisher (Ovidius University Press), and Language (English).

The main content area shows the author 'By: Koncsag, Claudia Irina; Popescu, Mariana; Balbae, Cornelia; Stanciu, Gabriela' and a summary of the paper. The keywords are 'petroleum cracking coking fraction thermocatalysis GC MS HPLC'. Below the text is a 'Full Text' button and an 'Expand All | Collapse All' link.

The 'Analytical Methods' section is expanded, showing a table of related methods:

Title	CAS Method Number
Analysis of Decyl butyrate in Gasoline by Gas chromatography-mass spectrometry	1-135-CAS-32545
Analysis of Decyl butyrate in Petroleum fractions by HPLC	1-135-CAS-38904
Analysis of Decyl butyrate in Gasoline by Gas chromatography	1-135-CAS-66100

Other sections include 'Concepts', 'Substances', and 'Cited Documents'.

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 $\mu\text{L}/100\text{ mL}$; 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 $\mu\text{L}/100\text{ mL}$ 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 shows the CAS SciFinderⁿ search results page. The interface includes a search bar at the top with the text 'Substances' and 'Enter a query...'. Below the search bar is a 'Filter Behavior' sidebar with various filter categories. The main area displays 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 1 through 6.

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)

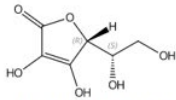
All Answer Types

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。

Q5: 有检索方面的服务吗?

A5: 可通过 CAS SCIENCE IP SERVICESSM 获取检索服务, 如需了解详情及检索服务联系方式请点击:

<https://www.cas.org/solutions/cas-custom-services/ip-services>