# CAS SciFinder Discovery Platform

# 全面高效获取科技信息

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# CAS SCIFINDER DISCOVERY PLATFORM™

## 2024专题论坛直播时间表

结合CAS信息科学家精心撰写的相关洞察报告，了解不同领域的研究进展、趋势与创新、挑战与机会，同时进行安全的专利布局和侵权风险管理，助力自信应对立项布局、研发流程和专利调研相关的信息挑战。

**9月26日｜药物立项调研策略**

**11月14日｜电池及电化学能源材料**

**10月24日｜聚合物的研发与应用**

**12月19日｜专利查新与规避专利侵权风险**

**CAS SciFinder Discovery Platform**

**9 月至12 月的四场专题论坛**

**直播时间为周四15:00 - 16:00。扫描二维码注册，观看直播有机会获得CAS定制纪念品，欢迎**在直播中提问互动。

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# 大纲

- CAS及CAS SciFinder Discovery Platform 简介
- 科研信息的高效查阅
  - 全面的文献调研与拓展助力开题
  - 多角度出发检索物质结构及相关属性
  - 生物序列检索方法与结果分析
  - 探索实验方案以获取制备及其他实验详情
- 常见问题Q&A




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# CAS 具有最全面的学科连接内容合集


Over
**50K**
scientific journals and documents
超过5万种科技期刊

Over
**279**
million substances
2.79亿种数据

Over
**50**
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50多种语言

Over
**109**
patent offices worldwide
109个专利授权机构




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# CAS独特的内容合集


来源：
https://www.cas.org/cas-data
https://www.cas.org/about/cas-content




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# CAS 内容合集来源于化学、超越化学

## 5大类80小类

- **生物化学：**
  - 药理学、农化产品管控信息、生化遗传学、发酵、免疫化学
- **有机化学各领域：**
  - 有机金属化合物、脂肪/环族化合物、杂环化合物、生物分子、碳水化合物
- **大分子化学各领域：**
  - 合成高聚物化学；塑料的制造、加工、成型与应用；涂料、墨水
  - 染料、有机颜料；合成橡胶；纺织品、纤维
- **应用化学各领域：**
  - 大气污染、陶瓷、精油、化妆品、化石燃料、黑色金属、合金
- **物理、无机、分析化学各领域：**
  - 电化学、表面化学、催化剂、相平衡、核现象

来源：https://www.cas.org/support/documentation/references/ca-sections




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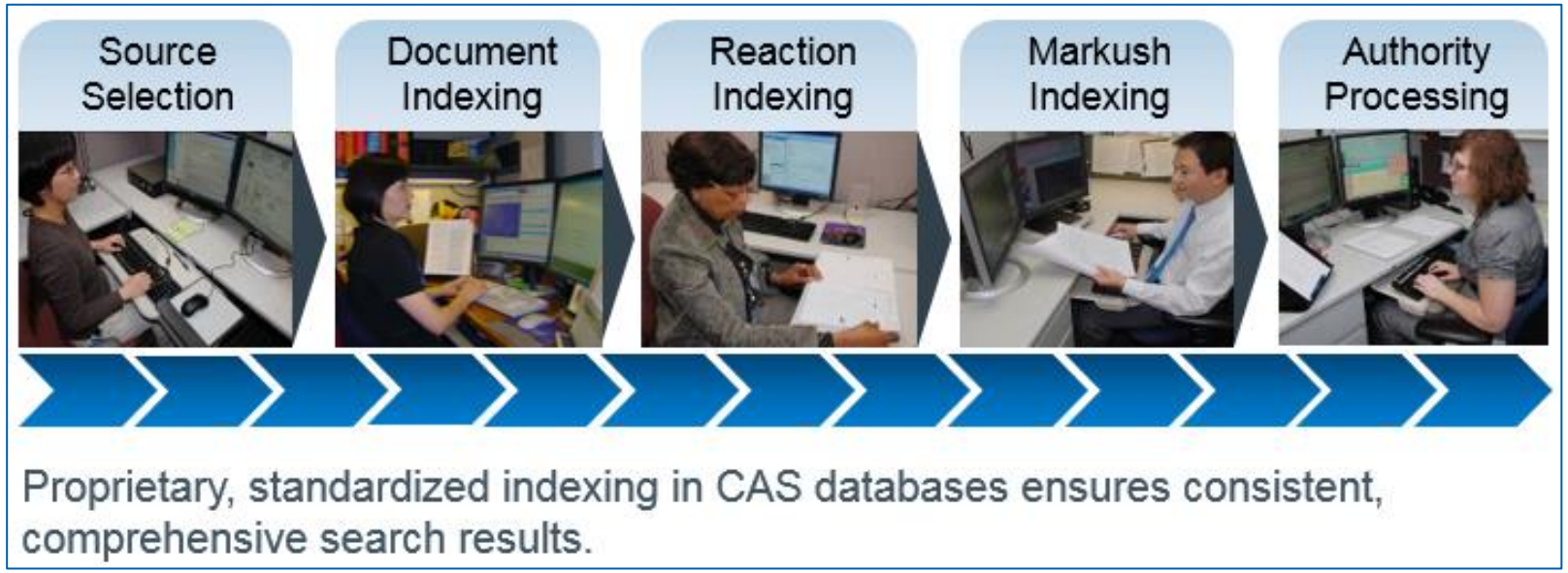
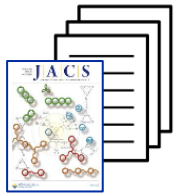
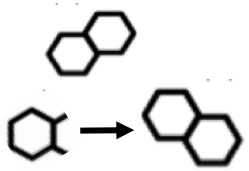
# CAS科学家的智力标引

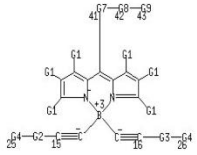



Data pre-repository




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科学家增值的文献研究

例: 专利WO2018152134

**改写的标准和摘要，尽可能揭示专利核心价值**

**丰富的增值标引信息：**

***19** Concepts*

***163** Substances*

***625** Reactions*

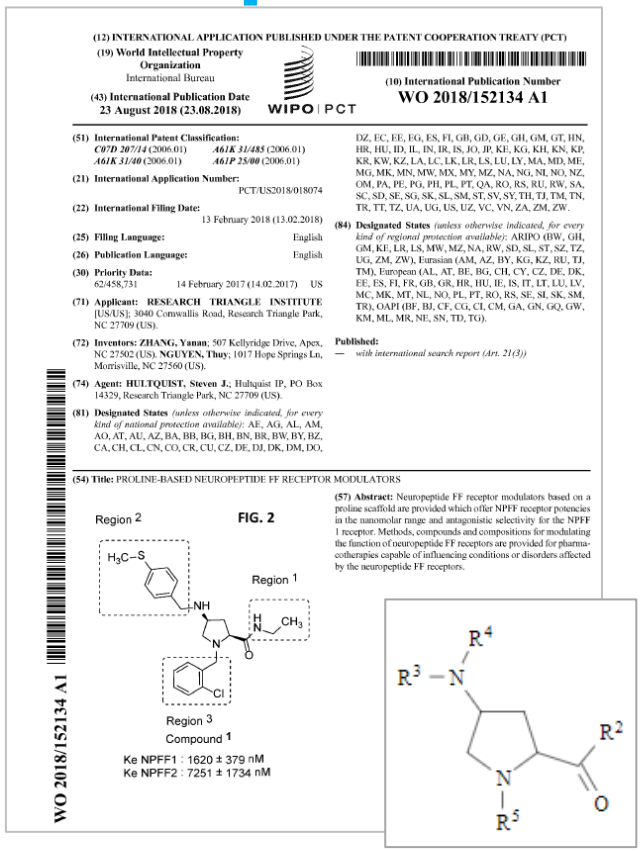
***13** Patent Family Members*

***3** Formulations*

***1** Markush structure*

***18** SAR data points*

***141** ADME data points*



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

(19) World Intellectual Property Organization
International Bureau

(43) International Publication Date
23 August 2018 (23.08.2018)

WIPO | PCT

(10) International Publication Number
WO 2018/152134 A1

(51) International Patent Classification:
*C07D 207/14* (2006.01) *A61K 31/485* (2006.01)
*A61K 31/40* (2006.01) *A61P 25/00* (2006.01)

(21) International Application Number:
PCT/US2018/018074

(22) International Filing Date:
13 February 2018 (13.02.2018)

(25) Filing Language: English

(26) Publication Language: English

(30) Priority Data:
62/458,731 14 February 2017 (14.02.2017) US

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(74) Agent: **HULTQUIST, Steven J.**; Hultquist IP, PO Box 14329, Research Triangle Park, NC 27709 (US).

(81) Designated States *(unless otherwise indicated, for every kind of national protection available)*: AE, AG, AL, AM, AO, AT, AU, AZ, BA, BB, BG, BH, BN, BR, BW, BY, BZ, CA, CH, CL, CN, CO, CR, CU, CZ, DE, DJ, DK, DM, DO, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, GT, HN, HR, HU, ID, IL, IN, IR, IS, JO, JP, KE, KG, KH, KN, KP, KR, KW, KZ, LA, LC, LK, LR, LS, LU, LY, MA, MD, ME, MG, MK, MN, MW, MX, MY, MZ, NA, NG, NI, NO, NZ, OM, PA, PE, PG, PH, PL, PT, QA, RO, RS, RU, RW, SA, SC, SD, SE, SG, SK, SL, SM, ST, SV, SY, TH, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, ZA, ZM, ZW.

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Published:
— *with international search report (Art. 21(3))*

(54) Title: PROLINE-BASED NEUROPEPTIDE FF RECEPTOR MODULATORS

(57) Abstract: Neuropeptide FF receptor modulators based on a proline scaffold are provided which offer NPFF receptor potencies in the nanomolar range and antagonistic selectivity for the NPFF 1 receptor. Methods, compounds and compositions for modulating the function of neuropeptide FF receptors are provided for pharmacotherapies capable of influencing conditions or disorders affected by the neuropeptide FF receptors.

WO 2018/152134 A1

Region 2

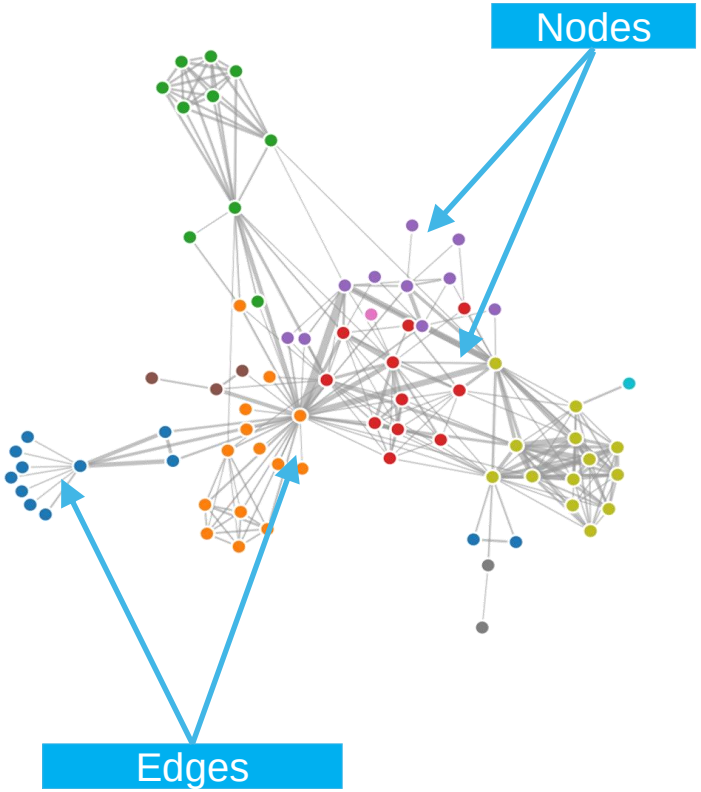
FIG. 2

Region 1

Region 3

Compound 1

Ke NPFF1 : 1620 ± 379 nM
Ke NPFF2 : 7251 ± 1734 nM



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# CAS SciFinder Discovery Platform (Academic)平台解决方案

## CAS SciFinder ——加速科学发现的业界领先的科学工具

业界最领先的相关性搜索引擎，提供和化学相关的各学科的文献、物质、反应和生物序列等检索内容，检索智能、高效、简单。可用于基金申请的文献准备、为新课题制定实验计划、寻求学术合作者、进行逆合成分析以及更多其他的教学和科研活动。

## CAS Analytical Methods ——借助CAS科学家深度加工的科学方法，提升研究效率

分析方法解决方案涵盖来自期刊中的化学分析方法，提供检索和对比功能，可快速获得能直接在实验室操作的分析方法。可为法医学、食品科学、农学、制药、环境等学科的教学和实验提供帮助。

## CAS Formulus ——助力开发安全、有效的产品

集成配方（制剂）数据与工作流程的解决方案，提供来自期刊、专利和产品说明中的配方详情。可检索制药、化妆品、食品、农化、油墨、涂料等众多领域中的配方，及其工艺、成分、目标成分的常见配伍成分、设计配方、和探索合规要求等。




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**使用说明：**

**1、CAS SciFinder-n 账号注册须知**

读者在使用CAS SciFindern之前须用江南大学的学校域名邮箱地址注册账号（如果已经注册了CAS SciFinder账号，请用该账号直接登录CAS SciFinder-n），根据提示输入相应信息，提交注册申请后系统将自动发送一个链接到您所填写的邮箱中，进入邮箱激活此链接即可完成注册。

**2、SciFinder账号注册链接**

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**3、CAS SciFinder-n检索网址**

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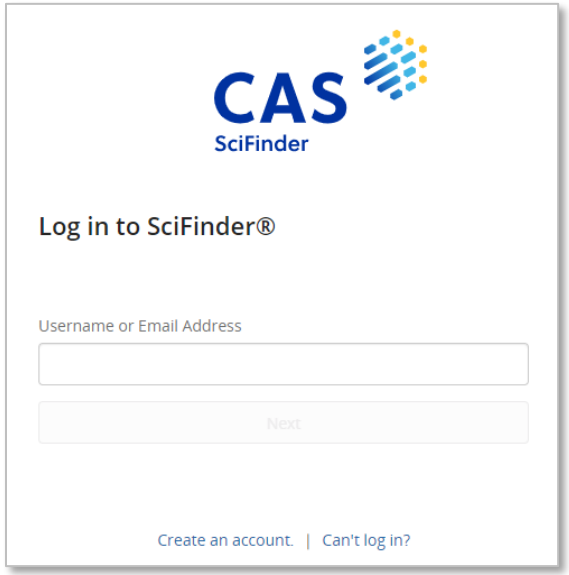
请注意：
1.必须输入真实姓名和学校邮箱。
2.用户名必须是唯一的，且包含 5-15 个字符。它可以只包含字母或字母组合、数字和/或以下特殊字符：
- -（破折号）
- _（下划线）
- .(句点)
- @（表示“at”的符号）

3.密码必须包含 7-15 个字符，并且至少包含三种以下字符：
- 字母
- 混合的大小写字母
- 数字
- 非字母数字的字符（例如 @、#、%、&、*）

例：abc@123
4.从下拉列表中选择一个密码提示问题并给出答案。
单击 Register（注册）。

点击激活链接后注册成功

通过https://SciFinder-n.cas.org访问





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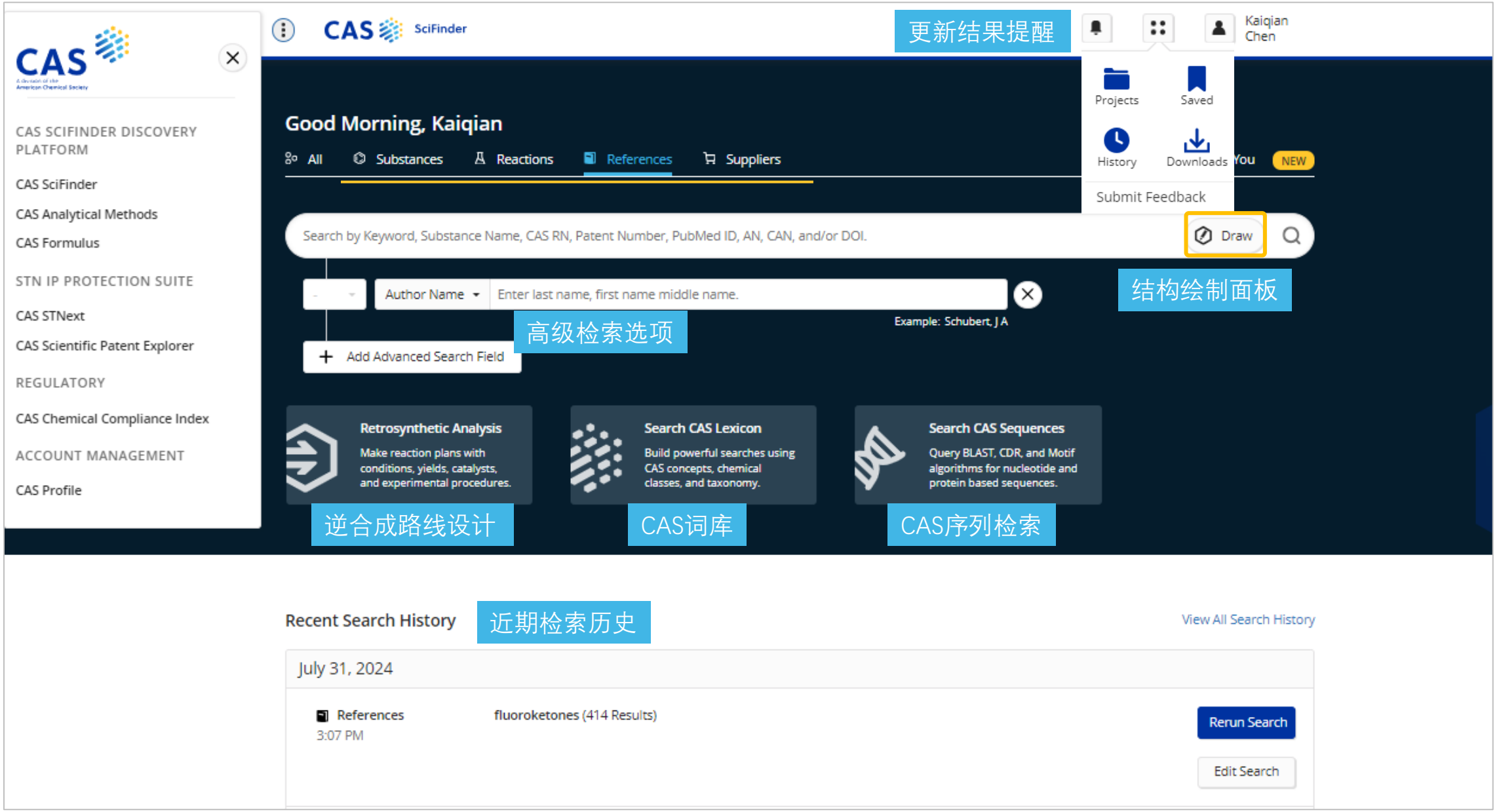
# CAS SciFinder主界面



# 大纲

- CAS及CAS SciFinder Discovery Platform (Academic)简介
- 科研信息的高效查阅
  - 全面的文献调研与拓展助力开题
  - 多角度出发检索物质结构及相关属性
  - 生物序列检索方法与结果分析
  - 探索实验方案以获取制备及其他实验详情
- 常见问题Q&A

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# 您可能会感兴趣：

- **主题词**怎么选择？如何构建？
- 如何**筛选**文献？追踪最新进展？
- 如何关注某篇文献的**被引文献**和**引文**？
- 如何快速获取**专利文献**中的关键信息？




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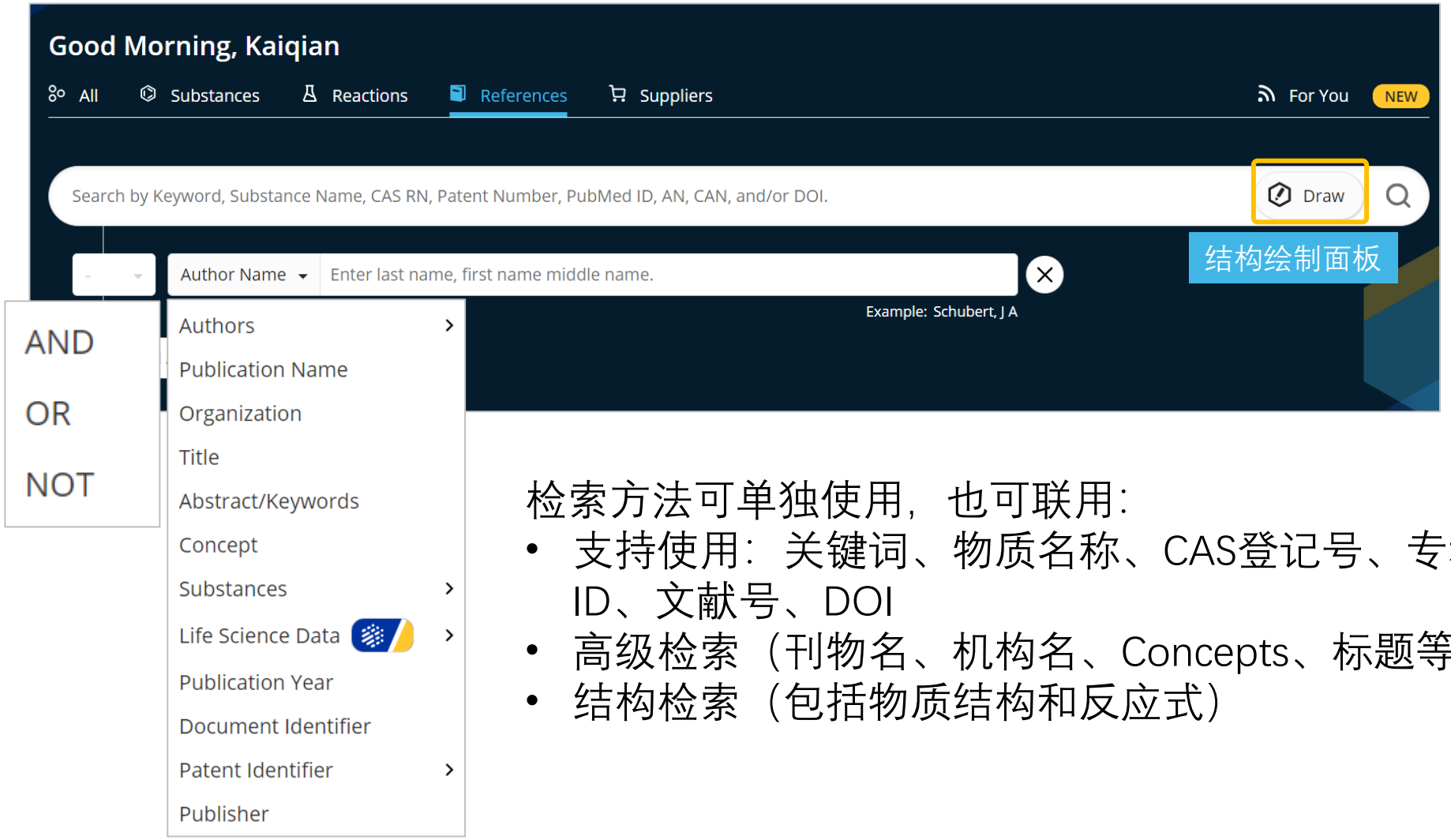
# 文献检索方式




检索方法可单独使用，也可联用：

- 支持使用：关键词、物质名称、CAS登记号、专利号、PubMed ID、文献号、DOI
- 高级检索（刊物名、机构名、Concepts、标题等）；
- 结构检索（包括物质结构和反应式）

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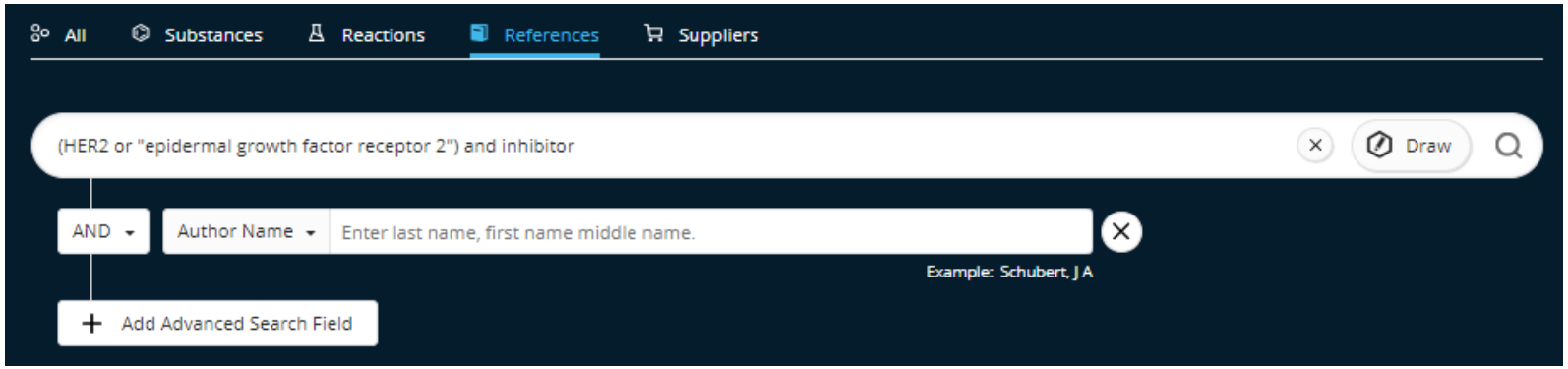
# 如何构建检索主题?


- 支持布尔逻辑运算符(and, or, not) , 默认运算顺序or > and > not
- “”不允许词形变化，但可出现单数或复数
- ()优先运算，括号中表达式还可以和其他术语交互
- 支持通配符*或？（*代表0或多个字符；？代表0或1个字符）

e.g., (HER2 or "epidermal growth factor receptor 2”) and inhibitor







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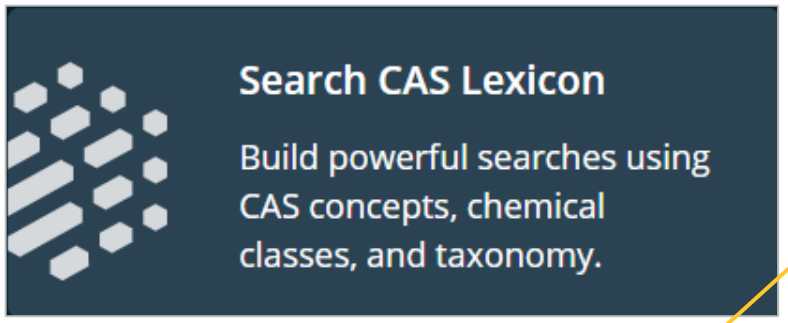
# CAS Lexicon 快速开启检索

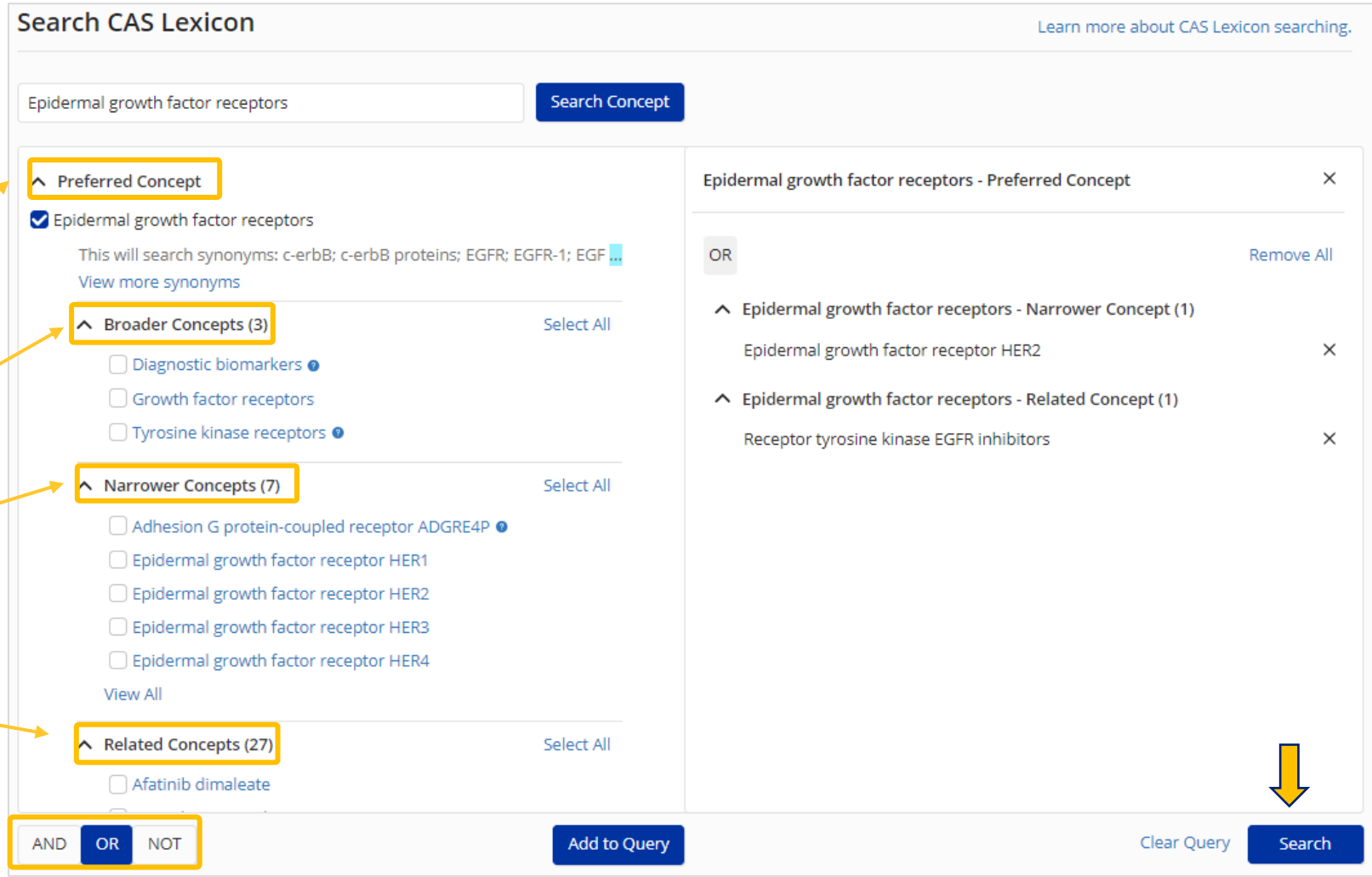
对新的研究方向了解不深，不知道从何入手？

主题词示例：
Epidermal growth factor receptors

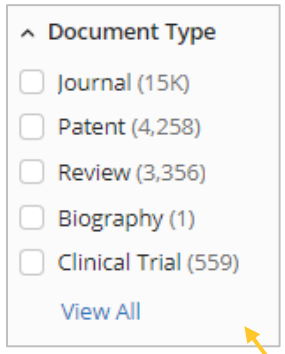



在CAS Lexicon词库层中选择适合的主题词：

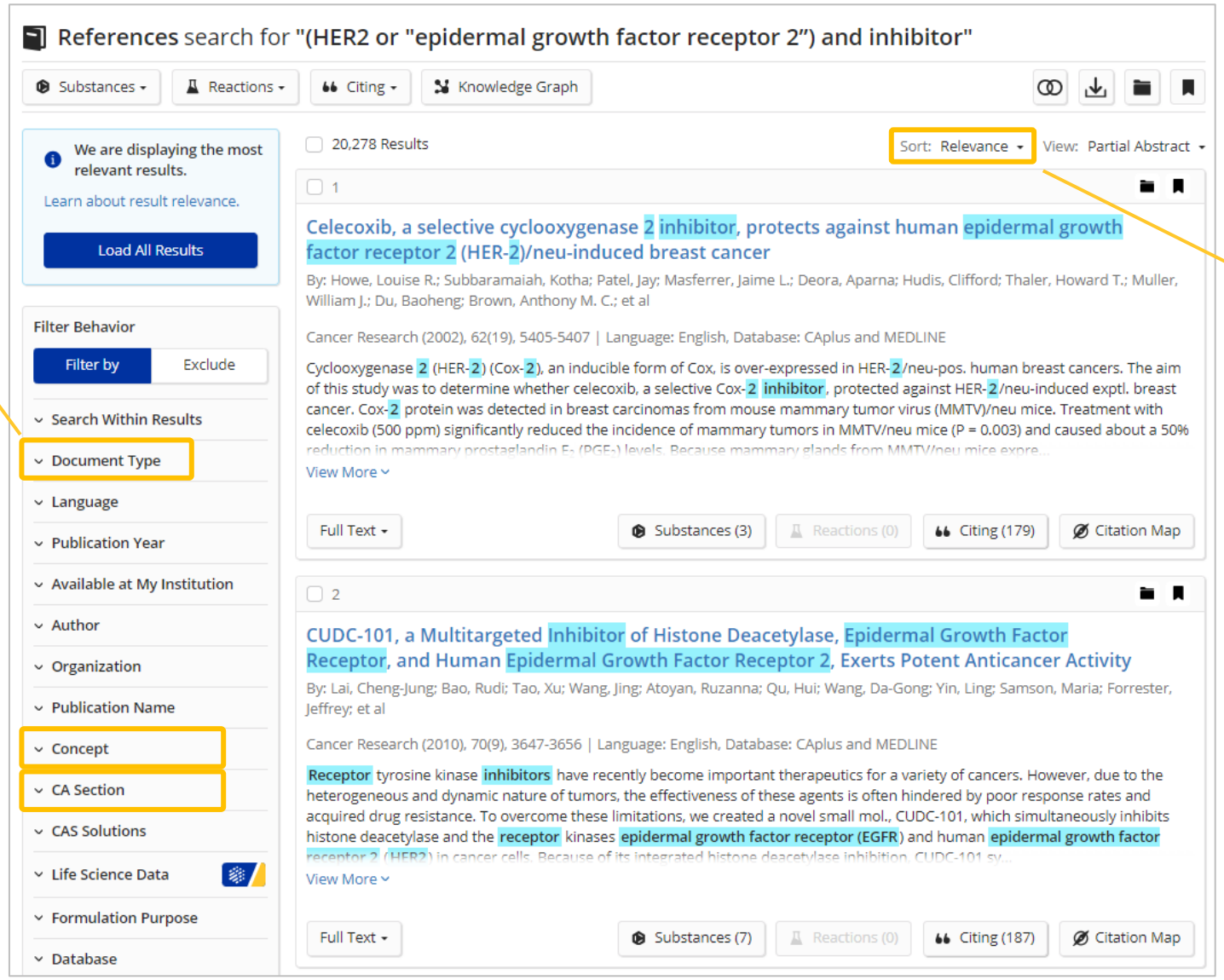
- 同义词
- 上位词
- 下位词
- 相关词



# 筛选文献结果




二次筛选
**文献类型**
文献语言
发表年份
作者
发表机构
期刊名称
**核心研究点**
**学科研究方向**
CAS解决方案
制剂/配方目的
来源数据库
……





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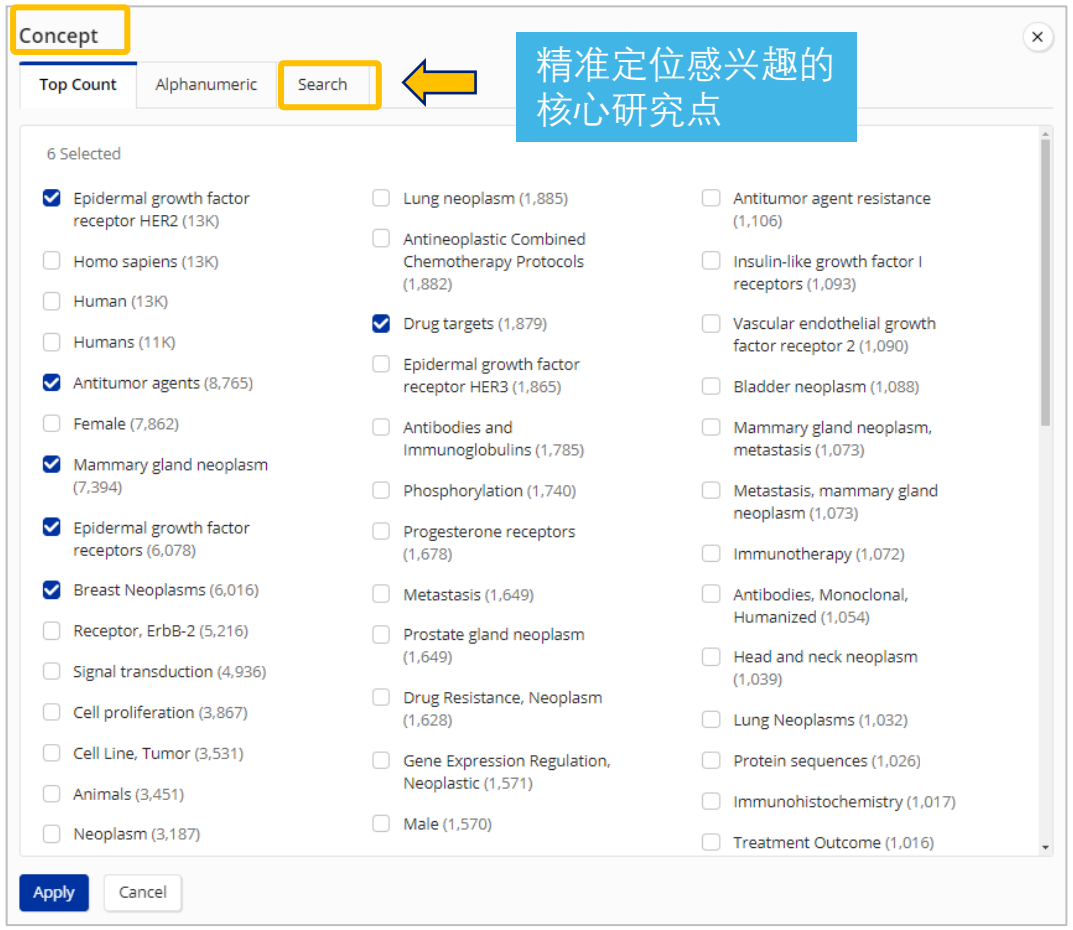
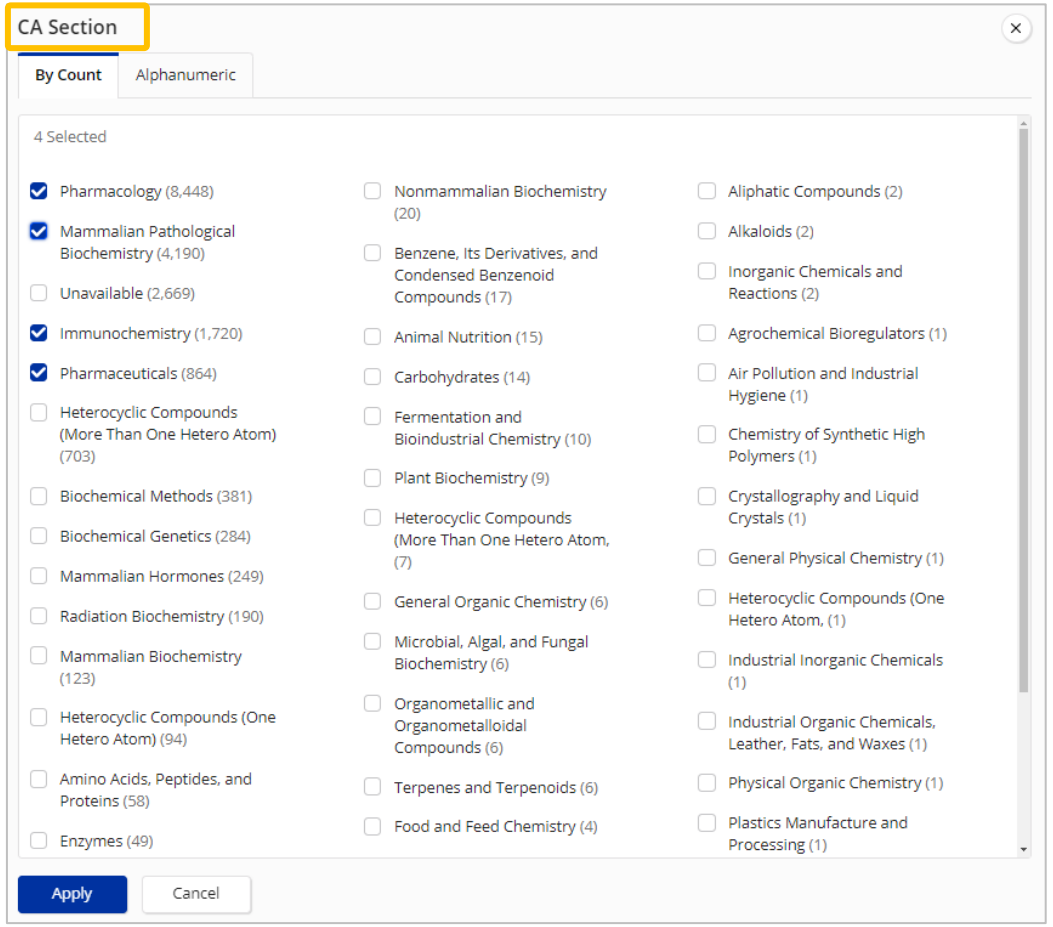
# 筛选工具 CAS Section & Concept

CAS标引的核心研究点




CAS标引的学科研究方向







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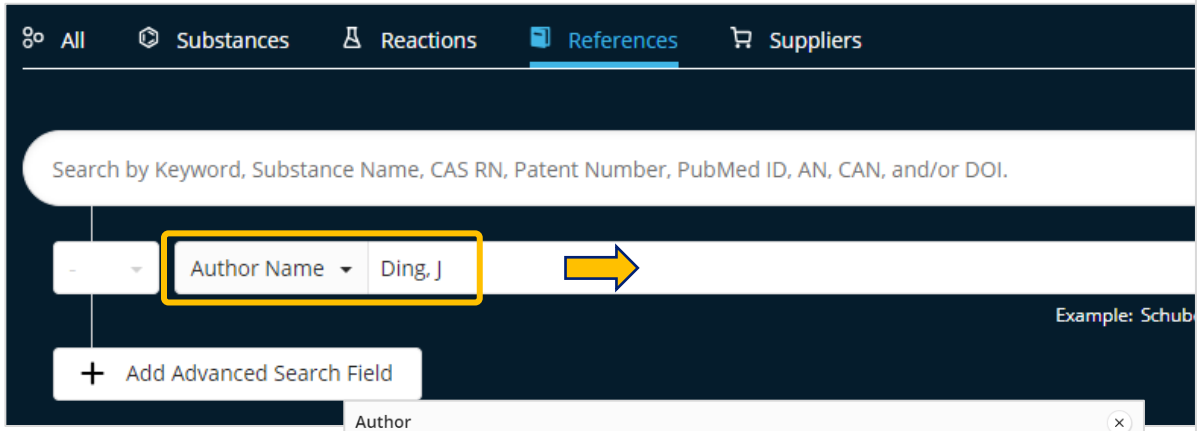
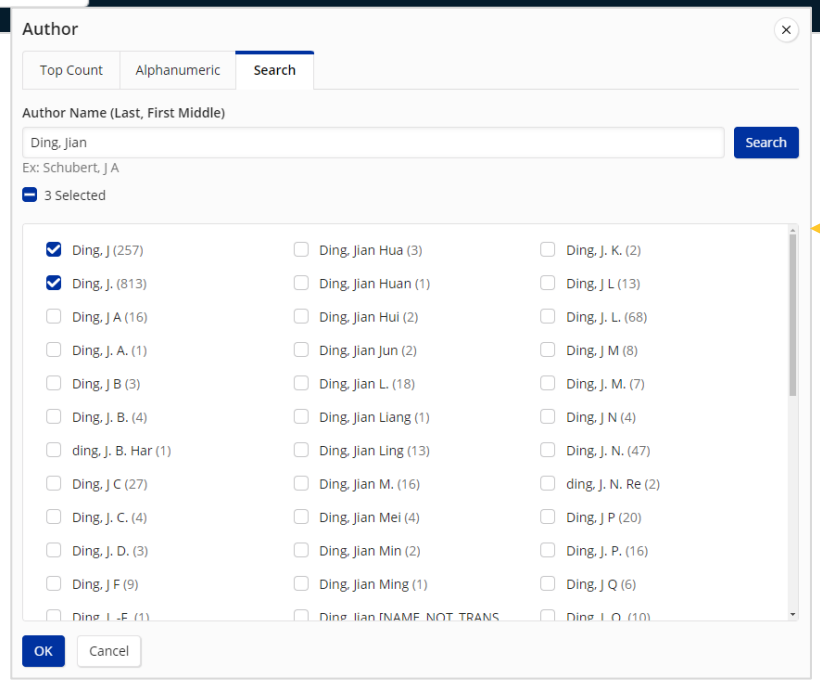
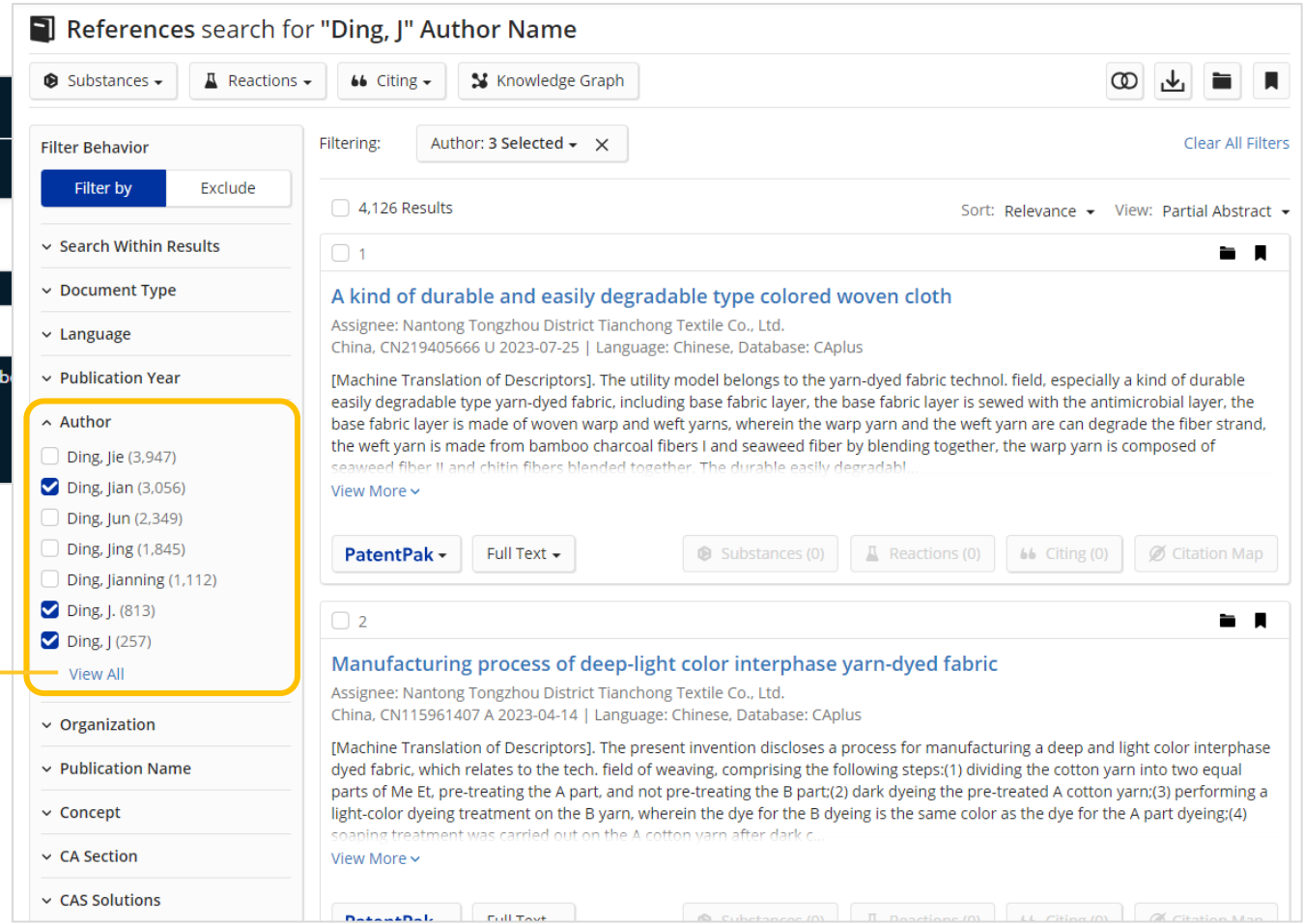
# 关注某作者的研究

## 高级检索选项，细化检索区域




**先全面检索，再筛选精炼**



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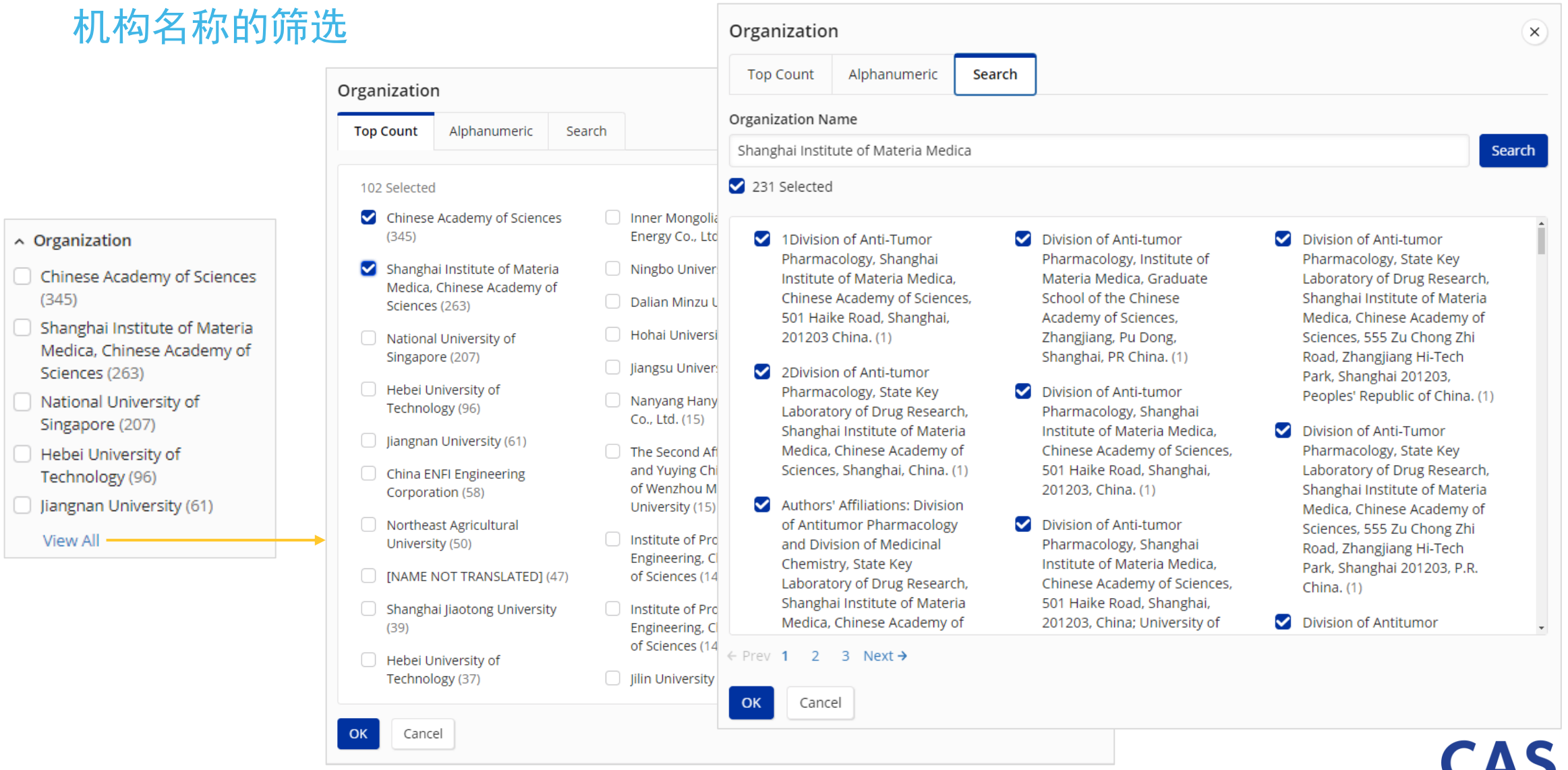
# 关注某作者的研究

## 机构名称的筛选



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# 文献详情

检索范围：标题，摘要，关键词，CAS标引的核心研究点、物质信息等

## BIBW2992, an irreversible EGFR/HER2 inhibitor highly effective in preclinical lung cancer models

6 | 0 | 1,133 | Citation Map | 引文地图

**In this Reference**

- Concepts
- Substances
- Biomarkers
- Cited Documents

By: Li, D.; Ambrogio, L.; Shimamura, T.; Kubo, S.; Takahashi, M.; Chirieac, L. R.; Padera, R. F.; Shapiro, G. I.; Baum, A.; Himmelsbach, F.; et al
View All

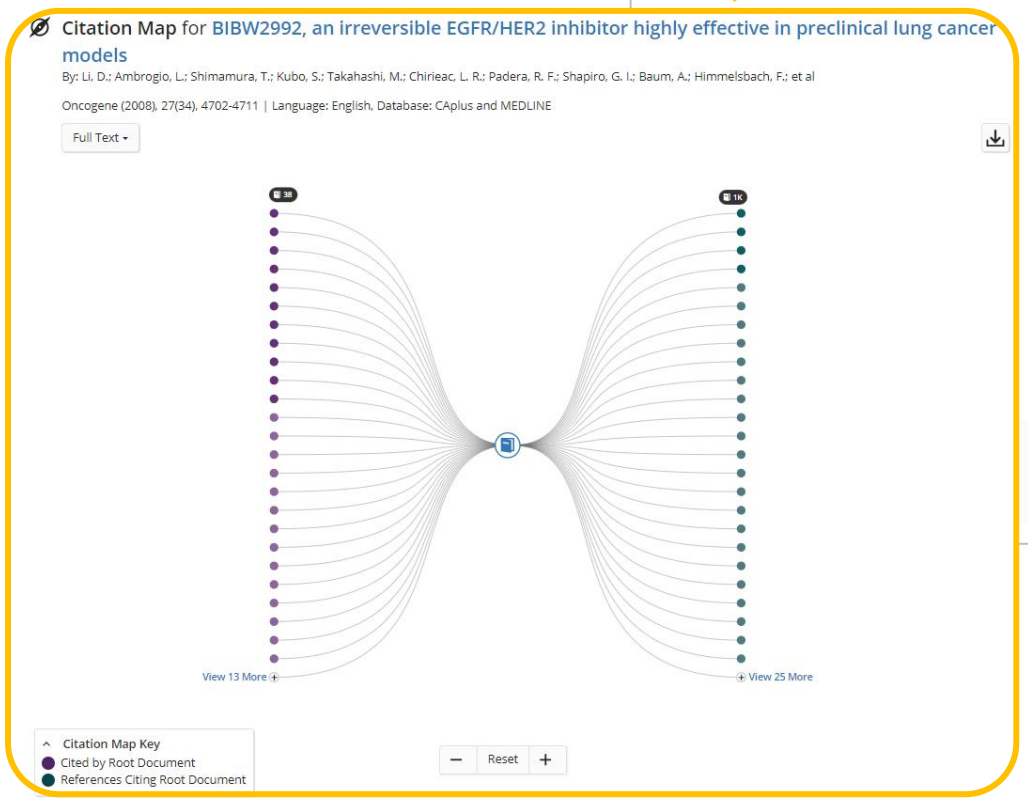
**DOI:** 10.1038/onc.2008.109

Genetic alterations in the kinase domain of the epidermal growth factor receptor (EGFR) in non-small cell lung cancer (NSCLC) patients are associated with sensitivity to treatment with small mol. tyrosine kinase inhibitors. Although first-generation reversible, ATP-competitive inhibitors showed encouraging clin. responses in lung adenocarcinoma tumors harboring such EGFR mutations, almost all patients developed resistance to these inhibitors over time. Such resistance to first-generation EGFR inhibitors was frequently linked to an acquired T790M point mutation in the kinase domain of EGFR, or upregulation of signaling pathways downstream of HER3. Overcoming these mechanisms of resistance, as well as primary resistance to reversible EGFR inhibitors driven by a subset of EGFR mutations, will be necessary for development of an effective targeted therapy regimen. Here, we show that BIBW2992, an anilino-quinazoline designed to irreversibly bind EGFR and HER2, potently suppresses the kinase activity of wild-type and activated EGFR and HER2 mutants, including erlotinib-resistant isoforms. Consistent with this activity, BIBW2992 suppresses transformation in isogenic cell-based assays, inhibits survival of cancer cell lines and induces tumor regression in xenograft and transgenic lung cancer models, with superior activity over erlotinib. These findings encourage further testing of BIBW2992 in lung cancer patients harboring EGFR or HER2 oncogenes. Oncogene (2008) 27, 4702-4711; doi:10.1038/onc.2008.109; published online 14 Apr. 2008.

**Keywords:** antitumor resistance anilinoquinazoline derivative BIBW2992 EGFR HER2 lung cancer

View Source | Full Text

Journal View More







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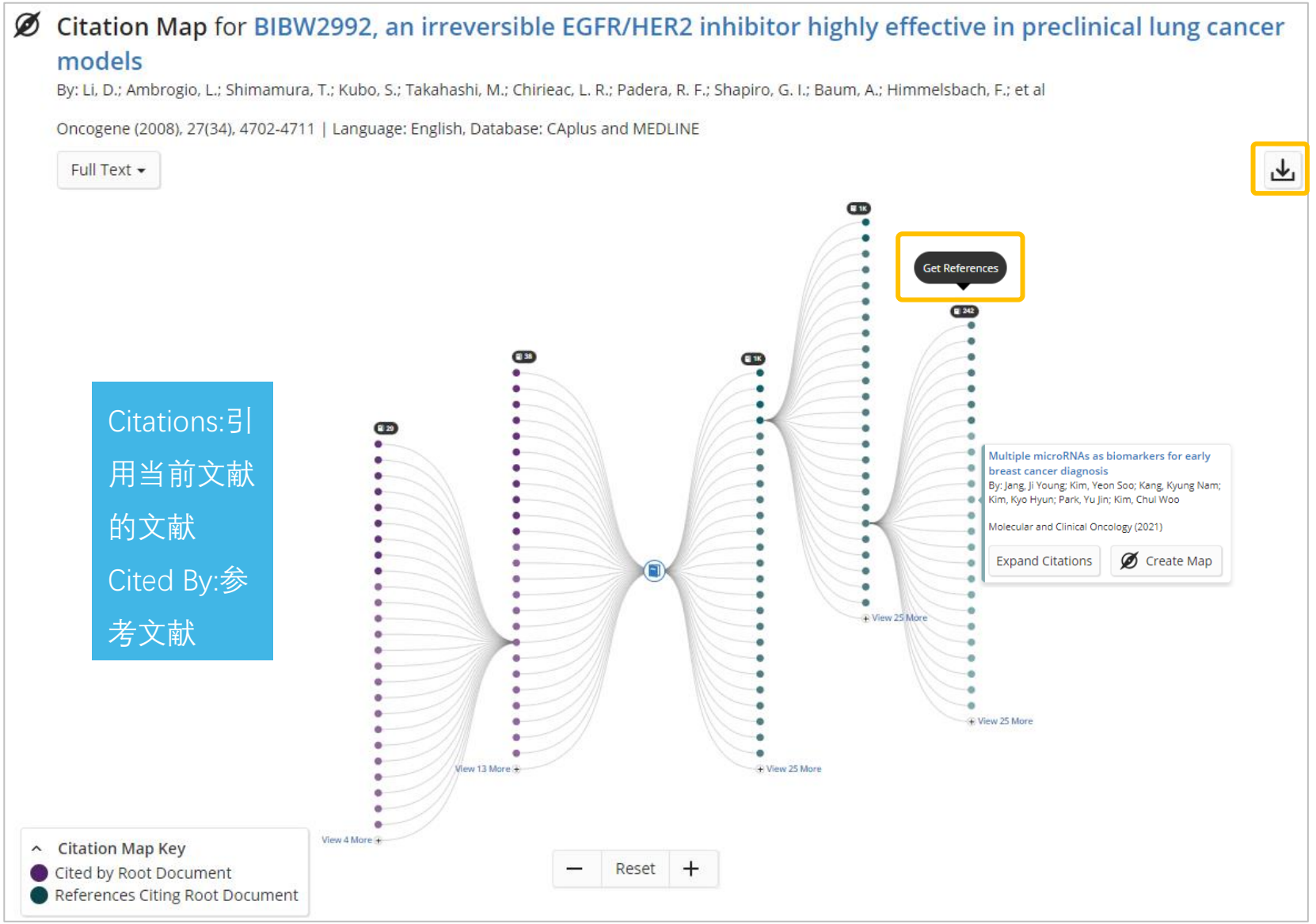
# 引文地图——便捷获取引文信息

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- 可直接进入文献详情页面



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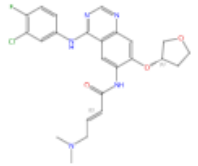
# 文献详情

## Substances

原文中重点研究的物质信息

850140-72-6

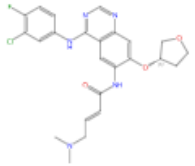


Absolute stereochemistry shown
Double bond geometry shown

$C_{24}H_{25}ClFN_5O_3$
Afatinib

**Role:** Unspecified

439081-18-2



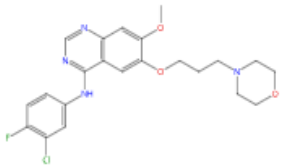
Absolute stereochemistry shown
Double bond geometry unknown

$C_{24}H_{25}ClFN_5O_3$
*N*-[4-[(3-Chloro-4-fluorophenyl)amino]-7-[[(3*S*)-tetrahydro-3-furanyl]oxy]-6-quina...

**Role:** Pharmacological Activity, Therapeutic Use, Biological Study, Uses

物质角色

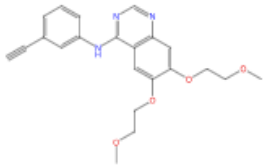
184475-35-2



$C_{22}H_{24}ClFN_4O_3$
Gefitinib

**Role:** Pharmacological Activity, Therapeutic Use, Biological Study, Uses

183321-74-6



$C_{22}H_{23}N_3O_4$
Erlotinib

**Role:** Pharmacological Activity, Therapeutic Use, Biological Study, Uses

## CAS Concepts

CAS标引的核心研究点

| | |
|---|---|
| Antitumor agent resistance | Epidermal growth factor receptors<br>Role: Biological Study, Unclassified |
| Antitumor agents | Homo sapiens |
| Covalent inhibitors | Human |
| Drug targets | Mutation<br>Modifier: EGFR and HER2 |
| Epidermal growth factor receptor HER2<br>Role: Biological Study, Unclassified | Non-small-cell lung carcinoma |
| Epidermal growth factor receptor HER3<br>Role: Biological Study, Unclassified | Protein phosphorylation |

## Reactions

原文中重点研究的反应信息

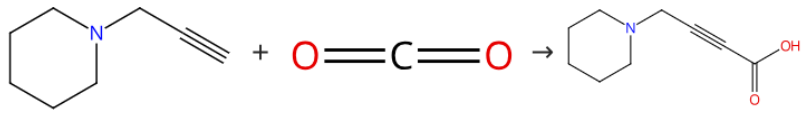
244

31-320-CAS-11506461

**Steps:** 1 **Yield:** 100%

View Experimental Protocols

1.1 Reagents: Butyllithium
Solvents: Tetrahydrofuran, Hexane
1.2 -

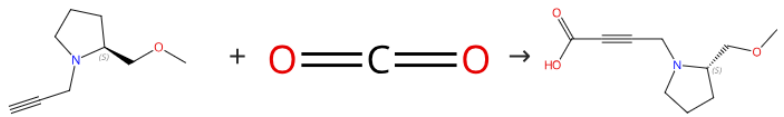


31-320-CAS-8784633

**Steps:** 1 **Yield:** 99%

View Experimental Protocols

1.1 Reagents: Butyllithium
Solvents: Tetrahydrofuran, Hexane
1.2 -



Absolute stereochemistry shown

Absolute stereochemistry shown

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# 专利文献详情

## Combination of a purine-based CDK inhibitor with a tyrosine kinase inhibitor and use thereof in the treatment of proliferative disorders

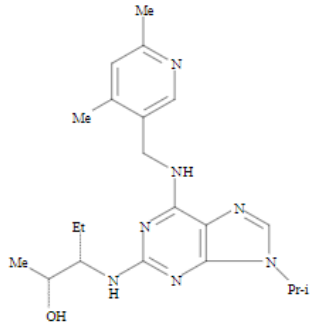
51 | 30 | 7 | Citation Map

**In this Reference**

- IPC Data
- CAS Concepts
- Substances
- Reactions
- Formulations
- Cited Documents

By: Green, Simon; Frame, Sheelagh; Fleming, Ian

The present invention relates to combination comprising (i) an ErbB inhibitor; and (ii) a CDK inhibitor, or a pharmaceutically acceptable salt thereof, selected from: (a) roscovitine; (b) 3-{9-isopropyl-6-[(pyridin-3-yl-methyl)-amino]-9H-purin-2-yl-amino)- 2-methyl-pentan-2-ol; (c) 3-{9-isopropyl-6-[(pyridin-3-ylmethyl)-amino]-9H-purin-2- yl-amino}-pentan-2-ol; and (d) (2R,3S)-3-(6-(4,6-dimethyl-pyridin-3-yl-methylamino)-9-isopropyl-9H-purin-2-yl-amino)pentan-2-ol. Further aspects of the invention relate to pharmaceutical products and pharmaceutical compositions comprising combinations according to the invention, and methods of treatment using the same. Thus, the combination of trastuzumab (an ErbB2 inhibitor) and seliciclib (a CDK inhibitor) produced greater downregulation of the HER2 receptor in breast cancer cell lines than either single agent treatment alone, suggesting that the drugs synergistically downregulate the levels of this receptor.




Keywords: DK kinase ErbB tyrosine kinase inhibitor proliferative disorder; purine CDK kinase inhibitor tyrosine kinase inhibitor proliferative disorder

PatentPak Viewer | Get Prior Art Analysis | Full Text

题录信息

CAS PatentPak

Publication Information • Patent — View More

Patent Family 专利家族

| Patent | Language | Kind Code | PatentPak Opt | Publication Date | Application Number | Application Date |
|---|---|---|---|---|---|---|
| WO2008122779 | English | A1 | PDF \| PDF+ Viewer | 2008-10-16 | WO2008-GB1189 | 2008-04-02 |
| EP2139486 | English | A1 | | 2010-01-06 | EP2008-718990 | 2008-04-02 |
| CN101678029 | Chinese | A | | 2010-03-24 | CN2008-80018864 | 2008-04-02 |
| JP2010523536 | Japanese | T | | 2010-07-15 | JP2010-501589 | 2008-04-02 |

### IPC Data

IPC信息

| Patent | Class | Patent Family Classification Codes |
|---|---|---|
| WO2008122779 | IPCI | A61K 0031/52; A61K 0031/517; A61K 0045/00; A61K 0045/06; A61P 0035/00 |
| EP2139486 | IPCI | A61K 0031/52; A61K 0031/517; A61K 0045/00; A61K 0045/06; A61P 0035/00 |
| CN101678029 | IPCI | A61K 0031/52; A61K 0031/517; A61K 0045/00; A61K 0045/06; A61P 0035/00 |
| JP2010523536 | IPCI | A61K 0031/52; A61K 0045/00; A61K 0031/517; A61K 0039/395; A61K 0031/5377; A61P 0043/00; A61P 0035/00 |

### CAS Concepts

CAS标引的核心研究点

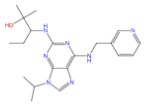
| | |
|---|---|
| Antitumor agents | Head and neck neoplasm |
| Apoptosis | Homo sapiens |
| Combination chemotherapy | Human |
| Drug delivery systems<br>Modifier: kits | Lung neoplasm |
| Drug interactions, synergistic | Mammary gland neoplasm |

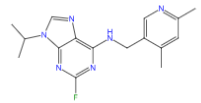
### Substances

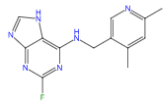
51

物质信息

1070912-92-3
Image Not Available
Unspecified PKI
PatentPak
Role: Pharmacological Activity, Therapeutic Use, Biological Study, Uses

1070862-90-6

$C_{20}H_{29}N_7O$
2-Methyl-3-[[9-(1-methylethyl)-6-[(3-pyridinylmethyl)amino]-9*H*-purin-2-yl]amino]...
PatentPak
Role: Pharmacological Activity, Therapeutic Use, Biological Study, Uses

1070791-10-4

$C_{16}H_{19}FN_6$
*N*-[(4,6-Dimethyl-3-pyridinyl)methyl]-2-fluoro-9-(1-methylethyl)-9*H*-purin-6-amine
PatentPak
Role: Properties, Reactant, Synthetic Preparation, Reactant or Reagent, Preparation

1070791-09-1

$C_{13}H_{13}FN_6$
*N*-[(4,6-Dimethyl-3-pyridinyl)methyl]-2-fluoro-9*H*-purin-6-amine
PatentPak
Role: Properties, Reactant, Synthetic Preparation, Reactant or Reagent, Preparation

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# CAS PatentPak：高效浏览专利

一键定位专利原文中的核心研究物质

CAS PatentPak：
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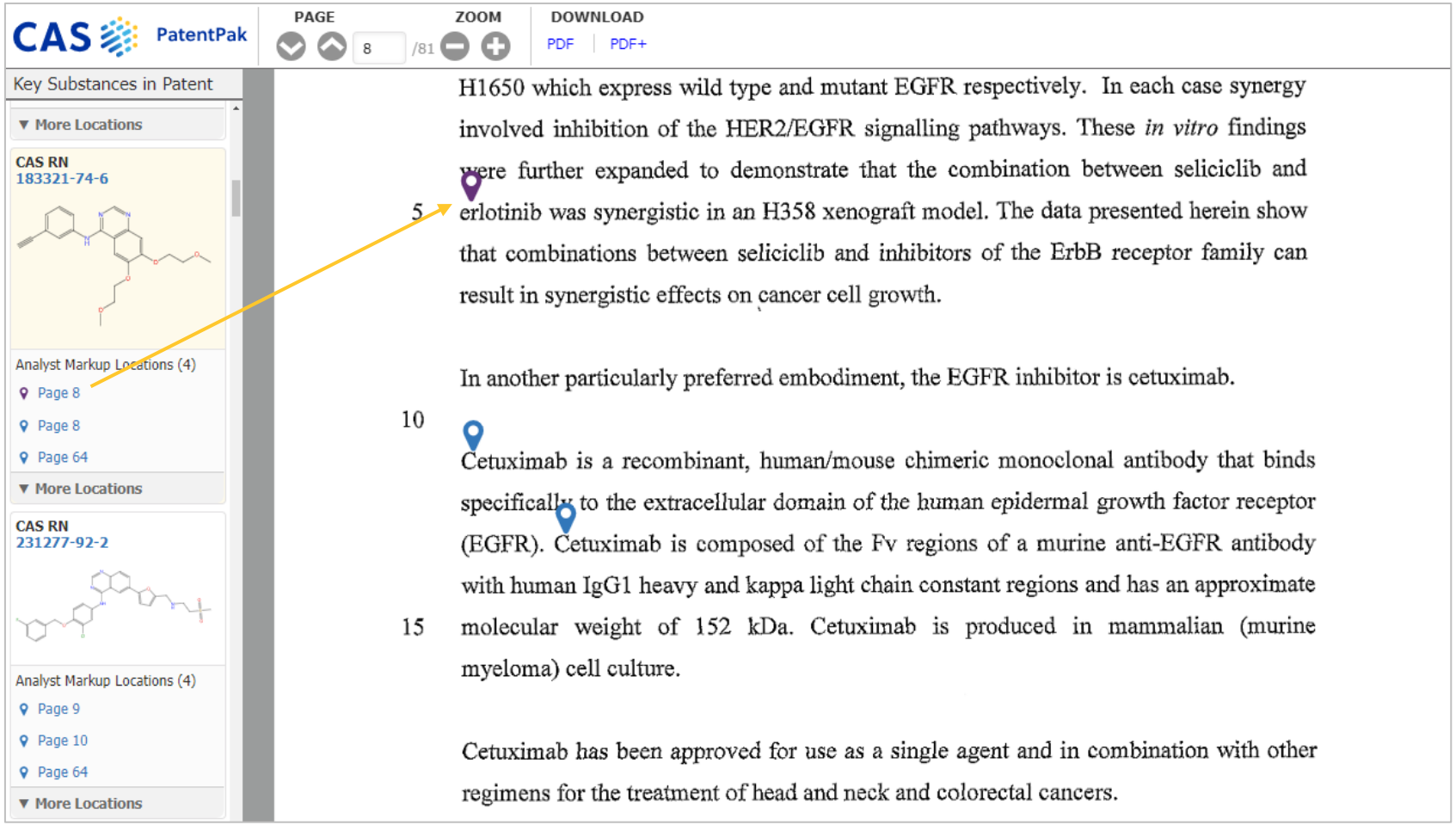
- 阅读其他语言撰写的等同专利







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# 小结

- 灵活构建检索主题：布尔逻辑运算符支持的灵活主题词构建，全面精准获取最相关的研究文献，高效获取领域研究前沿及全貌信息。
- CAS Lexicon：便捷获取CAS科学家标引的层级词库，拓展领域标准词，简便快速开启自动检索。
- 检索结果的分析与精炼：丰富的聚类分析选项，如Concept、CA Section等，快速缩小文献范围，细化研究热点及领域，多维度了解技术布局情况，并聚焦最感兴趣的文献，加速突破技术瓶颈。
- 文献详情速览：基于CAS的数据关联，从最相关的研究文献中获取重要的信息。利用引文地图拓展文献检索。
- CAS PatentPak：高效阅读专利原文，定位其中的关键物质；重点专利现有技术分析。节省查阅全文所需的时间和精力，专注于研发与创新工作。

# 大纲

- CAS及CAS SciFinder Discovery Platform (Academic)简介
- 科研信息的高效查阅
  - 全面的文献调研与拓展助力开题
  - 多角度出发检索物质结构及相关属性
  - 生物序列检索方法与结果分析
  - 探索实验方案以获取制备及其他实验详情
- 常见问题Q&A




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# 您可能会感兴趣：

- 检索完整**分子结构**？**通式结构**？或含有某些片段的物质？
- 结构式**信息不足**该如何检索？
- 利用**谱图数值**确认产物或杂质？从**属性值**出发，调研某类材料？
- 如何确认结构**新颖性**和**可专利性**？




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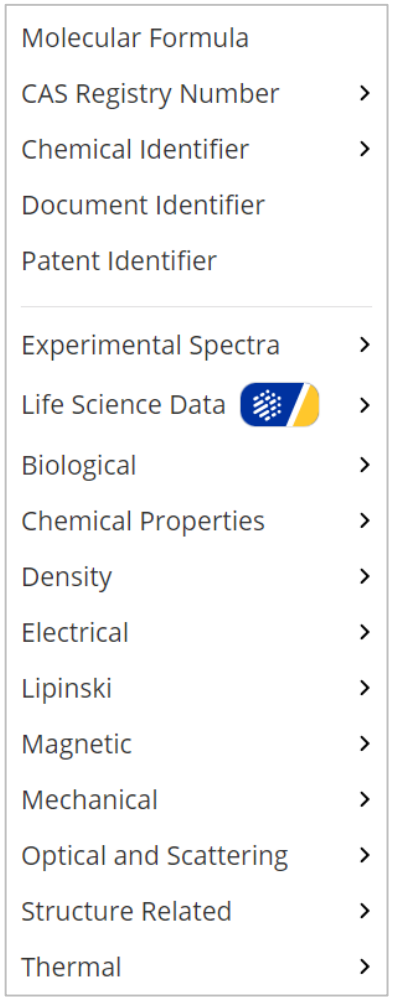
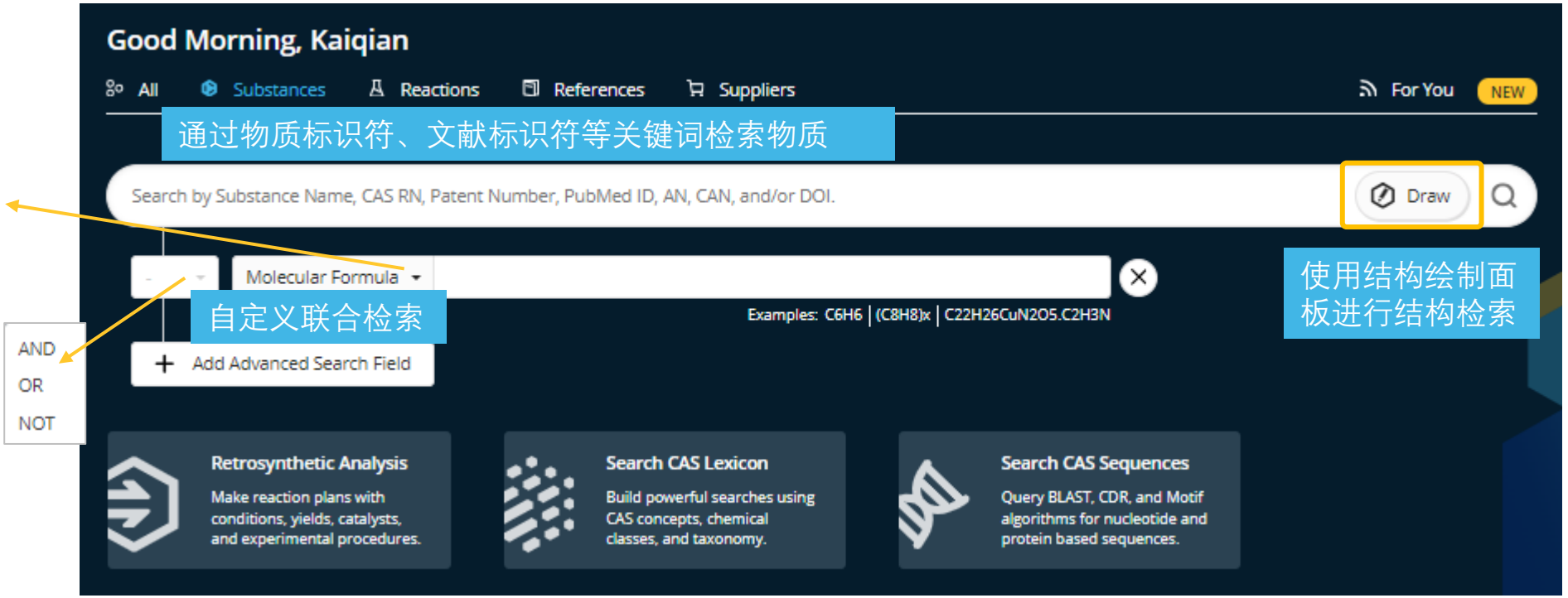
# 物质检索的方式

灵活的检索方式，满足各种物质类别的检索




- 检索策略推荐
  - 有机化合物，金属配合物，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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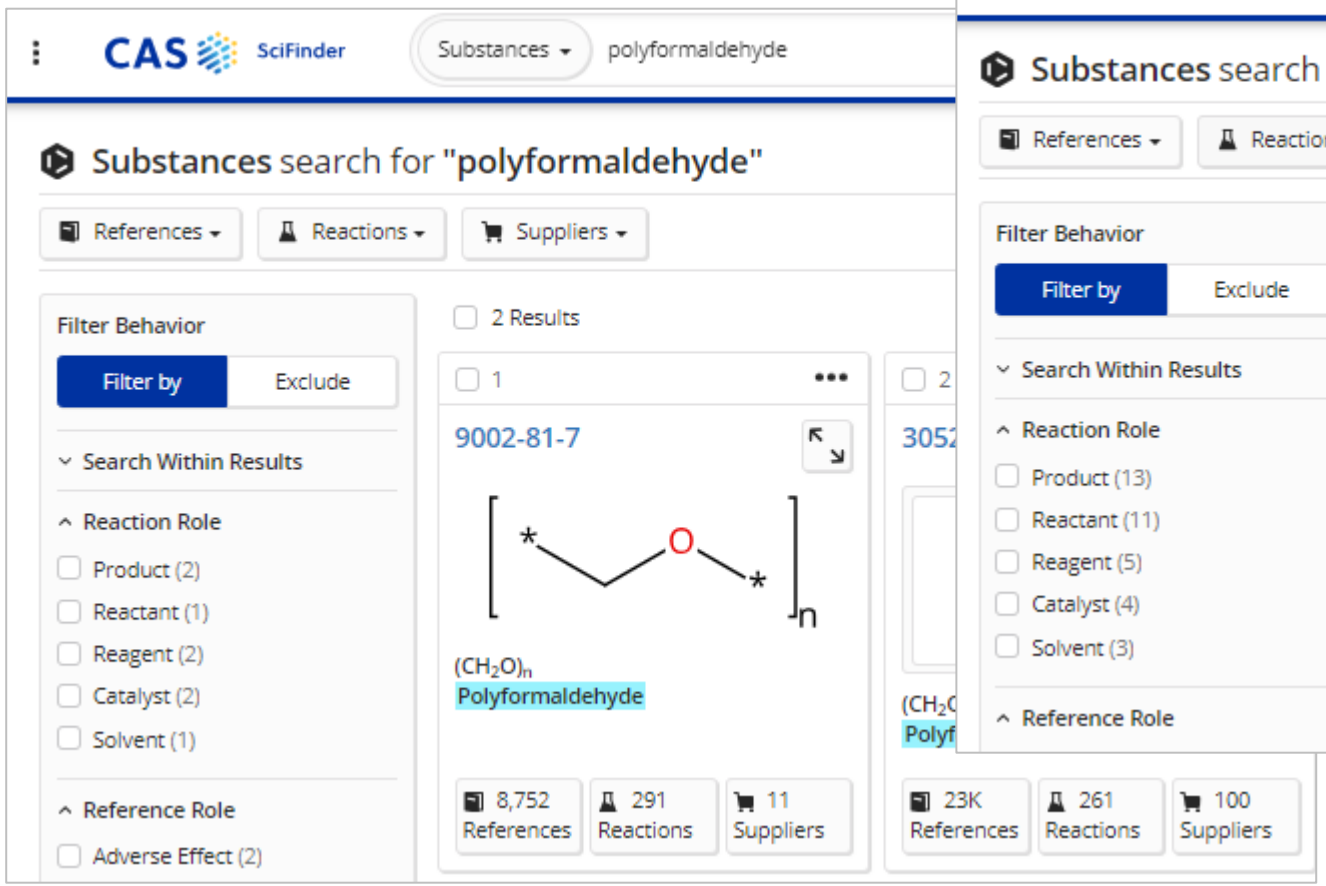
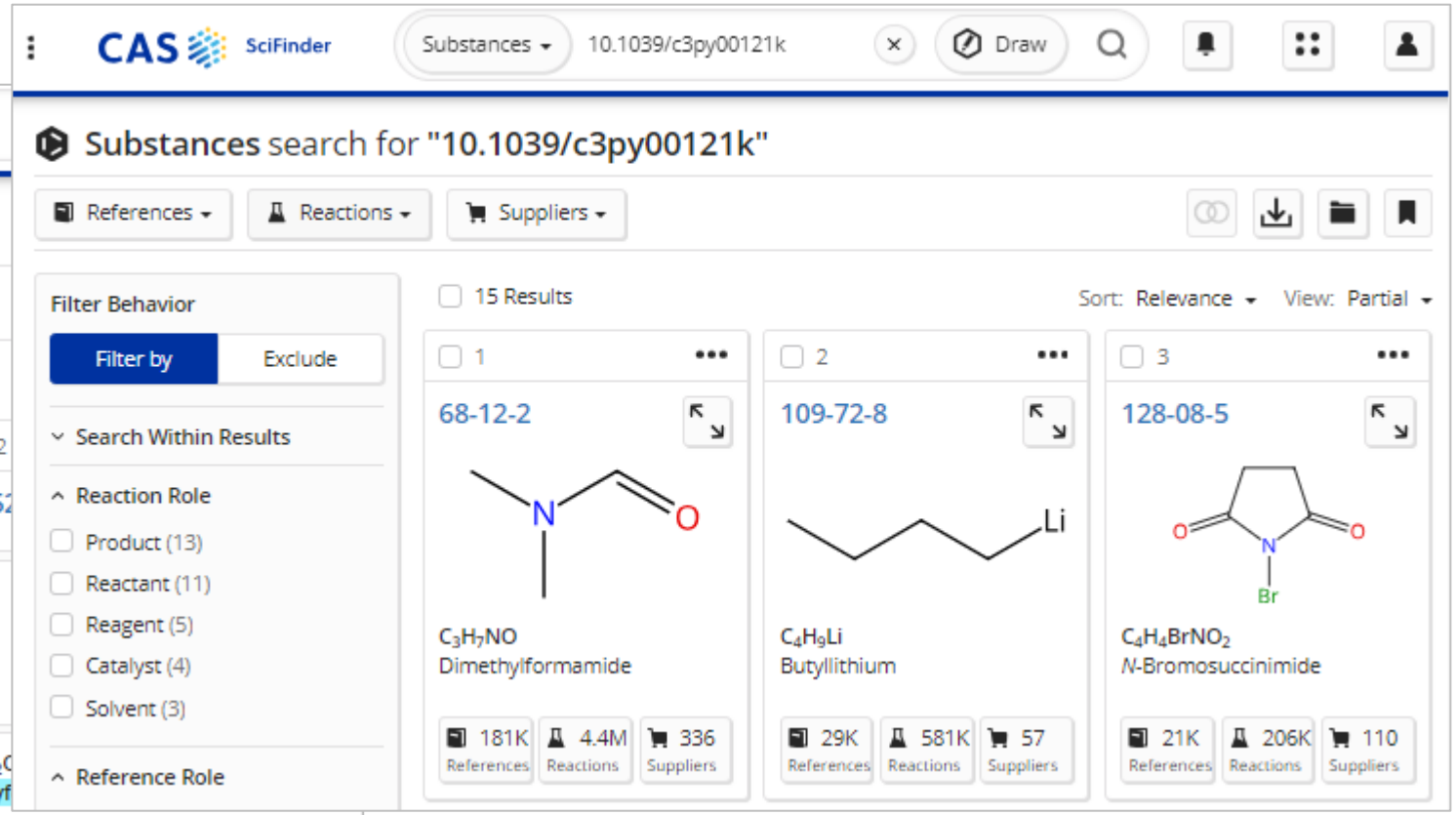
# 物质检索—物质/文献标识符

- 可同时检索多个物质识别符（物质名称或CAS RN）
- 不同物质使用空格隔开（<2000个字符

- 迅速获得关注文献中的物质信息







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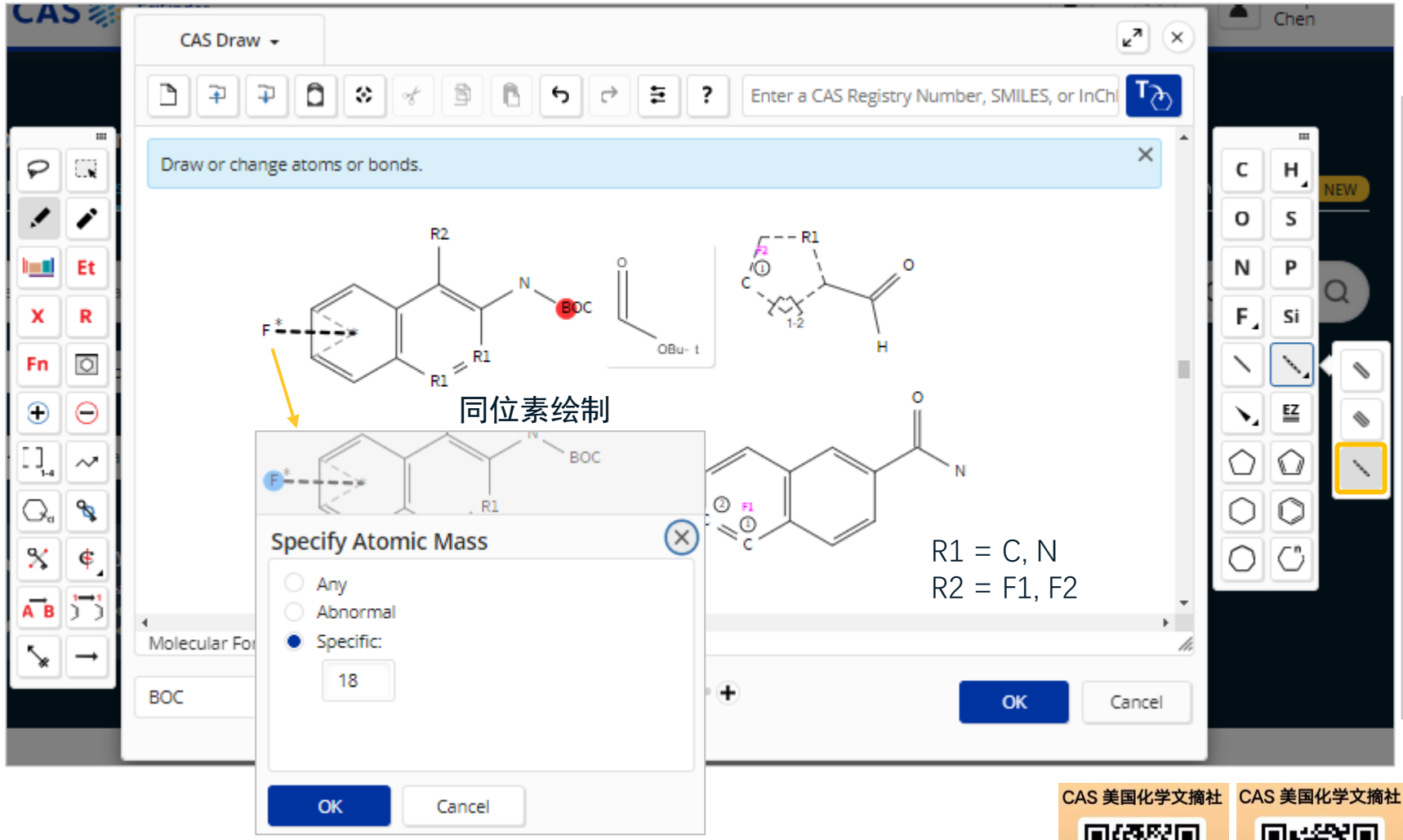
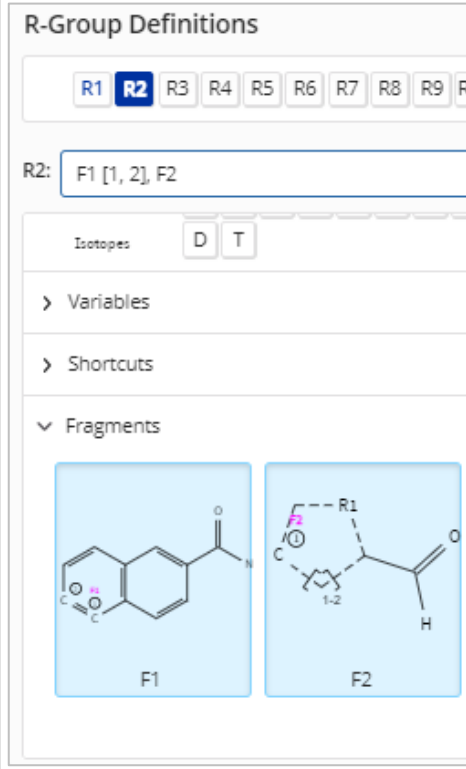
# 物质检索—CAS Draw：结构绘制面板

重要结构绘制工具注释：

- X 选择可变基团
- R 自定义R基团
- Fn 片段结构
- 重复工具
- 取代位置可变
- 环锁定工具
- 原子锁定工具




线上学习短视频：

CAS 美国化学文摘社 CAS 美国化学文摘社

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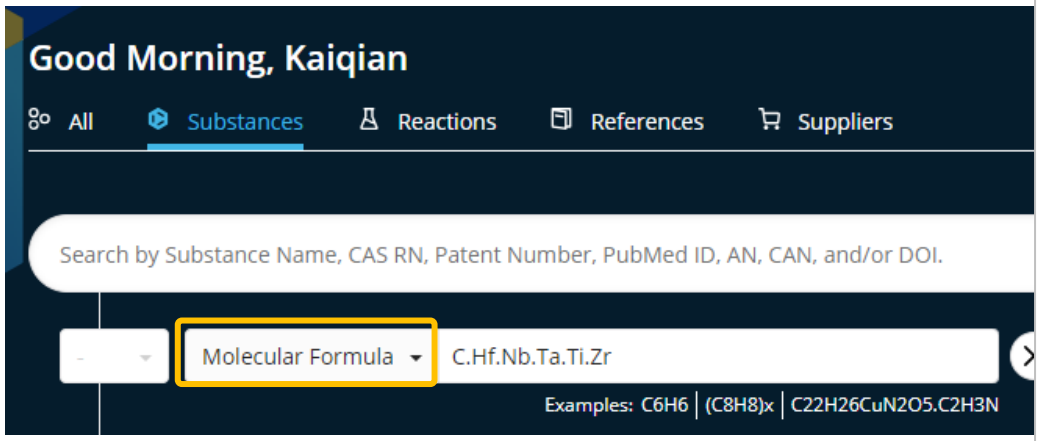
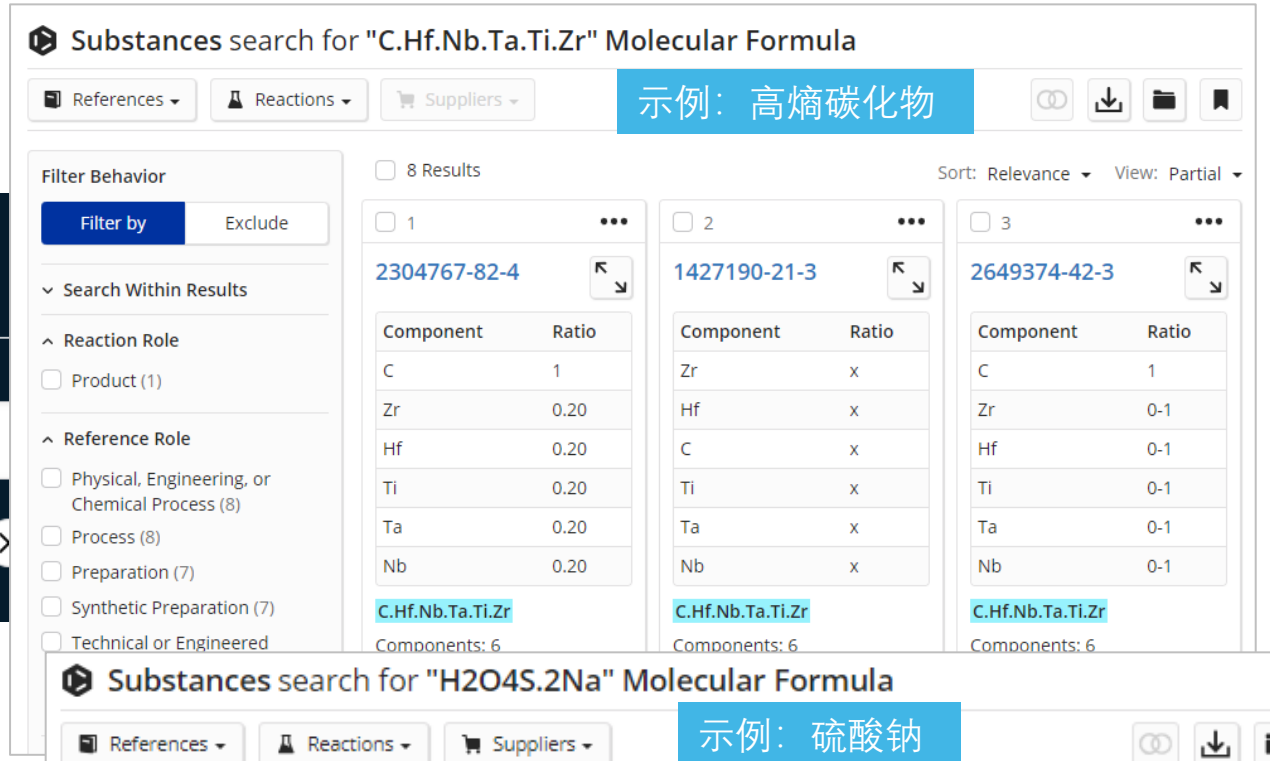
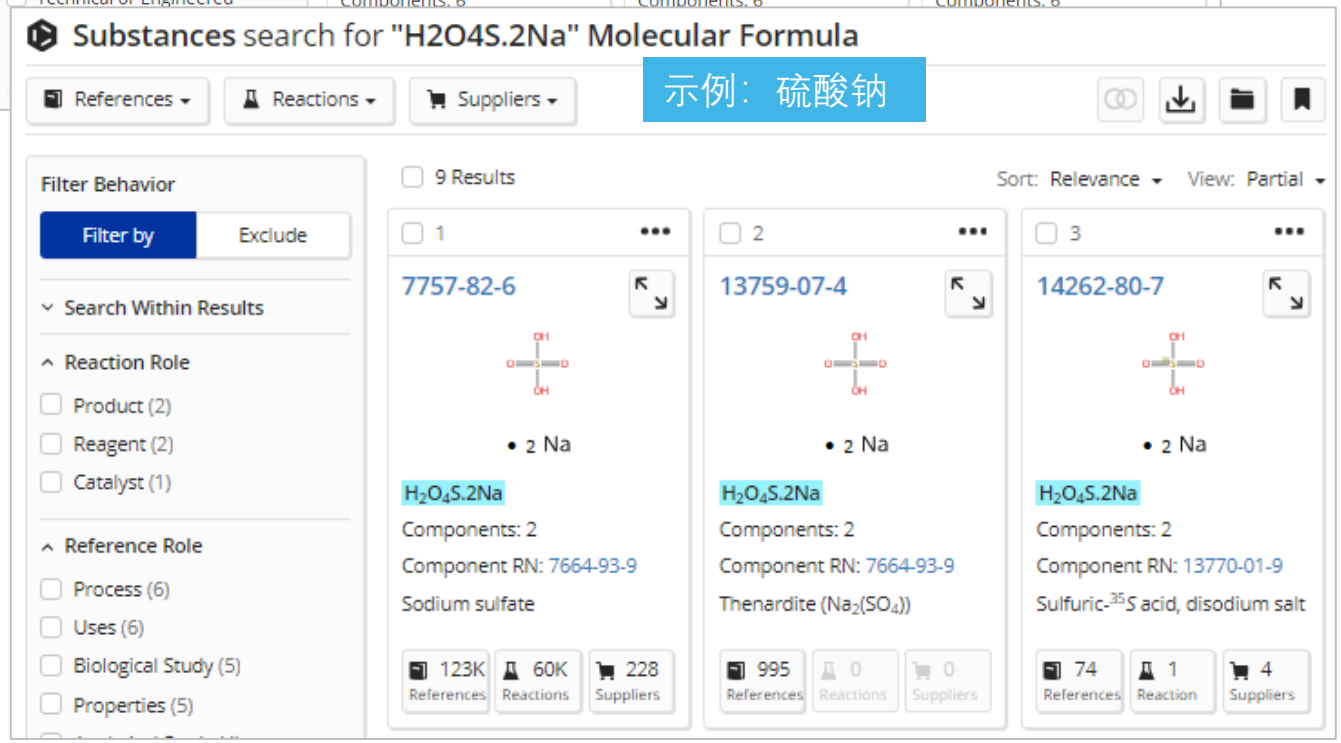
# 物质检索—分子式检索

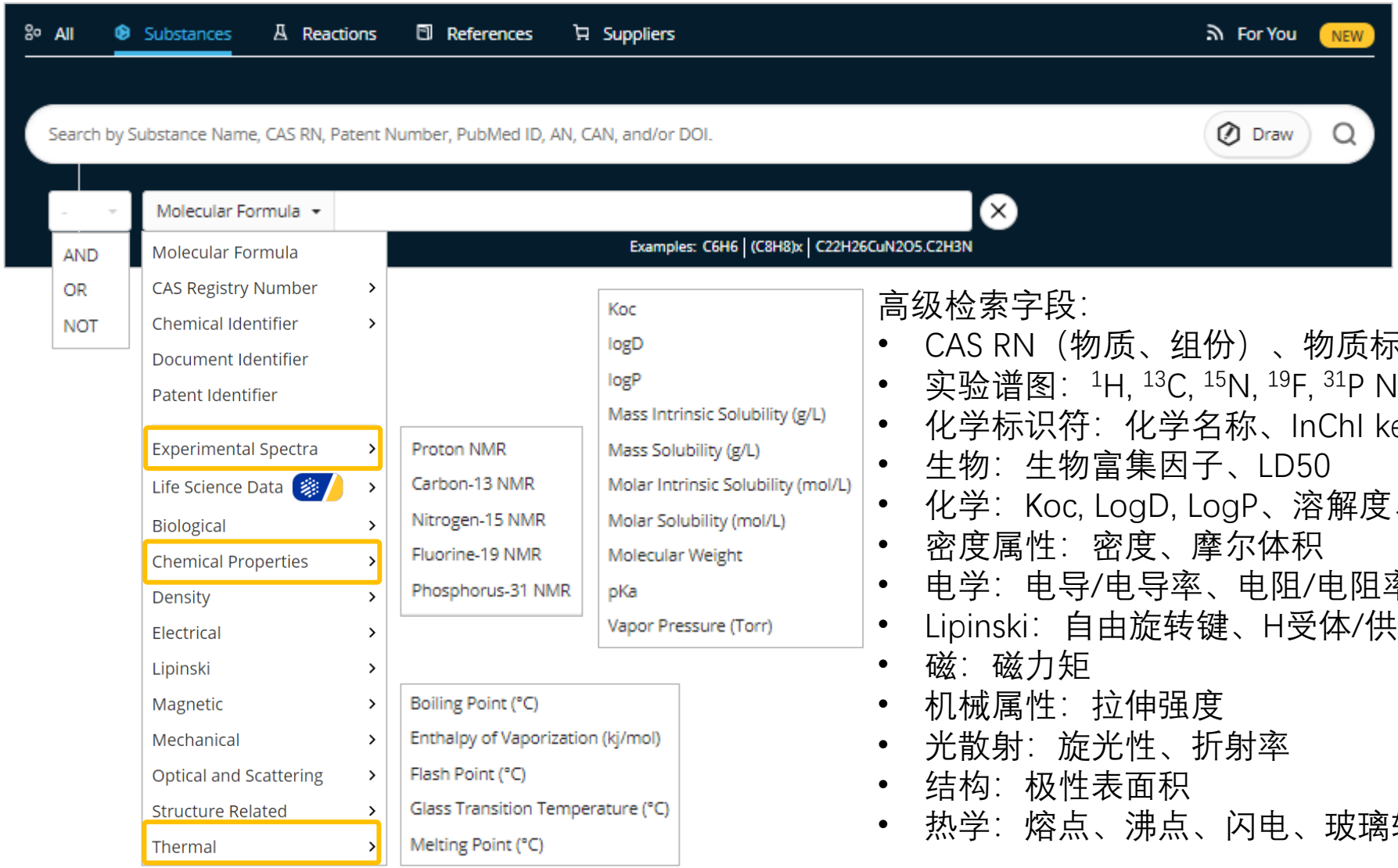



- **希尔(Hill)排序规则：**C排首位，H排第二，其他元素符号按照首字母顺序进行排列。当化学式不含C时，所有元素（包括H）按字母顺序列出。
- 不同组分之间用“.”隔开，如：高熵碳化物 C.Hf.Nb.Ta.Ti.Zr
- 无机含氧盐：阳离子和阴离子用点（.）分开；阴离子以氢补齐至电中性

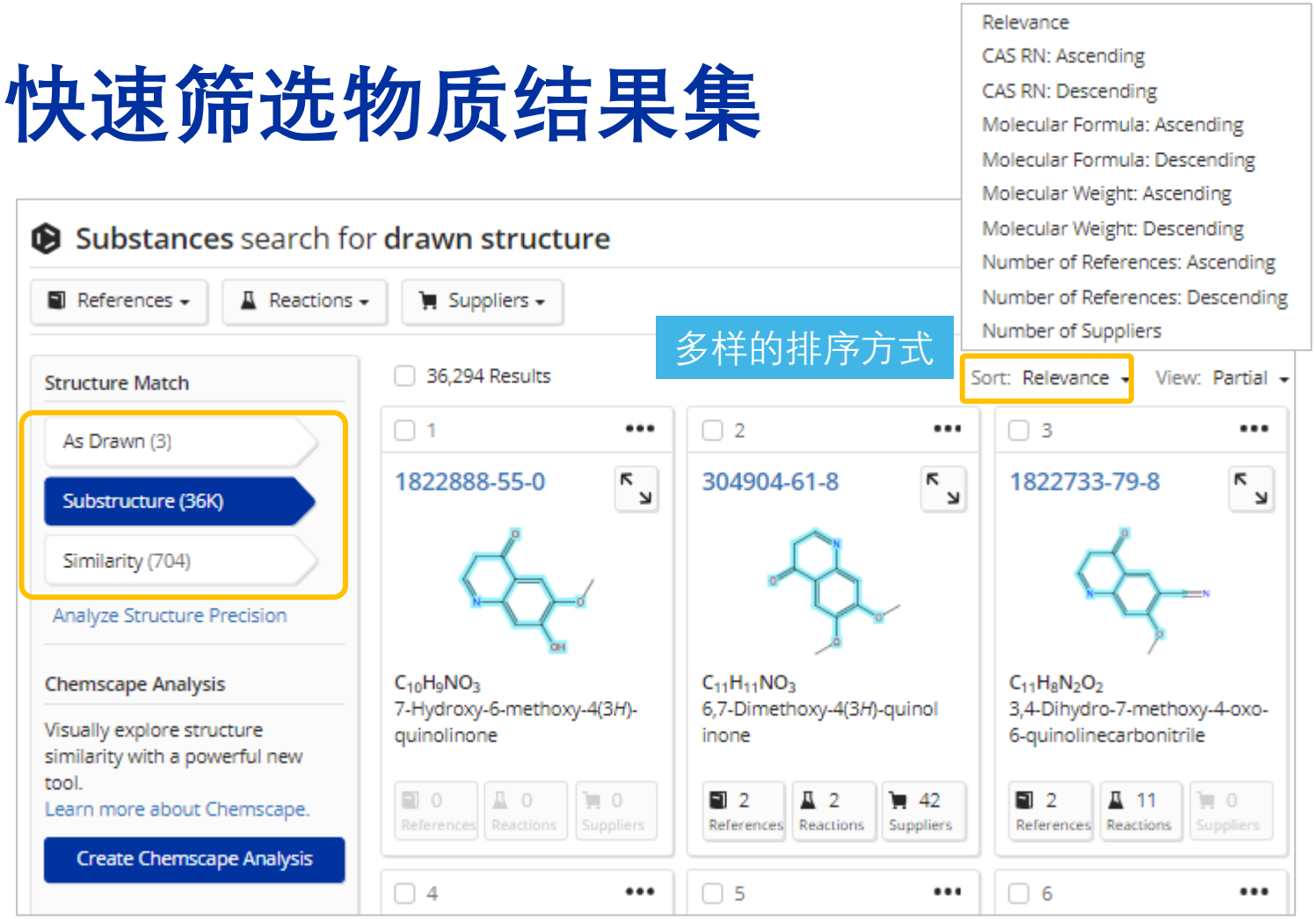
# 物质检索—属性值、谱图数值联用检索

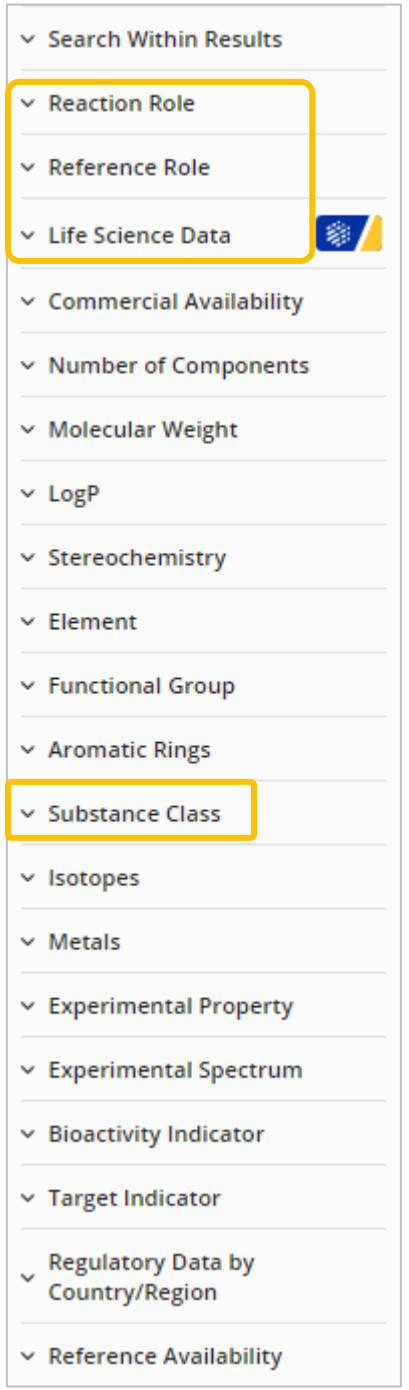



高级检索字段：

- CAS RN（物质、组份）、物质标识符、分子式、文献号、专利号
- 实验谱图：$^{1}H$, $^{13}C$, $^{15}N$, $^{19}F$, $^{31}P$ NMR
- 化学标识符：化学名称、InChI key
- 生物：生物富集因子、LD50
- 化学：Koc, LogD, LogP、溶解度、分子量、pKa、蒸汽压
- 密度属性：密度、摩尔体积
- 电学：电导/电导率、电阻/电阻率
- Lipinski：自由旋转键、H受体/供体
- 磁：磁力矩
- 机械属性：拉伸强度
- 光散射：旋光性、折射率
- 结构：极性表面积
- 热学：熔点、沸点、闪电、玻璃转化温度、蒸发焓

# 快速筛选物质结果集




物质筛选类别:
二次筛选
**反应角色**
**研究角色**
**生物活性数据**
组分数量
分子量
立体化学
含有元素
取代基
芳环数量
**物质类别**
同位素
含有金属
实验属性
实验谱图
GHS危害信息
……

结构检索类别:

- As Drawn：可变结构可变，其他位点锁环锁原子。
- Substructure 亚结构：包含As Drawn结果，有取代基。
- Similarity 相似结构：母体结构可以被取代，也可以被改变的相似结果。

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# 聚类分析选项

**Reaction Role**

- Product (193K)
- Reactant (81K)
- Reagent (7,923)
- Catalyst (5,952)
- Solvent (2,374)

**Substance Class**

- Organic/Inorganic Small Molecule (227K)
- Manual Registration (150K)
- Nucleic Acid Sequence (94K)
- Protein/Peptide Sequence (81K)
- Salt and Compound With (11K)

View All

**Life Science Data**

- Pharmacological Data (1,951)
- ADME (242)
- Toxicity (50)

**Reference Role**

物质在文献中的研究角色

By Count | Alphanumeric

0 Selected

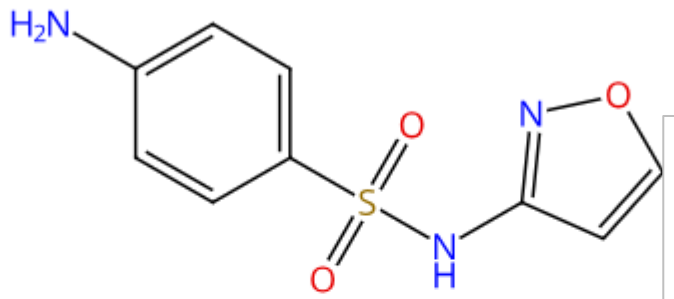
- Preparation (25K)
- Synthetic Preparation (25K)
- Biological Study (20K)
- Uses (20K)
- Therapeutic Use (20K)
- Pharmacological Activity (17K)
- Reactant (5,173)
- Reactant or Reagent (5,173)
- Biological Study, Unclassified (2,998)
- Prophetic Synthesis or Use (1,289)
- Properties (1,003)
- Pharmacokinetics (445)
- Industrial Manufacture (282)
- Analytical Study (262)
- Analyte (228)
- Adverse Effect (194)
- Agricultural Use (130)
- Purification or Recovery (113)
- Process (105)
- Physical, Engineering, or Chemical Process (75)
- Technical or Engineered Material Use (70)
- Combinatorial Study (67)
- Occurrence (58)
- Natural Product Occurrence (52)
- Biological Use, Unclassified (42)
- Modifier or Additive Use (31)
- Analytical Role, Unclassified (27)
- Analytical Reagent Use (26)
- Nanoscale (24)
- Diagnostic Use (18)
- Formation, Non-preparative (18)
- Removal or Disposal (14)
- Byproduct (13)
- Formation, Unclassified (13)
- Cosmetic Use (12)
- Food or Feed Use (10)
- Pollutant (6)
- Reagent (6)
- Analytical Matrix (4)
- Other Use, Unclassified (4)
- Biosynthetic Preparation (3)
- Polymer in Formulation (2)
- Biochemical Process (1)
- Miscellaneous (1)
- Occurrence, Unclassified (1)

Apply | Cancel

# 物质检索—详情页面

CAS Registry Number: 723-46-6

28K | 1,029 | 125



$C_{10}H_{11}N_3O_3S$

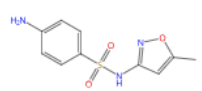
Benzenesulfonamide, 4-amino-*N*-(5-methyl-3-isoxazolyl)- (9CI, ACI)

重要物理性质

| Key Physical Properties | Value | Condit |
|---|---|---|
| Molecular Weight | 253.28 | - |
| Melting Point (Experimental) | 167 °C | - |
| Boiling Point (Predicted) | 482.1±55.0 °C | Press: |
| Density (Experimental) | 1.08 g/cm³ | - |
| pKa (Predicted) | 5.81±0.50 | Most A |

Experimental Properties | Spectra

723-46-6

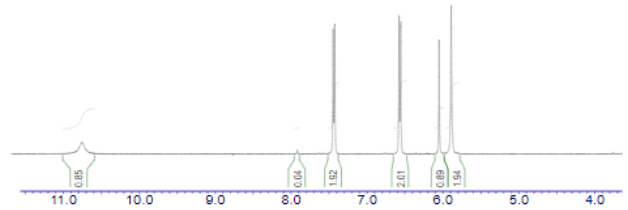


$C_{10}H_{11}N_3O_3S$

CAS Name
Sulfamethoxazole

Conditions
Working Frequency
400 MHz
Solvent
Dimethyl sulfoxide (67-68-5)
Carbon tetrachloride (56-23-5)
Temperature
20 °C

Spectrum Summary
Spectrum ID
F0175-0013
Source
Spectral data were obtained from Life Chemicals




实验谱图

Reset

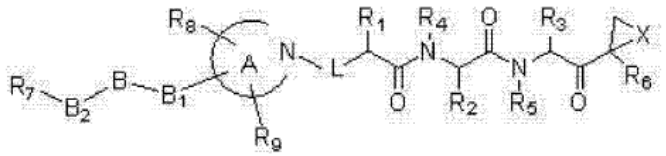
实验属性

- Other Names and
- Experimental Properties
- Experimental Spectra
- Pharmacological Data — CAS LIFE SCIENCES
- ADME — CAS LIFE SCIENCES
- Toxicity — CAS LIFE SCIENCES
- Predicted Properties
- Predicted Spectra
- Bioactivity Indicators
- Target Indicators
- Regulatory Information
- GHS Hazard Statements
- Additional Details

# CAS Markush检索，助力结构查新



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

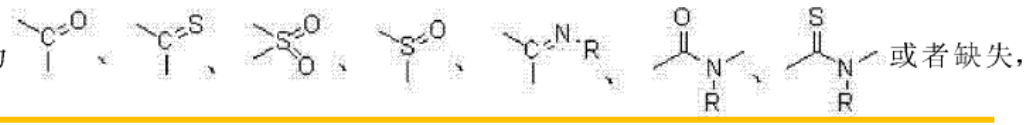
其中：

$R_1$，$R_2$，$R_3$ 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

## 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 登记号

## 预测性物质[Prophetic Substance]

- 使用Markush结构陈述的预测物质，一个Markush可以陈述上千甚至更多的结构
- 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登记号
- Markush检索，能检索到通过Substance可能检索不到的结构

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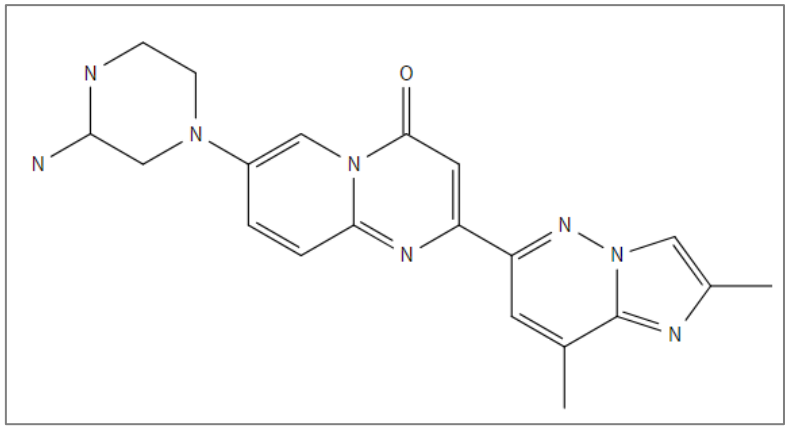
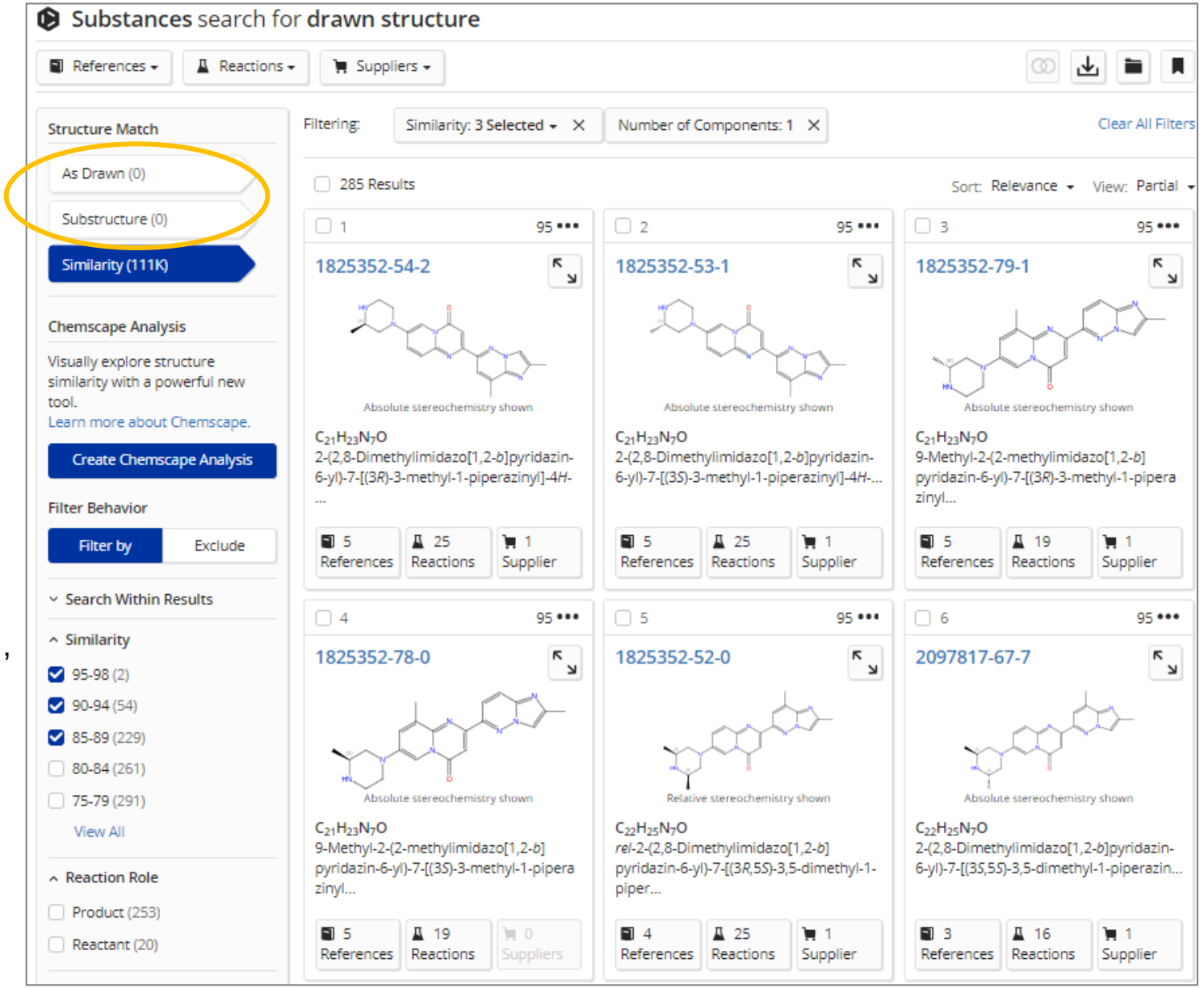
# CAS Markush检索

该结构进行精准结构，亚结构均无结果，能够确定它没有被公开吗？

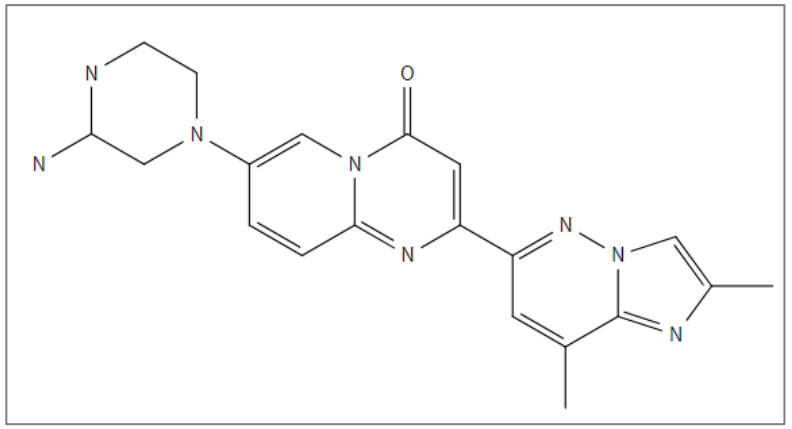


此时您检索的是CAS REGISTRY数据合集，它是专利审查员的重要参考依据之一。



# CAS Markush检索

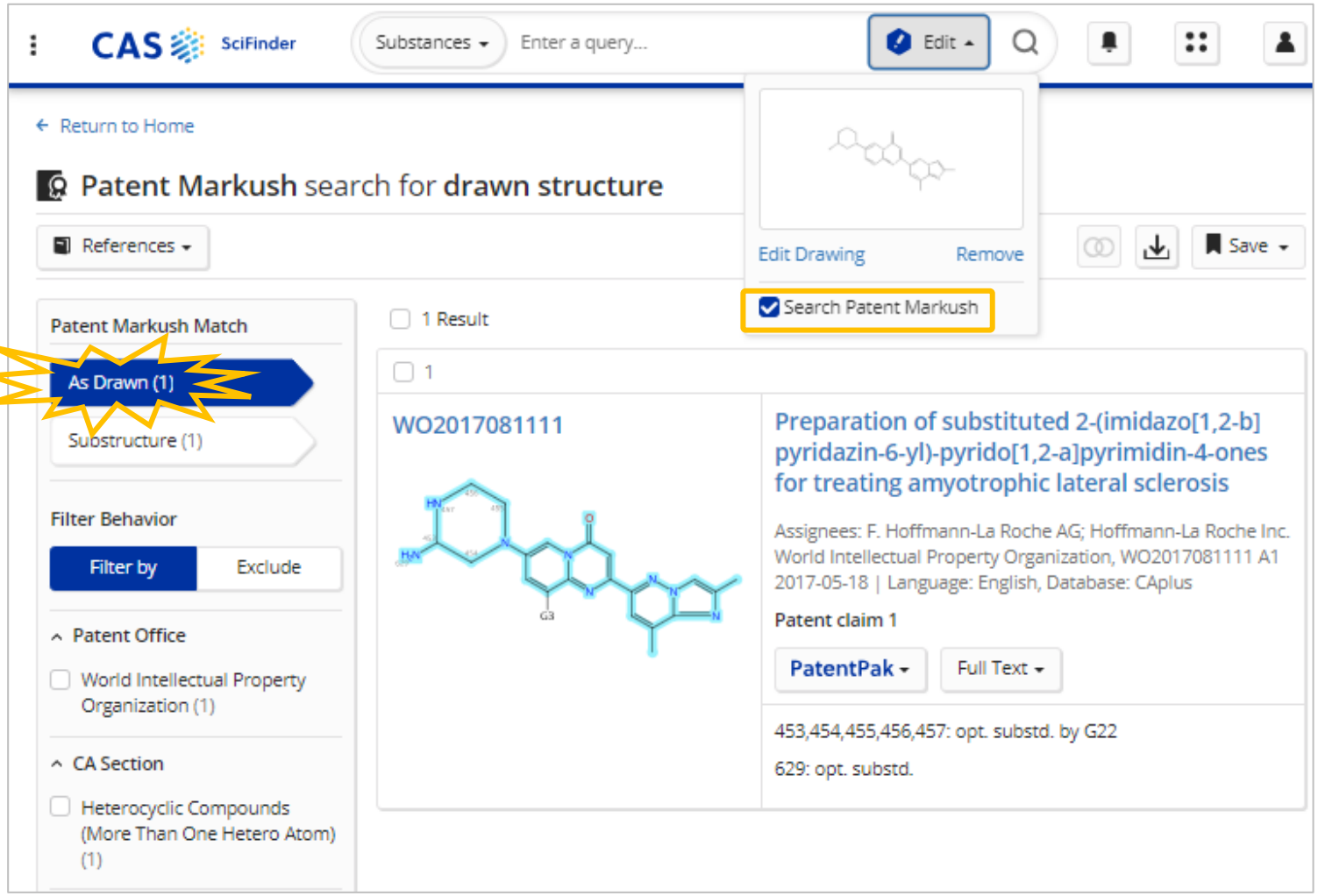
通过专利Markush结构检索，获得高度相关的专利结果



此时您检索的是Markush数据合集，

它也是专利审查员的重要参考依据。

为了尽可能完整地获得公开的结构信息，需要同时进行Substance和Markush结构检索；根据需要，可进行文献检索补充。







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# 小结

- 物质的检索方式：灵活使用CAS科学家增值标引的信息，充分利用结构绘制工具，合理扩大或限定结构检索范围
- 检索结果的筛选：丰富的聚类分析选项，如Substance Role、Reference Role、Substance Class等。
- 物质详情速览：物质详情页解读，快速便捷地获取物质理化性质及实验谱图等。
- CAS Markush (MARPAT)：REGISTRY与MARPAT等数据库是专利审查员进行专利实查的重要参考依据，可以通过结构检索获取确切结构和预测结构两部分结果，合并后即可获取结构查新全景。

# 大纲

- CAS及CAS SciFinder Discovery Platform (Academic)简介
- 科研信息的高效查阅
  - 全面的文献调研与拓展助力开题
  - 多角度出发检索物质结构及相关属性
  - 生物序列检索方法与结果分析
  - 探索实验方案以获取制备及其他实验详情
- 常见问题Q&A

# 您可能会感兴趣：

- 如何从已知序列片段出发，检索**对应序列**？
- 如何获取序列相同但**修饰不同**的结果？
- 对含有**可变部分**的生物序列，如何进行检索？
- 如何对多个**CDR**序列进行检索？
- 如何通过**物质**或**文献**调研感兴趣的序列？
- ……




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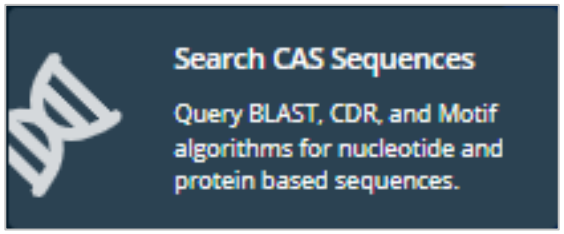
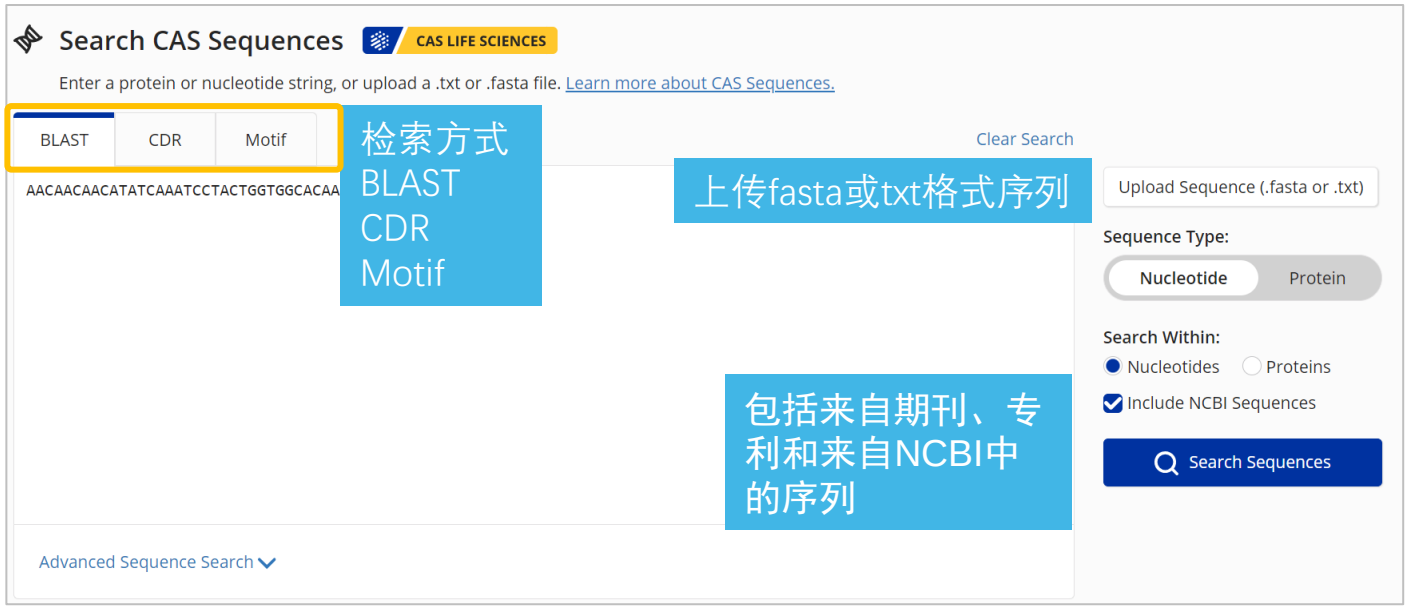
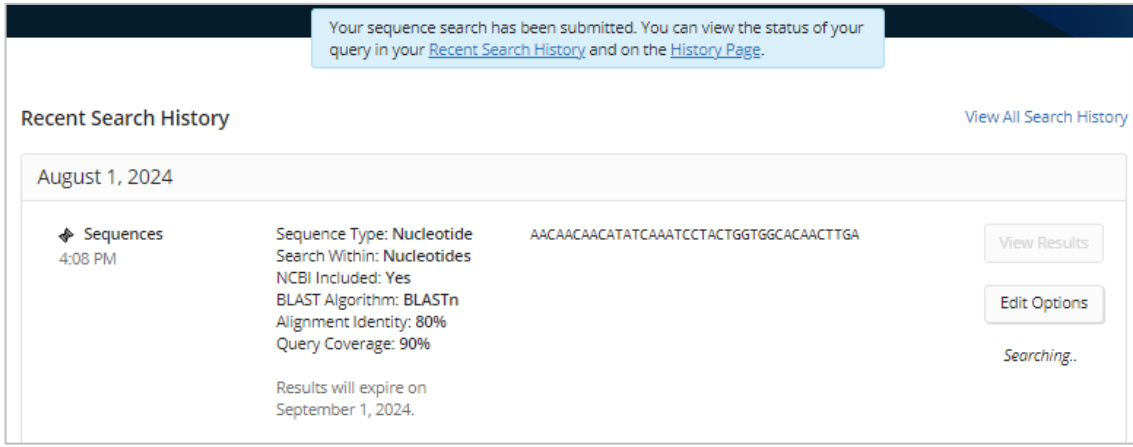
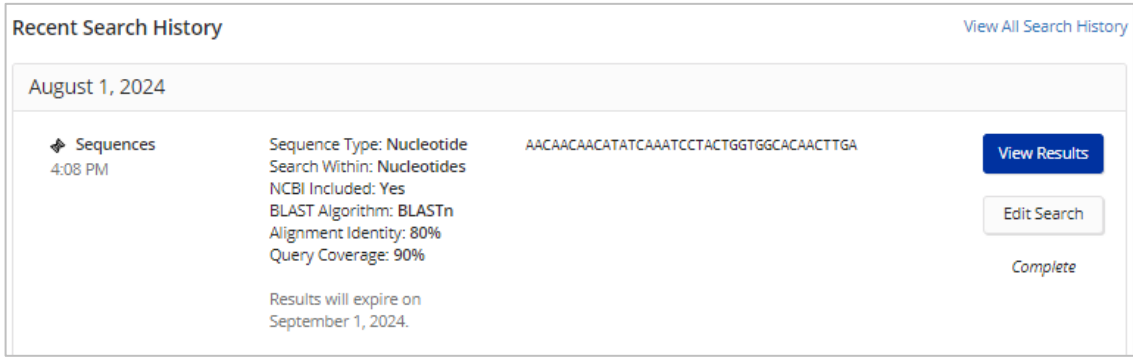
# CAS Sequences——序列检索




支持四种检索选择：
Protein-Protein
Protein-Nucleotides
Nucleotide-Nucleotides
Nucleotide-Proteins







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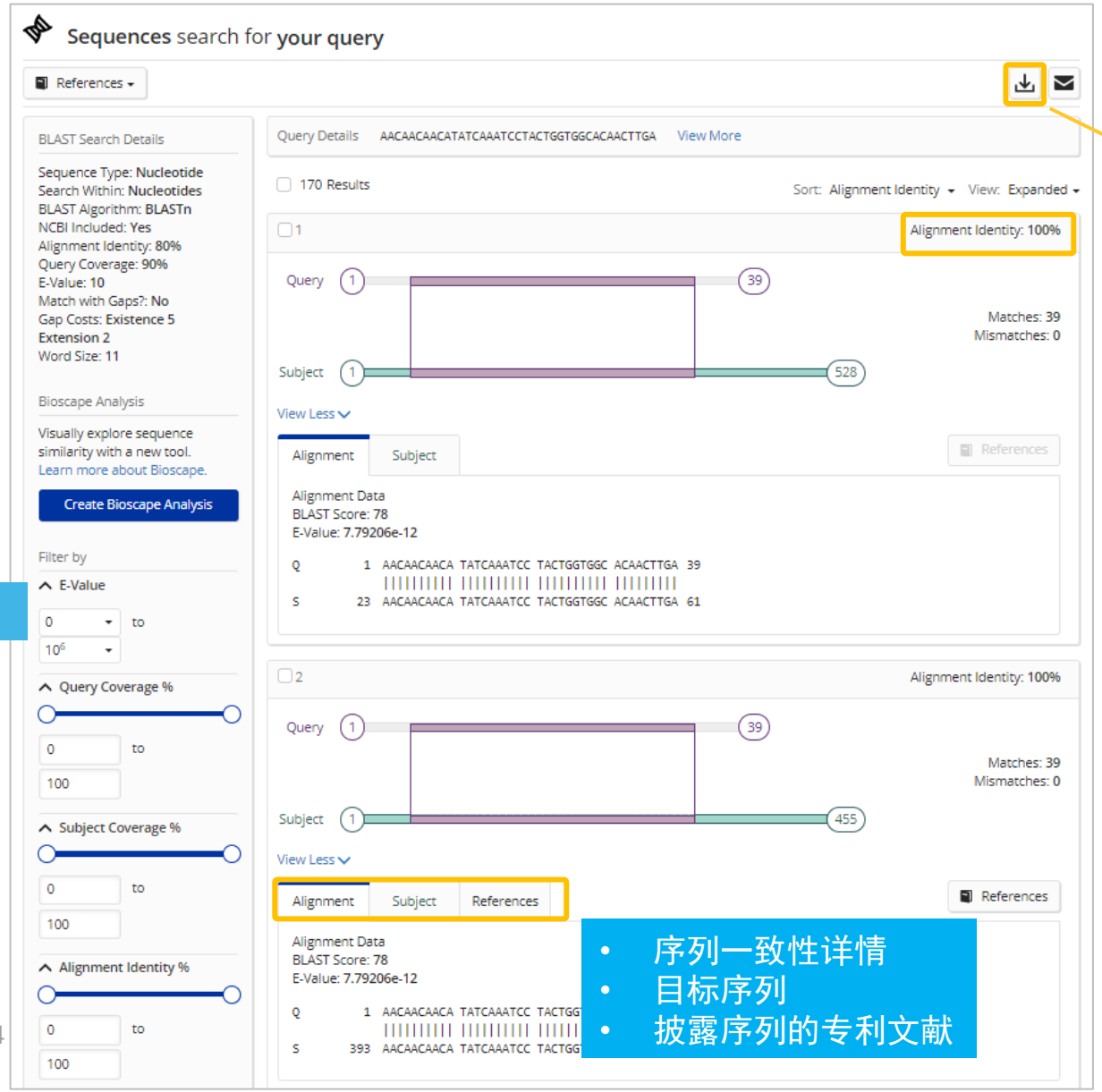
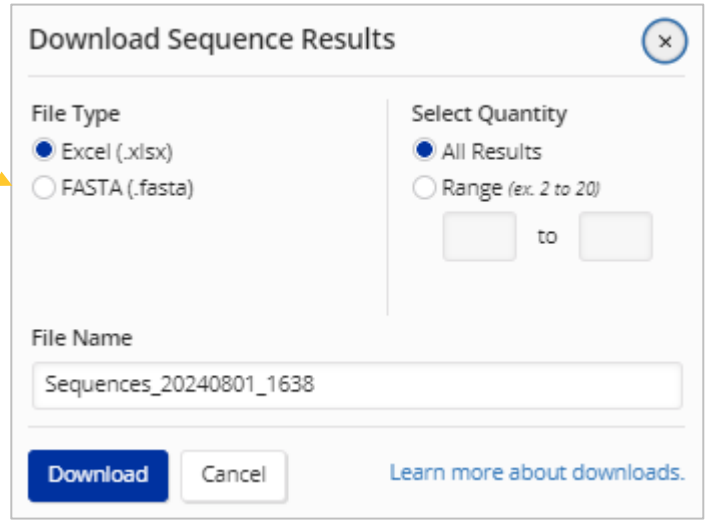
# CAS Sequences——BLAST检索结果




结果筛选




检索结果下载：
- 比对详情
- 序列长度参数
- 相关专利号
- 专利中的序列编号等

支持Excel或FASTA格式

- 序列一致性详情
- 目标序列
- 披露序列的专利文献

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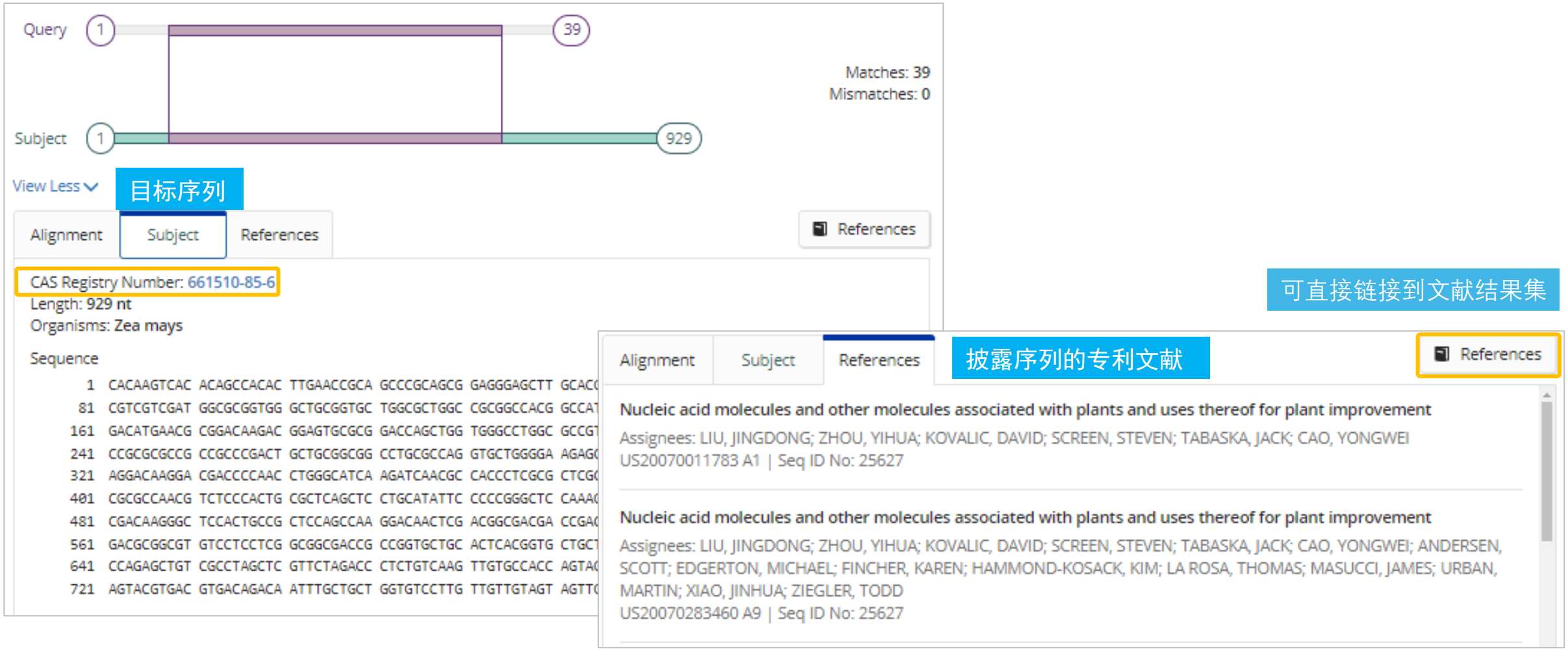
# CAS Sequences——BLAST检索结果







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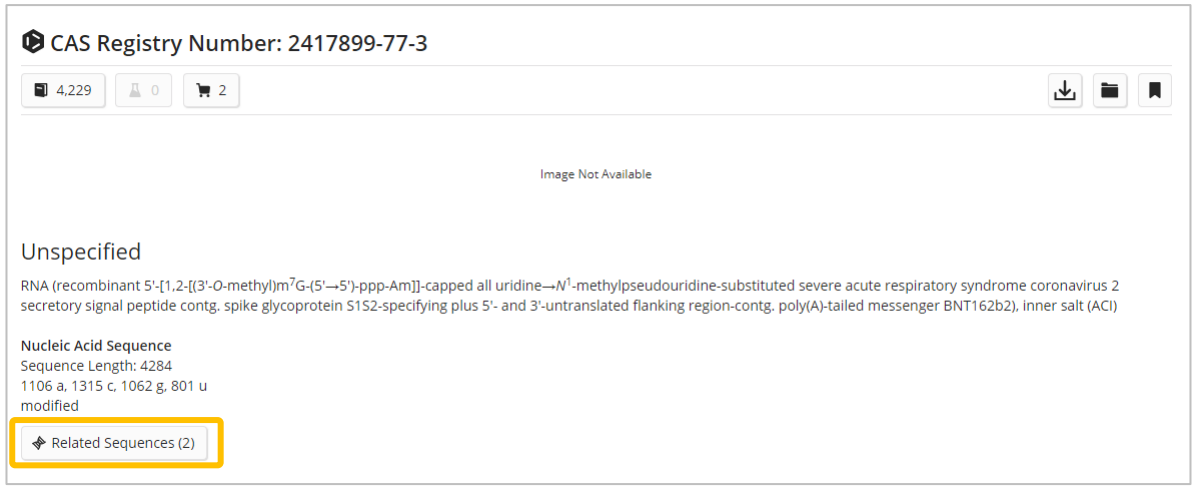
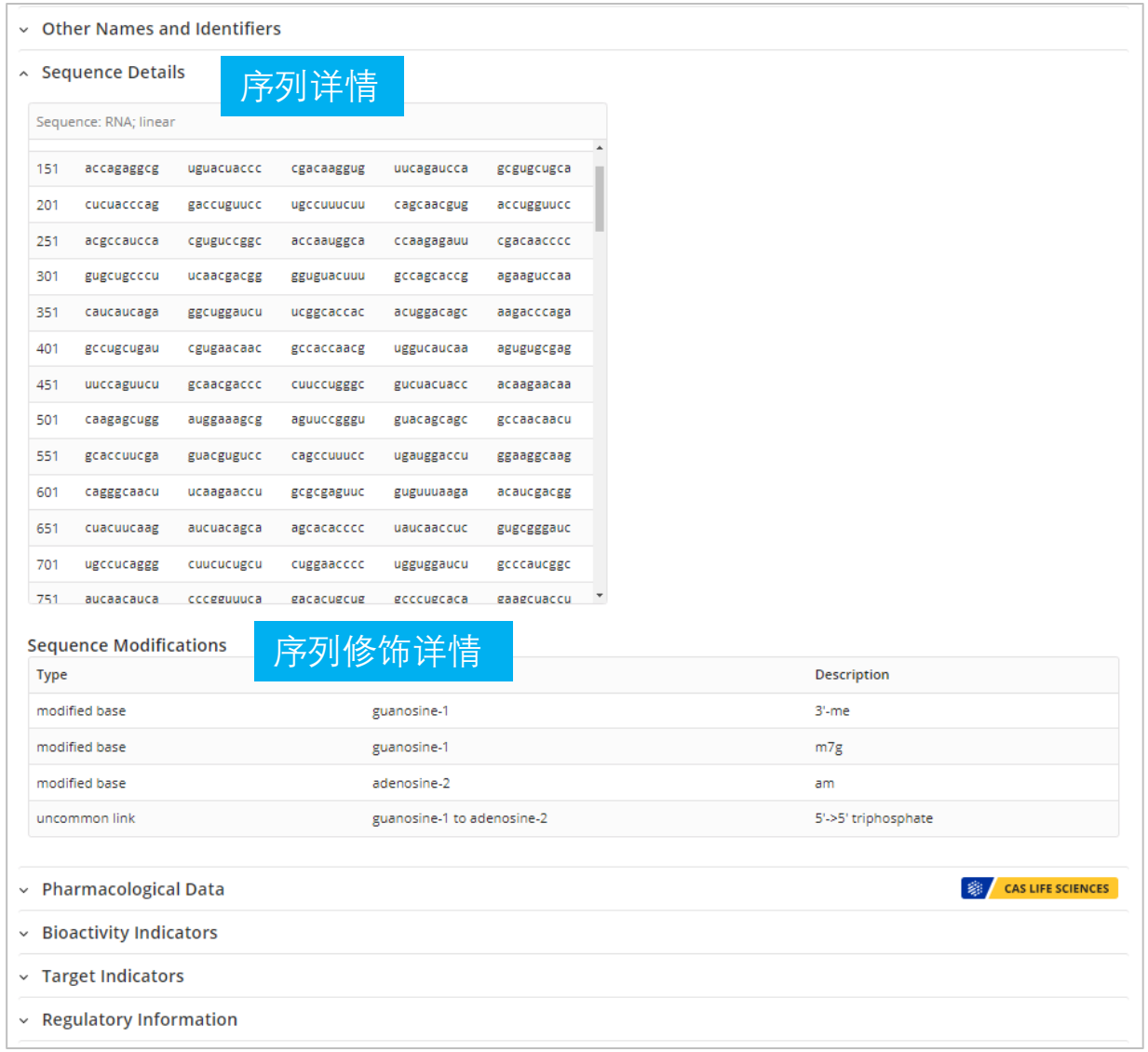
# 序列详情及相关序列




获取序列一致、修饰不同或来自不同文献的相关序列







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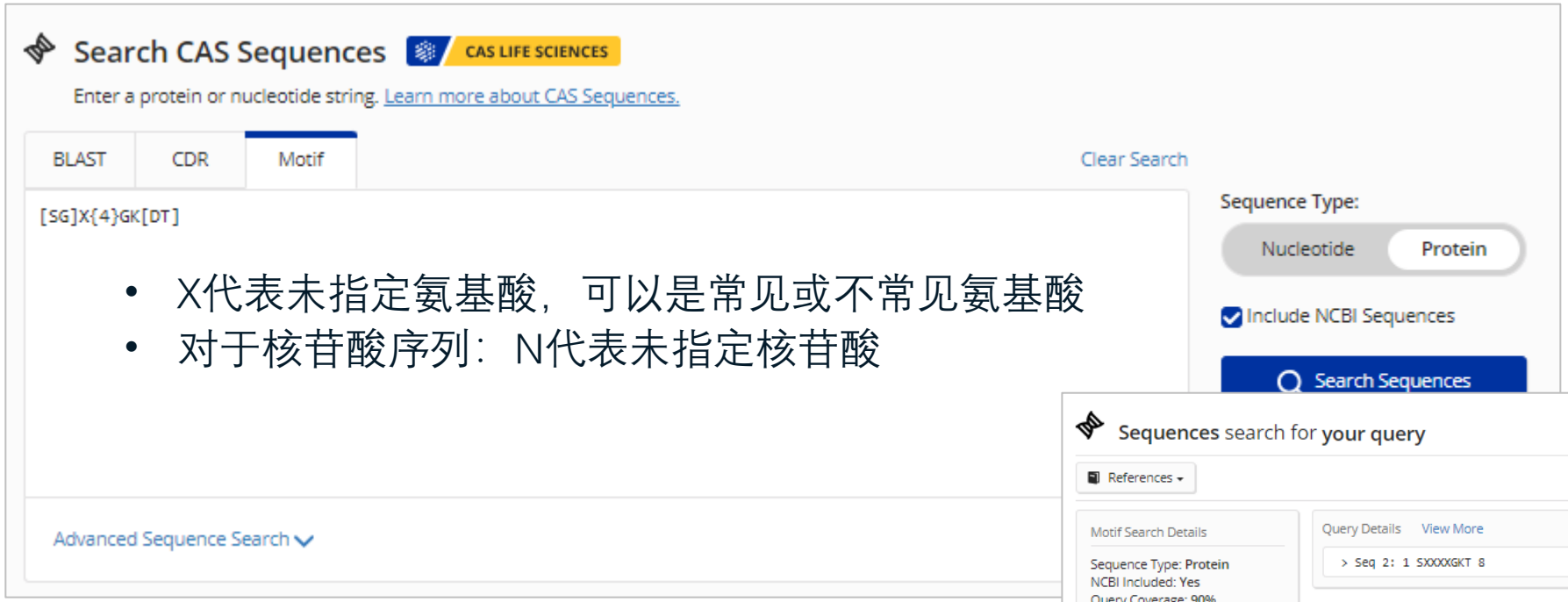
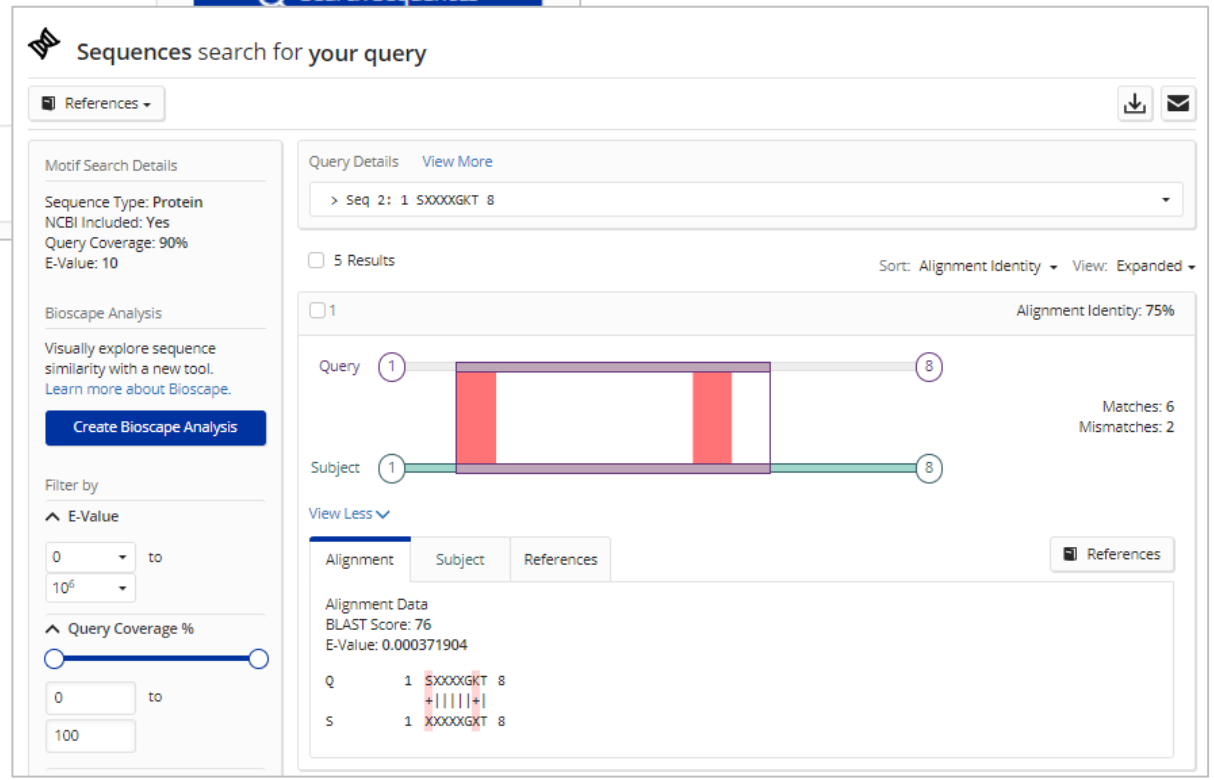
# CAS Sequences——Motif检索结果




- X代表未指定氨基酸，可以是常见或不常见氨基酸
- 对于核苷酸序列：N代表未指定核苷酸

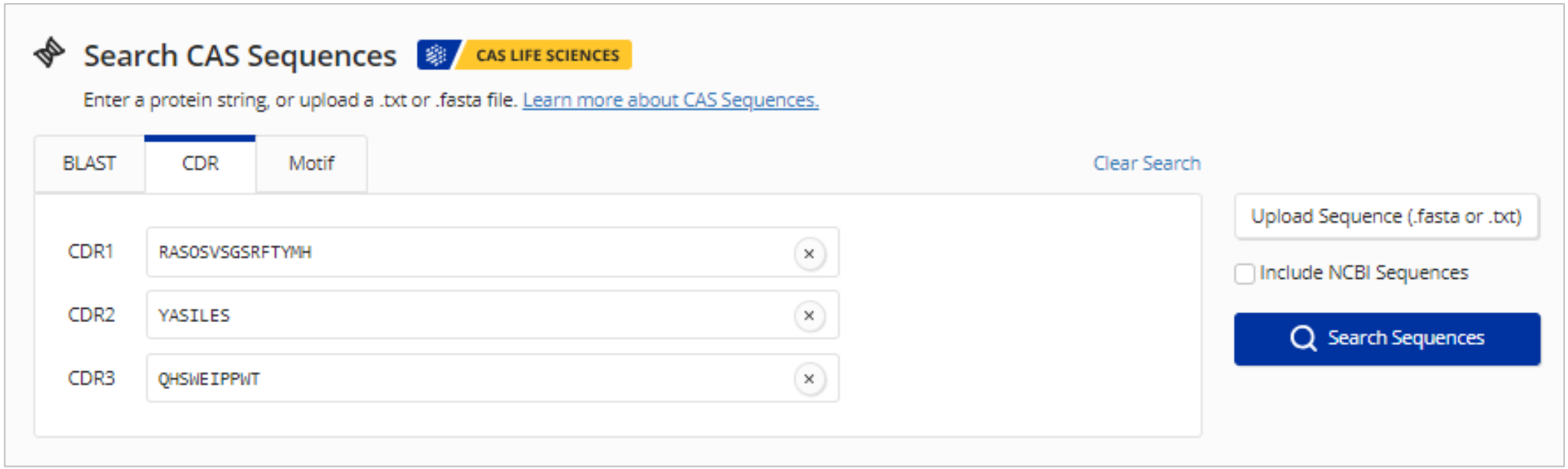



Motif中有可变部分，可借助符号来表示：

- **“[ ]”中括号**：代表或者，表示出现在该位置的氨基酸或核苷酸是括号中的任意一个
- **“{ }”大括号**：代表氨基酸或核苷酸的重复次数。其中字段可用逗号隔开，{2,6}表示在大括号左边紧密相连的氨基酸可重复2-6次

# CAS Sequences——CDR检索结果

CDR (complementarity – determining regions): 抗体或细胞中的互补决定区




支持单个或多个CDR序列检索并用

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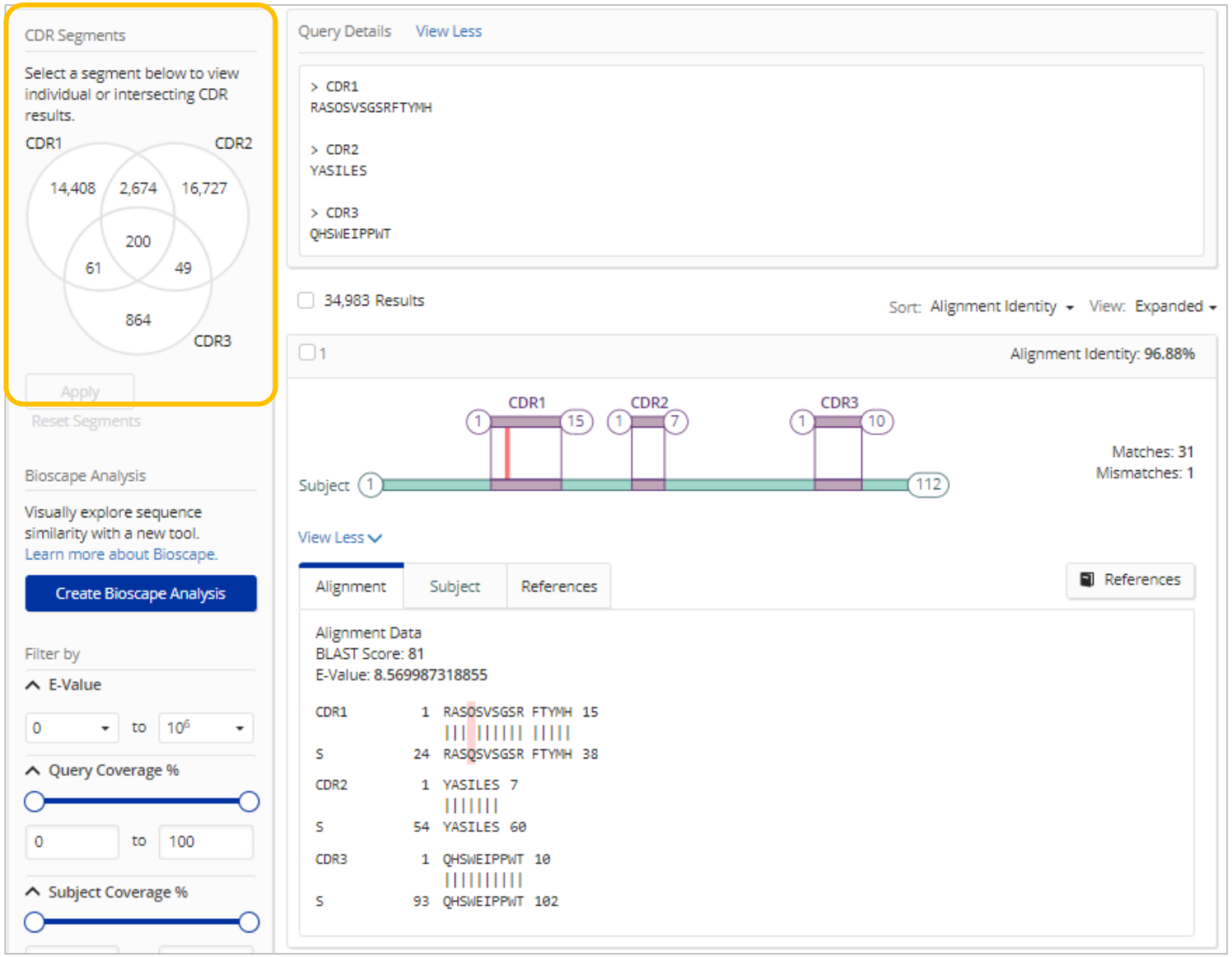
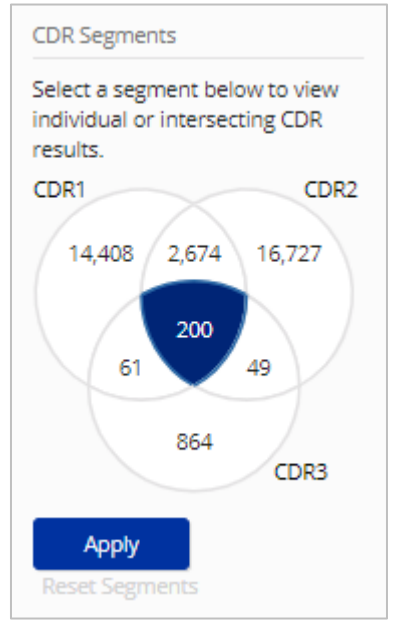
# CAS Sequences——CDR检索结果




CDR Segments：

- 匹配到一个或者多个CDR的subject序列的序列数量
- 可根据已知信息和需求查看1-3个CDR被包含的序列结果

Reset segments：

- 重新选择查看匹配的序列结果

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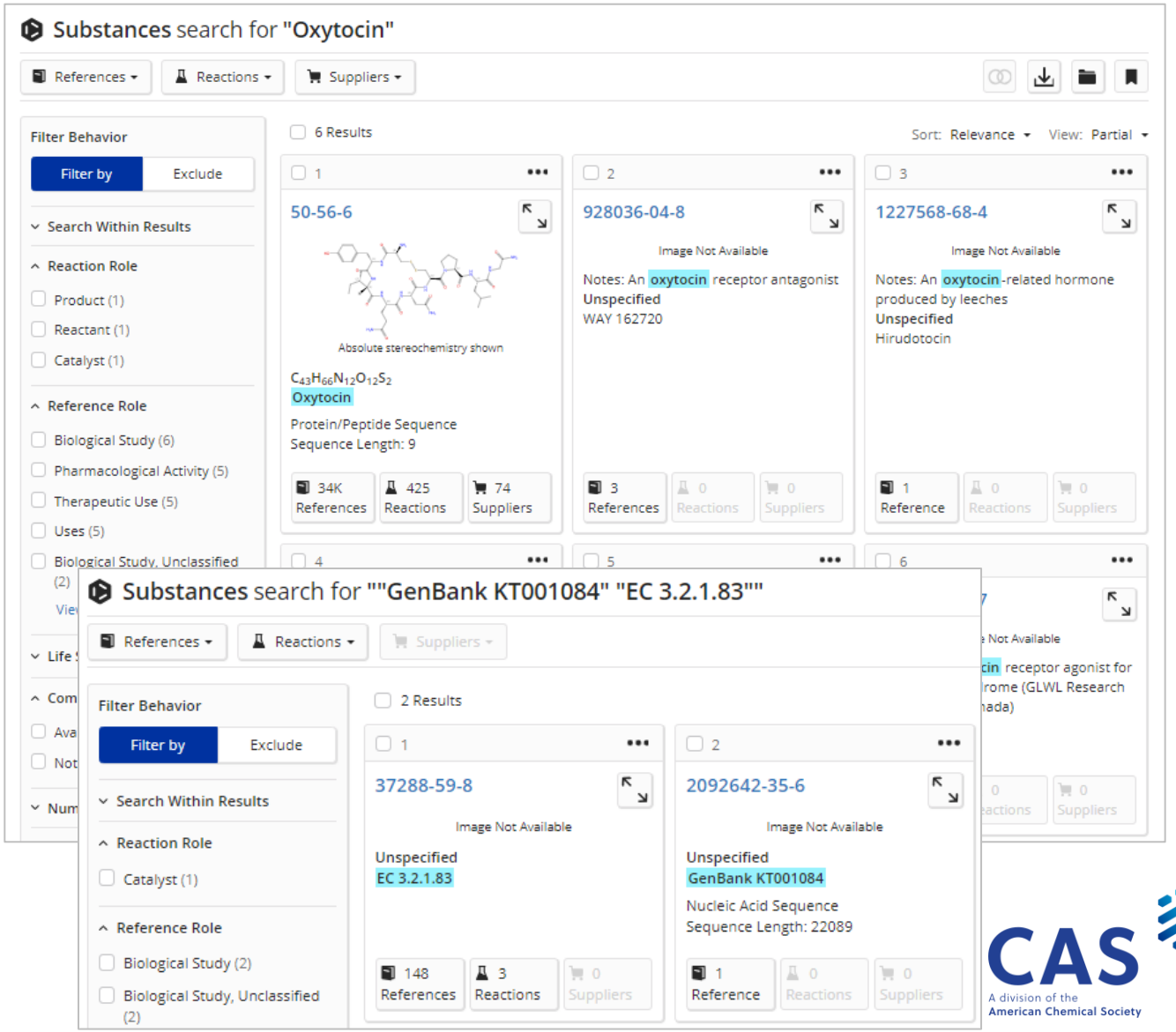
# 根据物质名称和识别符进行生物分子检索

- Common name: e.g. Oxytocin
- Brand name (drug name): e.g. Rituxan
- Generic name: e.g. Adalimumab
- CAS Registry Number: e.g. 219808-29-4
- GenBank Number: e.g. GenBank KT001084
- EC number：e.g. EC 3.2.1.83







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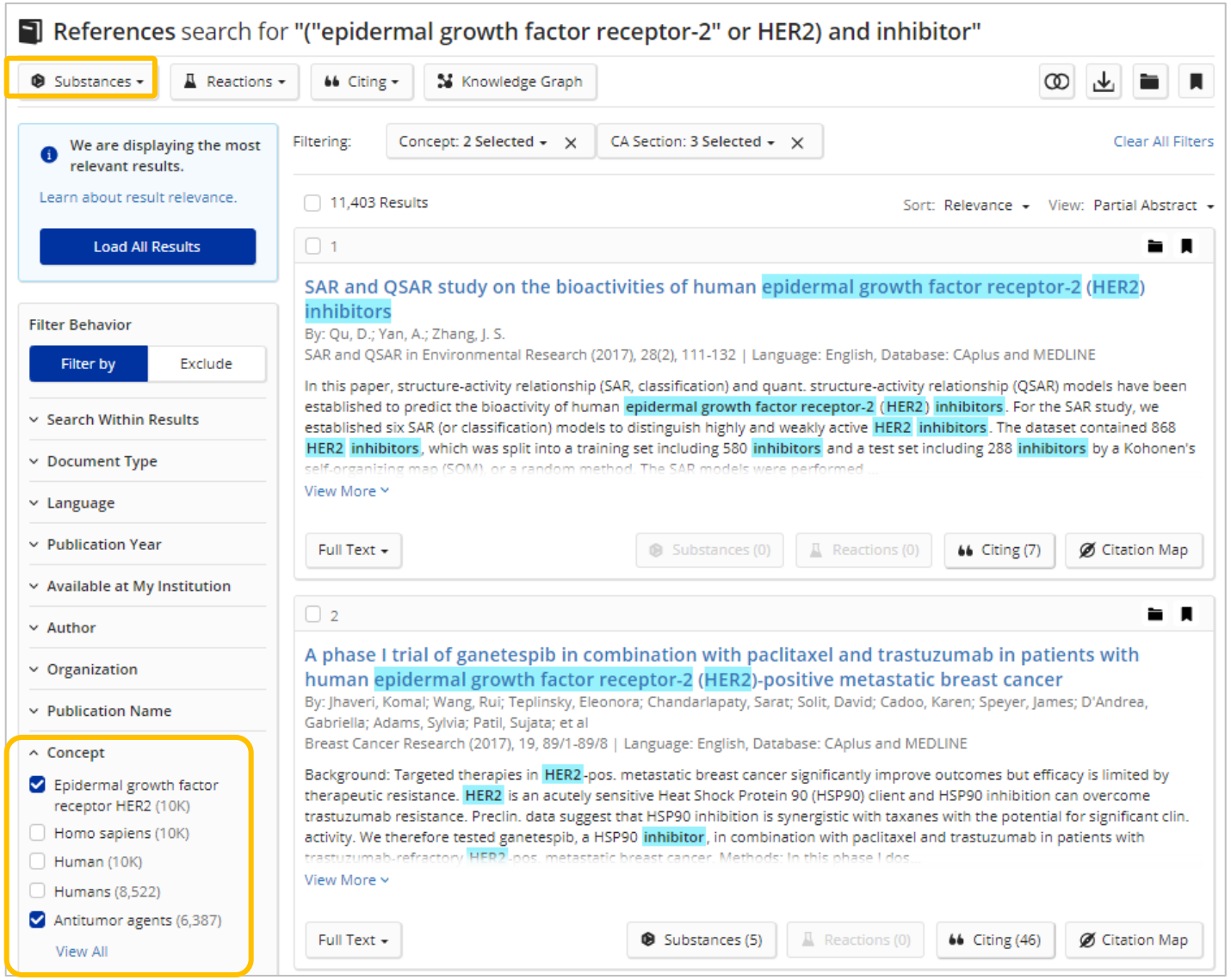
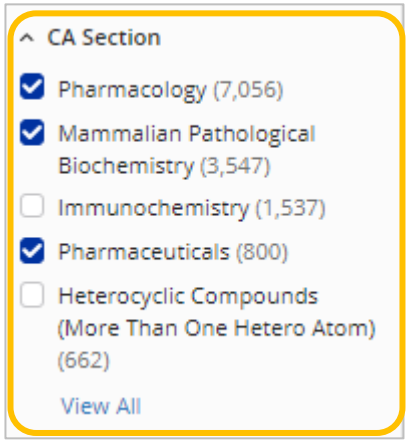
# 根据文献主题词检索，再获取物质信息

主题词示例：

("epidermal growth factor receptor-2" or HER2) and inhibitor







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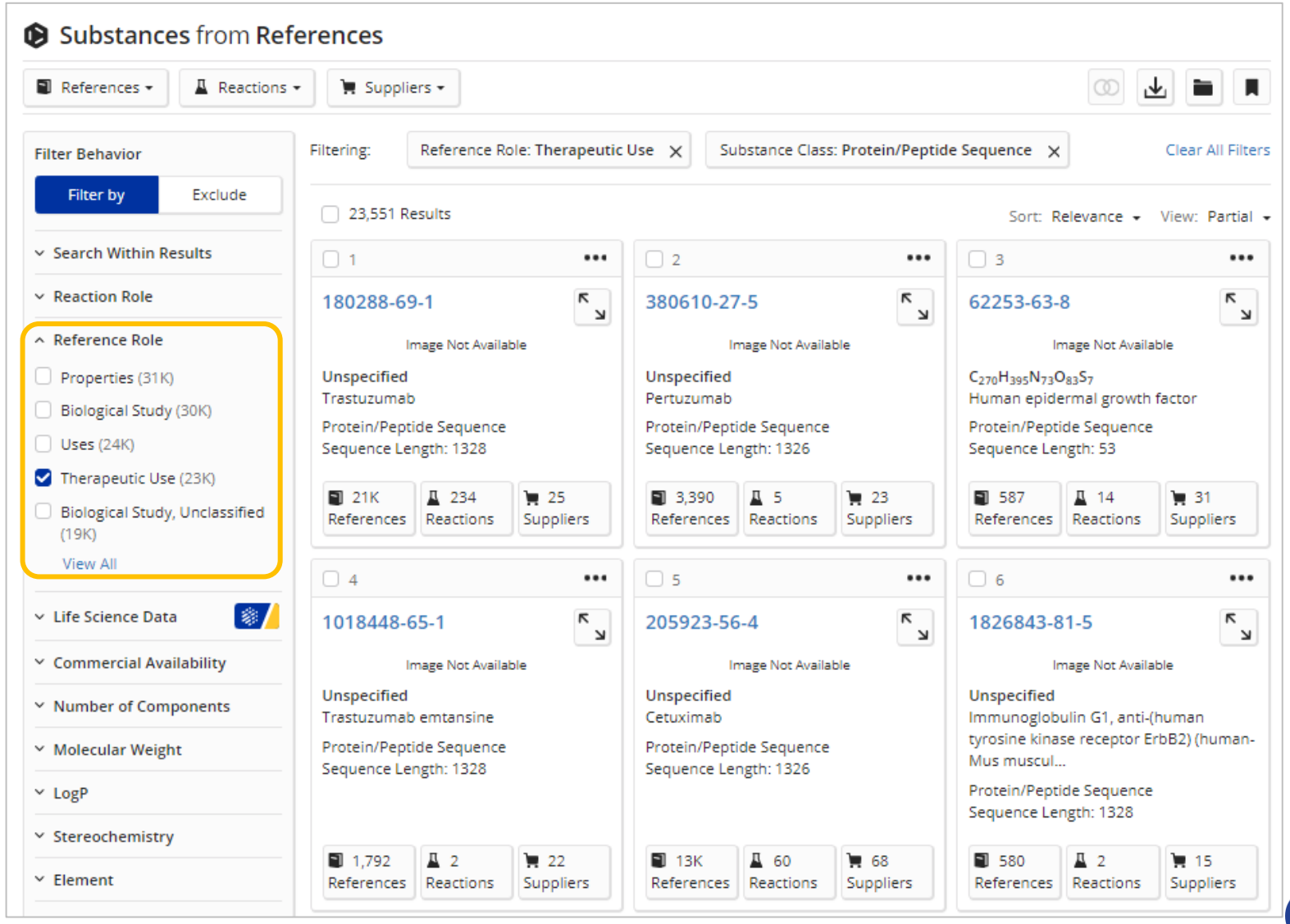
# 根据文献主题词检索，再获取物质信息







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# 小结

- CAS Sequences检索：BLAST, CDR, Motif，可以针对DNA/RNA的核苷酸、多肽/蛋白的氨基酸序列进行检索，也可以对相同序列不同修饰的结果进行拓展。Motif适合短序列检索，并且支持可变部分输入。CDR可根据已知信息和需求查看1-3个CDR被包含的序列结果。
- 通过物质检索序列：通过常用名，品牌名，通用名，CAS登记号，GenBank编号，EC编号等直接检索序列。
- 通过文献间接获取序列：基于CAS的数据关联，从相关的研究文献中获取序列相关信息，并通过聚类分析选项进行筛选。

# 大纲

- CAS及CAS SciFinder Discovery Platform (Academic)简介
- 科研信息的高效查阅
  - 全面的文献调研与拓展助力开题
  - 多角度出发检索物质结构及相关属性
  - 生物序列检索方法与结果分析
  - 探索实验方案以获取制备及其他实验详情
- 常见问题Q&A

# 您可能会感兴趣：

- 如何从我感兴趣的底物、产物或催化剂出发，找到**关联的反应**？
- 如何查找涉及**机理研究**的反应？或**人名反应**？
- 如何在大量反应结果中，**快速找到**最想要的反应？
- 如何设计新化合物的**逆合成**路线？
- 具体的**实验方案**怎么查、怎么选？
- ……




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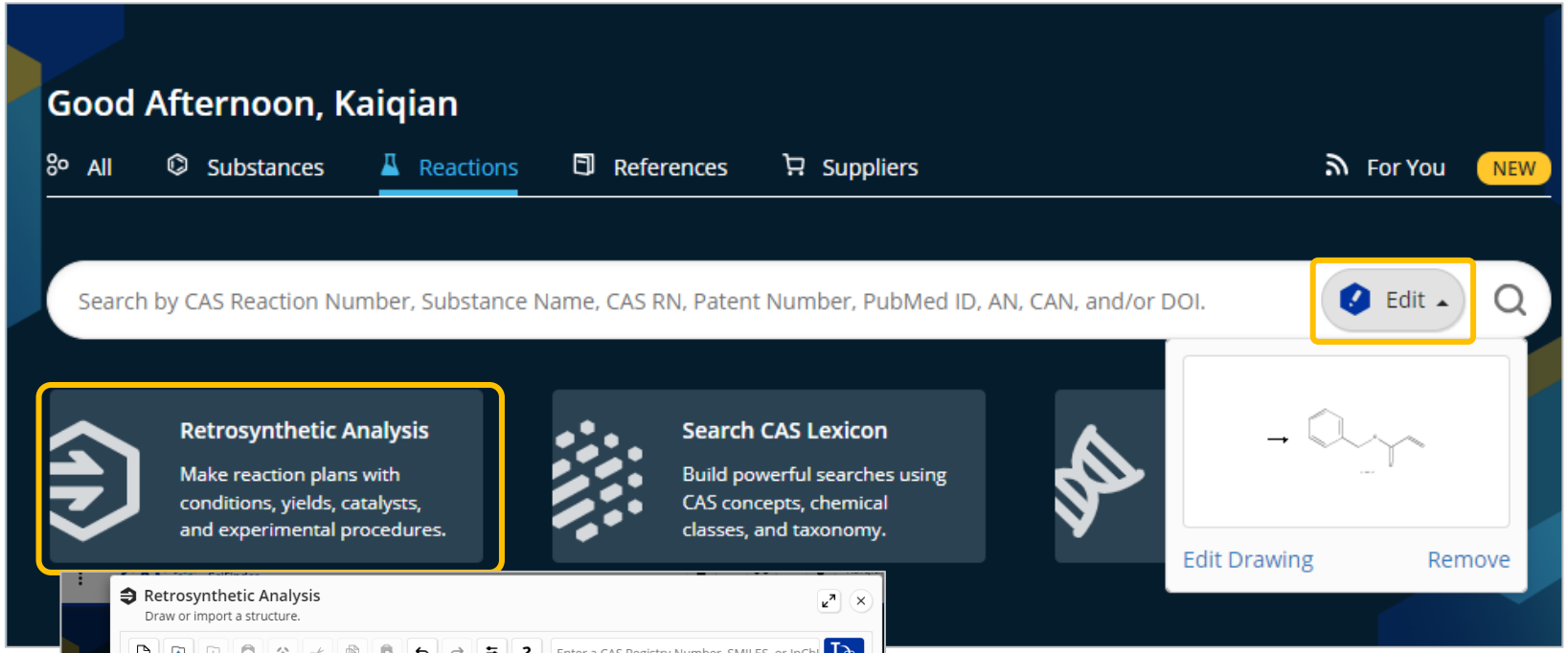
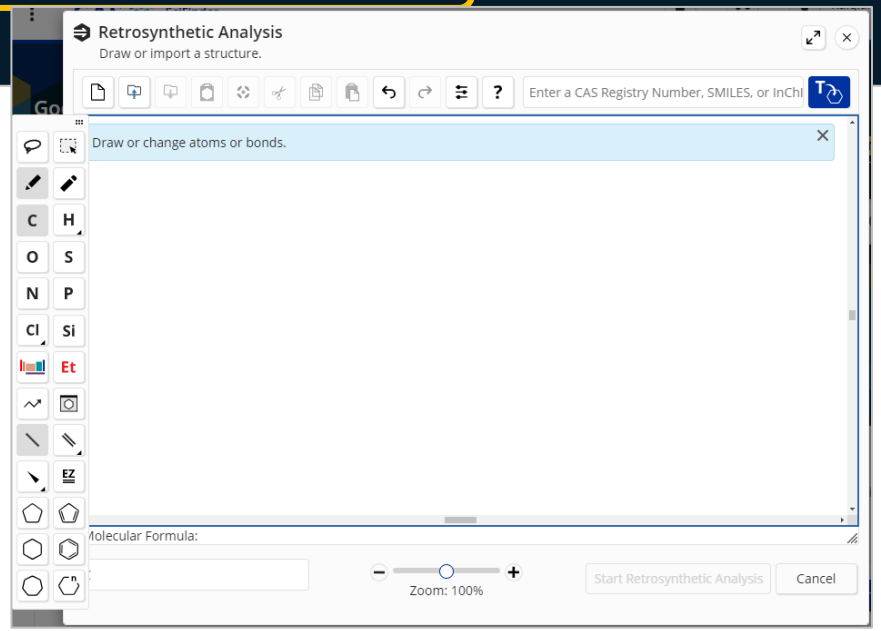
# 反应的获取方法——直接检索




直接进行Reaction检索




通过Retrosynthesis Plan
获取逆合成反应路线



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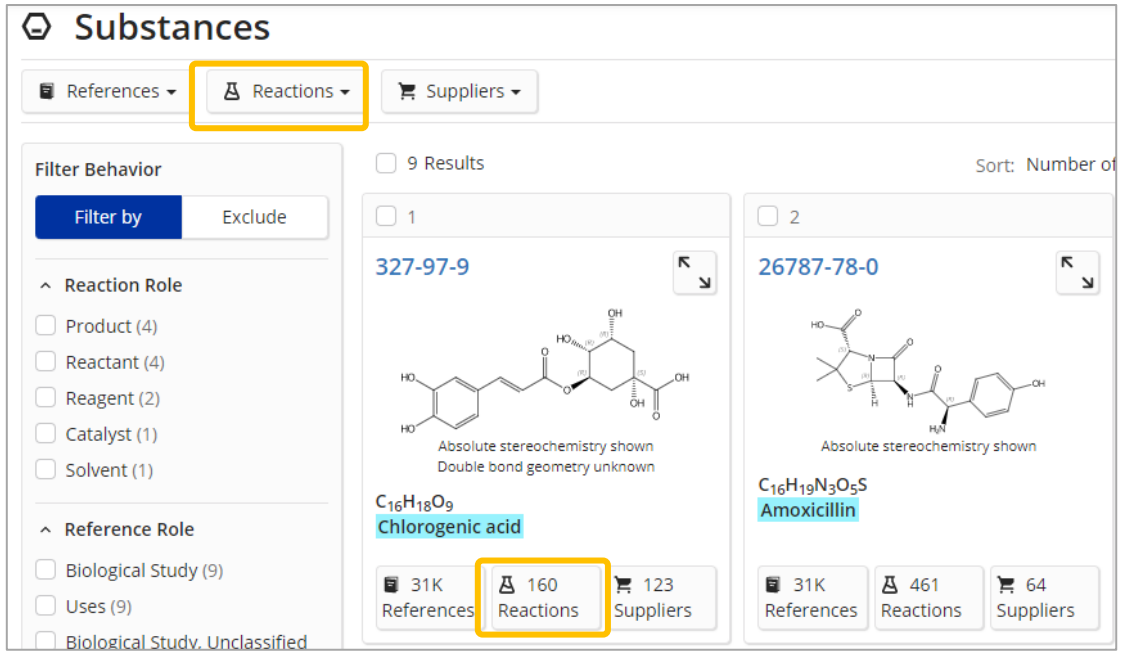
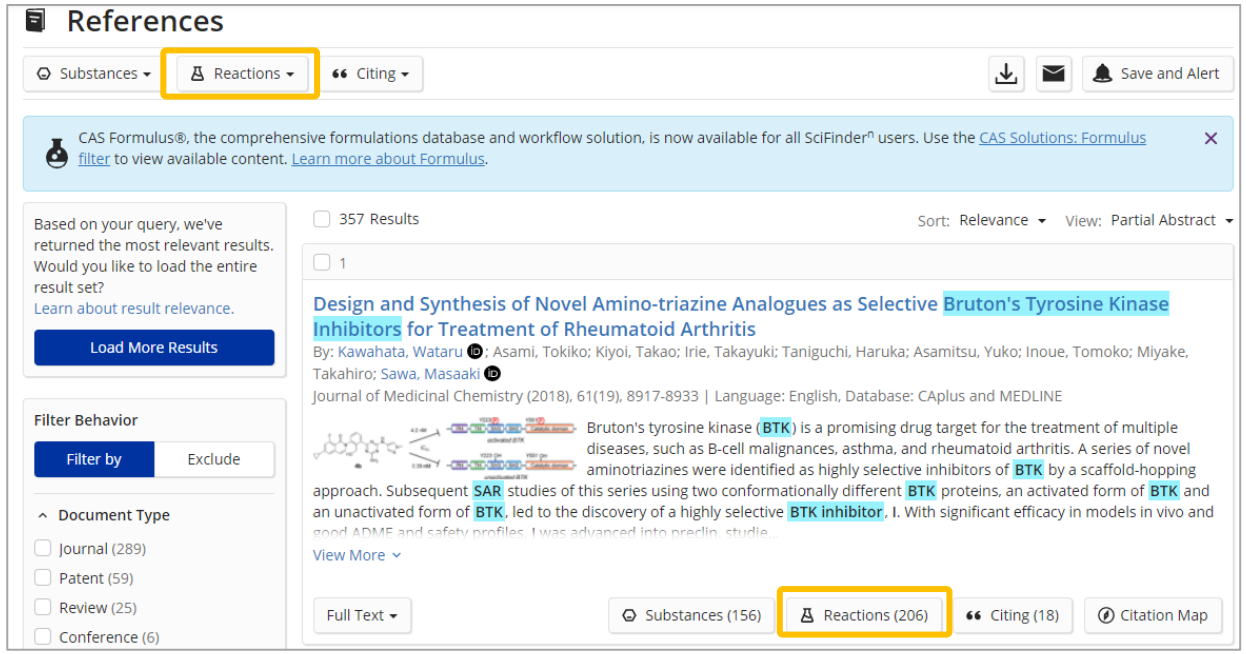
# 反应的获取方法——间接检索

通过物质获取反应




通过文献获取反应







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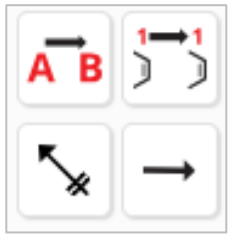
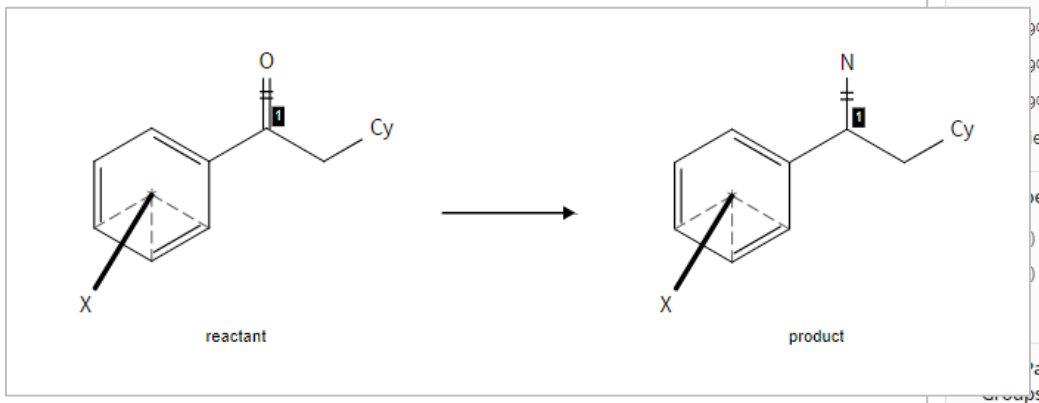
# 使用绘制反应式、底物或产物检索反应

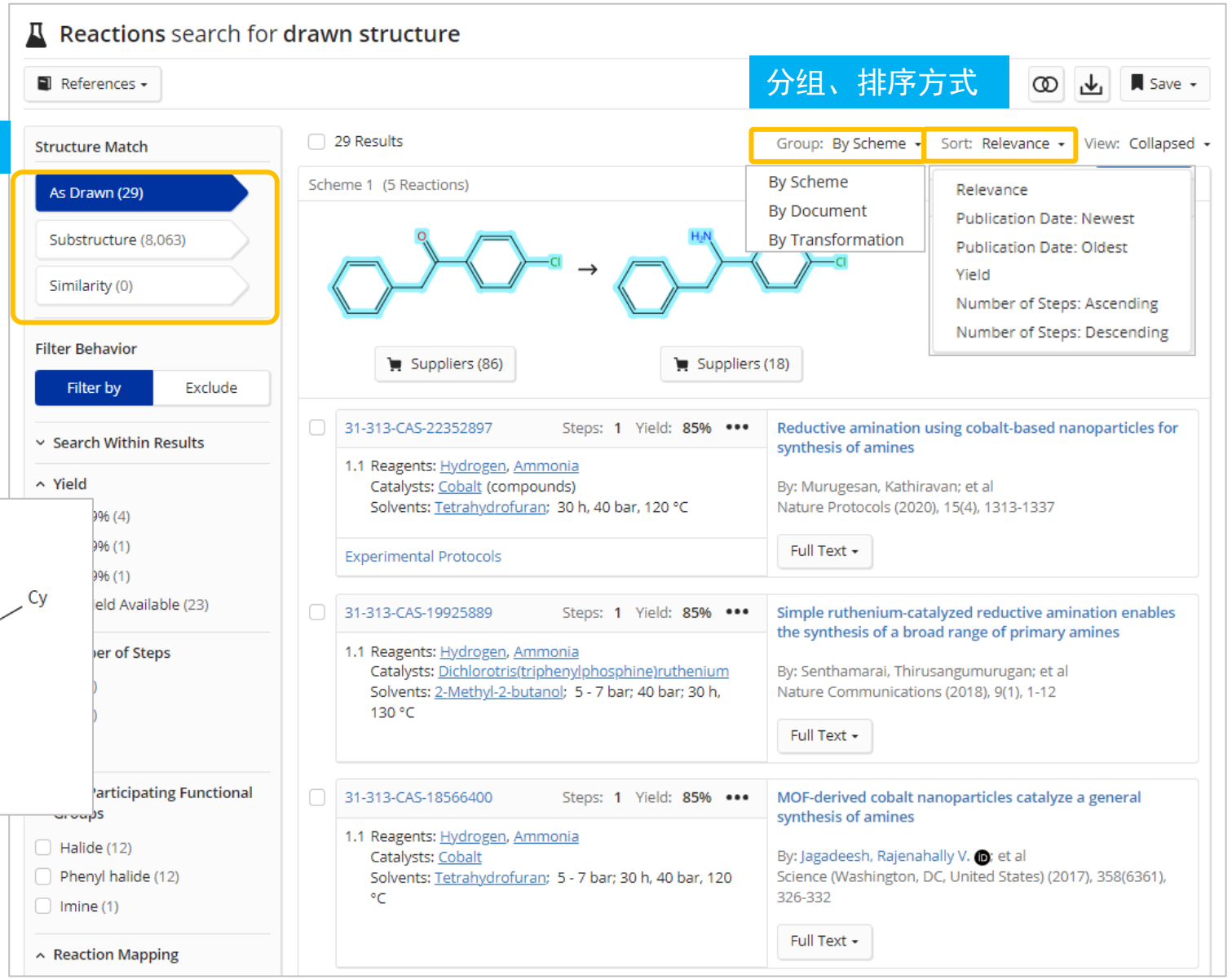




反应角色定义工具
反应原子标记工具
化学键标记工具
反应箭头

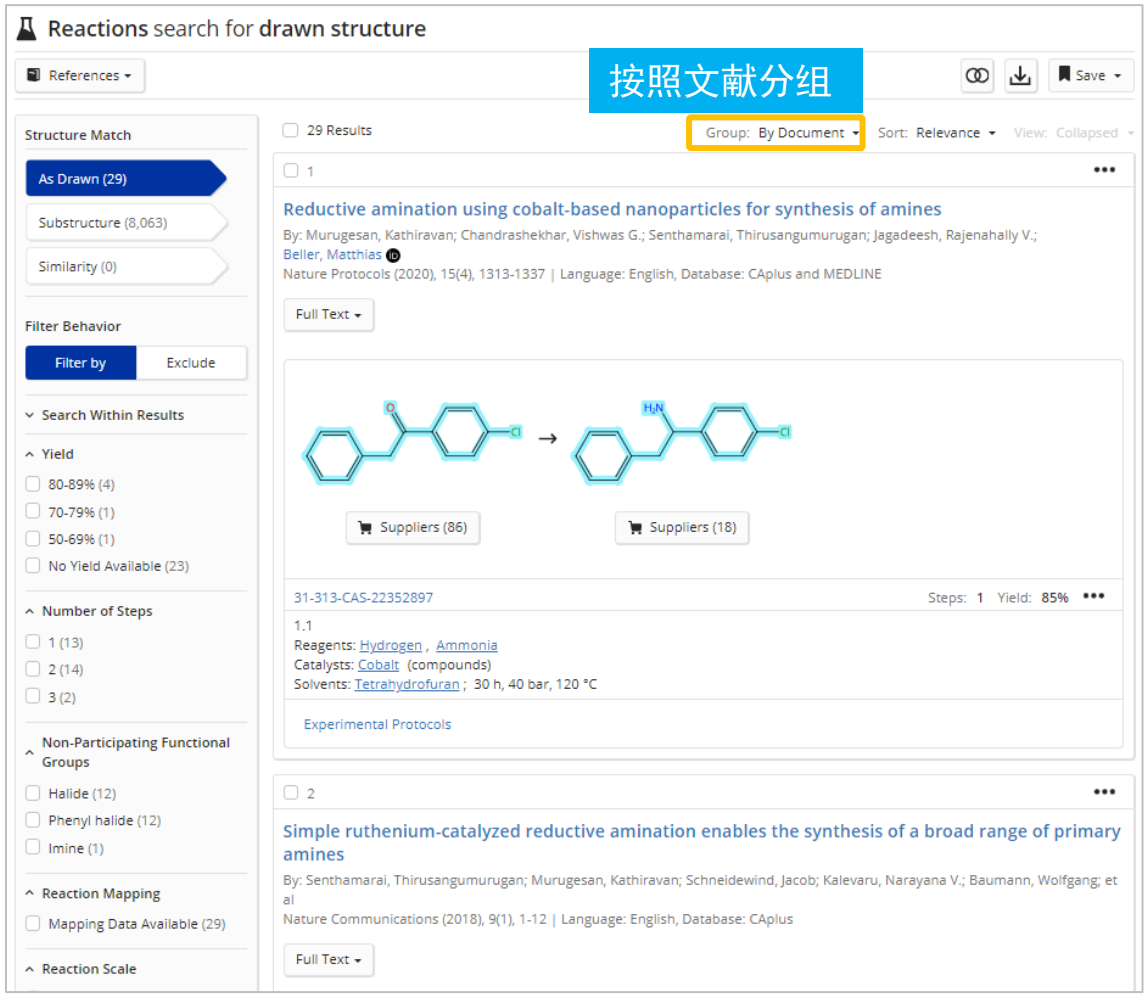


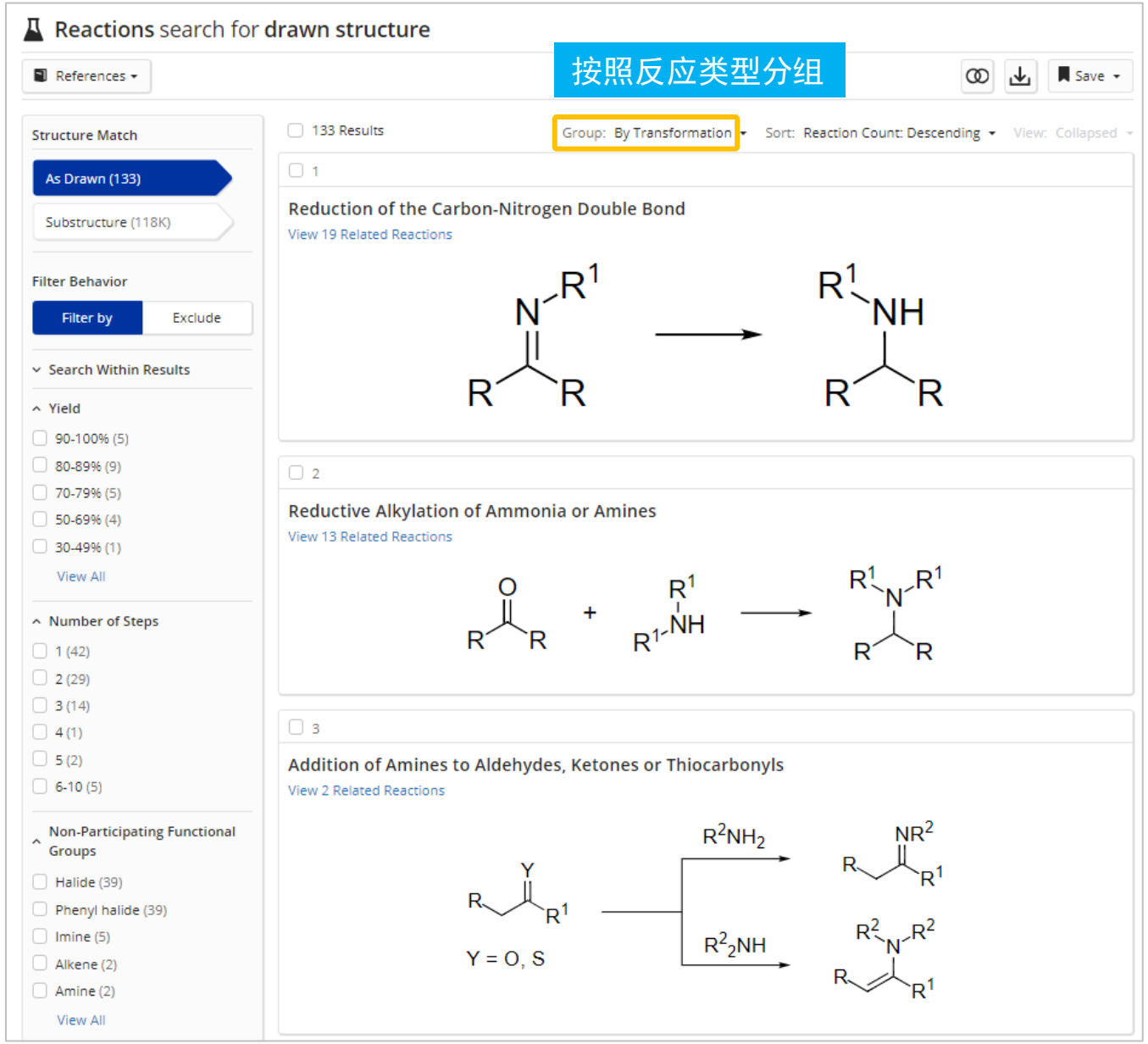

结构匹配度

分组、排序方式



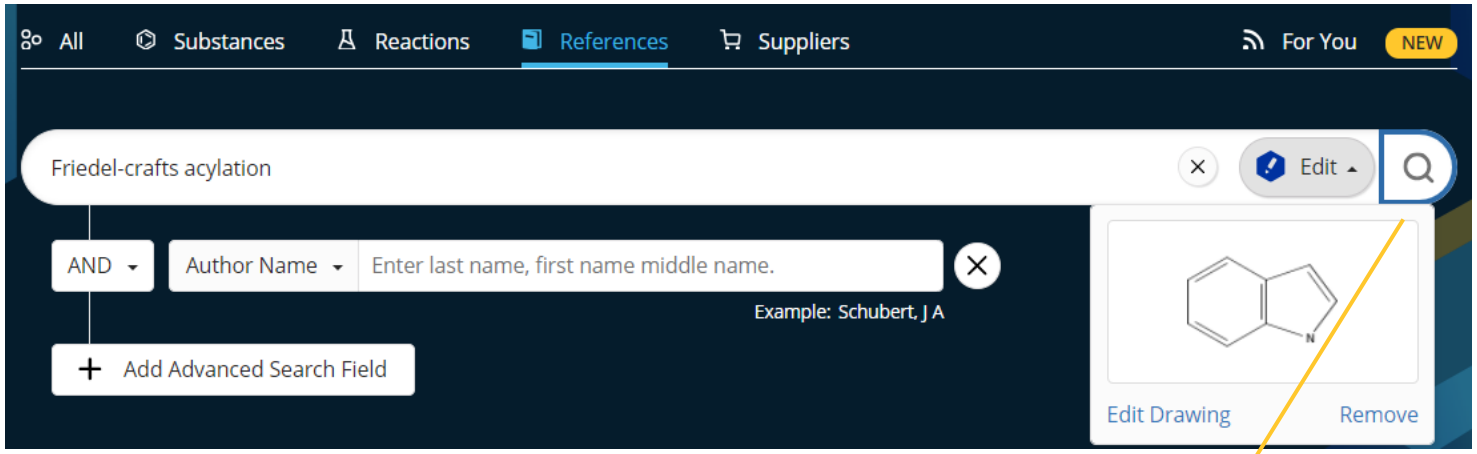
# 反应检索结果集的分组

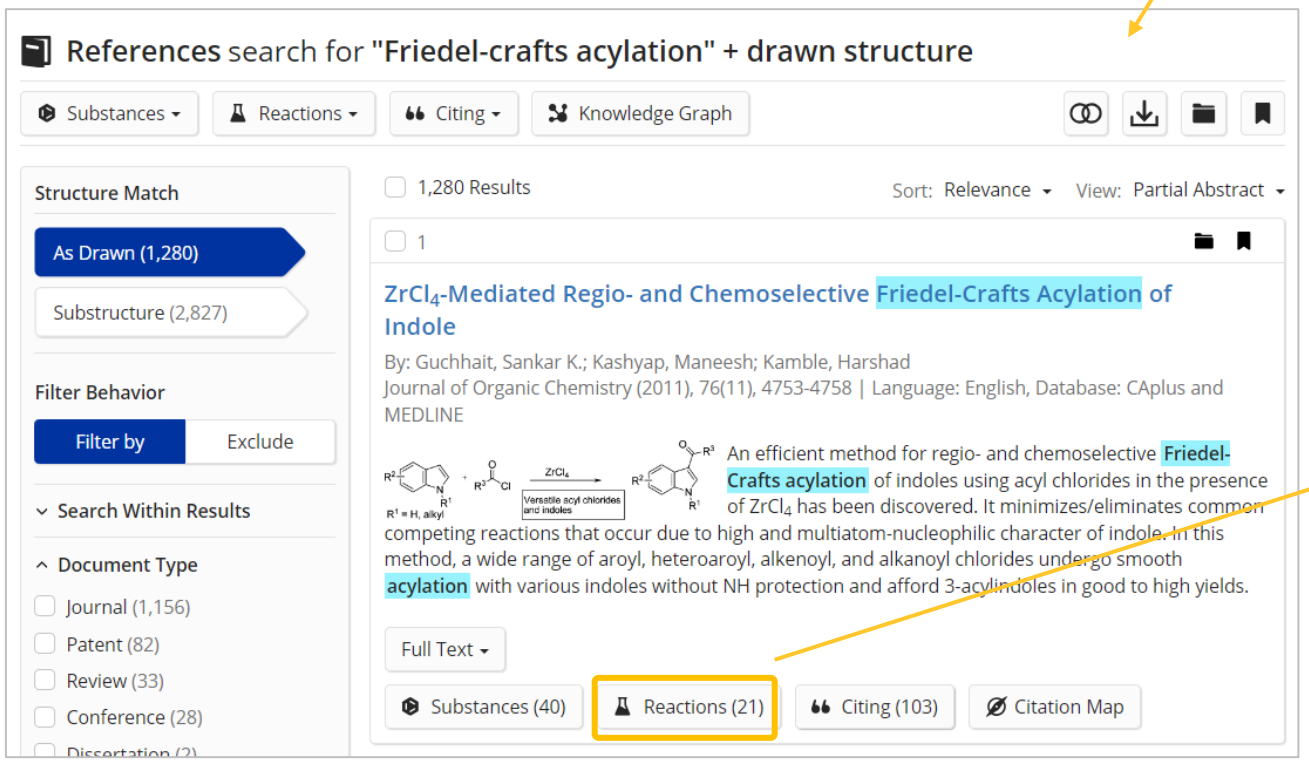


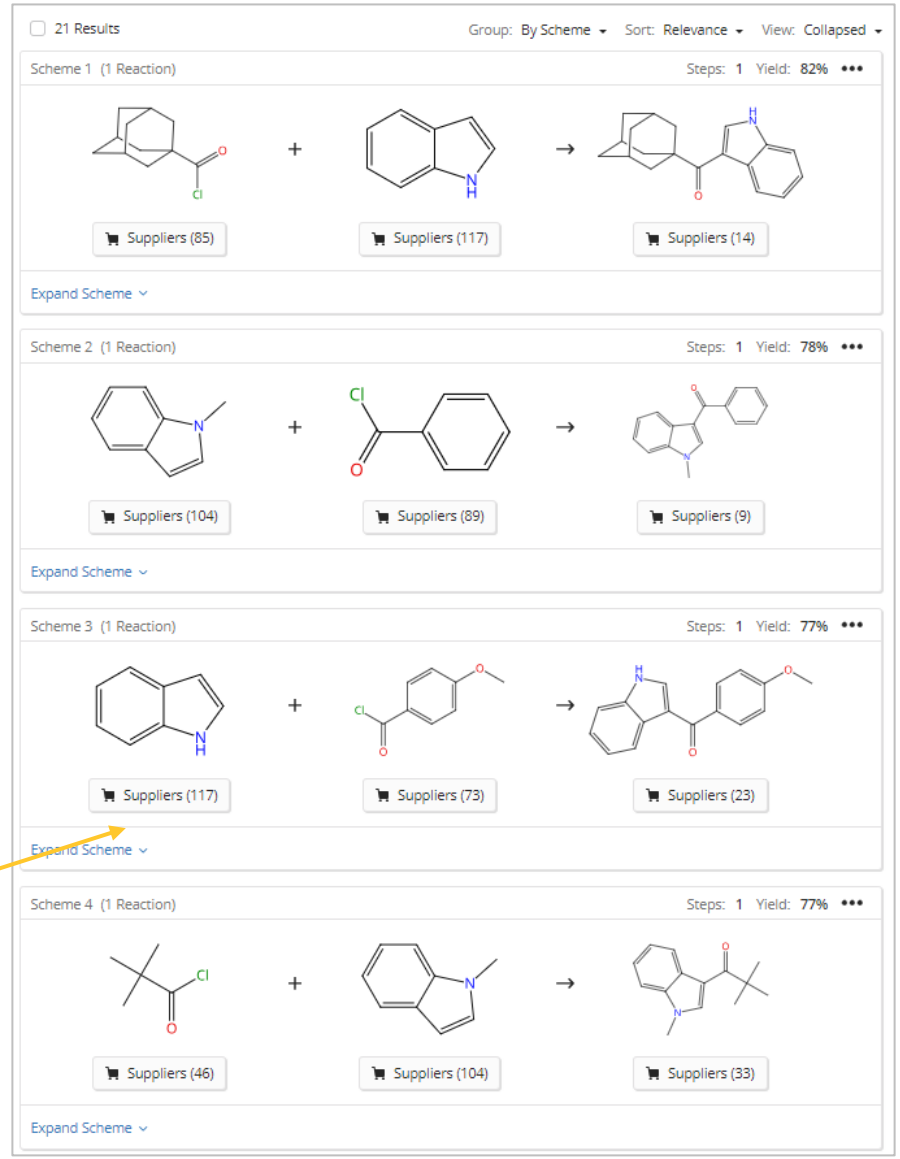



# 使用联用检索——结构与关键词检索反应

联用检索提高检索效率

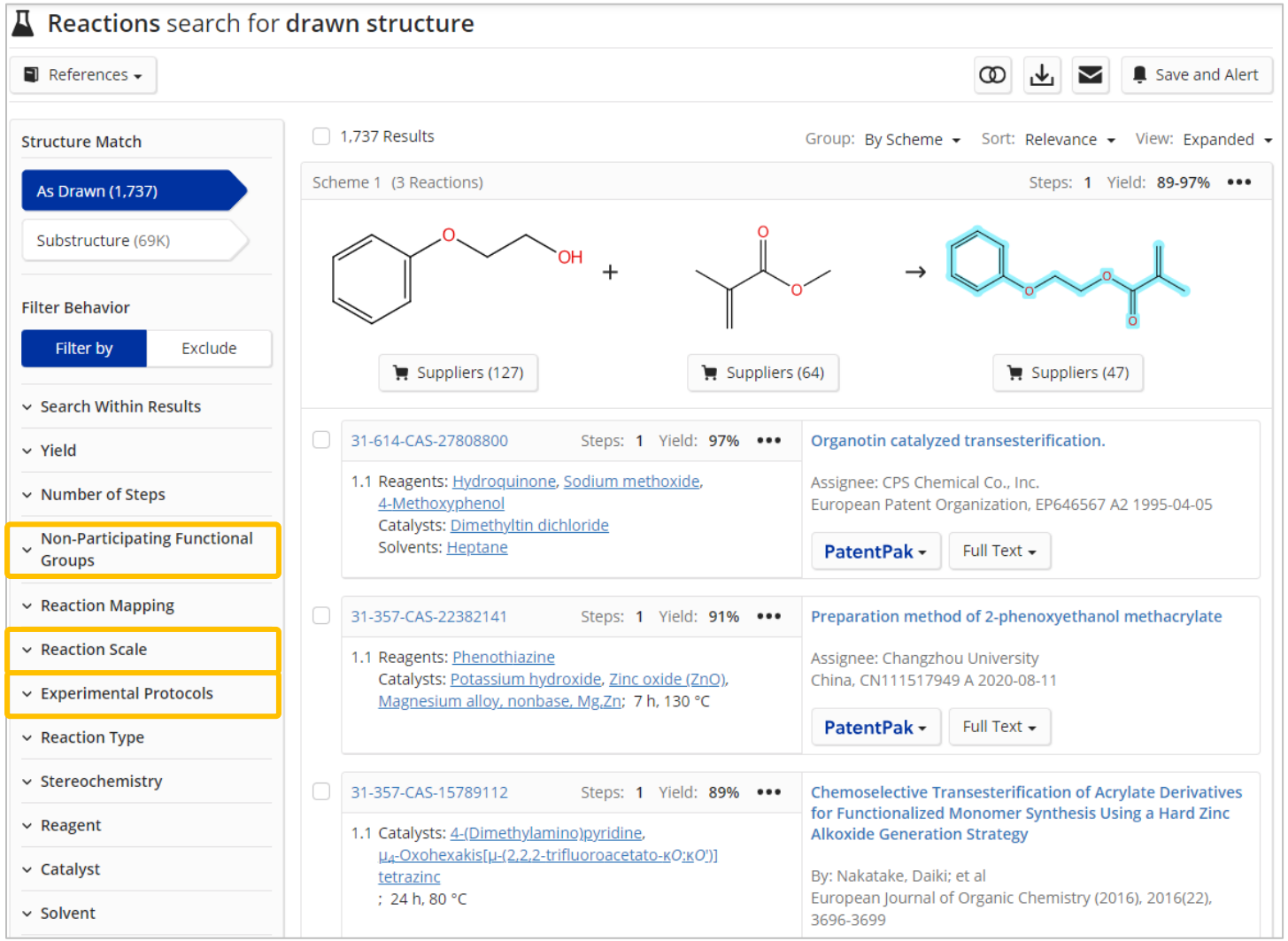


# 反应结果的筛选

二次筛选
产率
反应步骤数
**不参与反应官能团**
反应原子标记
**反应规模**
**实验步骤**
反应类型
立体化学
试剂
催化剂
溶剂
……




**Non-Participating Functional Groups**

- Acyclic alkene (11)
- Alkene (11)
- Ether (11)

**Reaction Scale**

- Milligram (9)
- Gram (6)
- No Scale Provided (1,760)

**Experimental Protocols**

- Synthetic Methods (33)
- Experimental Procedure (107)

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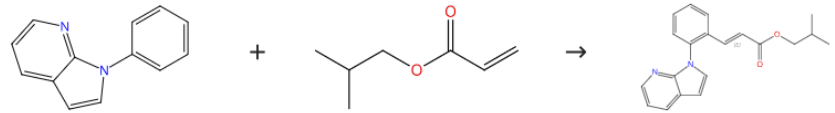
# 反应的详情页

Synthetic Methods——CAS科学家增值标引的合成制备详情

CAS Reaction Number: 31-177-CAS-21171434

Get Similar Reactions | Save




Suppliers (5) | Suppliers (41) | 99%

**Reaction Overview**

Steps: 1 Yield: 99%

**JOURNAL**

Rhodium(III)-catalyzed mono- and dialkenylation of N-phenyl-7-azaindoles via regioselective C-H bond cleavage

By: Morioka, Ryosuke; et al
View All
Chemistry Letters (2016), 45(6), 682-684

View PDF | Full Text

**Company/Organization**

Department of Applied Chemistry, Graduate School of Engineering
Osaka University
Suita, Osaka 565-0871
Japan

Step 1

| Stage | Reagents | Catalysts | Solvents | Conditions |
|---|---|---|---|---|
| 1 | Silver acetate | Tris(acetonitrile)[(1,2,3,4,5-η)-1,2,3,4,5-pentamethyl-2,4-cyclopentadien-1-yl]rhodium(2+) | 1,2-Dimethoxyethane | 3 h, 40 °C |

Alternative Steps (0)

Experimental Protocols

Synthetic Methods

| | |
|---|---|
| Products | 2-Methylpropyl (2*E*)-3-[2-(1*H*-pyrrolo[2,3-*b*]pyridin-1-yl)phenyl]-2-propenoate, Yield: 99% |
| Reactants | Isobutyl acrylate<br>1-Phenyl-1*H*-pyrrolo[2,3-*b*]pyridine |
| Reagents | Silver acetate |
| Catalysts | Tris(acetonitrile)[(1,2,3,4,5-η)-1,2,3,4,5-pentamethyl-2,4-cyclopentadien-1-yl]rhodium(2+) |
| Solvents | 1,2-Dimethoxyethane |

**Procedure**

1. Stir a mixture of N-phenyl-7-azaindole (0.2 mmol), the corresponding alkene (0.2 mmol), $[Cp^*Rh(MeCN)_3][SbF_6]_2$ (0.008 mmol, 6.7 mg), AgOAc (0.4 mmol, 67 mg), and 1-methylnaphthalene (ca. 30 mg) as internal standard in DME (2 mL) under nitrogen at 40 °C for 3 hours.
2. Cool the mixture.
3. Extract the mixture with ethyl acetate (100 mL).
4. Dry the crude product over $Na_2SO_4$.
5. Evaporate the solvents under vacuum.
6. Purify the crude product by column chromatography on silica gel using hexane-ethyl acetate (10:1, v/v) as eluent to obtain isobutyl (E)-3-(2-(1H-Pyrrolo[2,3-b]pyridin-1-yl)phenyl)acrylate.

易于阅读的实验操作流程

**Transformation** Arylation and Alkylation of Alkenes/ Heck Reaction

**Characterization Data** 产物表征数据

2-Methylpropyl (2*E*)-3-[2-(1*H*-pyrrolo[2,3-*b*]pyridin-1-yl)phenyl]-2-propenoate

| | |
|---|---|
| Proton NMR Spectrum | (400 MHz, $CDCl_3$) δ 0.84 (d, *J*= 6.7 Hz, 6H), 1.85 (sep, *J*= 6.7 Hz, 1H), 3.85 (d, *J*= 6.8 Hz, 2H), 6.39 (d, *J* = 15.9 Hz, 1H), 6.67 (d, *J*= 3.5 Hz, 1H), 7.13 (dd, *J*= 7.7, 4.7 Hz, 1H), 7.28 (d, *J*= 3.5 Hz, 1H), 7.34 (d, *J*= 16.0 Hz, 1H), 7.43-7.58 (m, 3H), 7.82 (dd, *J*= 8.0, 1.3 Hz, 1H), 7.99 (dd, *J*= 7.9, 1.6 Hz, 1H), 8.32 (dd, *J*= 4.7, 1.5 Hz, 1H) |
| Carbon-13 NMR | (100 MHz, $CDCl_3$) δ 19.0, 27.7, 70.5, 101.7, 116.7, 120.3, 120.7, 127.4, 128.4, 128.8, 129.2, 129.7, 130.8, 131.9, 137.6, 139.9, 144.0, 148.6, 166.5 |
| HRMS | *m/z*calcd for $C_{20}H_{21}N_2O_2$ ($[M+H]^+$) 321.1598, found 321.1619 |
| State | yellow oil |

CAS Method Number 3-177-CAS-21171434

反应转化类型

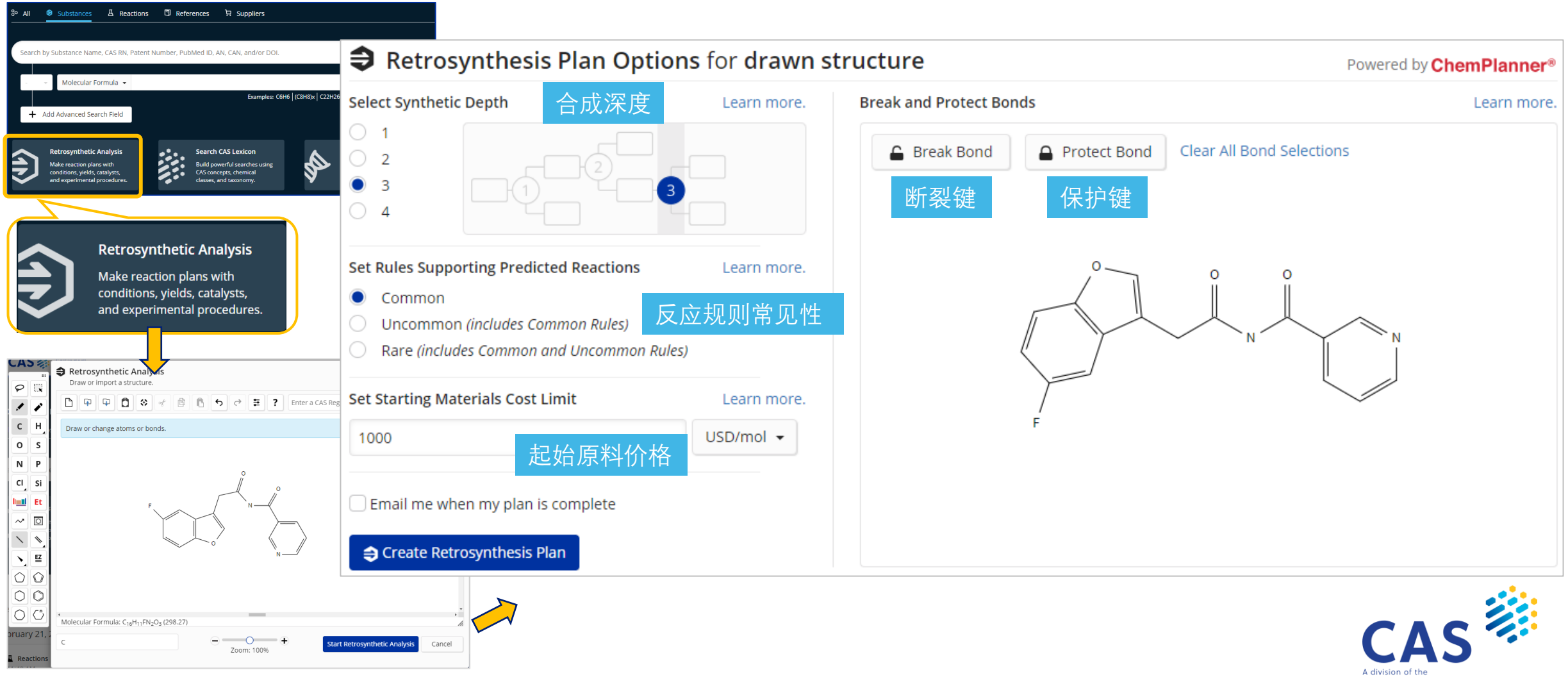
**Transformations**
1. Arylation and Alkylation of Alkenes/ Heck Reaction

反应注释

**Reaction Notes**
regioselective, stereoselective

# Retrosynthetic Analysis——逆合成路线分析

结合先进的AI技术和CAS科学家标引的高质量反应数据，为已知/未知分子设计的合成路线

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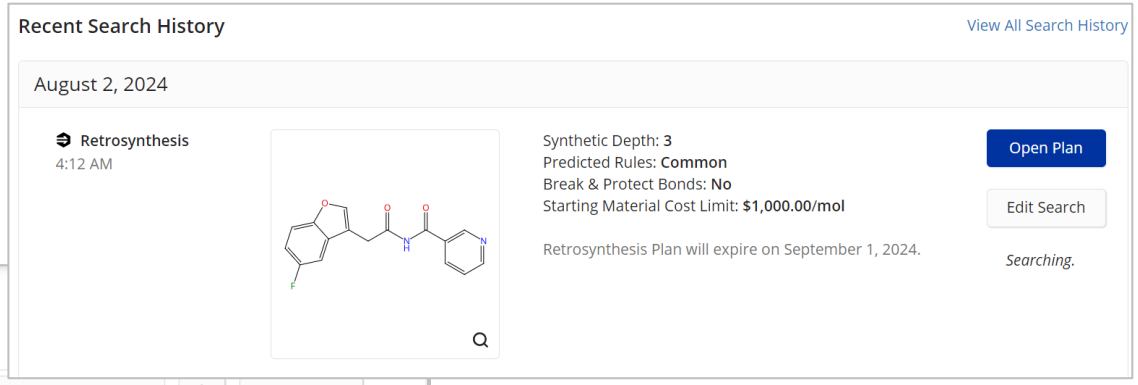
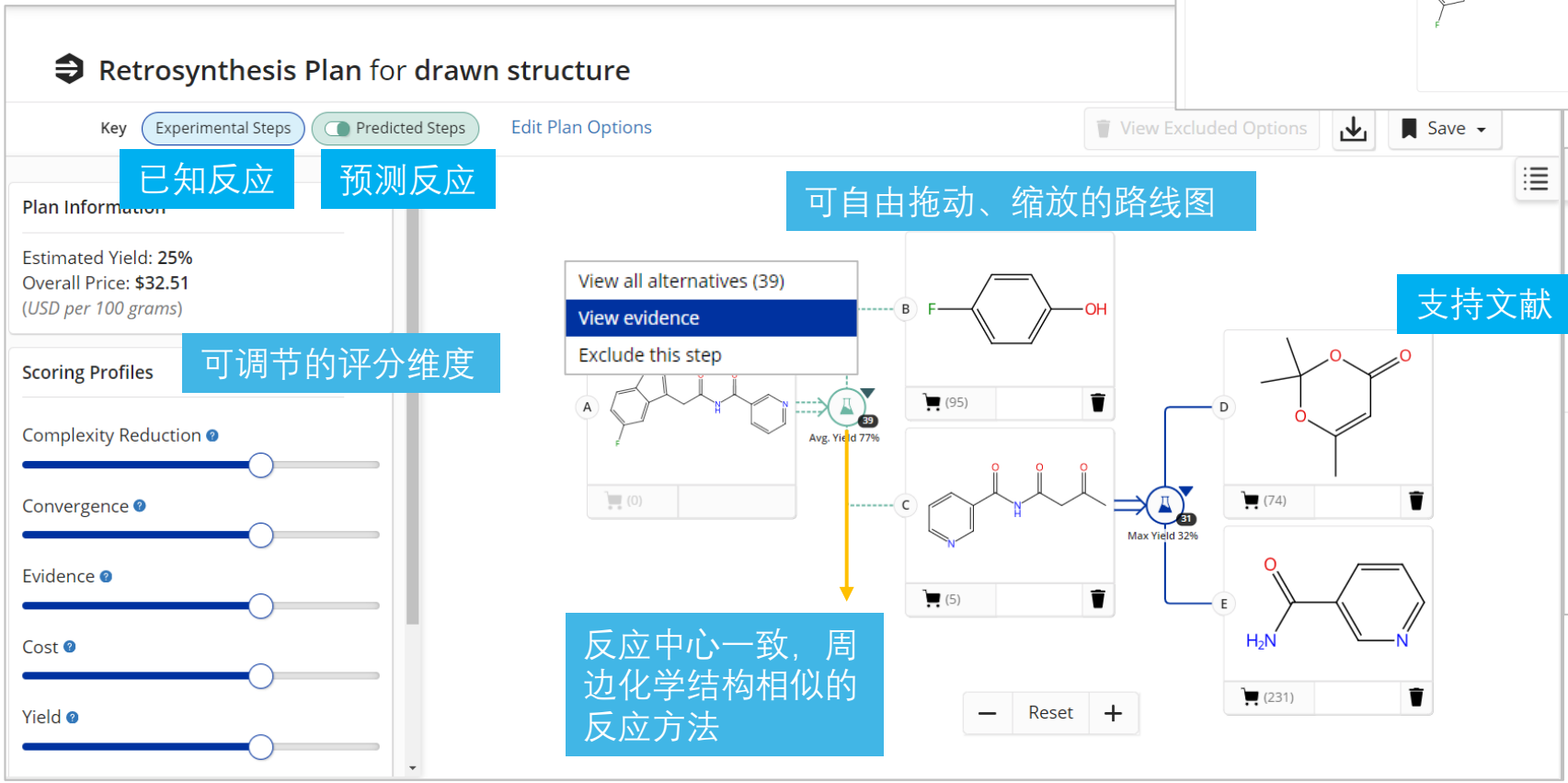
# Retrosynthetic Analysis——路线结果呈现

可查看每步反应的文献支持与详细条件

点击Alternative Steps查看并选择替换路线，
得到自定义的合成路线





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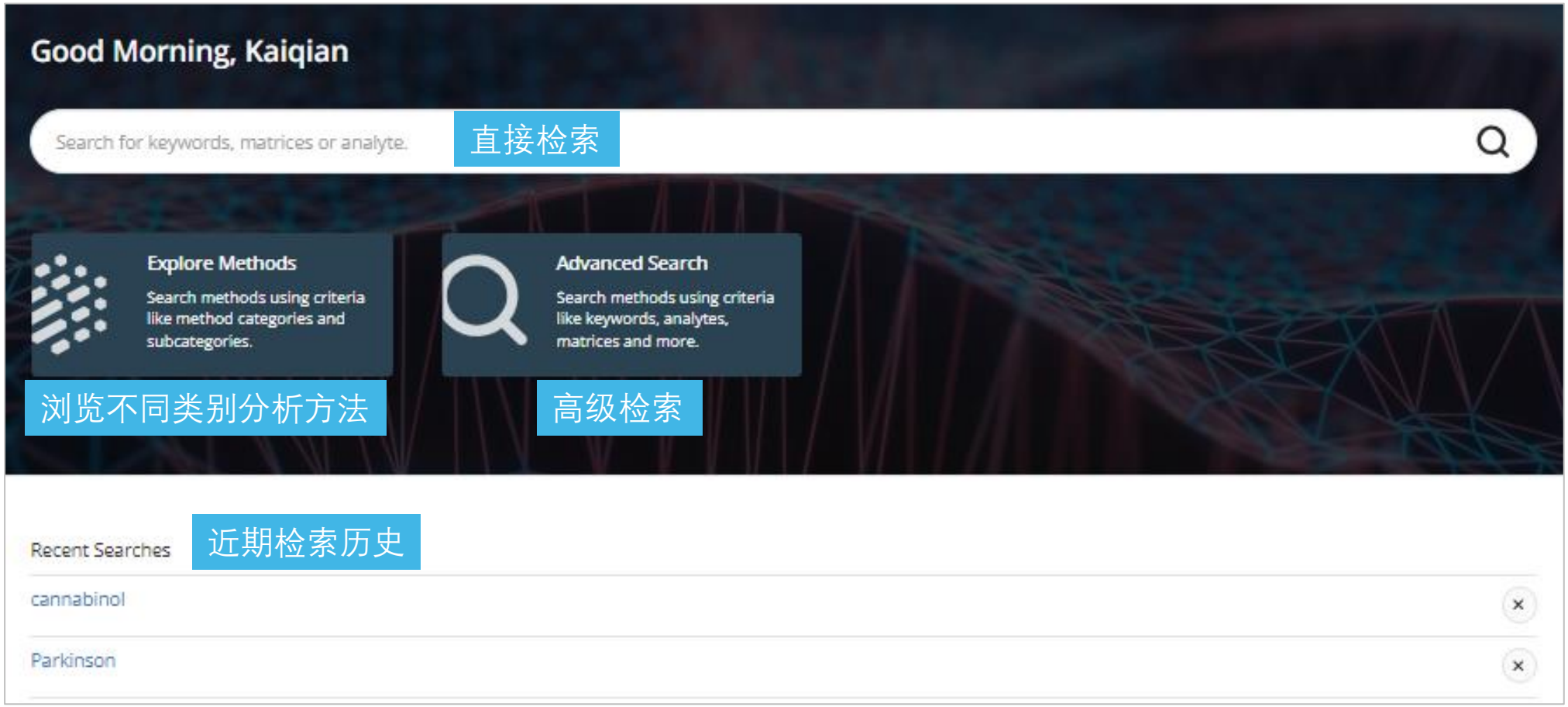
# CAS Analytical Methods - 分析方法

- 访问网址：https://methods.cas.org/







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# 分析方法结果集

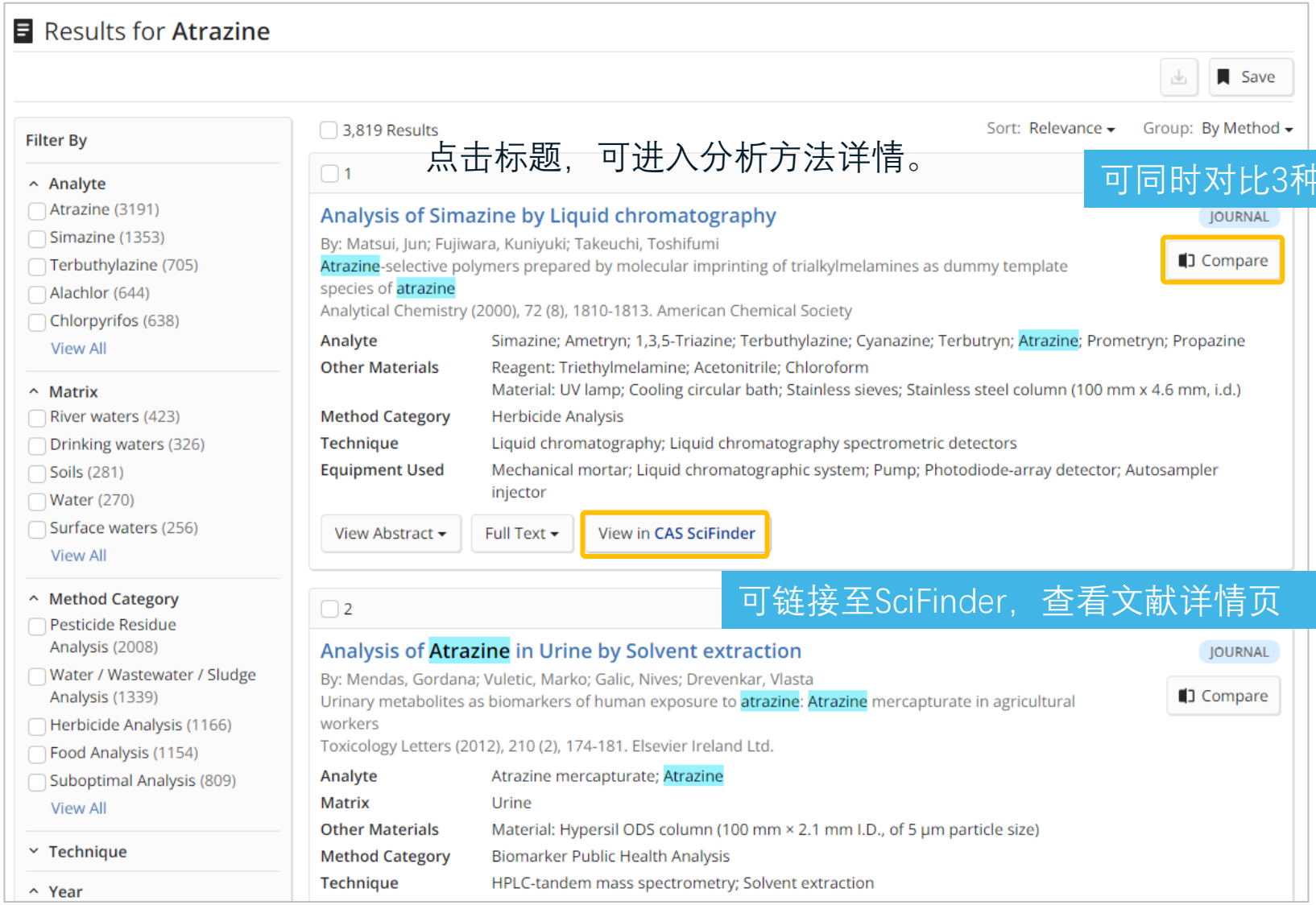
示例：莠去津

分析物

基质

方法类别

所用技术
发表年份







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# 分析方法详情

示例：利用液液微萃取技术分析废水中残余的莠去津

## Analysis of Atrazine in Wastewater by Liquid-liquid microextraction

Save

| CAS Method Number | Method Category | Technique |
|---|---|---|
| 1-143-CAS-148147 | Water / Wastewater / Sludge Analysis; Herbicide Analysis | Liquid-liquid microextraction; Liquid chromatography spectrometric detectors; HPLC |

| Analyte | Matrix | Material | Reagent | Biological Reagent |
|---|---|---|---|---|
| Deethylatrazine<br>Atrazine<br>Deisopropylatrazine | Wastewater<br>Groundwaters | Hollow fibers 150 × 4.6mm I.D. $C_{18}$ column (Zorbax RX-C18, 5 µm particles) | Hydrochloric acid<br>Acetonitrile<br>1-Octanol<br>Sodium chloride | - |

分析物
分析基质
所用材料

所用仪器

## Equipment Used

Liquid chromatographic instrument, LC-VP, Shimadzu, Japan

Diode array detector, SPD-M10Avp, Shimadzu, Japan

HPLC system controller, SCL-10Avp, Shimadzu, Japan

HPLC pump, LC-10ATvp, Shimadzu, Japan

Source

文献来源

JOURNAL

Determination of atrazine, desethyl atrazine and desisopropyl atrazine in environmental water samples using hollow fiber-protected liquid-phase microextraction and high performance liquid chromatography

Peng, Jinfeng; Lue, Jianxia; Hu, Xialin; Liu, Jingfu; Jiang, Guibin

Microchimica Acta (2007), 158 (1-2), 181 - 186. Springer Wien

CODEN : MIACAQ | ISSN : 00263672 | DOI : 10.1007/s00604-006-0692-9

View Abstract ▾ Full Text ▾

Instructions 无需阅读原文，即可获取方法详情。

### Preparation of water samples

1. Collect wastewater and ground water samples.
2. Store the samples at 4 °C.

### Preparation of atrazine stock solutions

1. Prepare standard stock solutions (100 mg/L) of atrazine (ATR), desethylatrazine (DEA) and desisopropyl atrazine (DIA) by dissolving 0.25 mg of the compounds in 2.5 mL acetonitrile.
2. Store the solutions in brown glass bottles at 4 °C.
3. Prepare fresh working solutions daily by appropriate dilution of the stock solutions.

### Preparation of polyvinylidene fluoride (PVDF) fiber

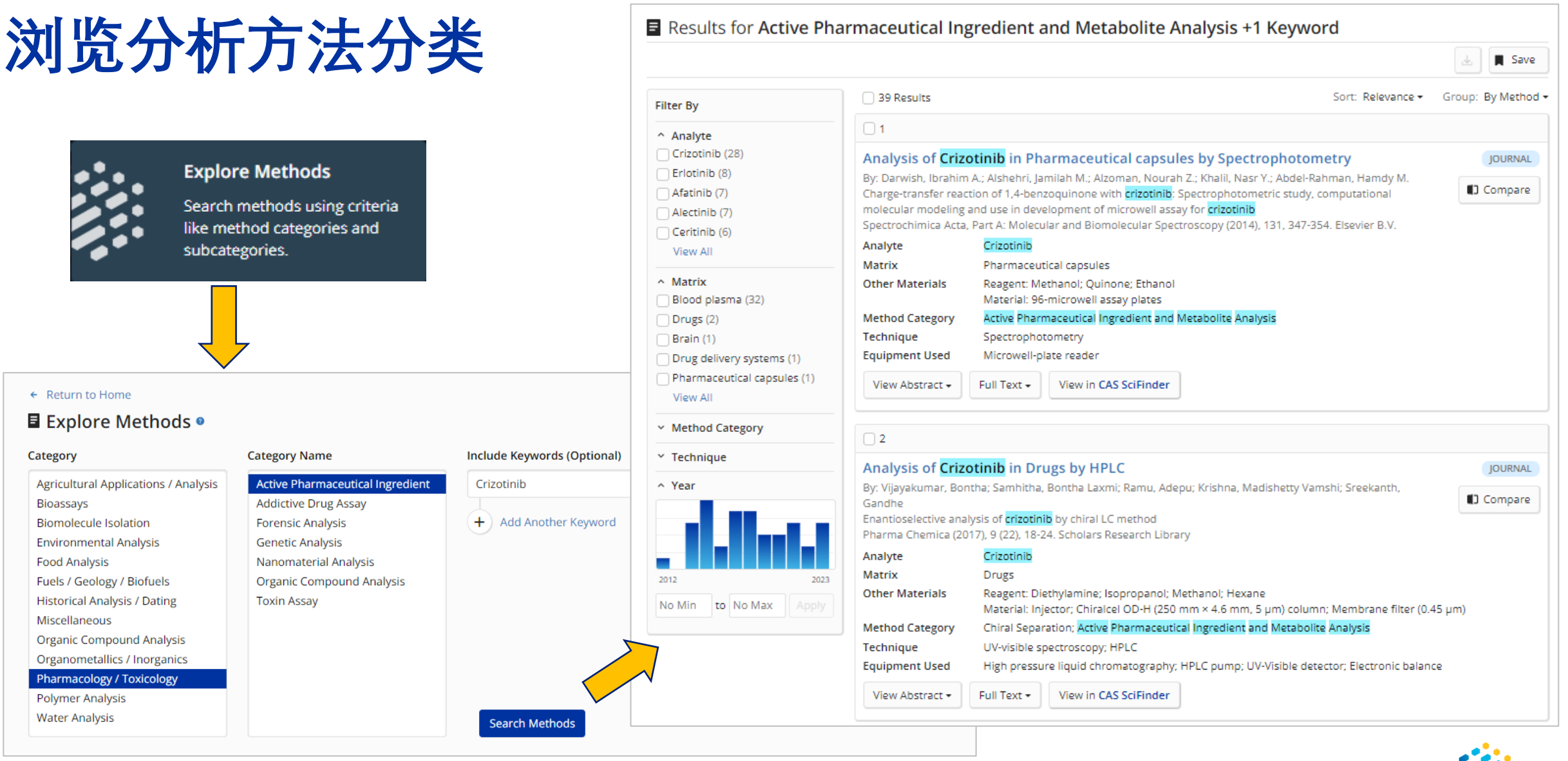
1. Cut PVDF porous hollow fiber membrane (inner diameter 450 µm, wall thickness 125 µm, pore size 2.5 µm) manually into 5.1 cm length.
2. Immerse the fiber in 1-octanol for 10 min.
3. Take out the hollow fiber.
4. Flush the outside and inside of the fiber five times with water in a washing bottle and water in a 0.5 mL microsyringe, respectively.
5. Connect the hollow fiber with the needle of the microsyringe holding ~20 µL acceptor solution (4 M HCl).
6. Depress the plunger of the microsyringe to flush out ~20 µL acceptor solution to wash and fill the lumen of the hollow fiber without any air bubbles.
7. Seal the two ends of the fiber with heated tweezers.
8. Obtain the hollow fiber protected liquid-phase microextraction device with an effective fiber length of ~5.0 cm with acceptor phase volume of ~8 µL ready for extraction.

详细直观的实验步骤

### Liquid-phase microextraction procedure

1. Perform extraction with PVDF fiber at a middle-stirring rate.
2. Extract 50 mL volume of aqueous solution in a 100 mL petri dish with addition of 20% sodium chloride.
3. Cover the petri dish with glass cap.
4. After extracting for 30 min, take out the hollow fiber from the aqueous solution.
5. Cut open one sealed end of the fiber for connecting with the microsyringe.
6. Cut open the other sealed end to facilitate flushing out the acceptor solution into 200 µL glass vial with the microsyringe.
7. Add 8 µL of sodium hydroxide into the glass vial to neutralize the acid acceptor solution.
8. Finally, retract the total solution of ~16 µL into an 25 µL HPLC microsyringe for analysis.

# 浏览分析方法分类







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# CAS Formulus - 制剂/配方

- 访问网址：https://formulus.cas.org/




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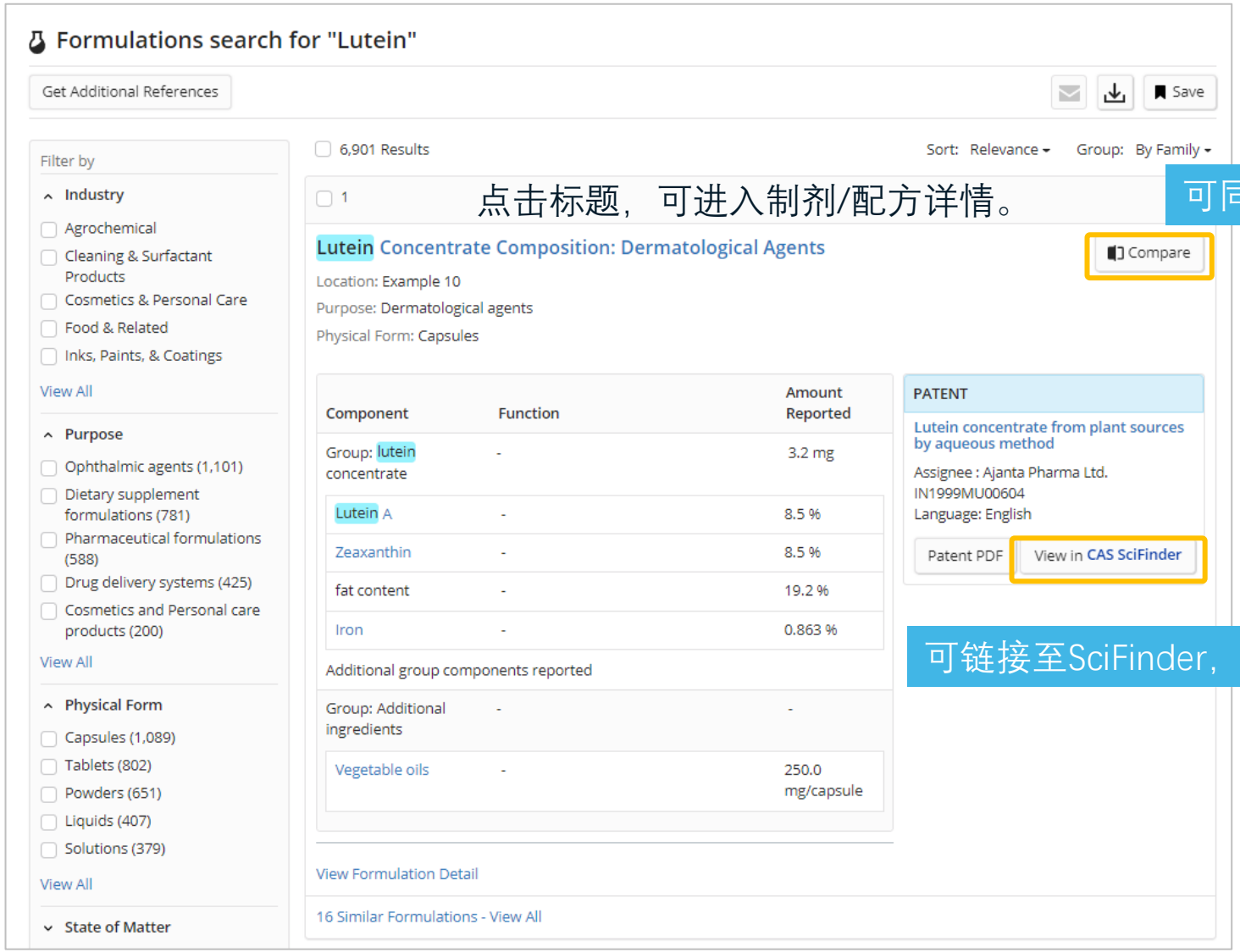
# 制剂/配方结果集

领域

用途
物理形态
物质状态
递送途径

所含信息
文献类型
机构/组织
语言
发表年份



# 制剂/配方详情

## Soft Capsule Formulation: Food

配方用途

Save

| Purpose | Target | Delivery Route | Physical Form | Source |
|---|---|---|---|---|
| Food | Homo sapiens, reaggregation | Oral drug delivery systems | Capsules | |

Predicted value

配方成分

### Formulation Ingredients

| Component | Function |
|---|---|
| Group: hardly soluble component | Formulation active agents |
| Lutein A | - |
| Capsanthin | pigment |
| Diacetyltartaric acid | - |
| saffron oil | - |
| Group: Coating materials | Coating materials |
| gelatin BCN 200 S | Coating materials |
| Glycerol | Food additives |
| caramel BD-2 | pigments |

无需阅读原文，即可获取配方详情

### Process

hardly soluble component, organic acid monoglyceride, hydrophilic emulsifier, glycerin fatty acid ester/polyglycerin fatty acid ester and other components were mixed and then each component as a film was coated to obtain a soft capsule preparation

详细、直观的操作步骤与实验数据

### Effective Dose

| Descriptor | Solvent | Details |
|---|---|---|
| separation of oily components containing sparingly soluble components is slight, but to the first solution of disintegration test dispersibility is uniform good | Water | - |

**Experimental Activity**

| Descriptor | Notes | Details |
|---|---|---|
| dispersibility test | visual observation of dispersibility in water were evaluated | - |

### Experimental Activity

### Source Patent

Pharmaceutical oral agent comprising sparingly soluble component with organic acid monoglyceride and hydrophilic emulsifier

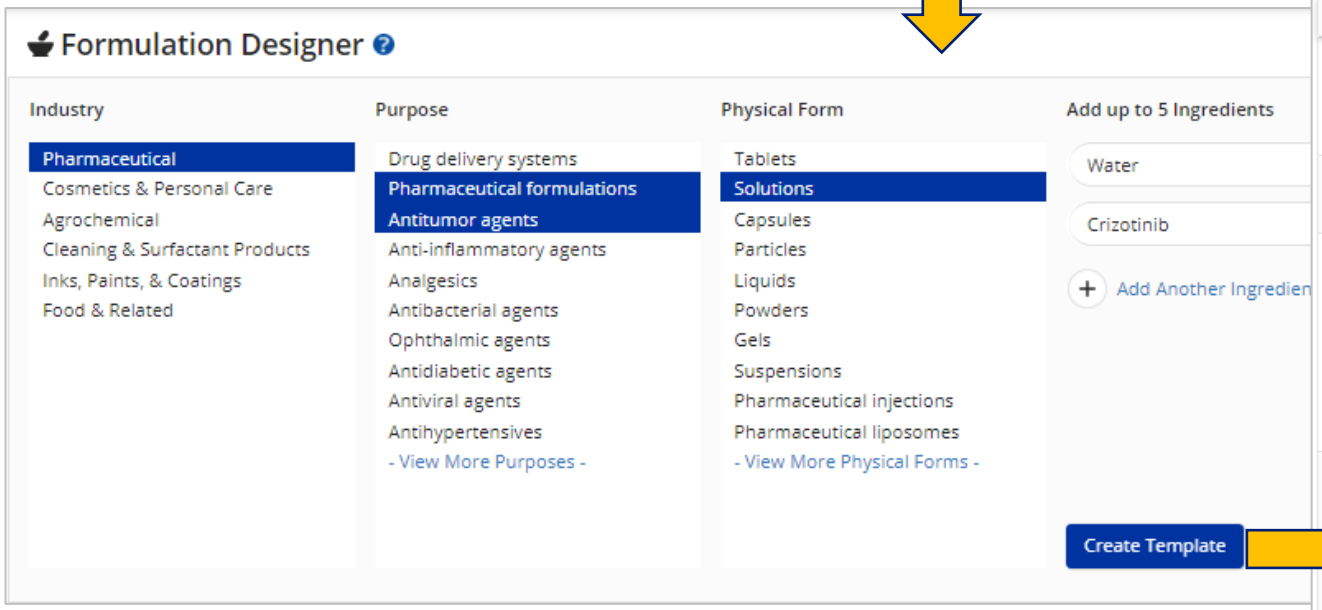
Assignee : Lion Corporation
WO2018101267
Language: Japanese
**Location:** Table 5, Example 29

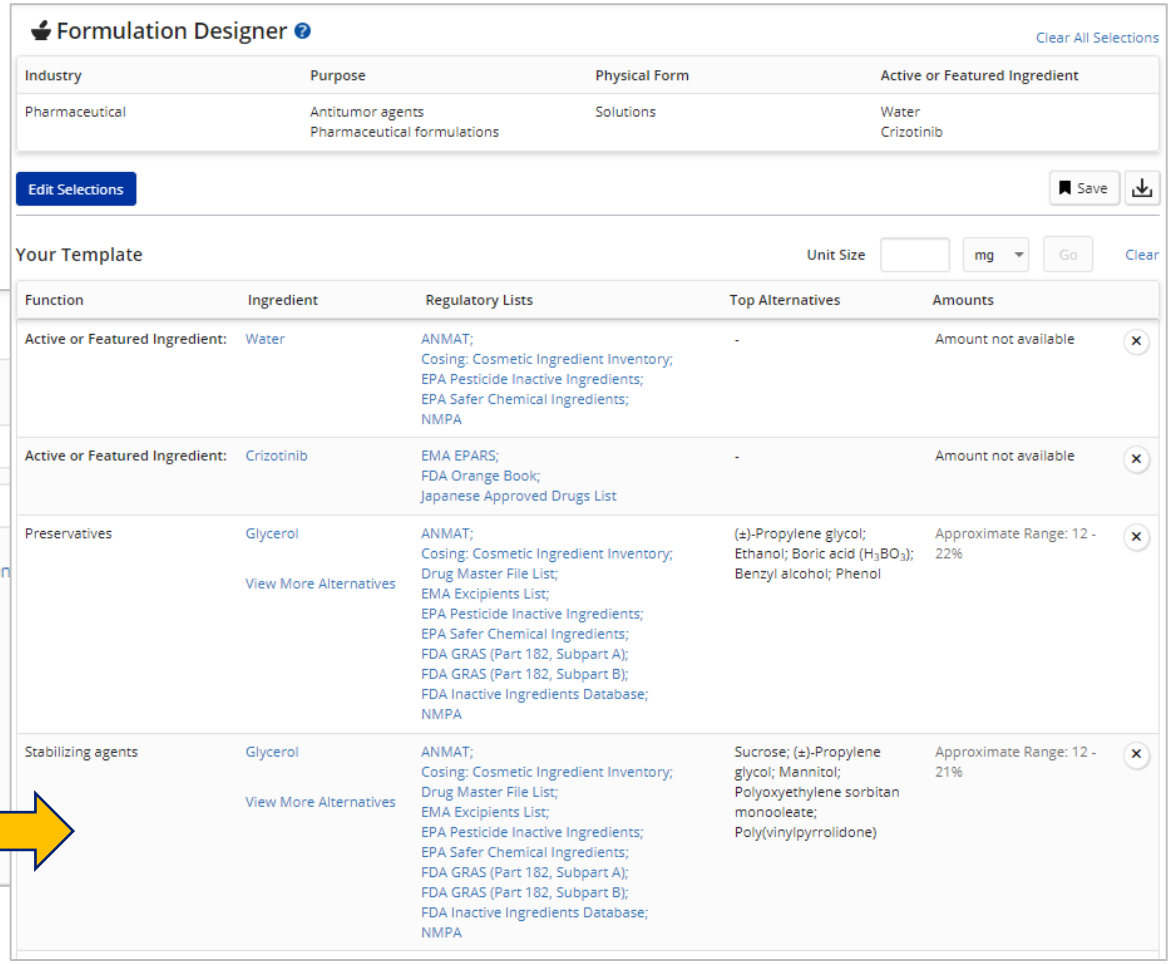
文献来源

Patent PDF | View in CAS SciFinder

# Formulation Designer辅助设计制剂、配方

## 启发制剂配方设计


基于期刊、专利和产品说明书中标引的制剂、配方数据，获得见解。

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# 小结

- 反应的检索方式：使用标识符，结构绘制以及关键词联用等方式，关注筛选目标反应信息。
- 信息之间的深度关联：从关注的物质/文献，一键链接到相关反应，高效完成信息检索。
- 反应检索及路线设计：多元的检索方式，逆合成路线分析，反应结果的筛选和详情查看。
- 反应检索结果筛选及详情速览：Synthetic Methods，通过CAS科学家的标引，无需阅读原文，直接获取实验步骤详情及产物表征信息。
- CAS Analytical Methods：分析方法解决方案，支持直接检索、高级检索及按不同类别浏览，提供分析方法详情和方法对比。
- CAS Formulus：制剂/配方解决方案，支持制剂/配方及成分的检索，提供详情和详情对比，以及协助设计制剂/配方。

# 总结

- CAS 内容合集来源于化学并超越于化学，支持多学科、跨学科研发创新
- 全面覆盖的内容确保不遗漏任何重要的信息
- CAS 科学家人工智慧与先进专有技术结合标引的数据，能够揭示隐藏在数据间的隐秘关联
- 强大的功能确保降低文献检索和分析的时间，将更多宝贵的时间应用于创新工作中，提升科研创新效率

# 大纲

- CAS及CAS SciFinder Discovery Platform (Academic)简介
- 科研信息的高效查阅
  - 全面的文献调研与拓展助力开题
  - 多角度出发检索物质结构及相关属性
  - 生物序列检索方法与结果分析
  - 探索实验方案以获取制备及其他实验详情
- 常见问题Q&A




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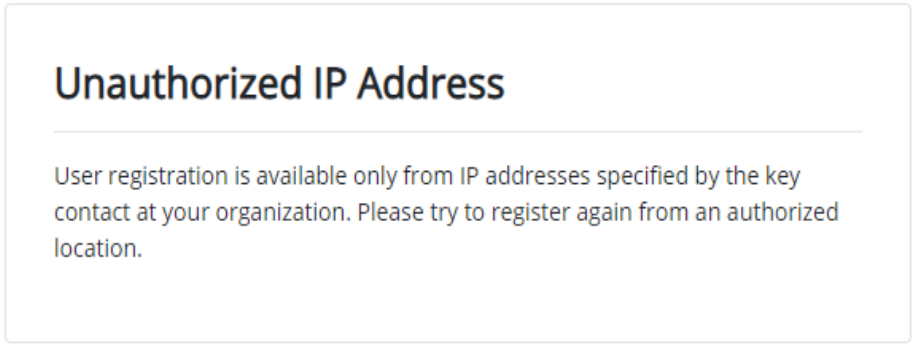
# CAS SciFinder检索浏览器推荐

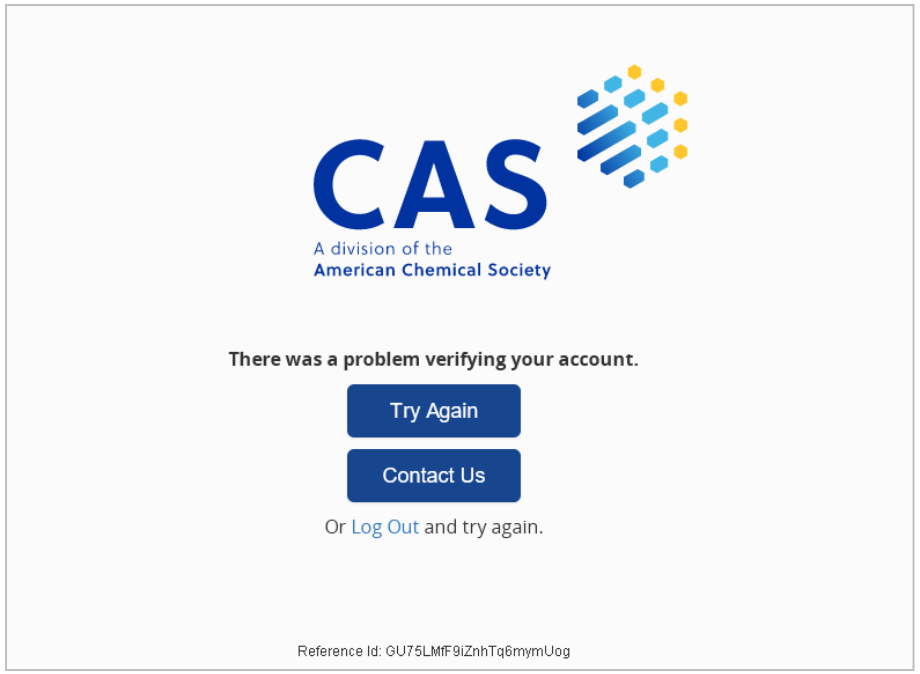
浏览器推荐：

- Windows (7, 8.1, 10)：Chrome 60及更高版本，Firefox 55及更高版本，Firefox 52 (ESR)、Edge 15及更高版本
- Mac OS X (10.11, 10.12, 10.13)：Safari 9.3及更高版本，Chrome 60及更高版本，Firefox 55及更高版本，Firefox 52 (ESR)
- **不建议使用360浏览器，相关功能或插件会被自动拦截**

# 常见登录问题




- 检查注册链接是否正确
- 确认连入校园网，且不是通过VPN连接
- 如果链接正确，且在校园内，请联系图书馆或china@acs-i.org

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# Between problems and progress are connections that matter

# 谢谢！

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