CAS SciFinder

疑难检索案例分析

2021.5

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大纲

- CAS及CAS SciFinder介绍
- 文献相关信息的检索策略
  - 利用Index Term修正检索词
  - 巧用CAS Role
  - 善用Categorize
  - 如何高效阅读专利文献详情(CAS PatentPak)
- 物质相关信息的检索策略
  - 检索具有相同结构特征的物质
  - Markush检索
  - 如何筛选天然产物
  - 无机复合物、聚合物的检索
- 反应相关信息的检索策略
  - 如何检索化学选择性反应
  - 直接检索反应受限时如何处理
  - 新化合物的合成路线设计
  - 案例分析
  - 如何高效获取反应详情
- 获取分析方法的策略（CAS Analytical Methods）

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CAS致力于提高创新效率

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

HINDSIGHT

Connecting past discoveries
to build a better future

连接前人的发现，建设更美好的未来

INSIGHT

Revealing unseen relationships that spark ideas and speed discovery

揭示能激发想法和加速发现的，未预见的联系

FORESIGHT

Identifying trends and emerging opportunities to accelerate growth

确定加速增长的趋势和新机遇

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CAS具有最全面的学科连接内容合集

ACTIVE PHARMA INGREDIENT
COSMETIC FORMULATIONS
INFRARED DATA
ANALYTICAL METHODS PROTOCOLS
GLOBAL REGULATIONS
SPECTRAL DATA
STRUCTURES
REACTIONS
PHARMACOLOGY / TOXICOLOGY
PROCESSES
STRUCTURE-ACTIVITY-RELATIONSHIP
PROPERTIES
IP CLAIMS
INGREDIENT FUNCTIONS
DNA / RNA SEQUENCES
MARKUSH
DISEASES
UVCB SUBSTANCES
NMR DATA
FORMULATIONS
CELL LINES / TYPES
POLYMER PROPERTIES
MASS SPEC DATA
BIOMOLECULE ISOLATION
TARGETS
AGRICULTURE FORMULATIONS
PROTOCOLS
ORGANOMETALLICS / INORGANICS
BIOASSAYS

Over **50K** scientific journals and documents

Over **250** million substances

Over **50** languages translated

64 patent offices worldwide

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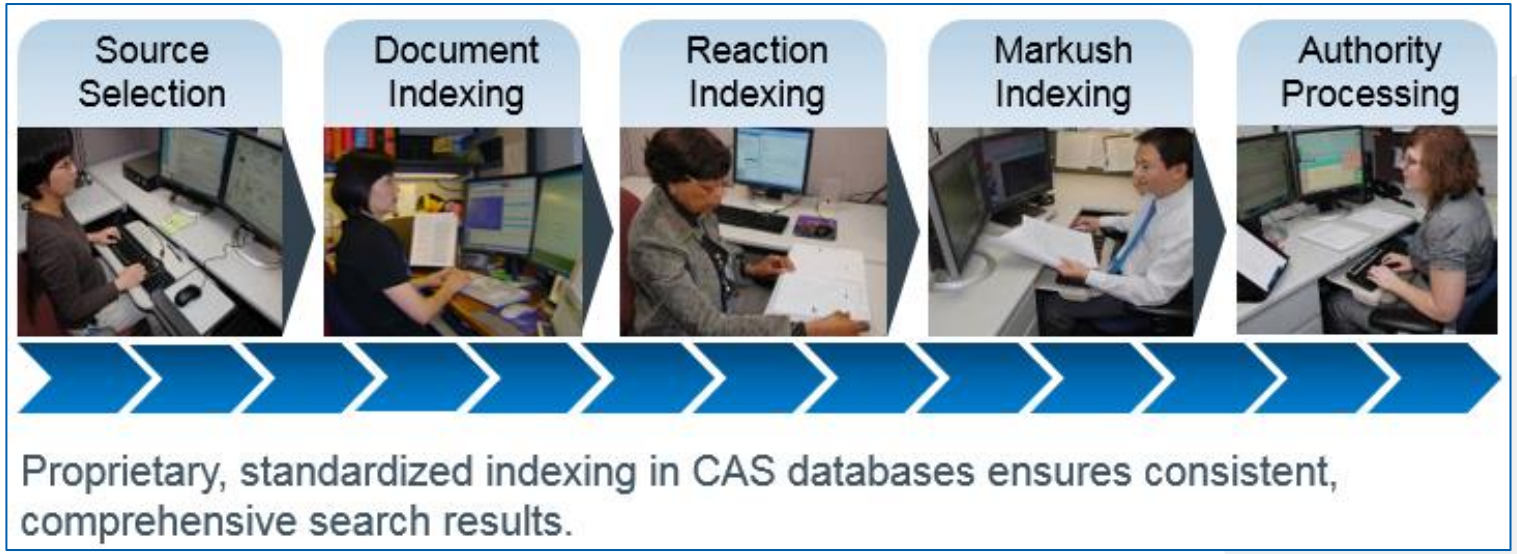
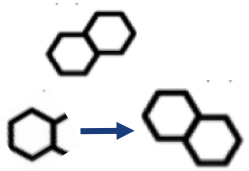
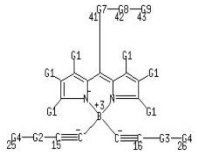
CAS科学家的智力标引



1990
Smith, M.
anthracene





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

CAS科学家利用人类智慧对公开内容进行揭示，使相关信息更容易被挖掘

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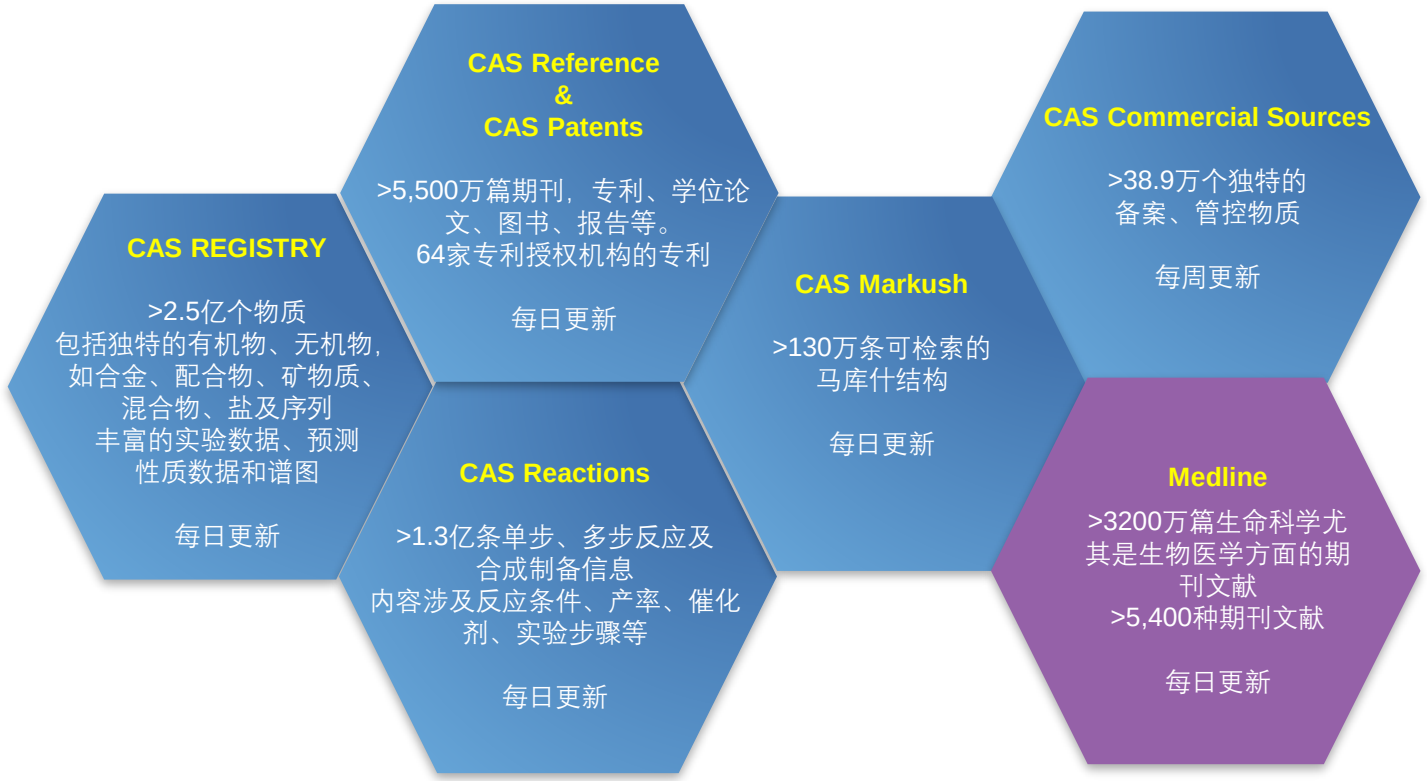
CAS内容合集--CAS SciFinder



CAS SciFinder是提供经CAS科学家人工标引内容的工具型解决方案。

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CAS解决方案与服务

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Customized data, analytics and insights to maximize the value of information assets and fuel digitalization success

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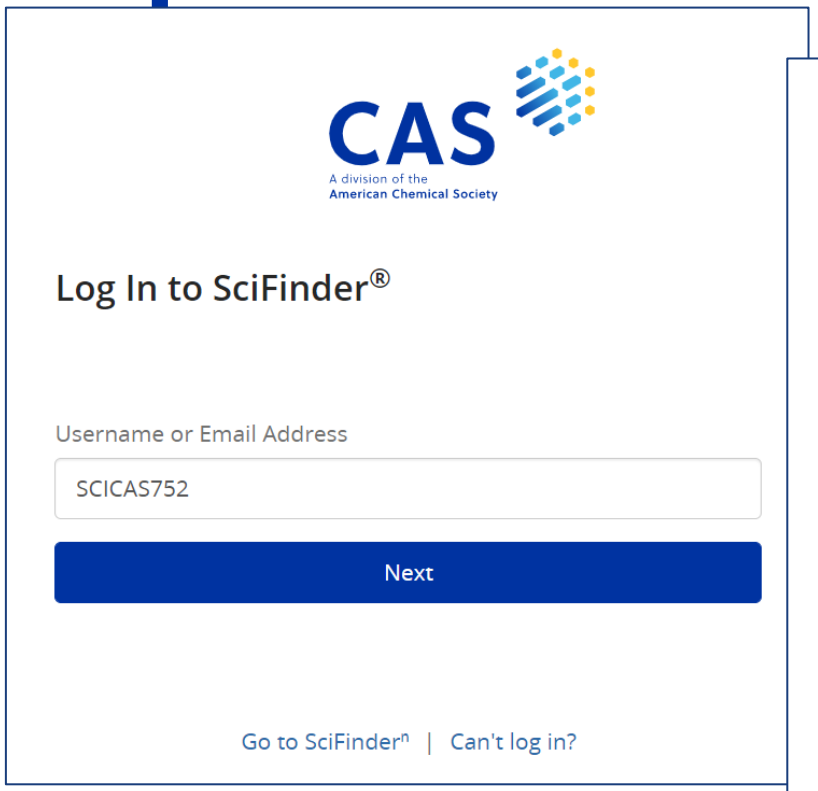
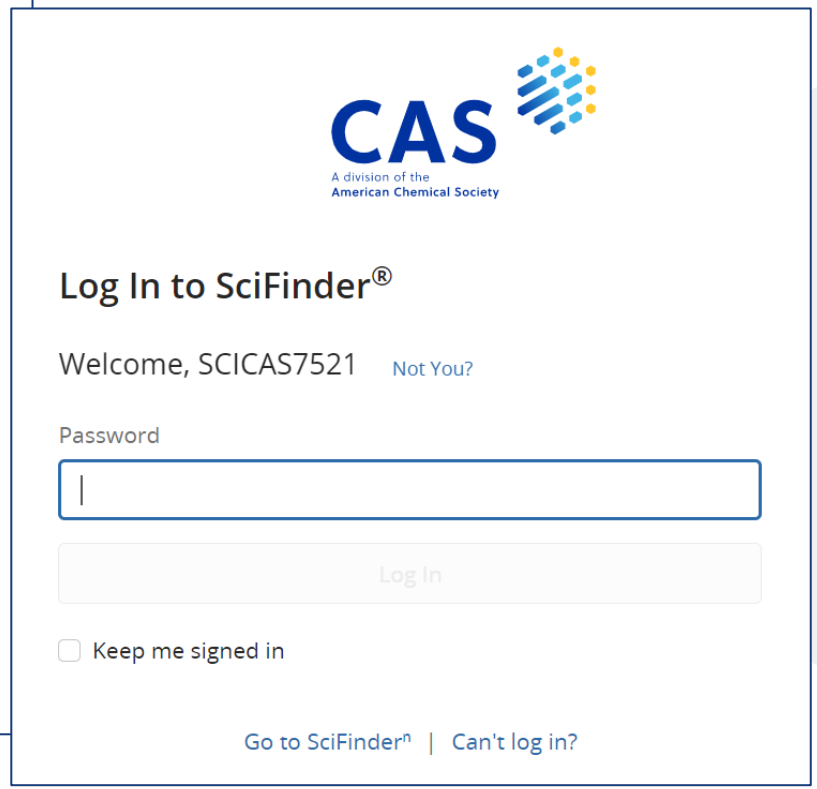
CAS SciFinder登录网址

https://SciFinder.cas.org





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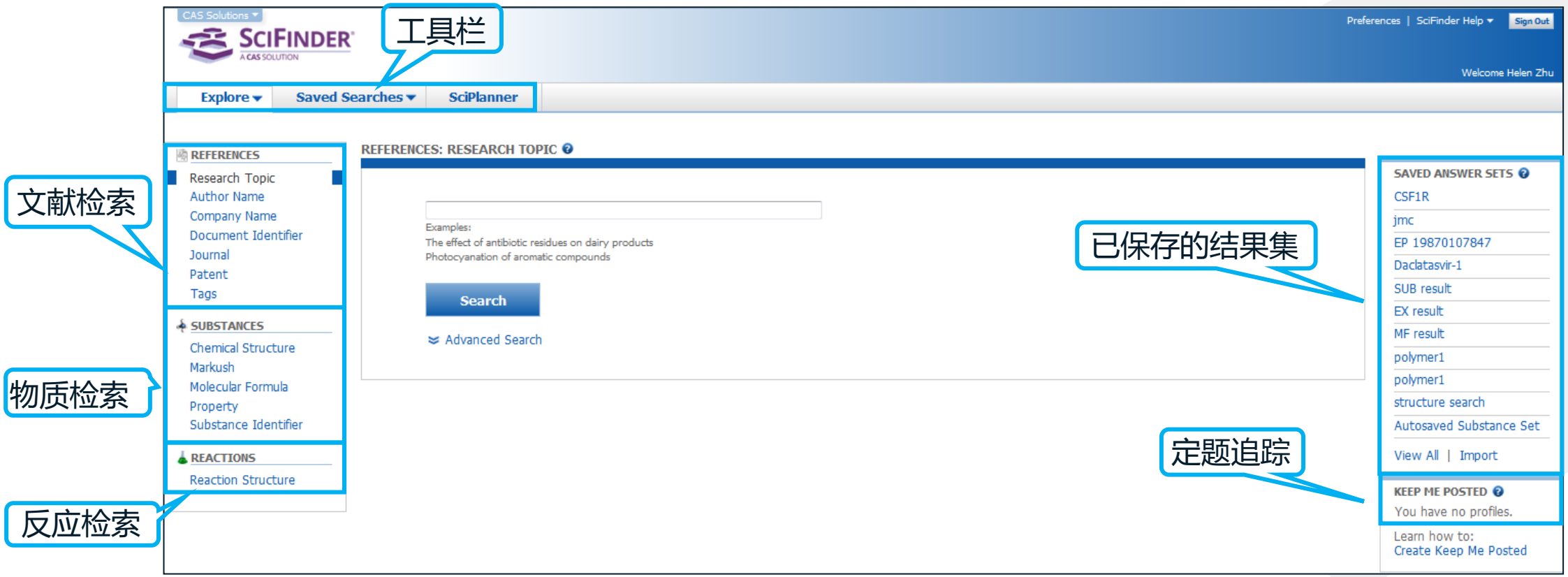
CAS SciFinder主界面



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大纲

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- 文献相关信息的检索策略
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  - 善用Categorize
  - 如何高效阅读专利文献详情(CAS PatentPak)
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CAS SciFinder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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利用Index Term选词

主题检索：植物中天然活性成份的抗癌研究

检索式： Nature Active Component with Anti Cancer

关键词之间用介词连接：in, with, of…

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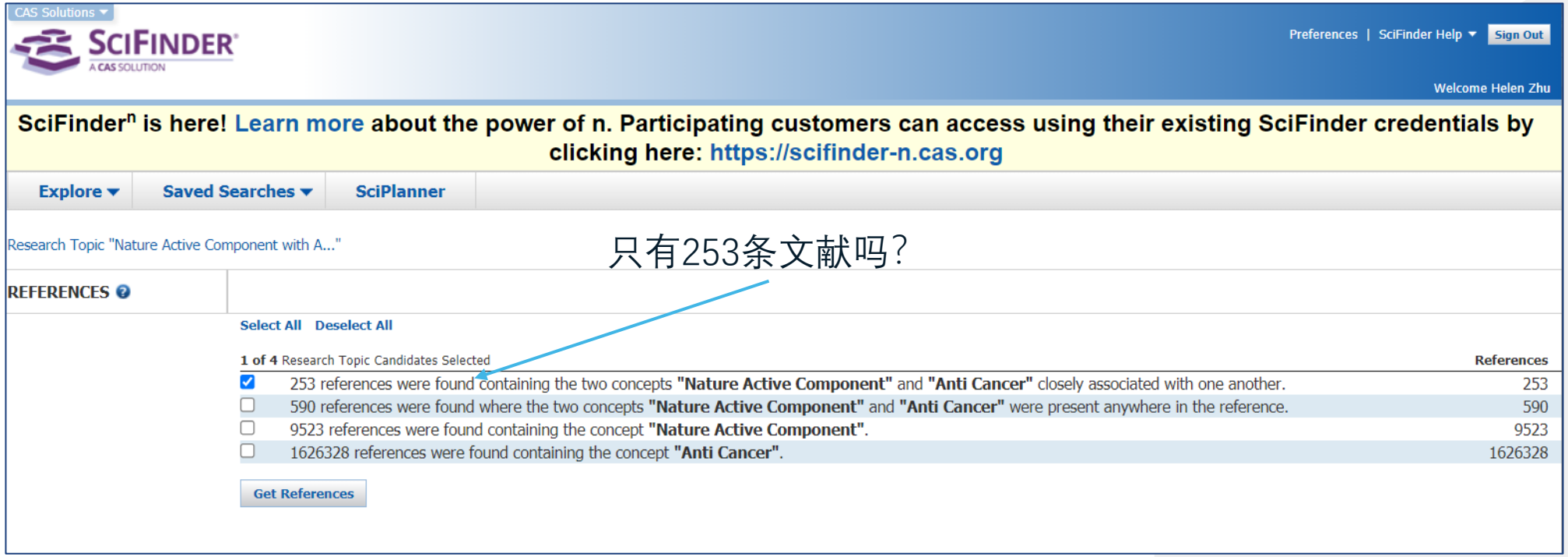
利用Index Term选词



只有253条文献吗？

"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；

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利用Index Term选词

文献筛选工具

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ore | Saved Searches | SciPlanner | Save | Print | Export

27 duplicates were automatically removed.

Research Topic "Nature Active Component with A..." > references (226)

REFERENCES | Get Substances | Get Reactions | Get Related Citations | Tools | Create Keep Me Posted Alert | Send to SciPlanner

Analyze | Refine | Categorize

Sort by: Accession Number | Display Options

Analyze by: Author Name

Zhang Yaozhou	4
Chen Jianqing	3
Chen Yujiao	3
Cheng Jianjun	3
Cheng Yiyu	3
Cui Jinsong	3
Dou Jing	3
Gao Jiayu	3
Ge Zhiwei	3
He Qing	3

Show More

0 of 226 References Selected | Page: 1 of 12

1. Fucoidan induces apoptosis in A2058 cells through ROS-exposed activation of MAPKs signaling pathway
Quick View | Other Sources
By Ryu, Yea Seong; Hyun, Jin Won; Chung, Ha Sook
From Natural Product Sciences (2020), 26(3), 191-199. | Language: English, Database: CAPLUS
Fucoidan, a **natural component** of brown seaweed, has various biol. **activities** such as **anti-cancer activity**, **anti**-oxidant, and **anti**-inflammatory against various **cancer** cells. However, the fucoidan has been implicated in melanoma cells via apoptosis signaling pathway. Therefore, we investigated apoptosis with fucoidan in A2058 human melanoma cells with dose- and time-dependent manners. In our results, A2058 cells viability decreased at relatively short-time and low-concn. through fucoidan. This effects of fucoidan on A2058 cells appeared to be mediated by the induction of apoptosis, as manife...

2. Traditional chinese medicine-based pharmaceutical composition [Machine Translation].
Quick View | PATENTPAK
By Cai, Haide; Cai, Xin
From Faming Zhuanli Shenqing (2021), CN 112587560 A 20210402. | Language: Chinese, Database: CAPLUS
[Machine Translation of Descriptors]. The pharmaceutical compn. provided by the present invention combines a medicine for cell nutrition and cell stabilization, a medicine for **anti**-platelet aggregation, and **anti-cancer** metastasis, and a medicine for regulating the balance of YIN and YANG of the human body, supplementing blood and clearing blood, supplementing QI and ventilating, dredging the meridians, and **reducing** blood lipid.The invention has the advantages that the **activity** of the inherent pluripotent stem cells in the blood of the human body is **activated**, the **activated** pluripotent stem ce...

3. Exploring the self-assembly mechanism and effective synergistic antitumor chemophototherapy of a biodegradable and glutathione responsive ursolic acid prodrug mediated photosensitive nanodrug
Quick View | Other Sources
By Cheng, Jianjun; Wang, Shu; Zhao, Haitian; Liu, Yan; Yang, Xin
From Biomaterials Science (2021), Ahead of Print. | Language: English, Database: CAPLUS
Supermolecularly assembled photochemotherapeutic nanocomposites composed of pure drug small mols. are promising for synergistically improved **tumor** therapy, yet potential multiple challenges remain to be addressed. Herein, we rationally designed a novel multifunctional small mol. disulfide modified **natural** pentacyclic triterpene of ursolic acid (UASS) that simultaneously possesses self-assembly ability, glutathione (GSH) responsivity, **anticancer activity**, biocompatibility and biodegradability and further constructed carrier-free GSH-sensitive photosensitive nanocomposite UASS-Ce_6 NPs for safe ...

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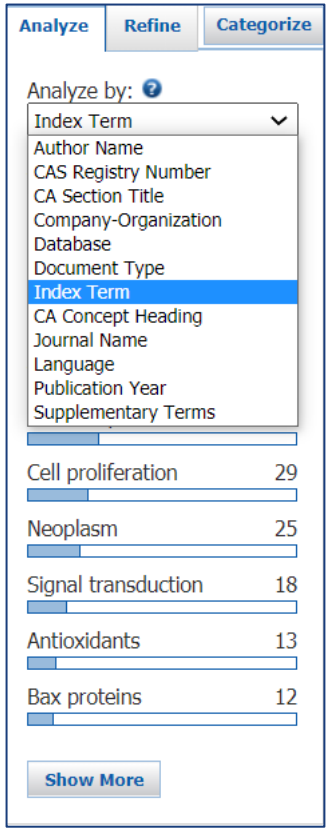
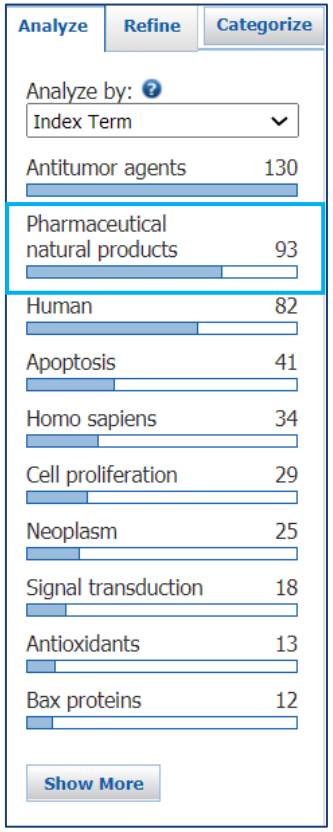
利用Index Term选词





Index Term基于内容的分析工具，发现natural products, Pharmaceutical这个和”天然活性成分”很相关的词

是否用这个词去检索，效果会更好?

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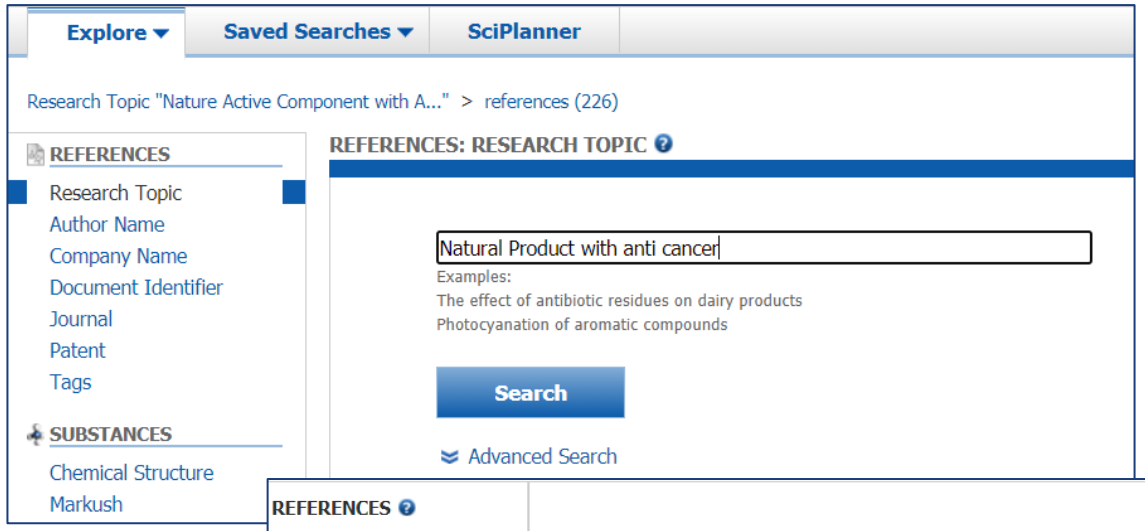
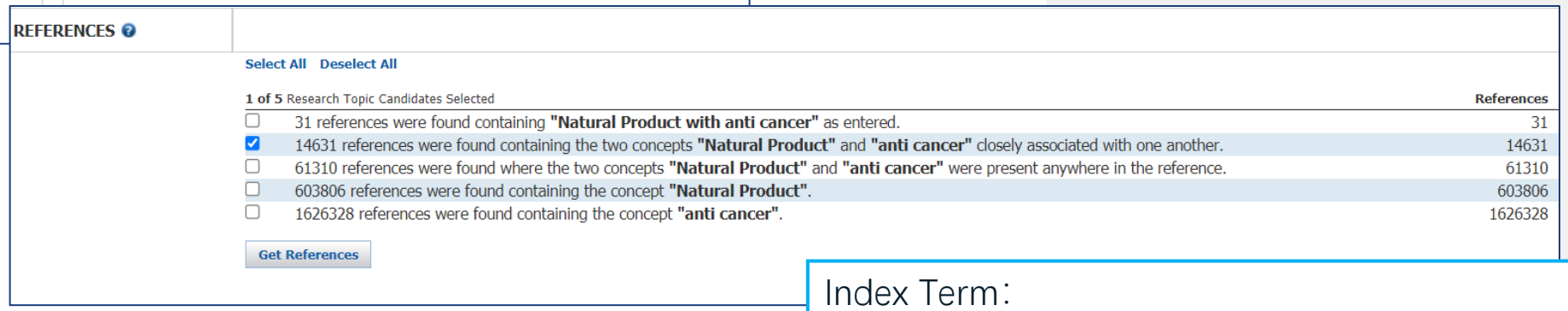
利用Index Term选词



新的检索式：

Natural Product with anti cancer



更换检索词后，结果放大近60倍

Index Term：

帮助用户了解涉及到的重要技术术语，并修正检索词

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STN中的CAS Role

ANST Analytical Study

Analyte	ANT
Analytical Matrix	AMX
Analytical Reagent Use	ARG
Analytical Role, Unclassified	ARU

PREP Preparation

Bioindustrial Manufacture	BMF
Biosynthetic Preparation	BPN
Byproduct	BYP
Industrial Manufacture	IMF
Preparation, Unclassified	PNU
Purification or Recovery	PUR
Synthetic Preparation	SPN

PROC Process

Biochemical Process	BCP
Biological Process	BPR
Geological or Astronomical Process	GPR
Physical, Engineering, or Chemical Process	PEP
Removal or Disposal	REM

BIOL Biological Study

Adverse Effect, Including Toxicity	ADV
Agricultural Use	AGR
Biological Activity or Effector, Except Adverse	BAC
Biochemical Process	BCP
Bioindustrial Manufacture	BMF
Biological Occurrence	BOC
Biosynthetic Preparation	BPN
Biological Process	BPR
Biological Study, Unclassified	BSU
Biological Use, Unclassified	BUU
Cosmetic Use	COS
Diagnostic Use	DGN
Food or Feed Use	FFD
Natural Product Occurrence	NPO
Pharmacological Activity	PAC
Pharmacokinetics	PKT
Therapeutic Use	THU

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STN中的CAS Role

FORM	**Formation, Nonpreparative**	
	Formation, Unclassified	FMU
	Geological or Astronomical Formation	GFM
NANO	**Nanomaterial**	
OCCU	**Occurrence**	
	Biological Occurrence	BOC
	Geological or Astronomical Occurrence	GOC
	Natural Product Occurrence	NPO
	Occurrence, Unclassified	OCU
	Pollutant	POL

RACT	**Reactant or Reagent**	
	Reactant	RCT
	Reagent	RGT
USES	**Uses**	
	Agricultural Use	AGR
	Analytical Reagent Use	ARG
	Biological Use, Unclassified	BUU
	Catalyst Use	CAT
	Cosmetic Use	COS
	Diagnostic Use	DGN
	Food or Feed Use	FFD
	Modifier or Additive Use	MOA
	Other Use, Unclassified	NUU
	Polymer in Formulation	POF
	Technical or Engineered Material Use	TEM
	Therapeutic Use	THU

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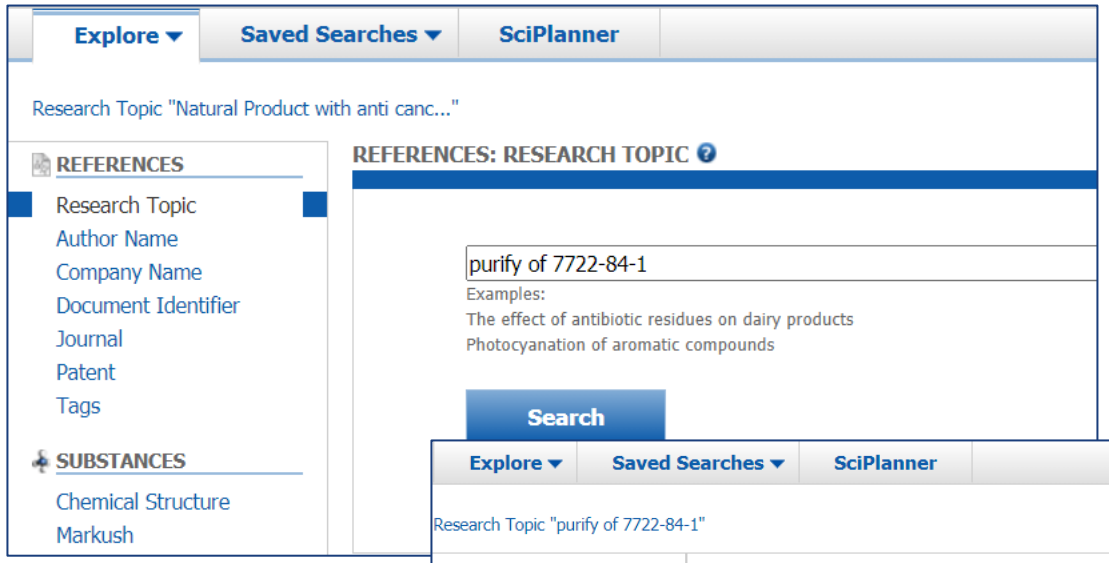
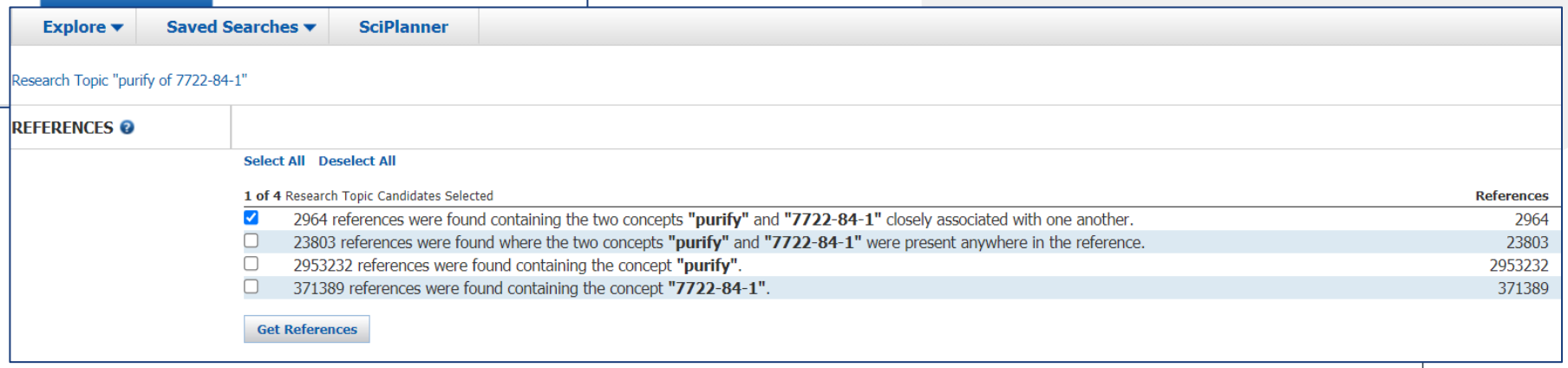
巧用CAS Role

查找纯化双氧水（7722-84-1）的文献





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巧用CAS Role

1. Material preparation method with visible light catalysis for purifying indoor air and sterilizing

By: Huang, Aimin
Assignee: Hebei Yuqing Environmental Protection Equipment Co., Ltd., Peop. Rep. China

The invention discloses a material prepn. method with visible light catalytic purifn. of indoor air and sterilization, which has good purifn. effect on formaldehyde, excellent sterilization performance, high visible light utilization rate and low cost. The material is a composite formed by loading Ag^+/Cu-$BiVO_4$ on sepiolite.

Patent Information

Patent No.	PatentPak Options	Kind	Language	Date	Application No.	Date
CN 112691683	PDF	A		Apr 23, 2021	CN 2020-11545149	Dec 24, 2020

Priority Application

CN 2020-11545149	Dec 24, 2020

Indexing

Catalysis, Reaction Kinetics, and Inorganic Reaction Mechanisms (Section67)

Concepts

Composites
Heat treatment
Stirring
Volatile organic compounds
Drying process
Roasting
Vibration

material prepn. method with visible light catalysis for purifying indoor air and sterilizing

Substances

63800-37-3 Sepiolite

Catalyst support; material prepn. method with visible light catalysis for purifying indoor air and sterilizing

Catalyst use; Physical, engineering or chemical process; Process; Uses

14701-21-4

material prepn. method with visible light catalysis for purifying indoor air and sterilizing

Biological use, unclassified; Modifier or additive use; Biological study; Uses

7440-50-8P Copper

material prepn. method with visible light catalysis for purifying indoor air and sterilizing

Catalyst use; Modifier or additive use; Synthetic preparation; Preparation; Uses

7647-01-0 Hydrochloric acid
7697-37-2 Nitric acid
7722-84-1 Hydrogen peroxide

OH—OH

7761-88-8 Silver nitrate

material prepn. method with visible light catalysis for purifying indoor air and sterilizing

Physical, engineering or chemical process; Process

噪音信息

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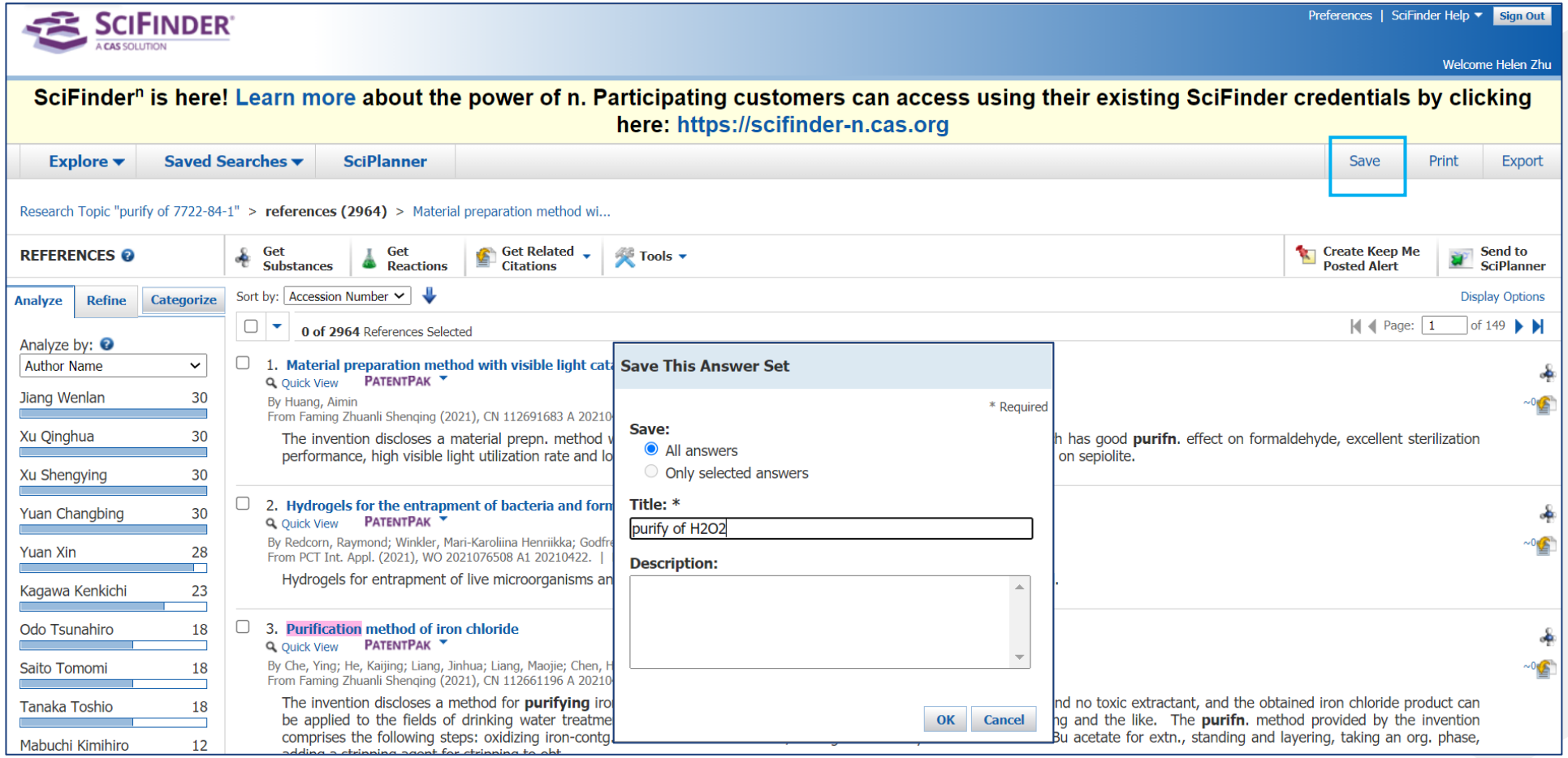

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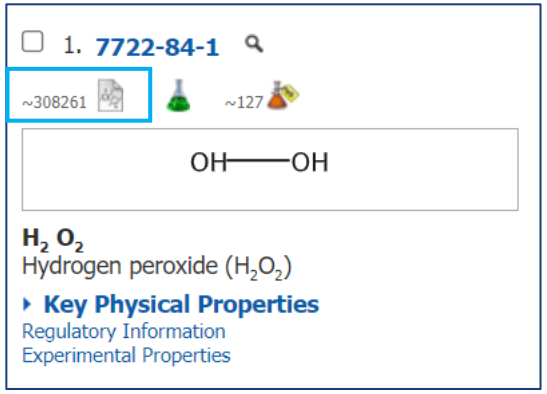
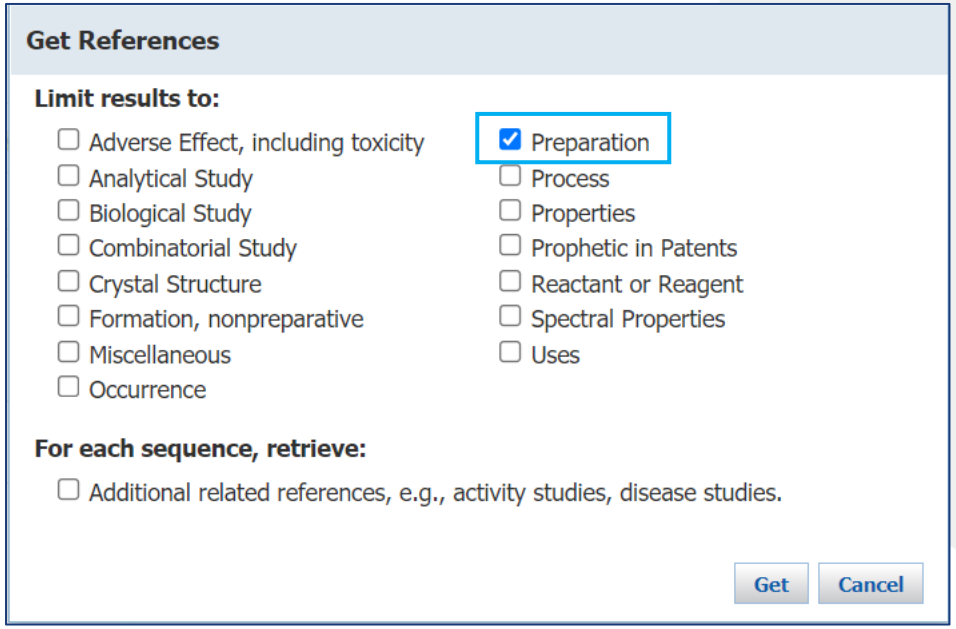
巧用CAS Role





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Duplicates not removed. Answer set exceeds 10,000 reference limit.

Substance Identifier "7722-84-1 " > substances (1) > **get references (18225)**

REFERENCES | Get Substances | Get Reactions | Get Related Citations | Tools | Create Keep Me Posted Alert | Send to SciPlanner

Tools: Remove Duplicates | Combine Answer Sets | Add Tag

Analyze | Refine | Categorize

Sort by: Accession Number | Display Options

0 of 18225 References Selected | Page: 1 of 912

Analyze by: Author Name

Hutchings Graham J	63
Wang Wei	56
Wang Li	55
Edwards Jennifer K	48
Wang Erzhong	45
Brillas Enric	39
Carley Albert F	36
Kornienko V L	35
Jia Liming	33

1. **Water-electrolysis bipolar plate structure for generating hydrogen peroxide**
   Quick View | PATENTPAK
   By Park, Kyuwon; Park, Seogwon; Kim,
   From PCT Int. Appl. (2021), WO 202108
   The present invention relates t… electrolysis bipolar plate structu… pos. electrode; and an elec. shi… electrode and the neg. electrode… electrode and a neg. electrode, and provides an … ectrode (GDE); a pos. electrode part including a … de part to prevent elec. corrosion due to the pos.

2. **C70 Fullerene Catalyzed Photo…**
   Quick View | Other Sources
   By Kumar, Inder; Kumar, Rakesh; Gupta…
   From Journal of Organic Chemistry (202…
   …n explored here. The developed strategy's main … e and aldehydes. The reaction manifests broad … e. Further, sym. secondary amines can also be … ctional theory studies revealed that the current

Combine Answer Sets

Select saved answer set(s) to combine with your current answer set **(18225)**:

36 Answer Sets | 1 Selected

Reference Answer Set Details	Date Saved
purify of H2O2 (2964) Research Topic "purify of 7722-84-1" > references (2964)	May 17, 2021
黄芪 (4374) Research Topic "huangqi" > references (4374)	Dec 3, 2020
synthesis of Daclatasvir (24) Substance Identifier "Daclatasvir " > substances (1) > get reactions (156) > get references (24)	Nov 9, 2020
Jiangsu Univ-2001-2014 CAplus (13504) Opened saved answer set "Jiangsu Univ-~2014 CAplus" (13669) > refine "2000-" (13542) > refine "2001-" (13504)	Oct 12, 2020

Select an option for combining the answer sets:

- **Combine** — Include all answers from both sets
- **Intersect** — Include only answers that appear in both sets
- **Exclude** — Include only answers from **current answer set (18225)** that are not in **purify of H2O2 (2964)**
- **Exclude** — Include only answers from **purify of H2O2 (2964)** that are not in **current answer set (18225)**

Combine Answer Sets | Cancel

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Sort by: Accession Number

Display Options

Analyze by: Author Name

Tanaka Fujio	7
Huo Wenzhou	6
Li Huayi	6
Liu Ye	6
Lv Qinglin	6
Minamikawa Yoshitsugu	6
Murakami Shinichi	6
Kajiwara Shoichiro	5
Nagai Kazunori	5
Shi Ning	5

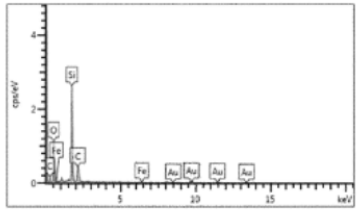
Show More

0 of 368 References Selected

Page: 1 of 19

1. **Process for providing anhydrous alkane sulfonic acids in purified form**
   Quick View PATENTPAK
   By Ott, Timo; Biertuempel, Ingo
   From PCT Int. Appl. (2020), WO 2020212298 A1 20201022. | Language: English, Database: CAPLUS
   The invention is related to a process for providing an anhyd. alkane sulfonic acid in purified form comprising: (i) providing a reaction mixt. comprising hydrocarbon, alkanesulfonic acid and disulfuric acid; (ii) adding an additive to the reaction mixt., the additive reacting with disulfuric acid to form sulfuric acid as well as a reaction product of SO_3 and the additive, the reaction product having a b.p. higher than SO_3; (iii) sepg. the hydrocarbon from the reaction mixt., followed by (iv) purifn. of the remaining reaction mixt. by distn. The advantage of the method of invention, is, that t...

2. **Droplet-impingement, flow-assisted electro-fenton purification using heterogeneous silica/iron nanocomposite catalyst**
   Quick View PATENTPAK
   By Basheer, Chanbasha; Haider, Muhammad Baseer; Nsubuga, Hakimu
   From U.S. Pat. Appl. Publ. (2020), US 20200321630 A1 20201008. | Language: English, Database: CAPLUS



   A droplet-impingement, flow-assisted electro-Fenton (DFEF) catalyst, system, and method can degrade to trace level org. materials, such as β-blockers in water. A silica/carbon-x % iron composite (RHS/C-x % Fe) can be made, e.g., from rice husks and iron ions into heterogeneous catalysts of varied iron content. The DFEF approach can improve oxygen satn., mass transfer of β-blockers at the cathode, and continuous electrogeneration of hydroxyl radicals (.OH) in soln. and at boron-doped anode surfaces. A central composite design (CCD) can reduce costs and increase efficiency. Beta-blockers can...

3. **Novel method for purifying hydrogen peroxide**
   Quick View PATENTPAK
   By Wang, Gang; Guo, Fumin; Liu, Qiong; Li, Suidang; Kou, Xiaokang
   From Faming Zhuanli Shenqing (2020), CN 111252740 A 20200609. | Language: Chinese, Database: CAPLUS
   The invention discloses a novel method for purifying hydrogen peroxide, which has the advantages of good prodn. safety and low cost. The method comprises using multi-way conversion valve system and hydrogen peroxide purifn. resin.

4. **Method for purifying hydrogen peroxide used in semiconductor device fabrication**
   Quick View PATENTPAK

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巧用CAS Role

1. Process for providing anhydrous alkane sulfonic acids in purified form

By: Ott, Timo; Biertuempel, Ingo
Assignee: BASF SE, Germany

The invention is related to a process for providing an anhyd. alkane sulfonic acid in purified form comprising: (i) providing a reaction mixt. comprising hydrocarbon, alkanesulfonic acid and disulfuric acid; (ii) adding an additive to the reaction mixt., the additive reacting with disulfuric acid to form sulfuric acid as well as a reaction product of SO_3 and the additive, the reaction product having a b.p. higher than SO_3; (iii) sepg. the hydrocarbon from the reaction mixt., followed by (iv) purifn. of the remaining reaction mixt. by distn. The advantage of the method of invention, is, that the formation of sulfur trioxide is avoided by adding an additive selected from hydrogen peroxide, sulfuric acid, alkane sulfonic acid, ALK-SO_2-O-O-X [ALK = Me, Et, Pr, Bu, C_{5-10} alkyl; X = H, alkali metals, earth alk. metals, aluminum, and zinc, as well as mixts. of two or more of them], or ALK-SO2-O-O-SO2-O-X,to the reaction mixt. prior to the removal of the non-reacted hydrocarbons.

Patent Information

Patent No.	PatentPak Options	Kind	Language	Date	Application No.	Date
WO 2020212298	PDF | PDF+ | Viewer	A1		Oct 22, 2020	WO 2020-EP60371	Apr 14, 2020

Priority Application

EP 2019-170171	A	Apr 18, 2019
EP 2019-176382	A	May 24, 2019

Indexing

Industrial Organic Chemicals, Leather, Fats, and Waxes (Section45-4)

Section cross-reference(s): 23

Concepts

Sulfonic acids

alkylper-, salts, reaction products with sulfur trioxide; process for providing anhyd. alkane sulfonic acids in purified form

Industrial manufacture; Preparation

Sulfonic acids

Substances

75-75-2P Methanesulfonic acid
7664-93-9DP Sulfuric acid, reaction products with sulfur trioxi
7722-84-1DP Hydrogen peroxide, reaction products with sulfu trioxide

process for providing anhyd. alkane sulfonic acid in purified f

Industrial manufacture; Preparation

5. Method for purifying hydrogen peroxide used in semiconductor device fabrication

By: Kim, Deokyun; Kim, Hyejin; Kim, Kyungyeol; Kim, Yongil
Assignee: OCI Company Ltd., S. Korea

The present invention relates to a method for purifying H_2O_2. More particularly, the method comprises: a step of purifying a crude product of H_2O_2 using a primary purifn. system; and a step of purifying the primarily-purified H_2O_2 soln. using a secondary purifn. system. One of the primary purifn. system and the secondary purifn. system comprises an electrodeionization system, and the other of the primary purifn. system and the secondary purifn. system comprises at least one of a distn. system, a resin system, a reverse osmosis system, and a combination system thereof.

Patent Information

Patent No.	PatentPak Options	Kind	Language	Date	Application No.	Date
WO 2020036274	PDF | PDF+ | Viewer	A1		Feb 20, 2020	WO 2019-KR1135	Jan 25, 2019
KR 2020020374	PDF | PDF+ | Viewer	A	Korean	Feb 26, 2020	KR 2018-96017	Aug 17, 2018
CN 112789241		A		May 11, 2021	CN 2019-80065196	Jan 25, 2019

Priority Application

KR 2018-96017	A	Aug 17, 2018
WO 2019-KR1135	W	Jan 25, 2019

Indexing

Industrial Inorganic Chemicals (Section49-8)

Section cross-reference(s): 76

Concepts

Semiconductor device fabrication

method for purifying hydrogen peroxide

Substances

7722-84-1P Hydrogen peroxide, preparation — Page 13 in PATENTPAK

method for purifying hydrogen peroxide

Purification or recovery; Technical or engineered material use; Preparation; Uses

都是需要的文献

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检索文献：

1. 去除N-甲基甲酰胺（123-39-7）的文献?

2. 用N-甲基甲酰胺（123-39-7）作洗脱剂的文献?

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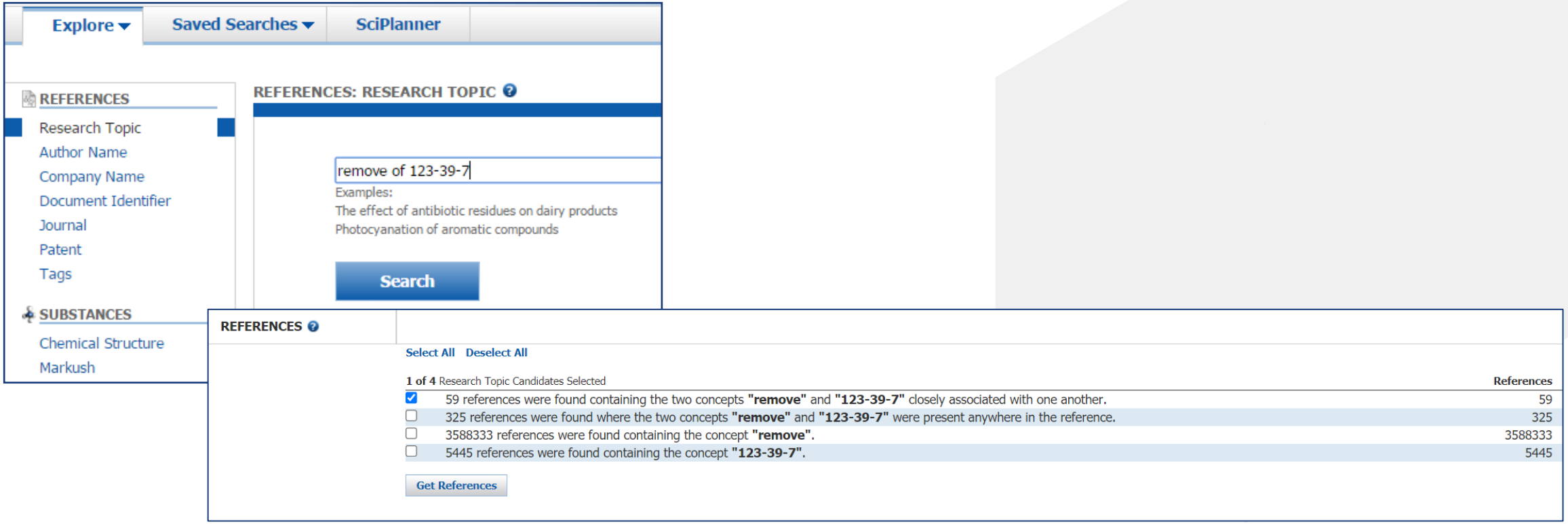
去除N-甲基甲酰胺（123-39-7）



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善用Categorize

1. Efficient organic piston ring decarburization repairing agent

By: Peng, Hongbin; Xiang, Hua
Assignee: Jiangxi Longwei Environmental Protection Technology Development Co., Ltd., Peop. Rep. China

The title repairing agent comprises (by wt. parts) carbon deposit dissolving agent (N,N-dimethylformamide, N,N-dimethylacetamide, etc.) 50-80, detergent dispersant (SURFONAMINE FL1000, SURFONAMINE B100 and/or T3595) 5-20, ester type lubricating tackifier (CRODA Perfad 3336, Ketjenlube 3700, etc.) 1-5, solvent-based surfactant (N,N-dimethyl-9-decenamide and/or STEPOSOL MET-10U) 1-10, oil fouling disintegration accelerator (triphenylphosphine and/or diphenyl-2-pyridylphosphine) 1-2, and additive 0.1-1. The additive includes antioxidant (2,6-di-tert-butyl-4-methylphenol and/or 2,6-di-tert-Bu mixed phenol) and rust inhibitor (T551, T561, etc.). The invention can improve carbon removal efficiency, soly., stability and corrosion resistance, and has high safety, simple recycling procedure and no wastewater discharge.

Patent Information

Patent No.	PatentPak Options	Kind	Language	Date	Application No.	Date
CN 111925844	PDF | PDF+ | Viewer	A		Nov 13, 2020	CN 2020-10654471	Jul 9, 2020

Priority Application

CN 2020-10654471	Jul 9, 2020

Indexing

Fossil Fuels, Derivatives, and Related Products (Section51-12)

Section cross-reference(s): 47

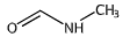
Concepts

Internal combustion engines
Piston rings
Lubricating oil additives

efficient piston ring org. carbon removal repairing agent for engine

Substances

68-12-2 N,N-Dimethylformamide, uses — Page 2 in PATENTPAK
79-16-3 N-Methylacetamide — Page 2 in PATENTPAK
88-12-0 N-Vinyl-2-pyrrolidone, uses — Page 2 in PATENTPAK
123-39-7 Methylformamide — Page 2 in PATENTPAK



127-19-5 N,N-Dimethylacetamide — Page 2 in PATENTPAK
128-37-0 2,6-Di-tert-butyl-4-methylphenol, uses — Page 2 in PATENTPAK
603-35-0 Triphenylphosphine, uses — Page 2 in PATENTPAK
616-45-5 2-Pyrrolidone — Page 2 in PATENTPAK
872-50-4 1-Methyl-2-pyrrolidone, uses — Page 2 in PATENTPAK
2687-91-4 1-Ethyl-2-pyrrolidone — Page 2 in PATENTPAK
3470-99-3 1-Propylpyrrolidin-2-one — Page 2 in PATENTPAK
6837-24-7 N-Cyclohexyl-2-pyrrolidone — Page 2 in PATENTPAK
14433-76-2 N,N-Dimethylcapramide — Page 2 in PATENTPAK
37943-90-1 Diphenyl-2-pyridylphosphine — Page 2 in PATENTPAK
150648-12-7 SURFONAMINE B100 — Page 2 in PATENTPAK
152618-68-3 T 561 — Page 2 in PATENTPAK
325737-17-5 T 747 (antirust additive) — Page 2 in PATENTPAK
1356964-77-6 N,N-Dimethyl-9-decenamide — Page 2 in PATENTPAK
1819965-72-4 Steposol MET 10U — Page 2 in PATENTPAK
1980862-50-7 T 746 (phosphate) — Page 2 in PATENTPAK
2566475-41-8 PE 3100 (polyester) — Page 2 in PATENTPAK

efficient piston ring org. carbon removal repairing agent for engine

Other use, unclassified; Uses

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Research Topic "remove of 123-39-7" > references (59) > Efficient organic piston ring ...

REFERENCES

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Analyze by: Author Name

- Egbe Matthew I 4
- Hara Yasushi 4
- Takahashi Fumiharu 4
- Bang Sun Hong 2
- Hong Heon Pyo 2
- Lee Dong Hoon 2
- Lee Woo Ram 2
- Legenza Michael Walter 2
- Park Tae Moon 2
- Ward Irl E 2

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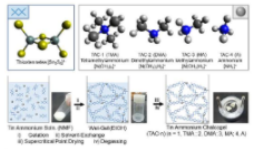
0 of 59 References Selected | Page: 1 of 3

1. Efficient organic piston ring decarburization repairing agent
   Quick View | PATENTPAK
   By Peng, Hongbin; Xiang, Hua
   From Faming Zhuanli Shenqing (2020), CN 111925844 A 20201113. | Language: Chinese, Database: CAPLUS
   The title repairing agent comprises (by wt. parts) carbon deposit dissolving agent (N,N-dimethylformamide, N,N-dimethylacetamide, etc.) 50-80, detergent dispersant (SURFONAMINE FL1000, SURFONAMINE B100 and/or T3595) 5-20, ester type lubricating tackifier (CRODA Perfad 3336, Ketjenlube 3700, etc.) 1-5, solvent-based surfactant (N,N-dimethyl-9-decenamide and/or STEPOSOL MET-10U) 1-10, oil fouling disintegration accelerator (triphenylphosphine and/or diphenyl-2-pyridylphosphine) 1-2, and additive 0.1-1. The additive includes antioxidant (2,6-di-tert-butyl-4-methylphenol and/or 2,6-di-tert-Bu mix...

2. Photoresist-removing stripper composition and method for stripping photoresist using same
   Quick View | PATENTPAK
   By Park, Tae Mun; Lee, Dong Hun; Song, Hyeon U.; Lee, U. Ram
   From Repub. Korean Kongkae Taeho Kongbo (2020), KR 2020112551 A 20201005. | Language: Korean, Database: CAPLUS
   The present invention relates to a photoresist-**removing** stripper compn. and a method for stripping photoresist using same, wherein the photoresist-**removing** stripper compn. has excellent photoresist stripping power, inhibits corrosion of a lower metal film during a stripping process, and is capable of effectively **removing** oxides.

3. Photoresist-removing stripper composition and method for stripping photoresist using same
   Quick View | PATENTPAK
   By Park, Tae Moon; Lee, Dong Hoon; Song, Hyun Woo; Lee, Woo Ram
   From PCT Int. Appl. (2020), WO 2020197014 A1 20201001. | Language: Korean, Database: CAPLUS
   The present invention relates to a photoresist-**removing** stripper compn. and a method for stripping photoresist using same, wherein the photoresist-**removing** stripper compn. has excellent photoresist stripping power, inhibits corrosion of a lower metal film during a stripping process, and is capable of effectively **removing** oxides.

4. Self-assembled radioactive cesium removal complex, its manufacturing method, and method for removing radioactive cesium using thereof
   Quick View | PATENTPAK
   By Oh, Yeong Tak; Lee, Hui Hyeon; Kim, Myeong Gil; Won, Jong Guk; Kang, Yeo Gyeong
   From Repub. Korean Kongkae Taeho Kongbo (2020), KR 2020064526 A 20200608. | Language: Korean, Database: CAPLUS
   The present invention relates to a radioactive cesium **removal** complex contg. self-assembled chalcogen compds.; and an ammonium group bound to the surface of the chalcogen compd.



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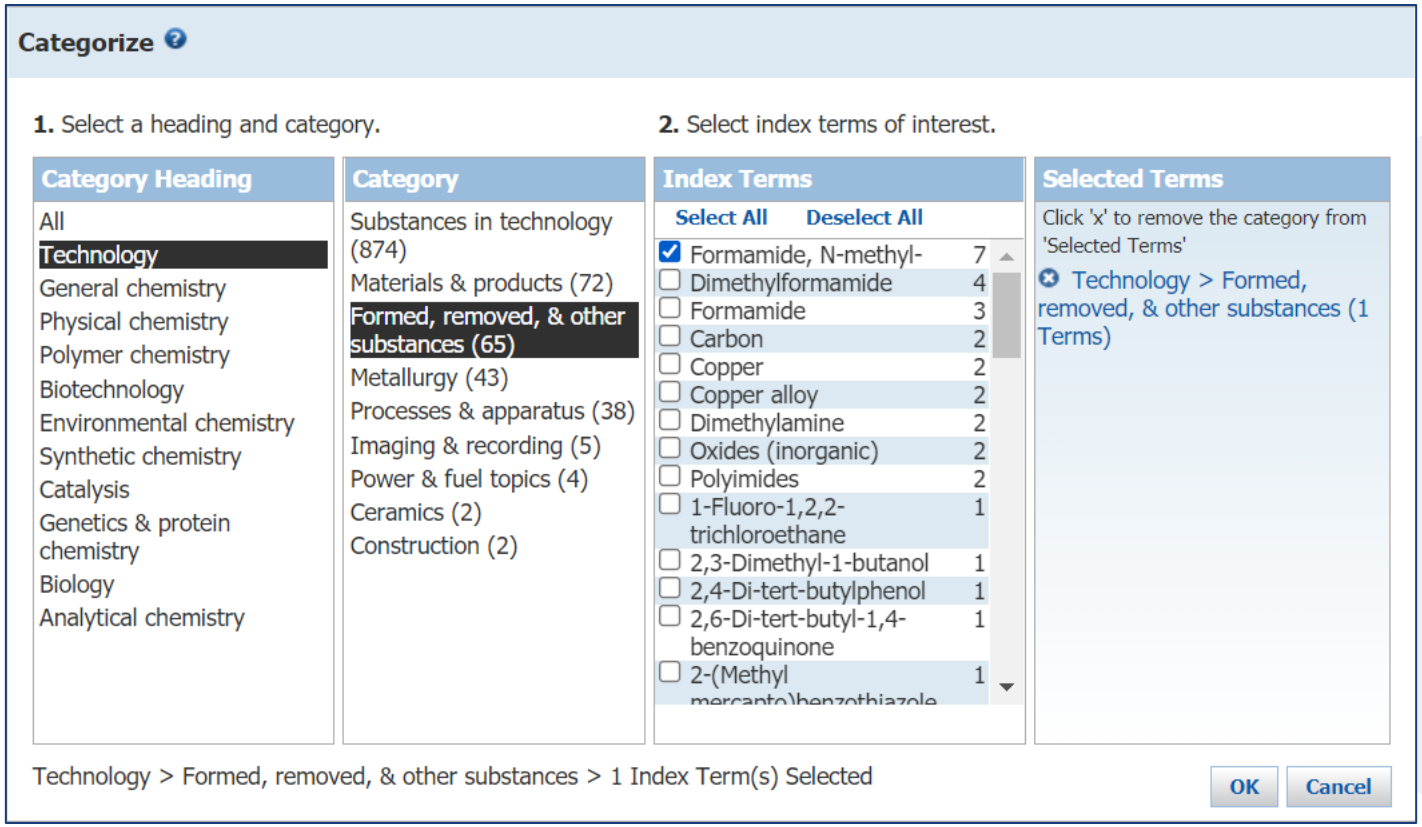

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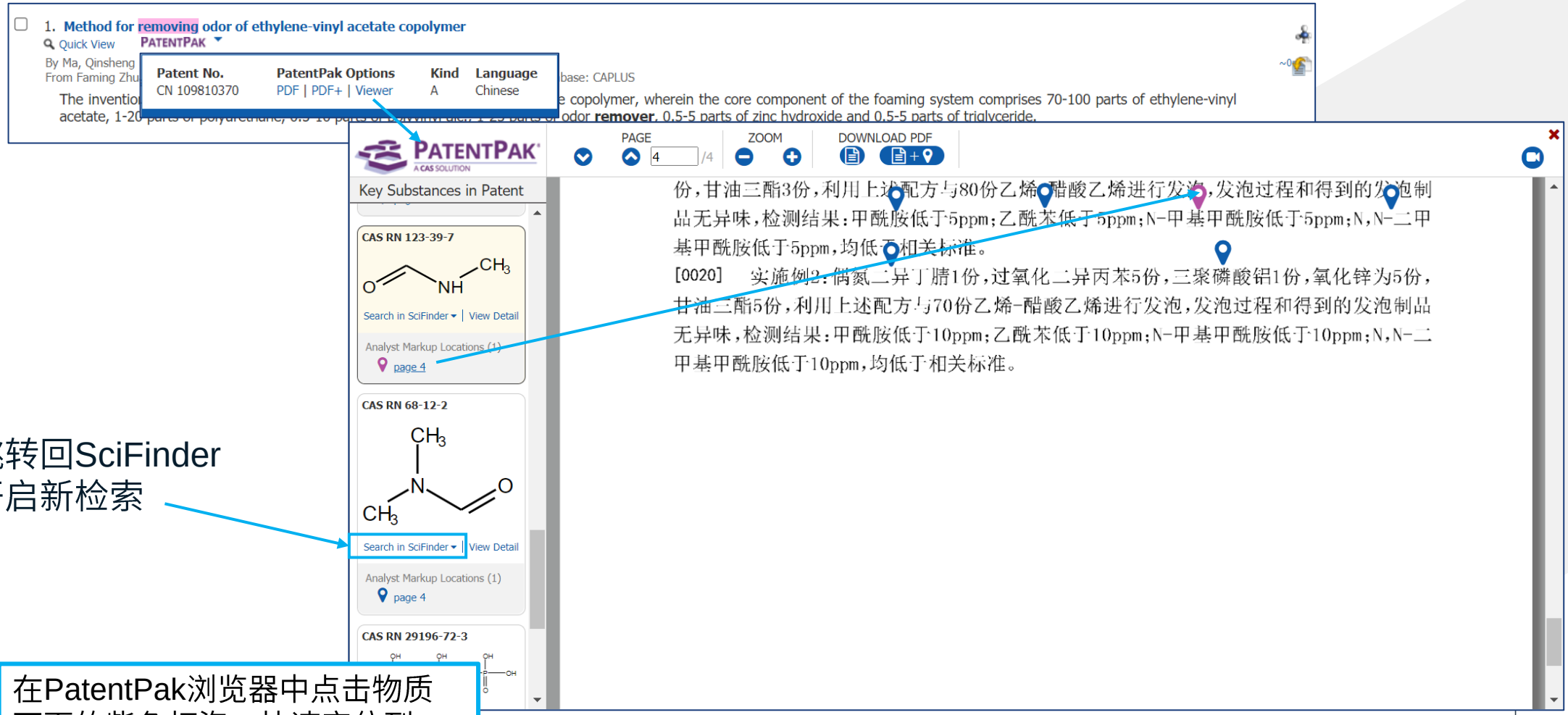

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2. 跟据检索要求选择合适的候选项
3. 通过SciFinder的Analyze/Refine功能来缩小检索的范围
4. 利用Analyze-Index Term查看更好的关键词
5. 使用Categorize可以让系统来实现自动分类
6. 利用CAS Role解决问题
7. 检索思路：初检—浏览结果集—修正检索式或考虑相应的筛选策略—得到更准确的结果集

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大纲

- CAS及CAS SciFinder介绍
- 文献相关信息的检索策略
  - 利用Index Term修正检索词
  - 巧用CAS Role
  - 善用Categorize
  - 如何高效阅读专利文献详情(CAS PatentPak)
- 物质相关信息的检索策略
  - 检索具有相同结构特征的物质
  - Markush检索
  - 如何筛选天然产物
  - 无机复合物、聚合物的检索
- 反应相关信息的检索策略
  - 如何检索化学选择性反应
  - 直接检索反应受限时如何处理
  - 新化合物的合成路线设计
  - 案例分析
  - 如何高效获取反应详情
- 获取分析方法的策略（CAS Analytical Methods）

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CAS SciFinder检索--物质检索

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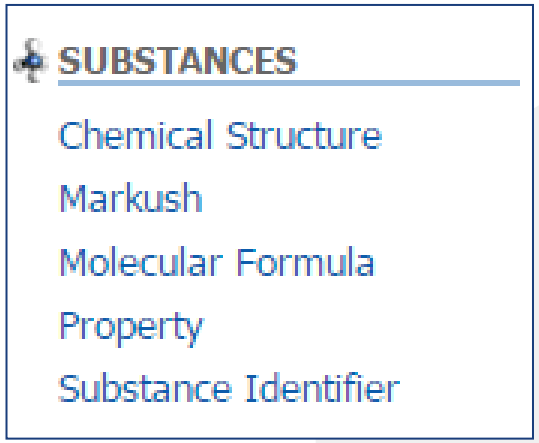
  - 结构式检索
  - 分子式检索
  - 理化性质（物质属性）检索
  - 物质标识符检索：化学名称、CAS RN
  - 从文献或反应结果获得
- 检索策略推荐
  - 有机化合物，天然产物：结构检索
  - 无机物，合金：分子式检索
  - 高分子化合物：分子式检索和结构检索



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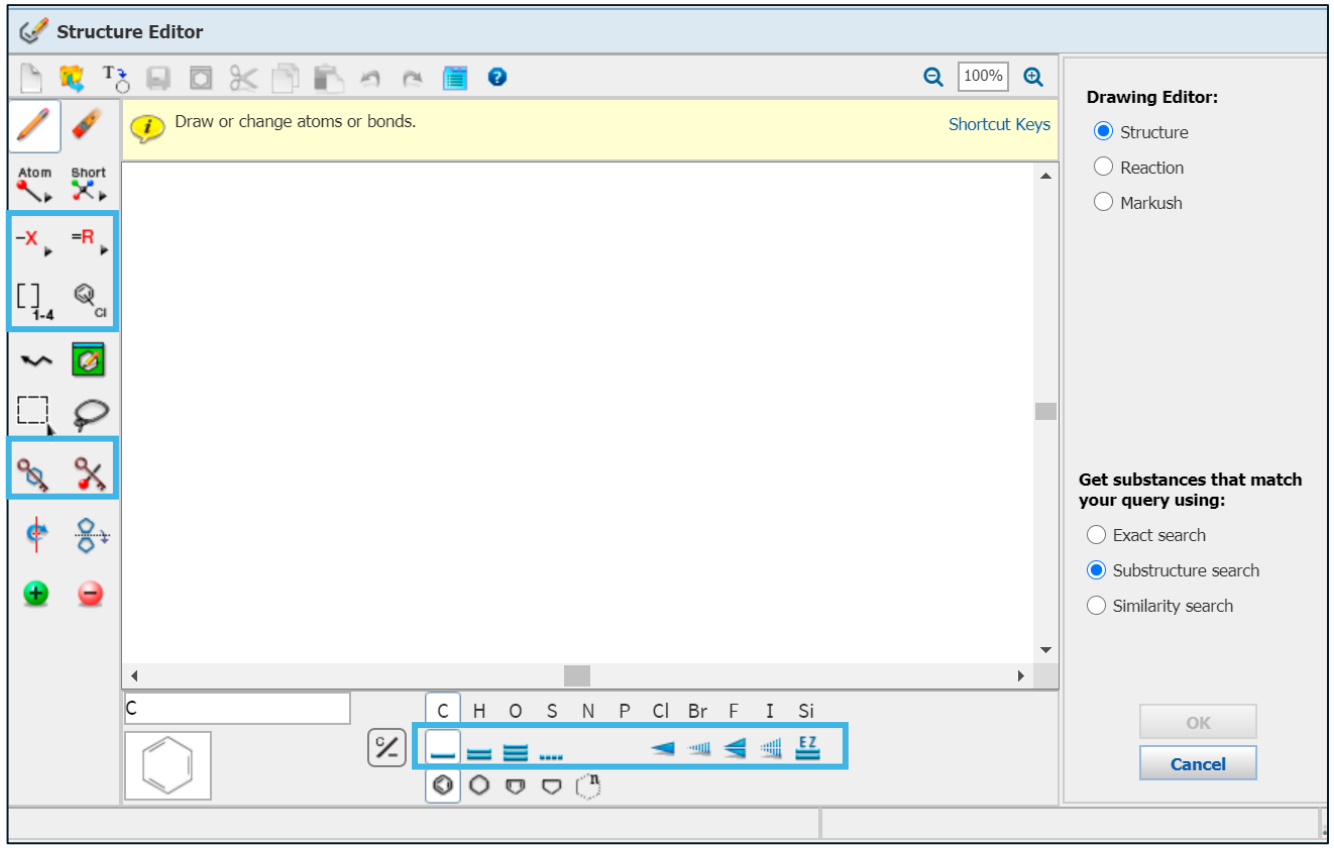

重要绘制工具注释

选择可变基团

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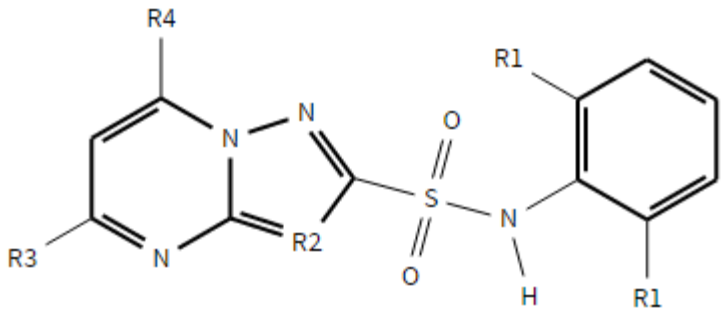

要求:

- R1 = X, H, -NO2, -CF3
- R2 = C 或 N
- R3 = 任意非氢原子
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(43) 申请公布日 2015.09.30

(21) 申请号 201410122313.4
(22) 申请日 2014.03.30
(71) 申请人 浙江大学
地址 310027 浙江省杭州市西湖区浙大路38号
申请人 中国科学院上海药物研究所
(72) 发明人 胡永洲 李佳 刘滔 张建康 周宇波 杨波 何俏军 许磊 胡小蓓
(74) 专利代理机构 杭州求是专利事务所有限公司 33200
代理人 张法高 赵杭丽
(51) Int.Cl.
C07K 5/087(2006.01)
C07K 5/083(2006.01)
C07K 1/16(2006.01)
C07K 1/06(2006.01)
A61K 38/06(2006.01)
A61P 35/00(2006.01)
A61P 35/02(2006.01)
A61P 25/28(2006.01)
A61P 37/02(2006.01)

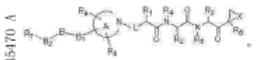
权利要求书3页 说明书24页 附图4页

(54) 发明名称

杂环构建的三肽环氧酮类化合物及制备和应用

(57) 摘要

本发明提供一种杂环构建的三肽环氧酮类化合物，以 Carfilzomib 为先导化合物，经缩合、酸性条件下脱去 Boc 保护基、碱性条件下反应得氨基酸甲酯异氰酸酯、水解、在缩合剂作用下获得。本发明是小分子短肽类蛋白酶体抑制剂。本发明化合物具有极强的蛋白酶体抑制活性及细胞增殖抑制活性，是有前景的蛋白酶体抑制剂，为癌症治疗药物的研究提供了新的思路。本发明化合物的合成所需原料易得，路线设计合理，反应条件温和，各步产率高，操作简便，适合工业化生产。具有下述式 I 的结构通式：



I

CN 104945470 A

具体实施方式

[0026] 本发明结合附图和实施例作进一步的说明，以下实施例仅是说明本发明，而不是以任何方式限制本发明。

[0027] 制备实施例 1、4-（吡嗪 -2- 基氨甲酰基）哌啶 -1- 甲酸叔丁酯（1a，1b）

将 1-（叔丁氧羰基）哌啶 -4- 甲酸（2.75g，12mmol）置于 50mL 三颈瓶中，N_2 保护下加入 25mL 无水 CH_2Cl_2，然后缓缓滴入吡啶（2.5mL，30mmol）和二氯亚砜（1.1mL，14mmol），该反应液置于室温反应半小时。随后，2- 氨基吡嗪（0.95g，10mmol）和三乙胺（5.7mL，40mmol）溶于 15mL CH_2Cl_2 后缓缓滴入上述反应液，室温反应 6 小时。反应液加 30mL 饱和食盐水稀释，分出有机层，水层 CH_2Cl_2 提取（15mL×3），合并有机层，无水硫酸钠干燥后减压除去溶剂，柱层析分离得白色固体 2.3g，收率 74%。m.p.：134-136℃；^{1}H NMR（500MHz，$CDCl_3$）：δ = 9.55（s，1H，pyrazine-H），8.35（d，1H，J=2.0Hz，pyrazine-H），8.23（s，1H，pyrazine-H），7.97（s，1H，NH），4.20（m，2H，CH_2），2.81（m，2H，CH_2），2.48（m，1H，CH），1.93（d，2H，J=12.5Hz，CH_2），1.76（m，2H，CH_2），1.47（s，9H，CH_3）ppm；ESI-MS：m/z = 307$[M+H]^+$。

[0028] 制备实施例 2、4-（吡嗪 -2- 酰基）哌嗪 -1- 甲酸叔丁酯（1c，1d）

吡嗪 -2- 羧酸（1.5g，12mmol）置于 50ml 反应瓶中，加入 35mL 无水 CH_2Cl_2 溶解，随即加入 1- 羟基苯并三氮唑（1.6g，12mmol）和 N-（3- 二甲氨基丙基）-N'- 乙基碳二亚胺盐酸盐（3.5g，18mmol），室温反应半小时。随后，哌嗪 -1- 甲酸叔丁酯（1.9g，10mmol）加入反应液中，室温反应 3 小时。反应液加入 30mL 饱和碳酸氢钠水溶液稀释，分出有机层，饱和食盐

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

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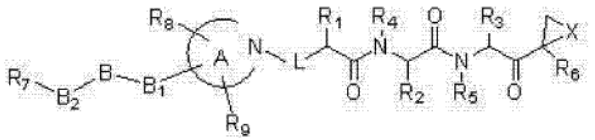
CAS Markush检索

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
- 被Markush结构包含，但未被实施或呈现在表格、权利要求书或说明书中的结构，不会被CAS分配CAS Registry Number
- Markush检索，能检索到通过结构检索检不到的专利

1. 一种杂环构建的三肽环氧酮类化合物，具有下述结构通式 I：



I

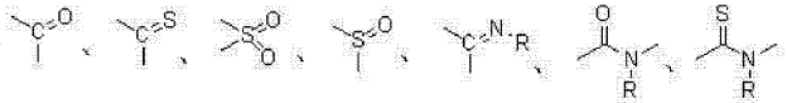
其中：

R_1，R_2，R_3 各自独立选自 H、C_{1-6} 烷基 -D、卤代的 C_{1-6} 烷基 -D、C_{1-6} 羟基烷基、C_{1-6} 巯基烷基、C_{1-6} 烷氧基烷基、芳基、芳烷基、杂芳基或杂芳烷基；其中：D 为 $N(R_a)(R_b)$ 或缺失，R_a，R_b 各自独立选自 H、OH、C_{1-6} 烷基、卤代的 C_{1-6} 烷基或 N 末端保护基；

R_4，R_5 各自独立选自 H、OH、C_{1-6} 烷基、卤代的 C_{1-6} 烷基或芳烷基；

R_6 选自 H，C_{1-6} 烷基，卤代的 C_{1-6} 烷基，C_{1-6} 羟基烷基，C_{1-6} 烷氧基，卤代的 C_{1-6} 烷氧基，$C(O)O-C_{1-6}$ 烷基，$C(O)NH-C_{1-6}$ 烷基，芳烷基；

X 为 O、S、NH、$N-C_{1-6}$ 烷基或 N- 卤代的 C_{1-6} 烷基；

L 为  或者缺失，

其中 R 选自 H、C_{1-6} 烷基或卤代的 C_{1-6} 烷基；

环 A 选自 5 ～ 7 元的饱和脂肪杂环、不饱和杂环、或者有取代的 5 ～ 7 元的饱和脂肪杂环、不饱和杂环，所述的杂环包含 0 ～ 3 个选自 O 、N 和 S 的杂原子并任选地被 R_8、R_9 和 B_1 基团取代；

R_8，R_9 分别独立选自 H、OH，C_{1-6} 烷基，C_{1-6} 烷氧基，C_{1-6} 羟基烷基，C_{1-6} 巯基烷基，C_{1-6} 烷基 -D，芳基，杂环芳基，环烷基和杂环基，这些基团可以被卤素、硝基、氨基、CN、C_{1-6} 烷基、卤代的 C_{1-6} 烷基，C_{1-6} 烷氧基或卤代的 C_{1-6} 烷氧基取代，每个基团可与一个或多个芳基或杂环

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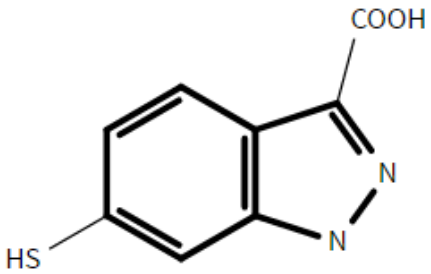
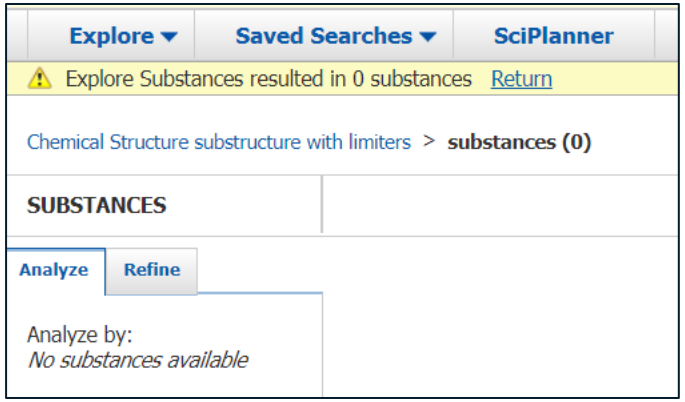
CAS Markush检索





Substance检索结果为0!

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CAS Markush检索

Markush substructure > references (69)

REFERENCES

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Analyze | Refine | Categorize

Sort by: Accession Number

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Page: 1 of 4

Analyze by: Author Name

- Boga Sobhana Babu 3
- Deng Yongqi 3
- Nan Yang 3
- Paliwal Sunil 3
- Shih Neng Yang 3
- Shipps Gerald W Jr 3
- Tsui Hon Chung 3
- Alhassan Abdul Basit 2
- Beier Norbert 2
- Bulawa Christine Ellen 2

Show More

1. **Preparation of ethynylheterocycles as rho-associated coiled-coil kinase (ROCK) inhibitors for the treatment of diseases**
   Quick View PATENTPAK
   By Li, An-Hu; Sakilam, Satish Kumar; Gadhiya, Satish Kumar; Lim, Dong Sung; Zong, Yao; Ponnala, Shashikanth; Zhang, Ying; Jung, Dawoon; Oehlen, Lambertus J. W. M.
   From PCT Int. Appl. (2021), WO 2021016256 A2 20210128. | Language: English, Database: CAPLUS
   The invention relates to prepn. of ethynylheterocycles of formula (I): and pharmaceutically acceptable salts thereof, wherein Cy^1, Cy^2, Cy^3 3 each independently represents an aryl, heteroaryl, or heterocyclic, which is optionally fused with a 3-8 membered cycloalkyl, 3-8 membered heterocycloalkyl, 6-membered aryl, or 5-6 membered heteroaryl; R, R^1, R^2, and R^3 each independently represents an aryl, heteroaryl, or heterocyclic, which is optionally fused with a 3-8 membered cycloalkyl, 3-8 membered heterocycloalkyl, 6-membered aryl, or 5-6 membered heteroaryl, and pharmaceutical compns. thereof, ...

2. **Indazoles and azaindazoles as LRRK2 inhibitors in the treatment of CNS disorders and their preparation**
   Quick View PATENTPAK
   By Garofalo, Albert W.; De Lombaert, Stephane; Schwarz, Jacob Bradley; Andreotti, Daniele; Sabbatini, Fabio Maria; Serra, Elena; Bernardi, Silvia; Migliore, Marco; Budassi, Federica; Beato, Claudia
   From PCT Int. Appl. (2021), WO 2021007477 A1 20210114. | Language: English, Database: CAPLUS
   The invention relates compds. of formula I, their prepn. and their use as inhibitors of LRRK2 in the treatment of CNS disorders. Compd. I, wherein A is halo, (un)subsititued C_{1-6} alkyl, (un)subsititued C_{2-6} alkenyl, etc.; ring B is Ph and 5- to 10-membered heteroaryl wherein said 5- to 10-membered heteroaryl comprises 1, 2 and 3 ring-forming heteroatoms independently864 selected from N, O and S; X^2 is N and CR^2; X^3 is N and CR^3; X^4 is N and CR^4; no more than two of X^2, X^3 and X^4 are simultaneously N; R^1 is independently H, halo, C_{1-6} alkyl, etc.; R^2 and R^4 are independently H, halo, C_{2-6} alke...

3. **Organic electroluminescent materials and devices**
   Quick View PATENTPAK
   By Ji, Zhiqiang; Boudreault, Pierre-Luc T.; Shih, Wei-Chun
   From U.S. Pat. Appl. Publ. (2020), US 20200358008 A1 20201112. | Language: English, Database: CAPLUS
   Provided are an organometallic compds. comprising novel ligands represented by a general chem. formula I (Y = R, OR, SR etc.; Z = O, S, NR''; X^{1-5} = C, N; R^A, R^B = substitution; R, R'' = alkyl, cycloakyl heteroalkyl etc.) as OLED materials for OLED.

为了尽可能全面地获得公开的结构信息，需要同时进行Substance和Markush结构检索

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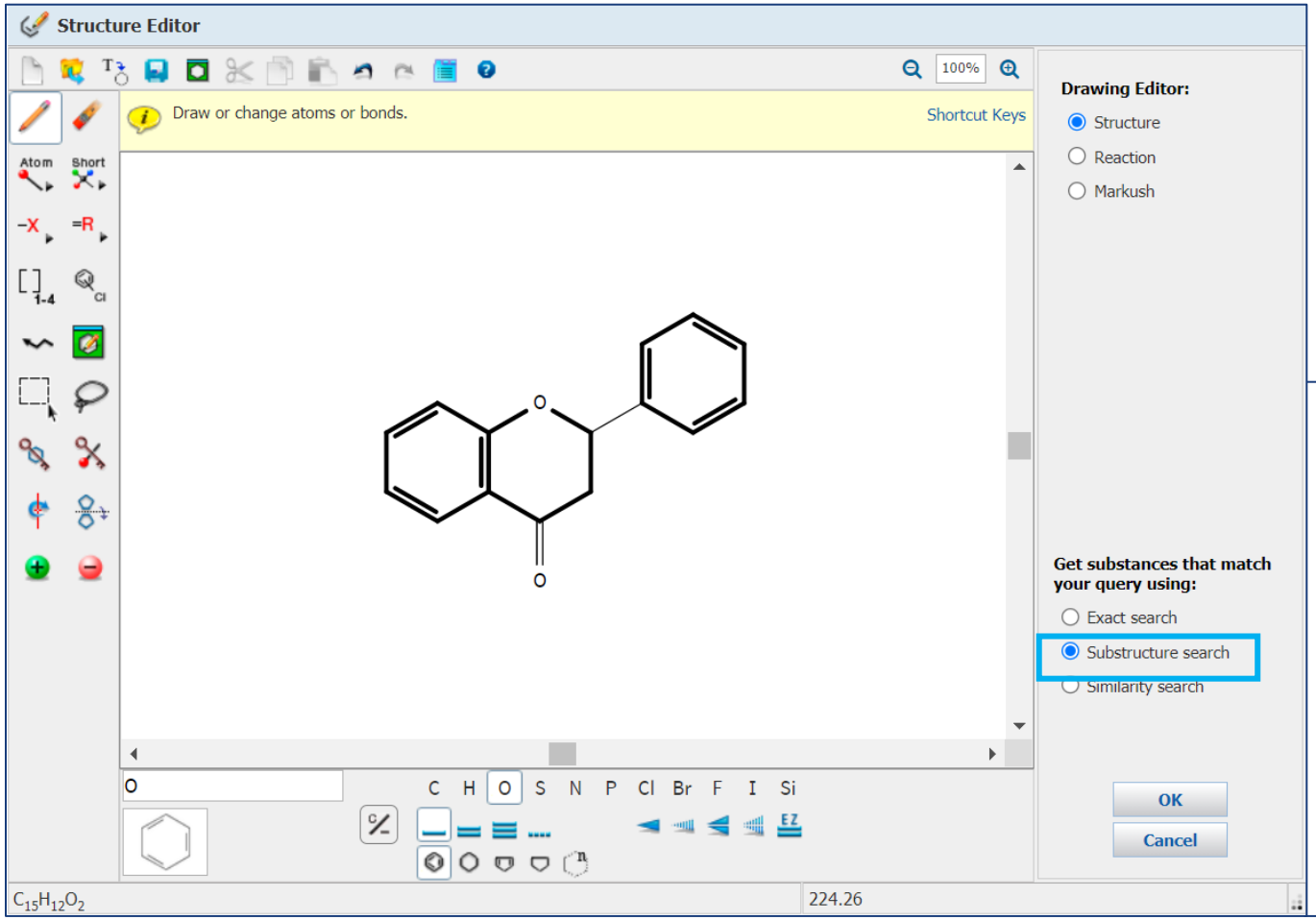
天然产物的筛选



Characteristics	☑ Single component
	☐ Commercially available
	☐ Included in references
Classes	☐ Alloys
	☐ Coordination compounds
	☐ Incompletely defined
	☐ Mixtures
	☐ Polymers
	☑ Organics, and others not listed
Studies	☐ Analytical
	☑ Biological
	☐ Preparation
	☐ Reactant or reagent

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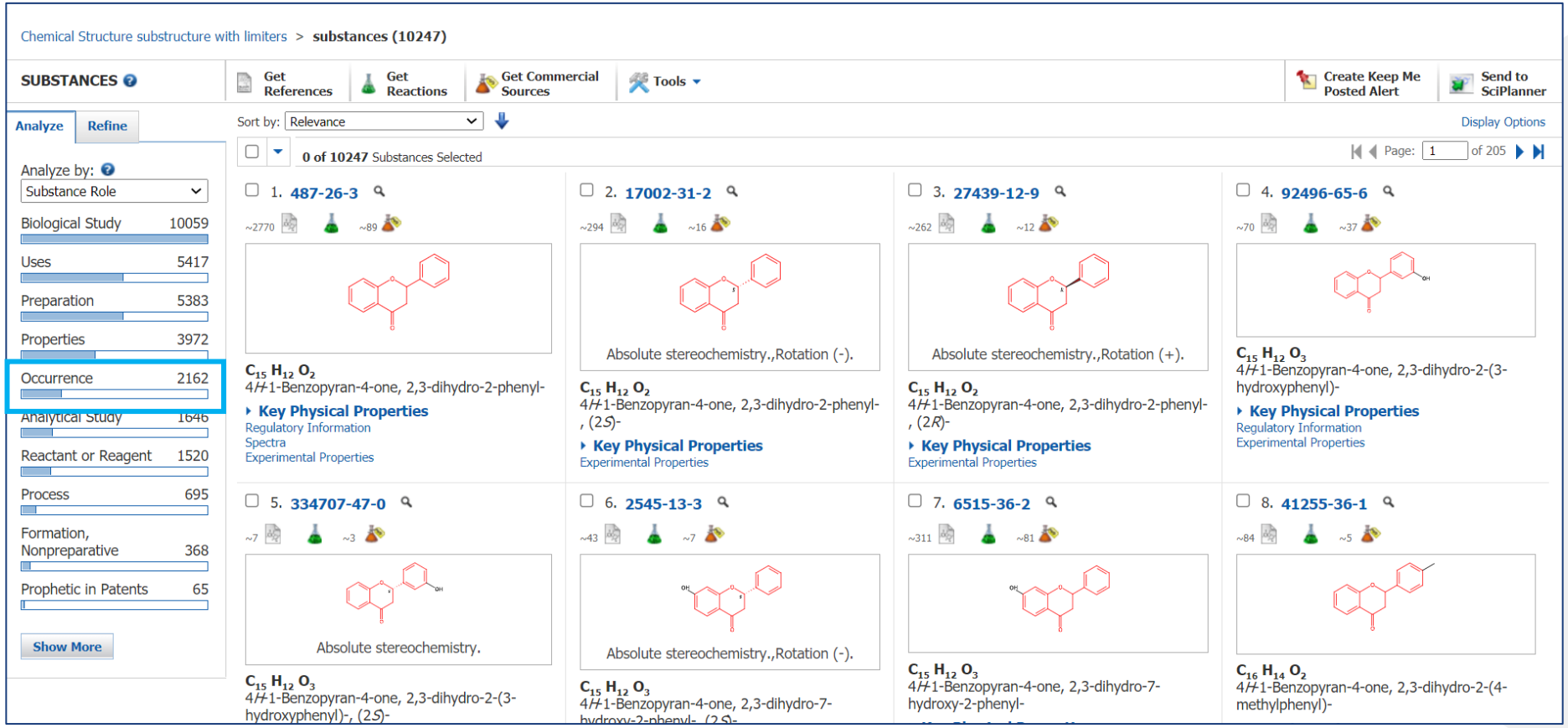
天然产物的筛选



哪些物质是天然存在的呢?

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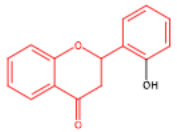
天然产物的筛选

22. **17348-76-4**

~147 ~63



$C_{15}H_{12}O_3$

4*H*-1-Benzopyran-4-one, 2,3-dihydro-2-(2-

Get References

Limit results to:

- ☐ Adverse Effect, including toxicity
- ☐ Analytical Study
- ☐ Biological Study
- ☐ Combinatorial Study
- ☐ Crystal Structure
- ☐ Formation, nonpreparative
- ☐ Miscellaneous
- ☑ Occurrence
- ☐ Preparation
- ☐ Process
- ☐ Properties
- ☐ Prophetic in Patents
- ☐ Reactant or Reagent
- ☐ Spectral Properties
- ☐ Uses

For each sequence, retrieve:

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

Get Cancel

Studies of structure-activity relationship on plant polyphenol-induced suppression of human liver cancer cells

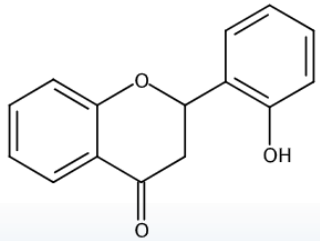
By: Loa, Jacky; Chow, Pierce; Zhang, Kai

To study anticancer activities of 68 plant polyphenols with different backbone structures and various substitutions and to analyze the structure-activity r
polyphenols on human liver cancer cells were screened by the 3-[4,5-dimethylthiazol-2-yl]-2,5-diphenyltetrazolium bromide method. Structure-activity
activities with selected structures. Cell cycle progression was assayed by flow cytometry anal. and apoptosis was analyzed by DNA fragment assay. Ba
were sub-classed to flavonoids (chalcones, flavanones, flavones and isoflavones), chromones and coumarins. The order of their potency to suppress th
chromones > isoflavones > flavanones > coumarins. Chalcones comprise the most potent group with IC_{50} values ranging from 21.69 to 197μM. Top n
hydroxylation at 2'-carbon position in B-ring. Flavones ranked second in their potencies. Quercetin, 4-hydroxyflavone and luteolin are three hydroxyfla
IC_{50} values are 30.81, 39.29 and 71.17μM, resp. Chromones, isoflavones, flavanones and coumarins showed much lower potencies when compared to
131 to >400, 138 to >400 and 360.85 to >400μM, resp. In mechanistic studies, the most potent chalcone, 2,2'-dihydroxychalcone could induce G2/M
anal. of structure-activity relationship showed that following structures are required for their inhibitory potencies on human liver cancer cells: (1) of the
unique backbone structure of chalcones with a open C-ring; (2) within the chalcone group, hydroxyl substitution at 2'-carbon of B-ring; (3) hydroxyl sub
However, some other structures were found to decrease their potencies: e.g. substitutions by sugar moieties in flavones. These data are valuable for
could be potential antiproliferative agents of cancer cells.

Indexing

Pharmacology (Section1-3)

17348-76-4 2'-Hydroxyflavanone



SAR showed that unique back bone structure of chalcones with open C-ring, within chalcone group, hydroxyl substitution of 2'-hydroxyflavanone from plant polyphenols was required for inhibiting human liver cancer cell

Natural product occurrence; Pharmacological activity; Therapeutic use; Biological study; Occurrence; Uses

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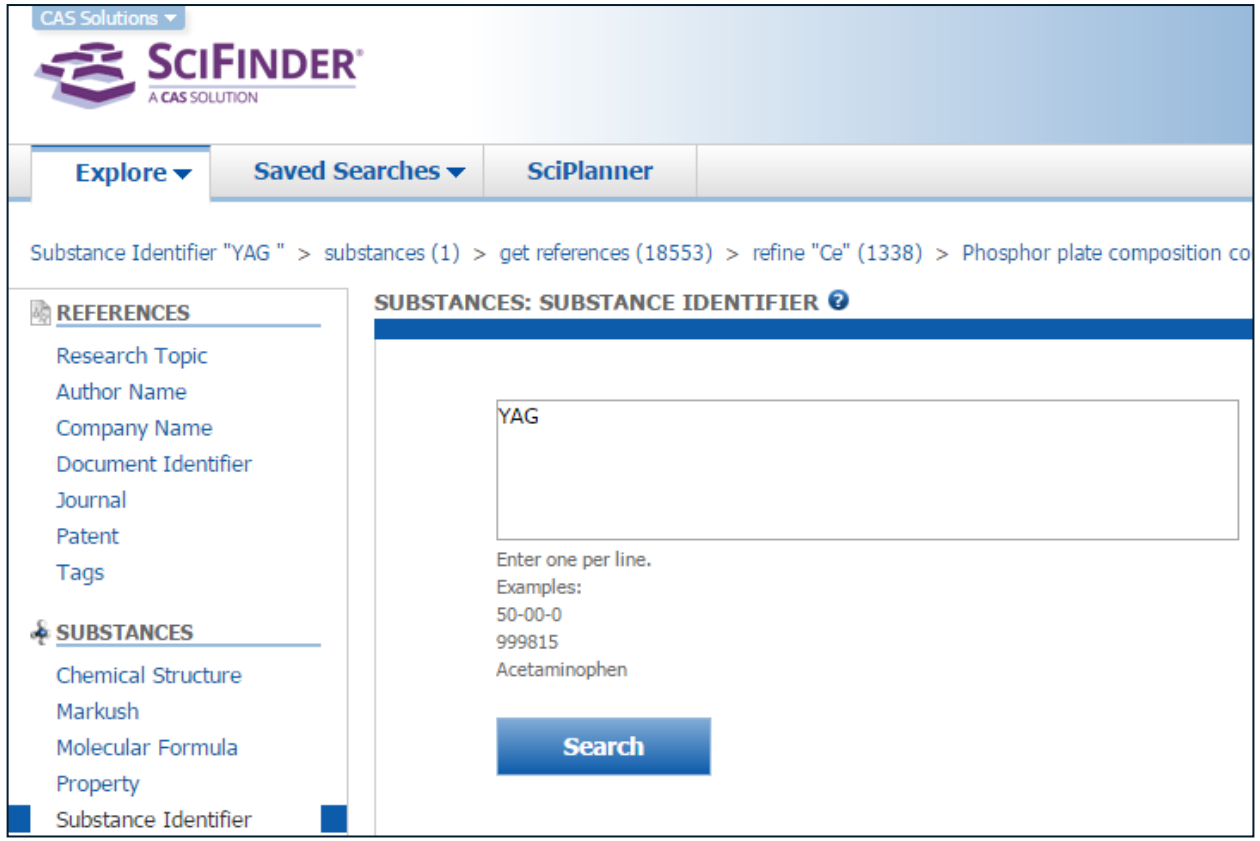
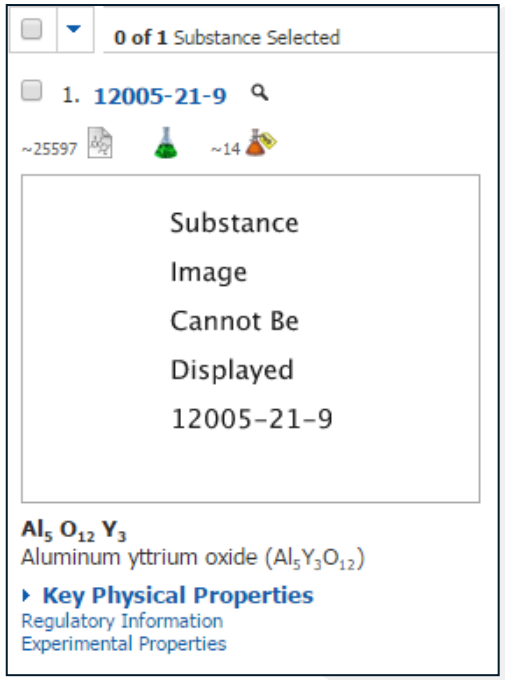
无机复合物的检索

检索YAG: Ce3+复合物及相关文献



先通过物质标识符检索底物YAG



了解YAG的分子式，
主要是元素组成 Al、O、 Y

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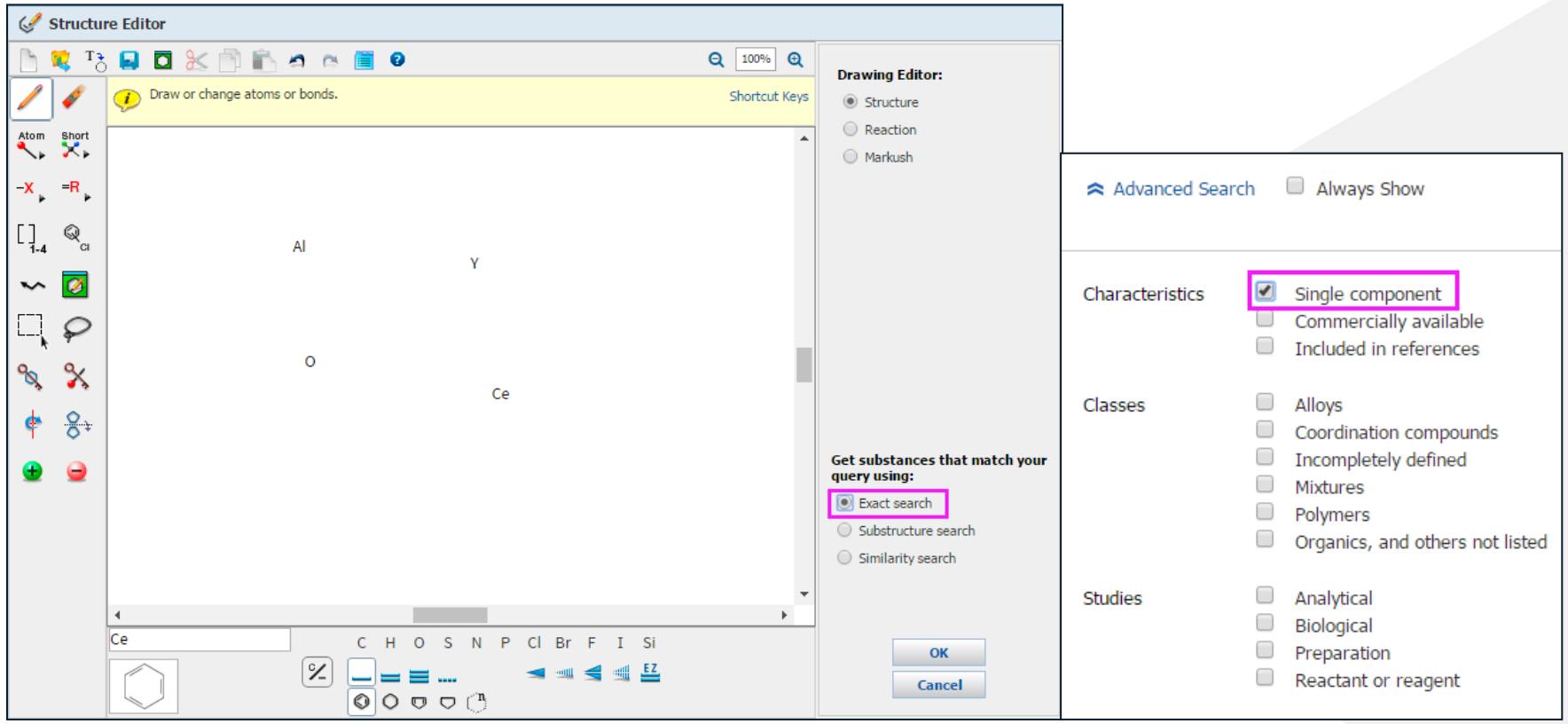
无机复合物的检索



画入所有原子，选择精确结构检索，随后选择单一组份

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无机复合物的检索

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0 of 111 Substances Selected Page: 1 of 3

1. 2055033-00-4

Component	Component Ratio
O	12
Y	1.5
Ce	1.5
Al	5

Al . Ce . O . Y
Aluminum cerium yttrium oxide
($Al_5Ce_{1.5}Y_{1.5}O_{12}$)

2. 1947312-57-3

Component	Component Ratio
O	12
Y	3
Ce	0.1
Al	5

Al . Ce . O . Y
Aluminum cerium yttrium oxide
($Al_5Ce_{0.1}Y_3O_{12}$)

3. 1879158-42-5

Component	Component Ratio
O	2
Y	0.1
Ce	0.8
Al	0.1

Al . Ce . O . Y
Aluminum cerium yttrium oxide
($Al_{0.1}Ce_{0.8}Y_{0.1}O_2$)

4. 1877290-93-1

Component	Component Ratio
O	12
Y	2.65
Ce	0.35
Al	5

Al . Ce . O . Y
Aluminum cerium yttrium oxide
($Al_5Ce_{0.35}Y_{2.65}O_{12}$)

5. 1821155-37-6

Component	Component Ratio
O	11.7
Y	2.98
Ce	0.02
Al	4.8

Al . Ce . O . Y
Aluminum cerium yttrium oxide
($Al_{4.8}Ce_{0.02}Y_{2.98}O_{11.7}$)

6. 1821155-35-4

Component	Component Ratio
O	12.3
Y	2.98
Ce	0.02
Al	5.2

Al . Ce . O . Y
Aluminum cerium yttrium oxide
($Al_{5.2}Ce_{0.02}Y_{2.98}O_{12.3}$)

7. 1693710-50-7

Component	Component Ratio
O	12
Y	2.1
Ce	0.9
Al	5

Al . Ce . O . Y
Aluminum cerium yttrium oxide
($Al_5Ce_{0.9}Y_{2.1}O_{12}$)

8. 1693710-49-4

Component	Component Ratio
O	12
Y	2.25
Ce	0.75
Al	5

Al . Ce . O . Y
Aluminum cerium yttrium oxide
($Al_5Ce_{0.75}Y_{2.25}O_{12}$)

9. 1693710-48-3 10. 1639807-13-8 11. 1639807-12-7 12. 1639807-11-6

人工通过列表上的比例判断目标物质，然后获取相关文献。

文献全吗？

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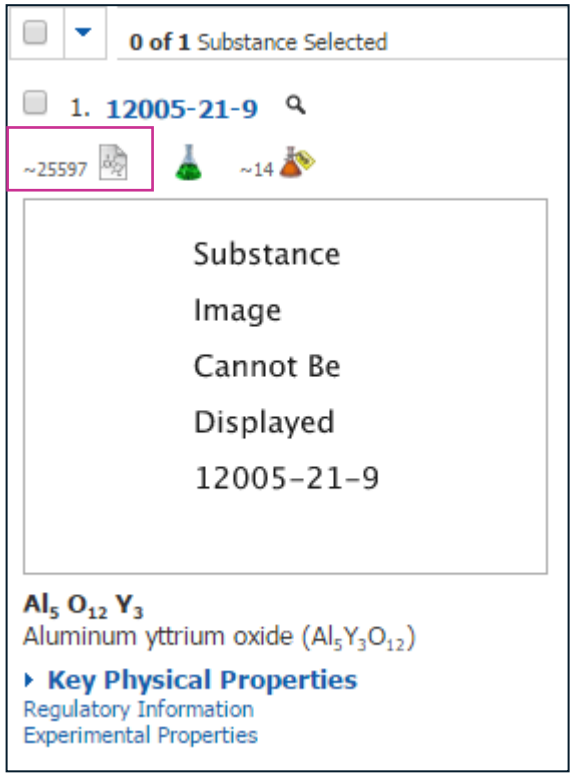

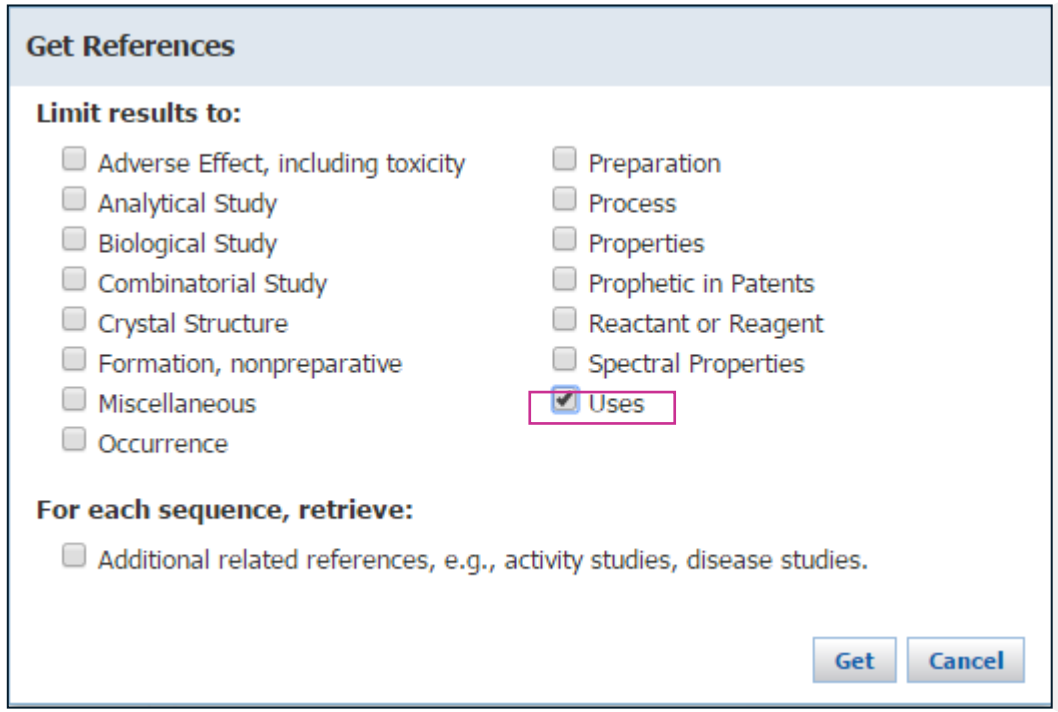

通过底物获得应用相关的文献

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无机复合物的检索

Substance Identifier "YAG " > substances (1) > **get references (18553)** > refine "Ce" (1338) > Phosphor plate composition com...

REFERENCES | Get Substances | Get Reactions | Get Related Citations | Tools | Create Keep Me Posted Alert | Send to SciPlanner

Analyze | Refine | Categorize

Refine by:
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- Author
- Company Name
- Document Type
- Publication Year
- Language
- Database

Research Topic
Ce

Examples:

The effect of antibiotic residues on dairy products

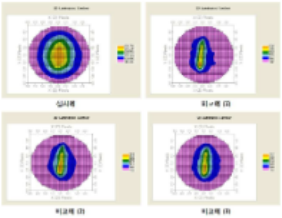
Photocyanation of aromatic compounds

Refine

Sort by: Accession Number ▼ | Display Options

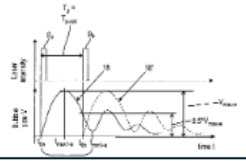
0 of 18553 References Selected | Page: 1 of 928

1. **Phosphor plate composition comprising phosphor powder and sintering agent for vehicle headlamp**
Quick View | PATENTPAK
By Won, Ju Yeon; Kim, Won Jin
From Repub. Korean Kongkae Taeho Kongbo (2017), KR 2017014153 A 20170208. | Language: Korean, Database: CAPLUS



An embodiment of the present invention relates to a phosphor plate compn. having wide luminescent region while improving brightness, comprising yttrium aluminum garnet (YAG) or gadolinium yttrium aluminum garnet (GdYAG) phosphor powders doped with at least one dopant selected from cesium (Ce), gadolinium (Gd) and neodymium (Nd); and at least one sintering agent selected from any one of lithium fluoride (LiF), magnesium oxide (MgO) and spinel ($MgAl_2O_4$).

2. **Cleaning system and method for operating the cleaning system**
Quick View | PATENTPAK
By Lukac, Nejc; Lukac, Matjaz; Jezersek, Matija; Gregorcic, Peter
From Eur. Pat. Appl. (2017), EP 3127502 A1 20170208. | Language: English, Database: CAPLUS



The invention relates to a cleaning system being configured for cleaning, including fragmentation, debridement, material removal, irrigation, disinfection and decontamination, of cavities filled with a liq.. The cleaning system comprises an electromagnetic radiation system and the liq. A treatment handpiece and its exit component are configured to irradiate the liq. within the cavity with the radiation beam, wherein a wavelength of the radiation beam is chosen for significant absorption of the radiation beam in the liq.. The electromagnetic radiation system is adapted to generate a first va...

用Ce限定文献

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无机复合物的检索

Substance Identifier "YAG " > substances (1) > get references (18553) > **refine "Ce" (1338)** > Phosphor plate composition com...

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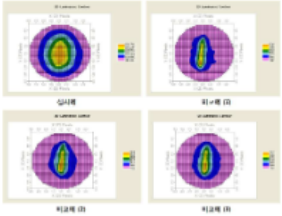
0 of 1338 References Selected | Page: 1 of 67

Analyze by: Author Name

Hirosaki Naoto	18
Takeda Takashi	14
Nikl M	12
Liang Xiaojuan	11
Xiang Weidong	11
Do Young Rag	10
Fujita Shunsuke	8
Funahashi Shiro	8
Mares J A	8
Nikl Martin	8

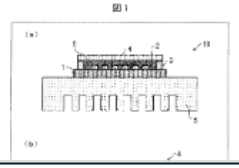
Show More

1. **Phosphor plate composition comprising phosphor powder and sintering agent for vehicle headlamp**
Quick View PATENTPAK
By Won, Ju Yeon; Kim, Won Jin
From Repub. Korean Kongkae Taeho Kongbo (2017), KR 2017014153 A 20170208. | Language: Korean, Database: CAPLUS



An embodiment of the present invention relates to a phosphor plate compn. having wide luminescent region while improving brightness, comprising yttrium aluminum garnet (YAG) or gadolinium yttrium aluminum garnet (GdYAG) phosphor powders doped with at least one dopant selected from cesium (**Ce**), gadolinium (Gd) and neodymium (Nd); and at least one sintering agent selected from any one of lithium fluoride (LiF), magnesium oxide (MgO) and spinel ($MgAl_2O_4$).

2. **Light emitting device improves heat dissipation efficiency of heat generated in wavelength converting member and illuminating device including light emitting device**
Quick View PATENTPAK
By Harada, Masamichi; Yoshimura, Kenichi; Onuma, Hiroaki
From Jpn. Kokai Tokkyo Koho (2017), JP 2017028097 A 20170202. | Language: Japanese, Database: CAPLUS



The present invention relates to a light emitting device and illuminating device including the light emitting device. Light emitting device comprises of multiple light emitting elements, substrate on which multiple light emitting elements are mounted, wavelength converting member for converting a wavelength of light emitted from multiple light emitting elements. The wavelength conversion member includes phosphor sealed with a sealing material for converting the wavelength of the light and a holding material for holding the phosphor. The holding material is characterized in that it contains ...

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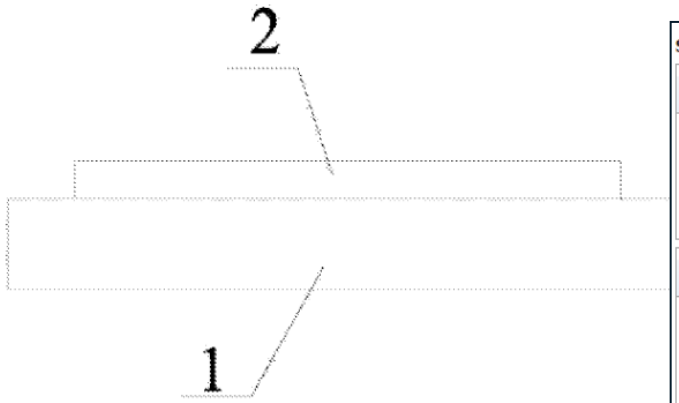
无机复合物的检索

5. Microchip composite luminescent structures based on Ce:YAG and having a wide luminescence spectrum, and their production method

By: Cao, Dun-Hua; Dong, Yong-Jun; Liang, Yue-Shan
Assignee: Peop. Rep. China

The present invention relates to a Ce:YAG wafer-based composite structure comprising a Ce:YAG wafer and a red light emitting layer fixed on the Ce:YAG wafer. The present invention also relates to a method for the prepn. of the Ce:YAG wafer-based composite structure. The optical composite structure realizes a wide waveband luminescence from green light to red light, and can be widely used in the fields of detection equipment and illumination devices.



Substances

7440-45-1 Cerium, properties — Page 7 in PATENTPAK

YAG doped with; microchip composite luminescent structures based on Ce:YAG and having a wide luminescence spectrum, and their prodn. method

Modifier or additive use; Properties; Technical or engineered material use; Uses

12005-21-9 YAG — Page 7 in PATENTPAK

cerium-doped, europium-doped; microchip composite luminescent structures based on Ce:YAG and having a wide luminescence spectrum, and their prodn. method

Properties; Technical or engineered material use; Uses

7440-53-1 Europium, properties — Page 6 in PATENTPAK

dopant; microchip composite luminescent structures based on Ce:YAG and having a wide luminescence spectrum, and their prodn. method

Modifier or additive use; Properties; Technical or engineered material use; Uses

1314-36-9 Yttrium oxide (Y_2O_3), properties — Page 6 in PATENTPAK

europium-doped; microchip composite luminescent structures based on Ce:YAG and having a wide luminescence spectrum, and their prodn. method

Properties; Technical or engineered material use; Uses

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却是我们需要的文献

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无机复合物的检索

PATENTPAK A CAS SOLUTION

PAGE 7 /7 ZOOM DOWNLOAD PDF

Key Substances in Patent

CAS RN 7440-53-1

Eu

Search in SciFinder | View Detail

Analyst Markup Locations (1)

page 6

CAS RN 1314-36-9

Yttrium oxide (Y_2O_3)

Search in SciFinder | View Detail

Analyst Markup Locations (1)

page 6

CAS RN 7440-45-1

Ce

US 2016/0341832 A1 Nov. 24, 2016
3

nm~700 nm, and thus achieving a wide waveband luminescence from green light to red light.

[0042] The purpose, technical solutions and beneficial effects of the present invention are described with reference to the above particular examples. Nevertheless, it will be understood that the above examples are not provided to limit the present invention. The invention is intended to cover various modifications and equivalent arrangements included within the spirit and scope of the claims.

1. A Ce:YAG wafer-based composite structure, wherein said composite structure comprises:

a Ce:YAG wafer; and

a red light emitting layer fixed on said Ce:YAG wafer.

2. The Ce:YAG wafer-based composite structure according to claim **1**, wherein the main emission peak of said red light emitting layer is at 580 nm–660 nm.

3. The Ce:YAG wafer-based composite structure according to claim **2**, wherein said red light emitting layer is a deposited film capable of emitting red light.

4. The Ce:YAG wafer-based composite structure according to claim **2**, wherein said red light emitting layer is a transparent colloid layer doped with red fluorescent powder.

5. The Ce:YAG wafer-based composite structure according to claim **2**, wherein said red light emitting layer is a crystalline, a ceramic or a glass doped with red light

6. A method for the preparation of a Ce:YAG wafer-based composite structure, comprising:

(1) producing a Ce:YAG wafer by Czochralski process, temperature gradient process or Kyropoulos process;

(2) grinding and polishing the Ce:YAG wafer produced in step (1) to obtain a fluorescent wafer having desired size; and

(3) adding a red light emitting layer on the fluorescent wafer obtained in step (2).

7. The method for the preparation of a Ce:YAG wafer-based composite structure according to claim **6**, wherein the red light emitting layer added in step (3) is a red light emitting film deposited by physical or chemical vapor deposition.

8. The method for the preparation of a Ce:YAG wafer-based composite structure according to claim **6**, wherein the red light emitting layer added in step (3) is a transparent colloid layer doped with red fluorescent powder.

9. The method for the preparation of a Ce:YAG wafer-based composite structure according to claim **6**, wherein the red light emitting layer added in step (3) is a crystalline, a ceramic or a glass doped with red light luminescence center of rare earth or transition metal and fixed on the fluorescent wafer.

专利中仅仅以文字方式提到此物质

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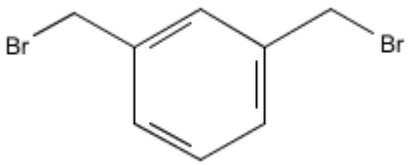
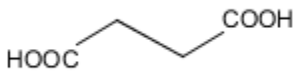
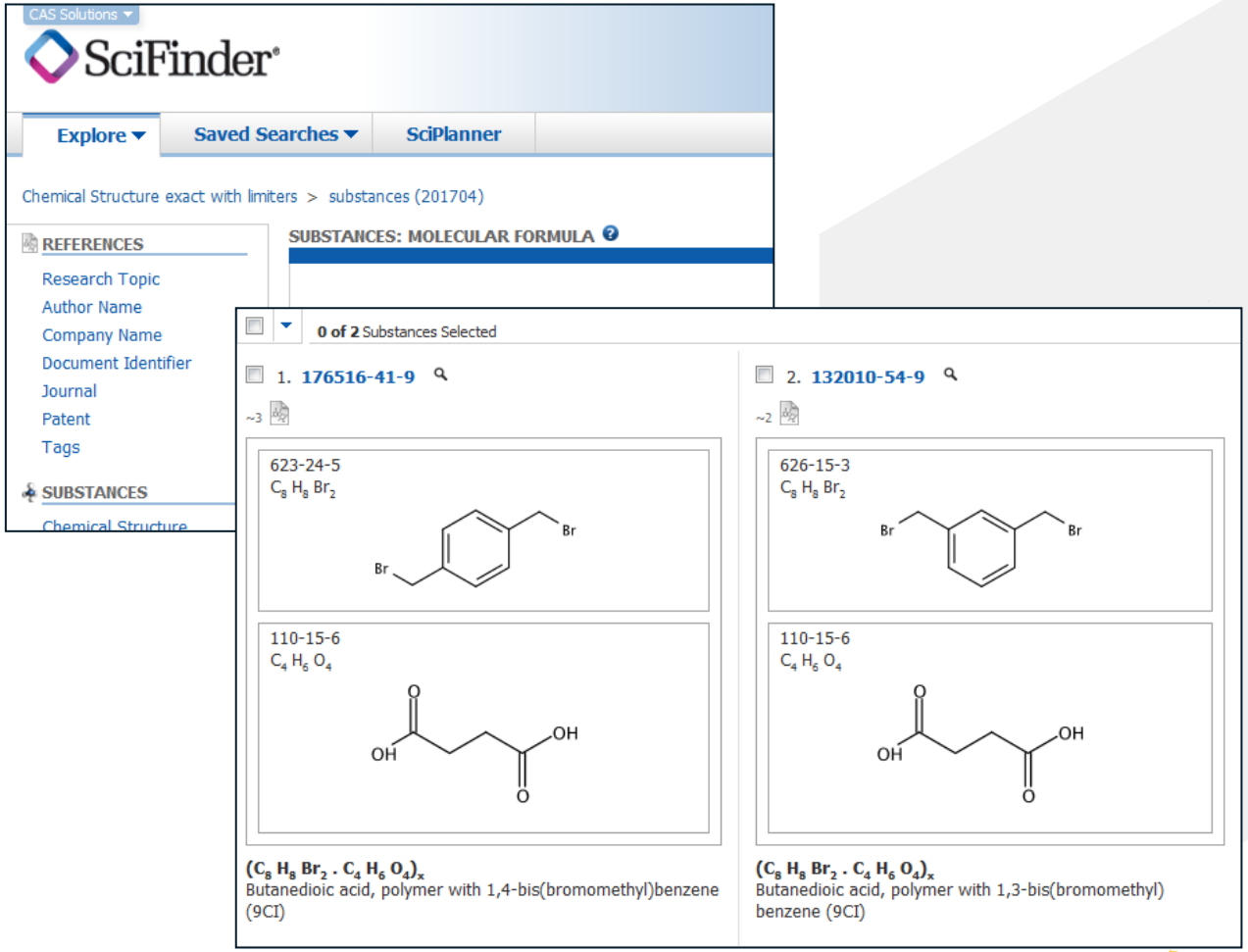
聚合物的检索

已知起始原料的聚合物





（C8 H8 Br2 . C4 H6 O4） x



分子式检索后会得到同分异构体

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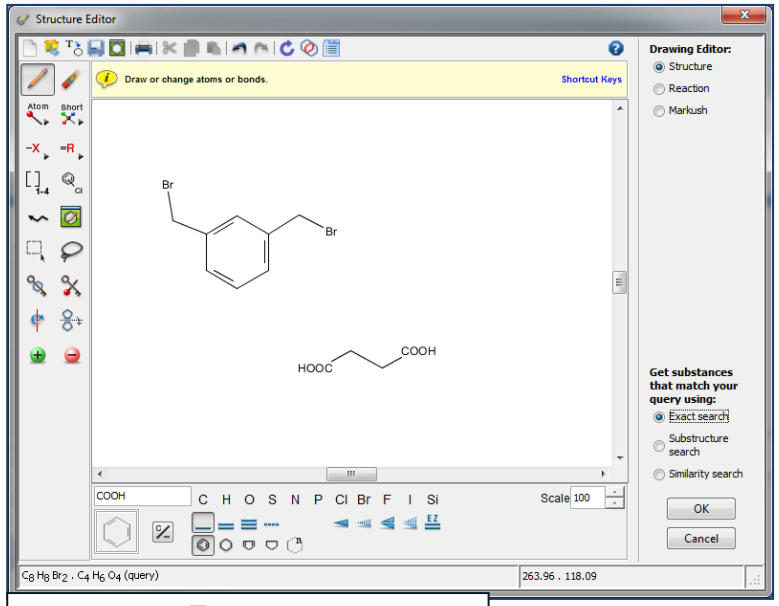
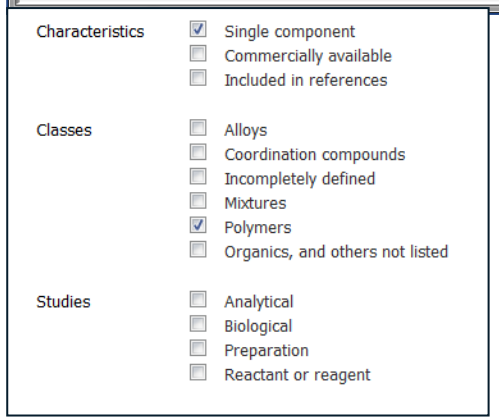
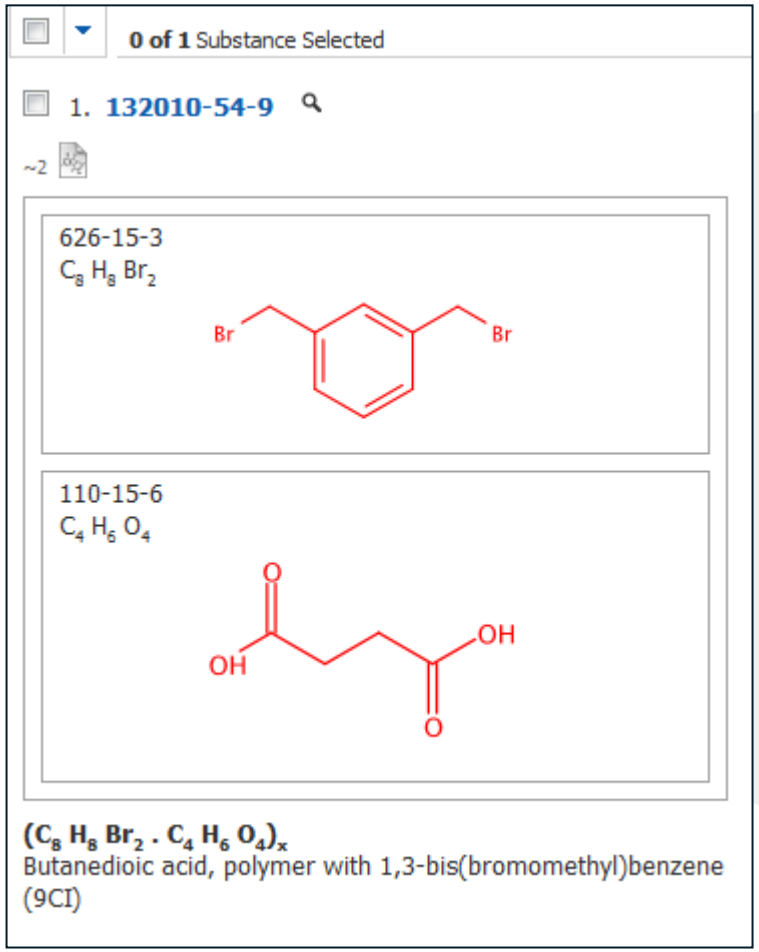
聚合物的检索





单一组分

聚合物



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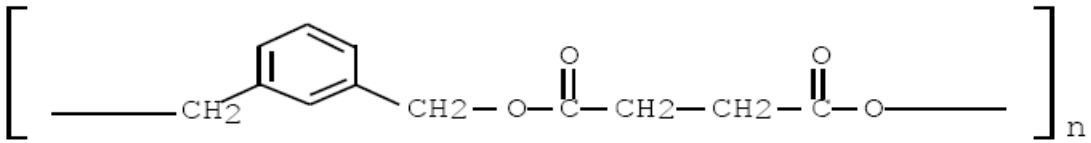
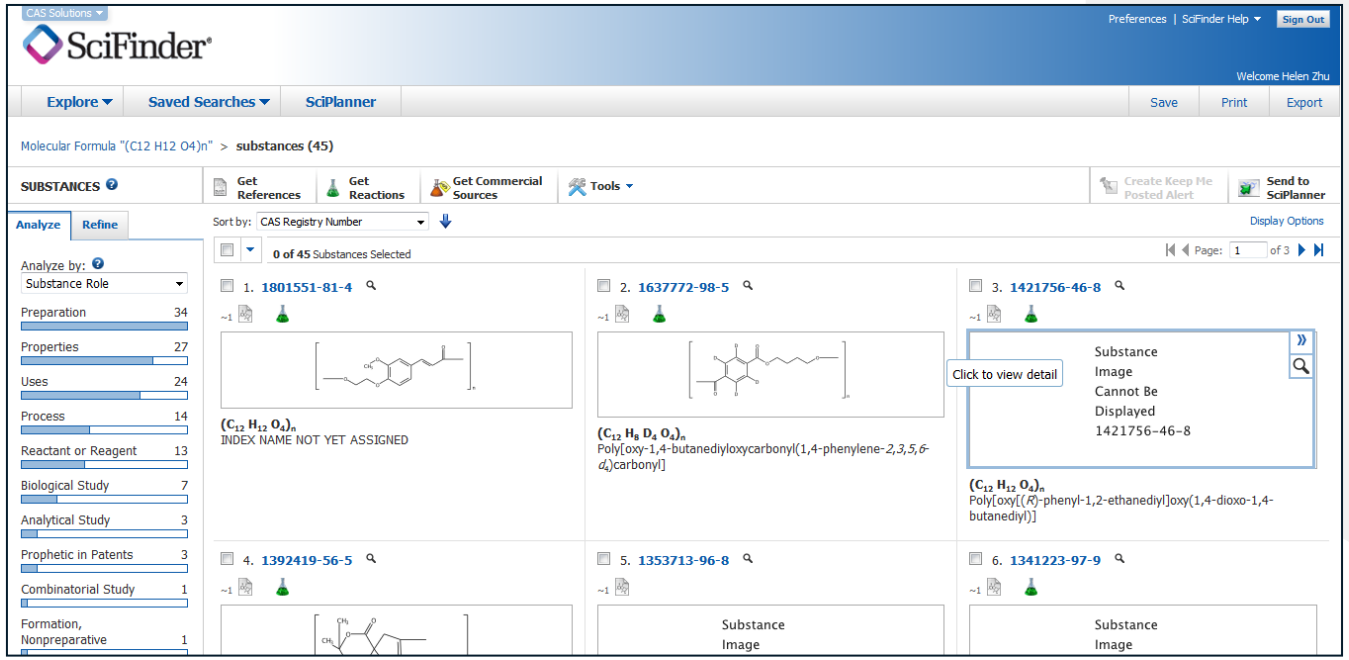
聚合物的检索

已知重复单元的聚合物



(C12 H12 O4)n



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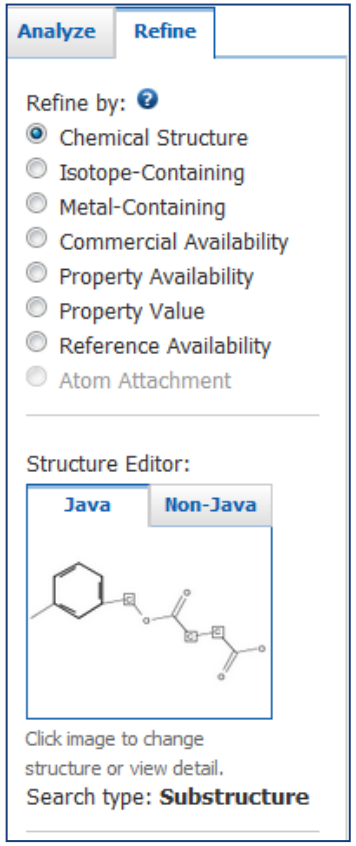
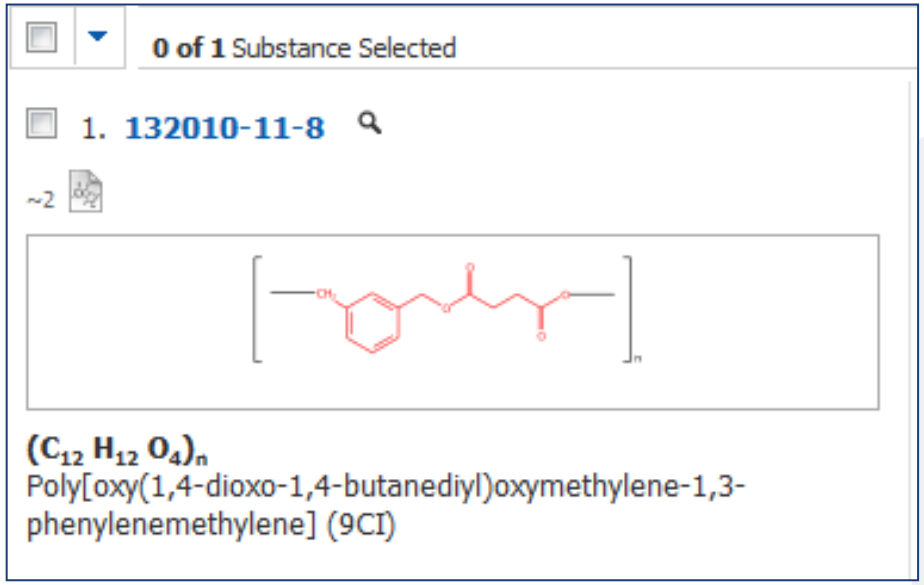
聚合物的检索





利用结构特征进行Refine，迅速查找需要的物质

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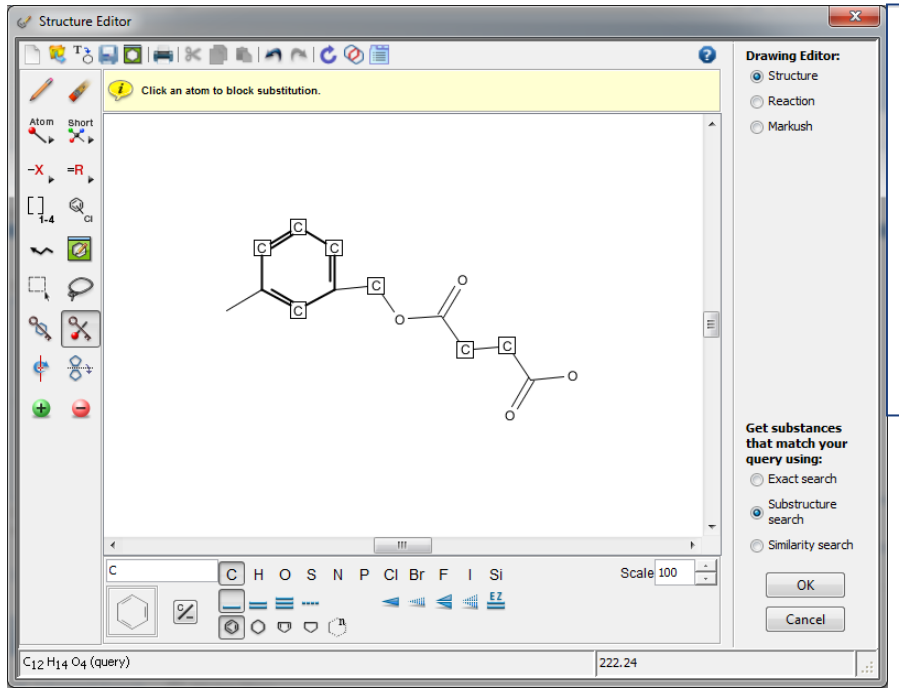
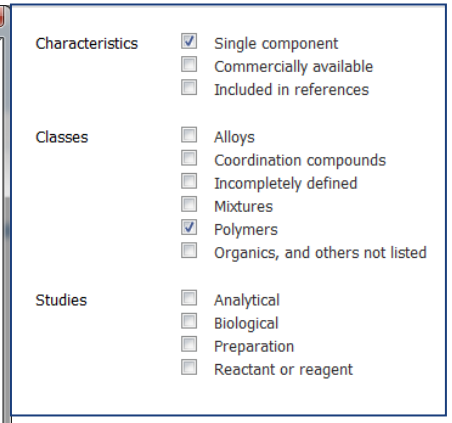
聚合物的检索



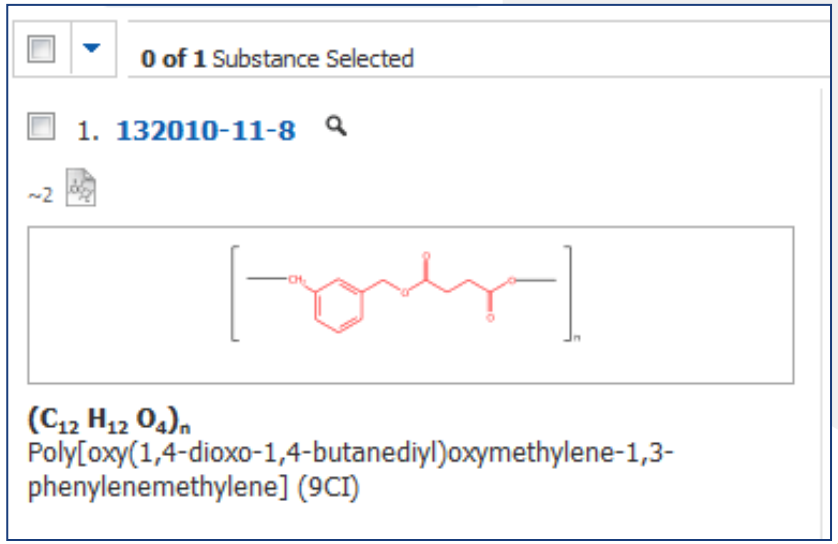


单一组分

聚合物

绘制好SRU后用亚结构检索

因为两段为开放状态



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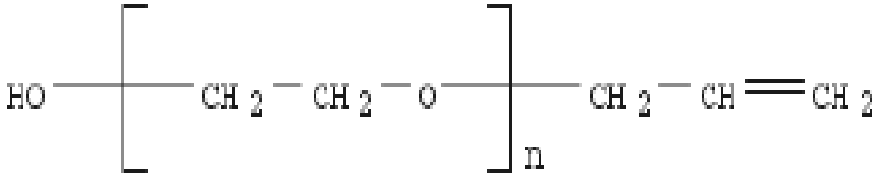
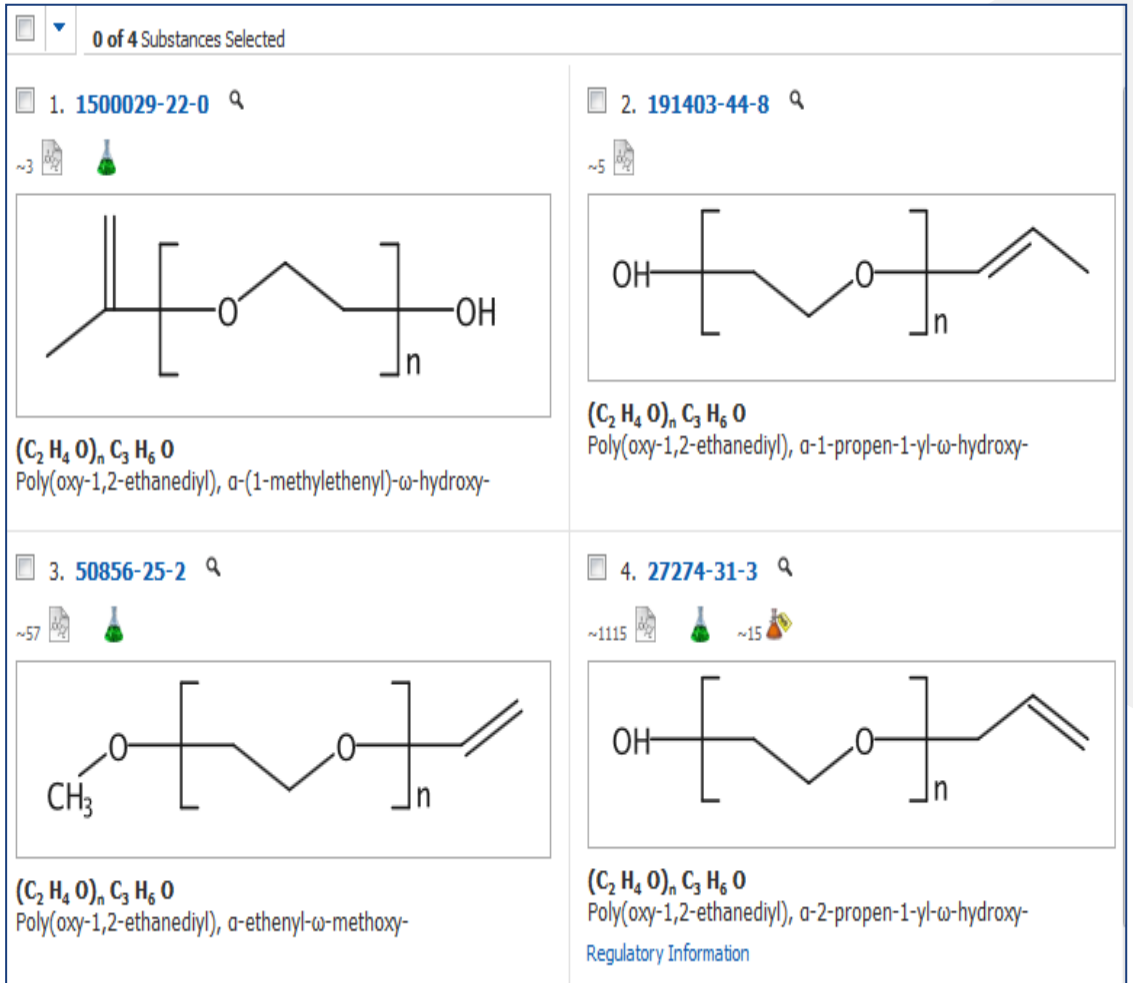
聚合物的检索

含端基和SRUs的聚合物

(C2 H4 O)n C3 H6 O

SRU部分　两端部分





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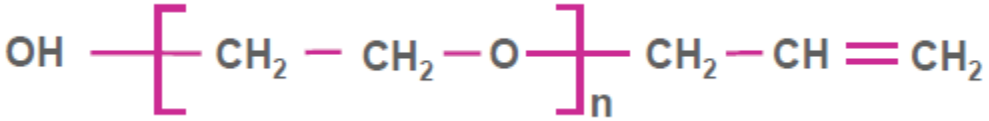
聚合物的检索

杂化聚合物的检索：

检索由以下聚合物和2-丙烯酸（C3H4O2）聚合生成的聚合物



检索策略：分子式检索

(C3 H4 O2. (C2 H4 O)n C3 H6 O)x

丙烯酸部分　**SRU部分**　**两端部分**

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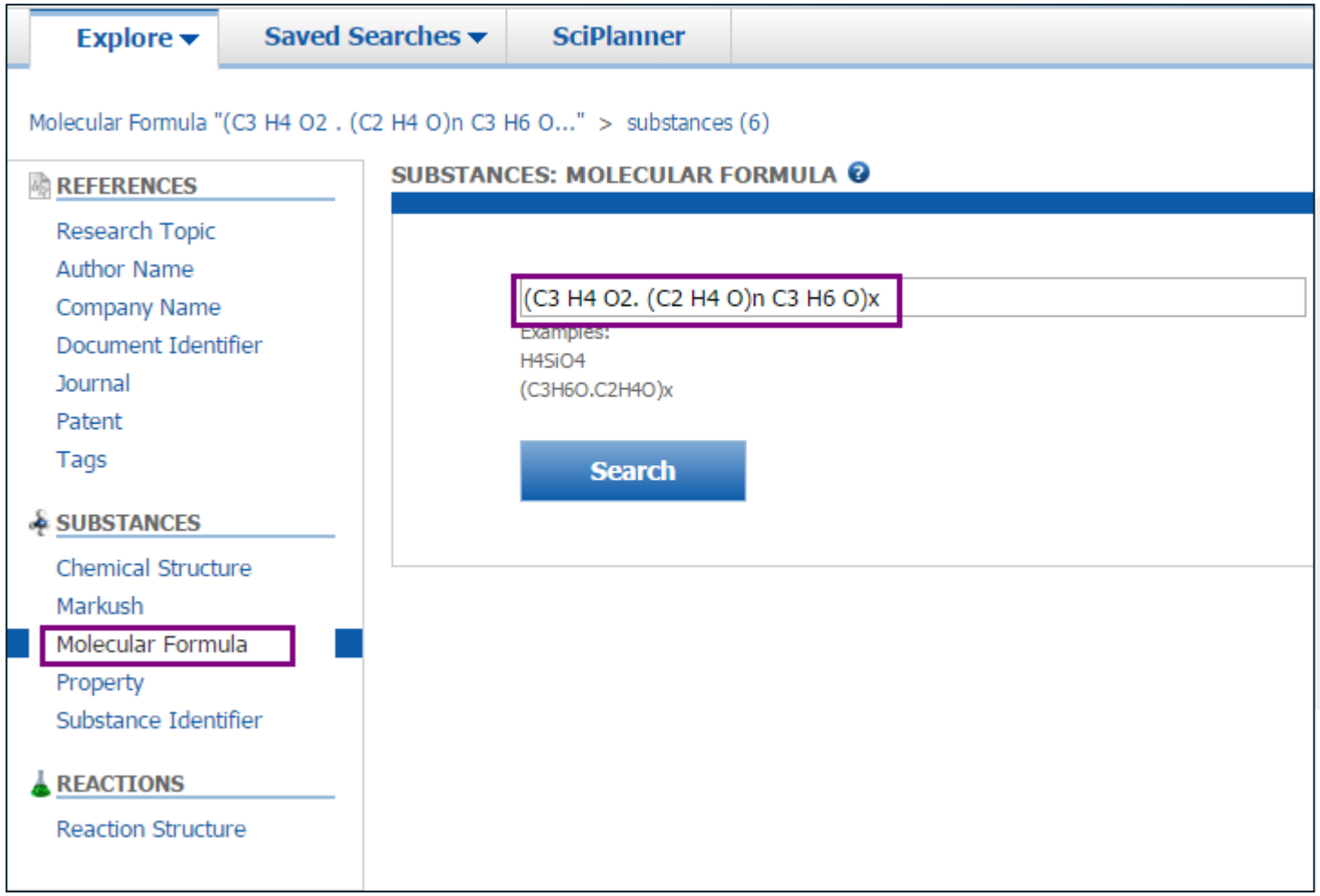
聚合物的检索



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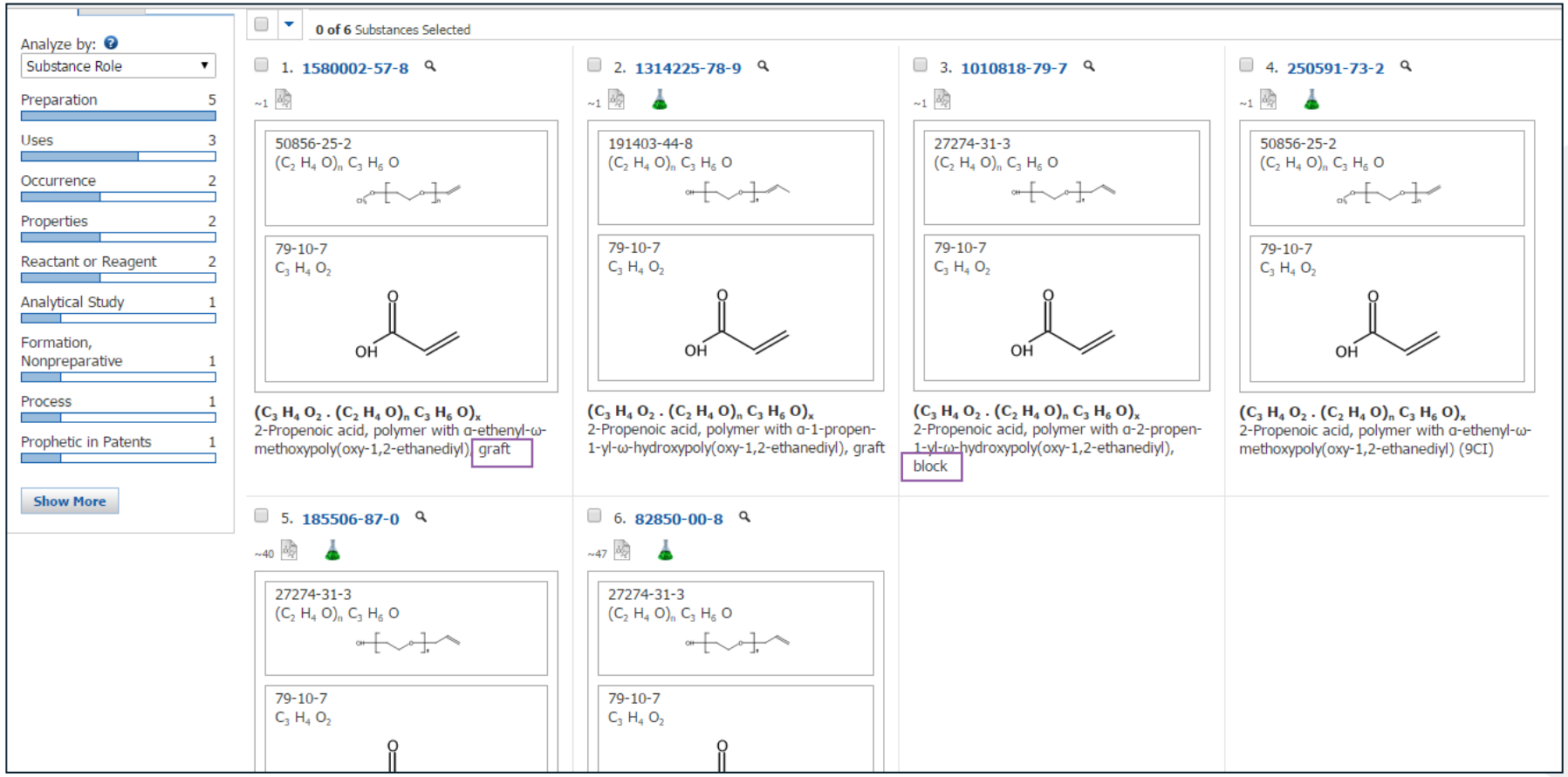
聚合物的检索



Block： 嵌段聚合物

Graft： 接枝聚合物

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聚合物的检索

后处理聚合物的检索：

检索对由2, 5-呋喃二酮和苯乙烯聚合而成的物质进行结构修饰的聚合物

检索策略：

1. 先检索由2, 5-呋喃二酮和苯乙烯聚合而成的物质，获得CAS登记号
2. 主题检索相应的CAS登记号加D
3. 如果有具体的修饰要求，可在topic中直接加入相应的词，

   如：sulfonated xxxx-xx-xd，ester xxxx-xx-xd

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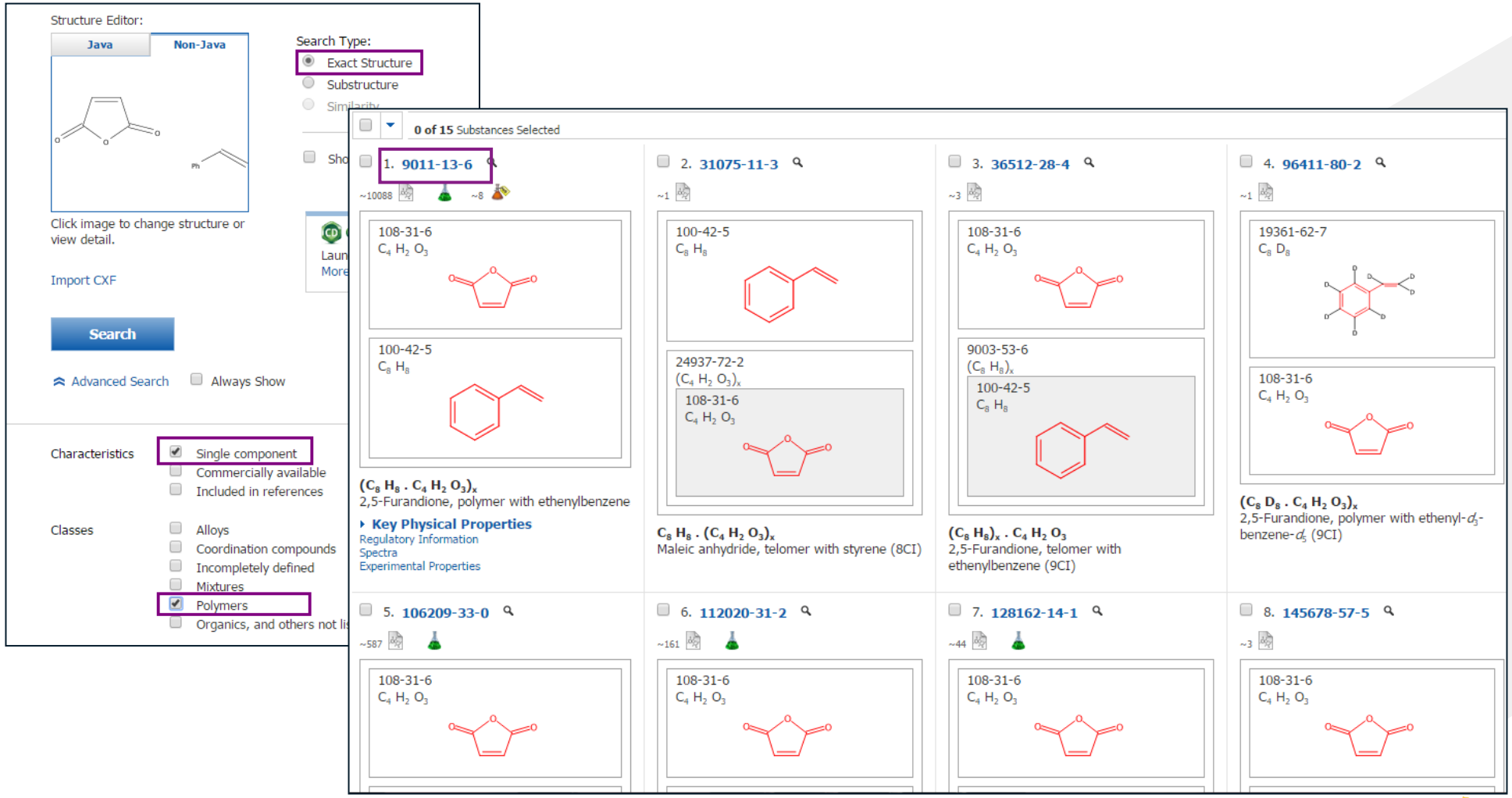
聚合物的检索



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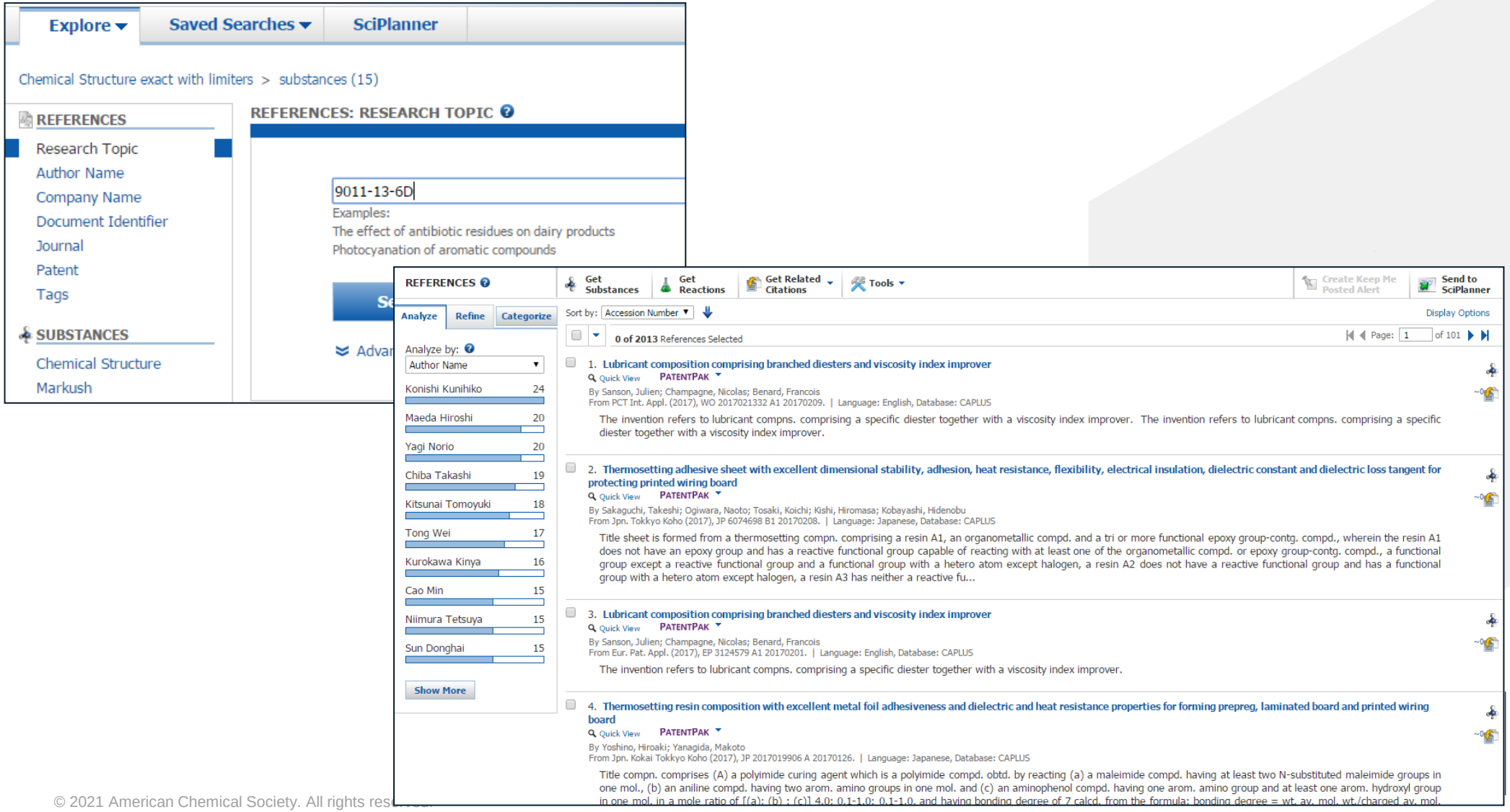
聚合物的检索



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聚合物的检索

1. Lubricant composition comprising branched diesters and viscosity index improver

By: Sanson, Julien; Champagne, Nicolas; Benard, Francois
Assignee: Total Marketing Services, Fr.

The invention refers to lubricant compns. comprising a specific diester together with a viscosity index improver. The invention refers to lubricant compns. comprising a specific diester together with a viscosity index improver.

Patent Information

Patent No.		Kind	Language	Date	Application No.	Date
WO 2017021332	PATENTPAK	A1		Feb 9, 2017	WO 2016-EP68229	Jul 29, 2016
EP 3124579	PATENTPAK	A1	English	Feb 1, 2017	EP 2015-179371	Jul 31, 2015

Priority Application

EP 2015-179371	A	Jul 31, 2015

Indexing

Fossil Fuels, Derivatives, and Related Products (Section51-8)

Concepts

Base oils
Lubricating oil additives
Crankcase oil
Transesterification

lubricant compn. comprising branched diesters and viscosity index improver

Polyolefins

lubricant compn. comprising branched diesters and viscosity index improver

Modifier or additive use; Uses

Lubricating oil additives

viscosity improvers; lubricant compn. comprising branched diesters and viscosity index

Substances

78-79-5D Isoprene, polymers
106-99-0D Butadiene, polymers
9003-31-0D Polyisoprene, hydrogenated
9011-13-6D Styrene-maleic anhydride copolymer, esters
25038-32-8D Isoprene-styrene copolymer, hydrogenated

lubricant compn. comprising branched diesters and viscosity index improver

Modifier or additive use; Uses

64-18-6 Formic acid
124-07-2 Octanoic acid
143-07-7 Dodecanoic acid
157336-71-5

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物质检索小结

1. 选择合适的检索方式
2. 利用结构绘制工具合理扩大结构检索范围：R基团、可变基团、可变位置取代等
3. 利用结构绘制工具适当限定检索结构：环锁工具、原子锁工具、EZ构型限定等
4. 正确理解Exact、Substructure、Similarity检索结果集的意义和范围
5. 利用CAS Markush检索尽可能全面的获得结构的公开信息

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大纲

- CAS及CAS SciFinder介绍
- 文献相关信息的检索策略
  - 利用Index Term修正检索词
  - 巧用CAS Role
  - 善用Categorize
  - 如何高效阅读专利文献详情(CAS PatentPak)
- 物质相关信息的检索策略
  - 检索具有相同结构特征的物质
  - Markush检索
  - 如何筛选天然产物
  - 无机复合物、聚合物的检索
- 反应相关信息的检索策略
  - 如何检索化学选择性反应
  - 直接检索反应受限时如何处理
  - 新化合物的合成路线设计
  - 案例分析
  - 如何高效获取反应详情
- 获取分析方法的策略（CAS Analytical Methods）

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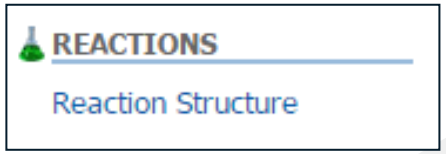
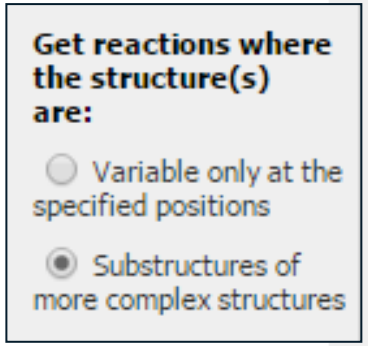
CAS SciFinder检索--反应检索

- 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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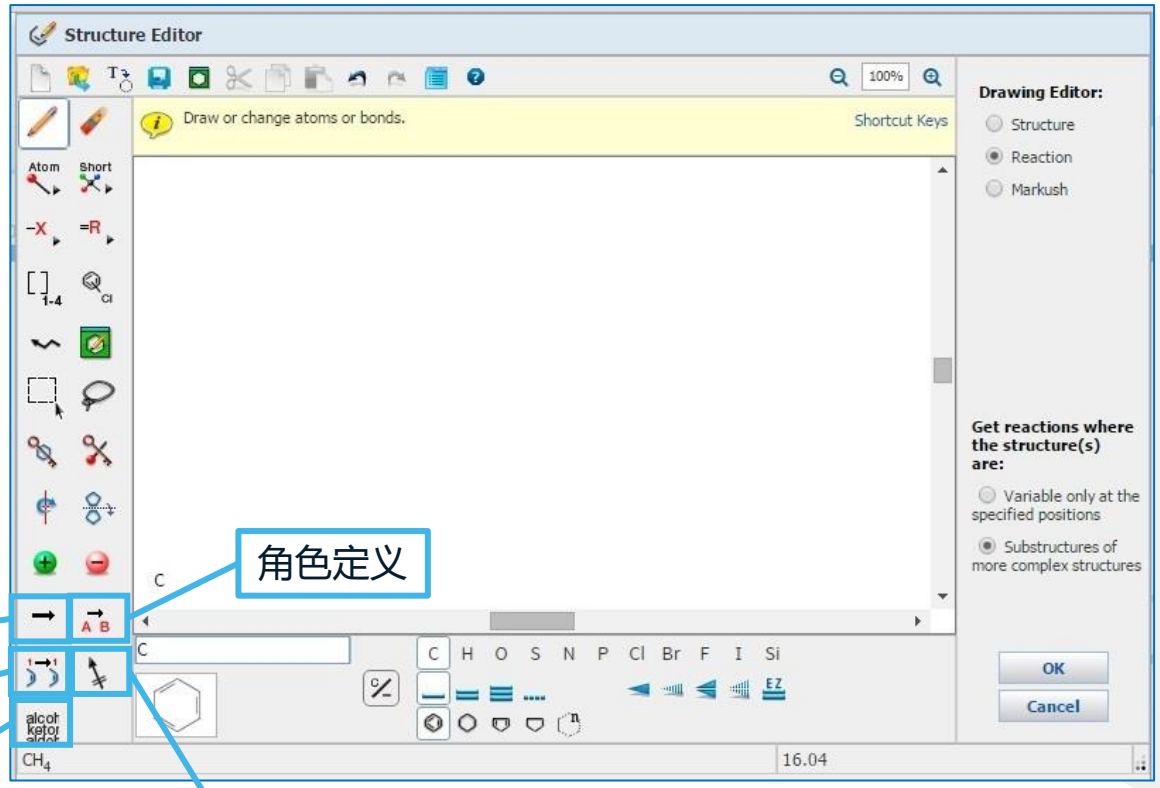
结构编辑器--绘制反应工具



角色定义

反应箭头

原子标记

官能团列表

化学键变化

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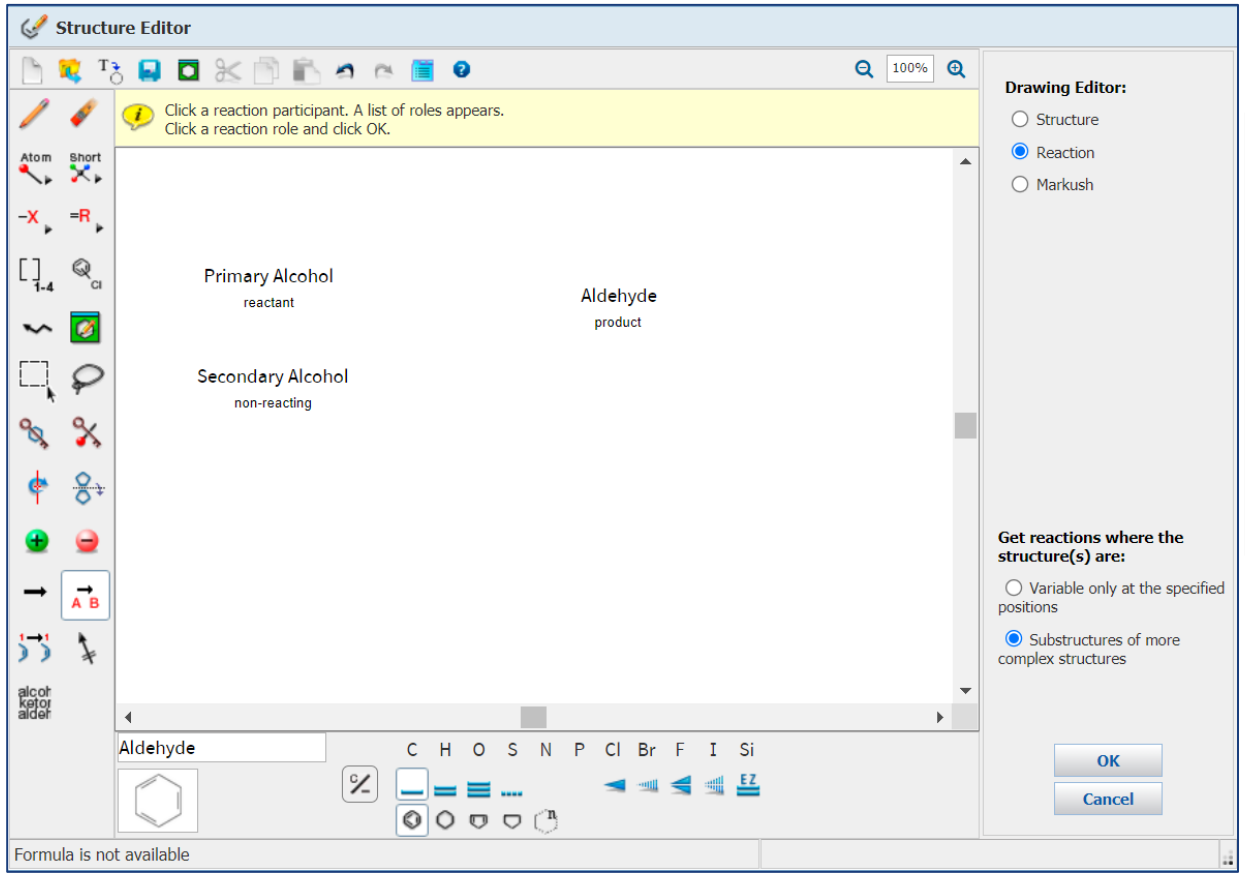
化学选择性反应的检索

问题：底物上有伯羟基和仲羟基，能否找到合适的氧化剂使伯羟基氧化成醛而仲羟基不受影响?



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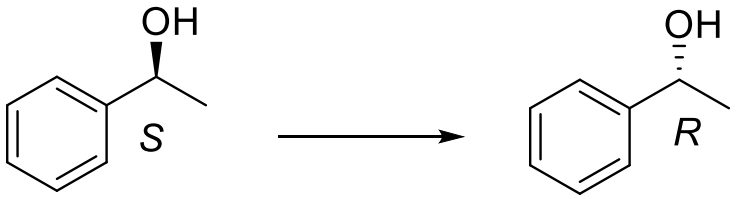
直接检索反应受限时如何处理

检索如下构型翻转的反应



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新化合物合成路线设计

检索思路1：检索结构相似的物质，获得有参考价值的合成路线；

检索思路2：检索通式结构，获得有参考价值的合成路线；

检索思路3：先自行做逆合成反应分析，然后验证相关的反应。

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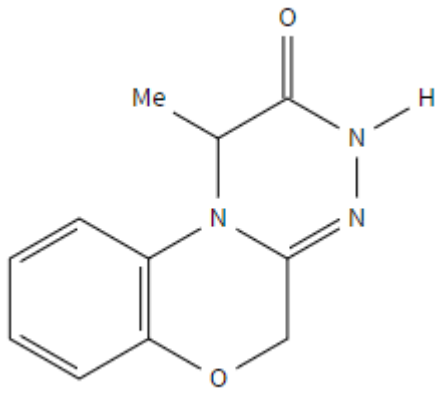
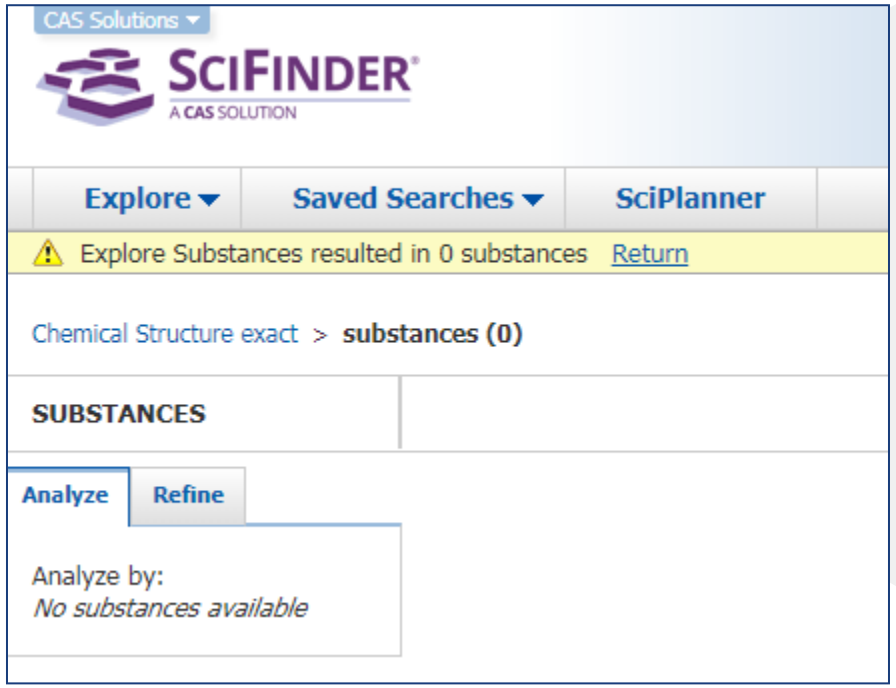
新化合物合成路线设计

检索思路1：相似结构检索，获得有参考价值的合成路线





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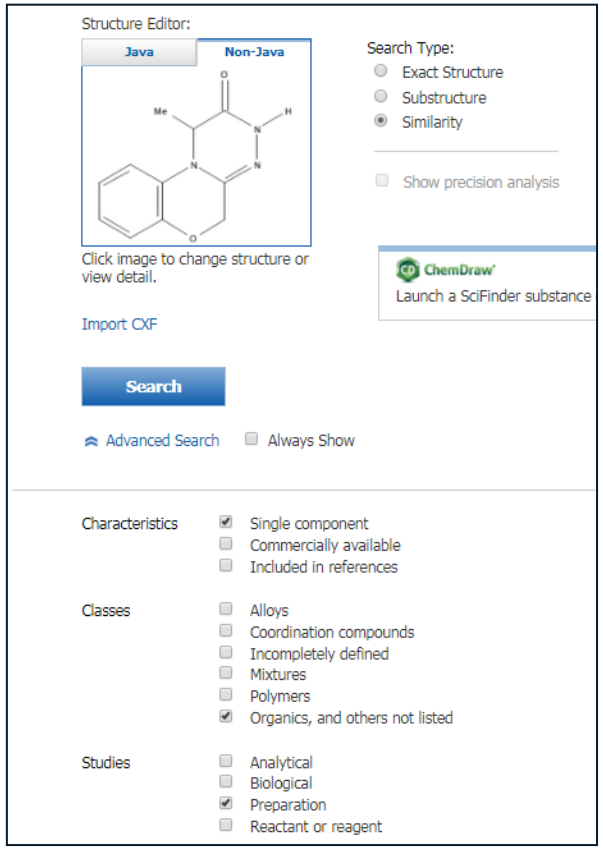
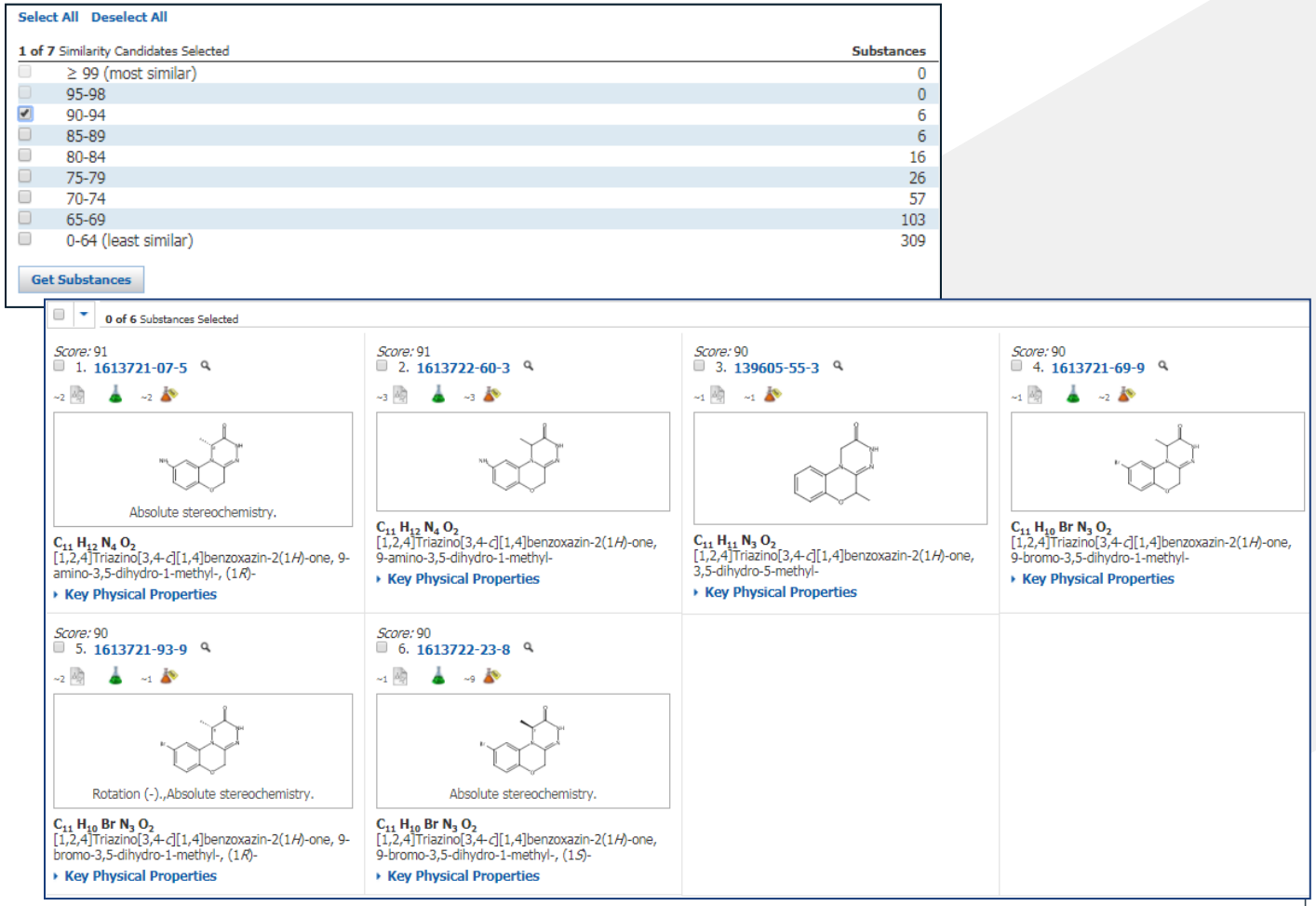
新化合物合成路线设计





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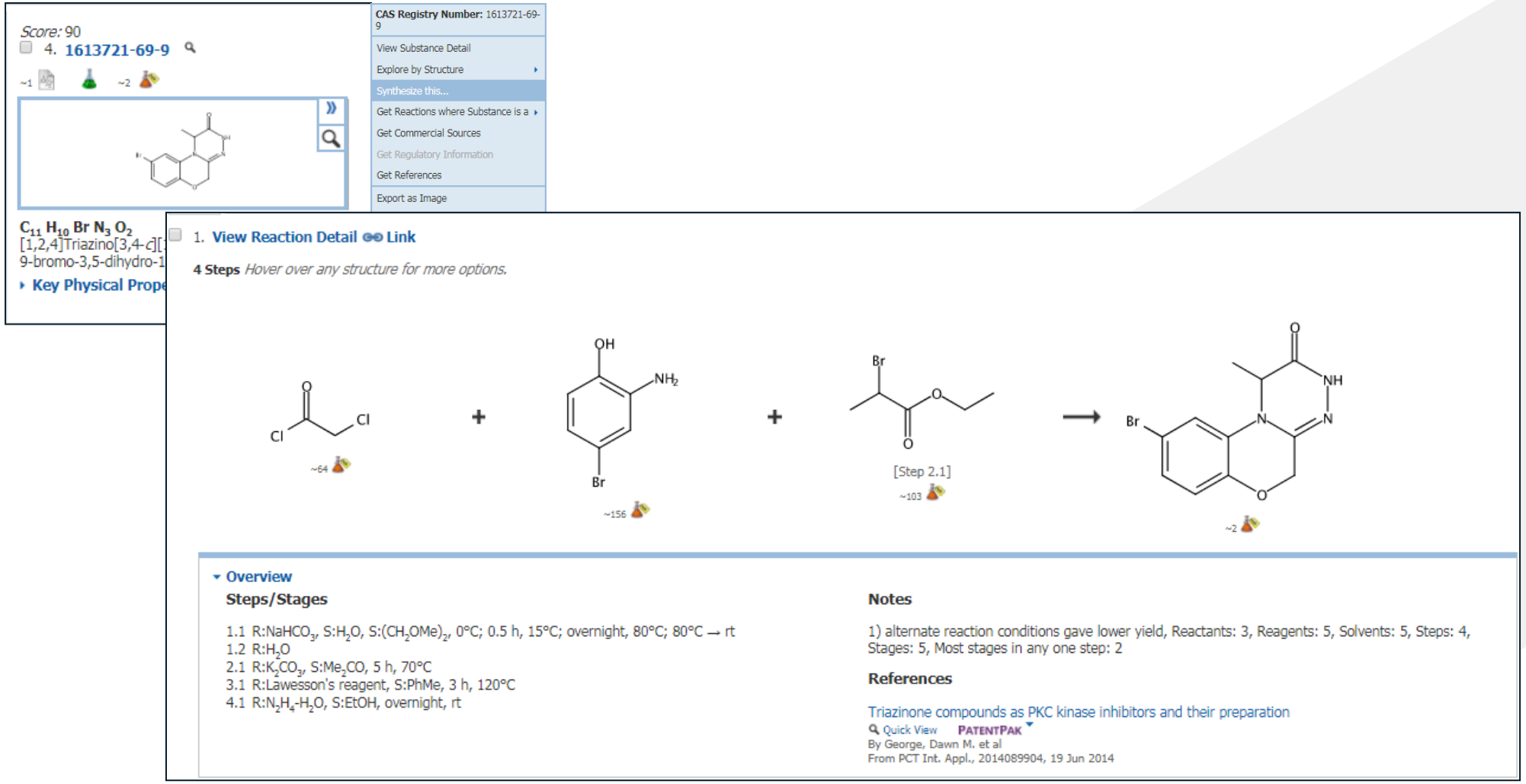
新化合物合成路线设计



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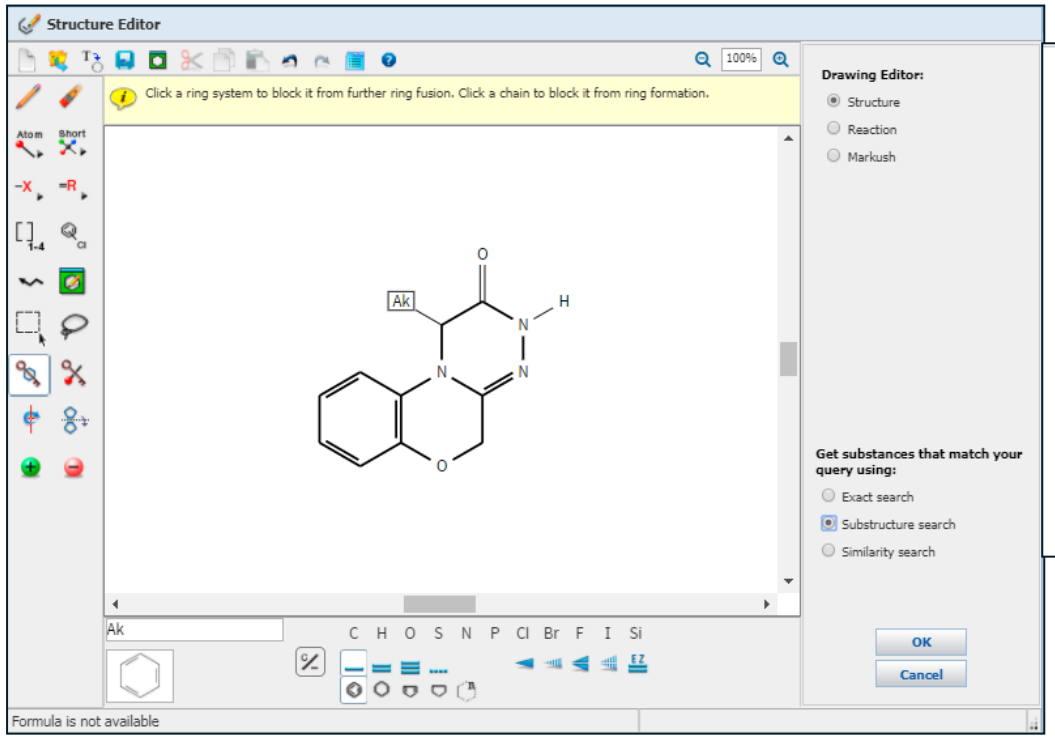
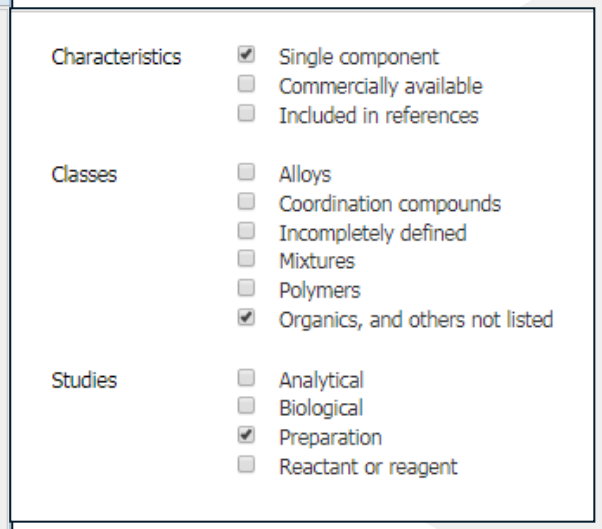
新化合物合成路线设计

检索思路2：通式结构检索，获得有参考价值的合成路线





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新化合物合成路线设计

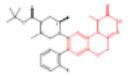
Sort by: CAS Registry Number

Display Options

0 of 424 Substances Selected

Page: 1 of 9

1. 1654735-60-0

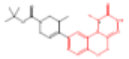


Absolute stereochemistry.

$C_{28}H_{34}FN_5O_4$
1-Piperazinecarboxylic acid, 4-[8-(2-fluorophenyl)-1,2,3,5-tetrahydro-1-methyl-2-oxo[1,2,4]triazino[3,4-*c*][1,4]benzoxazin-9-yl]-2,5-dimethyl-, 1,1-dimethylethyl ester, (2*S*,5*R*)-

Key Physical Properties

2. 1654735-59-7

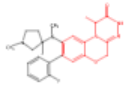


Absolute stereochemistry.

$C_{22}H_{28}N_4O_4$
1(2*H*)-Pyridinecarboxylic acid, 3,6-dihydro-3-methyl-4-[(1*R*)-1,2,3,5-tetrahydro-1-methyl-2-oxo[1,2,4]triazino[3,4-*c*][1,4]benzoxazin-9-yl]-, 1,1-dimethylethyl ester

Key Physical Properties

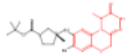
3. 1654735-57-5



$C_{24}H_{28}FN_5O_2$
[1,2,4]Triazino[3,4-*c*][1,4]benzoxazin-2(1*H*)-one, 9-[(1,3-dimethyl-3-pyrrolidinyl)methylamino]-8-(2-fluorophenyl)-3,5-dihydro-1-methyl-

Key Physical Properties

4. 1654735-48-4

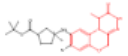


Absolute stereochemistry.

$C_{21}H_{28}BrN_5O_4$
1-Pyrrolidinecarboxylic acid, 3-[(8-bromo-1,2,3,5-tetrahydro-1-methyl-2-oxo[1,2,4]triazino[3,4-*c*][1,4]benzoxazin-9-yl)amino]-3-methyl-, 1,1-dimethylethyl ester, (3*R*)-

Key Physical Properties

5. 1654732-77-0

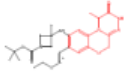


Absolute stereochemistry.

$C_{21}H_{28}BrN_5O_4$
1-Pyrrolidinecarboxylic acid, 3-[(8-bromo-1,2,3,5-tetrahydro-1-methyl-2-oxo[1,2,4]triazino[3,4-*c*][1,4]benzoxazin-9-yl)amino]-3-methyl-, 1,1-dimethylethyl ester, (3*S*)-

Key Physical Properties

6. 1654732-76-9

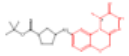


Double bond geometry as shown.

$C_{24}H_{33}N_5O_5$
1-Azetidinecarboxylic acid, 3-[[8-[(1*E*)-2-ethoxyethenyl]-1,2,3,5-tetrahydro-1-methyl-2-oxo[1,2,4]triazino[3,4-*c*][1,4]benzoxazin-9-yl]amino]-3-methyl-, 1,1-dimethylethyl ester

Key Physical Properties

7. 1654728-88-7

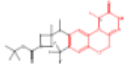


Absolute stereochemistry.

$C_{20}H_{27}N_5O_4$
1-Pyrrolidinecarboxylic acid, 3-[[(1*R*)-1,2,3,5-tetrahydro-1-methyl-2-oxo[1,2,4]triazino[3,4-*c*][1,4]benzoxazin-9-yl]amino]-, 1,1-dimethylethyl ester

Key Physical Properties

8. 1654728-63-8



Absolute stereochemistry.

$C_{23}H_{29}F_3N_4O_4$
1-Azetidinecarboxylic acid, 3-methyl-3-[1-[(1*R*)-1,2,3,5-tetrahydro-1-methyl-2-oxo-8-(trifluoromethyl)[1,2,4]triazino[3,4-*c*][1,4]benzoxazin-9-yl]ethyl]-, 1,1-dimethylethyl ester

Key Physical Properties

9. 1654725-00-4

10. 1632329-18-0

11. 1632329-17-9

12. 1632329-16-8

筛选结构相近的物质

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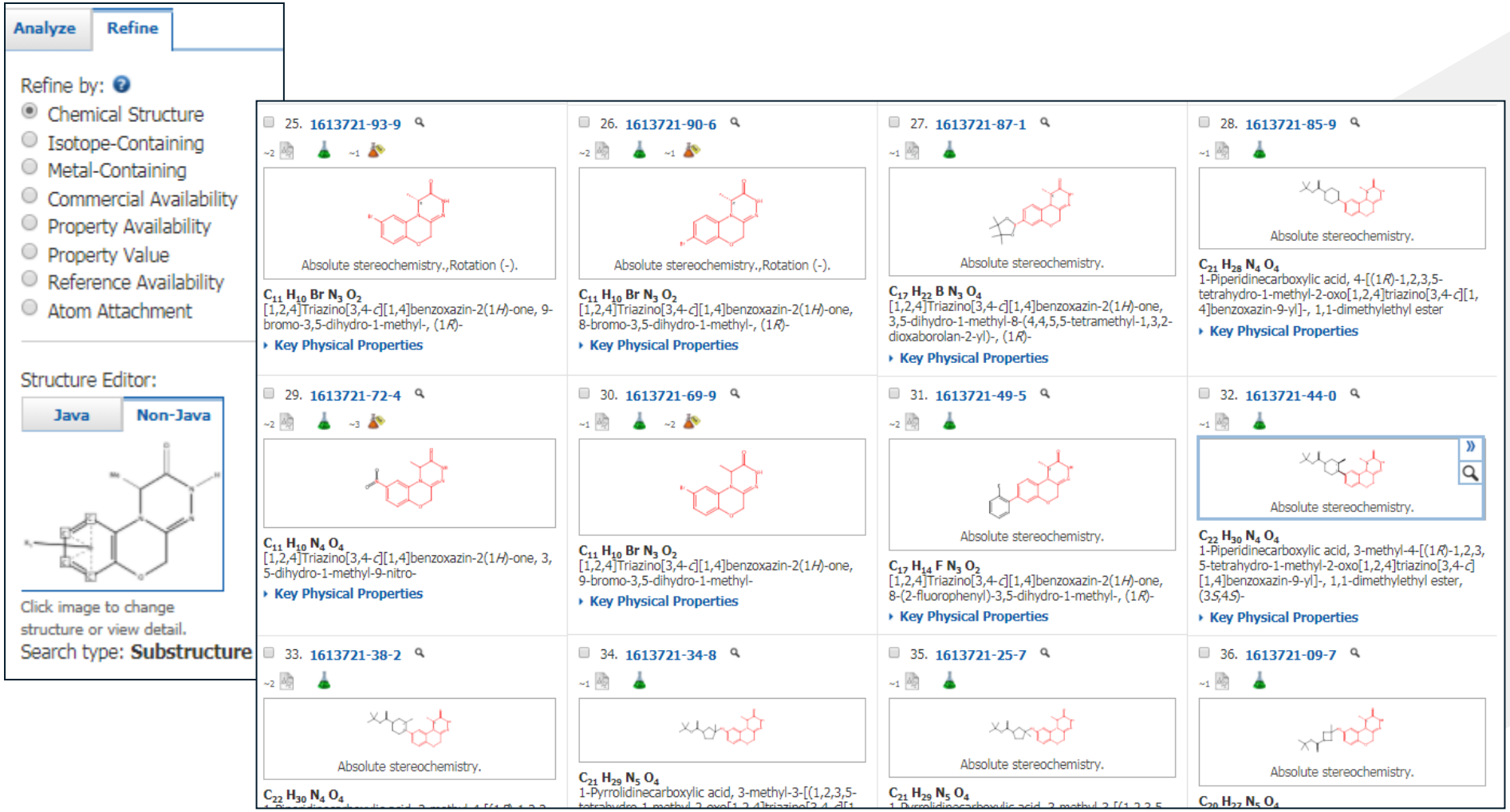
新化合物合成路线设计



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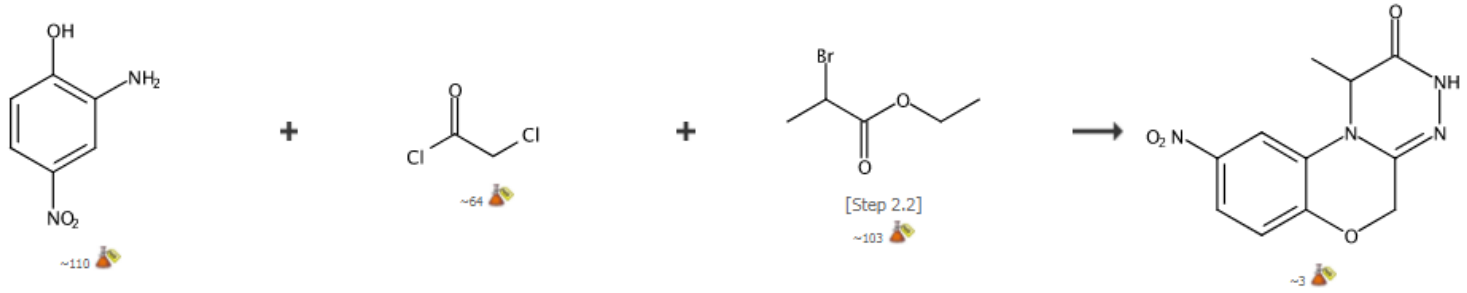
新化合物合成路线设计

Group by: No Grouping ▼ Sort by: Accession Number ▼ Display Options

0 of 8 Reactions Selected

1. View Reaction Detail Link

4 Steps *Hover over any structure for more options.*



Overview

Experimental Procedure

MethodsNow™

Procedure

1. Add 2-chloroacetyl chloride (83.6 mL, 1110 mmol) dropwise to a solution of 2-amino-4-nitrophenol (114.0 g, 740 mmol) , K_2CO_3 (306.2 g, 2220 mmol) and tetrabutyl ammonium bromide (23.8 g, 74 mmol) in acetonitrile (1.50 L) at 0 °C.
2. Heat the reaction mixture at 80 °C for 1 h.

View more...

Available Experimental Data

^{1}H NMR, R_f, State

View with MethodsNow

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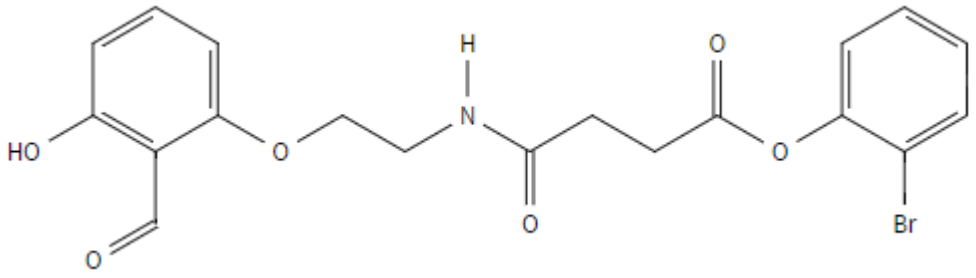
新化合物合成路线设计

检索思路3：先自行做逆合成反应分析，然后验证相关的反应。



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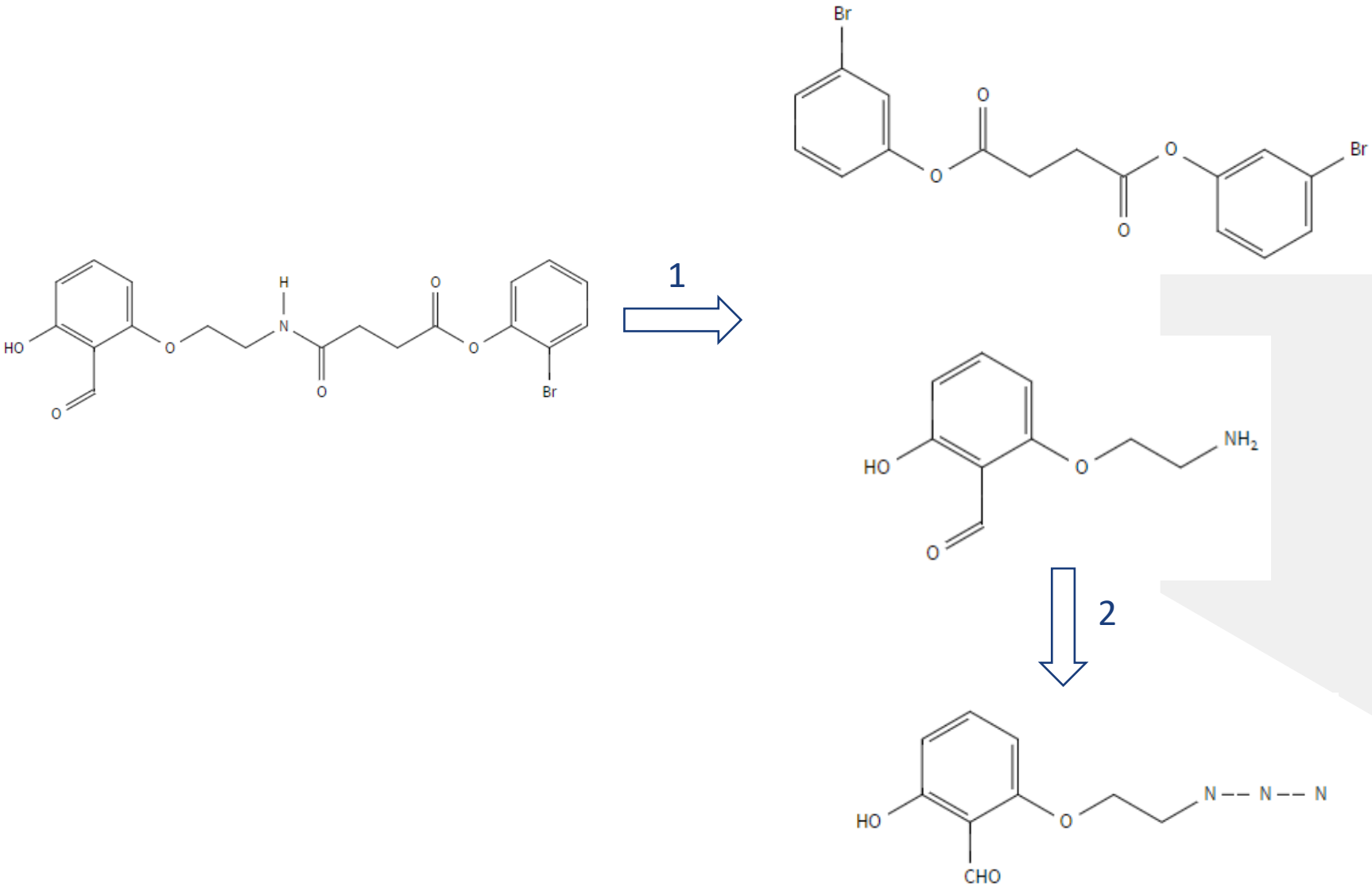
新化合物合成路线设计



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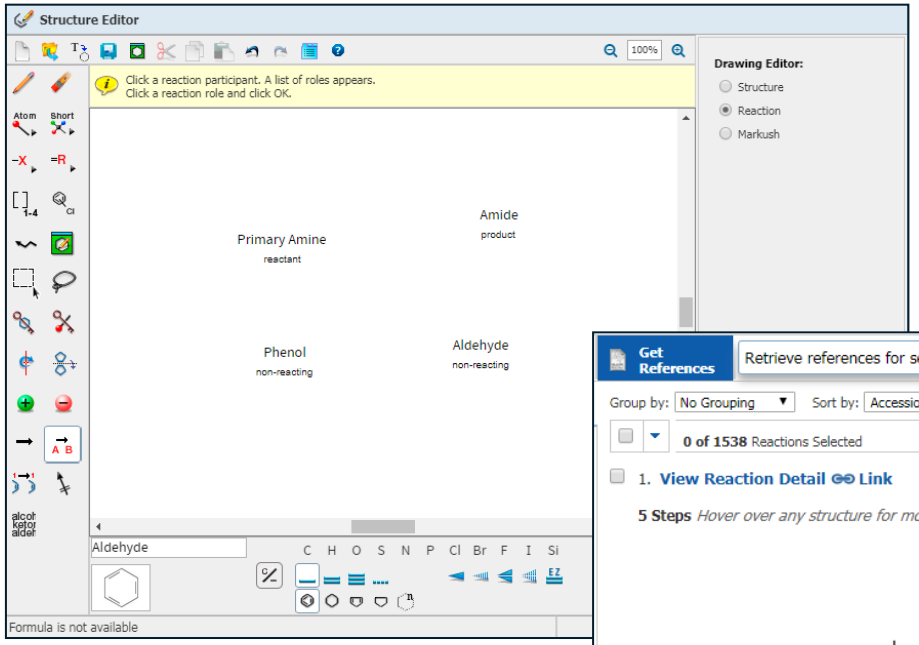
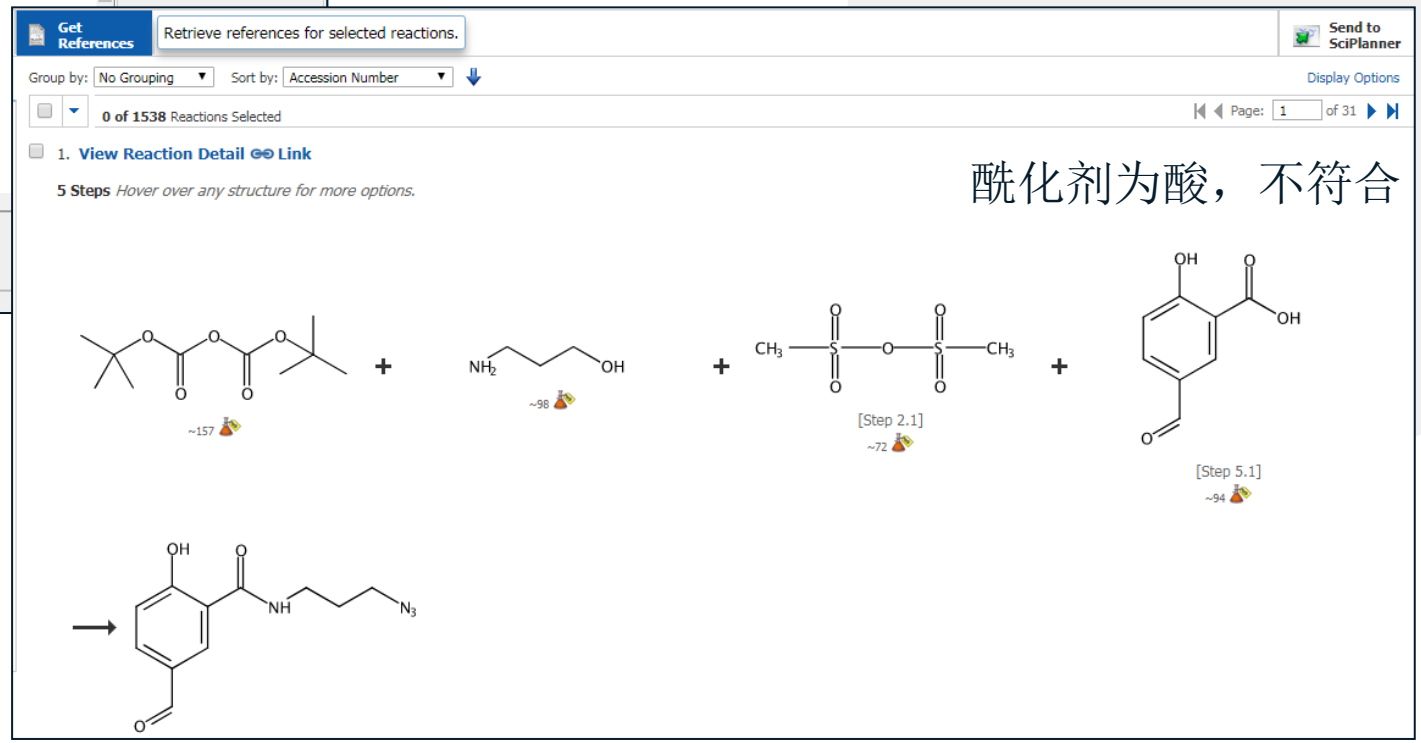
新化合物合成路线设计

反应1：





酰化剂为酸，不符合

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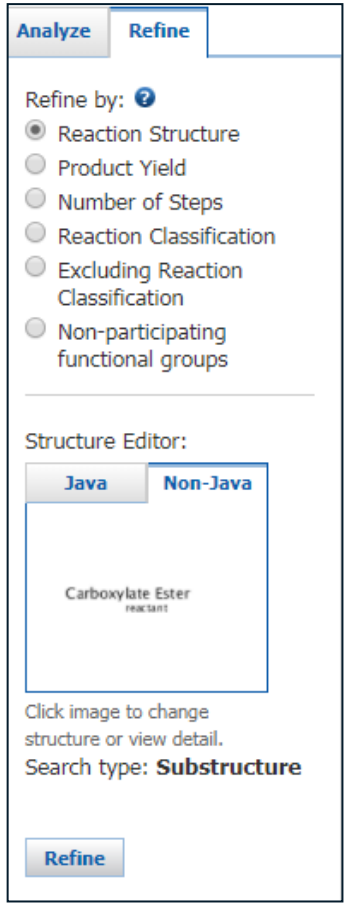
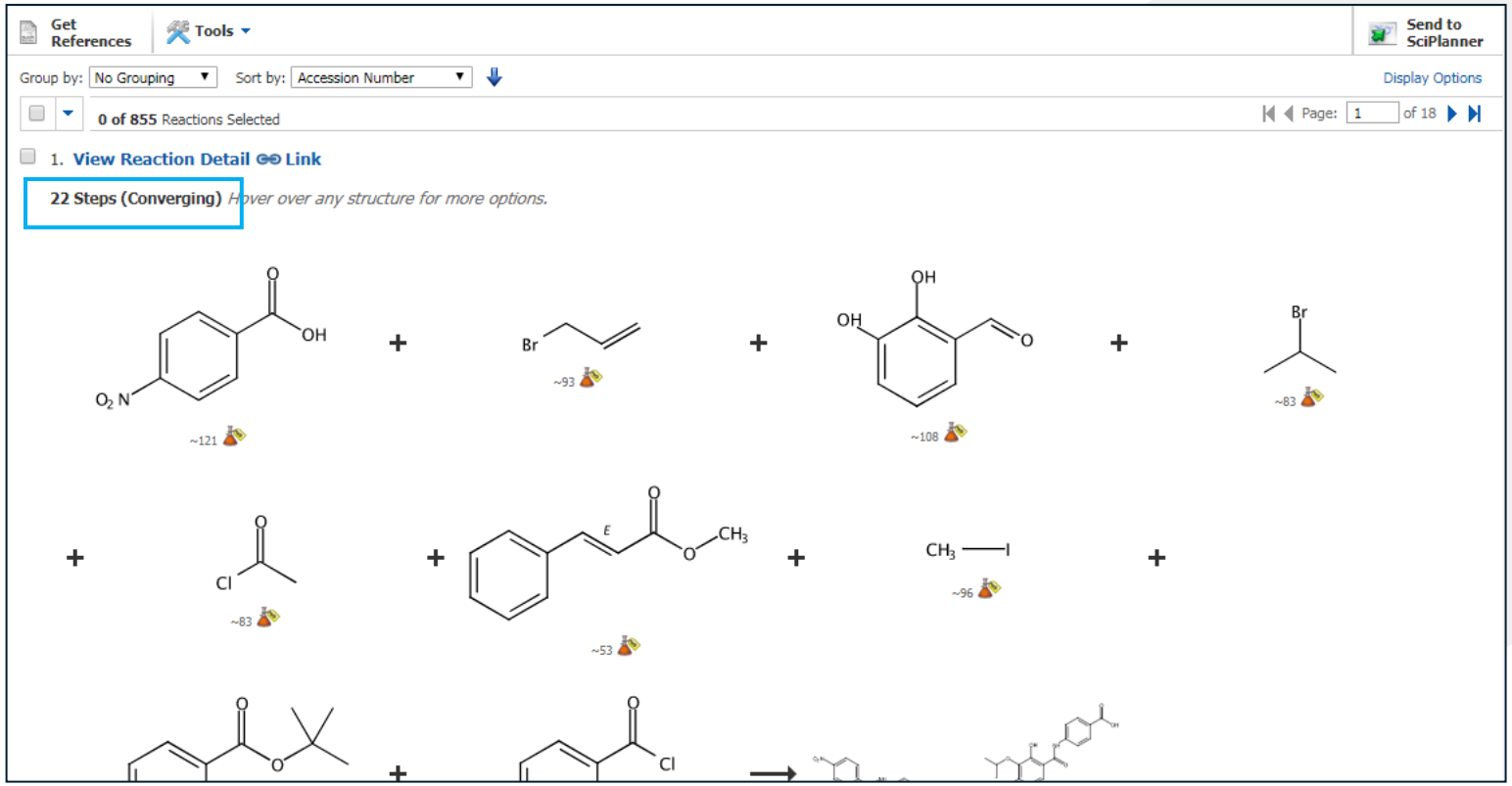
新化合物合成路线设计



不理想

问题：底物太多？步数太多！



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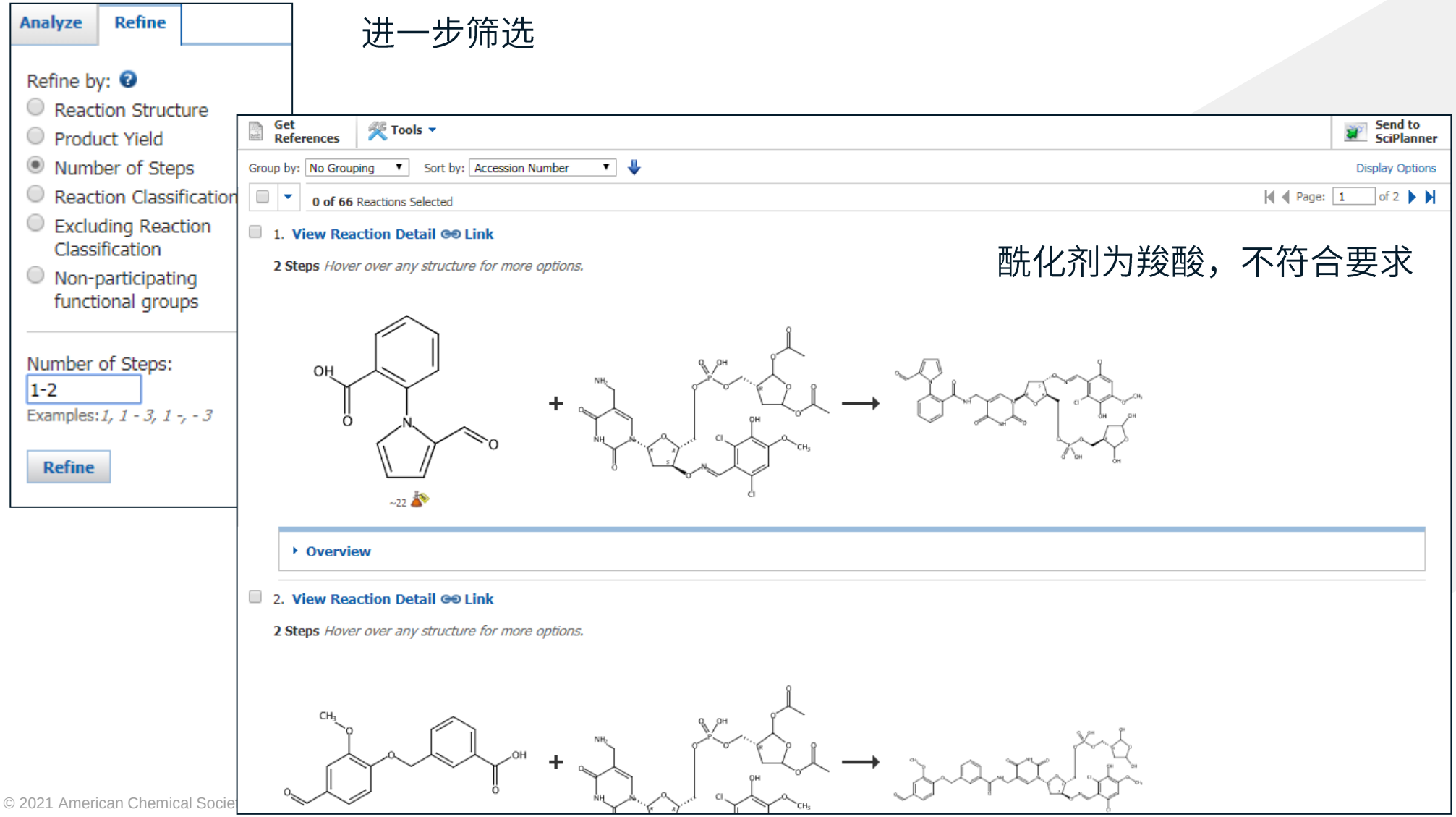
新化合物合成路线设计

进一步筛选

酰化剂为羧酸，不符合要求



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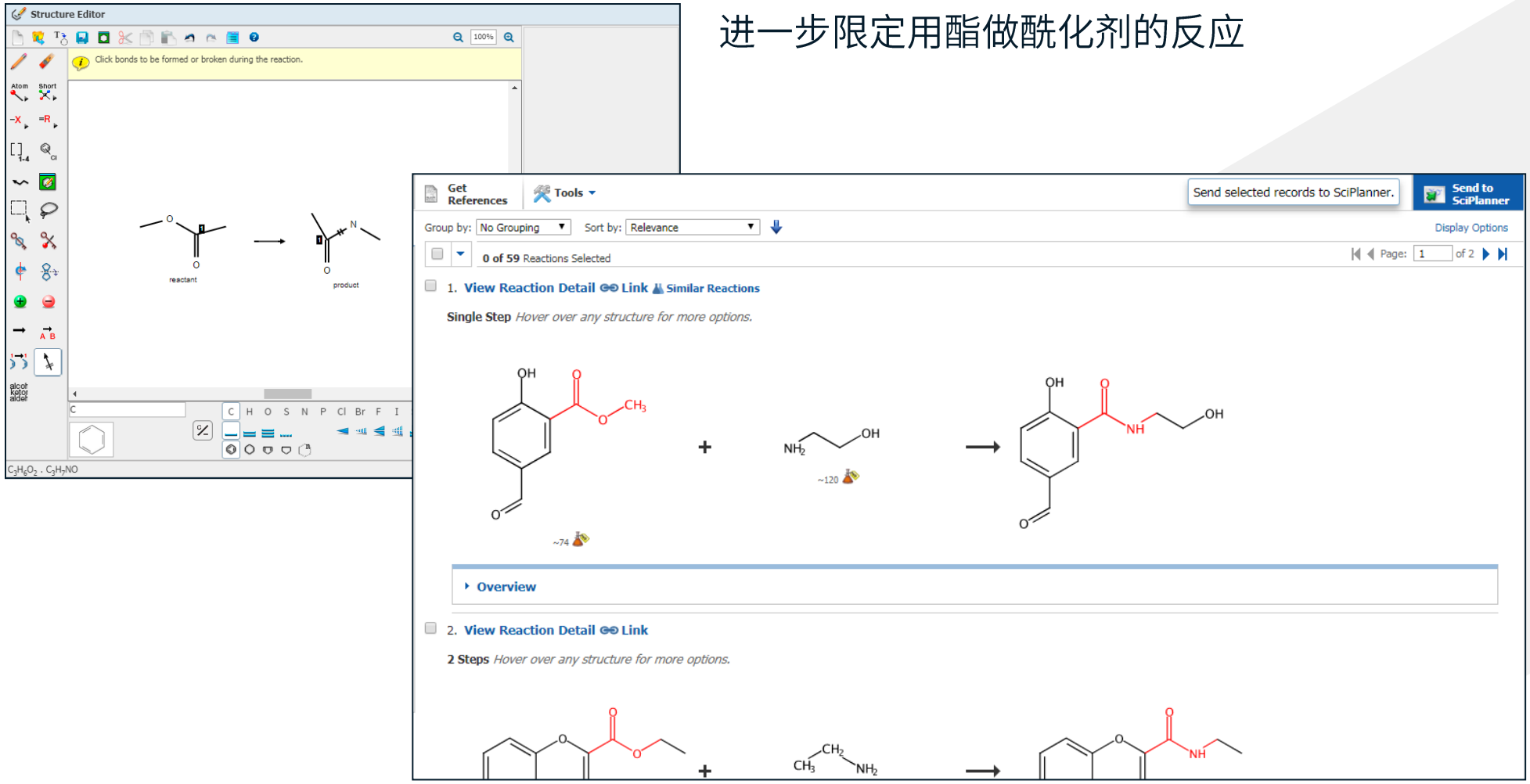
新化合物合成路线设计

进一步限定用酯做酰化剂的反应



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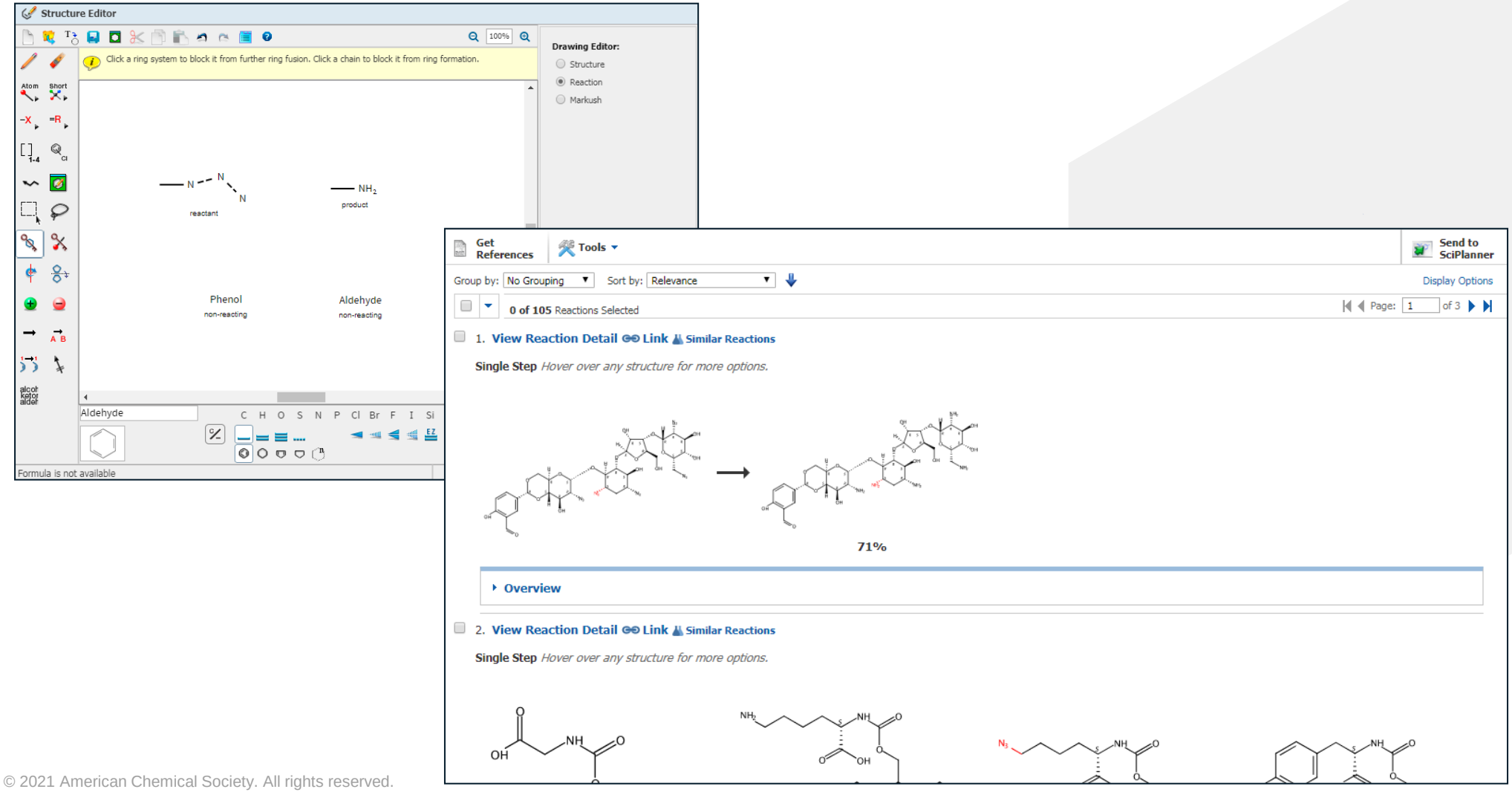
新化合物合成路线设计

反应2



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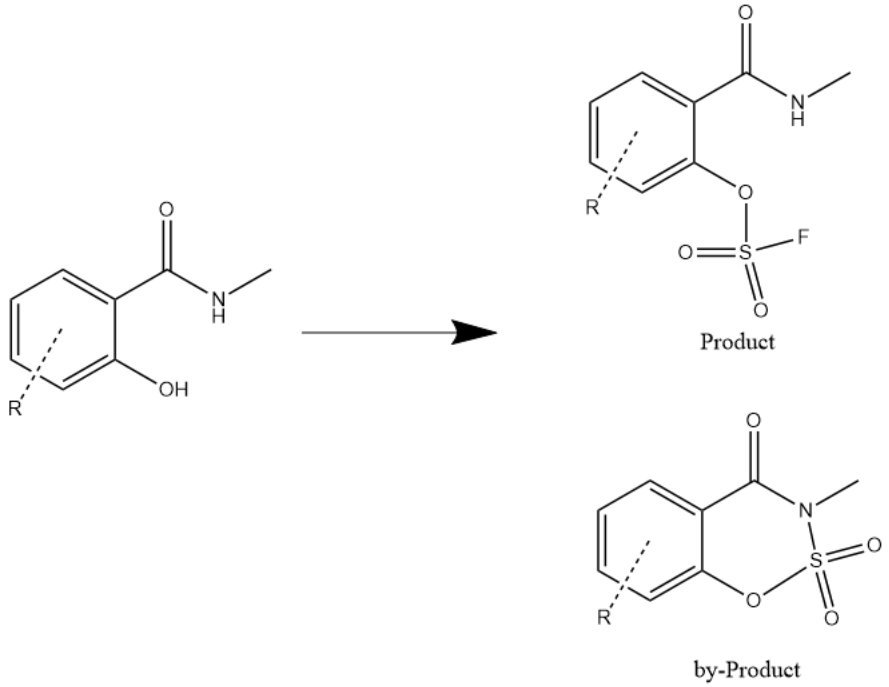
案例分析



如何提高主产物的收率?

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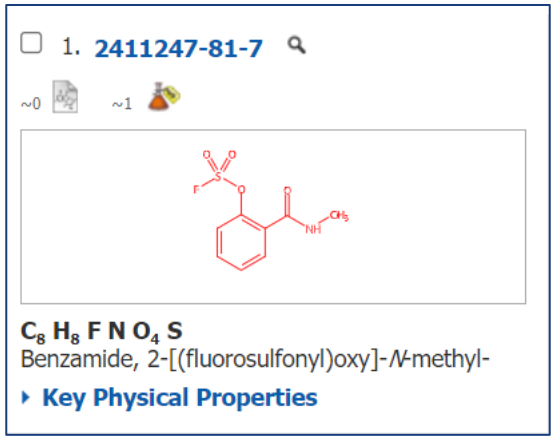
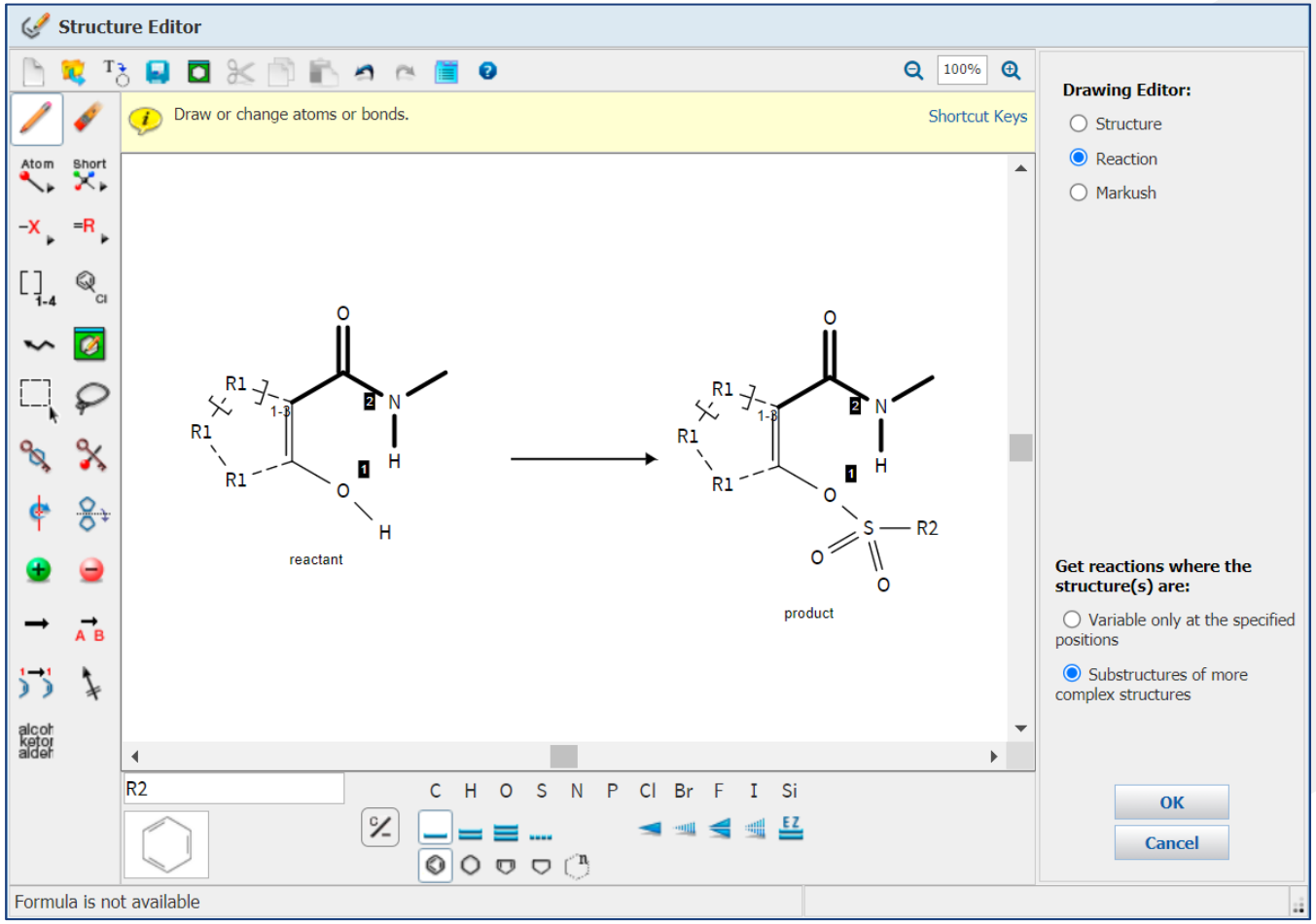
案例分析

1 .检索主产物



没有相关反应！

2. 扩大范围进行检索



R1=C、N、O；R2=X、OH

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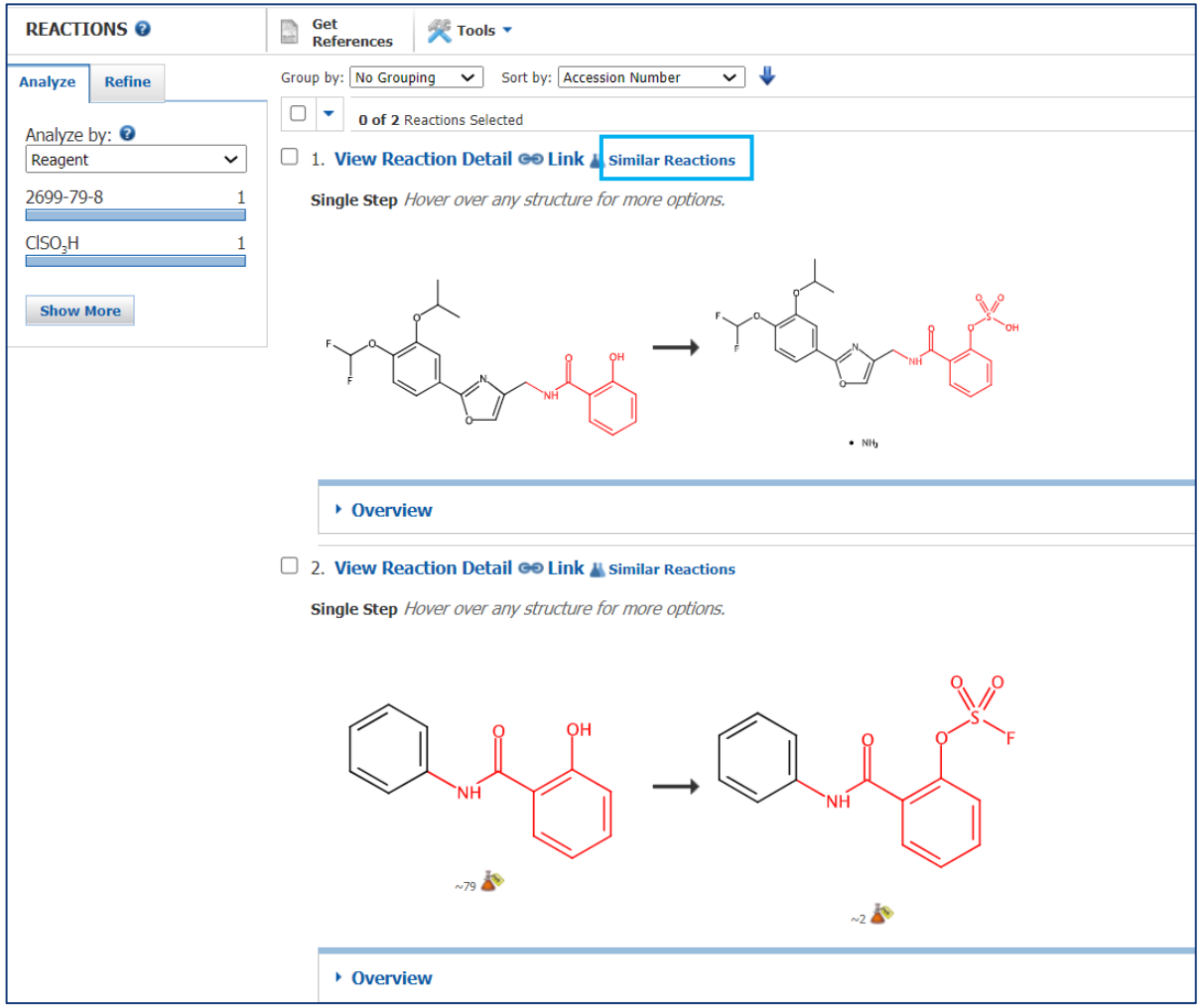
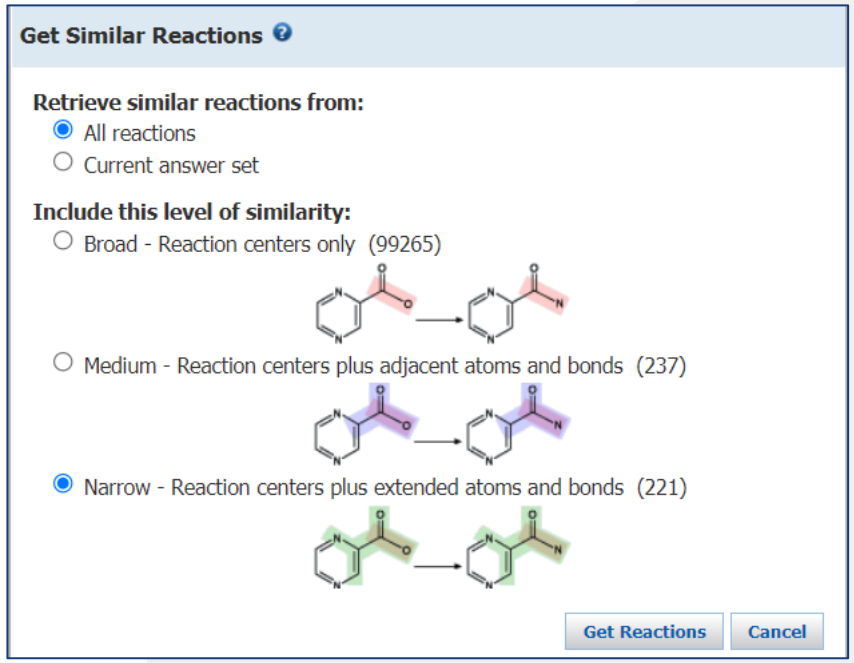
案例分析





Similar Reaction：获得更多相关反应信息

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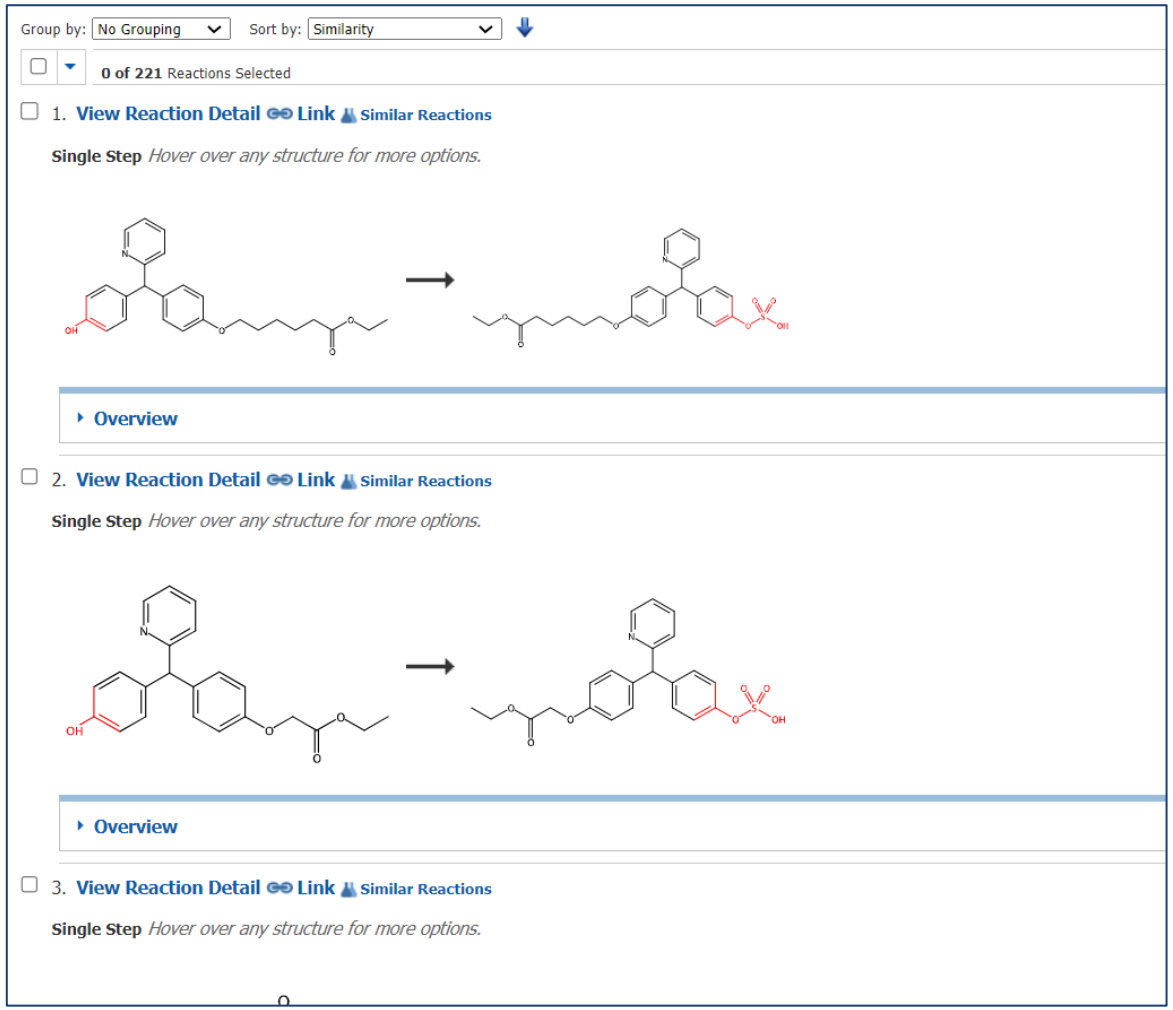
案例分析



如何获得相关度更大的反应信息?

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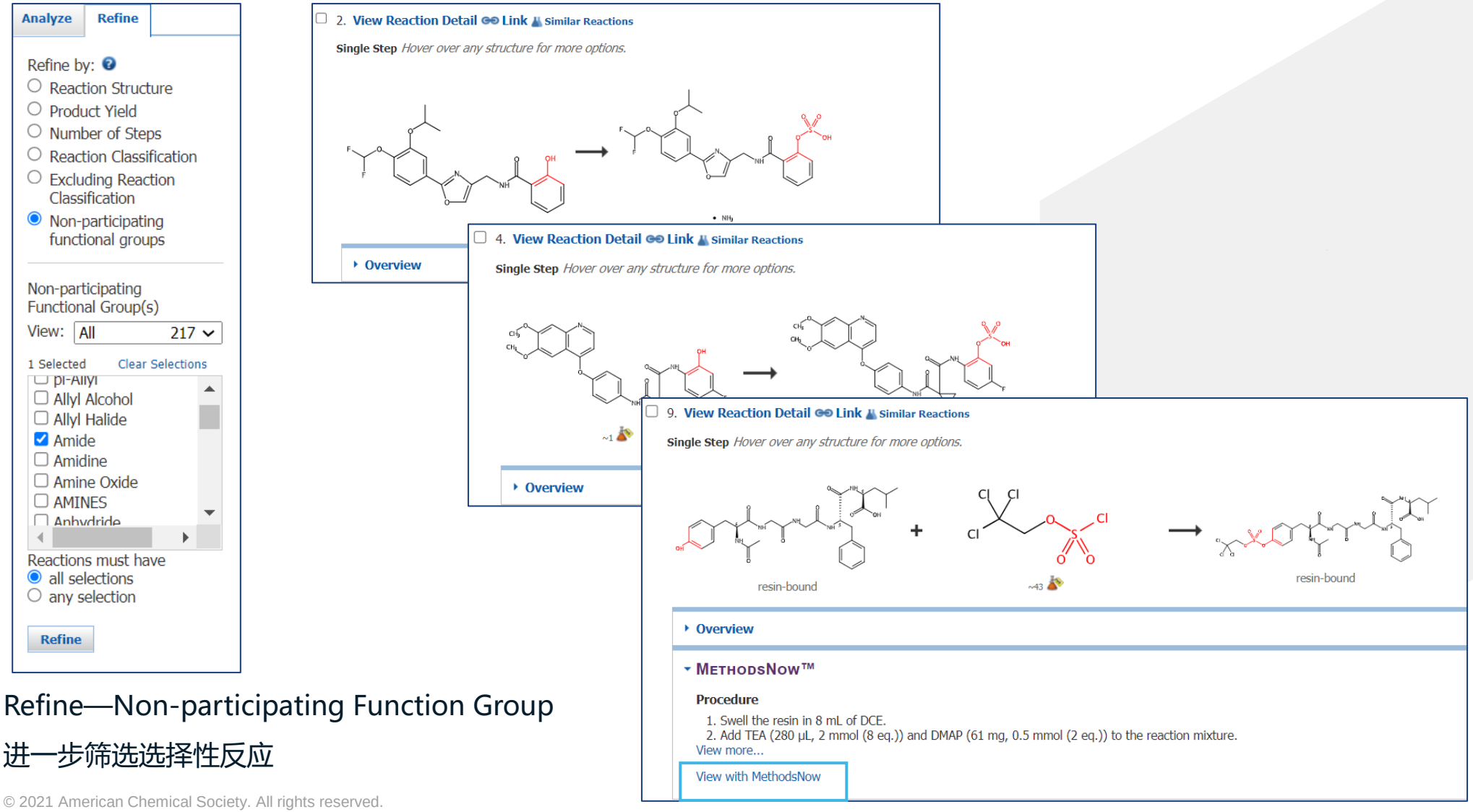
案例分析



Refine—Non-participating Function Group

进一步筛选选择性反应

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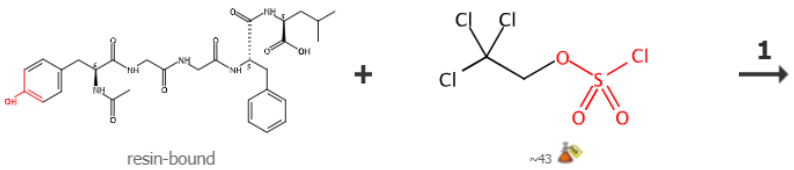
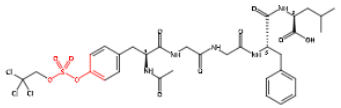
高效获取反应详情--MethodsNow

A general sequence independent solid phase method for the site specific synthesis of multiple sulfated-tyrosine containing peptides

By Bunschoten, Anton; Kruijtzer, John A. W.; Ippel, Johannes H.; de Haas, Carla J. C.; van Strijp, Jos A. G.; Kemmink, Johan; Liskamp, Rob M. J.
From Chemical Communications (Cambridge, United Kingdom), (21), 2999-3001; 2009
Published by Royal Society of Chemistry





Products	*N*-Acetyl-*O*-[(2,2,2-trichloroethoxy)sulfonyl]-L-tyrosylglycylglycyl-L-phenylalanyl-L-leucine, resin-bound, CAS RN: 1173091-38-7
Reactants	*N*-Acetyl-L-tyrosylglycylglycyl-L-phenylalanyl-L-leucine, resin-bound, CAS RN: 78922-82-4 Chlorosulfuric acid, 2,2,2-trichloroethyl ester, CAS RN: 764-09-0
Reagents	Triethylamine, CAS RN: 121-44-8 4-(Dimethylamino)pyridine, CAS RN: 1122-58-3
Solvents	1,2-Dichloroethane, CAS RN: 107-06-2
Procedure	1. Swell the resin in 8 mL of DCE. 2. Add TEA (280 µL, 2 mmol (8 eq.)) and DMAP (61 mg, 0.5 mmol (2 eq.)) to the reaction mixture. 3. Shake the mixture until complete dissolution. 4. Add 2,2,2-trichloroethyl chlorosulfate (265 µL, 2 mmol (8 eq.)) to the mixture. 5. Shake the reaction mixture overnight. 6. Wash the resin with DCE (3x), and ether (3x). 7. Dry the resin in vacuo over P_2O_5 to obtain the product.
Transformation	Preparation of Inorganic Esters from Alcohols
CAS Method Number	3-022-CAS-6472590

物质信息
名称
角色

实验过程

反应类型

MethodsNow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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反应检索小结

1. 反应检索方法汇总与区分
2. 反应绘制工具的灵活使用
3. 反应结果排序：Group by Transformation/Document
4. 反应结果的快速纵览及筛选，例如non-participating functional group；
5. 相似反应的获取获得更多启发
6. MethodsNow获取反应详情
7. SciPlanner工具助于自定义设计拟合成反应路线

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大纲

- CAS及CAS SciFinder介绍
- 文献相关信息的检索策略
  - 利用Index Term修正检索词
  - 巧用CAS Role
  - 善用Categorize
  - 如何高效阅读专利文献详情(CAS PatentPak)
- 物质相关信息的检索策略
  - 检索具有相同结构特征的物质
  - Markush检索
  - 如何筛选天然产物
  - 无机复合物、聚合物的检索
- 反应相关信息的检索策略
  - 如何检索化学选择性反应
  - 直接检索反应受限时如何处理
  - 新化合物的合成路线设计
  - 案例分析
  - 如何高效获取反应详情
- 获取分析方法的策略（CAS Analytical Methods）

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高效获取分析方法详情

CAS Analytical Methods

- CAS Analytical Methods介绍
- 关键词检索
- 检索结果的分析、精炼与详情
- 多个分析方法的对照

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CAS Analytical Methods分析方法类别

目前有13个大类，45个小类；某些子类属于多种方法分类：

Organic Compound Analysis: 天然产物分离分析，手性分离，活性药物成分及代谢产物分析…

Organometallics / Inorganics: 地质分析，无机物分析，金属有机化合物分析

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…

Water: 阴阳离子分析、环境分析、废水分析、微量元素分析…

Polymer: 聚合物分析…

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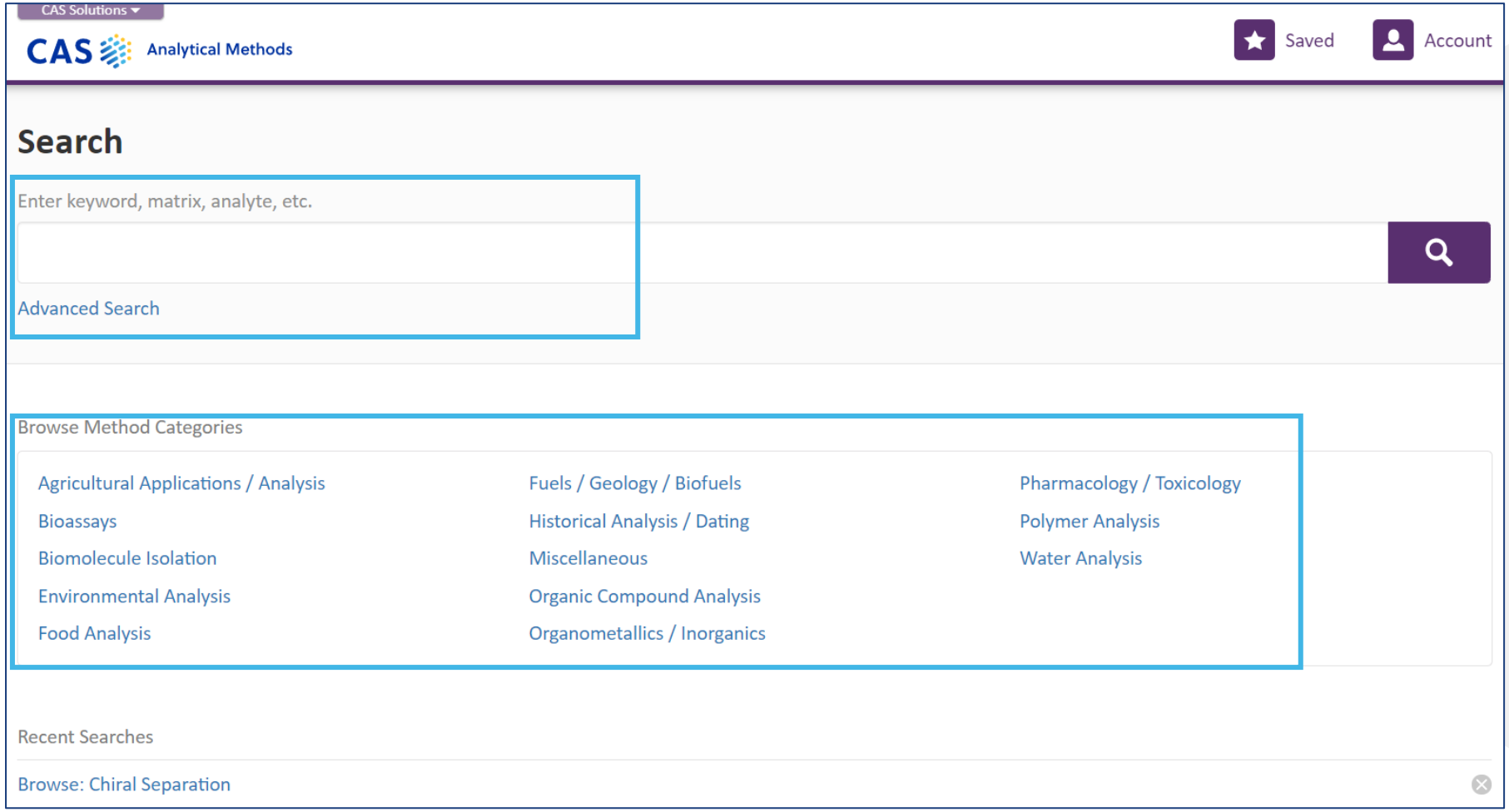
简洁易用的检索界面

CAS Analytical Methods登陆网址www.methodsnow.com



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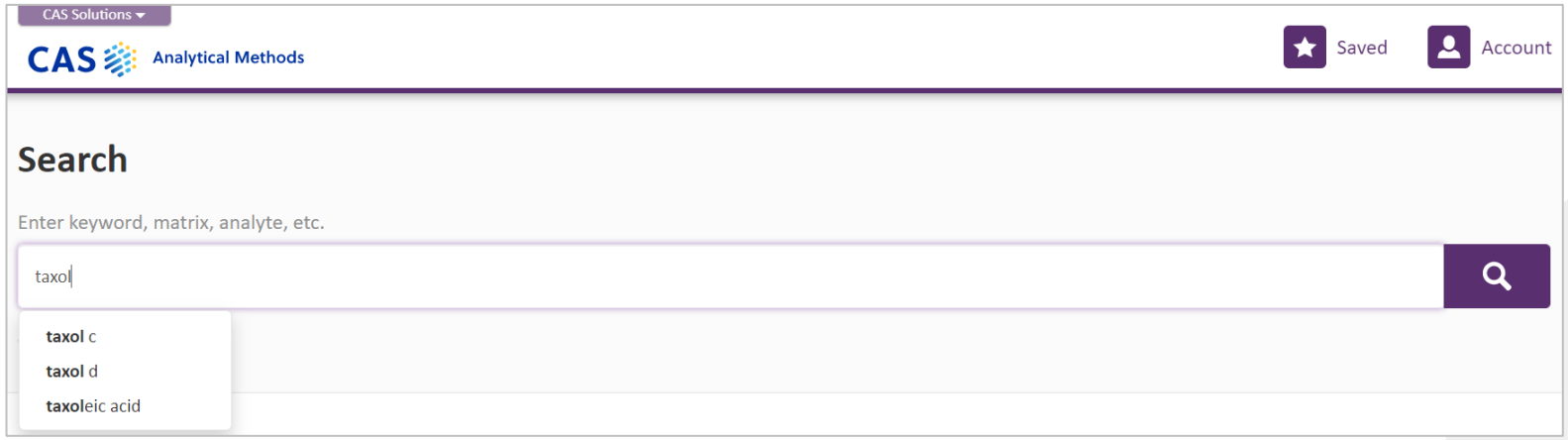
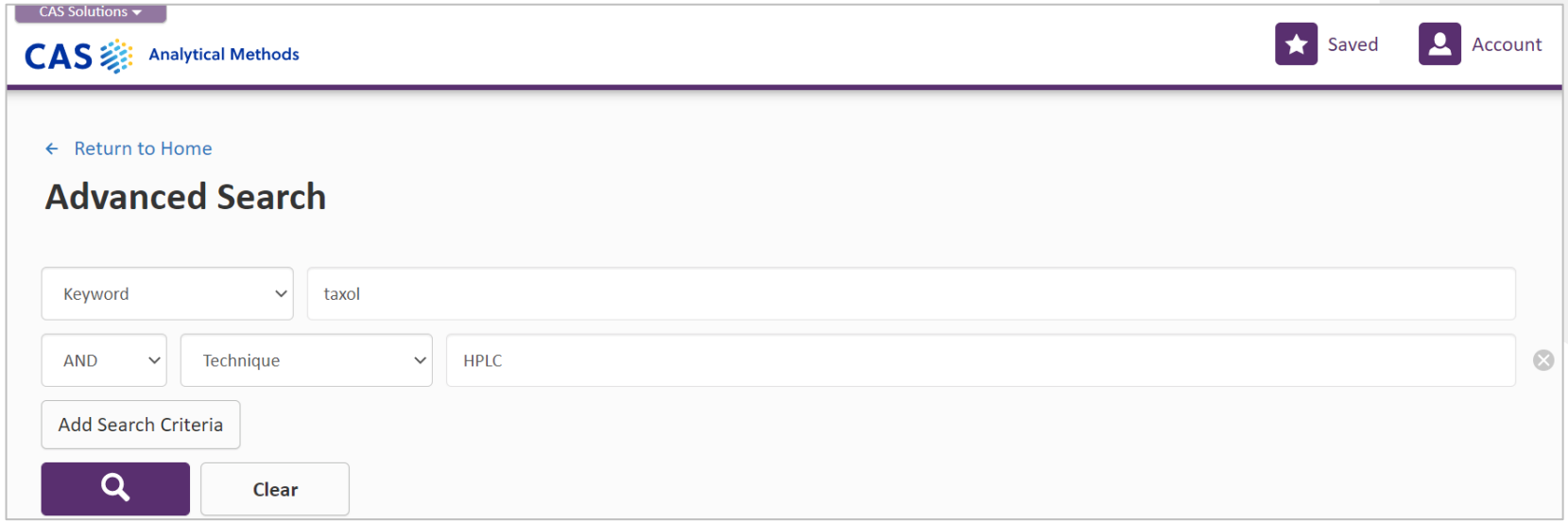
关键词检索分析方法





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检索结果分析与精炼

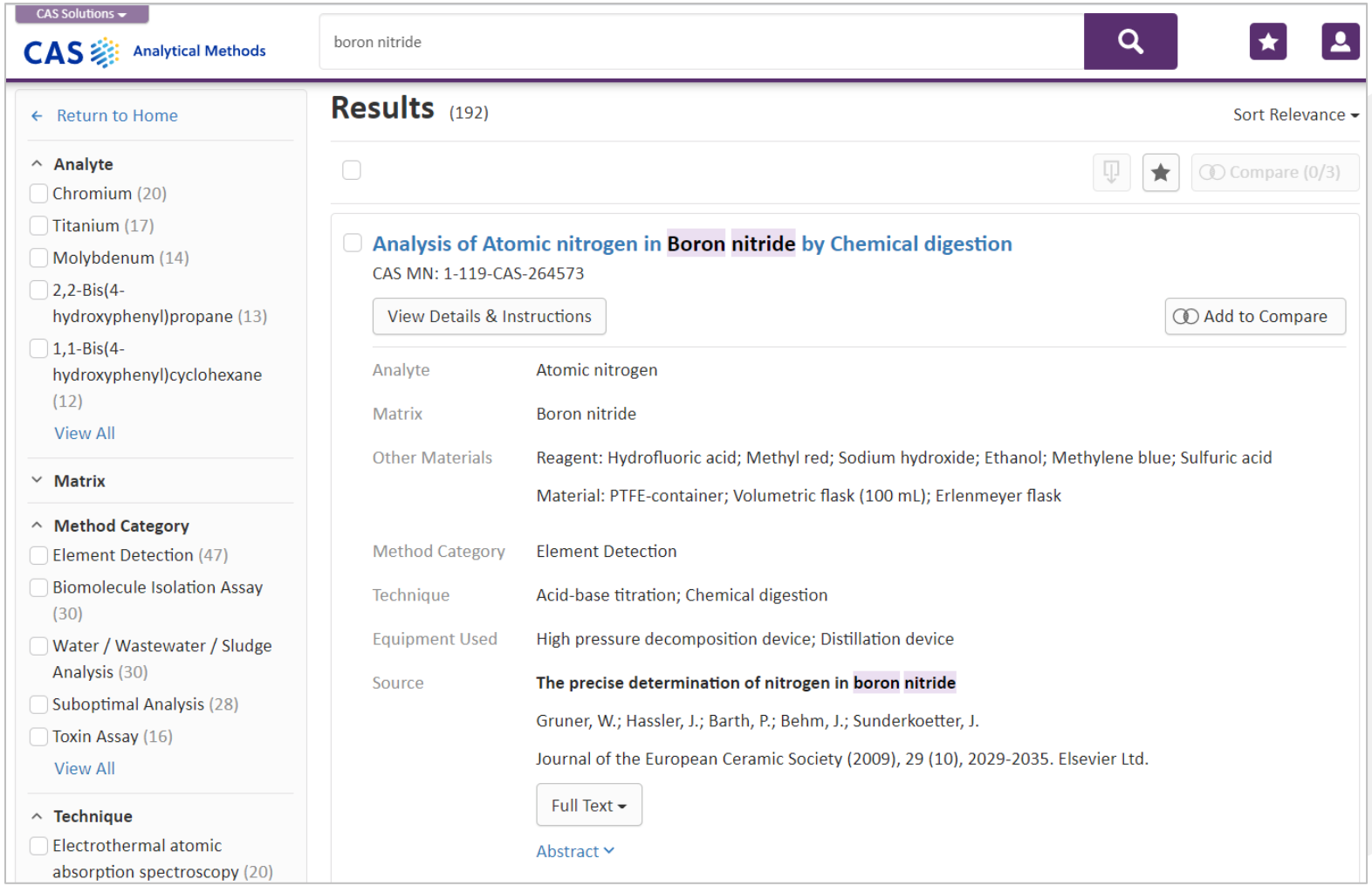
分析物

基质

方法分类

技术&仪器

年份



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分析方法详情

Method Detail (1 of 192)

← Prev Next →

Analysis of Atomic nitrogen in Boron nitride by Chemical digestion

CAS MN: 1-119-CAS-264573

Method Category: Element Detection
Technique: Acid-base titration; Chemical digestion

Materials	Role	Image	CAS RN
Atomic nitrogen	analyte	View Structure	17778-88-0
Boron nitride	matrix	View Structure	10043-11-5
PTFE-container	material		
Volumetric flask (100 mL)	material		
Erlenmeyer flask	material		
Hydrofluoric acid	reagent	View Structure	7664-39-3
Methyl red	reagent	View Structure	493-52-7
Sodium hydroxide	reagent	View Structure	1310-73-2
Ethanol	reagent	View Structure	64-17-5
Methylene blue	reagent	View Structure	61-73-4
Sulfuric acid	reagent	View Structure	7664-93-9

Source

The precise determination of nitrogen in boron nitride

Gruner, W.; Hassler, J.; Barth, P.; Behm, J.; Sunderkoetter, J.

Journal of the European Ceramic Society (2009), 29 (10), 2029 - 2035. Elsevier Ltd.

CODEN: JECSER | ISSN: 09552219 | DOI: 10.1016/j.jeurceramsoc.2008.12.021

Full Text

Abstract

To further improve the high performance ceramic material BN it is necessary to advance its analytics. The quant. determination of the nitrogen content as main component is compared by three methods: the carrier gas hot extraction, the LiOH fusion, and the Kjeldahl method. Thereby specific methodical aspects are critically highlighted with respect to the trueness and precision of the nitrogen anal. The "chem." plays a fundamental role in all methods. In the case of the instrumental anal. by CGHE important critical aspects are the calibration of CGHE measurements and the improvement of reproducibility which needs a much better understanding of the chem. reactions in the crucible. In case of the Kjeldahl method it is of decisive importance to apply an adequate high temperature of 260° for decomposition, whereas the melt-decomposition with LiOH is affected by melt additions

Equipment Used

High pressure decomposition device, Berghof Products and Instruments GmbH, Germany

Distillation device, Vapodest 3, erhardt Laboratory Systems, Germany

所用材料、标题摘要、著录信息、仪器

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分析方法详情

Instructions

Boron nitride sample

1. Collect boron nitride sample containing 0.1% soluble boric oxide, 0.7% oxygen for analysis.

Digestion

1. Weigh 0.2 g of the BN sample in a PTFE-container with 10 mL of HF-acid (40%).
2. Decompose the sample for 20 h at a temperature of 260 °C in a high pressure decomposition device (Berghof Products and Instruments GmbH, Germany).
3. Cool the solution and transfer into a volumetric flask (100 mL).

Acid-base titration using Kjeldahl method

1. Measure 20 - 30 mL of the solution in a sample cup and transfer into the Kjeldahl container built into the distillation device (Vapodest 3, erhardt Laboratory Systems, Germany).
2. Titrate 30 mL sulfuric acid (0.05 mol/L) into an Erlenmeyer flask and dilute with approximately 120 mL of water.
3. Add 2 - 3 mL of indicator solution (0.2% methyl red + 0.1% methylene blue in ethanol p.a.).
4. Apply the solution of sodium hydroxide (40%) to the sample and distill with steam into the Erlenmeyer flask.
5. Titrate excessive sulfuric acid with sodium hydroxide solution (0.1 mol/L).
6. Calculate the nitrogen content as wt.% using the following equation: N_{total}%: $(V_{H2SO4}f_{H2SO4} - V_{NaOH}f_{NaOH})F/m_S$: V_{acid}: consumption of 0.1 M H2SO4 [mL]; F: 70945 (titrimetric factor with 0.2 g solid sample); f_{H2SO4}: titration correction factor of H_2SO_4 solution; f_{NaOH}: titration correction factor of NaOH solution; ms: sample mass of taken liquid [mg].

Validation

Precision	0.20% (RSD)
Concentration	55.76 ± 0.11% wt

操作步骤和数据有效性验证

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浏览方法分类

Browse Method Categories

- Agricultural Applications / Analysis
- Bioassays
- Biomolecule Isolation
- Environmental Analysis
- Food Analysis
- Fuels / Geology / Biofuels
- Historical Analysis / Dating
- Miscellaneous
- Organic Compound Analysis
- Organometallics / Inorganics
- Pharmacology / Toxicology
- Polymer Analysis
- Water Analysis

Browse Method Categories > Organic Compound Analysis

- Active Pharmaceutical Ingredient and Metabolite Analysis
- Chiral Separation
- Natural Product Isolation Analysis
- Organic Compound Analysis

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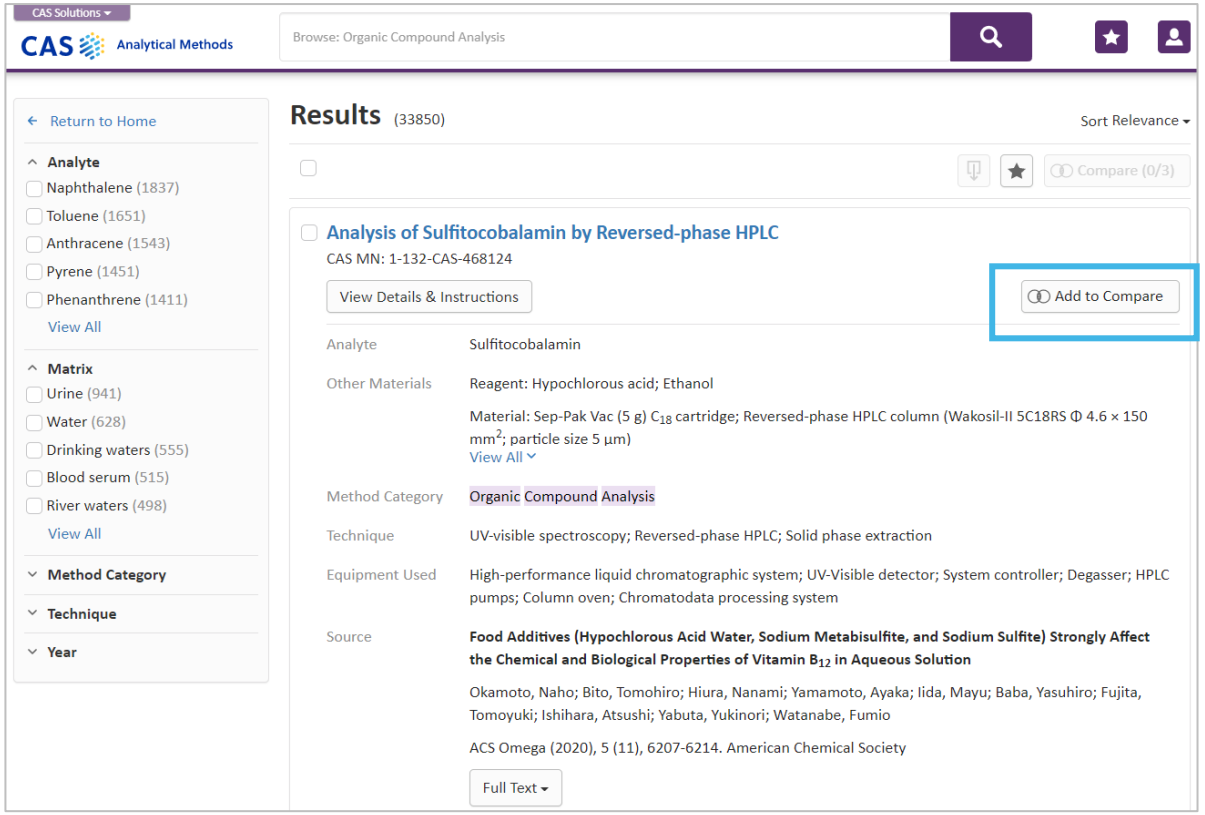
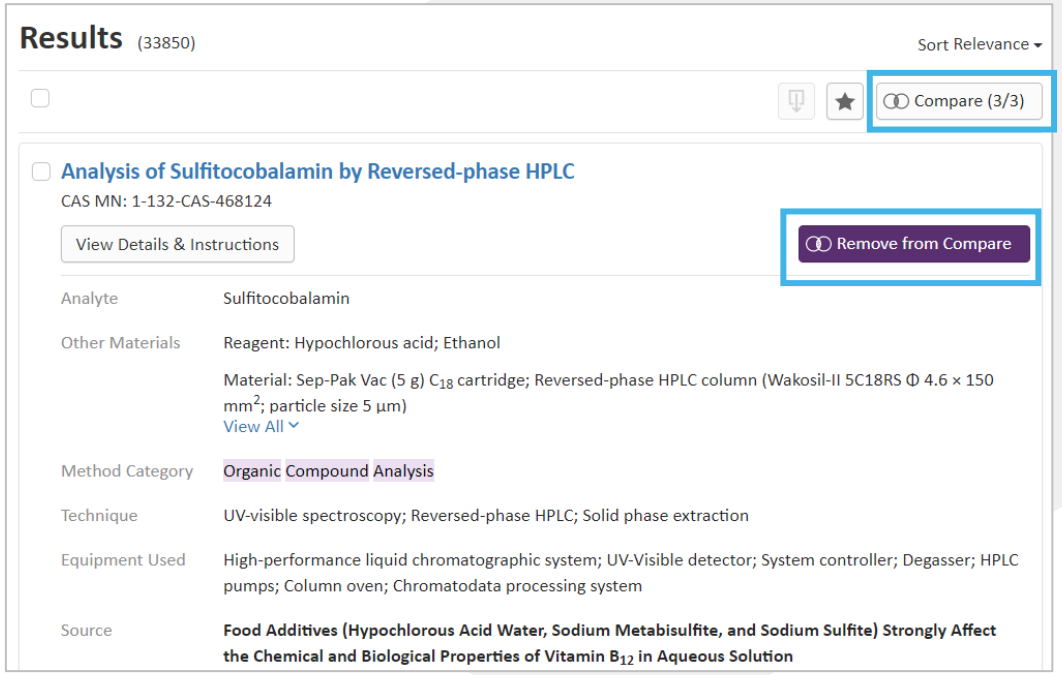
对照多个感兴趣的分析方法详情





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对照多个感兴趣的分析方法详情

Compare Methods

Expand All | Collapse All

	1	2	3
Title	**Analysis of Sulfitocobalamin by Reversed-phase HPLC**	**Analysis of Phenol by Spectrophotometry**	**Analysis of 2-Chlorophenol in Irrigation waters by Solid phase extraction**
CAS Method Number	1-132-CAS-468124	1-132-CAS-467381	1-132-CAS-466437
Method Category	Organic Compound Analysis	Organic Compound Analysis	Organic Compoun
Technique	UV-visible spectroscopy; Reversed-phase HPLC; Solid phase extraction	Spectrophotometry	Liquid chromatog detectors; Reverse phase extraction
Analyte	Sulfitocobalamin	Phenol	2-Chlorophenol; 2 Chlorophenol; 2,3 Chlorophenols
Matrix			Irrigation waters
Other Materials	Hypochlorous acid; Ethanol; Sep-Pak Vac (5 g) C_{18} cartridge; Reversed-phase HPLC column (Wakosil-II 5C18RS Φ 4.6 × 150 View All	3-Methyl-2-benzothiazolinone hydrazone; Phosphate; Glutaraldehyde; Reed	Hydrochloric acid; Triphenylbenzene chloride ($FeCl_3$); M View All
Equipment Used	High-performance liquid chromatographic system, Shimadzu; UV-Visible detector, SPD-10AV, Shimadzu; System controller, SCL-10A View All	UV-Vis spectrophotometer, Lambda 2, PerkinElmer, Waltham, MA	HPLC-DAD instrument, LC-20AT, Shimadzu, Japan
Source	**Food Additives (Hypochlorous Acid Water, Sodium Metabisulfite, and Sodium Sulfite) Strongly Affect the Chemical and Biological** View All	**Reed Membrane as a Novel Immobilization Matrix for the Development of an Optical Phenol Biosensor** View All	**Layered porous organic frameworks as a novel adsorbent for the solid phase extraction of chlorophenols prior to their** View All
Preparation		**Fabrication of the reed biosensor** 1. Peel a reed membrane carefully from reed View All	**Preparation of amorphous porous organic frameworks (A-POF)** 1. Dissolve $FeCl_3$ (4.87 g), 1,3,5- View All
Method	**Treatment cyanocobalamin ($CN-B_{12}$)** 1. Treat cyanocobalamin ($CN-B_{12}$) with hypochlorous acid water (an effective View All	**Analysis of phenol by spectrophotometry** 1. Perform the analysis on a UV-Vis spectrophotometer Lambda 2 View All	**Solid phase extraction** 1. Prepare the SPE cartridge by packing an empty 3 mL SPE cartridge with 30 View All
Retention Time	27.171 min		
Linearity Range		5 - 100 μM	
Limit of Detection		2.5 μM	
Recovery			30% in 80.0 ng/mL added concentration (read from figure), 2-chlorophenol, 39% in 80.0 ng/mL added concentration (read from View All

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CAS Analytical Methods使用方法小结：

1. CAS Analytical Methods目前有13个大类，45个小类；某些子类属于多种方法分类；
2. 可通过关键词检索，或者浏览方法分类来获取分析方法结果；
3. 检索结果可通过分析物、基质、方法分类、技术&仪器，以及年份来纵览或精炼；
4. 所有的分析方法都可获取详情，包括所用材料、标题摘要、著录信息、仪器、实验条件、操作步骤和数据有效性验证等信息；
5. 支持三种不同的分析方法之间的对照，以表格的形式清晰对比呈现所有的实验详情。

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浏览器选择建议

- Windows 7以上用户建议升级IE到10以上，不支持IE7、IE8
- 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

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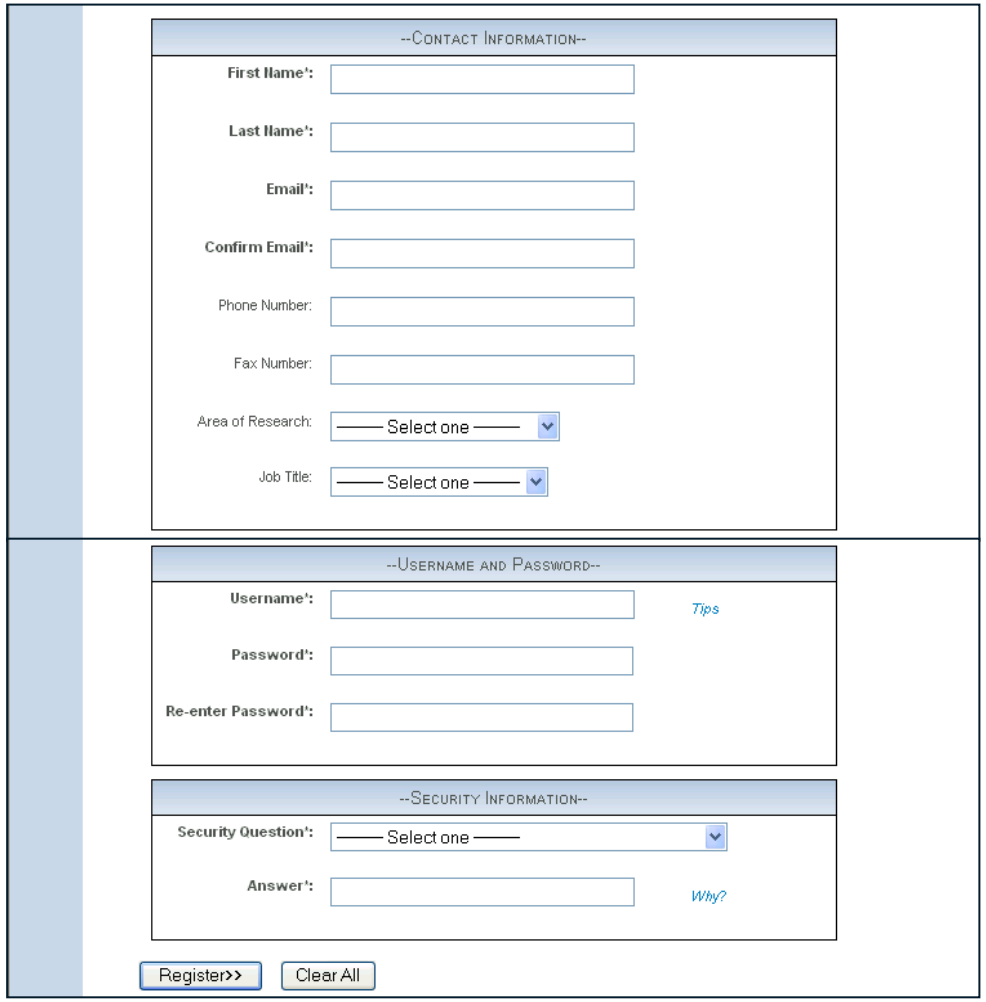
如何获取CAS SciFinder账号



请注意：
1.必须输入真实姓名和邮箱。
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）。

登录学校图书馆网站找到CAS SciFinder数据库说明页，按照提示进行注册

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使用注意事项

- 一人注册一个帐号
- 实名注册，请提供真实姓名信息（中文名用汉语拼音全拼）
- 不得过量下载（以电子形式存储不超过5,000条记录）
- 不得账号分享
- 不得将账号用于非学术研究

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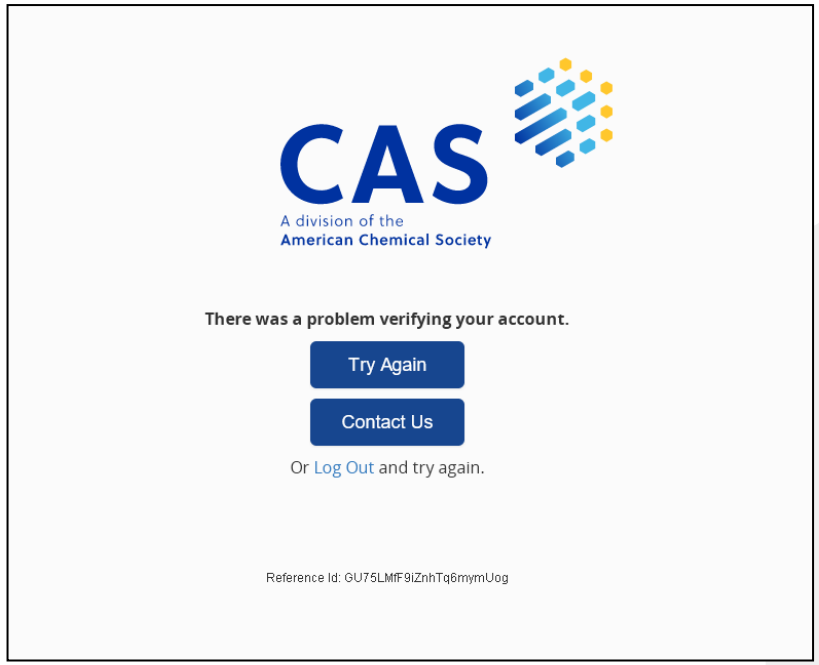
常见问题



- 确认账号密码是否正确
- 如果账号密码正确，请填写问题报告后联系图书馆或china@acs-i.org

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