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如何使用SciFinder获取科技信息

中南民族大学

2018.5.21



提纲

- 美国化学文摘社简介
- SciFinder简介及检索方式
 - 文献检索
 - 物质检索
 - Markush检索
 - 反应检索
 - SciPlanner
- SciFinder常见问题及解决

美国化学文摘社—Chemical Abstracts Service

- ACS的分支机构
- 创建于1907年，简称“CAS”
- 最早创立了《化学文摘》
- 密切关注，索引和提炼着全球化学相关的文献和专利
- 总部座落于俄亥俄州的哥伦布市



CAS——构建最高质量的化学数据库



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SCIFINDER[®]
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CAS——构建最高质量的化学数据库



CAS数据库——源于化学，超越化学

生物化学：

农化产品管控信息,生化遗传学,发酵,免疫化学,药理学

有机化学各领域：

氨基酸,生物分子,碳水化合物,有机金属化合物,类固醇

大分子化学各领域：

纤维素、木质素、造纸;涂料、墨水

染料、有机颜料;合成橡胶;纺织品、纤维

应用化学各领域：

大气污染,陶瓷,精油、化妆品,化石燃料,黑色金属、合金

物理、无机、分析化学各领域：

表面化学,催化剂,相平衡,核现象,电化学

CAS数据库最具价值的内容——人工索引


4. Process for preparation of novel sofosbuvir crystal

By: Zhou, Haohui; Lin, Guoliang; Wu, Yao; Zou, Wenjuan; Chan, Yunxia

Assignee: Beijing Winsunny Pharmaceutical Co., Ltd., Peop. Rep. China

The invention relates to a novel sofosbuvir crystal having high stability and soly. The novel sofosbuvir crystal is prepd. through crystg. sofosbuvir in pos. solvent and neg. solvent. The method has high repeatability, easy control, high yield, and high product purity.

Patent Information

Patent No.	Kind	Language	Date	Application No.	Date
CN 105732751  PATENTPAK	A		Jul 6, 2016	CN 2014-10742897	Dec 9, 2014

Priority Application

CN 2014-10742897	Dec 9, 2014
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Indexing


Carbohydrates (Section33-9)

Section cross-reference(s): 34, 63

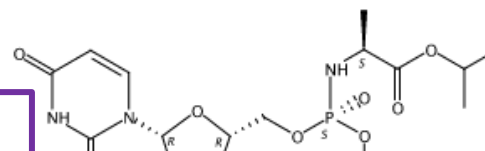
Concepts

Crystallization	Drug bioavailability
Hepatitis C	Hepatitis C virus
Homo sapiens	Human
Pharmaceutical coated tablets	

Substances

1190307-88-0P Sofosbuvir 
Absolute stereochemistry.

Page 2 in **PATENTPAK**



Tips:

1. 98%以上的文献，都经过人工索引
2. 用Index Term标引文献中的重要技术术语
3. 用CAS RN标引出文献中的重要物质
4. 用CAS Role标引文献中重要物质的研究领域

CAS人工标引解决的问题

- 检索词的同义词拓展：解决不同科研人员由于教育背景、语言、表达习惯不同导致的对同一个技术术语描述的差异。
- 用名称、分子式等检索化合物，会导致检索不全、不准的问题。CAS RN很好的解决了该问题，帮助检索人员实现精准定位化合物的目标。
- 利用SciFinder中的标引信息（Index Term，CAS RN，CAS Role），提高效率，启发思路。

CAS最新动向—解决方案

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CAS最新动向—解决方案

- CAS于2015年2月正式发布PatentPak™
- 专利工作流程解决方案
- 极大节约用户在研究专利时的时间
- 快速查找定位专利中的关键化学信息

6. Preparation of substituted nucleosides, nucleotides and analogs thereof as antiviral agents

Quick View PATENTPAK

By Beigelman, Le...
From PCT Int. App...

Disclosed he...
phosphate, R...
methods of...
medicament

Patent No.	Kind	Language
WO 2016100441	A1	English

Patent Family

Patent No.	Kind	Language
US 20160176911	A1	English

atkina, Natalia
Language: English, Database: CAPLUS

B is substituted purine and pyrimidine nucleobase; dashed bond between R and R⁴ is absent, then R is H, substituted each R⁶ and R⁷ are independently hydrogen or deuterium; R⁵ is -OH or F; methods of synthesizing nucleotide analogs and as a HCV infection with one or more nucleotide analogs. Thus, nucleotide II was prepd. and tested as antiviral agent and for a hepatitis C virus.

7. Process for preparation of sofosbuvir

Quick View PATENTPAK

By Li, Zebiao; Zhu, Mingmin; Zhang, Qinghai; Zhu, Gongfeng; Zhang, Zhaoguo; Lin, Yanfeng
From Faming Zhuanli Shenqing (2016), CN 105669804 A 20160615. | Language: Chinese, Database: CAPLUS

The prep. method comprises reaction of (2'R)-2'-deoxy-2'-fluoro-2'-methyluridine with

ZOOM

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8.

By...

From...

(12) INTERNATIONAL APPLICATION PUBLISHED UNDER THE PATENT COOPERATION TREATY (PCT)

(19) World Intellectual Property Organization
International Bureau

(43) International Publication Date
23 June 2016 (23.06.2016)

WIPO PCT

(51) International Patent Classification:
C07H 19/10 (2006.01) C07H 19/13 (2006.01)
C07H 19/20 (2006.01) A61K 31/702 (2006.01)
C07H 19/11 (2006.01) A61K 31/706 (2006.01)
C07H 19/213 (2006.01) A61K 31/708 (2006.01)
C07H 19/067 (2006.01) A61P 31/14 (2006.01)
C07H 19/073 (2006.01)

(81) Designated States (kind of national protection):
AO, AT, AU, AZ, BA, BB, BG, CA, CH, CL, CN, CZ, DE, DK, EC, EE, EG, ES, FI, FR, GB, GR, HK, HU, IL, IN, JP, KZ, LA, LC, LK, LT, LU, LV, MA, MD, ME, MK, MN, MW, MX, MY, NG, NI, NO, NZ, OM, PA, PE, PG, PH, PL, PT, RU, SE, SG, SK, SL, SM, ST, SV, SY, TH, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, ZA, ZM, ZW.

(84) Designated States (unless otherwise indicated, for every kind of regional protection available): ARIPO (BW, GH, GM, KE, LU, MG, MW, MZ, NA, NG, SD, SI, SZ, TZ, UG, ZM, ZW), EPO (AL, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, JP, KR, LK, LT, LU, LV, MA, MD, ME, MK, MN, MW, MX, MY, NG, NI, NO, NZ, OM, PA, PE, PG, PH, PL, PT, RU, SE, SG, SK, SL, SM, ST, SV, SY, TH, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, ZA, ZM, ZW).

(10) International Publication Number: WO 2016/100441 A1

(21) International Application Number: PCT/US2015/065981

(22) International Filing Date: 16 December 2015 (16.12.2015)

(25) Filing Language: English

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Analyst Markup Locations (1)

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CAS RN 1206126-39-7

Search in SciFinder | View Detail

Analyst Markup Locations (1)

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CAS RN 1206126-41-1

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Analyst Markup Locations (1)

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WO 2016/100441

PCT/US2015/065981

EXAMPLE 1
COMPOUND 1

HO-CH₂-CH₂-OH + HO-CH₂-CH₂-OH → HO-CH₂-CH₂-OH (1-1)

HO-CH₂-CH₂-OH (1-1) + HO-CH₂-CH₂-OH (1-2) → HO-CH₂-CH₂-OH (1-3)

HO-CH₂-CH₂-OH (1-3) + HO-CH₂-CH₂-OH (1-4) → HO-CH₂-CH₂-OH (1-5)

HO-CH₂-CH₂-OH (1-5) + HO-CH₂-CH₂-OH (1-6) → HO-CH₂-CH₂-OH (1-7)

Route 2

HO-CH₂-CH₂-OH (1-4a) + HO-CH₂-CH₂-OH (1-5a) → HO-CH₂-CH₂-OH (1-6a)

HO-CH₂-CH₂-OH (1-6a) + HO-CH₂-CH₂-OH (1-7a) → HO-CH₂-CH₂-OH (1-8a)

HO-CH₂-CH₂-OH (1-8a) + HO-CH₂-CH₂-OH (1-9a) → HO-CH₂-CH₂-OH (1-10a)

HO-CH₂-CH₂-OH (1-10a) + HO-CH₂-CH₂-OH (1-11a) → HO-CH₂-CH₂-OH (1-12a)

HO-CH₂-CH₂-OH (1-12a) + HO-CH₂-CH₂-OH (1-13a) → HO-CH₂-CH₂-OH (1-14a)

HO-CH₂-CH₂-OH (1-14a) + HO-CH₂-CH₂-OH (1-15a) → HO-CH₂-CH₂-OH (1-16a)

HO-CH₂-CH₂-OH (1-16a) + HO-CH₂-CH₂-OH (1-17a) → HO-CH₂-CH₂-OH (1-18a)

HO-CH₂-CH₂-OH (1-18a) + HO-CH₂-CH₂-OH (1-19a) → HO-CH₂-CH₂-OH (1-20a)

HO-CH₂-CH₂-OH (1-20a) + HO-CH₂-CH₂-OH (1-21a) → HO-CH₂-CH₂-OH (1-22a)

HO-CH₂-CH₂-OH (1-22a) + HO-CH₂-CH₂-OH (1-23a) → HO-CH₂-CH₂-OH (1-24a)

HO-CH₂-CH₂-OH (1-24a) + HO-CH₂-CH₂-OH (1-25a) → HO-CH₂-CH₂-OH (1-26a)

HO-CH₂-CH₂-OH (1-26a) + HO-CH₂-CH₂-OH (1-27a) → HO-CH₂-CH₂-OH (1-28a)

HO-CH₂-CH₂-OH (1-28a) + HO-CH₂-CH₂-OH (1-29a) → HO-CH₂-CH₂-OH (1-30a)

HO-CH₂-CH₂-OH (1-30a) + HO-CH₂-CH₂-OH (1-31a) → HO-CH₂-CH₂-OH (1-32a)

HO-CH₂-CH₂-OH (1-32a) + HO-CH₂-CH₂-OH (1-33a) → HO-CH₂-CH₂-OH (1-34a)

HO-CH₂-CH₂-OH (1-34a) + HO-CH₂-CH₂-OH (1-35a) → HO-CH₂-CH₂-OH (1-36a)

HO-CH₂-CH₂-OH (1-36a) + HO-CH₂-CH₂-OH (1-37a) → HO-CH₂-CH₂-OH (1-38a)

HO-CH₂-CH₂-OH (1-38a) + HO-CH₂-CH₂-OH (1-39a) → HO-CH₂-CH₂-OH (1-40a)

HO-CH₂-CH₂-OH (1-40a) + HO-CH₂-CH₂-OH (1-41a) → HO-CH₂-CH₂-OH (1-42a)

HO-CH₂-CH₂-OH (1-42a) + HO-CH₂-CH₂-OH (1-43a) → HO-CH₂-CH₂-OH (1-44a)

HO-CH₂-CH₂-OH (1-44a) + HO-CH₂-CH₂-OH (1-45a) → HO-CH₂-CH₂-OH (1-46a)

HO-CH₂-CH₂-OH (1-46a) + HO-CH₂-CH₂-OH (1-47a) → HO-CH₂-CH₂-OH (1-48a)

HO-CH₂-CH₂-OH (1-48a) + HO-CH₂-CH₂-OH (1-49a) → HO-CH₂-CH₂-OH (1-50a)

HO-CH₂-CH₂-OH (1-50a) + HO-CH₂-CH₂-OH (1-51a) → HO-CH₂-CH₂-OH (1-52a)

HO-CH₂-CH₂-OH (1-52a) + HO-CH₂-CH₂-OH (1-53a) → HO-CH₂-CH₂-OH (1-54a)

HO-CH₂-CH₂-OH (1-54a) + HO-CH₂-CH₂-OH (1-55a) → HO-CH₂-CH₂-OH (1-56a)

HO-CH₂-CH₂-OH (1-56a) + HO-CH₂-CH₂-OH (1-57a) → HO-CH₂-CH₂-OH (1-58a)

HO-CH₂-CH₂-OH (1-58a) + HO-CH₂-CH₂-OH (1-59a) → HO-CH₂-CH₂-OH (1-60a)

HO-CH₂-CH₂-OH (1-60a) + HO-CH₂-CH₂-OH (1-61a) → HO-CH₂-CH₂-OH (1-62a)

HO-CH₂-CH₂-OH (1-62a) + HO-CH₂-CH₂-OH (1-63a) → HO-CH₂-CH₂-OH (1-64a)

HO-CH₂-CH₂-OH (1-64a) + HO-CH₂-CH₂-OH (1-65a) → HO-CH₂-CH₂-OH (1-66a)

HO-CH₂-CH₂-OH (1-66a) + HO-CH₂-CH₂-OH (1-67a) → HO-CH₂-CH₂-OH (1-68a)

HO-CH₂-CH₂-OH (1-68a) + HO-CH₂-CH₂-OH (1-69a) → HO-CH₂-CH₂-OH (1-70a)

HO-CH₂-CH₂-OH (1-70a) + HO-CH₂-CH₂-OH (1-71a) → HO-CH₂-CH₂-OH (1-72a)

HO-CH₂-CH₂-OH (1-72a) + HO-CH₂-CH₂-OH (1-73a) → HO-CH₂-CH₂-OH (1-74a)

HO-CH₂-CH₂-OH (1-74a) + HO-CH₂-CH₂-OH (1-75a) → HO-CH₂-CH₂-OH (1-76a)

HO-CH₂-CH₂-OH (1-76a) + HO-CH₂-CH₂-OH (1-77a) → HO-CH₂-CH₂-OH (1-78a)

HO-CH₂-CH₂-OH (1-78a) + HO-CH₂-CH₂-OH (1-79a) → HO-CH₂-CH₂-OH (1-80a)

HO-CH₂-CH₂-OH (1-80a) + HO-CH₂-CH₂-OH (1-81a) → HO-CH₂-CH₂-OH (1-82a)

HO-CH₂-CH₂-OH (1-82a) + HO-CH₂-CH₂-OH (1-83a) → HO-CH₂-CH₂-OH (1-84a)

HO-CH₂-CH₂-OH (1-84a) + HO-CH₂-CH₂-OH (1-85a) → HO-CH₂-CH₂-OH (1-86a)

HO-CH₂-CH₂-OH (1-86a) + HO-CH₂-CH₂-OH (1-87a) → HO-CH₂-CH₂-OH (1-88a)

HO-CH₂-CH₂-OH (1-88a) + HO-CH₂-CH₂-OH (1-89a) → HO-CH₂-CH₂-OH (1-90a)

HO-CH₂-CH₂-OH (1-90a) + HO-CH₂-CH₂-OH (1-91a) → HO-CH₂-CH₂-OH (1-92a)

HO-CH₂-CH₂-OH (1-92a) + HO-CH₂-CH₂-OH (1-93a) → HO-CH₂-CH₂-OH (1-94a)

HO-CH₂-CH₂-OH (1-94a) + HO-CH₂-CH₂-OH (1-95a) → HO-CH₂-CH₂-OH (1-96a)

HO-CH₂-CH₂-OH (1-96a) + HO-CH₂-CH₂-OH (1-97a) → HO-CH₂-CH₂-OH (1-98a)

HO-CH₂-CH₂-OH (1-98a) + HO-CH₂-CH₂-OH (1-99a) → HO-CH₂-CH₂-OH (1-100a)

HO-CH₂-CH₂-OH (1-100a) + HO-CH₂-CH₂-OH (1-101a) → HO-CH₂-CH₂-OH (1-102a)

HO-CH₂-CH₂-OH (1-102a) + HO-CH₂-CH₂-OH (1-103a) → HO-CH₂-CH₂-OH (1-104a)

HO-CH₂-CH₂-OH (1-104a) + HO-CH₂-CH₂-OH (1-105a) → HO-CH₂-CH₂-OH (1-106a)

HO-CH₂-CH₂-OH (1-106a) + HO-CH₂-CH₂-OH (1-107a) → HO-CH₂-CH₂-OH (1-108a)

HO-CH₂-CH₂-OH (1-108a) + HO-CH₂-CH₂-OH (1-109a) → HO-CH₂-CH₂-OH (1-110a)

HO-CH₂-CH₂-OH (1-110a) + HO-CH₂-CH₂-OH (1-111a) → HO-CH₂-CH₂-OH (1-112a)

HO-CH₂-CH₂-OH (1-112a) + HO-CH₂-CH₂-OH (1-113a) → HO-CH₂-CH₂-OH (1-114a)

HO-CH₂-CH₂-OH (1-114a) + HO-CH₂-CH₂-OH (1-115a) → HO-CH₂-CH₂-OH (1-116a)

HO-CH₂-CH₂-OH (1-116a) + HO-CH₂-CH₂-OH (1-117a) → HO-CH₂-CH₂-OH (1-118a)

HO-CH₂-CH₂-OH (1-118a) + HO-CH₂-CH₂-OH (1-119a) → HO-CH₂-CH₂-OH (1-120a)

HO-CH₂-CH₂-OH (1-120a) + HO-CH₂-CH₂-OH (1-121a) → HO-CH₂-CH₂-OH (1-122a)

HO-CH₂-CH₂-OH (1-122a) + HO-CH₂-CH₂-OH (1-123a) → HO-CH₂-CH₂-OH (1-124a)

HO-CH₂-CH₂-OH (1-124a) + HO-CH₂-CH₂-OH (1-125a) → HO-CH₂-CH₂-OH (1-126a)

HO-CH₂-CH₂-OH (1-126a) + HO-CH₂-CH₂-OH (1-127a) → HO-CH₂-CH₂-OH (1-128a)

HO-CH₂-CH₂-OH (1-128a) + HO-CH₂-CH₂-OH (1-129a) → HO-CH₂-CH₂-OH (1-130a)

HO-CH₂-CH₂-OH (1-130a) + HO-CH₂-CH₂-OH (1-131a) → HO-CH₂-CH₂-OH (1-132a)

HO-CH₂-CH₂-OH (1-132a) + HO-CH₂-CH₂-OH (1-133a) → HO-CH₂-CH₂-OH (1-134a)

HO-CH₂-CH₂-OH (1-134a) + HO-CH₂-CH₂-OH (1-135a) → HO-CH₂-CH₂-OH (1-136a)

HO-CH₂-CH₂-OH (1-136a) + HO-CH₂-CH₂-OH (1-137a) → HO-CH₂-CH₂-OH (1-138a)

HO-CH₂-CH₂-OH (1-138a) + HO-CH₂-CH₂-OH (1-139a) → HO-CH₂-CH₂-OH (1-140a)

HO-CH₂-CH₂-OH (1-140a) + HO-CH₂-CH₂-OH (1-141a) → HO-CH₂-CH₂-OH (1-142a)

HO-CH₂-CH₂-OH (1-142a) + HO-CH₂-CH₂-OH (1-143a) → HO-CH₂-CH₂-OH (1-144a)

HO-CH₂-CH₂-OH (1-144a) + HO-CH₂-CH₂-OH (1-145a) → HO-CH₂-CH₂-OH (1-146a)

HO-CH₂-CH₂-OH (1-146a) + HO-CH₂-CH₂-OH (1-147a) → HO-CH₂-CH₂-OH (1-148a)

HO-CH₂-CH₂-OH (1-148a) + HO-CH₂-CH₂-OH (1-149a) → HO-CH₂-CH₂-OH (1-150a)

HO-CH₂-CH₂-OH (1-150a) + HO-CH₂-CH₂-OH (1-151a) → HO-CH₂-CH₂-OH (1-152a)

HO-CH₂-CH₂-OH (1-152a) + HO-CH₂-CH₂-OH (1-153a) → HO-CH₂-CH₂-OH (1-154a)

HO-CH₂-CH₂-OH (1-154a) + HO-CH₂-CH₂-OH (1-155a) → HO-CH₂-CH₂-OH (1-156a)

HO-CH₂-CH₂-OH (1-156a) + HO-CH₂-CH₂-OH (1-157a) → HO-CH₂-CH₂-OH (1-158a)

HO-CH₂-CH₂-OH (1-158a) + HO-CH₂-CH₂-OH (1-159a) → HO-CH₂-CH₂-OH (1-160a)

HO-CH₂-CH₂-OH (1-160a) + HO-CH₂-CH₂-OH (1-161a) → HO-CH₂-CH₂-OH (1-162a)

HO-CH₂-CH₂-OH (1-162a) + HO-CH₂-CH₂-OH (1-163a) → HO-CH₂-CH₂-OH (1-164a)

HO-CH₂-CH₂-OH (1-164a) + HO-CH₂-CH₂-OH (1-165a) → HO-CH₂-CH₂-OH (1-166a)

HO-CH₂-CH₂-OH (1-166a) + HO-CH₂-CH₂-OH (1-167a) → HO-CH₂-CH₂-OH (1-168a)

HO-CH₂-CH₂-OH (1-168a) + HO-CH₂-CH₂-OH (1-169a) → HO-CH₂-CH₂-OH (1-170a)

HO-CH₂-CH₂-OH (1-170a) + HO-CH₂-CH₂-OH (1-171a) → HO-CH₂-CH₂-OH (1-172a)

HO-CH₂-CH₂-OH (1-172a) + HO-CH₂-CH₂-OH (1-173a) → HO-CH₂-CH₂-OH (1-174a)

HO-CH₂-CH₂-OH (1-174a) + HO-CH₂-CH₂-OH (1-175a) → HO-CH₂-CH₂-OH (1-176a)

HO-CH₂-CH₂-OH (1-176a) + HO-CH₂-CH₂-OH (1-177a) → HO-CH₂-CH₂-OH (1-178a)

HO-CH₂-CH₂-OH (1-178a) + HO-CH₂-CH₂-OH (1-179a) → HO-CH₂-CH₂-OH (1-180a)

HO-CH₂-CH₂-OH (1-180a) + HO-CH₂-CH₂-OH (1-181a) → HO-CH₂-CH₂-OH (1-182a)

HO-CH₂-CH₂-OH (1-182a) + HO-CH₂-CH₂-OH (1-183a) → HO-CH₂-CH₂-OH (1-184a)

HO-CH₂-CH₂-OH (1-184a) + HO-CH₂-CH₂-OH (1-185a) → HO-CH₂-CH₂-OH (1-186a)

HO-CH₂-CH₂-OH (1-186a) + HO-CH₂-CH₂-OH (1-187a) → HO-CH₂-CH₂-OH (1-188a)

HO-CH₂-CH₂-OH (1-188a) + HO-CH₂-CH₂-OH (1-189a) → HO-CH₂-CH₂-OH (1-190a)

HO-CH₂-CH₂-OH (1-190a) + HO-CH₂-CH₂-OH (1-191a) → HO-CH₂-CH₂-OH (1-192a)

HO-CH₂-CH₂-OH (1-192a) + HO-CH₂-CH₂-OH (1-193a) → HO-CH₂-CH₂-OH (1-194a)

HO-CH₂-CH₂-OH (1-194a) + HO-CH₂-CH₂-OH (1-195a) → HO-CH₂-CH₂-OH (1-196a)

HO-CH₂-CH₂-OH (1-196a) + HO-CH₂-CH₂-OH (1-197a) → HO-CH₂-CH₂-OH (1-198a)

HO-CH₂-CH₂-OH (1-198a) + HO-CH₂-CH₂-OH (1-199a) → HO-CH₂-CH₂-OH (1-200a)

HO-CH₂-CH₂-OH (1-200a) + HO-CH₂-CH₂-OH (1-201a) → HO-CH₂-CH₂-OH (1-202a)

HO-CH₂-CH₂-OH (1-202a) + HO-CH₂-CH₂-OH (1-203a) → HO-CH₂-CH₂-OH (1-204a)

HO-CH₂-CH₂-OH (1-204a) + HO-CH₂-CH₂-OH (1-205a) → HO-CH₂-CH₂-OH (1-206a)

HO-CH₂-CH₂-OH (1-206a) + HO-CH₂-CH₂-OH (1-207a) → HO-CH₂-CH₂-OH (1-208a)

HO-CH₂-CH₂-OH (1-208a) + HO-CH₂-CH₂-OH (1-209a) → HO-CH₂-CH₂-OH (1-210a)

HO-CH₂-CH₂-OH (1-210a) + HO-CH₂-CH₂-OH (1-211a) → HO-CH₂-CH₂-OH (1-212a)

HO-CH₂-CH₂-OH (1-212a) + HO-CH₂-CH₂-OH (1-213a) → HO-CH₂-CH₂-OH (1-214a)

HO-CH₂-CH₂-OH (1-214a) + HO-CH₂-CH₂-OH (1-215a) → HO-CH₂-CH₂-OH (1-216a)

HO-CH₂-CH₂-OH (1-216a) + HO-CH₂-CH₂-OH (1-217a) → HO-CH₂-CH₂-OH (1-218a)

HO-CH₂-CH₂-OH (1-218a) + HO-CH₂-CH₂-OH (1-219a) → HO-CH₂-CH₂-OH (1-220a)

HO-CH₂-CH₂-OH (1-220a) + HO-CH₂-CH₂-OH (1-221a) → HO-CH₂-CH₂-OH (1-222a)

HO-CH₂-CH₂-OH (1-222a) + HO-CH₂-CH₂-OH (1-223a) → HO-CH₂-CH₂-OH (1-224a)

HO-CH₂-CH₂-OH (1-224a) + HO-CH₂-CH₂-OH (1-225a) → HO-CH₂-CH₂-OH (1-226a)

HO-CH₂-CH₂-OH (1-226a) + HO-CH₂-CH₂-OH (1-227a) → HO-CH₂-CH₂-OH (1-228a)

HO-CH₂-CH₂-OH (1-228a) + HO-CH₂-CH₂-OH (1-229a) → HO-CH₂-CH₂-OH (1-230a)

HO-CH₂-CH₂-OH (1-230a) + HO-CH₂-CH₂-OH (1-231a) → HO-CH₂-CH₂-OH (1-232a)

HO-CH₂-CH₂-OH (1-232a) + HO-CH₂-CH₂-OH (1-233a) → HO-CH₂-CH₂-OH (1-234a)

HO-CH₂-CH₂-OH (1-234a) + HO-CH₂-CH₂-OH (1-235a) → HO-CH₂-CH₂-OH (1-236a)

HO-CH₂-CH₂-OH (1-236a) + HO-CH₂-CH₂-OH (1-237a) → HO-CH₂-CH₂-OH (1-238a)

HO-CH₂-CH₂-OH (1-238a) + HO-CH₂-CH₂-OH (1-239a) → HO-CH₂-CH₂

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Reaction Structure substructure > reactions (9)
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REACTIONS 1

Analyze Surface

Analyze by: 1

Report

Et₃N 9

K₂CO₃ 6

EDM(Ph)₂ 2

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Group by: No Grouping Sort by: Relevance ▾

1 of 9 reactions Selected

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Single Step: Hover over any structure for more options.

Overview

MethodNow™

Procedure

1. Stir the mixture of 7-ethyl-4-methyl-2-methylcoumarin-3-one (400 mg, 1.65 mmol), 1-azidodecane (308 mg, 1.82 mmol), copper(II) sulfate pentahydrate (42 mg, 0.17 mmol), (+)-sodium-L-ascorbate (360 mg, 1.82 mmol) in t-BuOH/water (15 mL/25 mL) at room temperature for 4 hours.

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Available Experimental Data

¹H NMR, ¹³C NMR, IR, HRMS, Mass Spec, MP

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METHODS

Return to Home

- Analyte
 - Atorvastatin (227)
 - Atorvastatin calcium (211)
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 - Fenofibrate (46)
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- Matrix
 - Pharmaceutical tablets (293)
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- Method Category
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 - Reversed-phase HPLC (152)
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 - HPLC (57)
 - Liquid chromatographic UV detectors (43)
 - [View All](#)

Results (528) Sort Relevance

☐ ☐

☐ Analysis of Atorvastatin in Blood plasma by High-performance thin layer chromatography
CAS MN: 1-101-CAS-1389

Analyte	Atorvastatin
Matrix	Blood plasma
Other Materials	Material: 60 F ₂₅₄ silica gel HPTLC plates
Method Category	Active Pharmaceutical Ingredient and Metabolite Analysis
Technique	High-performance thin layer chromatography
Equipment Used	Automatic TLC Sampler 3
Source	HPTLC determination of atorvastatin in plasma Jamshidi, A.; Nateghi, A.R. Chromatographia (2007), 65 (11/12), 763-766. View at Verlag/GWV Fachverlage GmbH

单独的分析界面

提纲

- 美国化学文摘社简介
- SciFinder简介及检索方式
 - 文献检索
 - 物质检索
 - Markush检索
 - 反应检索
 - SciPlanner
- SciFinder常见问题及解决

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工具栏

The screenshot shows the SciFinder web interface. At the top, there is a header bar with the SciFinder logo and navigation links like 'Explore', 'Saved Searches', and 'SciPlanner'. A search input field is prominently displayed in the center, with a 'Search' button below it. On the left, a sidebar lists various search categories: REFERENCES, SUBSTANCES, and REACTIONS. On the right, there is a section for 'SAVED ANSWER SETS' showing a list of saved searches. Annotations in Chinese point to specific features: '检索入口' (Search Entry) points to the search input field; '工具栏' (Toolbar) points to the top navigation bar; '已保存的结果集' (Saved Results) points to the 'SAVED ANSWER SETS' section; '定题追踪' (Topic Tracking) points to the 'KEEP ME POSTED' section; and '检索完，请点击退出' (After search, click exit) points to the 'Sign Out' button in the top right corner.

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REFERENCES

- Research Topic
- Author Name
- Company Name
- Document Identifier
- Journal
- Patent
- Tags

SUBSTANCES

- Chemical Structure
- Markush
- Molecular Formula
- Property
- Substance Identifier

REACTIONS

- Reaction Structure

REFERENCES: RESEARCH TOPIC

Examples:
The effect of antibiotic residues on dairy products
Photocyanation of aromatic compounds

[Search](#)

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SAVED ANSWER SETS

- CSF1R
- jmc
- EP 19870107847
- Daclatasvir-1
- SUB result
- EX result
- MF result
- polymer1
- polymer1
- structure search
- Autosaved Substance Set

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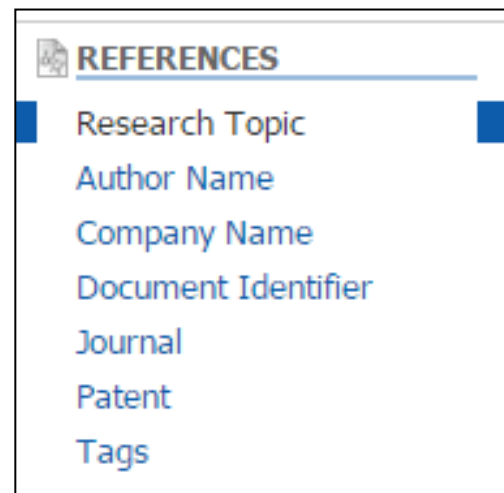
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- 机构名检索
- 文献标识符检索
- 期刊名称和专利信息（公开号，申请号等）
- 从物质，反应获得文献



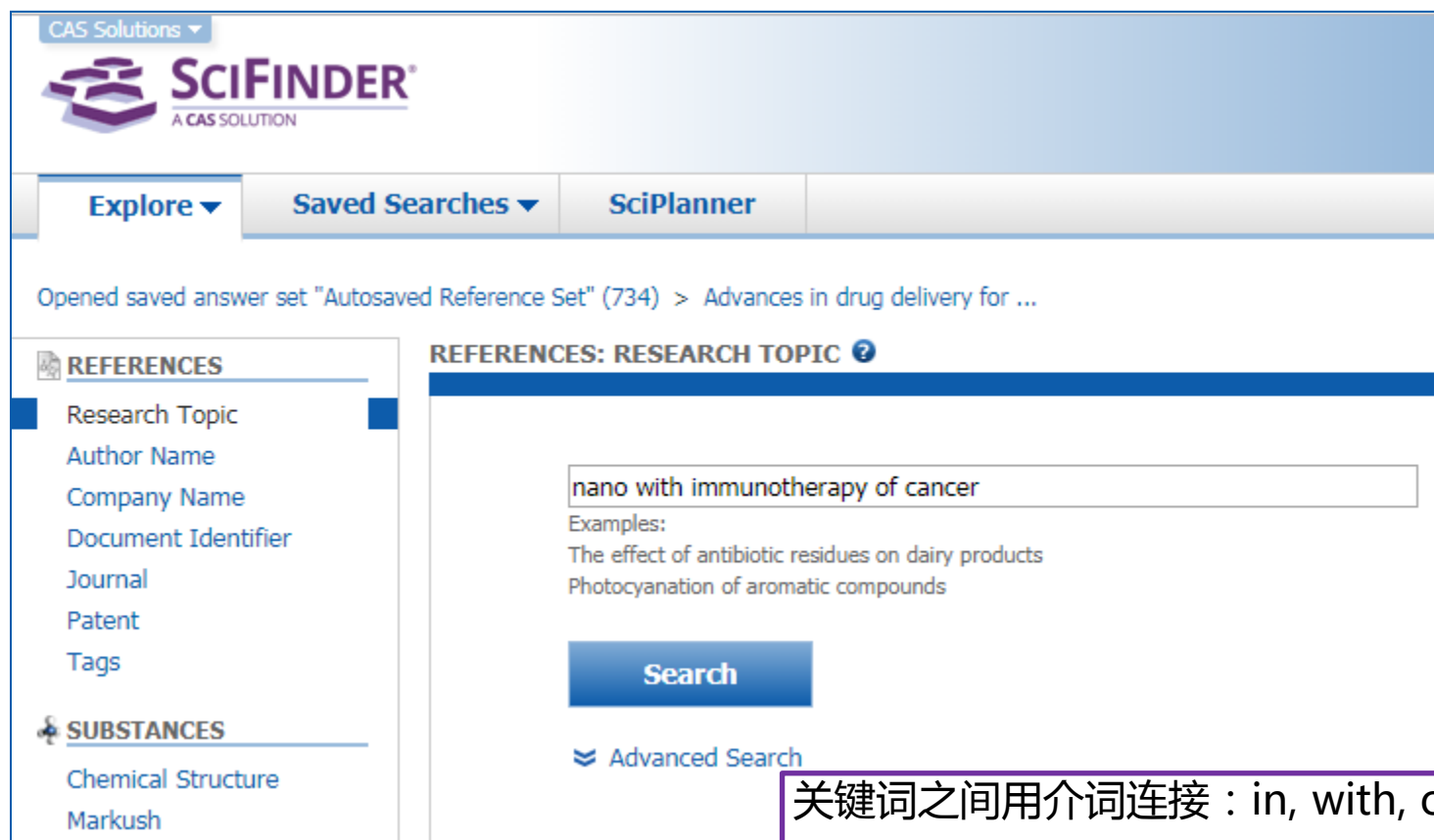
■ 检索策略推荐

- 关注某特定领域的文献：主题检索
- 关注物质有关的文献：先获得物质，再获得文献
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- 关注某机构科研进展：机构名检索

文献检索——主题

主题检索：纳米技术在癌症免疫疗法中的应用

检索式：nano with Immunotherapy of cancer




The screenshot displays the SciFinder web interface. At the top, the 'CAS Solutions' logo and 'SciFINDER A CAS SOLUTION' are visible. Below the header, there are tabs for 'Explore', 'Saved Searches', and 'SciPlanner'. The 'Explore' tab is active, showing a breadcrumb trail: 'Opened saved answer set "Autosaved Reference Set" (734) > Advances in drug delivery for ...'. On the left side, there is a sidebar with two main sections: 'REFERENCES' and 'SUBSTANCES'. Under 'REFERENCES', there is a list of search criteria: 'Research Topic', 'Author Name', 'Company Name', 'Document Identifier', 'Journal', 'Patent', and 'Tags'. Under 'SUBSTANCES', there are 'Chemical Structure' and 'Markush'. The main content area is titled 'REFERENCES: RESEARCH TOPIC ?'. It features a search input field containing the text 'nano with immunotherapy of cancer'. Below the input field, there are 'Examples:' listed as 'The effect of antibiotic residues on dairy products' and 'Photocyanation of aromatic compounds'. A blue 'Search' button is positioned below the examples. At the bottom of the main area, there is a link for 'Advanced Search'.

关键词之间用介词连接：in, with, of...

主题检索的候选项

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Research Topic "nano with immunotherapy of can..."

REFERENCES ?

Select All Deselect All

1 of 11 Research Topic Candidates Selected

		References
<input checked="" type="checkbox"/>	744 references were found containing all of the concepts "nano", "immunotherapy" and "cancer" closely associated with one another.	744
<input type="checkbox"/>	2734 references were found where all of the concepts "nano", "immunotherapy" and "cancer" were present anywhere in the reference.	2734
<input type="checkbox"/>	1697 references were found containing the two concepts "nano" and "immunotherapy" closely associated with one another.	1697
<input type="checkbox"/>	4144 references were found where the two concepts "nano" and "immunotherapy" were present anywhere in the reference.	4144
<input type="checkbox"/>	63058 references were found containing the two concepts "nano" and "cancer" closely associated with one another.	63058
<input type="checkbox"/>	109454 references were found where the two concepts "nano" and "cancer" were present anywhere in the reference.	109454
<input type="checkbox"/>	50122 references were found containing the two concepts "immunotherapy" and "cancer" closely associated with one another.	50122
<input type="checkbox"/>	97303 references were found where the two concepts "immunotherapy" and "cancer" were present anywhere in the reference.	97303
<input type="checkbox"/>	2318356 references were found containing the concept "nano".	2318356
<input type="checkbox"/>	187476 references were found containing the concept "immunotherapy".	187476
<input type="checkbox"/>	4775515 references were found containing the concept "cancer".	4775515

Get References

“Concepts”表示对主题词做了同义词的扩展；

“Closely associated with one another”表示同时出现在一个句子中；

“were present anywhere in the reference”表示同时出现在一篇文献中；

按被引次数排序— Citing References

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Research Topic "nano with immunotherapy of can..." > references (580)

REFERENCES ?

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Sort by: Citing References

Analyze by: Author Name

Lu Xiaoling 18

Zhao Yongxiang 17

Liu Zhuang 9

Lim Yong Taik 8

Santos Helder A 7

Xu Ligeng 7

Ito Atsuo 6

Shahbazi Mohammad Ali 6

Wang Chao 6

Wang Xiupeng 6

1. Photothermal Cancer Therapy: Impending Clinical Impact

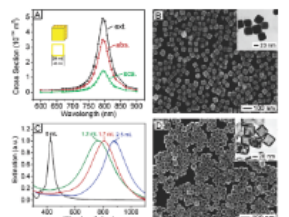
By Lal, Surbhi; Clare, Susan E.; Halas, Naomi J.
From Accounts of Chemical Research (2008), 41(12), 1842-1851. | Language: English, Database: CAPLUS

A review. Much of the current excitement surrounding **nanoscience** is directly connected to the promise of new **nanoscale** applications in **cancer** diagnostics and therapy. Because of their strongly resonant light-absorbing and light-scattering properties that depend on shape, noble metal **nanoparticles** provide a new and powerful tool for innovative light-based approaches. **Nanoshells**-spherical, dielec. core, gold shell **nanoparticles**-have been central to the development of photothermal **cancer** therapy and diagnostics for the past several years. By manipulating **nanoparticle** shape, researchers can tu...

2. Immuno Gold Nanocages with Tailored Optical Properties for Targeted Photothermal Destruction of Cancer Cells

By Chen, Jingyi; Wang, Danling; Xi, Jiefeng; Au, Leslie; Siekkinen, Andy; Warsen, Addie; Li, Zhi-Yuan; Zhang, Hui; Xia, Younan; Li, Xingde
From Nano Letters (2007), 7(5), 1318-1322. | Language: English, Database: CAPLUS

Gold **nanocages** with a relatively small size (e.g., ~45 nm in edge length) have been developed, and the structure of these **nanocages** was tailored to achieve strong absorption in the near-IR (NIR) region for photothermal **cancer** treatment. Numerical calcs. show that the **nanocage** has a large absorption cross section of $3.48 \times 10^{-14} \text{ m}^2$, facilitating conversion of NIR irradiation into heat. The gold **nanocages** were conjugated with monoclonal antibodies (anti-HER2) to target epidermal growth factor receptors (EGFR) that are overexpressed on the surface of breast **cancer** cells (SK-BR-3). Our preliminary p...



Citing Reference: 帮助找到最重要的文献

文献检索结果

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Research Topic "nano with immunotherapy of can..."

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Lu Xiaoling 18

Zhao Yongxiang 17

Liu Zhuang 9

Lim Yong Taik 8

Santos Helder A 7

Xu Ligeng 7

Ito Atsuo 6

Shahbazi Mohammad Ali 6

Wang Chao 6

Wang Xiupeng 6

1. Biodegradable Polymeric Nanoparticles for Therapeutic Cancer Treatments

Quick View Other Sources

By Karlsson, Johan; Vaughan, Hannah J.; Green, Jordan J.
From Annual Review of Chemical and Biomolecular Engineering (2018), Ahead of Print. | Language: English, Database: CAPLUS

Polymeric **nanoparticles** have tremendous potential to improve the efficacy of **therapeutic cancer** treatments by facilitating targeted delivery to a desired site. The phys. and chem. properties of polymers can be tuned to accomplish delivery across the multiple biol. barriers required to reach diverse subsets of cells. The use of biodegradable polymers as **nanocarriers** is esp. attractive, as these materials can be designed to break down in physiol. conditions and engineered to exhibit triggered functionality when at a particular location or activated by an external source. We present how biodeg...

2. Inactivated Sendai virus (HVJ-E) immobilized electrospun nanofiber for cancer therapy

Quick View Other Sources

By Okada, Takaharu; Niiyama, Eri; Uto, Koichiro; Aoyagi, Takao; Ebara, Mitsuhiro
From Materials (2016), 9(1), 12/1-12/11. | Language: English, Database: CAPLUS

Inactivated Hemagglutinating Virus of Japan Envelope (HVJ-E) was immobilized on electrospun **nanofibers** of poly(ε-caprolactone) by layer-by-layer (LbL) assembly technique. The precursor LbL film was first constructed with poly-L-lysine and alginate acid via electrostatic interaction. Then the HVJ-E particles were immobilized on the cationic PLL outermost surface. The HVJ-E adsorption was confirmed by surface wettability test, scanning laser microscopy, SEM, and confocal laser microscopy. The immobilized HVJ-E particles were released from the **nanofibers** under physiol. condition. In vitro cy...

3. A prospective highlight on exosomal nanoshuttles and cancer immunotherapy and vaccination

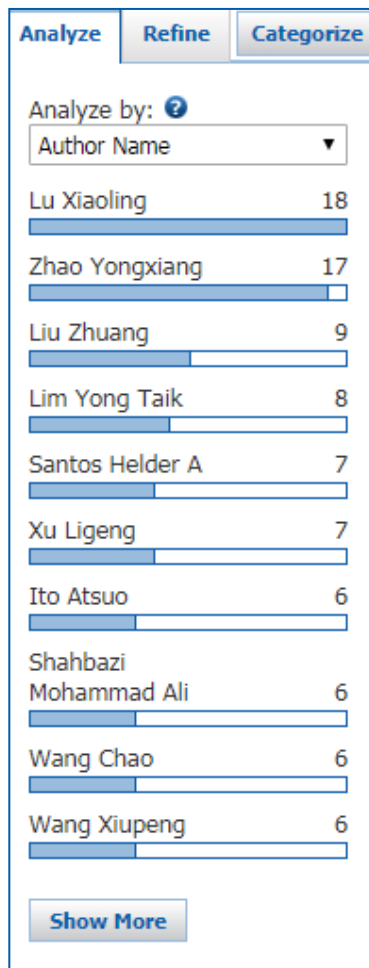
Quick View Other Sources

By Rafi, Mohammad A.; Omid, Yadollah
From BioImpacts (2015), 5(3), 117-122. | Language: English, Database: CAPLUS

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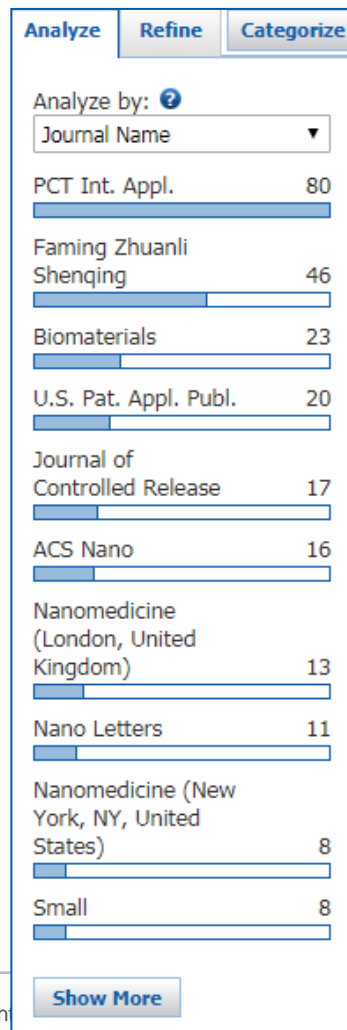
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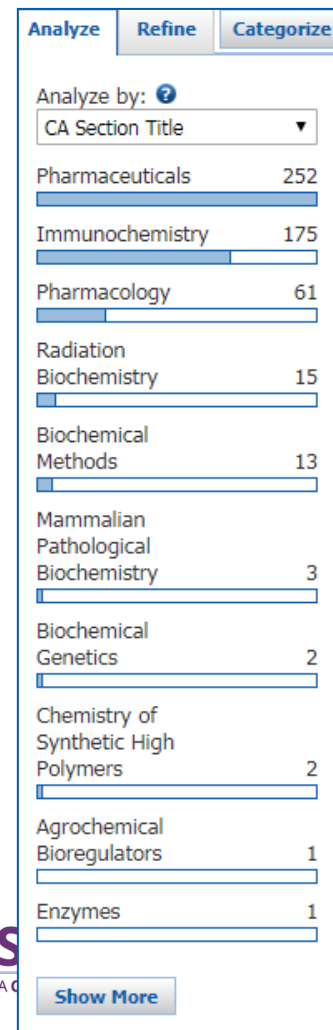
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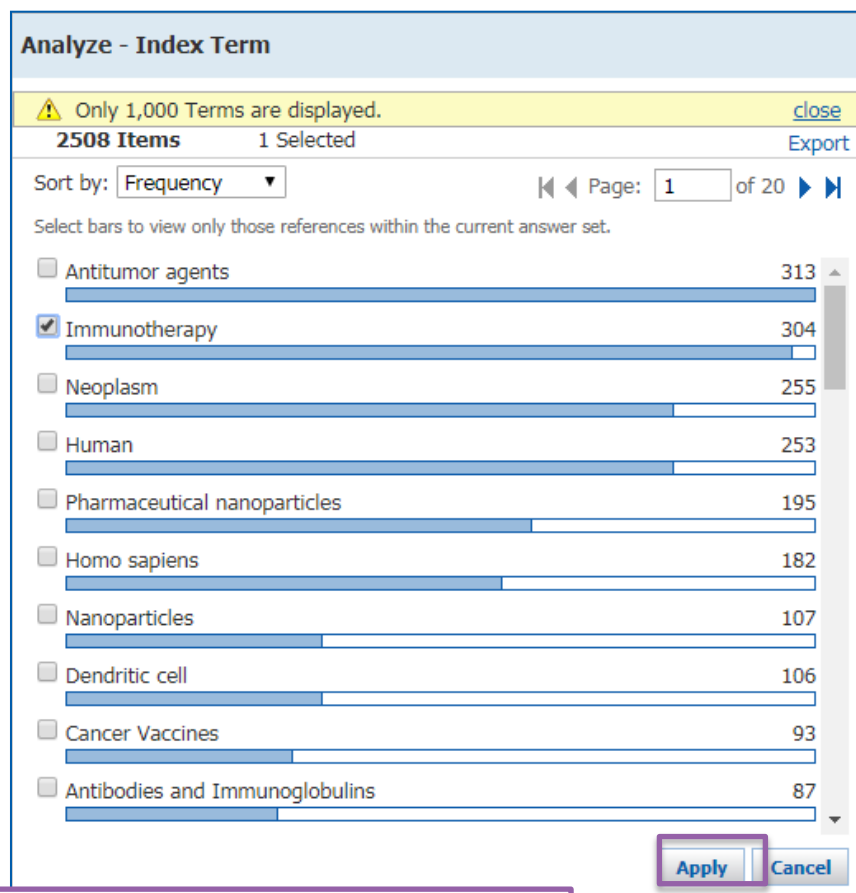
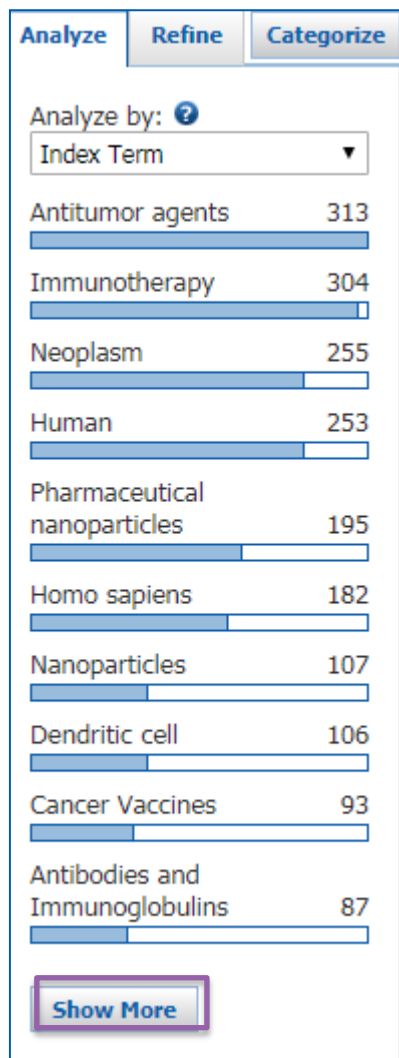
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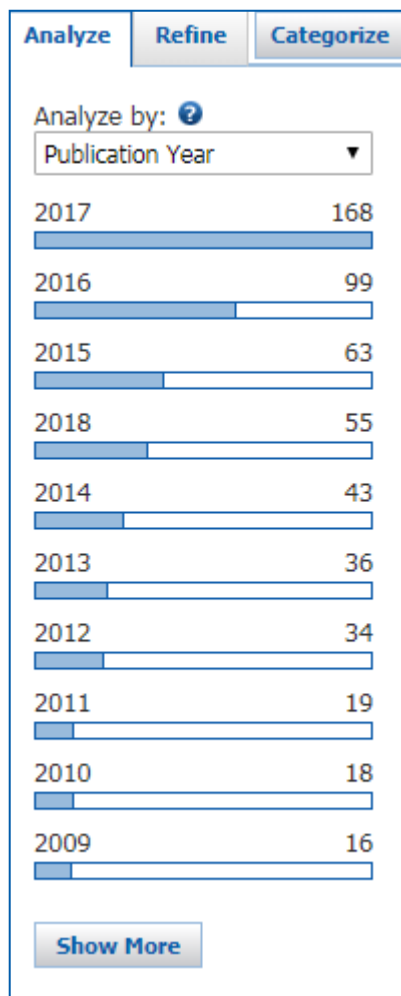


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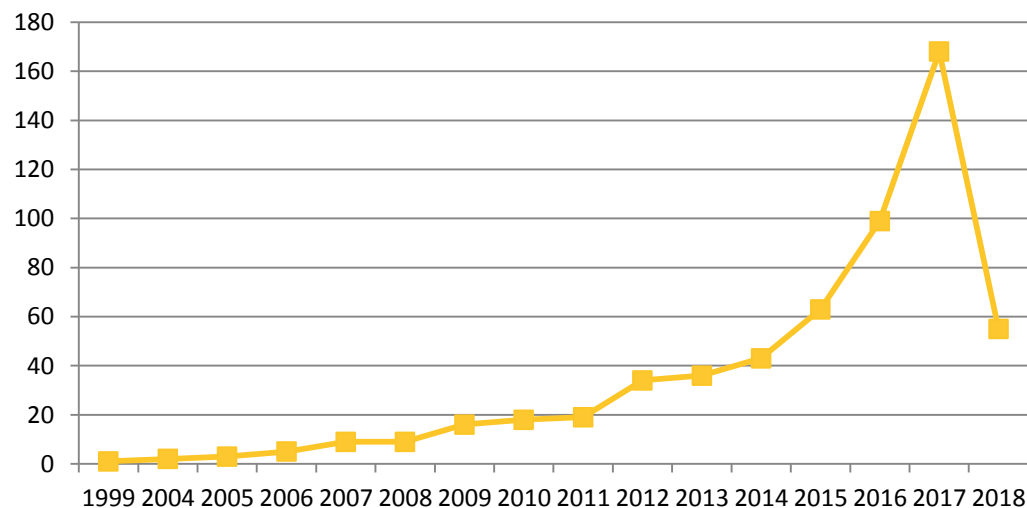


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Analyze **Refine** Categorize

Refine by: ?

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☐ Author

☐ Company Name

☒ Document Type

☐ Publication Year

☐ Language

☐ Database

Document Type(s)

☐ Biography

☐ Book

☐ Clinical Trial

☐ Commentary

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☐ Preprint

☐ Report

☒ Review

Refine

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1. **Nanoscale artificial antigen presenting cells for cancer immunotherapy**
Quick View Other Sources
By Rhodes, Kelly R.; Green, Jordan J.
From Molecular Immunology (2018), Ahead of Print. | Language: English, Database: CAPLUS
A review. Exciting developments in **cancer nanomedicine** include the engineering of **nanocarriers** to deliver drugs locally to tumors, increasing efficacy and reducing off-target toxicity assocd. with chemotherapies. Despite **nanocarrier** advances, metastatic **cancer** remains challenging to treat due to barriers that prevent **nanoparticles** from gaining access to remote, dispersed, and poorly vascularized metastatic tumors. Instead of relying on **nanoparticles** to directly destroy every tumor cell, **immunotherapeutic** approaches target immune cells to train them to recognize and destroy tumor cells, whic...

2. **Current trends and developments for nanotechnology in cancer**
Quick View Other Sources
By Ferreira, Monica; Almeida, Patrick; Shahbazi, Mohammad-Ali; Correia, Alexandra; Santos, Helder A.
Edited by Vale, Nuno
From Biomedical Chemistry (2016), 290-342. | Language: English, Database: CAPLUS
A review. In spite of the incessant development in medicine and technol., **cancer** continues to be one of the leading causes of death worldwide. Conventional systems for **cancer** therapy that are available in the market have limited and unspecific access to tumor sites. Thus, in the recent years, **nanotechnol.** has been applied to the field of medicine, opening new avenues to the treatment, diagnosis, and monitoring of **cancer** diseases. This horizon has become closer with a considerable no. of **nano**-formulations being recently approved for commercialization or reaching preclin. and clin. stages. ...

3. **Leveraging Engineering of Cells for Drug Delivery**
Quick View Other Sources
By Chen, Zhaowei; Hu, Quanyin; Gu, Zhen
From Accounts of Chemical Research (2018), 51(3), 668-677. | Language: English, Database: CAPLUS

Cell therapy has become a momentum-gathering treatment strategy for a variety of diseases, including **cancer**, diabetes, hemophilia, and cardiomyopathy. However, clin. applications of conventional cell therapies have often been compromised by rapid decline in viability and function of the transplanted cells due to host recognition and subsequent foreign body rejection. Along this line, cell engineering technologies such as cell encapsulation within microcapsules and immobilization in porous scaffolds have been implemented to address the immunosuppression concerns. As a recent emerging researc...

4. **The potential of nanoparticle vaccines as a treatment for cancer**

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主分类

学科领域
副分类

Index Term

选中的Index Term

Categorize ?

1. Select a heading and category.

Category Heading	Category
All	Substances in technology (926)
Genetics & protein chemistry	Materials & products (136)
Biotechnology	Processes & apparatus (78)
Biology	Metallurgy (73)
Physical chemistry	Imaging & recording (23)
Synthetic chemistry	Formed, removed, & other substances (32)
General chemistry	Ceramics (2)
Analytical chemistry	
Technology	
Polymer chemistry	
Environmental chemistry	
Catalysis	

2. Select index terms of interest.

Index Terms		Selected Terms
Select All	Deselect All	
<input type="checkbox"/>	Imaging agents 20	Click 'x' to remove the category from 'Selected Terms'
<input checked="" type="checkbox"/>	Tumor imaging 19	✖ Technology > Imaging & recording (1 Terms)
<input type="checkbox"/>	Imaging 17	
<input type="checkbox"/>	NMR imaging 14	
<input type="checkbox"/>	Fluorescence imaging 12	
<input type="checkbox"/>	Fluorescence microscopy 5	
<input type="checkbox"/>	Single-photon-emission computed tomography 5	
<input type="checkbox"/>	Infrared imaging 4	
<input type="checkbox"/>	NMR imaging agents 4	
<input type="checkbox"/>	Positron emission tomography 4	
<input type="checkbox"/>	Photoacoustic imaging 3	
<input type="checkbox"/>	Autoradiography 2	
<input type="checkbox"/>	Radiography 2	
<input type="checkbox"/>	Tomography 2	

Technology > Imaging & recording > 1 Index Term(s) Selected

OK Cancel

Categorize学科分类功能，基于Index Term，根据大学科方向对文献进行自动分类。

结果集的保存— Save, Print, Export

Searches ▾ SciPlanner Save Print Export

therapy of can..." > references (580) > refine by categories > Early cancer detection and enh...

Get Substances Get Reactions Get Related Citations Tools

Create Keep Me Posted Alert Send to SciPlanner

Sort by: Accession Number

0 of 19 References Selected

1. **Nanotechnology Strategies To Advance Outcomes in Clinical Cancer Care**
Quick View [f] Other Sources
By Hartshorn, Christopher M.; Bradbury, Michelle S.; Lanza, Gregory M.; Nel, Andre E.; Rao, Jianghong; Wang, Andrew Z.; Wiesner, Ulrich B.; Yang, Lily; Grodzinski, Piotr
From ACS Nano (2018), 12(1), 24-43. | Language: English, Database: CAPLUS

2. **Early cancer detection and enhanced immunotherapy/thermotherapy/ optionally gene delivery combination**
Quick View [f] Other Sources
By Peyman, Gholam A.
From U.S. Pat. Appl. Publ. (2017), US 20170172932 A1 20170622. | Language: English, Database: CAPLUS

3. **Nanomaterial-based cancer immunotherapy**
Quick View [f] Other Sources
By Luo, Lijia; Shu, Rui; Wu, Aiguo
From Journal of Materials Chemistry B: Materials for Biology and Medicine (2017), 5(28), 5517-5531. | Language: English, Database: CAPLUS

文献详细信息

Save : 保存在服务器上, 方便以后登陆查看, 每次可存2万条记录。

Export : 导出至本地电脑。

Print : 打印成PDF格式

Citation manager: 保存成RIS等格式, 可导入EndNote 等文献管理工具

Offline Review : 保存成PDF, RTF等格式, 用于脱机浏览

Export

Export:

☒ All
☐ Selected
☐ Range
Example: 2-20

For:

Citation Manager

☐ Citation export format (*.ris)
☐ Quoted Format (*.bt)
☐ Tagged Format (*.bt)

Offline review

☒ Portable Document Format (*.pdf)
☐ Rich Text Format (*.rtf)
☐ Answer Keys (*.bt)

Saving locally

☐ Answer Key eXchange (*.afx)

Details:

* Required

File Name: *

Reference_06_19_2012_100848

Format:

☐ Summary without abstracts
☐ Summary with partial abstracts
☒ Summary with full abstracts
☐ Detail (full record)

Include:

☐ Task History
☐ Tags
☐ Comments

Export Cancel

文献信息—题录、摘要、索引

2. Early cancer detection and enhanced immunotherapy/thermotherapy/ optionally gene delivery combination

By: Peyman, Gholam A.
Assignee: USA

Provided is a method of therapy for a tumor or other pathol. by administering a combination of thermotherapy and immunotherapy optionally combined with gene delivery. The controlled and precise application of thermal energy enhances gene transfer to any cell, whether the cell is a neoplastic cell, a pre-neoplastic cell, or a normal cell. The combination therapy beneficially treats the tumor and prevents tumor recurrence, either locally or at a different site, by boosting the patient's immune response both at the time or original therapy and/or for later therapy.

Patent Information

Patent No.	PatentPak Options	Kind	Language	Date	Application No.	Date
US 20170172932	PDF PDF+ Viewer	A1		Jun 22, 2017	US 2016-15143981	May 2, 2016
US 9849092	PDF	B2	English	Dec 26, 2017		
US 20170173191	PDF PDF+ Viewer	A1	English	Jun 22, 2017	US 2015-14976321	Dec 21, 2015

Priority Application


US 2015-14976321	A2	Dec 21, 2015
------------------	----	--------------

Indexing

Immunochimistry (Section15-3)
Section cross
Concepts 重要概念
Clustered regularly interspaced short palindromic repeat

Substances

重要物质

1425049-49-5 Cas9 nuclease  Page 21 in **PATENTPAK**

CRISPR/cas9 complex; early cancer detection and enhanced immunotherapy/thermotherapy/ optionally gene delivery combination

Therapeutic use; Biological study; Uses

QUICK LINKS

0 Tags, 0 Comments

PATENT INFORMATION

Jun 22, 2017
US 20170172932
A1

APPLICATION

May 2, 2016
US 2016-15143981

PRIORITY

Dec 21, 2015
US 2015-14976321

SOURCE

U.S. Pat. Appl. Publ.
22pp., Cont.-in-part of U.S.
Ser. No. 976,321.
Patent
2017
CODEN:USXXCO

ACCESSION NUMBER

2017:1034814
CAN167:99362
CAPLUS

LANGUAGE

English

文献详情界面包括：

1. 标题
2. 摘要
3. 文献中重要的技术术语
4. 文献中重要的物质
5. 书目信息
6. 获得文献中的物质，反应
7. 参考文献
8. 链接原文

文献检索小结

- 主题检索时，使用介词 in, with, of 等作为连接词
- 跟据检索要求选择合适的候选项
- 通过SciFinder 的Analyze/Refine功能来缩小检索的范围
- 尝试将不同的Analyze/Refine功能组合起来用，会有更多的收益
- 使用Categorize可以让系统来实现自动分类

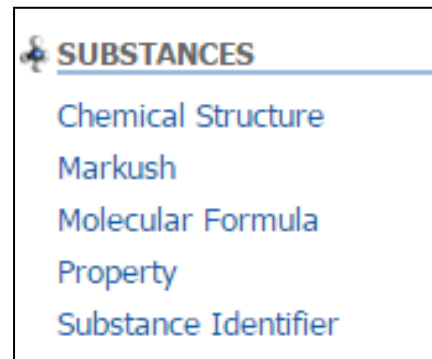
提纲

- 美国化学文摘社简介
- SciFinder简介及检索方式
 - 文献检索
 - 物质检索
 - Markush检索
 - 反应检索
 - SciPlanner
- SciFinder常见问题及解决

SciFinder检索选项——物质检索

■ 物质检索方法

- 结构式检索
- 分子式检索
- 理化性质检索
- 物质标识符检索：化学名称，CAS RN



■ 物质检索策略推荐

- 有机化合物，天然产物：结构检索
- 无机物，合金：分子式检索
- 高分子化合物：分子式检索和结构检索

物质检索——标识符检索



The screenshot displays the SciFinder web interface. At the top, there is a 'CAS Solutions' dropdown menu and the SciFinder logo with the tagline 'A CAS SOLUTION'. Below this is a navigation bar with 'Explore', 'Saved Searches', and 'SciPlanner' tabs. The left sidebar contains two main sections: 'REFERENCES' and 'SUBSTANCES'. Under 'REFERENCES', there are links for Research Topic, Author Name, Company Name, Document Identifier, Journal, Patent, and Tags. Under 'SUBSTANCES', there are links for Chemical Structure, Markush, Molecular Formula, Property, and Substance Identifier. The 'SUBSTANCES: SUBSTANCE IDENTIFIER' section is active, showing a search input field with the text 'qinghaosu'. Below the input field, there is a note 'Enter one per line.' and examples: '50-00-0', '999815', and 'Acetaminophen'. A blue 'Search' button is located at the bottom of the search area.

提示：

1. 一次最多可输入25个物质。
2. 每行一个物质标识符。

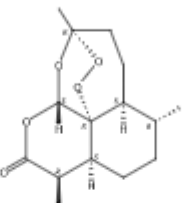
物质标识符包括CAS RN和化学名称，化学名称可以是通用名称、商品名、俗名。

SciFinder中的物质记录

点击CAS RN 获得物质详细信息

1. **63968-64-9** 🔍

~4864 📄 ~131 🧪



Absolute stereochemistry.

C₁₅ H₂₂ O₅
3,12-Epoxy-12H-pyrano[4,3-f]-1,2-benzodioxepin-10(3H)-one, octahydro-3,6,9-trimethyl-, (3R,5aS,6R,8aS,9R,12S,12aR)-

▶ **Key Physical Properties**
Regulatory Information
Spectra
Experimental Properties

CAS Registry Number: 63968-64-9

- View Substance Detail
- Explore by Structure ▶
- Synthesize this...
- Get Reactions where Substance is a ▶
- Get Commercial Sources
- Get Regulatory Information
- Get References
- Export as Image
- Export as molfile
- Send to SciPlanner

在SciFinder中，鼠标滑过物质，即可打开物质标准菜单，获得与物质相关的所有内容

SciFinder中的物质记录

SUBSTANCE DETAIL ?

Get References

Get Reactions

Get Commercial Sources

[Return](#)

CAS Registry Number 63968-64-1

~4,864 ~131

C₁₅ H₂₂ O₅
 3,12-Epoxy-12*H*-pyrano[4,3-*j*]-1,2-benzodioxepin-10(3*H*)-one,
 octahydro-3,6,9-trimethyl-, (3*R*,5*a*,6*R*,8*a*,9*R*,12*S*,12*a**R*)-

Molecular Weight
 282.33

Melting Point (Experimental)
 Value: 156-157 °C

Boiling Point (Predicted)
 Value: 389.9±42.0 °C | Condition: Press: 760 Torr

Density (Experimental)
 Value: 1.300 g/cm³

Other Names
 3,12-Epoxy-12*H*-pyrano[4,3-*j*]-1,2-benzodioxepin-10(3*H*)-one,
 octahydro-3,6,9-trimethyl-, [3*R*-(3*a*,5*a*β,6β,8*a*β,9*a*,12β,12*a**R*^{*})]-
 (3*R*,5*a*,6*R*,8*a*,9*R*,12*S*,12*a**R*)-Octahydro-3,6,9-trimethyl-3,12-epoxy-
 12*H*-pyrano[4,3-*j*]-1,2-benzodioxepin-10(3*H*)-one
 (+)-Arteannuin
 (+)-Artemisinin
 (+)-Qinghaosu
[View more...](#)

Absolute stereochemistry.

物质详情

通过物质获得文献

分析化学
生物研究

Get References

Retrieve references for:

☒ All substances
☐ Selected substances

Limit results to:

<input type="checkbox"/> Adverse Effect, including toxicity	<input type="checkbox"/> Preparation
<input type="checkbox"/> Analytical Study	<input type="checkbox"/> Process
<input type="checkbox"/> Biological Study	<input type="checkbox"/> Properties
<input type="checkbox"/> Combinatorial Study	<input type="checkbox"/> Prophetic in Patents
<input type="checkbox"/> Crystal Structure	<input type="checkbox"/> Reactant or Reagent
<input type="checkbox"/> Formation, nonpreparative	<input type="checkbox"/> Spectral Properties
<input type="checkbox"/> Miscellaneous	<input type="checkbox"/> Uses
<input type="checkbox"/> Occurrence	

For each sequence, retrieve:

☐ Additional related references, e.g., activity studies, disease studies.

制备
工艺

谱图数据
用途



SCIFINDER®
A CAS SOLUTION

EXPERIMENTAL PROPERTIES

EXPERIMENTAL SPECTRA

实验数据与实验谱图

¹H NMR **¹³C NMR** Hetero NMR IR Mass Raman UV and Visible Additional Spectra

¹³C NMR Properties

	Value	Condition	Note
Carbon-13 NMR Spectrum	See spectrum		(3)ACD
Carbon-13 NMR Spectrum	See spectrum		(4)ACD
Carbon-13 NMR Spectrum	See full text	1 of 8	(5)CAS

Notes

(3) ACD: Spectral data were obtained from Advanced Chemistry Development, Inc.

(4) Han, Jaehong; Journal of Natural Products 2001, V64(9), P1201-1205 CAPLUS 🔍

(5) Yadav, J. S.; Tetrahedron 2010, V66(11), P2005-2009 CAPLUS 🔍

预测数据与预测谱图

PREDICTED PROPERTIES

PREDICTED SPECTRA

¹H NMR **¹³C NMR**

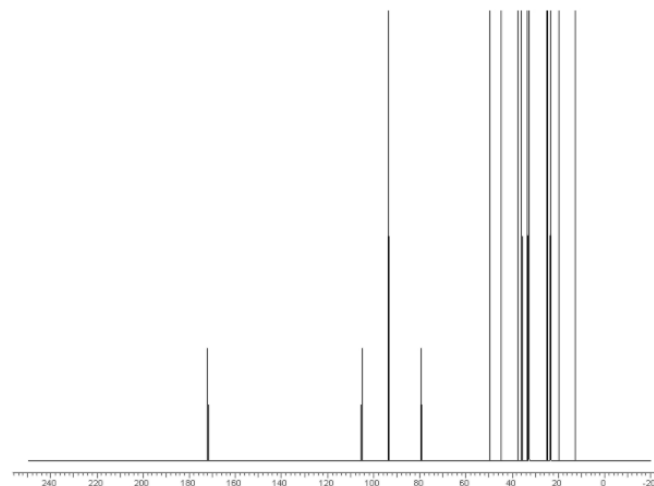
¹H NMR Properties

	Value
Proton NMR Spectrum	See spectrum

Notes

(28) Predicted NMR data calculated using Advanced Chemistry Development, Inc. (ACD/I

Carbon-13 NMR Spectrum



Print

SPECTRUM ID
7MED36_38.C

CAS REGISTRY NUMBER
63968-64-9

FORMULA
C₁₅ H₂₂ O₅

CAS INDEX NAME
3,12-Epoxy-12H-pyrano[4,3-β]-1,2-benzodioxepin-10(3H)-one, octahydro-3,6,9-trimethyl-, (3R,5aS,6R,8aS,9R,12S,12aR)-

NUCLEUS
13C

SOURCE
Spectral data were obtained from Advanced Chemistry Development, Inc.

物质检索——Property explore

https://scifinder.cas

CAS Solutions

SCIFINDER[®]
A CAS SOLUTION

Explore ▾ Saved Searches ▾

REFERENCES

- Research Topic
- Author Name
- Company Name
- Document Identifier
- Journal
- Patent
- Tags

SUBSTANCES

- Chemical Structure
- Markush
- Molecular Formula
- Property
- Substance Identifier

SUBSTANCE

Select Property...

- Bioconcentration Factor
- Boiling Point (°C)
- Density (g/cm³)
- Enthalpy of Vaporization (kJ/mol)
- Flash Point (°C)
- Freely Rotatable Bonds
- H Donor/Acceptor sum
- H Acceptors
- H Donors
- Koc
- logD
- logP
- Mass Intrinsic Solubility (g/L)
- Mass Solubility (g/L)
- Molar Intrinsic Solubility (mol/L)
- Molar Solubility (mol/L)
- Molar Volume (cm³/mol)
- Molecular Weight**
- pKa

Molecular Weight

250-400

Examples: 44, 25-35, >125

Search

nderExplore.jsf

Examples: 44, 25-35, >125

寻找分子量在250-400之间的物质

物质结果集的筛选——Refine

SUBSTANCES ?

Get References Get Reactions Get Commercial Sources Tools ▾

Analyze **Refine**

Sort by: CAS Registry Number ▾

☐ 0 of 45142315 Substances Selected

Refine by: ?

- ☒ Chemical Structure
- ☐ Isotope-Containing
- ☐ Metal-Containing
- ☐ Commercial Availability
- ☐ Property Availability
- ☐ Property Value
- ☐ Reference Availability
- ☐ Atom Attachment

Structure Editor:

Java Non-Java

Click to Edit

Search type: **Exact Structure**

Only retrieve substances

1. **1986293-22-4** 🔍

~0

C₁₅ H₁₇ Br N₂
3-Pyridinamine, 2-bromo-*N*-(3-phenylbutyl)-
▶ **Key Physical Properties**

2. **1986293-21-3** 🔍

~0

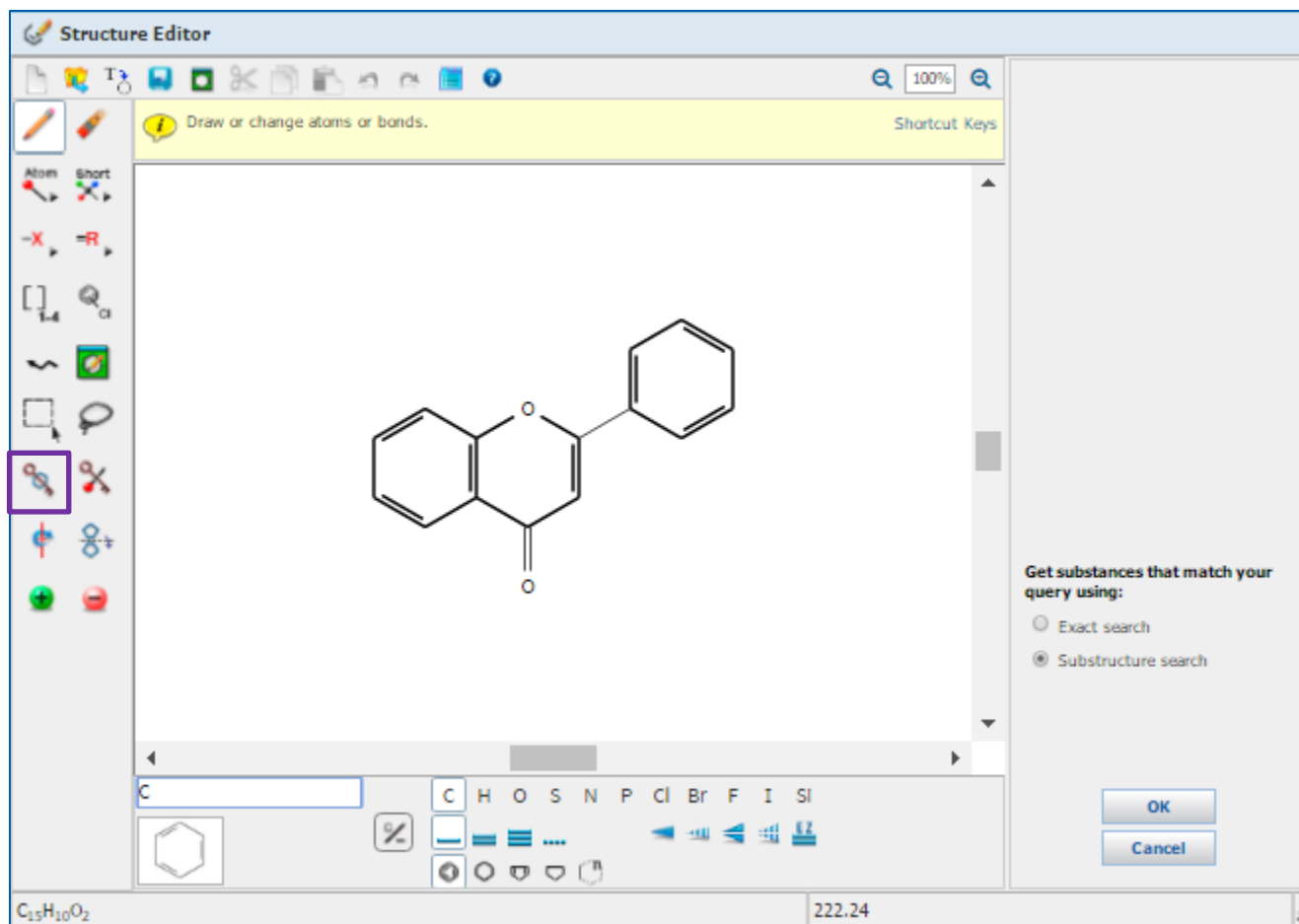
C₁₁ H₁₆ Cl F₂ N₃ O
4-Pyrimidinamine, *N*-(2-chloroethyl)-*N*-(2,2-difluoroethyl)-6-ethoxy-5-methyl-
▶ **Key Physical Properties**

4. **1986293-16-6** 🔍

5. **1986293-14-4** 🔍

4500多万个结构，
如何筛选黄酮类物质？

物质结果集的筛选——Refine



锁环工具：避免在被锁定的环结构上出现新的环结构

SUBSTANCES ?

Analyze Refine

Refine by: ?

- ☒ Chemical Structure
- ☐ Isotope-Containing
- ☐ Metal-Containing
- ☐ Commercial Availability
- ☐ Property Availability
- ☐ Property Value
- ☐ Reference Availability
- ☐ Atom Attachment

Structure Editor:

Java Non-Java

Click image to change structure or view detail.

Search type: **Substructure**

Only retrieve substances that:

- ☐ Have references
- ☐ Are commercially available
- ☒ Are a single component
- ☐ Are in specific substance classes
- ☐ Are in specific types of studies

Refine

物质检索结果集

Explore ▾ Saved Searches ▾ SciPlanner

Property "Predicted - Molecular Weight, ..." > substances (45142315) > refine "substructure" (16901)

SUBSTANCES ⓘ

Get References Get Reactions Get Commercial Sources Tools ▾

Analyze Refine

Sort by: Relevance ▾

0 of 16901 Substances Selected

Refine by: ⓘ

- Chemical Structure
- Isotope-Containing
- Metal-Containing
- Commercial Availability
- Property Availability
- Property Value
- Reference Availability
- Atom Attachment

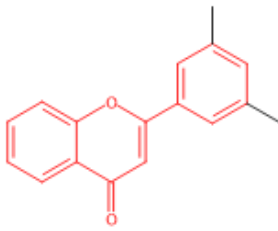
Structure Editor:

Java Non-Java

Click image to change structure or view detail.
Search type: Substructure

1. 1373355-19-1

~3

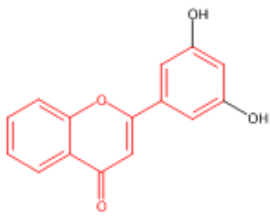


$C_{17}H_{14}O_2$
4/4'-1-Benzopyran-4-one, 2-(3,5-dimethylphenyl)-

Key Physical Properties

2. 912915-64-1

~6 ~3

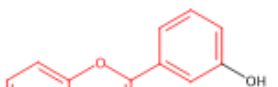


$C_{15}H_{10}O_4$
4/4'-1-Benzopyran-4-one, 2-(3,5-dihydroxyphenyl)-

Key Physical Properties

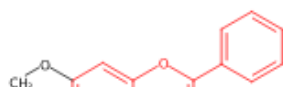
4. 6665-68-5

~38 ~7



5. 22395-22-8

~269 ~67



从4500多万个结构中
筛选出16901个黄酮类物质

物质检索——分子式

REFERENCES

- Research Topic
- Author Name
- Company Name
- Document Identifier
- Journal
- Patent
- Tags

SUBSTANCES

- Chemical Structure
- Markush
- Molecular Formula**
- Property
- Substance Identifier

REACTIONS

- Reaction Structure

SUBSTANCES: MOLECULAR FORMULA

Examples:
H4SiO4
(C3H6O,C2H4O)x

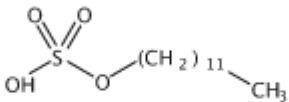
Search

无机金属盐：金属离子和阴离子间用点 (.) 分开

1. **151-21-3**

(Component: 151-41-7)

~84904 ~276



• Na

C₁₂H₂₆O₄S.Na
Sulfuric acid monododecyl ester sodium salt (1:1)

Key Physical Properties

- Regulatory Information
- Spectra
- Experimental Properties

分子式输入需要遵守Hill排序规则:不含碳化合物,按元素符号的字母顺序排列;分子式为含碳化合物时,则“C”在前;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

物质检索——结构

REFERENCES

- Research Topic
- Author Name
- Company Name
- Document Identifier
- Journal
- Patent
- Tags

SUBSTANCES

- Chemical Structure**
- Markush
- Molecular Formula
- Property
- Substance Identifier

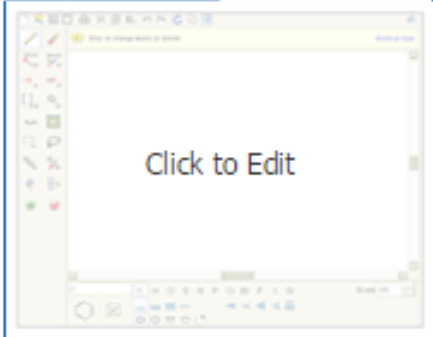
REACTIONS

- Reaction Structure

SUBSTANCES: CHEMICAL STRUCTURE ?

Structure Editor:


Java Non-Java



Search Type:


- ☐ Exact Structure
- ☒ Substructure
- ☐ Similarity

☐ Show precision analysis

 **ChemDraw**
Launch a SciFinder substance or reaction

Import CXF

Search

 Advanced Search ☒ Always Show

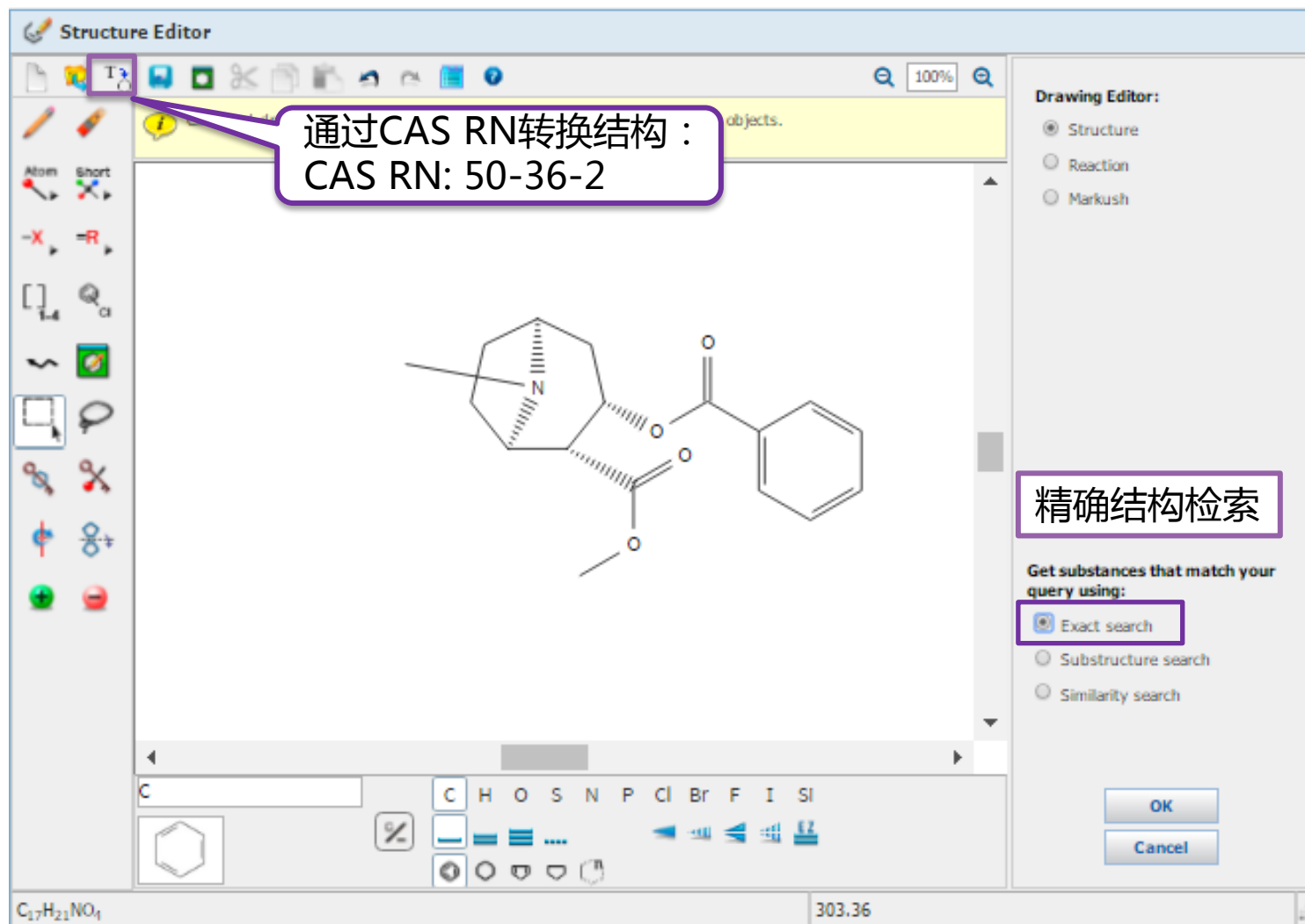
物质检索——结构

The image shows the SciFinder Structure Editor window with various tools and functions labeled in Chinese. The labels are as follows:

- 橡皮 (Eraser)
- 结构和反应切换功能 (Structure and Reaction Switching Function)
- 铅笔 (Pencil)
- 元素周期表 (Periodic Table)
- 可变基团 (Variable Group)
- 重复基团工具 (Repeat Group Tool)
- 碳链工具 (Carbon Chain Tool)
- 选择工具 (Selection Tool)
- 环锁定工具 (Ring Locking Tool)
- 旋转工具 (Rotation Tool)
- 正电子 (Positron)
- 负电子 (Negatron)
- C原子和单键恢复工具 (C Atom and Single Bond Restoration Tool)
- 常用基团 (Common Group)
- R基团定义工具 (R Group Definition Tool)
- 可变位置连接工具 (Variable Position Connection Tool)
- 模版工具 (Template Tool)
- 索套选择工具 (Loop Selection Tool)
- 原子锁定工具 (Atom Locking Tool)
- 镜面旋转工具 (Mirror Rotation Tool)
- 单双键, RS构型, 不确定键定义工具 (Single/Double Bond, RS Configuration, Uncertain Bond Definition Tool)
- 结构检索选择 (Structure Search Selection)
- 常见环, 多元环工具 (Common Ring, Polycyclic Ring Tool)

The interface includes a toolbar with icons for drawing and editing, a central workspace for the chemical structure, and a right-hand panel with search options (Exact search, Substructure search, Similarity search) and buttons for '确定' (OK) and '取消' (Cancel).

物质检索——精确结构检索



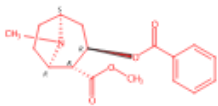
精确结构检索结果

Get References Get Reactions Get Commercial Sources Tools Create Posted

Sort by: Relevance 0 of 6 Substances Selected

1. **668-19-9**

~18 ~1



Absolute stereochemistry.

$C_{17}H_{21}NO_4$
8-Azabicyclo[3.2.1]octane-2-carboxylic acid, 3-(benzoyloxy)-8-methyl-, methyl ester, (1*R*, 2*R*, 3*R*, 5*S*)-

▶ Key Physical Properties
Spectra

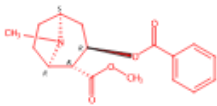
可卡因

2. **114599-38-1**

~5

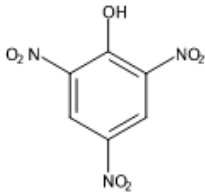
可卡因组合物

668-19-9
 $C_{17}H_{21}NO_4$



Absolute stereochemistry.

88-89-1
 $C_6H_3N_3O_7$

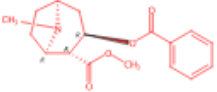


$C_{17}H_{21}NO_4 \cdot C_6H_3N_3O_7$
Alcococaine, picrate (6CI)

3. **109496-04-0**

(Component: 668-19-9)

~1



* HCl

Absolute stereochemistry.

$C_{17}H_{21}NO_4 \cdot ClH$
Alcococaine, hydrochloride (6CI)

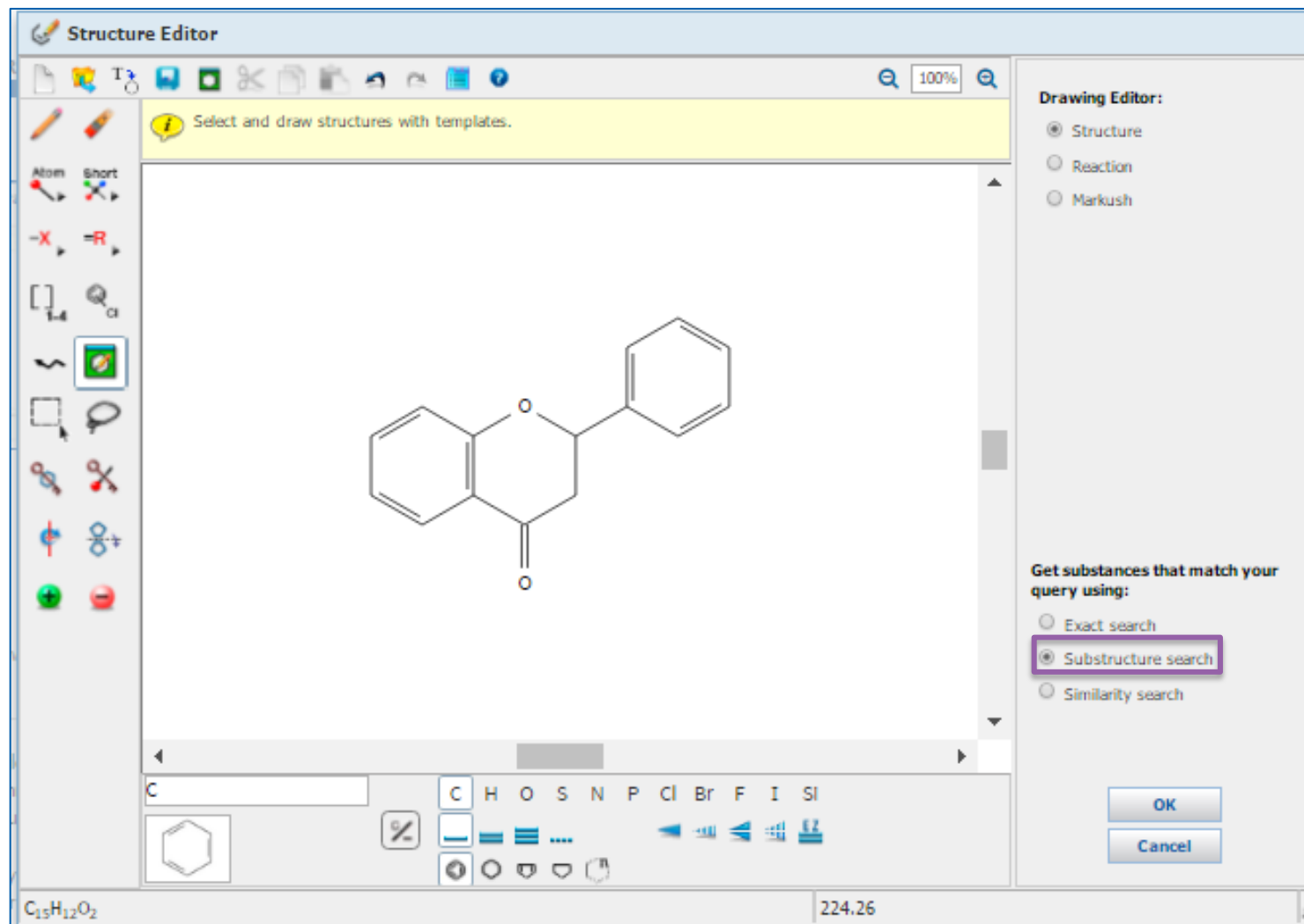
盐酸可卡因

物质检索——精确结构检索

精确结构检索：

获得被检索结构的盐，混合物，配合物，聚合物等，被检结构不能被取代

物质检索——亚结构检索

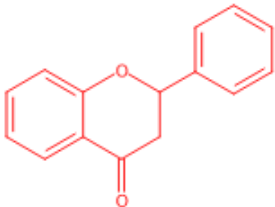


物质检索——亚结构检索

0 of 23824 Substances Selected

1. 487-26-3

~2093

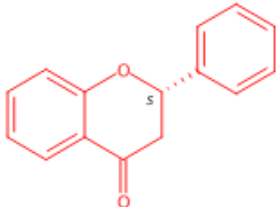


C₁₅H₁₂O₂
4-phenyl-4H-benzopyran-4-one, 2,3-dihydro-2-phenyl-

▶ **Key Physical Properties**
Regulatory Information
Spectra
Experimental Properties

2. 17002-31-2

~244



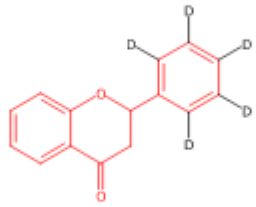
Absolute stereochemistry...Rotation (-).

C₁₅H₁₂O₂
4-phenyl-4H-benzopyran-4-one, 2,3-dihydro-

▶ **Key Physical Properties**
Experimental Properties

10. 146196-91-0

~1



C₁₅H₇D₅O₂
4-(2,3,4,5-tetradeuteriophenyl)-4H-benzopyran-4-one, 2,3-dihydro-2-(phenyl-d₄)- (9CI)

Spectra

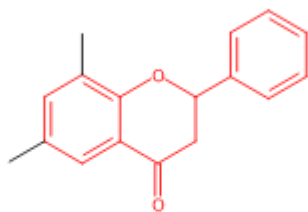
同位素

亚结构检索结果

281. 123251-10-5

~3 ~1

取代物



$C_{17}H_{16}O_2$

4H-1-Benzopyran-4-one, 2,3-dihydro-6,8-dimethyl-

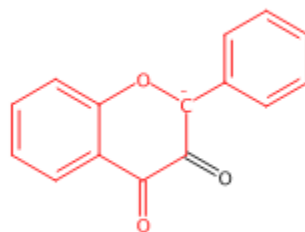
Key Physical Properties

Experimental Properties

295. 780723-19-5

~0

离子



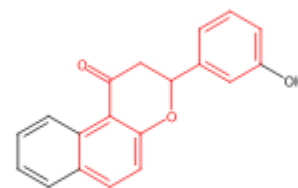
$C_{15}H_9O_3$

2H-1-Benzopyran-3,4-dione, 2-phenyl-, ion(1-)

284. 136116-23-9

~2

稠环物质



$C_{19}H_{14}O_3$

1H-Naphtho[2,1-b]pyran-1-one, 2,3-dihydro-3-(3-hydroxyphenyl)-

Key Physical Properties



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亚结构检索结果的限定

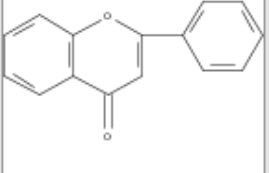
化学结构的再次限定

Analysis Refine

Refine by: ⓘ

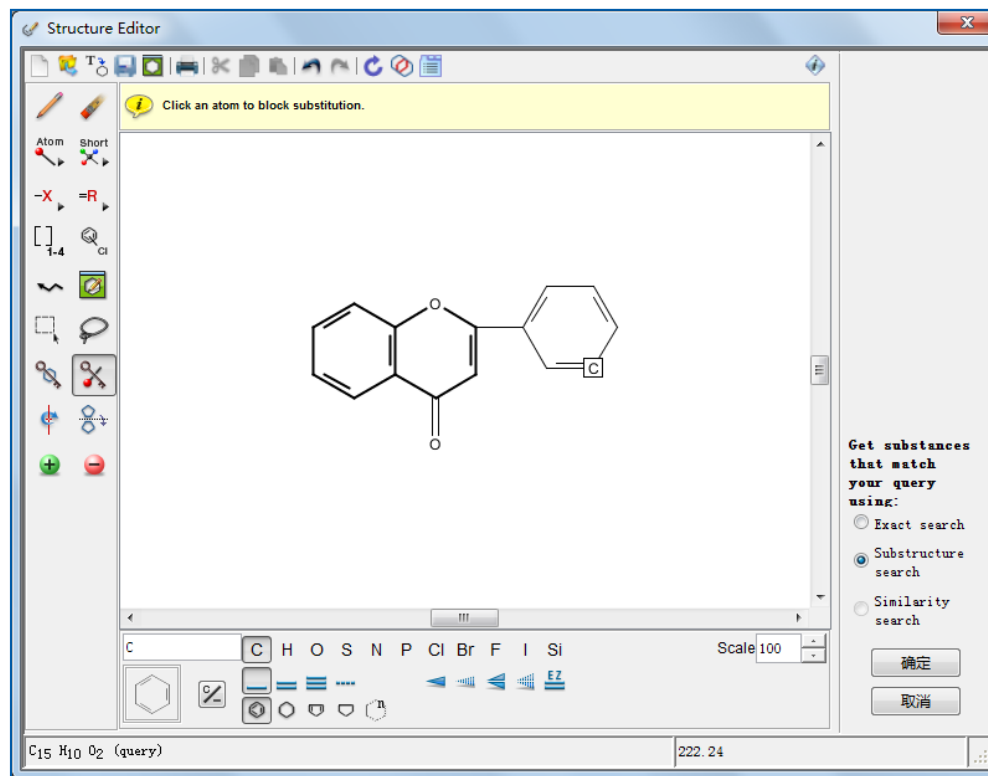
- ☒ Chemical Structure
- ☐ Isotope-Containing
- ☐ Metal-Containing
- ☐ Commercial Availability
- ☐ Property Availability
- ☐ Property Value
- ☐ Reference Availability
- ☐ Atom Attachment

Chemical Structure:



Click image to change structure or view detail

Search type: **Substructure**



环锁定

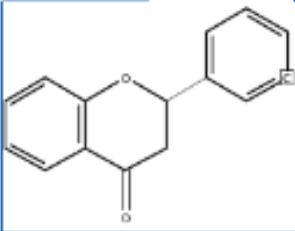


原子锁定

亚结构检索结果的限定

Structure Editor:

Java Non-Java



Click image to change structure or view detail.
Search type: **Substructure**

Only retrieve substances that:

- ☒ Have references
- ☐ Are commercially available
- ☒ Are a single component
- ☐ Are in specific substance classes
- ☐ Are in specific types of studies

Refine

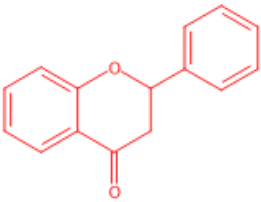
Get References Get Reactions Get Commercial Sources Tools

Sort by: Relevance

0 of 13826 Substances Selected

1. 487-26-3

~2093

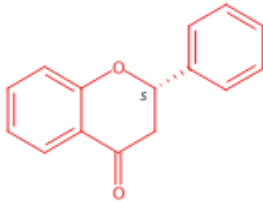


$C_{15}H_{12}O_2$
4H-1-Benzopyran-4-one, 2,3-dihydro-2-phenyl-

Key Physical Properties
Regulatory Information
Spectra
Experimental Properties

2. 17002-31-2

~244



Absolute stereochemistry., Rotation (-).

$C_{15}H_{12}O_2$
4H-1-Benzopyran-4-one, 2,3-dihydro-2-phenyl-, (2S)-

Key Physical Properties
Experimental Properties

4. 104550-32-5

~3

5. 75524-43-5

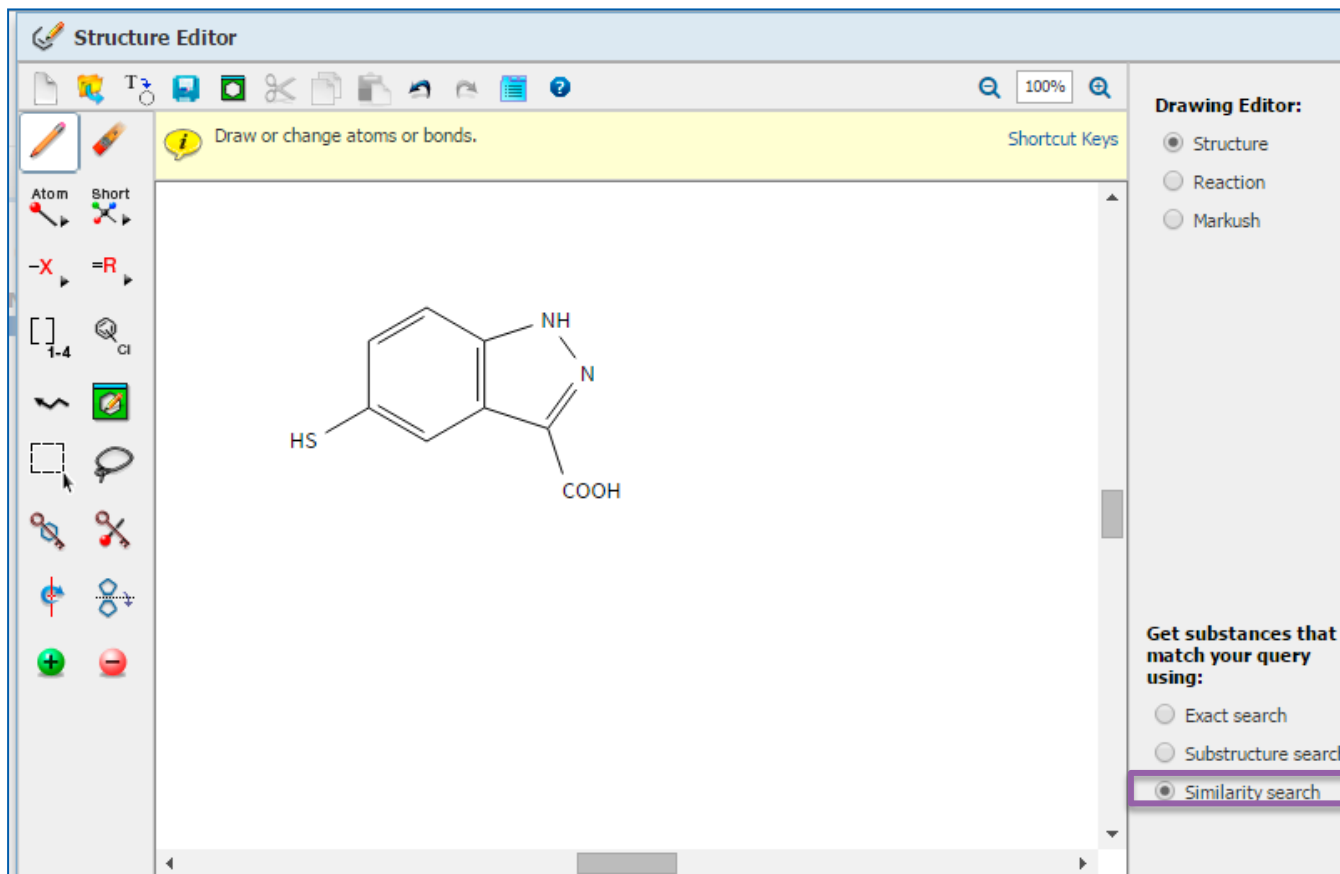
~2

物质检索——亚结构检索

- 亚结构检索：

包括精确结构检索结果，及被检索结构的修饰结构

物质检索——相似结构检索



相似结构检索结果

Select All Deselect All

0 of 6 Similarity Candidates Selected

	Substances
<input type="checkbox"/> ≥ 99 (most similar)	0
<input type="checkbox"/> 95-98	0
<input type="checkbox"/> 90-94	0
<input type="checkbox"/> 85-89	11
<input type="checkbox"/> 80-84	34
<input type="checkbox"/> 75-79	84
<input type="checkbox"/> 70-74	267
<input type="checkbox"/> 65-69	696
<input type="checkbox"/> 0-64 (least similar)	1818

Get Substances

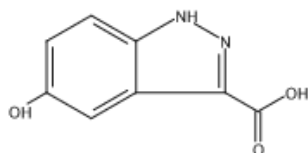
相似度越高，结构越相似

Score: 88

☐ 1. 885518-94-5

取代基变化

~1 ~35



$C_8H_6N_2O_3$

1H-Indazole-3-carboxylic acid, 5-hydroxy-

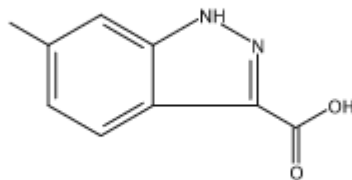
► Key Physical Properties

Score: 86

☐ 5. 858227-12-0

取代基位置变化

~7 ~41



$C_9H_8N_2O_2$

1H-Indazole-3-carboxylic acid, 6-methyl-

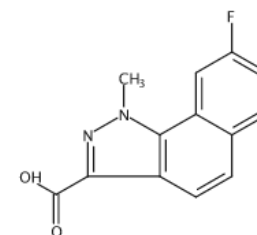
► Key Physical Properties

Score: 65

☐ 541. 1100422-

母体结构变化

~1



$C_{13}H_9FN_2O_2$

1H-Benz[g]indazole-3-carboxylic acid, 8-fluoro-1-methyl-

► Key Physical Properties



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物质检索——相似结构检索

- 相似结构检索：

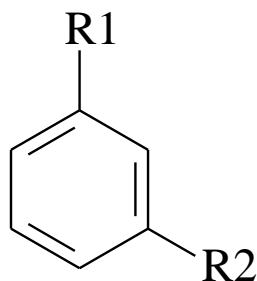
获得片段或整体结构与被检索结构相似的结果，母体结构可以被取代，也可以被改变

提纲

- 美国化学文摘社简介
- SciFinder简介及检索方式
 - 文献检索
 - 物质检索
 - Markush检索
 - 反应检索
 - SciPlanner
- SciFinder常见问题及解决

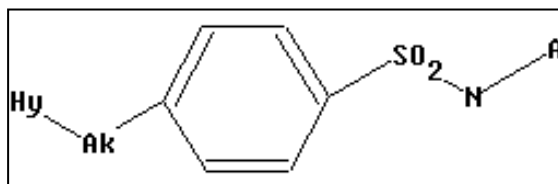
Markush检索

- 具体物质[Specific Substance]：
 - 以具体化学结构陈述的特定物质，会被分配CAS RN
- 预测性物质[Prophetic Substance]：
 - 使用Markush结构陈述的预测物质，一个Markush可以陈述上百或上千个化学物质
 - 专利中所陈述的预测物质，不会被分配CAS RN
 - Markush检索，能检索到通过结构检索检不到的专利




R1 = H, Br, Cl, I

R2 = Br, Cl, I, —CH₂—halogen, —CH(CH₃)—halogen,



可用SciFinder中的Markush检索
查看专利中化合物结构保护范围。

Markush检索


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Welcome Helen Zhu

Explore ▼ Saved Searches ▼ SciPlanner Save Print Export

Markush substructure > references (1969) > Compounds and methods for anti...

REFERENCES ⓘ

Get Substances
 Get Reactions
 Get Related Citations ▼
 Tools ▼

Create Keep Me Posted Alert
 Send to SciPlanner

Analyze Refine Categorize

Sort by: Accession Number ▼

0 of 1969 References Selected

Display Options

Page: 1 of 99

Analyze by:

Document Type ▼

Patent	1969
Journal	1

Show More

全部是专利

☐

1. Compounds and methods for anticoagulation therapy

Quick View PATENTPAK ▼

By Allende Rodriguez, Mikel; Hermida Santos, Jose; Montes Diaz, Ramon; Oyarzabal Santamarina, Julen
 From PCT Int. Appl. (2016), WO 2016120432 A1 20160804. | Language: English, Database: CAPLUS

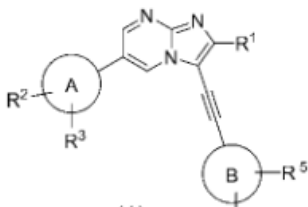
The invention relates to certain compds. that are inducers of Heat shock 70 kDa protein 1A/1B (HSPA1A/B) and their use for anticoagulation therapy; and to a method for anticoagulation therapy that comprises the administration of one of these inducer compds. It has been here proved that induction of Heat shock 70 kDa protein 1A/1B by administration of one of these inducer compds. has antithrombotic effects without accelerating or altering bleeding time.

☐


2. Preparation of new imidazopyrimidine derivatives as negative allosteric modulators of metabotropic glutamate receptor subtype 2 (mGlu2 receptor)

Quick View PATENTPAK ▼

By Urashima, Kuniko; Tojo, Kengo; Koike, Shoko; Masumoto, Shuji
 From Jpn. Kokai Tokkyo Koho (2016), JP 2016132660 A 20160725. | Language: Japanese, Database: CAPLUS



The title imidazo[1,2-a]pyrimidine derivs. I [R¹ = H or halogen; ring A Ph or pyridyl; R², R³ (same or different) = hydrogen, halogen, C₁₋₄ alkyl or C₁₋₄ alkoxy each optionally substituted with 1-5 halogen atoms; or in case where R² and R³ are at the adjacent substitution position, R² and R³ together with ring A form C₅₋₈ carbocyclic ring (optionally substituted with 1-5 halogen or 1-2 hydroxy group) or 5- or 6-membered satd. heterocyclic ring; ring B = Ph or pyridyl; R⁴, R⁵ (same or different) = H, halogen, hydroxy, amino, -C(O)OR^a, -C(O)NR^aR^b, SO₃H, SO₂NR^aR^b, SO₂R^b, or NR^aSO₂R^b; R^a, R^b (same...


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ACS / Proprietary and Confidential / Do Not Distribute

58

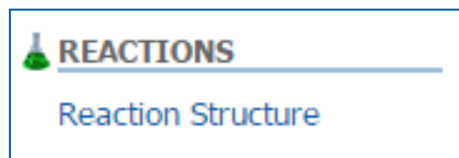
提纲

- 美国化学文摘社简介
- SciFinder简介及检索方式
 - 文献检索
 - 物质检索
 - Markush检索
 - 反应检索
 - SciPlanner
- SciFinder常见问题及解决

SciFinder检索选项——反应检索

- 反应检索方法

结构式



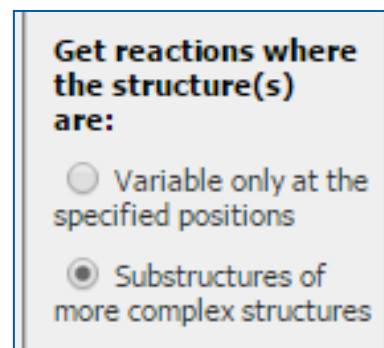
- 常用获取方法

已知物质：由物质获取反应

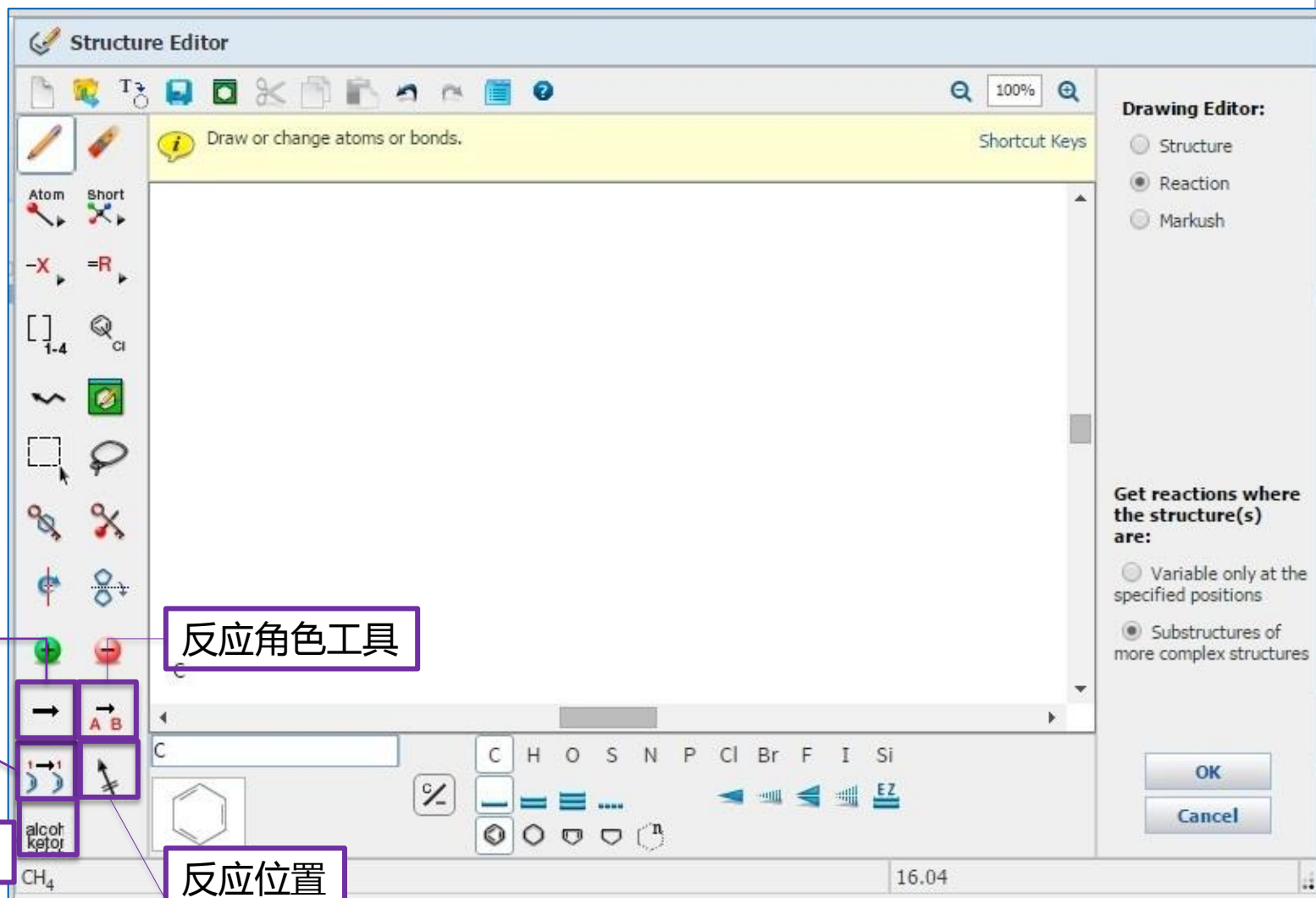
已知文献：从文献中获取反应

精确结构反应检索

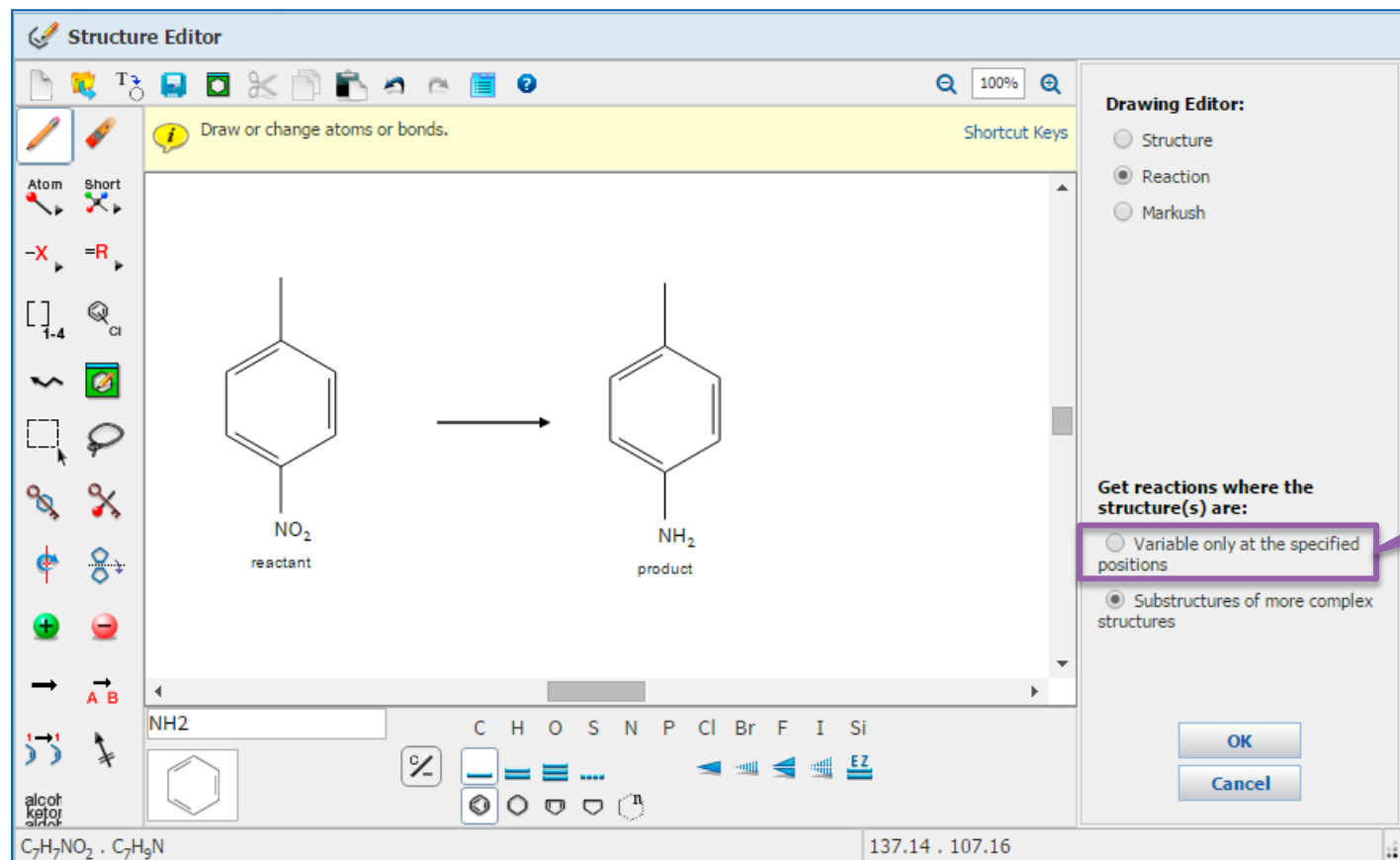
亚结构反应检索



反应绘制工具



SciFinder反应检索——精确反应检索



精确反应检索

反应检索结果

浏览记录，发现很多反应来自同一篇文献，
通过Group by Document合并。

Get References Tools





Group by: **No Grouping** | Sort by: Relevance

☐ No Grouping
☒ **Document**
☐ Transformation

Selected

1. [View Reaction Detail](#) [Link](#) [Similar Reactions](#)

Single Step Hover over any structure for more options.


~102  
100%
~122 

Overview

Steps/Stages

1.1 R:NaBH₄, C:1832616-28-0, C:Ru, S:H₂O, S:THF, 45 min, 25°C

Notes

solid-supported catalyst, ruthenium supported on porous organic polymer used, reusable catalyst, sealed tube used, scalable, Reactants: 1, Reagents: 1, Catalysts: 2, Solvents: 2, Steps: 1, Stages: 1, Most stages in any one step: 1

References

Fabrication of Ruthenium Nanoparticles in Porous Organic Polymers: Towards Advanced Heterogeneous Catalytic Nanoreactors

获取相似反应

选择相似反应的相似限制：

Broad：仅反应中心相似

Medium：反应中心及附属原子和键

Narrow：反应中心及扩展的原子和键

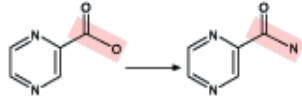
Get Similar Reactions ?

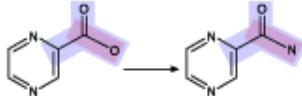
Retrieve similar reactions from:

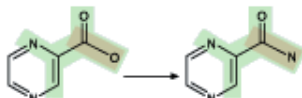
- ☒ All reactions
- ☐ Current answer set

Include this level of similarity:

- ☒ Broad - Reaction centers only (2934)


- ☐ Medium - Reaction centers plus adjacent atoms and bonds (109)


- ☐ Narrow - Reaction centers plus extended atoms and bonds (95)



Get Reactions

Cancel

按照反应类型排序

Group by: Transformation ▼ Sort by: Frequency ▼ ↓

☐ 0 of 560 Reactions Selected

☐ 1. Reduction of Nitro Compounds to Amines
538 Reactions

$$\text{R-NO}_2 \longrightarrow \text{R-NH}_2$$

☐ 2. Reduction of Nitro to Azo Compounds
11 Reactions

$$\text{Ar-NO}_2 \longrightarrow \text{Ar-N=N-Ar}$$

☐ 3. Reduction of Nitro to Azoxy Compounds
11 Reactions

$$\text{Ar-NO}_2 \longrightarrow \text{Ar-N}^+=\text{N-Ar} \begin{matrix} \text{O}^- \\ | \end{matrix}$$

更精确的查找需要的反应

反应检索结果的筛选

获得特定物质做还原剂的反应

REACTIONS ?

Get References Tools

Analyze Refine

Analyze by: Reagent

H ₂	148
NaBH ₄	51
N ₂ H ₄ ·H ₂ O	43
KOH	17
CO	16
HCO ₂ H	16
NH ₄ ⁺ ·HCO ₂ ⁻	16
H ₂ O	14
N ₂ H ₄	14
NaOH	14

Show More

Group by: No Grouping Sort by: Relevance

0 of 512 Reactions Selected

1. View Reaction Detail Link Similar Reactions

Single Step Hover over any structure for more options.

Overview

Steps/Stages

1.1 R:NaBH₄, C:1832616-28-0, C:Ru, S:H₂O, S:THF, 45 min, 25°C

Notes

solid-supported catalyst, ruthenium supported on porous organic polymer used, reusable catalyst, sealed tube used, scalable, Reactants: 1, Reagents: 1, Catalysts: 2, Solvents: 2, Steps: 1, Stages: 1, Most stages in any one step: 1

References

Fabrication of Ruthenium Nanoparticles in Porous Organic Polymers: Towards Advanced Heterogeneous Catalytic Nanoreactors

SciFinder囊括最大的反应实验过程合集

Single Step Hover over any structure for more options.



▼ Overview

Steps/Stages

1.1 R:H₂, R:Cs₂CO₃, C:1610424-70-8, C:1034343-98-0 (oxide), S:PhMe, 2 h, 100°C, 1 atm

Notes

solid-supported catalyst, palladium catalyst supported on graphene oxide prepared and used, reusable catalyst, Reactants: 1, Reagents: 2, Catalysts: 2, Solvents: 1, Steps: 1, Stages: 1, Most stages in any one step: 1

References

Catalyst Enhancement and Recyclability by Immobilization of Metal Complexes onto Graphene Surface by Noncovalent Interactions

[Quick View](#) [Other Sources](#)

By Sabater, Sara et al

From ACS Catalysis, 4(6), 2038-2047; 2014

▼ Experimental Procedure

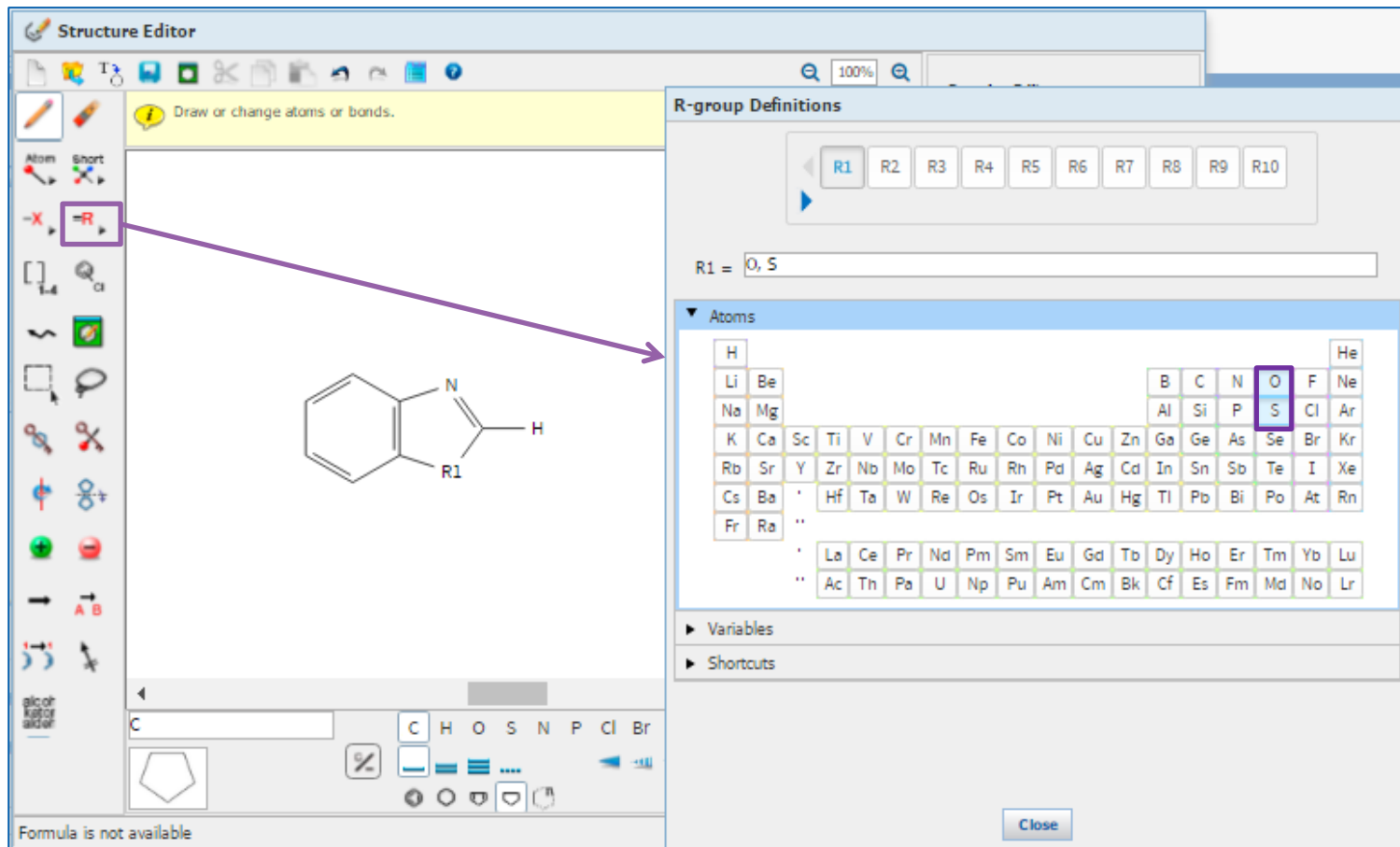


General/Typical Procedure: **General Procedure for Nitroarene Reductions.** Molecular hydrogen was added with a balloon filled with 1 atm of H₂ to a mixture of nitroarene (0.3 mmol), Cs₂CO₃ (0.3 mmol), anisole as internal standard (0.3 mmol), and NHC-Pd-rGO (6 × 10⁻³ mmol, based on metal) in toluene (5 mL). The system was then evacuated and backfilled with H₂ in cycles for three times before putting the reaction vessel in an oil bath at 100°C for 2h. Yields were determined by GC analyses using anisole (0.3 mmol) as internal standard. Products were identified according to spectroscopic data of the commercially available compounds. Entry: 4; Yield 100%.

不用阅读全文，直接获得包含实验过程的反应记录

亚结构反应检索

通过C-H活化对苯并噻唑或者恶唑进行烷基化



亚结构反应检索

The screenshot displays the 'Structure Editor' window. The main workspace shows a chemical reaction template: a benzimidazole derivative with an 'R1' substituent and a hydrogen atom at the 2-position, reacting to form a product where the hydrogen is replaced by a variable 'Ak'. A purple arrow points from the 'Ak' variable in the product to the 'Variables' panel on the right.

Structure Editor:

- ☐ Structure
- ☒ Reaction
- ☐ Markush

Variables:

X	Any halogen
M	Any metal
A	Any atom except H
Q	Any atom except C or H
Ak	Any carbon chain
Cy	Any cycle
Cb	Any carbocycle
Hy	Any heterocycle

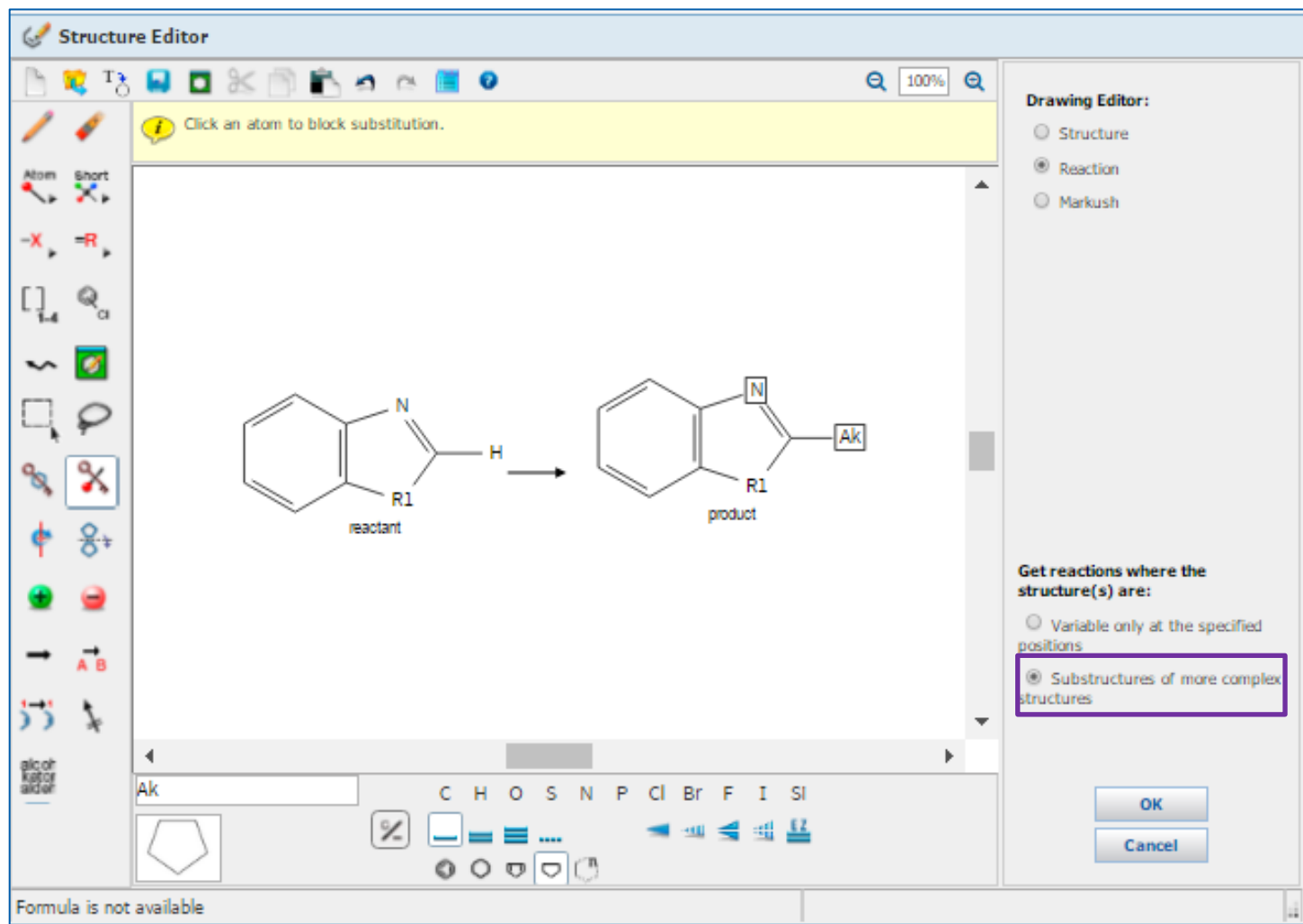
Get reactions where the structure(s) are:

- ☐ Variable only at the specified positions
- ☒ Substructures of more complex structures

Buttons: OK, Cancel, Close

Formula is not available

亚结构反应检索



通过后处理工具筛选反应--Analyze

通过催化剂筛选反应

REACTIONS ⓘ

Get References Tools ▾

Analyze Refine

Group by: No Grouping ▾ Sort by: Number of Steps ▾ ↑

0 of 249 Reactions Selected

1. View Reaction Detail ⓘ Link ⓘ Similar Reactions

Single Step Hover over any structure for more options.

~57 ~52 83%

▼ Overview

Steps/Stages

- 1.1 R:LiO-Bu-*t*, C:1905414-33-6, S:Dioxane, 16 h, 100°C
- 1.2 S:H₂O, rt
- 1.3 R:HCl, S:H₂O, neutralized

Notes

catalyst prepared and used, screw c
Reagents: 2, Catalysts: 1, Solvents:

References

Synthesis of quinoline-based NNN-p
for C-H bond alkylation of azoles wi
Quick View ⓘ Other Sources
By Patel, Ulhas N. et al
From Organometallics 35(11) 1785-1793

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提纲

- 美国化学文摘社简介
- SciFinder简介及检索方式
 - 文献检索
 - 物质检索
 - Markush检索
 - 反应检索
 - SciPlanner
- SciFinder常见问题及解决

SciPlanner使用简介

3. View Reaction Detail [Link](#) **勾选想要的反应**

3 Steps Hover over any structure for more options.

点击Send to SciPlanner

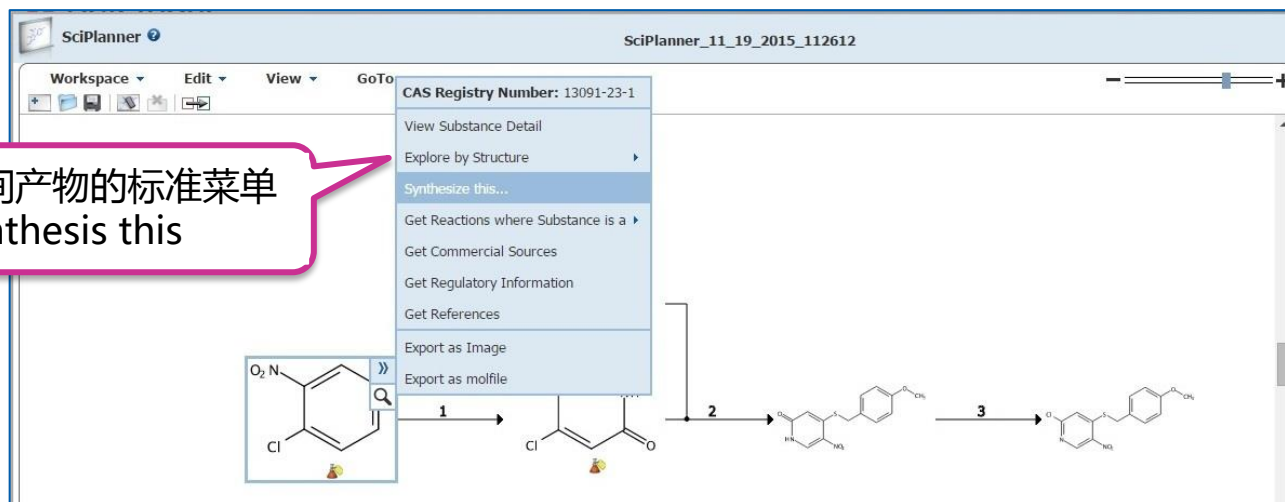
进入SciPlanner 新建文件

将刚推送过来的反应拖至编辑面板

The screenshot displays the SciPlanner web interface. At the top, a reaction scheme is shown: 5-chloro-2-nitropyridine (labeled ~192) reacts with 4-(methylthio)benzyl alcohol (labeled ~72, [Step 2.1]) to form 4-(4-methoxybenzylthio)-5-chloro-2-nitropyridine. Below the reaction, the 'Overview' section lists steps: 1.1 R: NH₃, R: t-BuOK, R: t-BuOOH, S: THF; 2.1 R: NaH, S: THF; 3.1 R: POCl₃, reflux. The 'Notes' section states: Reactants: 2, Reagents: 5, Solvents: 1, Steps: 3, Stages: 3, Most stages in any one step: 1. The 'References' section lists: Syntheses of 4- and 6-substituted thiazolo[4,5-c]pyridines. The bottom part of the image shows the SciPlanner workspace. The 'Workspace' menu is open, showing options: New, Open, Save, Duplicate, Import, Export, Print, Close. The workspace area contains the text: 'Your Workspace is empty. Drag items from the reference, substance, and reaction libraries (on the right) to this area.' On the right side, a small panel shows a reaction scheme being dragged into the workspace.

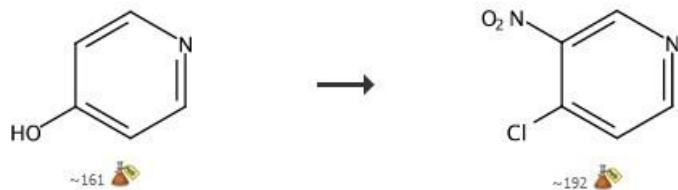
SciPlanner使用简介

打开中间产物的标准菜单
选择Synthesize this

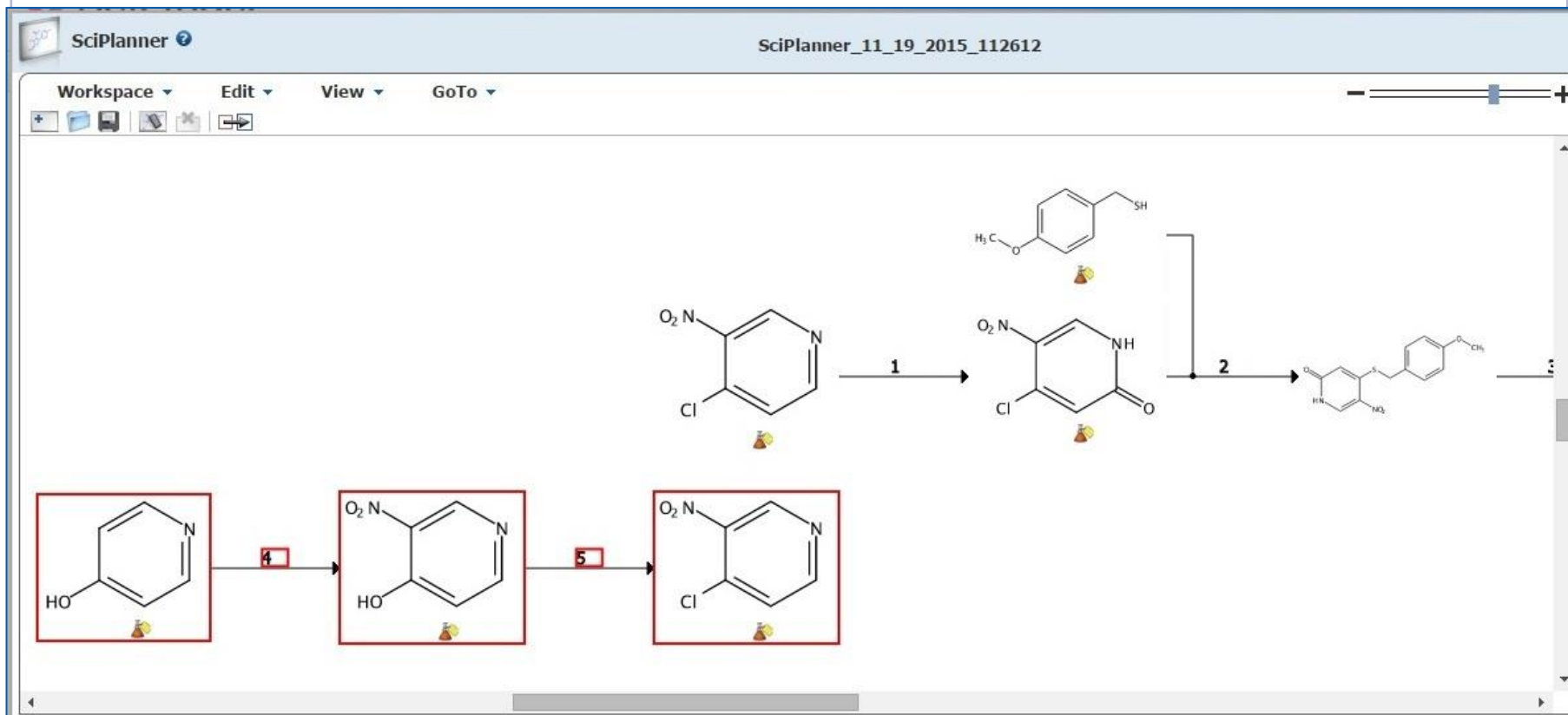


在检索到的反应中选择感兴趣的反应

继续推送到SciPlanner



SciPlanner使用简介



步骤同前，将推送过来的反应拖到编辑面板中，可以看到两条反应中存在同样的结构

SciPlanner使用简介

SciPlanner 11_19_2015_112612

Workspace Edit View GoTo

New
Open
Save
Duplicate
Import
Export
Print
Close

点击 Workspace, 选择 Export 导出结果

用鼠标将两个同样的结构拖至重叠, 两条反应合并

选择适当的输出格式, 输出结果

Export

For:

Offline Review

- ☒ Portable Document Format (*.pdf)
- ☐ Citations (*.ris)
- ☐ Image (*.png)

Saving Locally

- ☐ SciPlanner eXchange (*.pkx)

Details:

File Name: *
SciPlanner_11_19_2015_112612

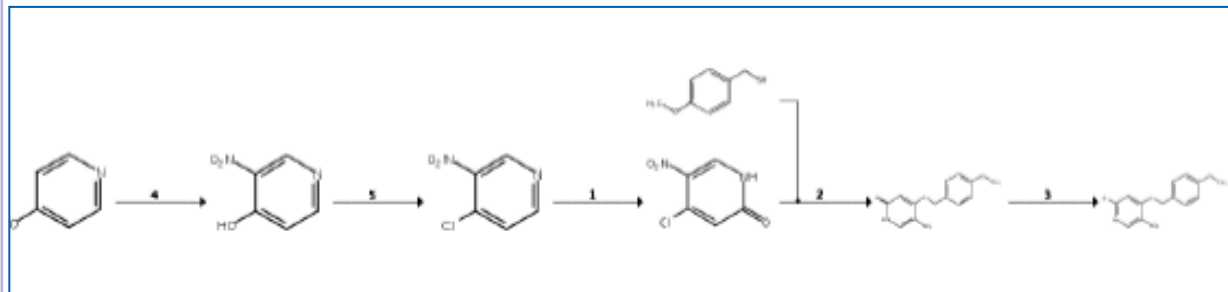
Title
[Empty field]

Include:

- ☒ SciPlanner Image
- ☒ Reaction Details
- ☒ Substance Details
- ☒ Reference Details

Export **Cancel**

SciPlanner导出结果



Reaction	Stages	Notes	Yield
5	1.1 R:POCl ₃ , S:PhMe, 0°C → rt; 16 h, rt → 110°C	Reactants: 1, Reagents: 2, Solvents: 2, Steps: 1, Stages: 2	90%
	1.2 R:K ₂ CO ₃ , S:H ₂ O, cooled, pH 10	Transformation: 1. Formation of Alkyl Halides from Alcohols	

References

High color rendering index and color stable hybrid white efficient OLEDs with a double emitting layer structure using a single phosphorescence dopant of heteroleptic platinum complexes

By Poloek, Anurach et al

From Journal of Materials Chemistry C: Materials for Optical and Electronic Devices, 2(48), 10343-10356; 2014

Substance Information		
<p>1228150-22-8</p> <p>C₁₃H₁₂N₂O₄S 2(1H)-Pyridone, 4-[[[4-methoxyphenyl)methyl]thio]-5-nitro- Related Info: ~ 2 References Reactions</p>	<p>1228150-23-9</p> <p>C₁₃H₁₁ClN₂O₄S Pyridine, 2-chloro-4-[[[4-methoxyphenyl)methyl]thio]-5-nitro- Related Info: ~ 2 References Reactions</p>	<p>13091-23-1</p> <p>C₅H₃ClN₂O₂ Pyridine, 4-chloro-3-nitro- Related Info: ~ 391 References Reactions ~ 190 Commercial Sources Regulatory Information</p>
<p>5435-54-1</p> <p>C₆H₄N₂O₃ 4-Pyridinol, 3-nitro- Related Info: ~ 113 References Reactions ~ 197 Commercial Sources Regulatory Information</p>	<p>6258-60-2</p> <p>C₈H₁₀O S Benzenemethanethiol, 4-methoxy- Related Info: ~ 749 References Reactions ~ 71 Commercial Sources Regulatory Information</p>	<p>626-64-2</p> <p>C₅H₅N O 4-Pyridinol Related Info: ~ 1351 References Reactions ~ 160 Commercial Sources Regulatory Information</p>
<p>850663-54-6</p> <p>C₆H₃ClN₂O₃ 2(1H)-Pyridone, 4-chloro-5-nitro- Related Info: ~ 22 References Reactions ~ 138 Commercial Sources</p>		

提纲

- 美国化学文摘社简介
- SciFinder简介及检索方式
 - 文献检索
 - 物质检索
 - Markush检索
 - 反应检索
 - SciPlanner
- SciFinder常见问题及解决

SciFinder浏览器选择建议

- Windows 7以上用户建议升级IE到10以上
- Chrome和FireFox浏览器在所有系统上的表现都优于IE浏览器
- 不建议使用360浏览器检索SciFinder，会被自动拦截相关功能或插件

如何获取SciFinder账号

点击注册链接，按照要求提交信息

<https://scifinder.cas.org/registration/index.html?corpKey=50B8E71AX86F3503FX3002D4D11EB02026EA>

如何获取SciFinder账号

The screenshot displays the SciFinder registration interface, organized into three main sections:

- CONTACT INFORMATION--**: Includes input fields for First Name, Last Name, Email, Confirm Email, Phone Number, and Fax Number. It also features dropdown menus for Area of Research and Job Title.
- USERNAME AND PASSWORD--**: Includes input fields for Username, Password, and Re-enter Password. A small "Tips" link is visible next to the Password field.
- SECURITY INFORMATION--**: Includes a dropdown menu for Security Question and an input field for the Answer. A small "Why?" link is visible next to the Answer field.

At the bottom of the form, there are two buttons: "Register>>" and "Clear All".

请注意：

1. 必须输入真实姓名和**学校**邮箱。
2. 用户名必须是唯一的，且包含 5-15 个字符。它可以只包含字母或字母组合、数字和/或以下特殊字符：

- - (破折号)
- _ (下划线)
- . (句点)
- @ (表示 "at" 的符号)

3. 密码必须包含 7-15 个字符，并且至少**包含三种以下字符**：

- 字母
- 混合的大小写字母
- 数字
- 非字母数字的字符 (例如 @、#、%、&、*)

例：abc@123

4. 从下拉列表中选择一个密码提示问题并给出答案。
单击 Register (注册)。

如何获取SciFinder账号

From: CAS

Dear user,

To complete your SciFinder registration, you must click the link provided below. By clicking the link, you agree to all of the following terms and conditions:

- I will not share my username and password with any other person.
- I will search only for myself and not for others or other organizations.
- I will not use any automated program or script for extracting or downloading CAS data, or any other systematic retrieval of data.
- I may retain a maximum of 5,000 Records at any given time for personal use or to share within a Project team for the duration of the Project.
- My organization's SciFinder License and the CAS Information Use Policies (<http://www.cas.org/legal/infopolicy.html>) apply to my use of SciFinder.
- I will contact my SciFinder Key Contact if I have questions.

If you do not accept these terms and conditions, do not click the link and delete this e-mail message.

<https://scifinder.cas.org/registration/completeRegistration.html?respKey=B8CB6727-86F3-F014-11E6-D312D80AC094>

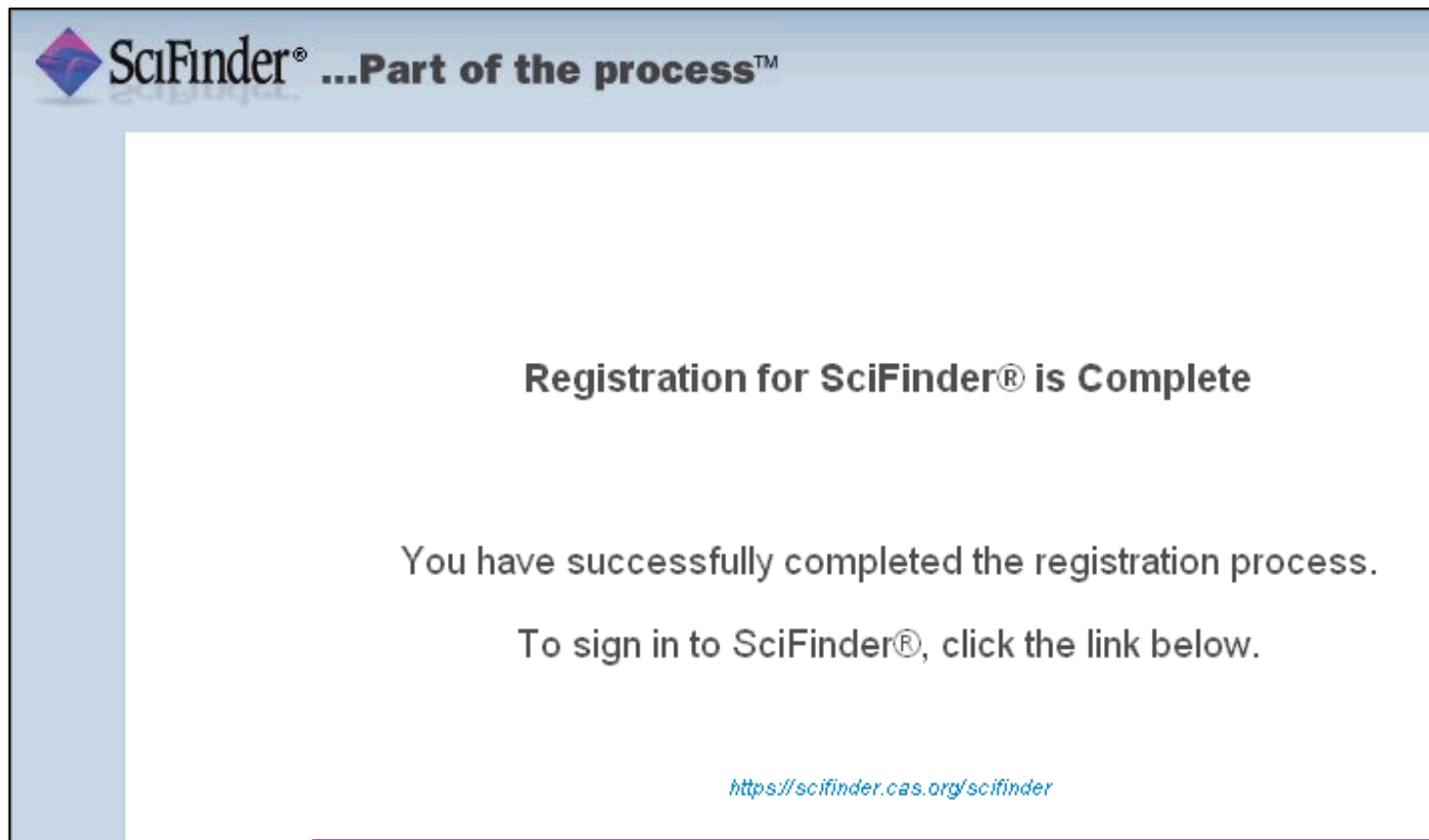
This link is valid for only one use and will expire within 48 hours.

If you need assistance at any time, consult the key contact at your organization.

打开并阅读 CAS 的电子邮件（必须在48小时内点击，否则需要重新注册）

注意垃圾邮件、未知邮件、订阅邮件等来自@cas.org的邮件

如何获取SciFinder账号



账号注册成功，登录scifinder.cas.org开始使用SciFinder

SciFinder使用注意事项

- 一人注册一个帐号
- 请提供真实姓名信息
- 严禁过量下载
- 严禁账号分享
- 严禁将账号用于非学术研究

更多培训资料请访问

www.cas-china.org

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