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美国化学文摘社北京代表处

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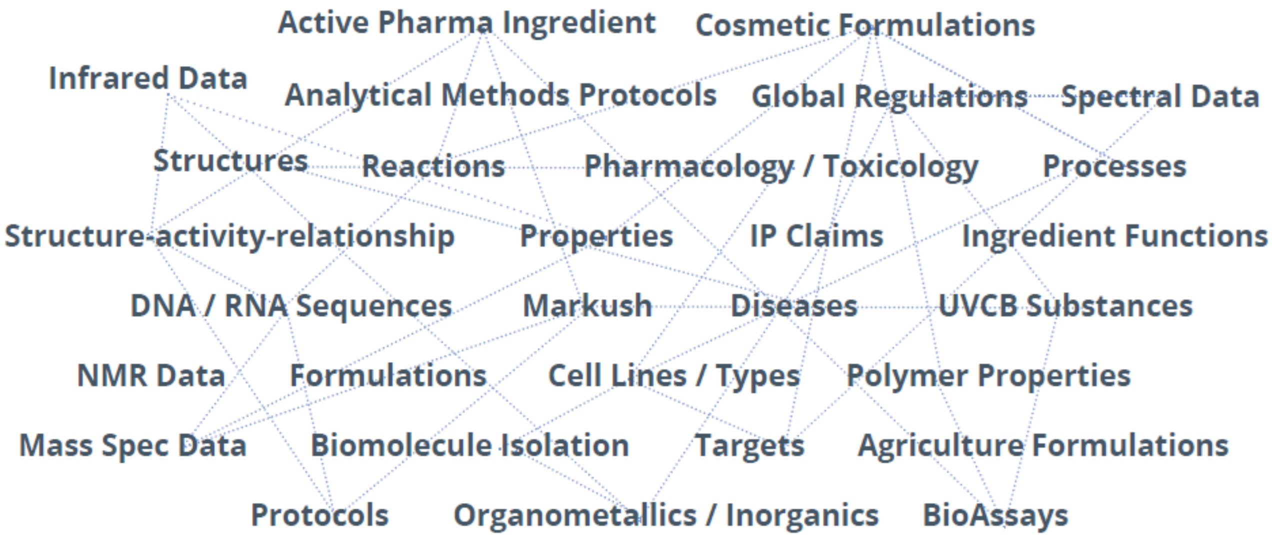

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(30) Priority Data:
62/265,780 10 December 2015 (10.12.2015) US

Row, San Diego, California 92121 (US). **GHOSH, Brahmananda**; 1400 McKean Road, Spring House, Pennsylvania 19477 (US). **HAO, Baoyu**; c/o Hutchinson Medipharma Limited, Building 4, 720 Cailun Road, Zhangjian Hi-Tech Park, Shanghai 201203 (CN). **KREUTTER, Kevin**; c/o Janssen Research & Development LLC, 1400 McKean Road, Spring House, Pennsylvania 19477 (US). **LI, Gang**; c/o Hutchinson Medipharma Limited, Building 4, 720 Cailun Road, Zhangjian Hi-Tech Park, Shanghai 201203 (CN). **TICHENOR, Mark S.**; 3210 Merryfield Row, San Diego, California 92121 (US). **VENABLE, Jennifer D.**; 3210 Merryfield Row, San Diego, California 92121 (US). **WEI, Jianmei**; 3210 Merryfield Row, San Diego, California

1000页！篇幅太长，难以短时间内理解其中的信息，是否太难？

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Table 2

近千个化合物，要确定其结构式和CAS号，是否太难？

Ex #	Compound Name	BTK_I_binding pIC50
1	N-((3R,5R)-1-Acryloyl-5-fluoropiperidin-3-yl)-5-(2-methyl-4-phenoxyphenyl)-4-oxo-4,5-dihydro-3H-1-thia-3,5,8-triazaacenaphthylene-2-carboxamide;	7.7
2	N-((3R,5S)-1-Acryloyl-5-hydroxypiperidin-3-yl)-5-(*S)-(2-methyl-4-phenoxyphenyl)-4-oxo-4,5-dihydro-3H-1-thia-3,5,8-triazaacenaphthylene-2-carboxamide;	8.2
974	(R)-N-(1-Acryloylpyrrolidin-3-yl)-5-(2-methyl-6-(pyridazin-3-yloxy)pyridin-3-yl)-4-oxo-4,5-dihydro-3H-1-thia-3,5,8-triazaacenaphthylene-2-carboxamide;	5.6
975	(R)-N-(1-Acryloylpiperidin-3-yl)-5-(2-methyl-6-(pyridazin-3-yloxy)pyridin-3-yl)-4-oxo-4,5-dihydro-3H-1-thia-3,5,8-triazaacenaphthylene-2-carboxamide;	5.0

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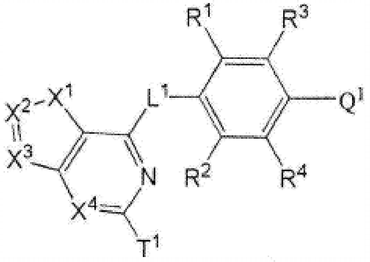
为什么需要美国化学文摘社（CAS）

CN 106232118 A　　权　利　要　求　书　　1/12 页

1.式I的化合物或其药学上可接受的盐用于治疗哺乳动物的D1-介导的(或D1-相关

障碍的用途：



I

结构式复杂，难以根据定义绘制其结构，是否太难？

L^1为O、S、NR^N、C(=O)、CH(OH)或$CH(OCH_3)$；

Q^1为含N的5元至10元杂芳基、含N的4元至12元杂环烷基或苯基，它们各自任选地被一个R^9取代且进一步任选地被1、2、3或4个R^{10}取代；

X^1为O、S、NH、N(C_{1-4}烷基)、N(环丙基)或N(-CH_2-环丙基)；

X^2为N或C-T^2；

X^3为N或C-T^3；

前提条件是当X^1为O或S时，则X^2和X^3中的至少一个不为N；

X^4为N或C-T^4；

T^1为H、-OH、卤素、-CN或任选被取代的C_{1-2}烷基；

T^2、T^3和T^4各自独立地选自由下列选项组成的组：H、-OH、卤素、-CN、任选被取代的C_{1-4}烷基、任选被取代的C_{3-4}环烷基、任选被取代的环丙基甲基以及任选被取代的C_{1-4}烷氧基；

R^N为H、C_{1-4}烷基、C_{3-4}环烷基或-C_{1-2}烷基-C_{3-4}环烷基，

R^1和R^2各自独立地选自由下列选项组成的组：H、卤素、-CN、C_{1-6}烷基、C_{1-6}卤代烷基、C_{1-6}烷氧基、C_{1-6}卤代烷氧基以及C_{3-6}环烷基，其中所述的C_{1-6}烷基和C_{3-6}环烷基各自任选地被各自独立地选自下列选项的1、2、3、4或5个取代基取代：卤代、-OH、-CN、C_{1-4}烷基、C_{1-4}卤代烷基、C_{1-4}烷氧基以及C_{1-4}卤代烷氧基；

R^3和R^4各自独立地选自由下列选项组成的组：H、卤素、-OH、-NH_2、-NH(CH_3)、-N$(CH_3)_2$、-NO_2、-CN、-SF_5、C_{1-6}烷基、C_{1-6}卤代烷基、C_{1-6}卤代烷氧基、C_{2-6}烯基、C_{2-6}炔基、C_{3-7}环烷基、4元至10元杂环烷基、-N(R^5)(R^6)、-N(R^7)(C(=O)R^8)、-C(=O)-N(R^5)(R^6)、-C(=O)-R^8、-C(=O)-OR^8、-N(R^7)(S(=O)$_2R^8$)、-S(=O)$_2$-N(R^5)(R^6)、-SR^8以及-OR^8，其中所述的C_{1-6}烷基、C_{3-7}环烷基及杂环烷基各自任选地被各自独立地选自由下列选项组成的组的1、2或3个取代基取代：卤素、-CN、-OH、C_{1-4}烷基、C_{1-4}烷氧基、C_{1-4}卤代烷基、C_{1-4}卤代烷氧基、C_{3-6}环烷基、-N(R^5)(R^6)、-N(R^7)(C(=O)R^8)、-C(=O)-OR^8、-C(=O)H、-C(=O)R^8、-C(=O)N(R^5)(R^6)、-N(R^7)(S

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为什么需要美国化学文摘社（CAS）

WO 2006/016684 PCT/JP2005/014867

1

DESCRIPTION

PDF原文中的标题和摘要

METHOD FOR SYNTHESIS OF AROMATIC AMINE

(57) Abstract: One embodiment of the present invention provides a method for synthesis of substituted secondary amine by the reaction of aniline with aryl halide by using a Pd catalyst including $(t\text{-Bu})_3P$ as a ligand.

Process for synthesis of substituted secondary amines via condensation of aniline with aryl halides with a palladium catalyst and (t-Bu)3P as a ligand as an electroluminescence source for display devices

CAS科学家改写的标题和摘要

By: Nakashima, Harue; Kawakami, Sachiko

Assignee: Semiconductor Energy Laboratory Co., Ltd., Japan

A process for the synthesis of secondary amines is presented via condensation of aniline with an aryl halide using palladium as a catalyst and $(t\text{-Bu})_3P$ as a ligand in the key step. Thus, N-(4-diphenylamino)phenylaniline is synthesized in 42% yield by condensation of N,N-diphenyl-N-(4-bromophenyl)amine with aniline. The process avoids protecting groups though the use of a palladium catalyst and $(t\text{-Bu})_3P$ as a ligand. N-(4-diphenylamino)phenylaniline can be used as an electroluminescence source for display devices including a light-emitting diodes, flat panel displays, liq. crystal display devices (no data).

CAS的科学家对专利进行必要改写，使其更容易被理解和获取

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Indexing

Heterocyclic Compounds (More Than One Hetero Atom) (Section28-16)

Section cross-reference(s): 1, 63

Concepts

Antirheumatic agents
Homo sapiens
Pharmaceutical excipients

Antitumor agents
Human

prepn. of oxodihydrothiatriazaacenaphthylenecarboxamides as inhibitors of Bruton's tyrosine kinase

CAS科学家标引的信息揭示了本专利的发明主题

Neoplasm
Rheumatoid arthritis

...ematosus

treatment of; prepn. of oxodihydrothiatriazaacenaphthylenecarboxamides as inhibitors of Bruton's tyrosine kinase

2101210-72-2P	Page 211 in PATENTPAK
2101210-73-3P	Page 211 in PATENTPAK
2101210-82-4P	Page 217 in PATENTPAK
2101211-31-6P	Page 257 in PATENTPAK
2101211-41-8P	Page 265 in PATENTPAK
2101211-62-3P	Page 280 in PATENTPAK
2101212-16-0P	Page 316 in PATENTPAK
2101212-26-2P	Page 323 in PATENTPAK
2101212-84-2P	Page 365 in PATENTPAK
2101214-41-7P	Page 493 in PATENTPAK
2101216-00-4P	Page 639 in PATENTPAK
2101216-02-6P	Page 640 in PATENTPAK
2101216-63-9P	Page 705 in PATENTPAK
2101216-66-2P	Page 706 in PATENTPAK
2101216-70-8P	Page 710 in PATENTPAK
2101216-72-0P	Page 714 in PATENTPAK
2101216-74-2P	Page 716 in PATENTPAK

CAS科学家标引的物质信息。此两组物质都为被制备的物质，有何异同？

prepn. of oxodihydrothiatriazaacenaphthylenecarboxamides as inhibitors of Bruton's tyrosine kinase

Pharmacological activity; Physical, engineering or chemical process; Synthetic preparation; Therapeutic use; Biological study; Preparation; Process; Uses

2101212-82-0P	Page 364 in PATENTPAK
2101212-92-2P	Page 370 in PATENTPAK
2101215-45-4P	Page 598 in PATENTPAK

prepn. of oxodihydrothiatriazaacenaphthylenecarboxamides as inhibitors of Bruton's tyrosine kinase

Pharmacological activity; Physical, engineering or chemical process; Reactant; Synthetic preparation; Therapeutic use; Biological study; Preparation; Process; Uses; Reactant or reagent

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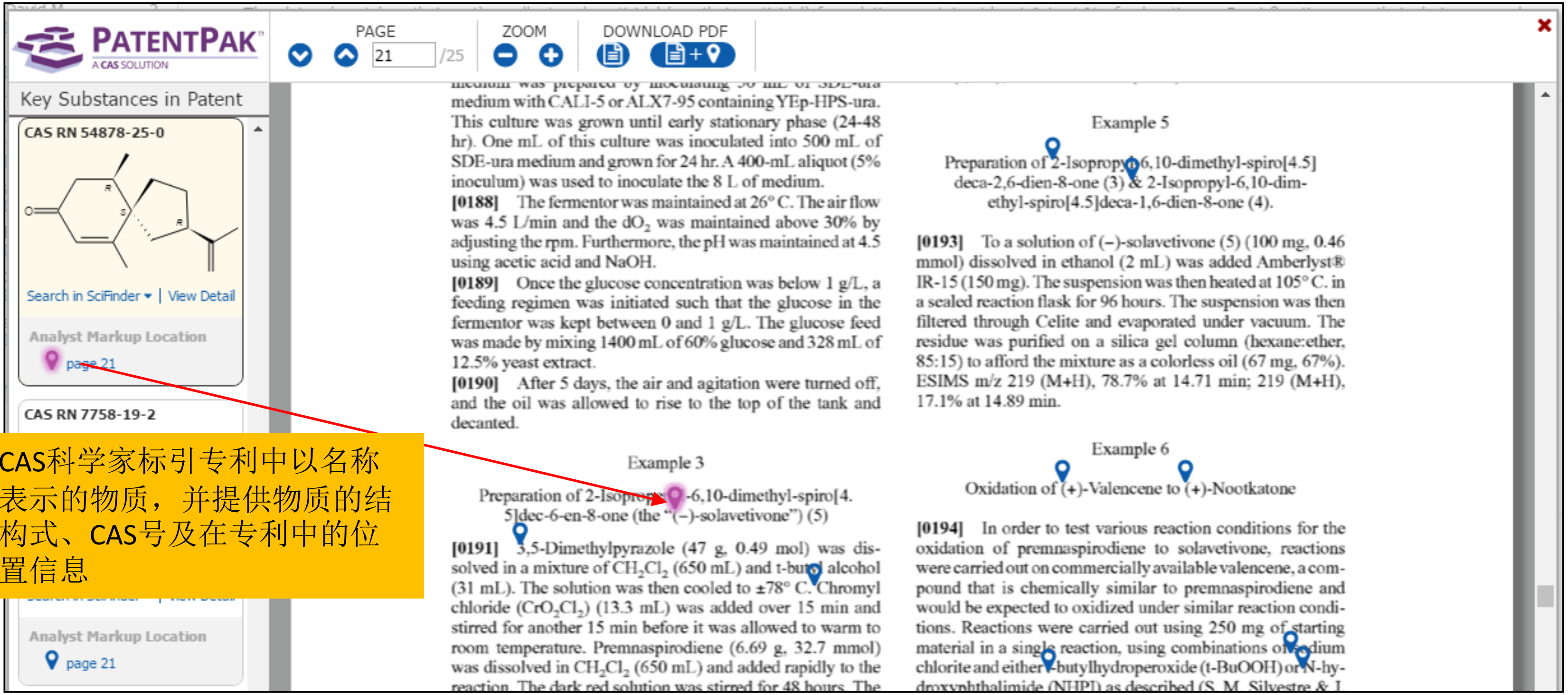

CAS科学家标引专利中以名称表示的物质，并提供物质的结构式、CAS号及在专利中的位置信息

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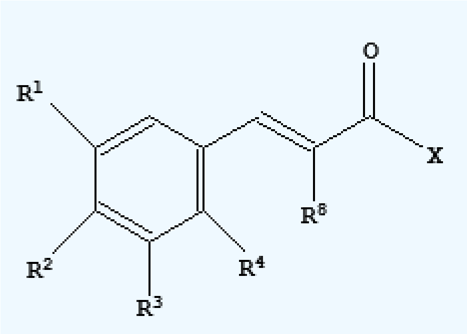
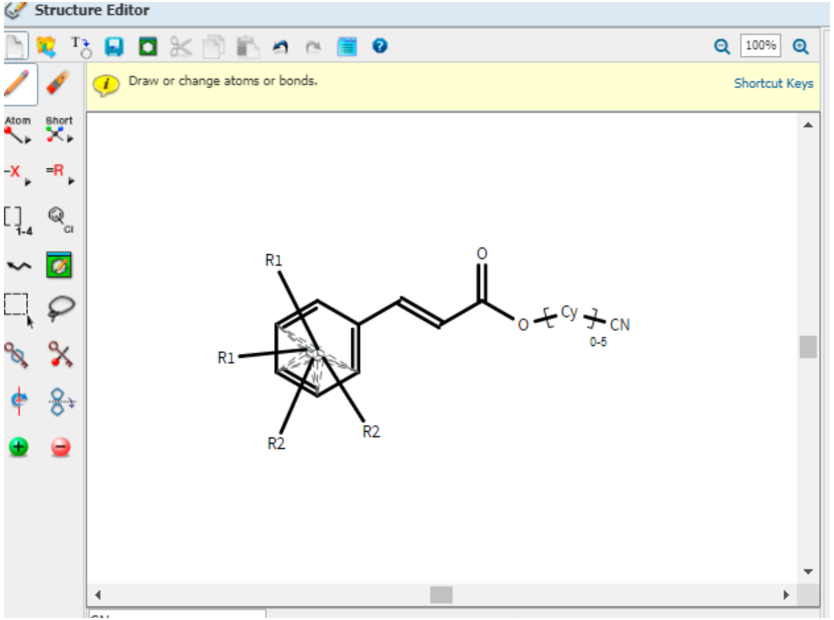
为什么需要美国化学文摘社(CAS)





R1-R4相同或不同，分别为H、F、Cl、Br

R1-R4至少有两个不能同为氢

X=O-[Ar]$_{0\text{-}5}$-CN

R8为任意原子

CAS的解决方案具有强大的结构绘制功能，能够绘制较复杂的结构

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- 数据平台
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- 技术评估
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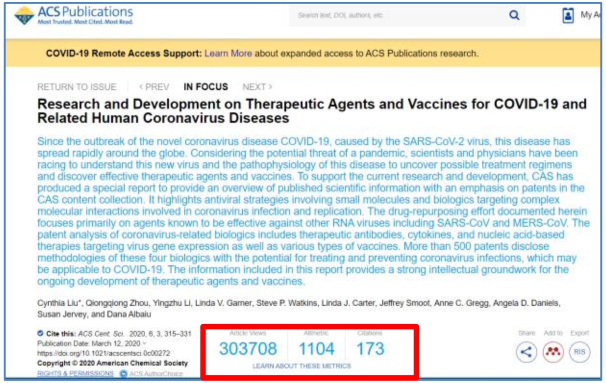
美国化学文摘社(CAS)为抗击新冠病毒发布的分析报告

COVID-19治疗药物及疫苗研发数据分析报告
ACS Cent. Sci. 2020, 6, 3, 315-331
发布日期：March 12, 2020
https://doi.org/10.1021/acscentsci.0c00272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Research and Development on Therapeutic Agents and Vaccines for COVID-19 and Related Human Coronavirus Diseases

Since the outbreak of the novel coronavirus disease COVID-19, caused by the SARS-CoV-2 virus, this disease has spread rapidly around the globe. Considering the potential threat of a pandemic, scientists and physicians have been racing to understand this new virus and the pathophysiology of this disease to uncover possible treatment regimens and discover effective therapeutic agents and vaccines. To support the current research and development, CAS has produced a special report to provide an overview of published scientific information with an emphasis on patents in the CAS content collection. It highlights antiviral strategies involving small molecules and biologics targeting complex molecular interactions involved in coronavirus infection and replication. The drug-repurposing effort documented herein focuses primarily on agents known to be effective against other RNA viruses including SARS-CoV and MERS-CoV. The patent analysis of coronavirus-related biologics includes therapeutic antibodies, cytokines, and nucleic acid-based therapies targeting virus gene expression as well as various types of vaccines. More than 500 patents disclose methodologies of these four biologics with the potential for treating and preventing coronavirus infections, which may be applicable to COVID-19. The information included in this report provides a strong intellectual groundwork for the ongoing development of therapeutic agents and vaccines.

Cynthia Liu*, Qiongqiong Zhou, Yingzhu Li, Linda V. Garner, Steve P. Watkins, Linda J. Carter, Jeffrey Smoot, Anne C. Gregg, Angela D. Daniels, Susan Jervey, and Dana Albaiu

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Publication Date: March 12, 2020
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Article Views 303708 | Altmetric 1104 | Citations 173
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Table 2. Key Proteins and Their Roles during the Viral Infection Process

target candidate	full name	role during viral infection	drug candidate
3CLpro	coronavirus main protease 3CLpro	a protease for the proteolysis of viral polyprotein into functional units	lopinavir[19,30]
PLpro	papain-like protease PLpro	a protease for the proteolysis of viral polyprotein into functional units	lopinavir[19,30]
RdRp	RNA-dependent RNA polymerase	an RNA-dependent RNA polymerase for replicating viral genome	remdesivir,[19,29,32] ribavirin[16,29,31]
S protein	viral spike glycoprotein	a viral surface protein for binding to host cell receptor ACE2	Arbidol[20,22,33a]
TMPRSS2	transmembrane protease, serine 2	a host cell-produced protease that primes S protein to facilitate its binding to ACE2	camostat mesylate[11]
ACE2	angiotensin-converting enzyme 2	a viral receptor protein on the host cells which binds to viral S protein	Arbidol[20,22,33a]
AT2	angiotensin AT2 receptor	an important effector involved in the regulation of blood pressure and volume of the cardiovascular system	L-163491[28]

[a]An inhibitor of viral entry to host cells. Its direct action on S protein and ACE2 is yet to be confirmed.

Table 8. Target Analysis of Patents on Developing Therapeutic Antibodies for SARS

patent number	antigen of SARS antibody	patent title	organization	priority date
EP2112164	lipid attachment signals or GPI	Antiviral peptides linked to a lipid attachment signals or GPI against enveloped virus such as HIV, avian flu, SARS or Ebola virus	Institute Pasteur of Shanghai	20080229
WO2009128963	spike protein	Cross-neutralizing human monoclonal antibodies to SARS-CoV and methods of use thereof	Institute for Research In Biomedicine	20080117
WO2009128963	spike protein	Cross-neutralizing human monoclonal antibodies to spike protein of SARS coronavirus and methods of use thereof	Humab, LLC	20080117
WO2008035894	viral infection	Preparation of antiviral antibody 3D8 fragments and their use in treatment of viral infection	Sung Kyun Kwan University; Ajou University; Invitroplant Co., Ltd.	20060919
WO2008060331	spike protein	Antibodies to SARS coronavirus	Amgen Inc.	20060519
WO2007044695	spike protein	Neutralizing monoclonal anti-spike protein antibodies for diagnosis and treatment of SARS-coronavirus-associated disease and screening of vaccine or anti-SARS agent	Dana-Farber Cancer Institute	20051007
CN1911963	RBD of S protein	Method for preparing neutralizing monoclonal antibody against severe acute respiratory syndrome coronavirus and its application	Chinese Academy of Sciences	20050810
CN1903878	spike protein	Fab fragment of human antibody IgG against SARS coronavirus	Fudan University	20050726
WO2006095180	S2 protein	Human monoclonal antibodies against SARS-associated coronavirus and treatment of patients with SARS	Ultra Biotech Ltd.; University of California	20050310
WO2006086561	spike protein	Neutralizing monoclonal antibodies against severe acute respiratory syndrome-associated coronavirus	New York Blood Center, Inc.	20050208

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美国化学文摘社(CAS)为抗击新冠病毒发布的分析报告

COVID-19诊断检测方法与技术开发

ACS Cent. Sci. 2020, 6, 5, 591-605
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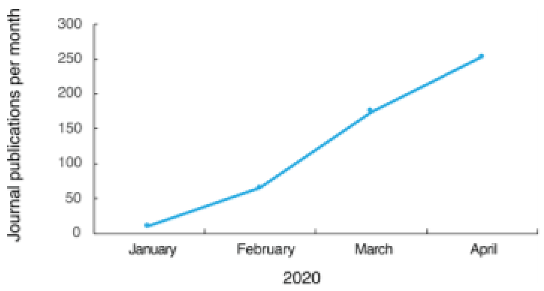

Figure 7. Monthly trend of journal publications related to COVID-19 diagnostics in 2020.

Table 4. Journal Articles with SARS-CoV-2-Related Sequences for Potential Applications in Diagnostics

publication date	title	journal	nucleic acids	proteins
2020	Nanopore Target Sequencing for Accurate and Comprehensive Detection of SARS-CoV-2 and Other Respiratory Viruses	*medRxiv*	40 primers	
2020	A Single and Two-Stage, Closed-Tube, Molecular Test for the 2019 Novel Coronavirus (COVID-19) at Home, Clinic, and Points of Entry	*ChemRxiv*	6 COVID-19 LAMP primers	
2020	Transmission and Clinical Characteristics of Coronavirus Disease 2019 in 104-Outside-Wuhan Patients, China	*medRxiv*	6 primers and probes	
2020	A Pneumonia Outbreak Associated with a New Coronavirus of Probable Bat Origin	*Nature*	4	50
2020	A New Coronavirus Associated with Human Respiratory Disease in China	*Nature*	1	10
2020	A Sequence Homology and Bioinformatic Approach Can Predict Candidate Targets for Immune Responses to SARS-CoV-2	*Cell Host & Microbe*		51
2020	Comparative Analysis of Primer-Probe Sets for the Laboratory Confirmation of SARS-CoV-2	*bioRxiv*	20 primers, 10 probes	
2020	Spike Protein Binding Prediction with Neutralizing Antibodies of SARS-CoV-2	*bioRxiv*		3
2020	SARS-CoV-2 Proteome Microarray for Mapping COVID-19 Antibody Interactions at Amino Acid Resolution	*bioRxiv*		11
2020	Evaluation of Recombinant Nucleocapsid and Spike Proteins for Serological Diagnosis of Novel Coronavirus Disease 2019 (COVID-19)	*medRxiv*	12 primers	
2020	RBD Mutations from Circulating SARS-CoV-2 Strains Enhance the Structure Stability and Infectivity of the Spike Protein	*bioRxiv*		8
2020	Teicoplanin Potently Blocks the Cell Entry of 2019-nCoV	*bioRxiv*	14	134
2020	Differential Antibody Recognition by SARS-CoV-2 and SARS-CoV Spike Protein Receptor Binding Domains: Mechanistic Insights and Implications for the Design of Diagnostics and Therapeutics	*bioRxiv*		7
2020	A Proposal of an Alternative Primer for the ARTIC Network's Multiplex PCR to Improve Coverage of SARS-CoV-2 Genome Sequencing	*bioRxiv*	2	
2020	First 12 Patients with Coronavirus Disease 2019 (COVID-19) in the United States	*medRxiv*	12	109

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美国化学文摘社(CAS) 为抗击新冠病毒提供数据集

CAS 抗新冠病毒数据集

50,000候选化合物

包括已知或潜在的抗病毒活性物质以及相关的数据，以支持研究，数据挖掘和分析应用

下载网址： https://www.cas.org/covid-19-antiviral-compounds-dataset

```
L-Alanine, N-[(S)-hydroxyphenoxyphosphinyl]-, 2-ethylbutyl ester, 6-ester
C27H35N6O8P
1809249-37-3 Copyright (C) 2020 ACS
42 45  0  0  1  0  0  0  0  0999 V2000
24113.740225083.5116    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
24738.466831027.3695    0.0000 N   0  0  0  0  0  0  0  0  0  0  0  0
14556.860113339.0458    0.0000 O   0  0  0  0  0  0  0  0  0  0  0  0
35135.6204 8964.8958    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
41864.271512849.6839    0.0000 O   0  0  0  0  0  0  0  0  0  0  0  0
48592.9226 8964.8958    0.0000 P   0  0  1  0  0  5  0  0  0  0  0  0
48592.922616734.4721    0.0000 O   0  0  0  0  0  0  0  0  0  0  0  0
53768.806911953.1943    0.0000 N   0  0  0  0  0  0  0  0  0  0  0  0
48592.9226 2988.2986    0.0000 O   0  0  0  0  0  0  0  0  0  0  0  0
58944.6882 8964.8958    0.0000 C   0  0  1  0  0  0  0  0  0  0  0  0

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L-Alanine, N-[(S)-hydroxyphenoxyphosphinyl]-, 2-ethylbutyl ester, 6-ester with 2-C-(4-
aminopyrrolo[2,1-f][1,2,4]triazin-7-yl)-2,5-anhydro-D-altrononitrile

> <molecular.formula>
C27H35N6O8P

> <molecular.weight>
602.58

> <density.predicted>
1.47Â±0.1 g/cm3    Temp: 20 Â°C; Press: 760 Torr

> <pka.predicted>
12.00Â±0.70    Most Acidic Temp: 25 Â°C
```

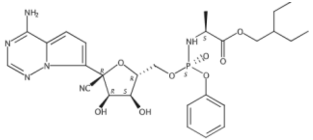

Absolute stereochemistry.

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美国化学文摘社(CAS) 为抗击新冠病毒提供数据集

COVID-19
Protein Target Thesaurus

CAS 抗新冠病毒候选靶向蛋白数据集
包括SARS-CoV-2 病毒蛋白，病毒入侵所依赖的宿主蛋白，宿主免疫反应相关蛋白等，下载网址：https://www.cas.org/covid-19-protein-target-thesaurus

63个靶向蛋白以及它们的常用名

5	328404-18-8	Angiotensin-converting enzyme 2	Carboxypeptidase, angiotensin-converting enzyme-related Angiotensin-converting enzyme-related carboxypeptidase Carboxypeptidase ACE2 ACE2 APN 01 Angiotensin I converting enzyme II Angiotensin I converting enzyme 2 Angiotensin 1 converting enzyme 2 Angiotensin 1 converting enzyme II E.C. 3.4.17.23 EC 3.4.17.23 ACE-II ACE-2 Angiotensin-converting enzyme II ACEII

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大纲

- 美国化学文摘社(CAS)内容特色及定制服务
- 为什么需要SciFinder^n

为什么需要SciFinder^n

- SciFinder^{n}完全涵盖SciFinder中的内容
- SciFinder^{n}整合了专利流程解决方案PatentPak，利于快速定位专利中的关键信息及节省阅读、理解专利原文所花费的时间
- SciFinder^{n}整合了方法学解决方案MethodsNow-Synthesis，无需获取全文即可获得合成方法所需的详细信息
- 采用先进的技术和算法，可按相关性排列检索结果，提高获取信息的效率
- 多样化的聚类选项，细化研究，拓展思路
- 利用CAS的大数据及新技术，提供逆合成设计工具Retrosynthesis，触发创新灵感

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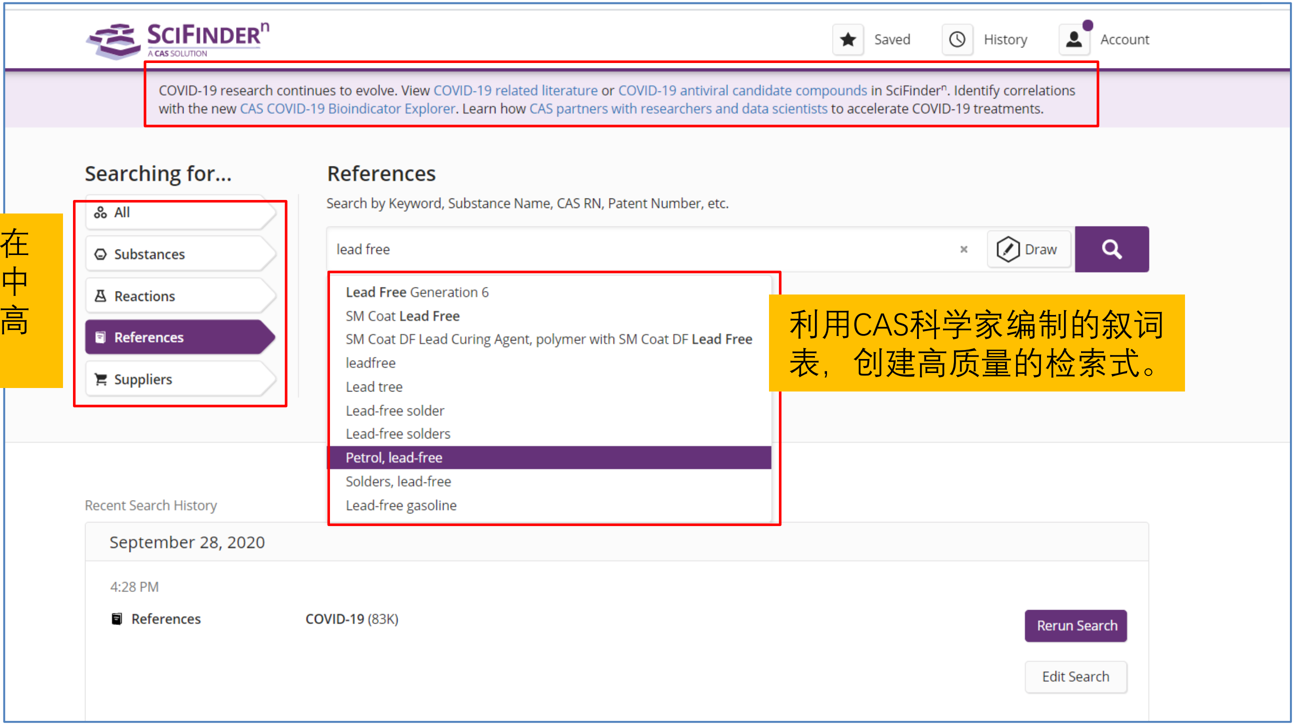
为什么需要SciFinder^n

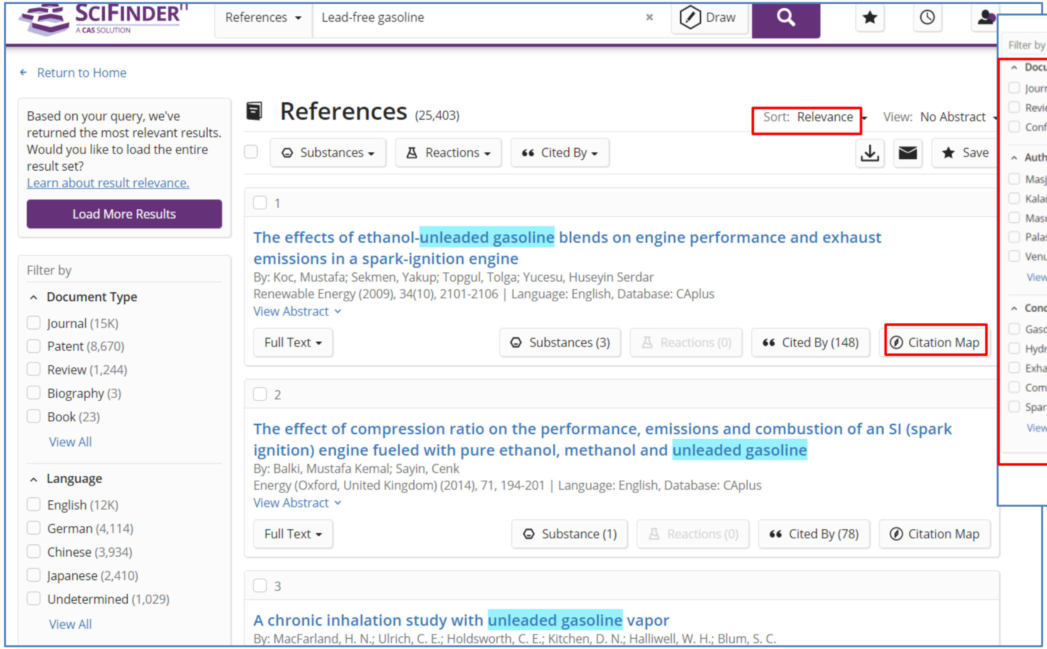
无需逐步在不同信息中检索，提高检索效率



利用CAS科学家编制的叙词表，创建高质量的检索式。

为什么需要SciFinder^{n}

按相关性排序，无需花费
更多时间查找相关信息



在一个页面获取完整的前向、后向引文，并有多个聚类选项对引文进行筛选

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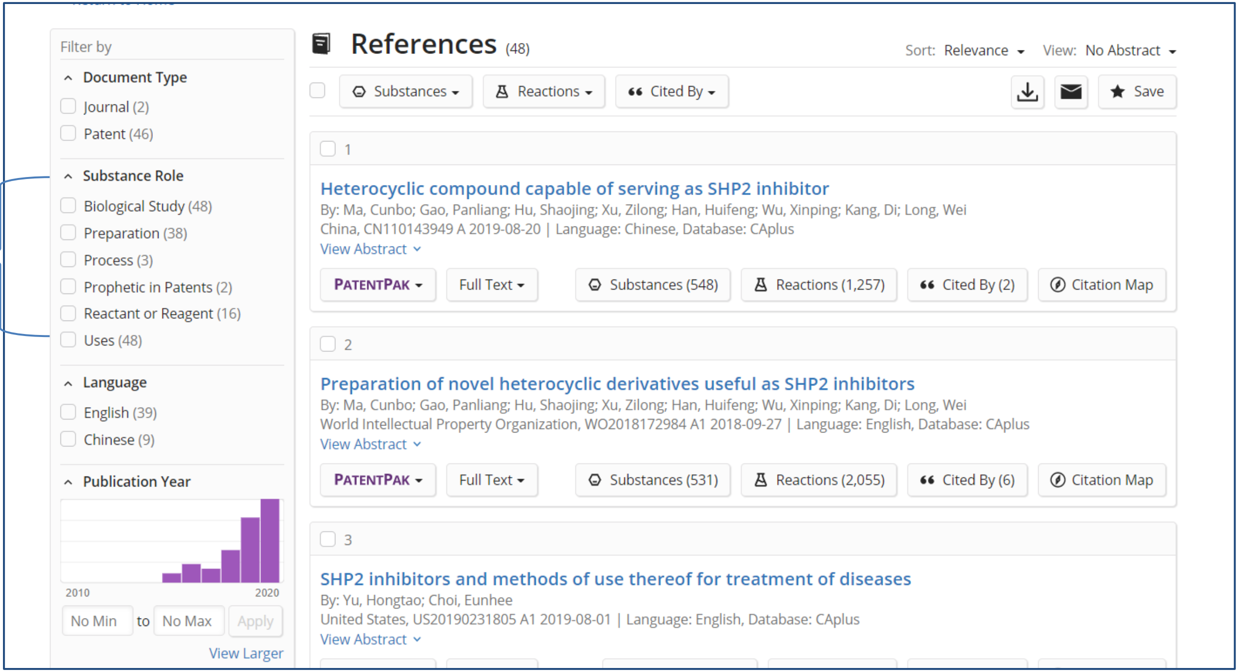
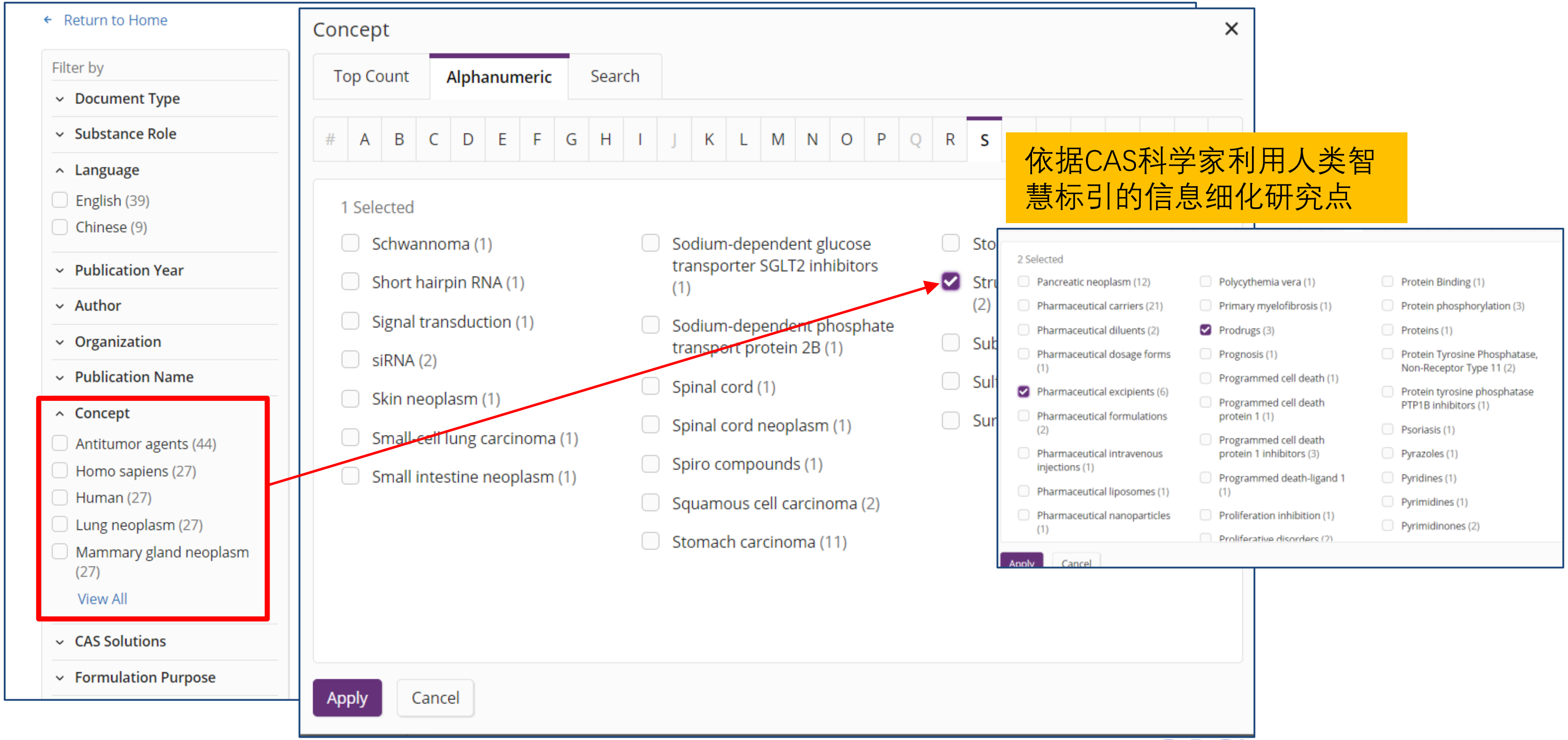
为什么需要SciFinder^{n}

依据CAS科学家利用人类智慧标引的信息，精准定位文献



为什么需要SciFinder^n



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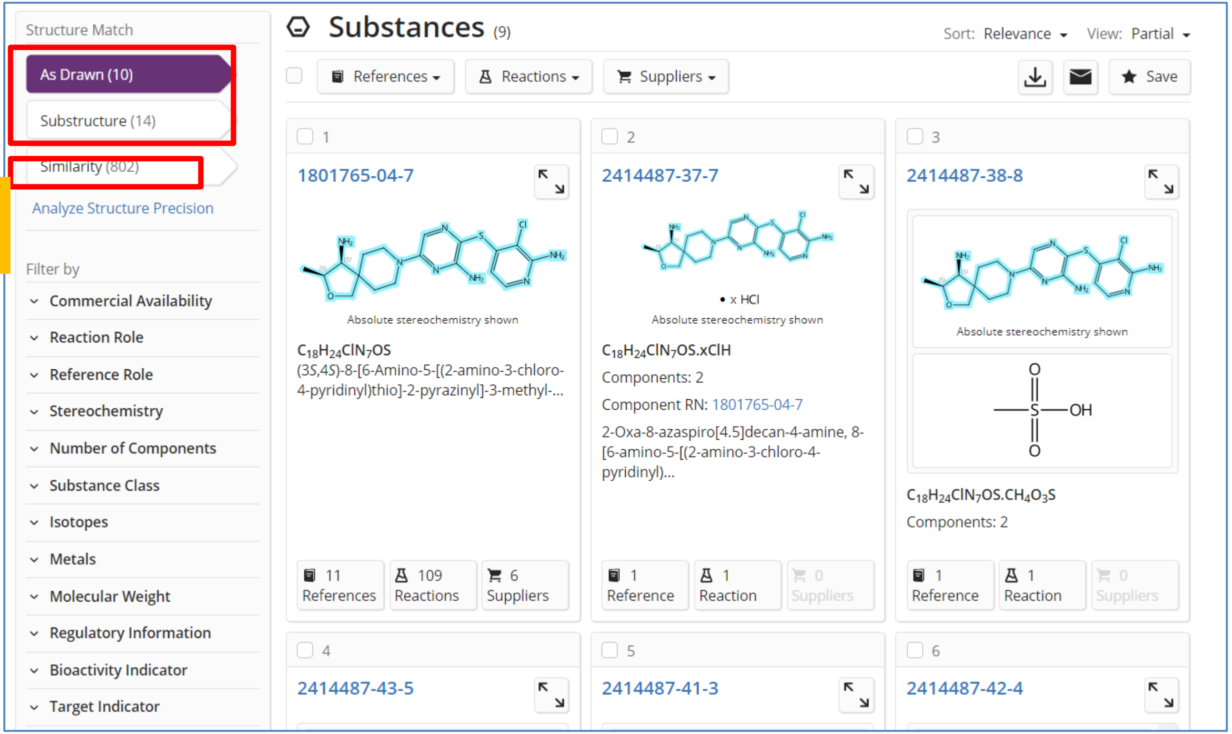
为什么需要SciFinder^{n}

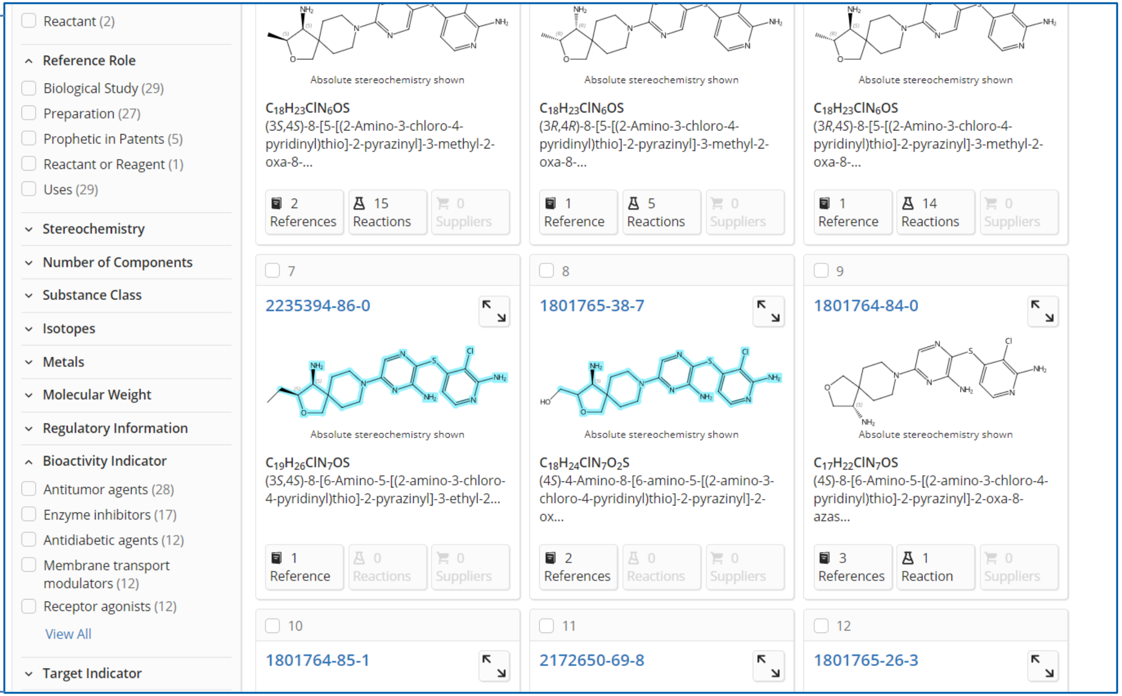
化合物新颖性的依据

为化合物设计提供新的想法



为什么需要SciFinder^n

聚类筛选项节省时间，一目了然。无需逐步二次检索和限定，直接勾选即可定位所需信息



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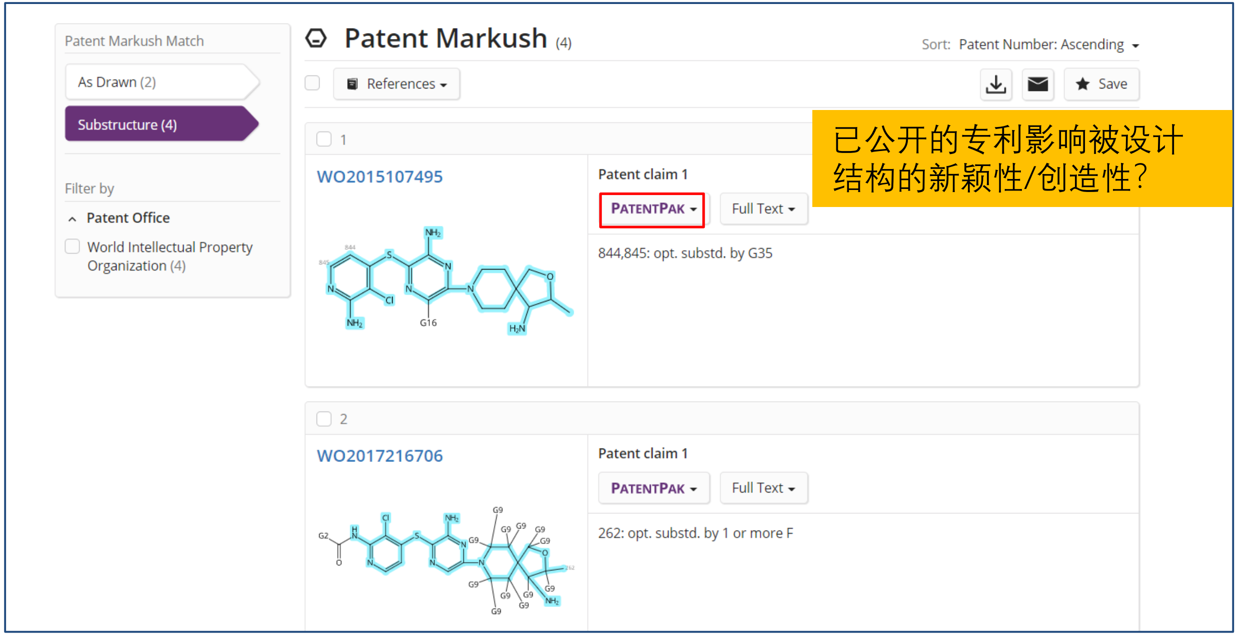
为什么需要SciFinder^{n}



已公开的专利影响被设计结构的新颖性/创造性？

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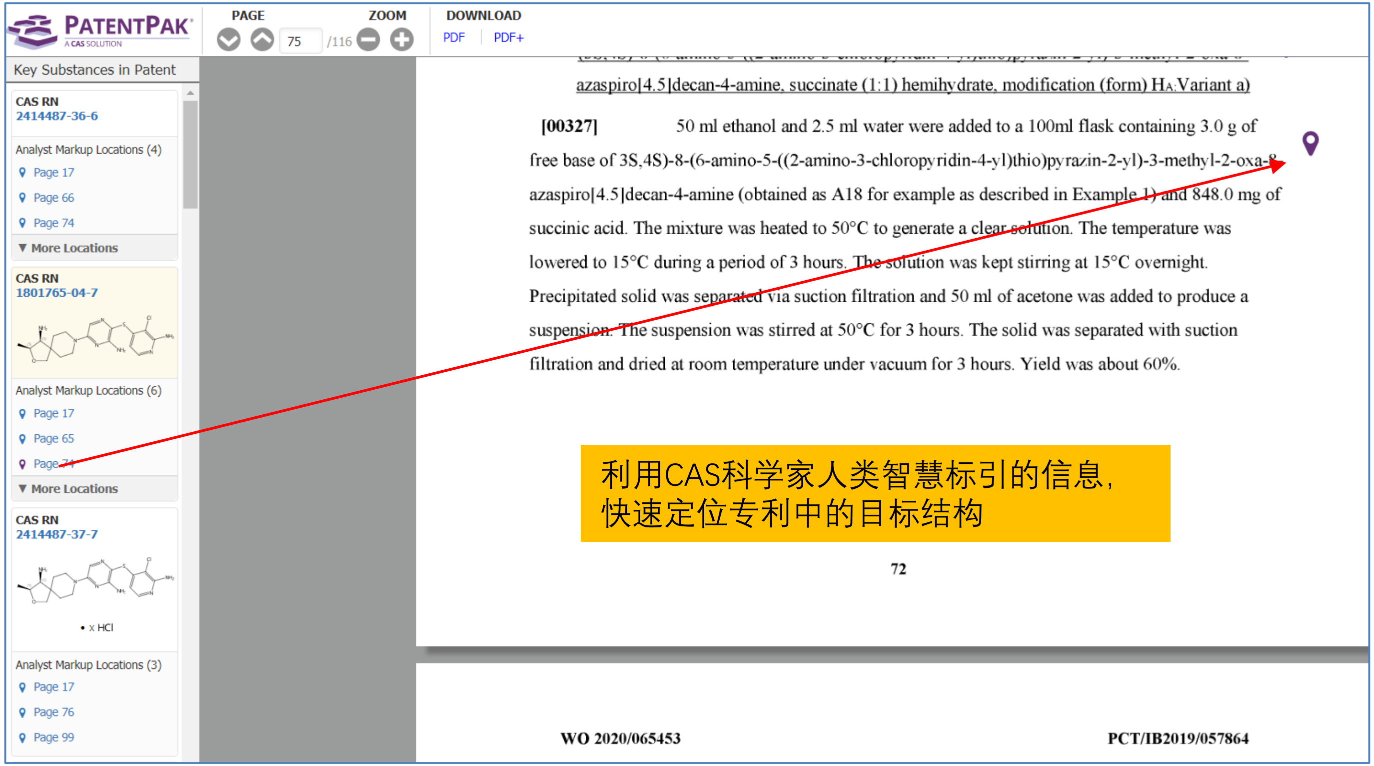
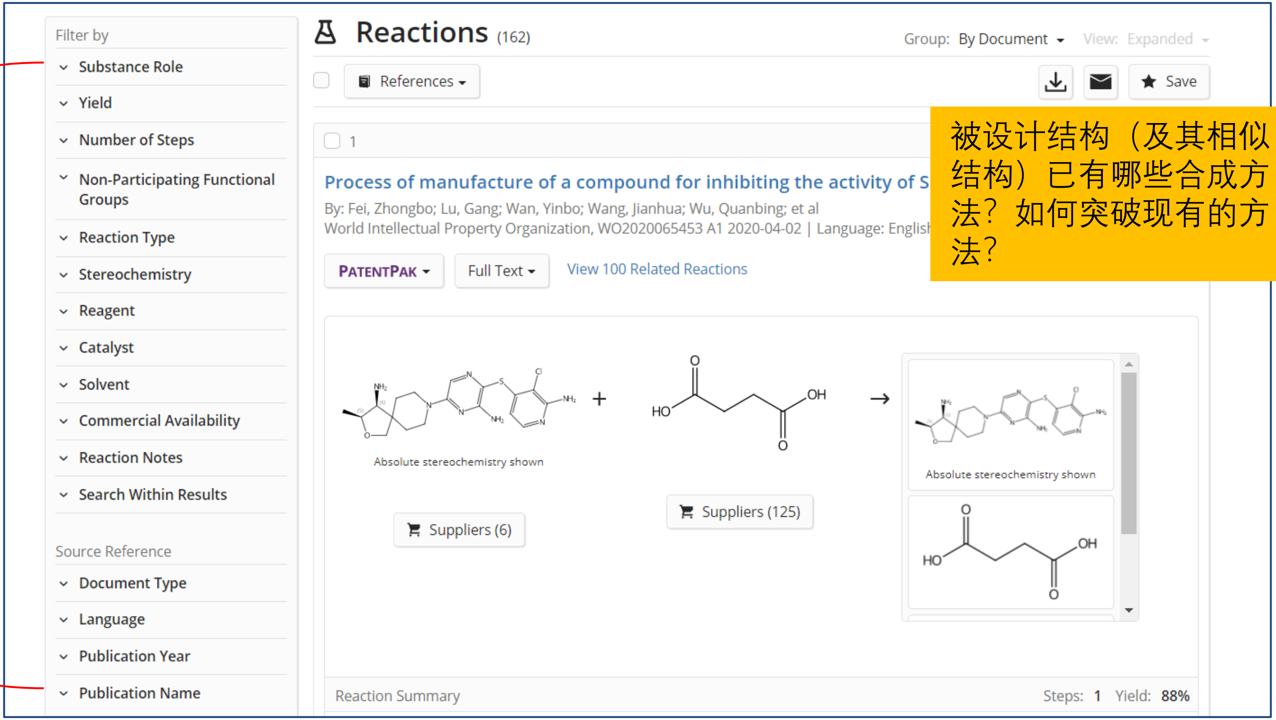
为什么需要SciFinder^n



利用CAS科学家人类智慧标引的信息，
快速定位专利中的目标结构

为什么需要SciFinder^n

筛选合成方法的多个聚类选项



被设计结构（及其相似结构）已有哪些合成方法？如何突破现有的方法？

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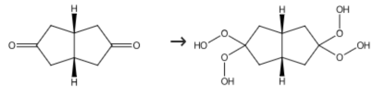
Reaction Detail (Scheme 1, Reaction 1 of 1)

← Prev Next →

Save



Relative stereochemistry shown Relative stereochemistry shown

64%

Suppliers (53)

Steps: 1

Yield: 64%

Step 1

Alternative Steps (0)

Stage	Reagents	Catalysts	Solvents	Conditions
1	Hydrogen peroxide	Iodine	Acetonitrile Water	5 h, 23 °C

CAS Reaction Number: 31-207-CAS-18256071

Notes

safety

提供反应安全信息，提高实验安全性

Experimental Protocols

MethodsNow™

Products	1803406-76-9 , Yield: 64%
Reactants	*cis*-Tetrahydro-2,5(1*H*,3*H*)-pentalenedione
Reagents	Hydrogen peroxide
Catalysts	Iodine

Reference

Less sensitive oxygen-rich organic peroxides containing geminal hydroperoxy groups

View Reference Detail

By: Gamage, Nipuni-Dhanesha H.; et al

View All

Chemical Communications (Cambridge, United Kingdom) (2015), 51(68), 13298-13300

Full Text

Company/Organization

Department of Chemistry
Wayne State University
Detroit, Michigan 48202
United States

Solvents	Acetonitrile Water
Procedure	1. Charge a 50 ml round bottomed flask with a magnetic stir bar, I_2 (0.010 g, 0.040 mmol) in CH_3CN (1 mL). 2. Add a 50 wt.% aqueous solution of H_2O_2 (0.10 mL, 1.7 mmol) to the reaction mixture. 3. Add cis-1,5-dimethylbicyclo[3.3.0]octane-3,7-dione (0.20 mmol) to the solution. 4. Stir the reaction mixture at room temperature (23 °C) for 5 hours. 5. At this point, concentrate the reaction mixture under reduced pressure. 6. Dissolve the reaction mixture in 1 mL of DCM: CH_3OH (20:1). 7. Purify the product by silica gel column chromatography with 4:1 CH_2Cl_2 : EtOAc.
Safety Information	Caution: the H_2O_2 solutions are strong oxidizers that may cause explosions. All organic peroxides are potentially explosive and require handling with extreme care. Reactions and manipulations should be run in fume hoods behind blast shields. Personal safety gear should include a face shield, lether gloves, a lether apron and hearing protection. Peroxide compound should not come into contact with strong acid, metal salts, or easily oxidized species. All reaction should be run at or below room temperature and performed on small scales. Specifically, 3 exploded upon concentrating a solution containing approximately 30 mg of crystals on the walls of the flask and shattered the flask and damaged the stir bar and but an explosion occurred upon solvent removal under reduced pressure, the flask shattered and even the stir bar was damaged. View Less
Transformation	Formation of Hydroperoxides/ Autoxidation
Scale	milligram

实验详情，无需获取或阅读全文即可获得实验所需的信息

Characterization Data

1803406-76-9

Proton NMR Spectrum	(400 MHz, CD_3OD, 23 °C, δ) OOH resonances not observed due to exchange with CD_3OD, 2.722.56 (m, 2H, CH), 2.18 (d of d, 4H, J= 14.4, 8.8 Hz), 1.86 (d of d, 4H, J= 14.4, 5.6 Hz).
Carbon-13 NMR	(101 MHz, CD_3OD, 23 °C, ppm) 122.10 (peroxy C), 40.54 (CH), 39.03 (CH_2).
Elemental Analysis	$C_8H_{14}O_8$: C, 40.34; H, 5.92. Found: C, 39.98; H, 5.77.
State	white solid.

CAS Method Number 3-614-CAS-2972525

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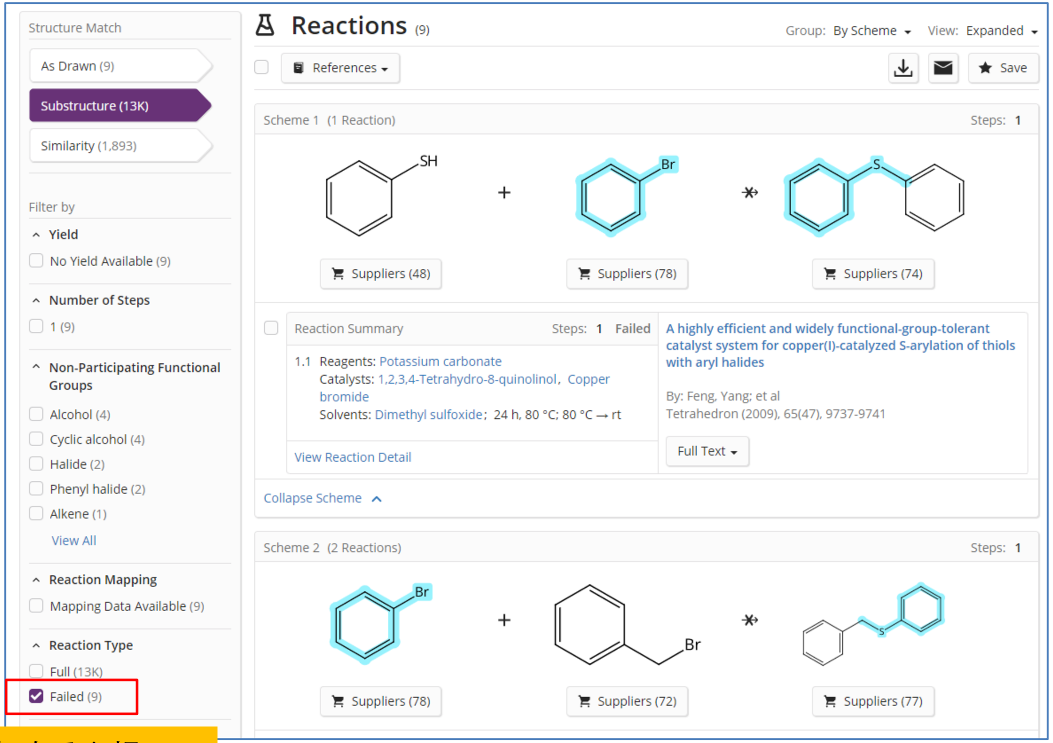

失败反应提醒，
避免走弯路

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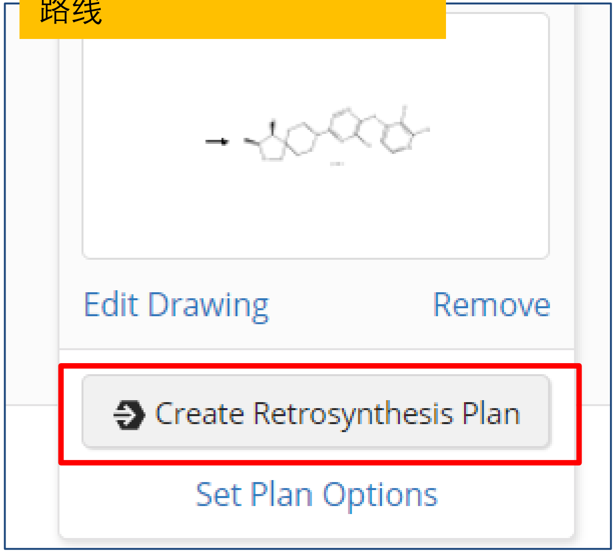
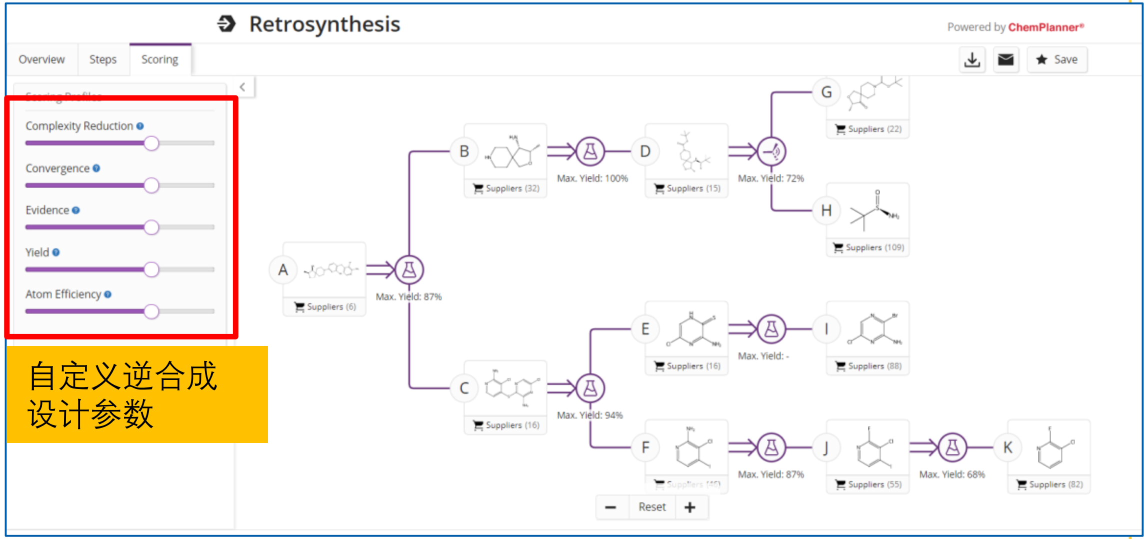
为什么需要SciFinder^n

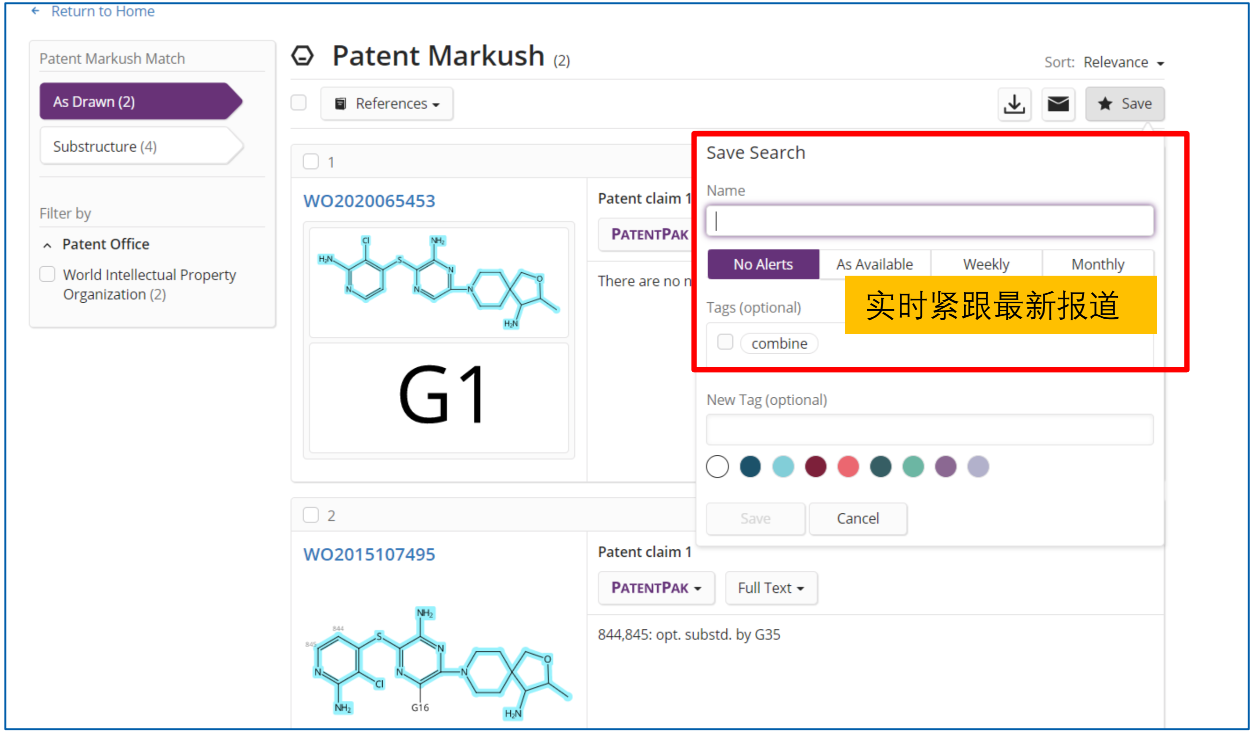
利用逆合成工具，突破现有合成方法，寻找最优的合成路线





自定义逆合成设计参数

为什么需要SciFinder^n



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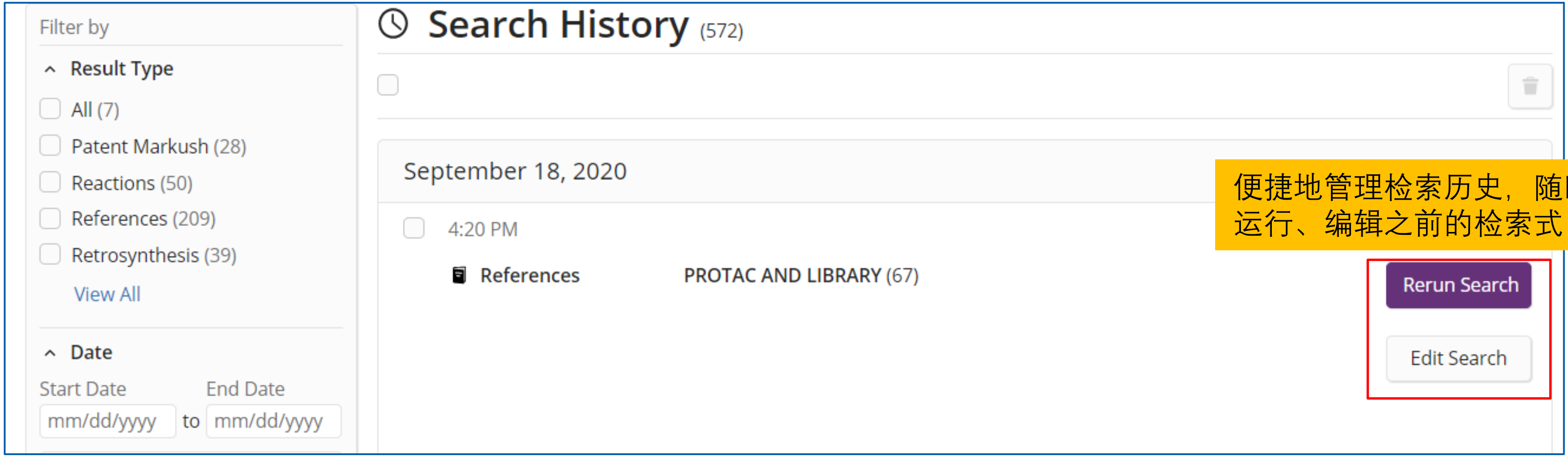
为什么需要SciFinder^{n}



便捷地管理检索历史，随时运行、编辑之前的检索式

为什么需要SciFinder^n

- CAS**科学家解读**的科技信息，有助于提高获取信息的效率
- **多种聚类筛选项**，一目了然，节省逐步筛选/二次检索的时间
- 数据的**全面**性和**及时**性，有助于确定研究的新颖性，避免潜在的专利风险
- 利用CAS大数据和先进技术的**逆合成设计工具**有助于突破现有合成方法，为获得最优方法提供见解和思路
- CAS科学家利用**人类智慧标引**的信息，有助于细化研究点
- 便捷地**管理检索历史**

SciFinder^n ——最先进的化学信息检索工具

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