朱传娴
hzhu@acs-i.org

美国化学文摘社(CAS)持续推动科技创新

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大纲

- 为什么需要美国化学文摘社
- CAS主要产品
  - SciFinder Web （简称SciFinder）
  - SciFinder^{n}
  - PatentPak
  - MethodsNow

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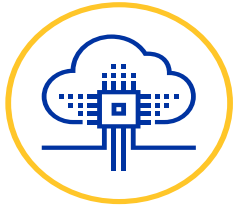
美国化学文摘社(CAS)隶属美国化学会(ACS)，致力于追踪、收录、标引科学信息

- 拥有超过110年的经验；创立权威化学索引《化学文摘》（CA）
- 密切追踪、标引和提炼着全球化学相关的文献（包括专利）
- 提供各种科学信息和相关技术产品与服务
- 协助创新和保护创新，助力于解决科研方面的难题与挑战

UNPARALLELED
SCIENTIFIC CONTENT



SPECIALIZED
TECHNOLOGY

UNMATCHED
HUMAN EXPERTISE

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CAS数据覆盖学科

- **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

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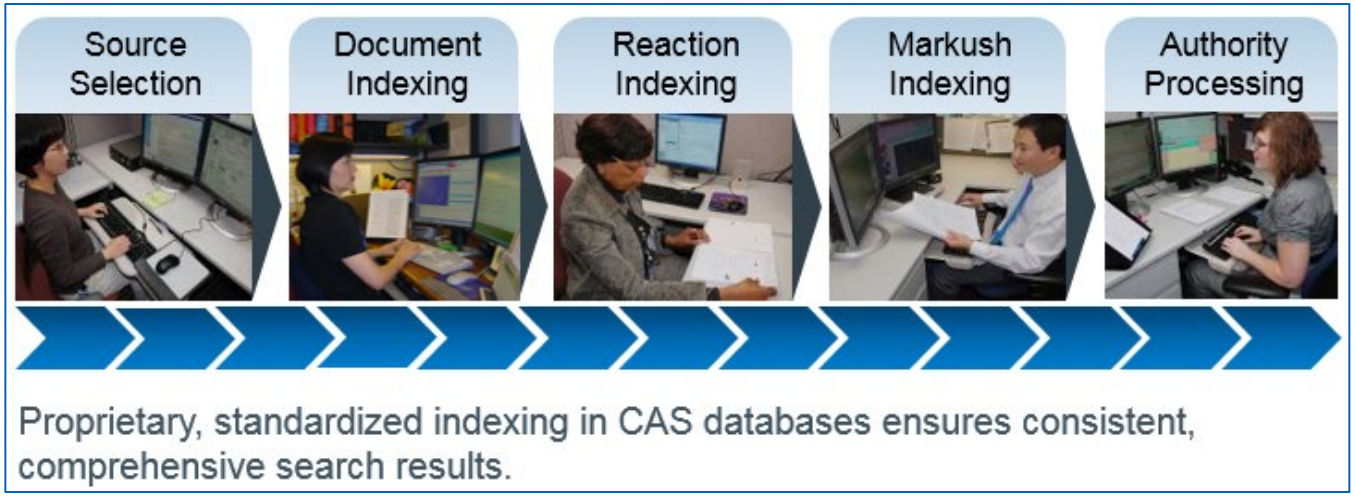
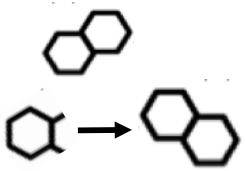
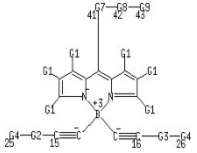


Data pre-repository

1990
Smith, M.
anthracene





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

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- 人工标引——精准揭示关键技术信息
- 数千名科学家组成的编辑团队深刻理解客户的实际需求
- 审阅、筛选、摘要、标引以覆盖并揭示全球所有已公开的化学及相关信息
- CAS登记号——物质的黄金标准
- CAS Roles (CAS物质角色)——生物研究、性能用途、分析检测、合成制备
- CAS Index Terms (CAS技术词语标准)——揭示技术词语相互间的关联
- CA Sections (CAS学科分类，80个类别)——精准定位具体研究领域

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CAS各类科学信息研究工具

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LIMITLESS POSSIBILITIES 无限可能

定制服务应对挑战.

CONTENT SERVICES 内容服务

- 定制数据集合
  Content licensing
- 数据结构
  Data structure
- 数据平台
  Data platforms

TECHNOLOGY SERVICES 技术服务

- 数据架构
  Data architecture
- 平台整合
  Platform integration
- 检索引擎
  Search engines
- 定制解决方案
  Custom solutions

KNOWLEDGE SERVICES 知识服务

- 外包IP检索
  Outsourced IP search
- 数据分析
  Analytics
- 机会分析
  Opportunity exploration
- 技术评估
  Technical Assessment

PROFESSIONAL SERVICES 专业服务

- 人员派遣
  Talent augmentation
- 咨询
  Consulting
- Technical writing
  科技写作
- Scientific analysis
  科研分析

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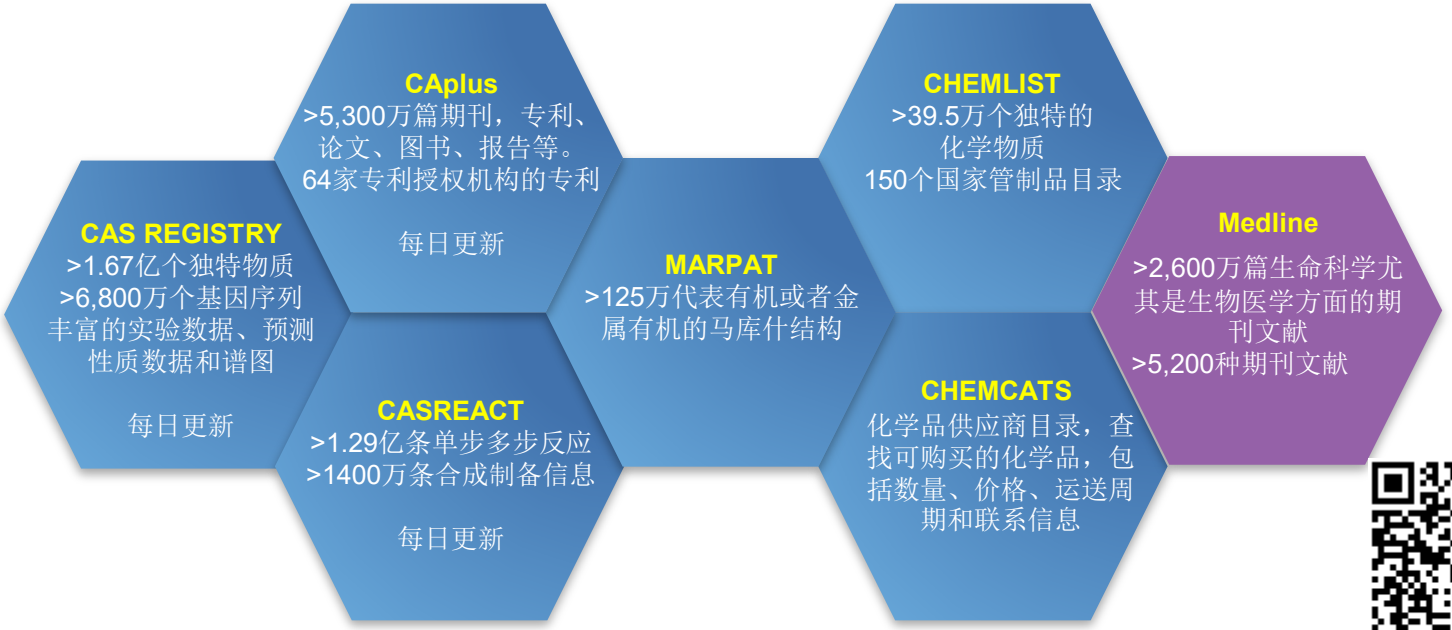
SciFinder覆盖的数据库



SciFinder是提供经CAS科学家人工标引内容的工具型数据库。

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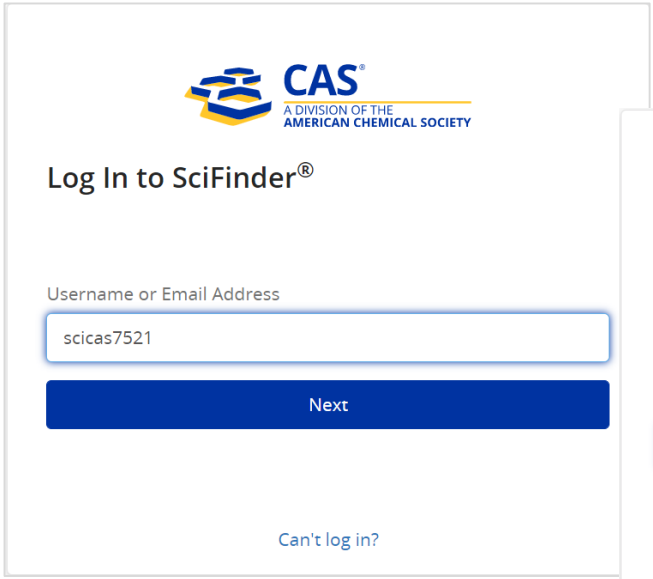

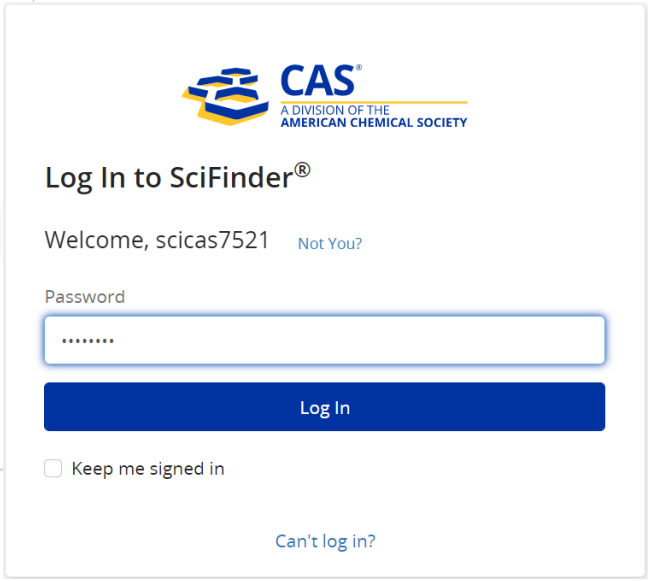

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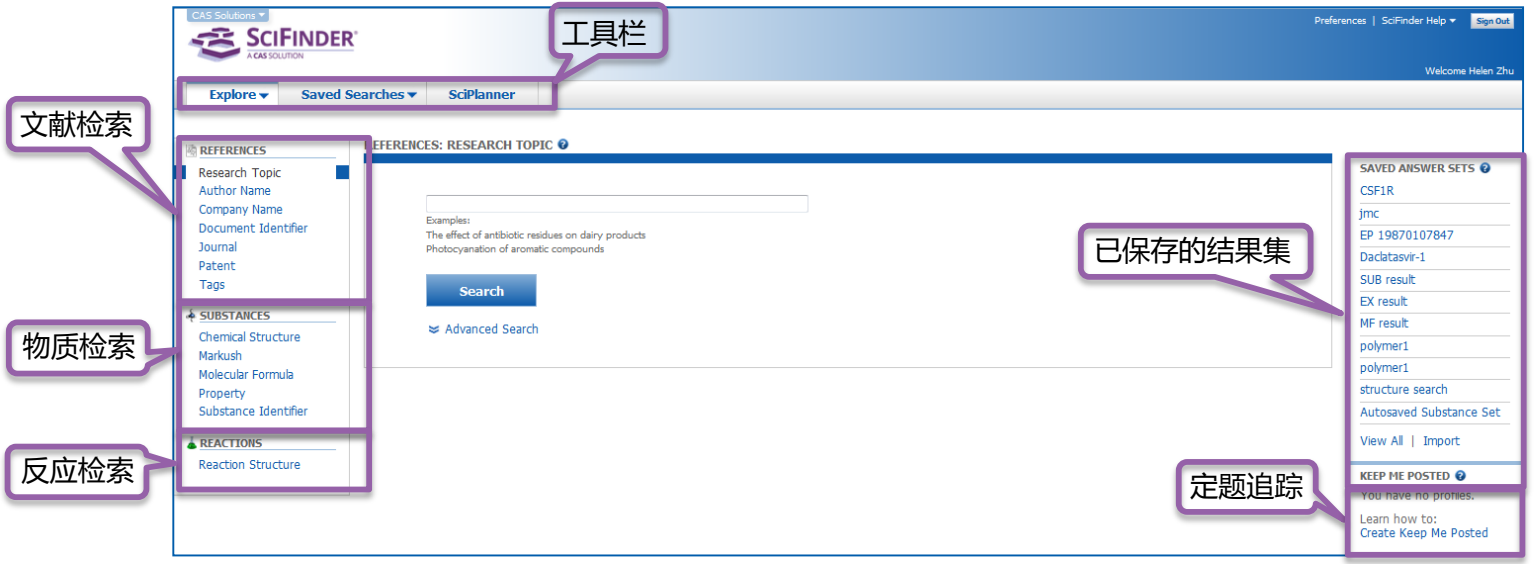
SciFinder Web主界面



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SciFinder Web检索——文献检索

- 文献检索方法
  - 主题检索
  - 作者名检索
  - 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
  - 关注某科研人员的文献：作者名检索
  - 关注某机构科研进展：机构名检索

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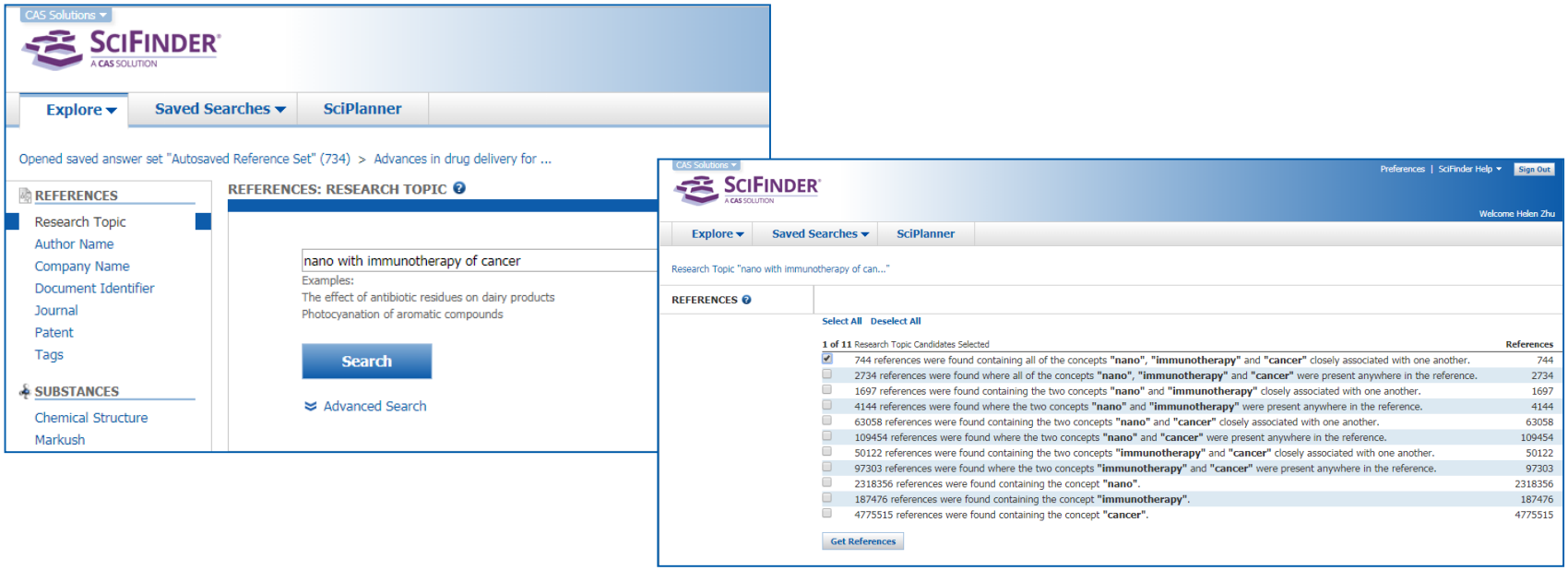
SciFinder Web检索——文献检索



输入关键词检索，之后根据检索要求勾选候选项

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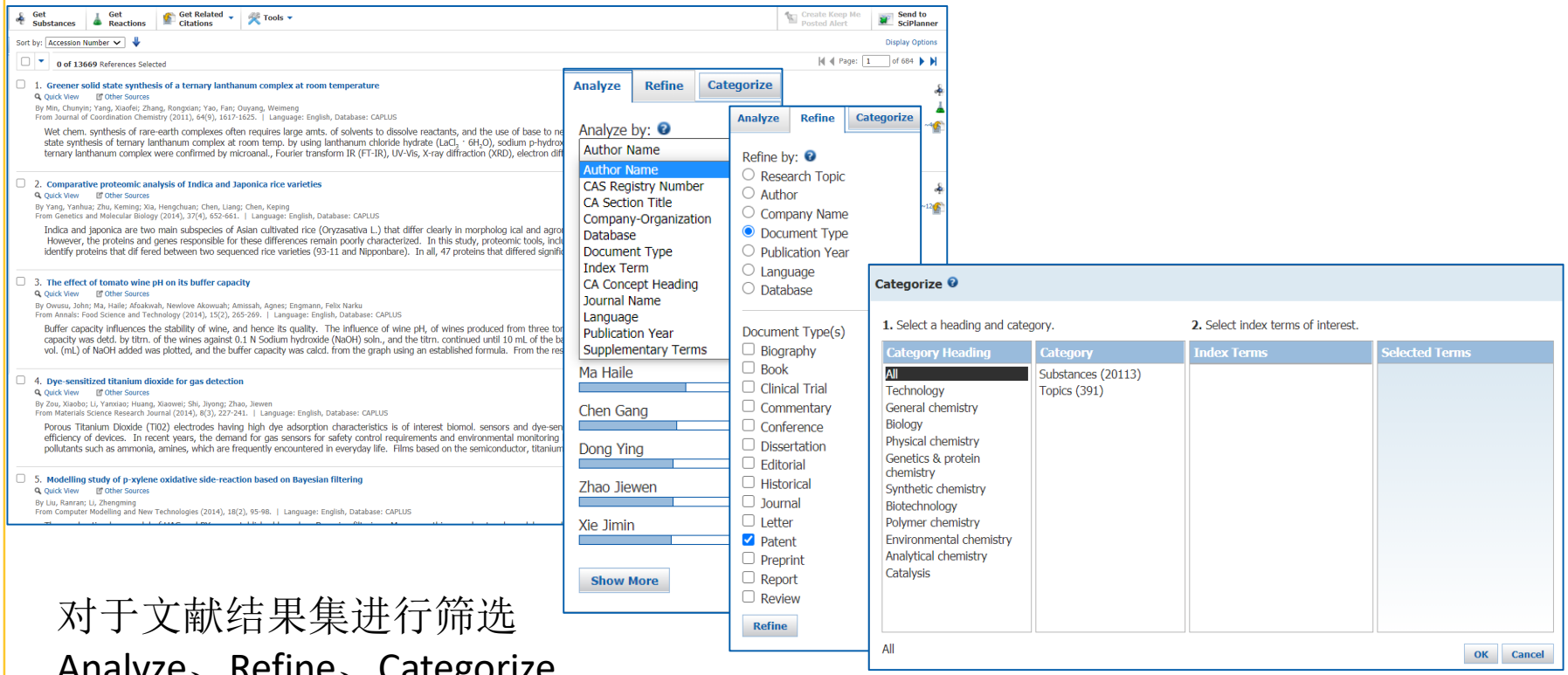
SciFinder Web检索——文献检索



对于文献结果集进行筛选

Analyze、Refine、Categorize

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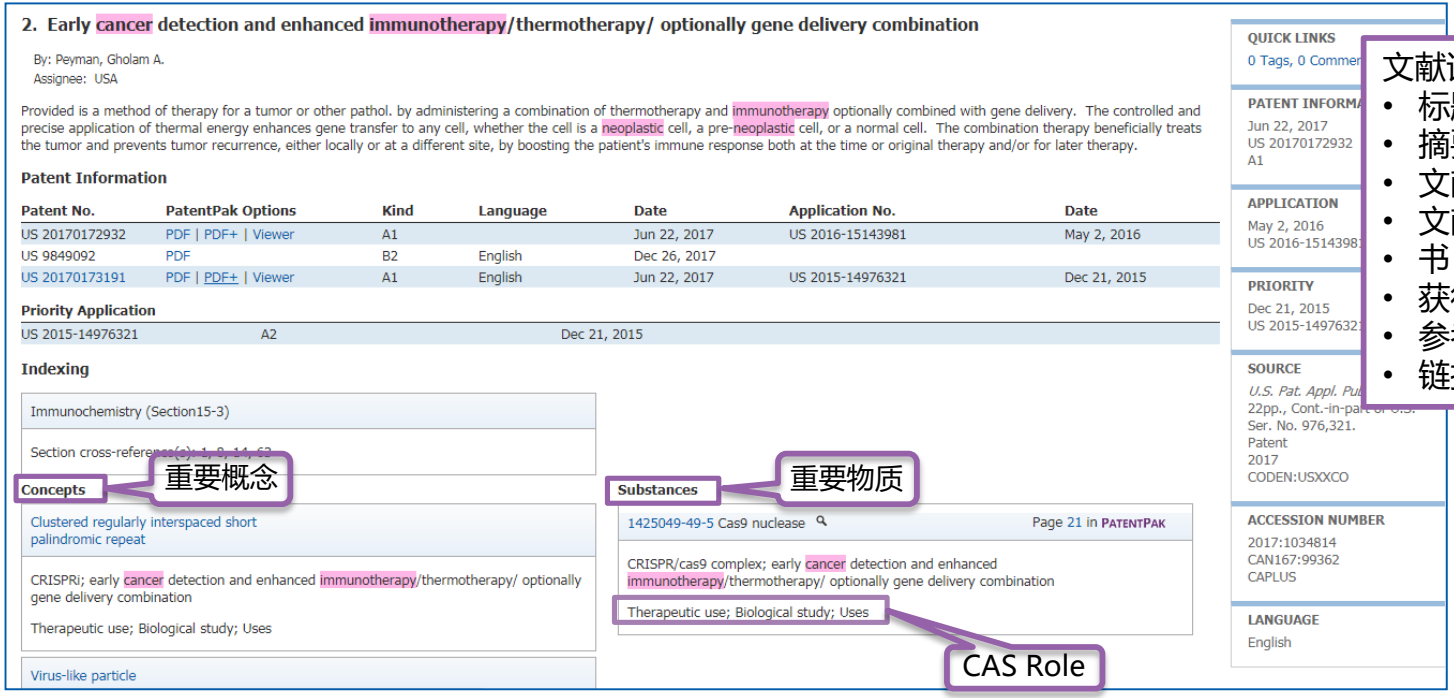
SciFinder Web检索——文献记录



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

Immunochemistry (Section15-3)

Section cross-reference(s): 1, 9, 14, 63

Concepts

Clustered regularly interspaced short palindromic repeat

CRISPRi; early cancer detection and enhanced immunotherapy/thermotherapy/ optionally gene delivery combination

Therapeutic use; Biological study; Uses

Virus-like particle

Substances

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 Commer

PATENT INFORMA
Jun 22, 2017
US 20170172932
A1

APPLICATION
May 2, 2016
US 2016-1514398

PRIORITY
Dec 21, 2015
US 2015-1497632

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

ACCESSION NUMBER
2017:1034814
CAN167:99362
CAPLUS

LANGUAGE
English

重要概念

重要物质

CAS Role

文献详情界面包括：

- 标题
- 摘要
- 文献中重要的技术术语
- 文献中重要的物质
- 书目信息
- 获得文献中的物质、反应
- 参考文献
- 链接原文

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SciFinder Web检索——物质检索

- 物质检索方法

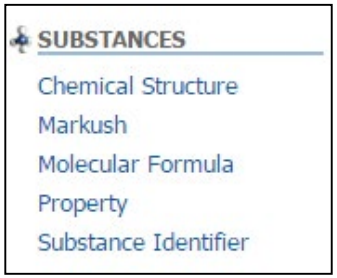
—结构式检索

—分子式检索

—理化性质（物质属性）检索

—物质标识符检索：化学名称，CAS RN

—从文献或反应结果获得



- 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

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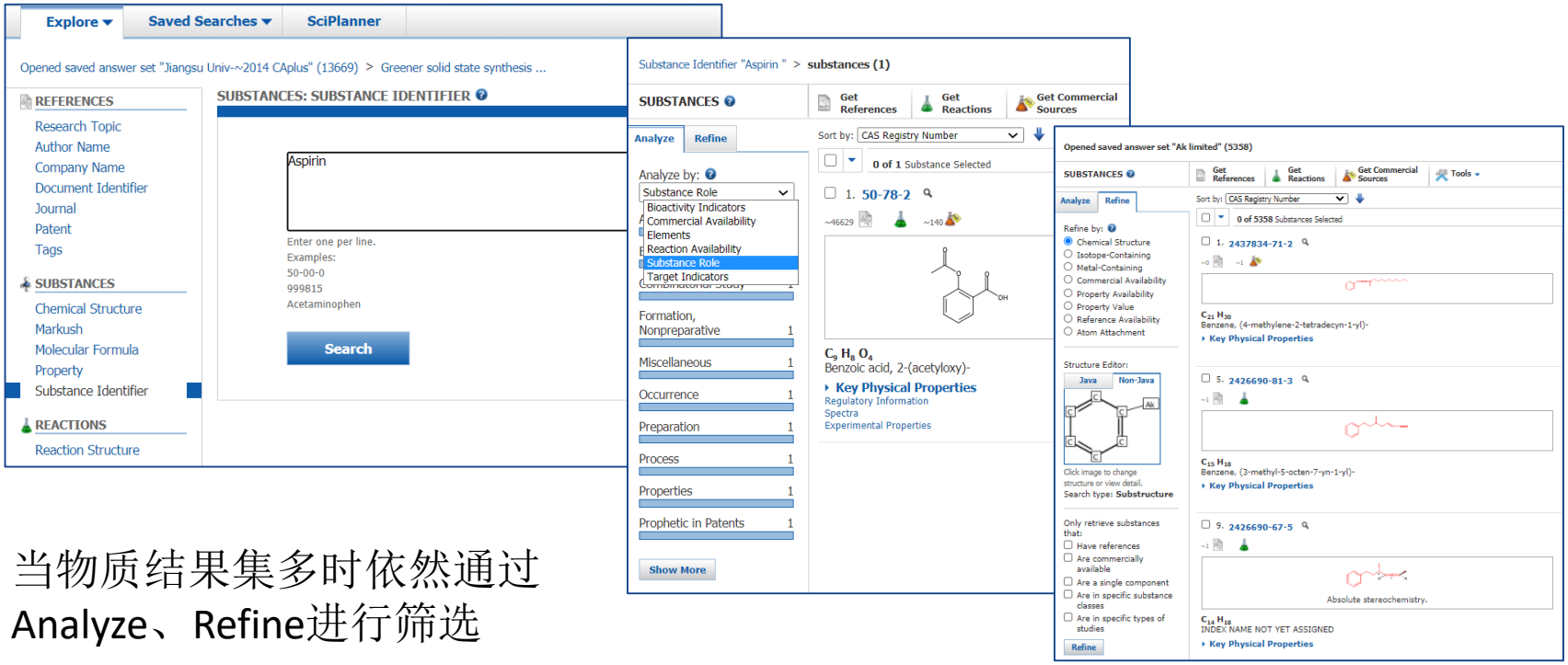


当物质结果集多时依然通过Analyze、Refine进行筛选

SciFinder Web检索——物质记录

CAS Registry Number 50-78-2

~46,629 ~140

$C_9 H_8 O_4$

Benzoic acid, 2-(acetyloxy)-

Molecular Weight
180.16

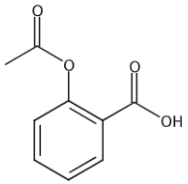
Melting Point (Experimental)
Value: 135 °C

Boiling Point (Experimental)
Value: 197-200 °C | Condition: Press: 7 Torr

Density (Experimental)
Value: 1.40 g/cm3

pKa (Predicted)
Value: 3.48±0.10 | Condition: Most Acidic Temp: 25 °C

Other Names
Rhodine (7CI)
Salicylic acid acetate (8CI)
2-(Acetyloxy)benzoic acid
2-Acetoxybenzoic acid
2-Carboxyphenyl acetate
View more...



▸ EXPERIMENTAL PROPERTIES	实验属性
▸ EXPERIMENTAL SPECTRA	实验谱图
▸ PREDICTED PROPERTIES	预测属性
▸ PREDICTED SPECTRA	预测谱图
▸ REGULATORY INFORMATION	管制信息
▸ BIOACTIVITY INDICATORS	生物活性指示剂
▸ TARGET INDICATORS	生物靶点指示剂
▸ CAS REFERENCE ROLES	文献研究类别
▸ ADDITIONAL DETAILS	其他

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SciFinder Web检索——反应检索

- 反应检索方法

  结构式

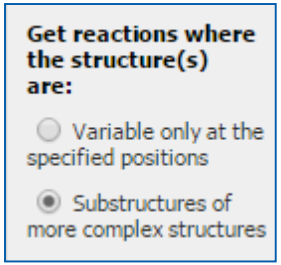
- 常用获取方法

  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



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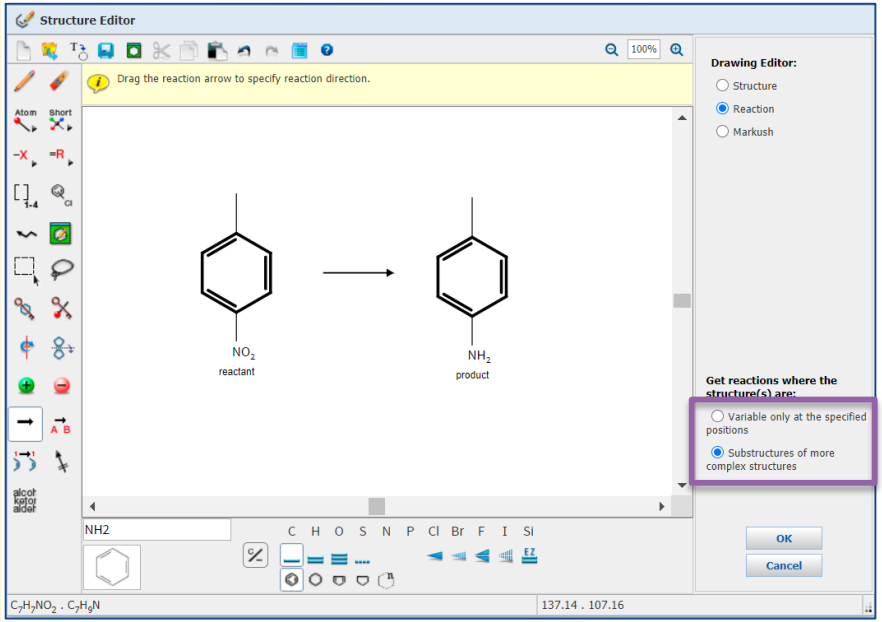

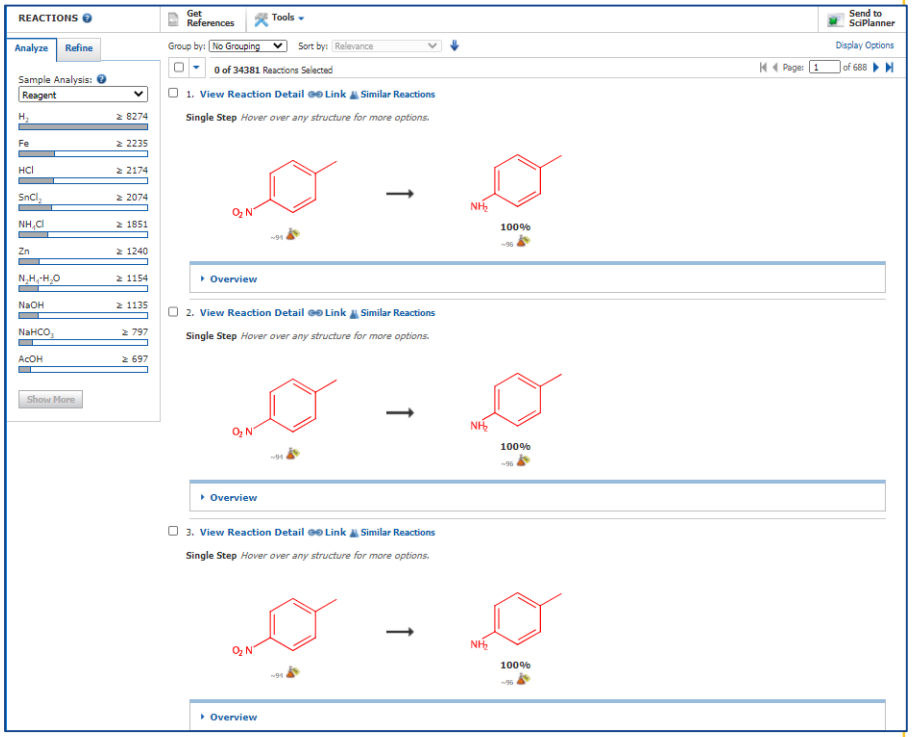

当反应结果集多时通过
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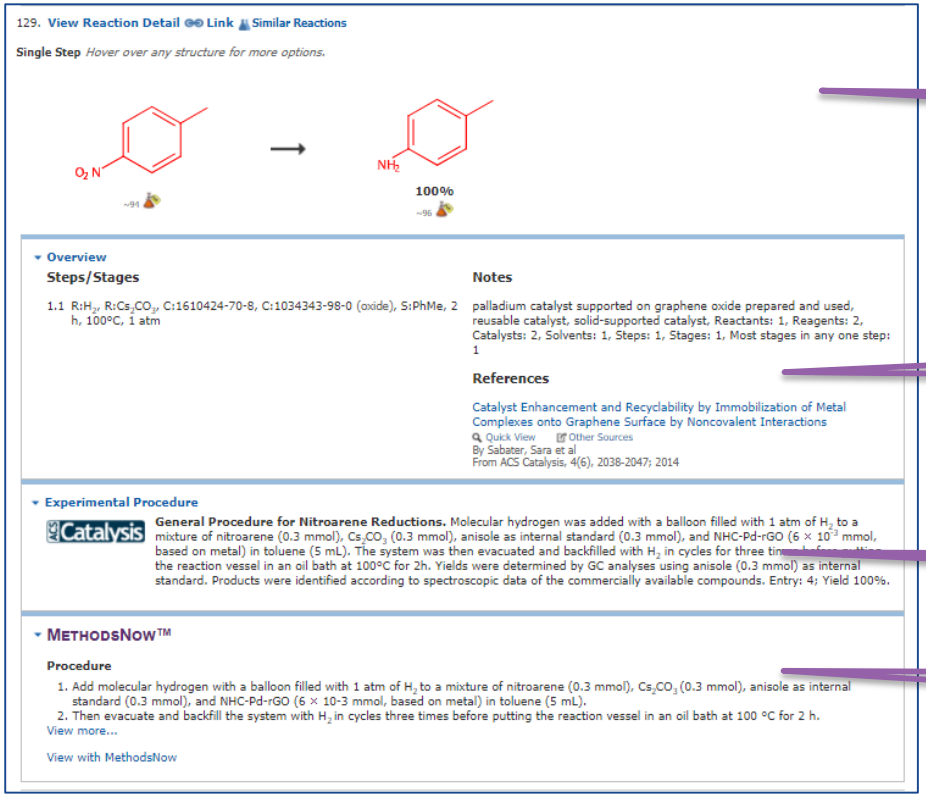

反应式

概览：步骤、反应试剂、溶剂、催化剂、温度、文献来源等

实验详情：来自原文

操作步骤：CAS编辑根据原文进行加工整理

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- 先进的平台不仅需要实现信息的获取，还要帮助用户发现最佳起点
- CAS的化学信息历史积累、系统知识和人工智力能够加速您的工作

用户需求的演进、内容的增长和广度的扩展推动
新的技术解决方案的出现！

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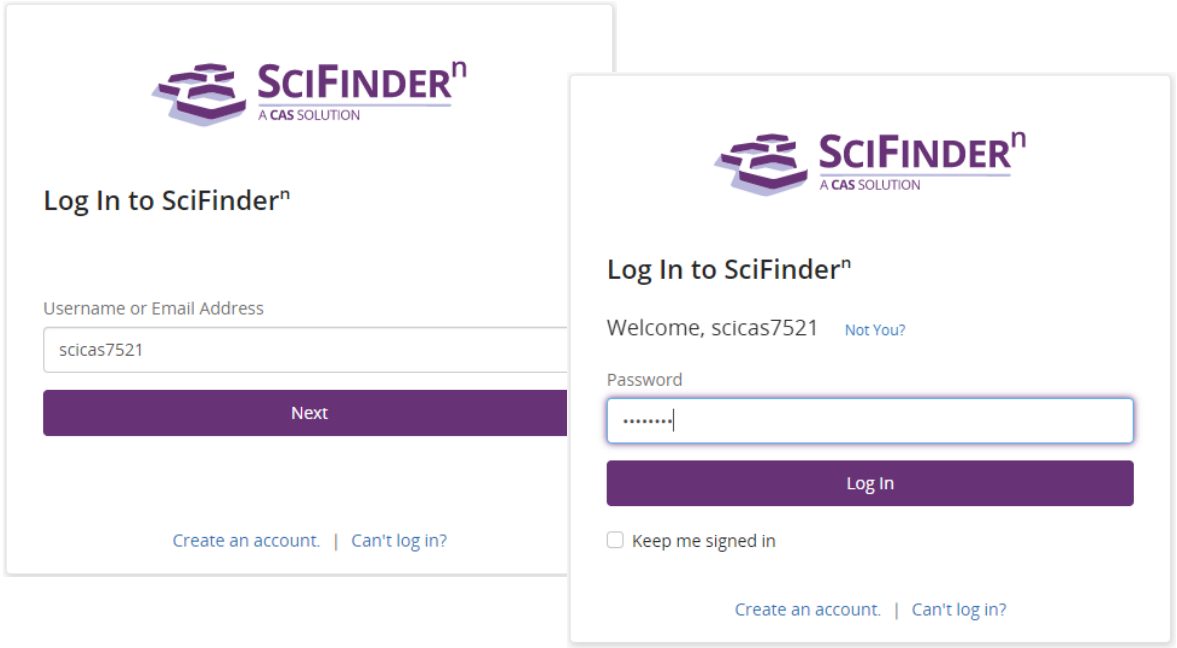

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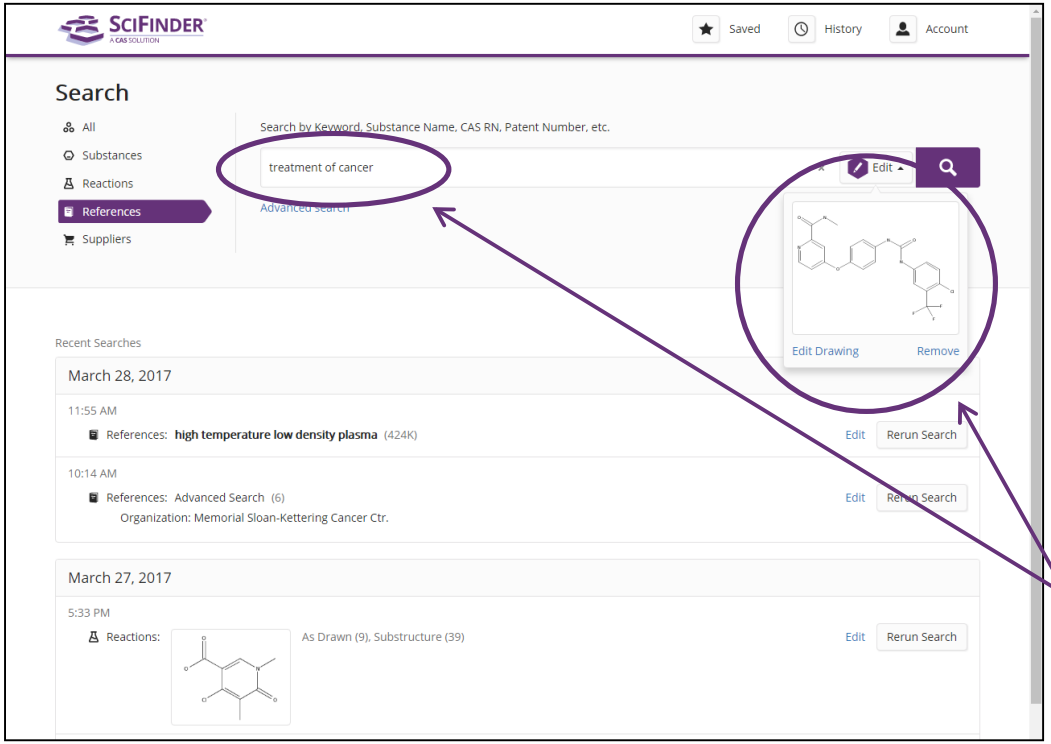
简化的界面，快速执行检索

灵活的检索选项

快速运行之前的检索项目



便捷地合并文本与结构检索

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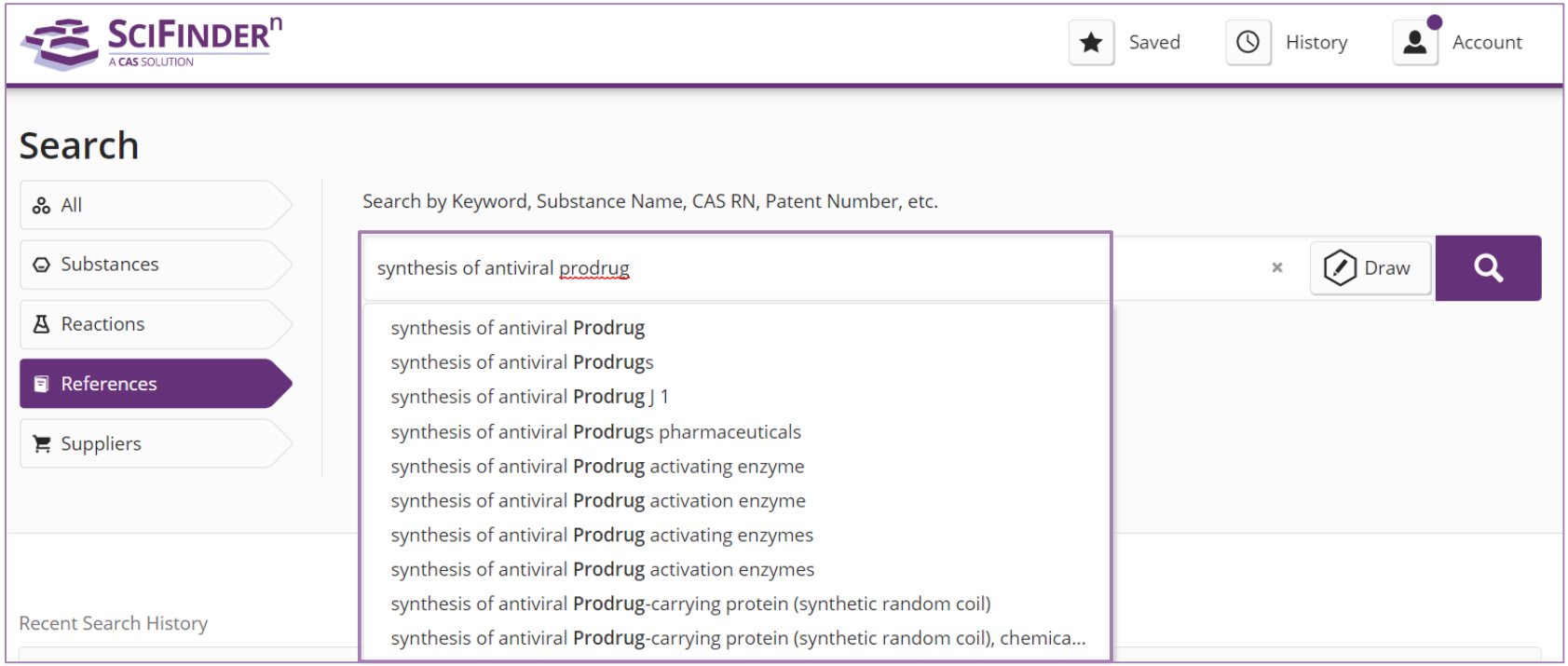
自动提示词，启发灵感; 同时支持自然语言和布尔逻辑运算符



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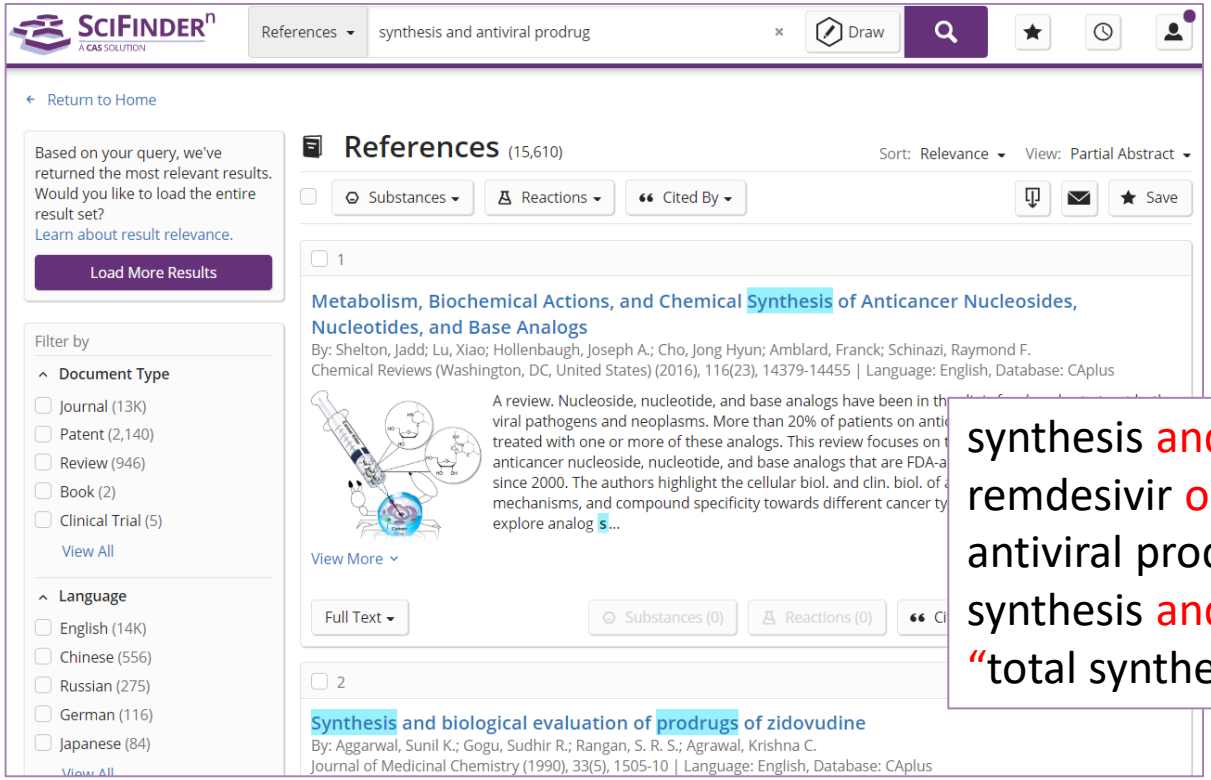
支持布尔逻辑运算符及双引号，提高检索准确性



synthesis and antiviral prodrug
remdesivir or cinanserin
antiviral prodrug not antitumor drug
synthesis and (remdesivir or cinanserin)
“total synthesis” of taxol

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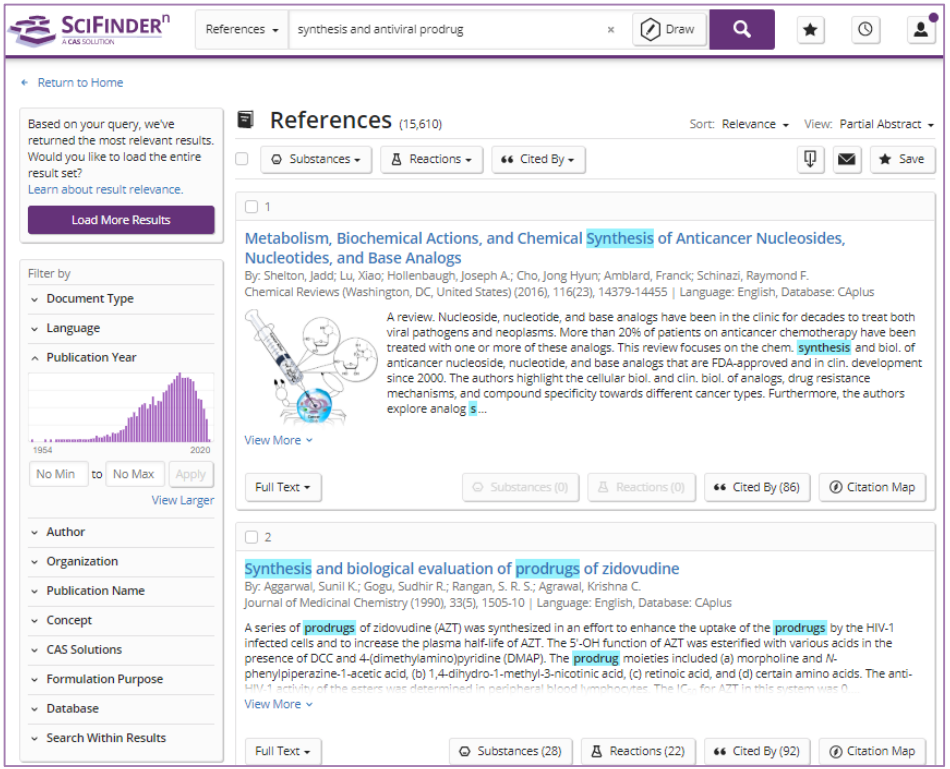
直观的结果页面，丰富的聚类分析



直观、丰富的聚类分析，
助于快速分析和筛选

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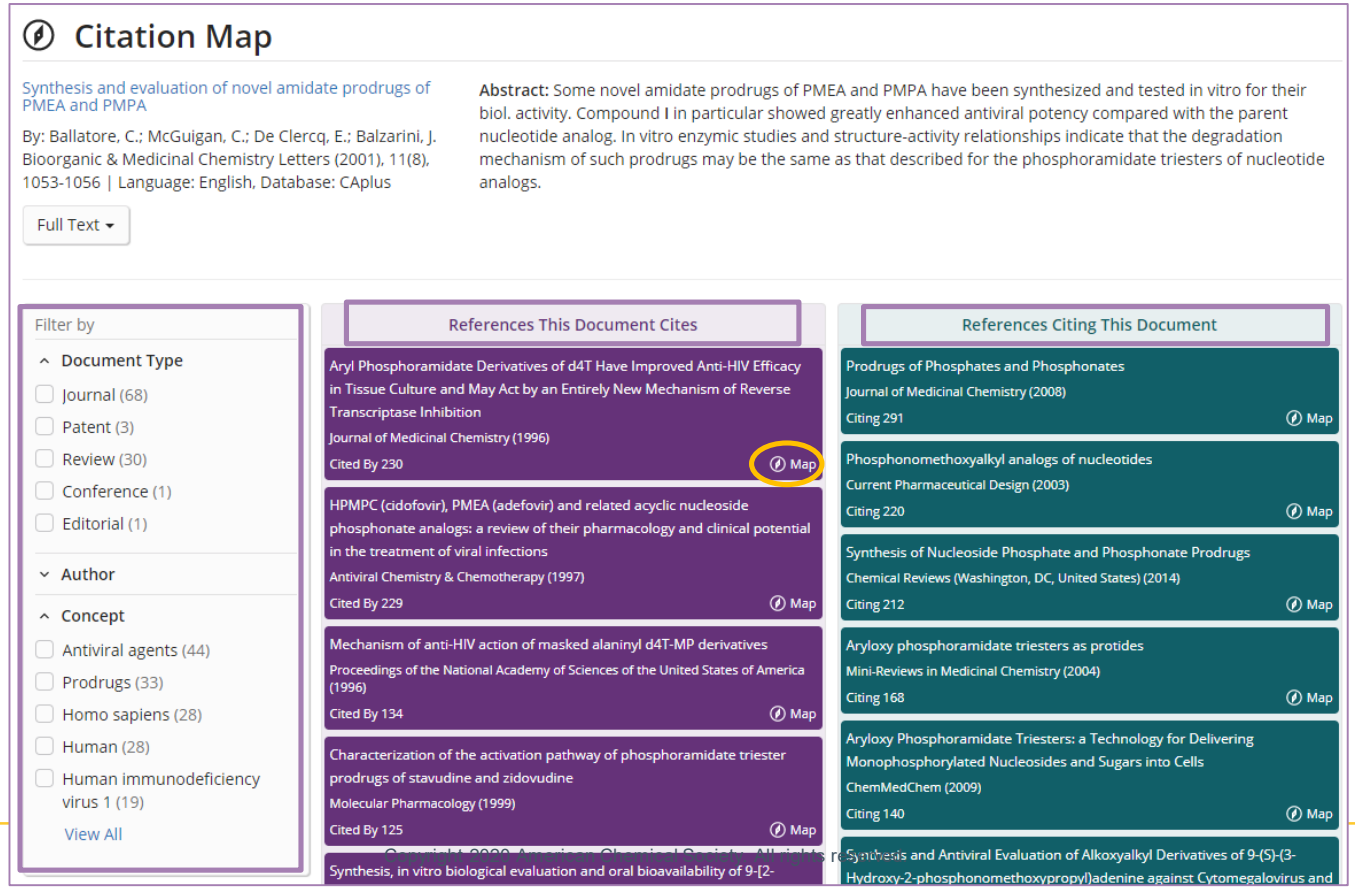
Citation Map: 引文地图，发现相关的研究方向



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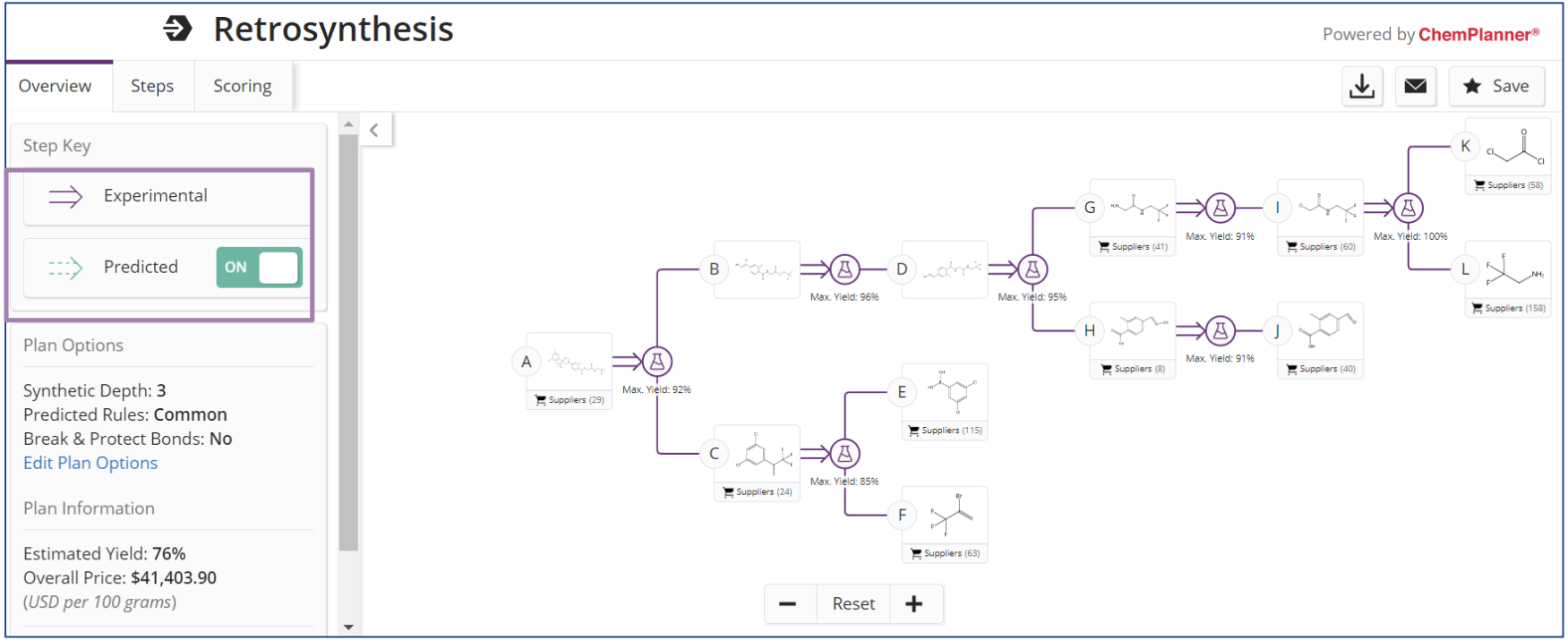
Retrosynthesis：高效获取逆合成反应路线



对已知化合物，Retrosynthesis既可以获取其已经报道的逆合成实验路线，
也可以查看其预测的路线

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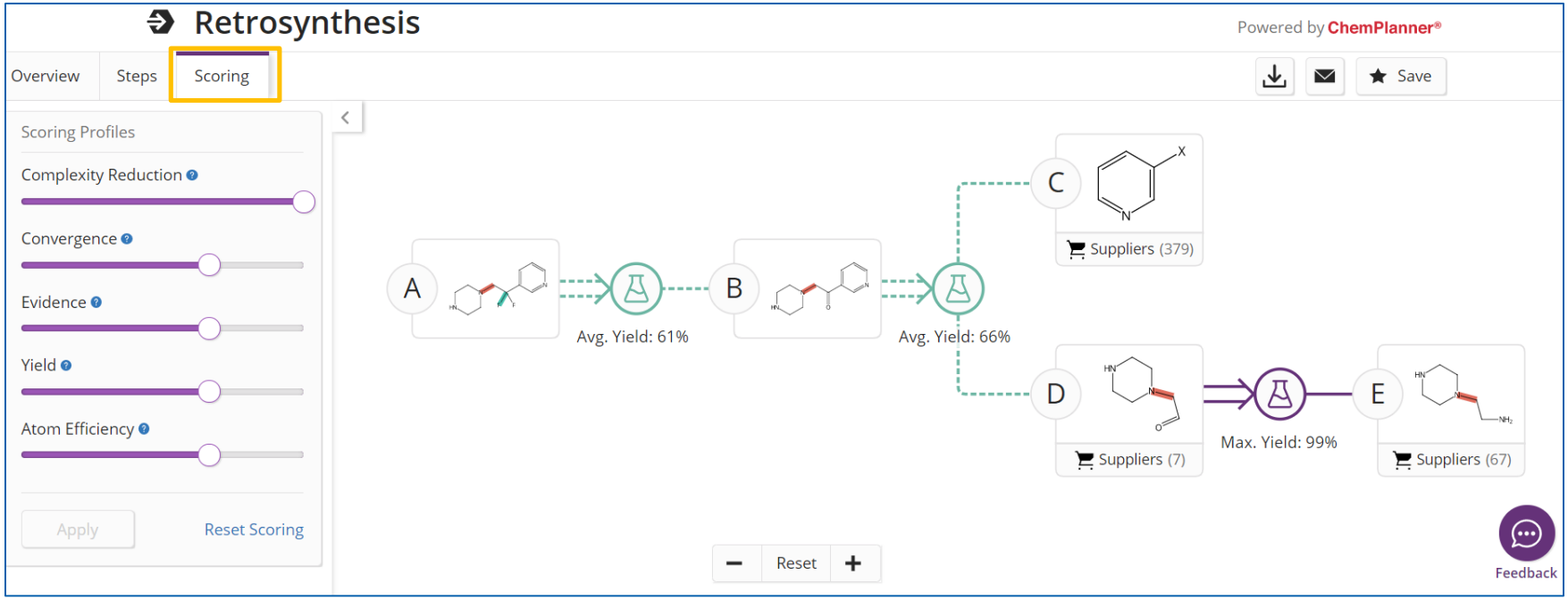
预测的逆合成实验路线结果



预测新化合物的合成路线后，可继续通过Scoring灵活调整预测参数

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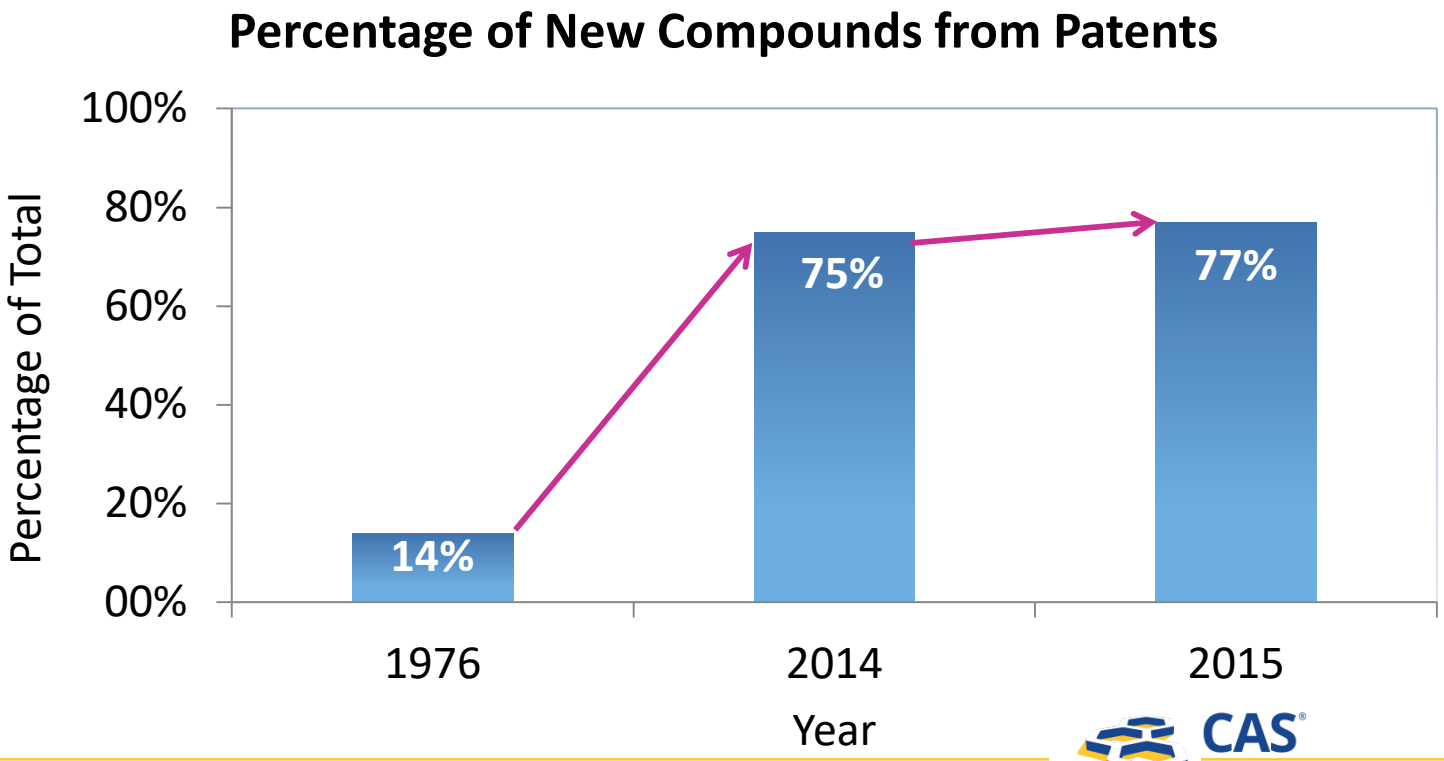
越来越多的新化合物倾向于首先通过专利公布



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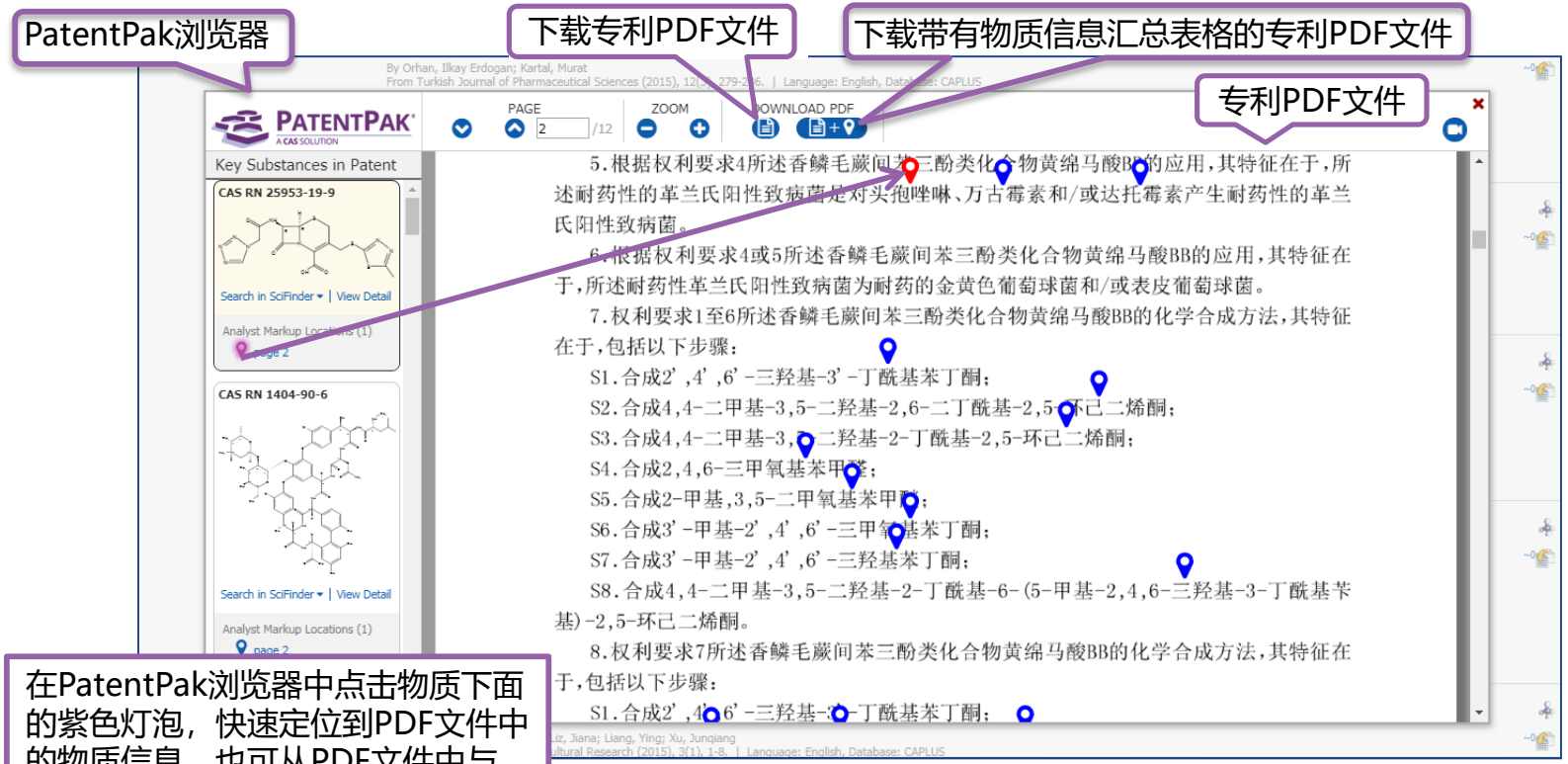

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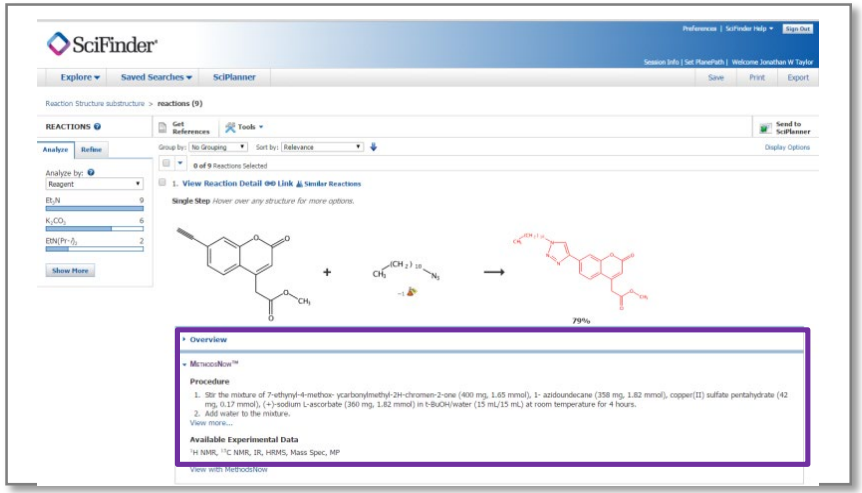

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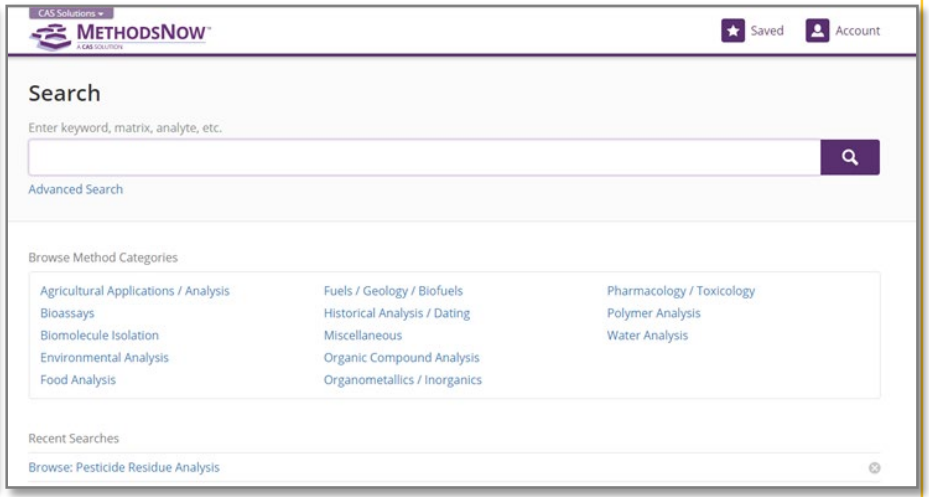

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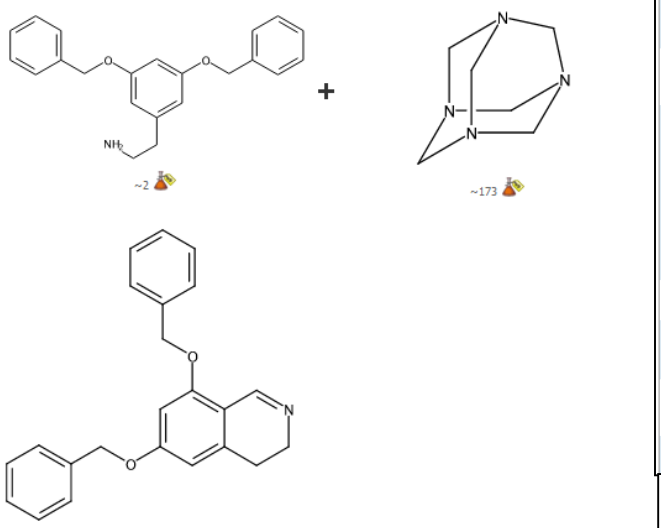
Asymmetric formal synthesis of schulzeines A and C

By Jang, Jaebong; Jung, Jong-Wha; Ahn, Jaeseung; Sim, Jaehoon; Chang, Dong-Jo; Kim, Dae-Duk; Suh, Young-Ger
From Organic & Biomolecular Chemistry, 10(27), 5202-5204; 2012
Published by Royal Society of Chemistry

Reaction Steps 1 2 3 4 5 6 7 8 9 10 11



Products	Isoquinoline, 3,4-dihydro-6,8-bis(phenylmethoxy)-, 95%, CAS RN: 1384461-35-1
Reactants	Benzeneethanamine, 3,5-bis(phenylmethoxy)-, CAS RN: 188662-05-7 Hexamethylenetetramine, CAS RN: 100-97-0
Solvents	Trifluoroacetic acid, CAS RN: 76-05-1 Acetic acid, CAS RN: 64-19-7
Procedure	1. Add hexamethylenetetramine (3.1 g, 22.1 mmol) to the mixture of 2-(3,5-bis(benzyloxy)phenyl)ethylamine (2.0 g, 11.0 mmol), AcOH (12 mL) and TFA (3 mL) under argon 2. Stir the mixture for 3hours at 90EC. 3. Dilute the reaction mixture with H_2O. 4. Basify with potassium carbonate and extract with CH_2Cl_2. 5. Wash the combined organic layers with brine. 6. Dry over $MgSO_4$ and concentrate in vacuo. 7. Purify the residue by column chromatography on silica gel (5 to 10% EtOAc in hexane) to obtain 6,8-bis(benzyloxy)-3,4-dihydroisoquinoline.
Scale	gram
^{1}H NMR	($CDCl_3$, 400 MHz) δ 8.69 (s, 1H), 7.43 - 7.29 (m, 10H), 6.45 (d, *J* = 1.88 Hz, 2H), 6.36 (s, 1H), 5.05 (s, 2H), 5.04 (s, 2H), 3.67 (t, 2H), 2.65 (t, 2H)
^{13}C NMR	($CDCl_3$, 100 MHz) δ 161.9, 157.7, 155.2, 140.0, 136.3, 128.6, 128.5, 128.1, 128.0, 127.4, 127.1, 111.9, 105.3, 98.5, 70.1, 46.5, 26.0
IR	(thin film, neat) ν_{max} 3062, 3032, 2935, 1736, 1620, 1603, 1575, 1497, 1442, 1377, 1351, 1309 cm^{-1}
HRMS	(FAB+) calcd for $C_{23}H_{22}NO_2$ ($M+H^+$) 344.1651; found 344.1658
Mass Spec	(FAB+) *m/z* 344 ($M+H^+$)
	yellow solid
er	3-614-CAS-200055

Print/Export Clos

多步反应中，原文没有
描述的实验过程以灰色展示

物质信息
名称、角色

实验过程

图谱信息

保存/导出

MethodsNow Synthesis中的实验详情不仅包含原文中描述的实验内容，**还包括supporting information中涉及的实验内容**

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MethodsNow – Analysis (www.methodsnow.com)

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Pharmacology / Toxicology: 成瘾药物检测，有毒物检测…

Bioassays: 生物探针，生物标定细胞实验，生物标定药物实验，生物医学材料分析，生物分子/生物组织分离测定…

Water Analysis: 阴阳离子分析，元素测定，痕量元素分析，废水分析，生物标记公共卫生分析…

Historical Analysis / Dating: 考古分析，同位素分析

Environmental Analysis: 土壤/空气/水分析，农药残留分析…

Agricultural Applications / Analysis: 除草剂分析…

Food Analysis: 脂肪酸分析，脂肪酸酯分析，蛋白质分析…

Fuels / Geology / Biofuels: 生物燃料分析，油气分析，石油产品分析，煤炭加工…

Miscellaneous: 化妆品分析，爆炸物分析，纳米材料分析…

目前有13个大类，45个小类。某些子项目属于多种方法分类！

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MethodsNow – Analysis (www.methodsnow.com)

Analysis of Nitric oxide in Blood plasma by Electrochemical biosensors

改写的标题

CAS MN: 2-114-CAS-117192

Method Category: Biomolecule Isolation Assay; Gas Analysis
Technique: Electrochemical biosensors

Materials	Role
Nitric oxide	analyte
Blood plasma	matrix
Catheters	materi
Nitric oxide (NO) sensor (700 µm in diameter at the detection tip)	materi
4-French (4-Fr) catheter (1,200 mm long)	materi
7-Fr JR catheter	materi
Doppler guide wire	materi
Silicon	reagen
Isosorbide dinitrate	reagen
Acetylcholine	reagen
Ketamine	reagen
N^G-Monomethyl-L-arginine	reagen
Heparin	reagen
Pentobarbital sodium	reagen
Physiological saline solutions	reagen
Polyurethanes	reagen

实验的材料

Source

文献信息

Evaluation of bioavailability of nitric oxide in coronary circulation by direct measurement of plasma nitric oxide concentration

Neishi, Yoji; Mochizuki, Seiichi; Miyasaka, Takehiro; Kawamoto, Takahiro; Kume, Teruyoshi; Sukmawan, Renan; Tsukiji, Miwako; Ogasawara, Yasuo; Kajiya, Fumihiko; Akasaka, Takashi; Yoshida, Kiyoshi; Goto, Masami

Proceedings of the National Academy of Sciences of the United States of America (2005), 102 (32), 1

CODEN: PNASA6 | ISSN: 00278424 | DOI: 10.1073/pnas.0501392102

Full Text

Abstract

Although bioavailability of NO in the coronary circulation is commonly evaluated by acetylcholine (AC
relation to the flow response after injection of ACh are still unknown. Thus, the authors directly mea
NO sensor for coronary sinus. An NO-sensitive sensor was located and fixed in a 4-Fr catheter with a
pure water, the catheter-type NO sensor was located in the coronary sinus in anesthetized dogs. The
Intracoronary injection of ACh (0.4 and 1.0 µg/kg) increased plasma NO concentration in a dose-dep
no significant difference between the two ACh doses. After ACh, the peak value of plasma NO concer
synthase inhibitor) decreased basal NO concentration by 3 nM and suppressed the ACh-induced NO
conclude that production of NO in the coronary circulation can be evaluated in the coronary sinus. A
NO concentration in terms of magnitude and time course. Direct measurement of plasma NO concer
NO in the coronary circulation.

Equipment Used

Nitric oxide (NO) monitor, inNO-T, Innovative Instruments, Tampa, FL

Respirator pump, VS-600, Instrumental Development, Pittsburgh

Strain gauge pressure transducer, TP-400T, Nihon Kohden, Tokyo

实验仪器

Instructions

详细步骤

Preparation of animals

1. Sedate the adult mongrel dogs (n = 7) with ketamine (200 mg i.m.).
2. Anesthetize with pentobarbital sodium (30 mg/kg i.v.).
3. Heparinize the each dog by injecting 100 units/kg of heparin.
4. Ventilate the animals by using a respirator pump (model VS-600, Instrumental Development, Pittsburgh).
5. Place the NO sensor in the coronary sinus through a 7-Fr JR catheter (Bright Chip, Cordis, Miami) from the right jugular vein.
6. Place a doppler guide wire (FloWire, JoMed, Rancho Cordova, CA) in the left anterior descending artery through another 7-Fr JR catheter inserted in the right carotid artery under cinefluorography.

Preparation of nitric oxide (NO) sensor

1. Mount the NO sensor (amiNO-700 XL, Innovative Instruments, Tampa, FL; 700 µm in diameter at the detection tip) in a 4-Fr catheter (1,200 mm long; Hirakawa Hewtech, Tokyo).
2. Fix with silicon adhesive.
3. Attach soft protection tip of polyurethane at the edge of the detection tip to protect the vessel wall.
4. Attach two metal wires along the detection tip to protect the detection tip.
5. Monitor oxidative current of NO by using an NO monitor (model inNO-T, Innovative Instruments).
6. Calibrate each sensor by using an NO-saturated pure water.
7. Prepare NO-saturated pure water by bubbling pure NO gas in oxygen-free pure water.
8. Inject 5 µL into a well stirred saline solution (50 mL) using a gas-tight syringe and immerse NO sensor (final NO concentration: 190 nM).

Determination of nitric oxide (NO)

1. Monitor plasma NO concentration in the coronary sinus using NO sensor, phasic coronary blood flow by the doppler guide wire in the left anterior descending artery and aortic pressure by a strain gauge pressure transducer (model TP-400T, Nihon Kohden, Tokyo).
2. Measure average peak velocity (APV) as coronary flow velocity.
3. Inject saline (vehicle) and acetylcholine (ACh) of 0.4 µg/kg and 1.0 µg/kg from the left coronary artery (LCA) for 20 s.
4. Dilute each solution to 5 mL with saline.
5. Administrate N^G-methyl-L-arginine (L-NAME, 10 µg/kg/min) into the LCA for 20 min to inhibit NO synthesis.
6. Repeat the ACh injection at two doses (0.4 µg/kg and 1.0 µg/kg).
7. Inject NO donor, isosorbide dinitrate (ISDN, 0.5 mg).

Validation

数据有效性

Sensitivity	366 ± 122 pA/nM
Concentration	1.9 ± 0.6 nM vs. 5.0 ± 2.7 nM (After L-NAME vs. control) at 0.4 µg/kg 2.8 ± 0.8 nM vs. 7.3 ± 3.5 nM (After L-NAME vs. control) at 1.0 µg/kg

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