

CAS定制服务及 CAS SciFinderⁿ新功能、 新特色

CAS 致力于提高创新效率

CAS的数据和服务是基于对以往知识经验的回顾，对当代前沿研究的洞察，以及对未来发展趋势的前瞻



HINDSIGHT

Connecting past discoveries to build a better future

连接前人的科学发现，建设更美好的未来

INSIGHT

Revealing unseen relationships that spark ideas and speed discovery

揭示未被发现的数据关联，激发创新火花、加速科学突破

FORESIGHT

Identifying trends and emerging opportunities to accelerate growth

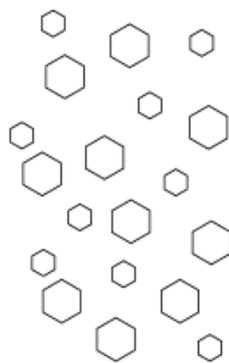
预见加速增长的趋势和新机遇

数据必须经过治理，才能为研发带来价值

PUBLISHED SCIENCE



DATA



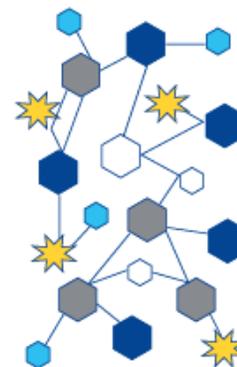
INFORMATION



HINDSIGHT



INSIGHT



FORESIGHT



CURATION
(& data
governance)

数据收
录、标
引、解
读，形成
信息

CONNECTING
建立数据
间的关联

ANALYZING
分析数据

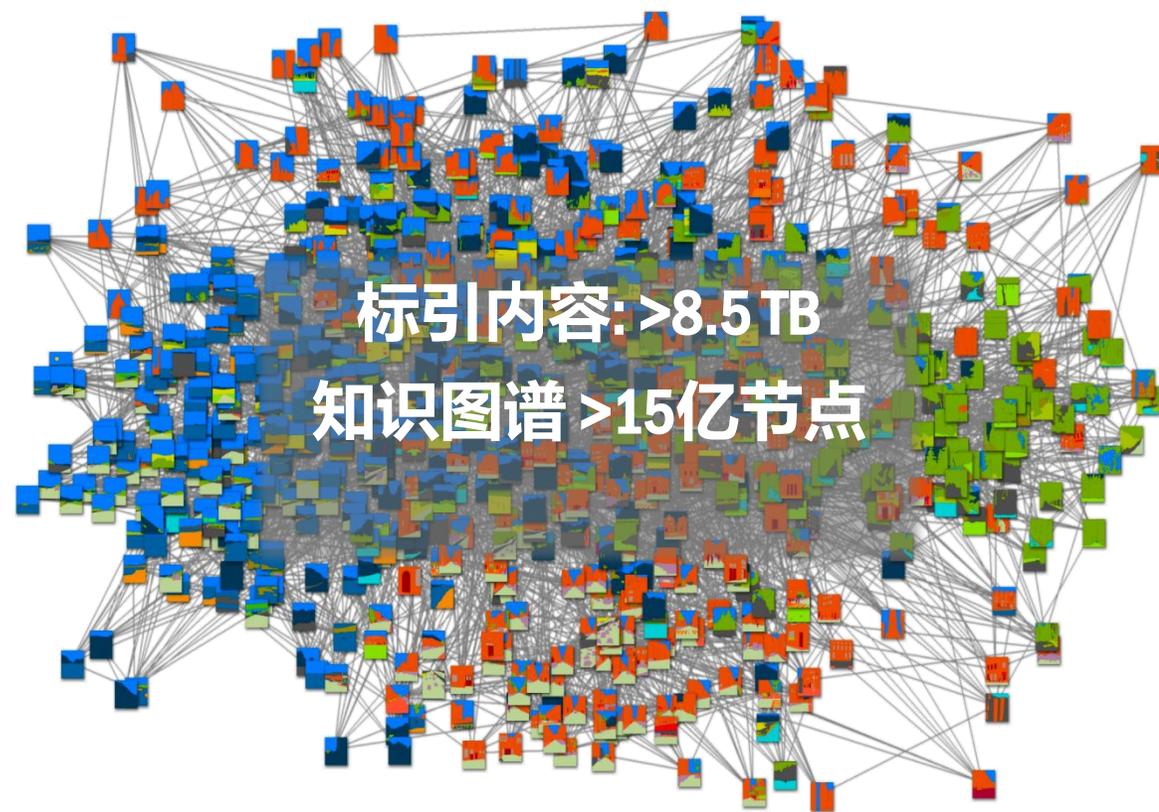
**INSIGHT-LED
DECISION SUPPORT**
形成见解，支撑决策

大数据基础架构和专有技术揭示了重点发展领域

CAS一直引领着化学信息存储和检索技术的创新：

- 完善了使化学结构可机读的算法
- 开发摩根指纹
- 创建CAS登记号（物质数据库）
- 引领化学结构检索
- 物质、反应和马库什一站检索

CAS持续创新，以解决研究团队面临的最大科技信息挑战



数据与洞见

科学家无处不在

在 CAS, 科学家标引科学出版物, 揭示未被发现的数据关联

- CAS Registry Numbers®
- STNext®
- CAS SciFinderⁿ
- **Your custom project**



CAS定制服务致力于实现科学数据的最大化价值

CAS在何处提供创新动力？

独特内容

科学家创建的高质量内容，能够提供解决用户主要难题的定制化内容

专业技术

专业的定制内容交付渠道无缝集成到现有工作流程中，提高AI、机器学习和预测分析的效率和成功率

专业知识

500多名全球科学家和技术人员揭示了超越算法的见解，他们在管理科学信息方面具有独特的经验，熟练掌握50多种语言

Predict activity and properties | Break down data silos | Data integration for ELNs and inventory systems | Much more...

与CAS定制服务合作，推动数据分析取得成功

AI & 机器学习

高级分析

CAS IP
ServicesSM

整合工作流程

知识管理

CAS Registry
ServicesSM

利用强大的预测能力揭示
最佳的研究起点

获取用于数据驱动决策的可
执行见解

用于商业决策的检索 &
见解

快速访问信息，提高
研发效率

建立、维护、建立科学信息
秩序

建立、维护、建立您所在机
构的科学信息秩序

- 定制化数据集
- 数据构架
- 分子描述符
- 咨询

- 预测 & 洞见
- 趋势分析
- 决策分析

- 聚焦研发方向
- 发现新的业务机会
- 优化IP投资组合

- API integration
- 标准化数据
- 数据整合
- 定制化标引

- 咨询与培训
- 数据管理
- 数据治理
- 定制化检索工具

- 分子命名与注册服务
- 监管提交支持
- 数据许可

数据质量对机器学习预测的影响

目标

与剑桥大学合作，测试给定算法所使用的化学描述符的质量对机器学习预测的影响。

挑战

对复杂化学物质进行编码并表示为机器可读，对于成功的预测应用至关重要。

大多数分子表达通过算法生成，具有局限性，不适合所有的模型。

解决方案

利用相同的SVM（支持向量机）算法将预测其生物活性的1万个化学实体按照靶点分为5组。利用CAS科学家创建的“CAS专有指纹”替代化学描述符 (Morgan)。

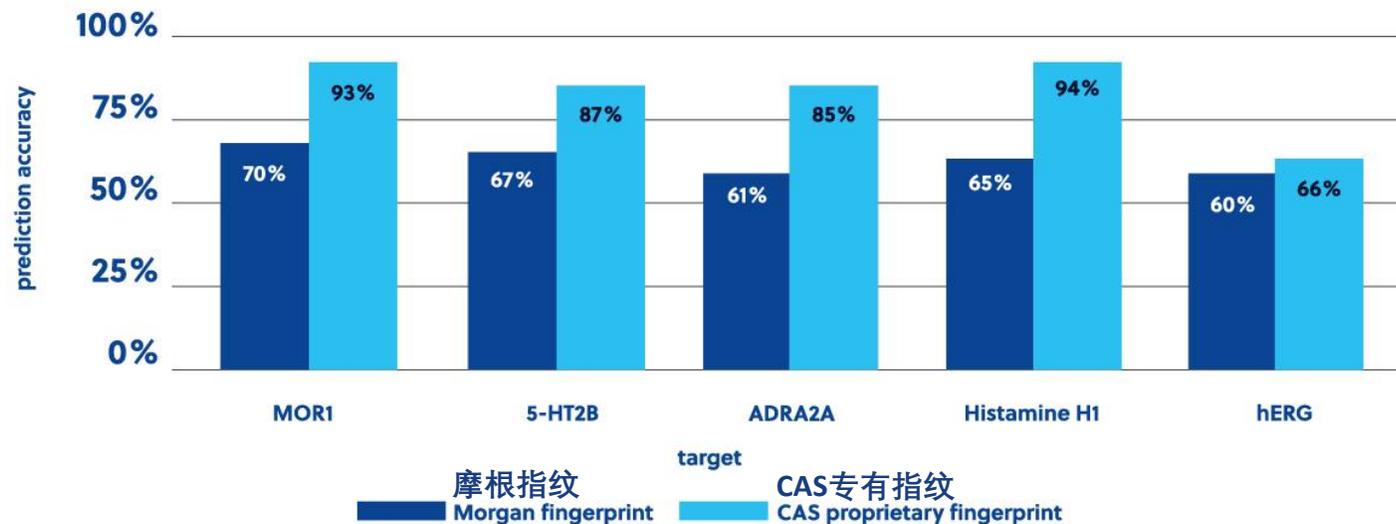
定制服务案例一

数据质量对机器学习预测的影响

结果

使用高质量的CAS数据时，分类精度提升30%。

这种精确度的提高使团队能够探索更广阔的领域，减少误报，并将精力集中在最有前景的化合物上。



“More and better data is obvious. What isn’t obvious is how data is interpreted. Encoding requires expert chemistry knowledge. CAS descriptors get better results because of the expertise of their scientists.”

“更多更好的数据是显而易见的。不明显的是如何解读数据。编码需要专业的化学知识。CAS描述符获得更好结果的原因是因为其科学家们的专业知识。”

Dr. Alpha Lee
Co-founder/Chief Scientific Officer, PostEra



数据质量对机器学习预测的影响

研究扩大

- 88个靶点
- 15万个化合物
- 4种算法
- 符号检验:

detects consistent differences and evaluates quality by “wins against”

CAS专有指纹优于常用的其他指纹

Average Sign Test Score

Fingerprint	Logistical Regression	Naïve Bayes	Tanimoto	Forest
CAS	74%	58%	67%	73%
MACCS	33%	51%	21%	47%
Avalon	52%	27%	50%	53%
RDK6	35%	40%	58%	48%
Morgan	45%	64%	52%	20%
Hashap	55%	56%	50%	53%

As measured by AUC-ROC



Morgan



MACCS



Avalon



CAS



RDK6



ACS
International



CAS为南京大学化学百年定制出版“科学文献典藏：南京大学”系列图书

目标

南京大学化学学科创立100周年，展示100年以来化学学科的贡献

挑战

时间跨度大、学校多次更名、抗战期间学校搬迁到多个地址、解放前作者英文名为民国拼音。获得全面精准的检索结果难度极大

解决方案

专家团队、CAS机构名词库、专业检索平台

CAS为南京大学化学百年定制出版“科学文献典藏：南京大学”系列图书

结果

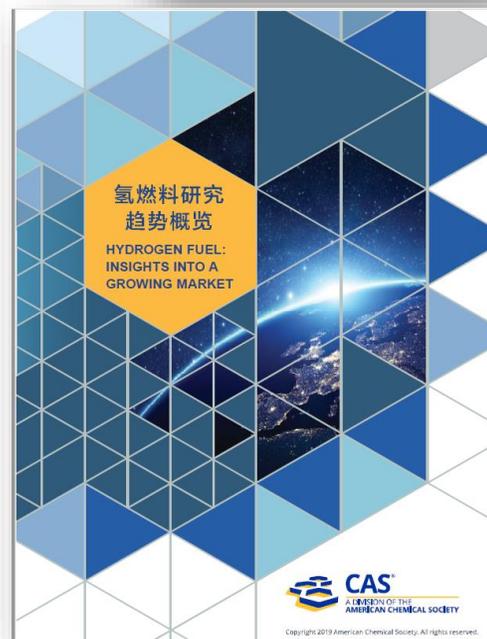
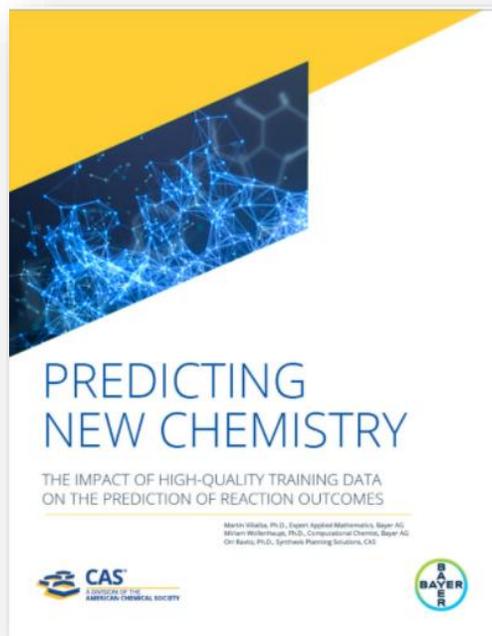
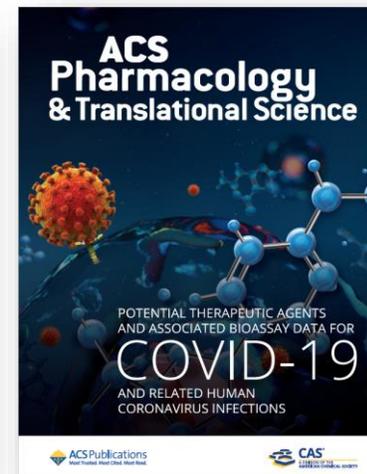
该专辑将南京大学百年以来所发表的、由“化学文摘”收录的所有化学及相关学科的学术期刊文章及专利结集出版，共计33卷，成果52,024项，跨越1919到2020年。



Case Study

CAS定制服务

提供免费数据分析报告，洞察研发态势



中科院信息素养大讲堂

CAS定制服务

为抗击新冠，免费提供定制数据集



CAS 抗新冠病毒数据集 50,000候选化合物

包括已知或潜在的抗病毒活性物质以及相关的数

以支持研究，数据挖掘和分析应用下载网址：
<https://www.cas.org/covid-19-sar-dataset>

```
L-Alanine, N-[(S)-hydroxyphenoxyphosphinyl]-, 2-ethylbutyl ester, 6-ester  
C27H35N6O8P  
1809249-37-3 Copyright (C) 2020 ACS  
42 45 0 0 1 0 0 0 0 0 0999 v2000  
24113.740225083.5116 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
24738.466831027.3695 0.0000 N 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
14556.860113339.0458 0.0000 O 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
35135.6204 8964.8958 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
41864.271512849.6839 0.0000 O 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
48592.9226 8964.8958 0.0000 P 0 0 1 0 0 5 0 0 0 0 0 0 0 0  
48592.922616734.4721 0.0000 O 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
53768.806911953.1943 0.0000 N 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
48592.9226 2988.2986 0.0000 O 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
58944.6882 8964.8958 0.0000 C 0 0 1 0 0 0 0 0 0 0 0 0 0 0
```

```
> <cas.index.name>  
L-Alanine, N-[(S)-hydroxyphenoxyphosphinyl]-, 2-ethylbutyl ester, 6-ester with 2-C-(4-  
aminopyrrolo[2,1-f][1,2,4]triazin-7-yl)-2,5-anhydro-D-altronitrile  
  
> <molecular.formula>  
C27H35N6O8P  
  
> <molecular.weight>  
602.58  
  
> <density.predicted>  
1.47Å±0.1 g/cm3 Temp: 20 Å°C; Press: 760 Torr  
  
> <pka.predicted>  
12.00Å±0.70 Most Acidic Temp: 25 Å°C
```

CAS定制服务

为抗击新冠，免费提供定制数据集

COVID-19 Protein Target Thesaurus

63个靶向蛋白以及它们的常用名

5	328404-18-8	Angiotensin-converting enzyme 2	Carboxypeptidase, angiotensin-converting enzyme-related Angiotensin-converting enzyme-related carboxypeptidase Carboxypeptidase ACE2 ACE2 APN 01 Angiotensin I converting enzyme II Angiotensin I converting enzyme 2 Angiotensin 1 converting enzyme 2 Angiotensin 1 converting enzyme II E.C. 3.4.17.23 EC 3.4.17.23 ACE-II ACE-2 Angiotensin-converting enzyme II ACEII
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CAS 抗新冠病毒候选靶向蛋白数据集

包括SARS-CoV-2 病毒蛋白，病毒入侵所依赖的宿主蛋白，宿主免疫反应相关蛋白等，下载网址：

<https://www.cas.org/covid-19-protein-target-thesaurus>

CAS SciFinderⁿ新内容、新特色

- CAS SciFinderⁿ含盖独特的专利流程解决方案— CAS PatentPak
- CAS SciFinderⁿ含盖独特的合成方法详情解决方案—Synthetic Methods
- CAS SciFinderⁿ含盖独特的逆合成工具—CAS Retrosynthesis Tool
- CAS SciFinderⁿ含盖独特的分子生物学解决方案— Biosequences Search
- CAS SciFinderⁿ界面友好、易于使用，提供多个聚类筛选项，减少二次检索、分析所花费的时间

CAS SciFinderⁿ含盖的独特专利解决方案— CAS PatentPak

- 来自CAS收录的64家专利局中 46 家主要专利局，1,800多万件专利全文，专利数量持续增加
- 多种语种撰写的专利，包括但不限于英语、德语、中文、日语、法语、韩语、俄语、西班牙语、保加利亚语等
- CAS科学家增值标引了物质在专利中的位置信息，同时提供其结构、CAS登记号等信息
- 可直接下载带有CAS增值的物质位置标记信息、结构式等在内的专利全文（PDF文件）

CAS SciFinderⁿ定含盖的独特专利解决方案— CAS PatentPak

The screenshot displays the CAS PatentPak interface. On the left, there is a sidebar with 'Key Substances in Patent' and several chemical structures with their respective CAS RNs and analyst markup locations. The main area shows a list of chemical substances, each with a blue location pin icon. A blue line connects one of the pins to the corresponding chemical structure in the sidebar. The list of substances includes: inhibitors, imitocan (CI-101), SN-38, carboplatin, nadirone, camptothecins, cyclophosphamide, crizotinib, cytarabine, dacarbazine, dasatinib, dinaciclib, docetaxel, dactinomycin, daunorubicin, doxorubicin, 2-pyrrolinodoxorubicine (2P-DOX), cyano-morpholine doxorubicin, doxorubicin glucuronide, epirubicin glucuronide, erlotinib, estramustine, epidophyllotoxin, erlotinib, entinostat, estrogen receptor binding agents, etoposide (VP16), etoposide glucuronide, etoposide phosphate, exemestane, fingolimod, flavopiridol, floxuridine (FUdR), 3',5'-O-dioleoyl-FudR (FUdR-dO), fludarabine, flutamine, farnesyl-protein transferase inhibitors, fostamatinib, ganetespib, GDC-0834, GS-1101, gefitinib, gemcitabine, hydroxyurea, ibrutinib, idarubicin, idelalisib, ifosfamide, imatinib, L-asparaginase, lapatinib, lenolidamide, leucovorin, LFM-A13, lomustine, mechlorethamine, melphalan, mercaptopurine, 6-mercaptopurine, methotrexate, mitoxantrone, mithramycin, mitomycin, mitotane, navelbine, neratinib, nilotinib, nitrosurea, olaparib, plicomycin, procarbazine, paclitaxel, PCI-32765, pentostatin, PSI-341, raloxifene, semustine, sorafenib, streptozocin, SU11248, sunitinib, tamoxifen, temazolomide (an aqueous form of DTIC), transplatinum, thalidomide, thioguanine, thiotepa, teniposide, topotecan, uracil mustard, vatalanib, vinorelbine, vinblastine, vincristine, vinca alkaloids and ZD1839.

- 快速定位专利中重要物质
- 选择下载熟识语种撰写的专利
- 直接下载专利的PDF全文

CAS SciFinderⁿ 涵盖的独特逆合成工具—CAS Retrosynthesis Tool

Retrosynthesis

Powered by ChemPlanner[®]

Overview Steps

Predicted Results ON

Plan Information

Estimated Yield: 44%
Overall Price: \$158.50
(USD per 100 grams)

Commercially Available:
A, B, C, D, E, F, G, H

Plan Options

Synthetic Depth: 3
Predicted Rules: Common
Break & Protect Bonds: No
Edit Plan Options

Scoring Profiles

Complexity Reduction ●

Convergence ●

Evidence ●

Cost ●

Yield ●

Retrosynthesis Step Key

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

Experimental Steps

Predicted Steps

Reset

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

Maximum Yield: 93%
Evidence (31,929)
Alternative Steps (88)

B ⇒ C + D

Maximum Yield: 88%
Evidence (534)
Alternative Steps (111)

C ⇒ E + F

Maximum Yield: 69%
Evidence (1)
Alternative Steps (58)

E ⇒ G + H

Maximum Yield: 78%
Evidence (1)
Alternative Steps (15)

- 已公开报道及全新分子的逆合成路线
- 同时提供被文献报道的路线和预测合成路线
- 节省时间、提高效率

CAS SciFinderⁿ 含盖独特的合成方法详细信息— Synthetic Methods

Reaction Detail (Document 1, Reaction 17 of 245)

← Prev Next →

↓ ✉ ★ Save

Steps: 1
Yield: 97%

Suppliers (106) Suppliers (82) Suppliers (79)

Step 1

Stage	Reagents	Catalysts	Solvents	Conditions
1	Benzytriethylammonium chloride Sodium hydroxide	-	Dichloromethane	1 - 2 h, rt

CAS Reaction Number: 31-081-CAS-14407309

Alternative Steps (89)

Experimental Protocols

Synthetic Methods Experimental Procedure

Products	1-(Phenylsulfonyl)indole, Yield: 97%
Reactants	Benzenesulfonyl chloride Indole
Reagents	Benzytriethylammonium chloride Sodium hydroxide
Solvents	Dichloromethane

Reference

Synthesis and Quantitative Structure-Activity Relationship (QSAR) Study of Novel N-Arylsulfonyl-3-acetylindole Arylcarbonyl Hydrazone Derivatives as Nematocidal Agents

By: Che, Zhiping; et al
View All

Journal of Agricultural and Food Chemistry (2013), 61(24), 5696-5705

Full Text

Company/Organization

Laboratory of Pharmaceutical Design and Synthesis, College of Sciences
Northwest A&F University
Shaanxi Province 712100
China

Procedure

1. Stir a mixture of reactant (1 mmol), benzytriethylammonium chloride (TEBA, 0.1 mmol), NaOH (1.8 mmol), and arylsulfonyl chlorides (1.2 mmol) in dry CH₂Cl₂ (5 mL) at room temperature.
2. Stir for 1-2 h.
3. Add water (10 mL) to the mixture.
4. Extract with CH₂Cl₂ (30 mL × 3).
5. Wash the combined organic phase by brine (30 mL).
6. Dry over anhydrous Na₂SO₄ and concentrate under reduced pressure.

Transformation

Sulfonation of Aromatic Compounds
Formation of Sulfonamides

Characterization Data

1-(Phenylsulfonyl)indole

Proton NMR Spectrum	(400 MHz, CDCl ₃) δ 7.99 (dd, J = 8.4, 4.0 Hz, 1H), 7.87 (d, J = 8.0 Hz, 2H), 7.56 (d, J = 3.6 Hz, 1H), 7.50 (d, J = 8.0 Hz, 2H), 7.40 (d, J = 7.6 Hz, 2H), 7.29 (d, J = 8.4 Hz, 1H), 7.21 (d, J = 7.6 Hz, 1H), 6.66 (d, J = 2.8 Hz, 1H);
Mass Spectrum	EI-MS, (%) 257 (M ⁺ , 85) .
Melting Point	= 78-79 °C
State	white solid

CAS Method Number 3-081-CAS-14407309

- 科学家提炼的实验详细信息
- 可读性高
- 无需再查找原文进行提炼和总结

CAS SciFinderⁿ 含盖独特的分子生物学信息— Biosequences Search

Searching for...

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

Biosequences

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

BLAST CDR Motif

```
GSETATSGSETAGTSESATSESGAGSTAGSETSTEAGTSESATSESGAGSETATSGSETAGSETATSGSETAGTSTEASE  
GSASGTSTEASEGSASGTSESATSESGAGSETATSGSETAGTSTEASEGSASGTAGSETSTEAGTSESAT
```

Sequence Type:

Search Within:
 Nucleotides Proteins

Limit Total Sequence Results to:

[Advanced Biosequence Search](#) v

- 超过5亿8千万条序列
- 含盖专利、非专利文献披露的序列
- 可实现新颖性、创造性检索

CAS SciFinder[®] 含盖独特的分子生物学信息— Biosequences Search

BLAST Search Details

Sequence Type: Protein
Search Within: Proteins
BLAST Algorithm: BLASTp
Alignment Identity: -
Query Coverage: 90%
E-Value: 10
Match with Gaps?: No
Gap Costs: Existence 11
Extension 1
Word Size: 3

Bioscape Analysis

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

Create Bioscape Analysis

Filter by

E-Value

0 to 10⁶

Query Coverage %

0 to 100

Subject Coverage %

0 to 100

Alignment Identity %

0 to 100

Apply Reset Filters

Biosequences (100)

Sort: Alignment Identity View: Collapsed

Query Details GSETATSGSETAGTSESATS ESGAGSTAGS ETSTEAGTSE SATSESGAGS ETATSGSETA GSETATSGSE...

1 Alignment Identity: 100%

Query 1 151

Subject 1 890

Matches: 151
Mismatches: 0

View Less

Alignment Subject References

References

Alignment Data
BLAST Score: 711
E-Value: 2.34675e-74

```
Q 1 GSETATSGSE TAGTSESATS ESGAGSTAGS ETSTEAGTSE SATSESGAGS ETATSGSETA GSETATSGSE 70
  |||
S 1 GSETATSGSE TAGTSESATS ESGAGSTAGS ETSTEAGTSE SATSESGAGS ETATSGSETA GSETATSGSE 70

Q 71 TAGTSTEASE GSASGTSTEA SEGSASGTSE SATSESGAGS ETATSGSETA GTSTEASEGS ASGSTAGSET 140
  |||
S 71 TAGTSTEASE GSASGTSTEA SEGSASGTSE SATSESGAGS ETATSGSETA GTSTEASEGS ASGSTAGSET 140

Q 141 STEAGTSESA T 151
  |||
S 141 STEAGTSESA T 151
```

2 Alignment Identity: 100%

Query 1 151

Subject 1 935

Matches: 151
Mismatches: 0

View More

3 Alignment Identity: 100%

可视化地图

结果筛选

导出Excel格式的序列
检索结果

获取CAS SciFinder[®]中
披露该序列的文献

CAS SciFinderⁿ新内容、新特色

- CAS SciFinderⁿ含盖独特的专利流程解决方案— CAS PatentPak
- CAS SciFinderⁿ含盖独特的合成方法详情解决方案—Synthetic Methods
- CAS SciFinderⁿ含盖独特的逆合成工具—CAS Retrosynthesis Tool
- CAS SciFinderⁿ含盖独特的分子生物学解决方案— Biosequences Search
- CAS SciFinderⁿ界面友好、易于使用，提供多个聚类筛选项，减少二次检索、分析所花费的时间

简单易用的界面，快速执行检索

保存、提醒、历史、账号管理

The screenshot displays the CAS SciFinder web interface. At the top, the CAS SciFinder logo is on the left, and navigation links for 'Saved', 'History', and 'Account' are on the right. A purple banner below the header contains a message about COVID-19 research. The main content area is divided into two sections: 'Searching for...' on the left and 'References' on the right. The 'Searching for...' section features a vertical list of search categories: 'All', 'Substances', 'Reactions', 'References' (highlighted in purple), 'Suppliers', and 'Biosequences'. The 'References' section includes a search input field with the placeholder 'Enter a query...', a 'Draw' button, and a search icon. Below the input field, there is a link to 'Advanced Search' for Author, Journal, or Organization. At the bottom of the interface, a 'Recent Search History' section shows a search performed on May 4, 2021, at 10:12 AM, with the query 'nano and lipid and carrier (699)' and a 'Rerun Search' button.

丰富的检索项
支持多途径检索

近期检索记录

使用布尔逻辑运算符，精准构建检索式

The screenshot shows the CAS SciFinder search interface. At the top, there are navigation links for 'Saved', 'History', and 'Account'. A banner message states: 'You can now use BLAST search to mine our newly enhanced collection of more than 500M proteins and nucleotides from 60+ patent authorities dating back to 1957. Plus visually review sequence similarity and frequency across your patent search results.' Below this, the 'Searching for...' sidebar is visible with options: All, Substances, Reactions, References (selected), Suppliers, and Biosequences. The main search area shows the query '(ADC or "antibody drug conjugate") and toxin' in the search bar. A dropdown menu displays several suggestions, including '(ADC or "antibody drug conjugate") Multidrug and toxin extrusion 2-K', '(ADC or "antibody drug conjugate") Coptis and toxin-resolving decoction', '(ADC or "antibody drug conjugate") Multidrug and toxin extrusion proteins', '(ADC or "antibody drug conjugate") Multidrug and toxin extrusion protein 1', '(ADC or "antibody drug conjugate") Multidrug and toxin extrusion protein 2', '(ADC or "antibody drug conjugate") Multidrug and toxin extrusion protein 1 (MATE...', '(ADC or "antibody drug conjugate") Multidrug and toxin extrusion protein 2 (MATE...', '(ADC or "antibody drug conjugate") Protein ZmMATE (corn multidrug and toxin-extr...', '(ADC or "antibody drug conjugate") DNA (corn multidrug and toxin-extrusion prote...', and '(ADC or "antibody drug conjugate") DNA (synthetic onconase and toxin transmembra...'. The interface also includes 'Draw' and search icons.

- 基于科学家创建的叙词表，充分利用自动提示检索词，启发检索思路
- 支持布尔逻辑运算符
- “ ” 不允许词形变化，但可出现单数或复数。实现精准检索

文本与结构联用，减少检索步骤，提高检索效率

The screenshot displays the CAS SciFinder search interface. At the top, the CAS SciFinder logo is on the left, and navigation links for 'Saved', 'History', and 'Account' are on the right. A purple banner below the header provides information about the CAS Formulus module. The main search area is titled 'References' and includes a search bar with the query '(ADC or "antibody drug conjugate") and toxin'. Below the search bar, there are options for 'Advanced Search' and a search button. A chemical structure drawing is overlaid on the search results, with 'Edit Drawing' and 'Remove' buttons. On the left side, a 'Searching for...' sidebar lists various search categories: All, Substances, Reactions, References (highlighted), Suppliers, and Biosequences.

文本和结构检索可以单独使用；也可灵活联用，同时识别检索关键词和结构信息，高效获得最相关的信息

CAS SciFinderⁿ的Filter合并了SciFinder中的Analyze和Refine选项，提高了检索效率

The screenshot displays the CAS SciFinderⁿ interface. At the top, the search bar contains the query "(ADC or "antibody drug conjugate") and toxin". The left sidebar features a "Filter Behavior" panel with a "Filter by" button highlighted in a blue box. Below this, various filter categories are listed, including Document Type, Substance Role, Language, and Publication Year. A histogram shows the distribution of results from 1976 to 2021. The main content area shows search results for "References (734)". The first result is titled "Synthesis of the death-cap mushroom toxin α -amanitin" and includes a chemical structure diagram. The second result is titled "Highly Potent, Anthracycline-based Antibody-Drug Conjugates Generated by Enzymatic, Site-specific Conjugation".

丰富直观的聚类分析, 高效直观地纵览检索结果, 便捷地选择或排除结果

引文地图，便捷地获取关联研究文献

1

Synthesis of the death-cap mushroom toxin α -amanitin

By: Matinkhoo, Kaveh; Pryyma, Alla; Todorovic, Mihajlo; Patrick, Brian O.; Perrin, David M.
Journal of the American Chemical Society (2018), 140(21), 6513-6517 | Language: English, Database: CAPLUS and MEDLINE

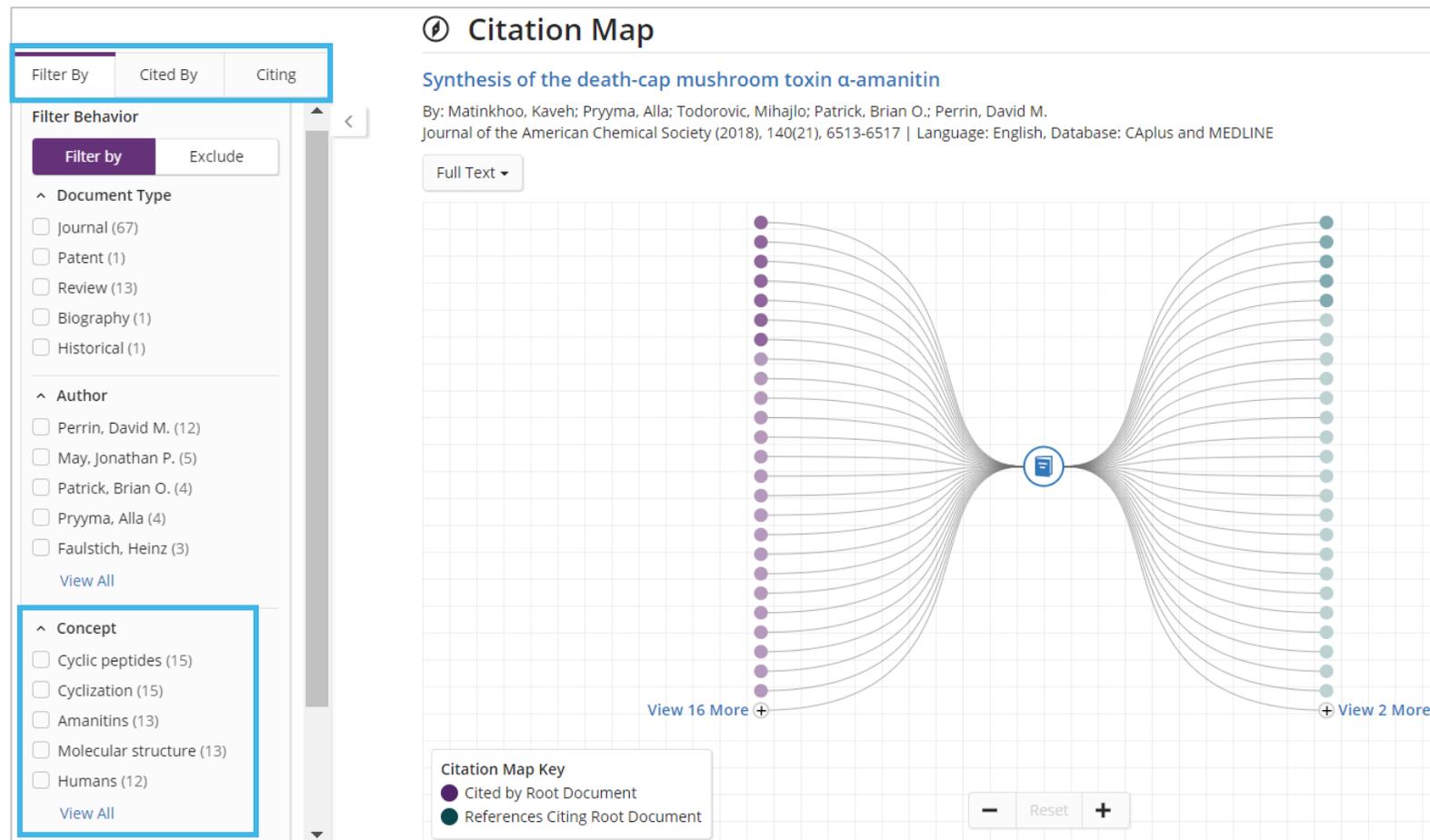


α -Amanitin is an extremely toxic bicyclic octapeptide isolated from the death-cap mushroom, *Amanita phalloides*. As a potent inhibitor of RNA polymerase II, α -amanitin is toxic to eukaryotic cells. Recent interest in α -amanitin arises from its promise as a payload for **antibody-drug conjugates**. For over 60 years, *A. phalloides* has been the only source of α -amanitin. Here we report a synthesis of α -amanitin, which surmounts the key challenges for installing the 6-hydroxy-trypathionine sulfoxide bridge, an antipolarizable synthesis of (2S,3R,4R)-4,5-dihydroxy-isoleucine, and diastereoselective sulf-

View More \downarrow

Full Text \downarrow Substances (47) Reactions (471) Cited By (27) Citation Map

Citation Map: 引文地图，
发现前向、后向研究



一步检索即可获得不同类型的结果集

The screenshot displays the CAS SciFinder search results page. At the top, there is a search bar with the text 'Enter a query...' and a search icon. Below the search bar, the 'Structure Match' section is highlighted with a blue border. It contains three options: 'As Drawn (1)', 'Substructure (6,359)', and 'Similarity (51K)'. The 'As Drawn (1)' option is selected. The main content area shows the search results for 'As Drawn', including a chemical structure of 3-(3-pyridinyl)-1H-indole, its molecular formula $C_{13}H_{10}N_2$, and its name. There are also buttons for 'References', 'Reactions', and 'Suppliers'.

- As Drawn：绘制结构中可出现R基团、可变基团。绘制结构中价态未达饱和的原子只能接氢，环系（如有）不能与其他的环稠合或成桥环。
- Substructure：包括As Drawn的检索结果，另外价态未达饱和的原子可以连接氢以外的其他原子，环系（如有）可以与其他环稠合或成桥环。
- Similarity：绘制结构中不能出现R基团、可变基团，绘制的结构必须是一个确定的结构。获得片段或整体结构与被检索结构相似的物质，母体结构可以被取代，也可以被改变。

Structure Match Introduction
https://scifinder-n.cas.org/help/#t=Working_with_Search_Results%2FSubstances%2FStructure_Match.htm&rhsearch=as%20drawn

Markush结构检索直接呈现专利中的通式结构，快速判定专利的相关性，有利于对化合物的新颖性/创造性/侵权进行判断

CAS SciFinder® Substances Enter a query... Edit

Return to Home

Patent Markush Match

As Drawn (54)

Substructure (712)

Filter Behavior

Filter by Exclude

Patent Office

- World Intellectual Property Organization (32)
- China (9)
- United States (6)
- Japan (5)
- European Patent Organization (1)
- Germany (1)

Patent Markush (54)

References

Sort: Patent Number: Descending

Edit Drawing Remove

Search Patent Markush

1

WO9942092

Patent claim 1

PATENTPAK Full Text

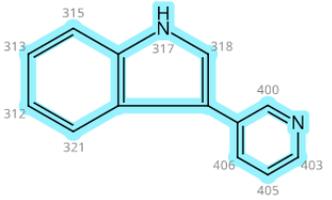
312,313,315,317,318,321: opt. substd.

400,403,405,406: opt. substd.

PATENTPAK Full Text

Patent Language Kind Code PatentPak Options

WO9942092 English A2 PDF | PDF+ | View



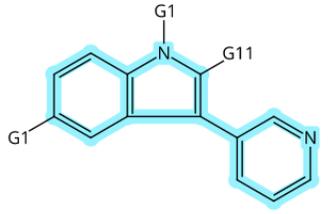
2

WO9829408

Patent claim 1

PATENTPAK Full Text

There are no notes to display for this structure.



WO 99/42092 PCT/US99/03655

16

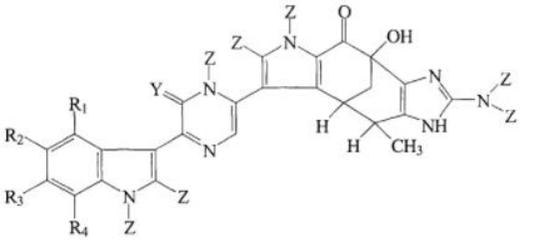
Claims

1. A method of treating inflammation in a human or animal, wherein said method comprises administering to said human or animal an effective amount of a compound having the following formula:

$$A_1-M-A_2$$

wherein each of A_1 and A_2 is a heterocycle; and M is a core moiety linking A_1 and A_2 .

2. The method, according to claim 1, wherein said compound has the following structure:



(I)

3 R_{1-4} are the same or different and are selected from the group consisting of -H, -OH, halogen, -R, -OR, -OCOR, -OA, and NZZ (wherein the Zs can be the same or different);

4 Y is the single group =O, or the single group =NZ, or two groups, same or different, selected from the group consisting of -H, -OH, -OR, -OCOR, and NZZ (wherein the Zs can be the same or different);

5 Z is independently selected from the group consisting of -H, -R, -OH, and -COR; and

6 R is C1-C8 alkyl or C1-C8 alkoxy, mesyl, or tosyl; and A is -R-phenyl.

Save & Alerts: 结果的保存与设置提醒

The screenshot displays the CAS SciFinder search results page for the query "(ADC or 'antibody drug conjugate') and toxin". The interface includes a search bar, navigation options, and a list of results. A 'Save Search' dialog box is open, allowing the user to save the search and set up alerts. The dialog box contains the following fields and options:

- Name:** (ADC or "antibody drug conjugate") and toxin
- Alert Frequency:** No Alerts, As Available (selected), Weekly, Monthly
- Tags (optional):** 13 PATENTS, 13 substructure, 29 as drawn, 602 as drawn Markush, ANTIBODY (selected)
- New Tag (optional):** ADC

The background shows search results for "Synthesis of the death-cap mushroom toxin α -amanitin" and "Highly Potent, Anthracycline-based Antibody-Targeted Drug Conjugates".

便捷地将CAS SciFinder中保存的结果迁移至CAS SciFinderⁿ中

The screenshot displays the CAS SciFinder web interface. At the top, the search bar contains the query "(ADC or 'antibody drug conjugate') and toxin". A star icon in the top navigation bar is highlighted with a blue box, indicating the 'Saved' section. On the left, a 'Filter by' sidebar lists various categories like 'Result Type', 'Alerts', and 'Tags'. Below this, there are buttons for 'Combine Saved Results' and 'Migrate Alerts & Saved Results', with the 'Migrate' button highlighted by a blue box. The main content area, titled '★ Saved (330)', lists three saved search results:

- Search 1: "(ADC OR 'antibody drug conjugate') AND toxin" (References), dated April 28, 2021, 10:45 AM. Includes a 'Rerun Search' button and a tag 'ADC'.
- Search 2: "H2O4S.2Na" (Substances), dated April 27, 2021, 5:12 PM. Includes a 'Rerun Search' button and the molecular formula H2SO4.2Na.
- Search 3: "'antibody-drug conjugate'2" (References), dated April 26, 2021, 9:00 PM. Includes a 'Rerun Search' button.

便捷地管理检索历史

CAS SciFinder®

References ▾ Enter a query...

Draw 🔍 ⭐ 🕒 👤

Filter by

^ Result Type

- All (305)
- Biosequences (48)
- Patent Markush (258)
- Reactions (622)
- References (3,295)
- Retrosynthesis (193)
- Substances (1,913)
- Suppliers (73)

[View Fewer](#)

^ Date

Start Date mm/dd/yyyy to End Date mm/dd/yyyy

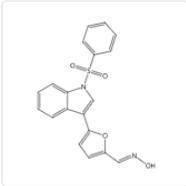
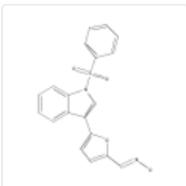
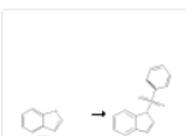
May, 2021

SU	MO	TU	WE	TH	FR	SA
25	26	27	28	29	30	1
2	3	4	5	6	7	8
9	10	11	12	13	14	15
16	17	18	19	20	21	22
23	24	25	26	27	28	29
30	31	1	2	3	4	5

🕒 Search History (6,707)

1 Selected

May 6, 2021

- 6:46 PM
 - Retrosynthesis Synthetic Depth: 3
Predicted Rules: Common
Break & Protect Bonds: No
 - 
 - Retrosynthesis Plan will expire on Aug 4, 2021.
 - [Open Plan](#)
 - [Edit Options](#)
 - Generating Plan
- 6:46 PM
 - Patent Markush As Drawn (0)
Substructure (0)
 - 
 - [Rerun Search](#)
 - [Edit Search](#)
- 6:11 PM
 - Reactions As Drawn (105)
Substructure (100K)
Similarity (146)
 - 
 - [Rerun Search](#)
 - [Edit Search](#)

学习资源

1. 关注“ACS美国化学会”微信公众号, 搜索**SciFinder-n**, 查看检索技巧、检索视频, 以及论坛回放视频



2. CAS SciFinderⁿ网络在线演示培训资料
<https://www.cas.org/about/events/scifinder-webinars>

3. CAS官网上的培训资料
<https://www.cas.org/support/training/scifinder-n>

4. CAS SciFinderⁿ Help使用指南
https://scifinder-n.cas.org/help/#t=Searching_in_SciFinder-n%2FIntroduction_to_searching.htm

网络公开培训

	日期	主题	主讲人
基础 培训	1月18日	SciFinder ⁿ 入门使用技能	余敏
	3月30日	SciFinder ⁿ 新内容、新功能	钱欣
功能 详解	4月13日	文献检索方法	朱传娴
	4月27日	物质检索方法	朱传娴
	5月18日	反应检索方法（包括Retrosynthesis功能）	程小燕
	6月3日	专利信息检索方法	余敏
	6月22日	如何管理检索结果集	匡金海
检索 案例	7月6日	聚合物相关信息获取策略	程小燕
	7月20日	无机与金属有机化合物相关信息获取策略	钱欣
	8月10日	光电材料相关信息获取策略	程小燕
	8月24日	农化相关信息获取策略	钱欣
	9月28日	药物结构设计与合成	程小燕
	10月19日	天然植物化学相关信息获取策略	钱欣
11月23日	生物序列相关信息获取策略（包括Biosequences）	余敏	



关注公众号：**ACS美国化学会**
随时观看回放，了解直播信息



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谢谢关注！



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