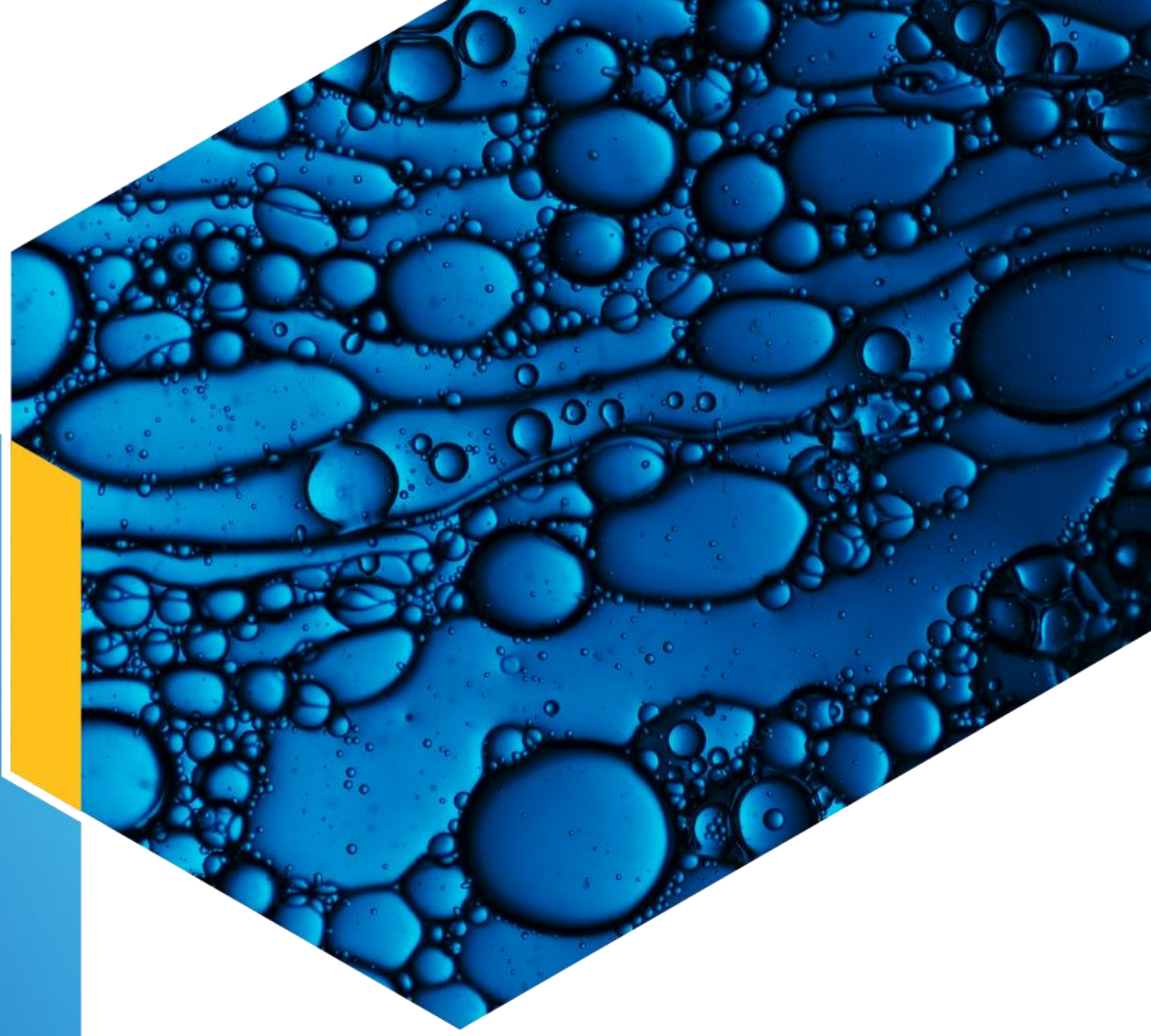

CAS SciFinder

全程助力医药科学研究

客户顾问：匡金海
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- **CAS及CAS SciFinder介绍**
- **文献相关信息的获取策略**
  - 文献检索方法
  - 文献结果排序、筛选和详情
  - 如何高效阅读专利文献详情(CAS PatentPak)
- **物质相关信息的获取策略**
  - 常见的物质检索方法
  - 物质结果排序、筛选和详情
- **反应相关信息的获取策略**
  - 反应的获取方法
  - 反应结果排序、筛选和详情
  - 如何高效获取反应详情（Synthetic Methods）
- **分析相关信息的获取 (CAS Analytical Methods)**

CAS致力于提高创新效率

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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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Over **50** languages translated

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CAS SciFinder覆盖的学科

- **生物化学：**
  - 农化产品管控信息、生化遗传学、发酵、免疫化学、药理学
- **有机化学各领域：**
  - 氨基酸、生物分子、碳水化合物、有机金属化合物、类固醇
- **大分子化学各领域：**
  - 纤维素、木质素、造纸；涂料、墨水
  - 染料、有机颜料； 合成橡胶； 纺织品、纤维
- **应用化学各领域 ：**
  - 大气污染、陶瓷、精油、化妆品、化石燃料、黑色金属、合金
- **物理、无机、分析化学各领域：**
  - 表面化学、催化剂、相平衡、核现象、电化学

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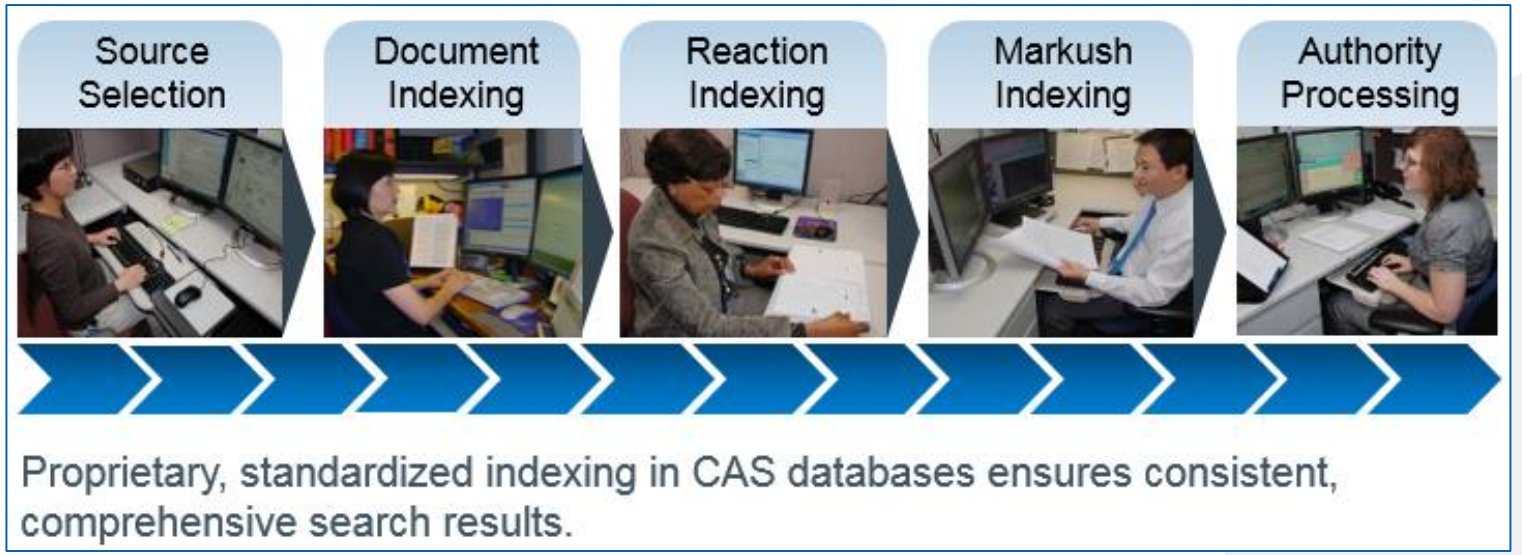
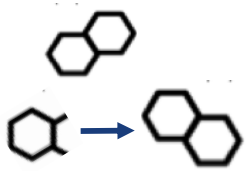
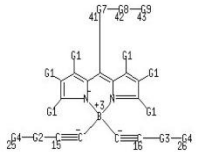
CAS科学家的智力标引



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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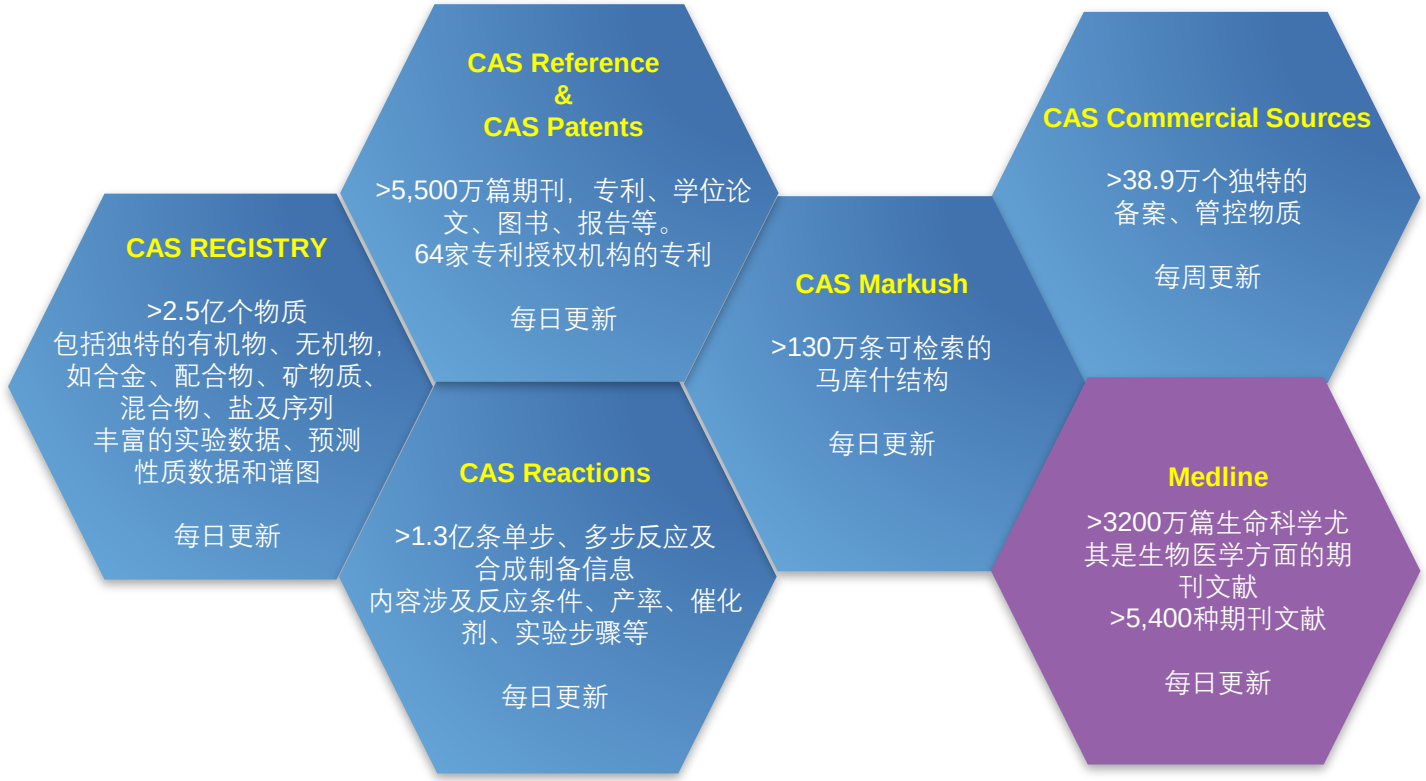
CAS内容合集--CAS SciFinder



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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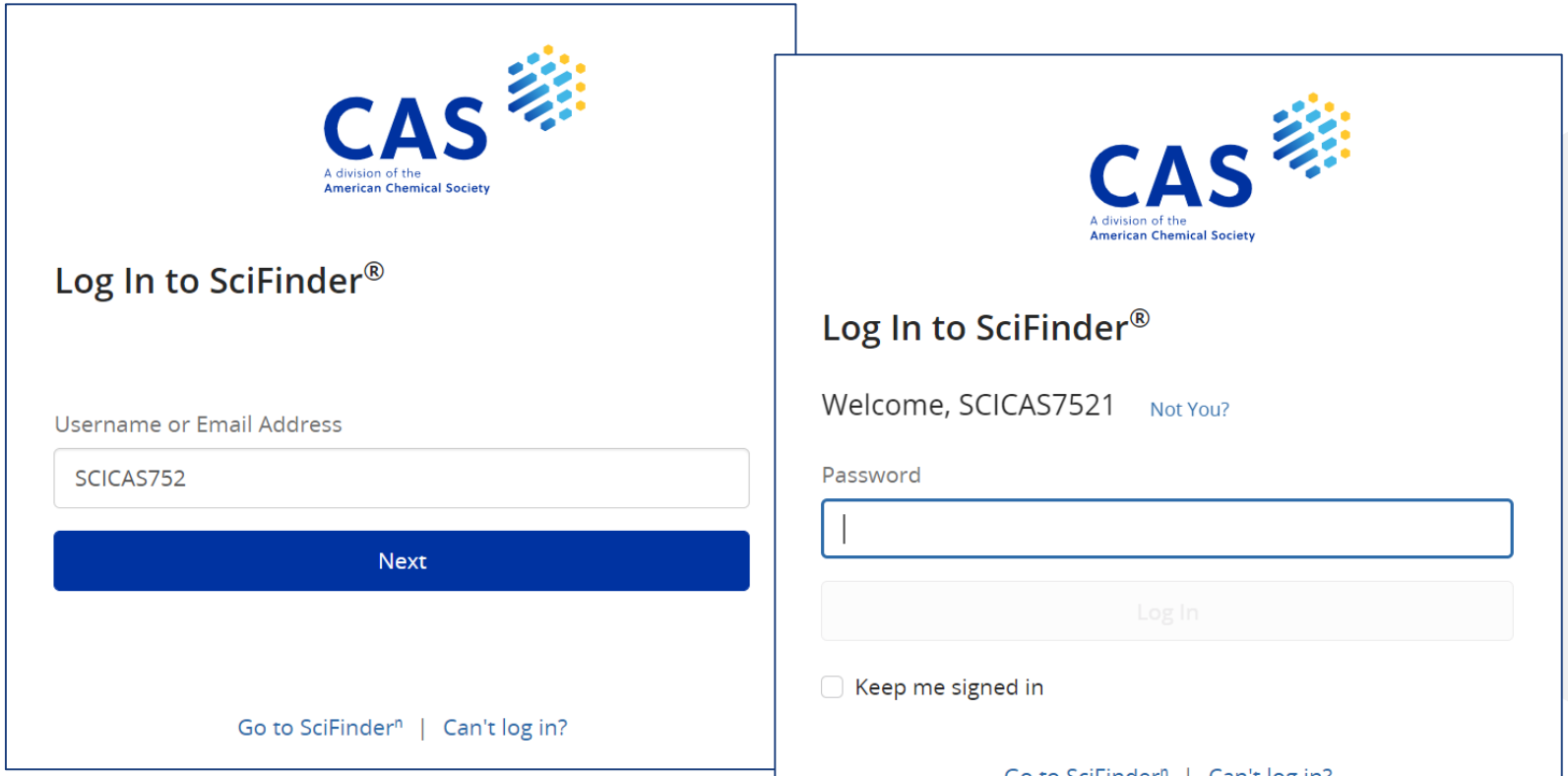
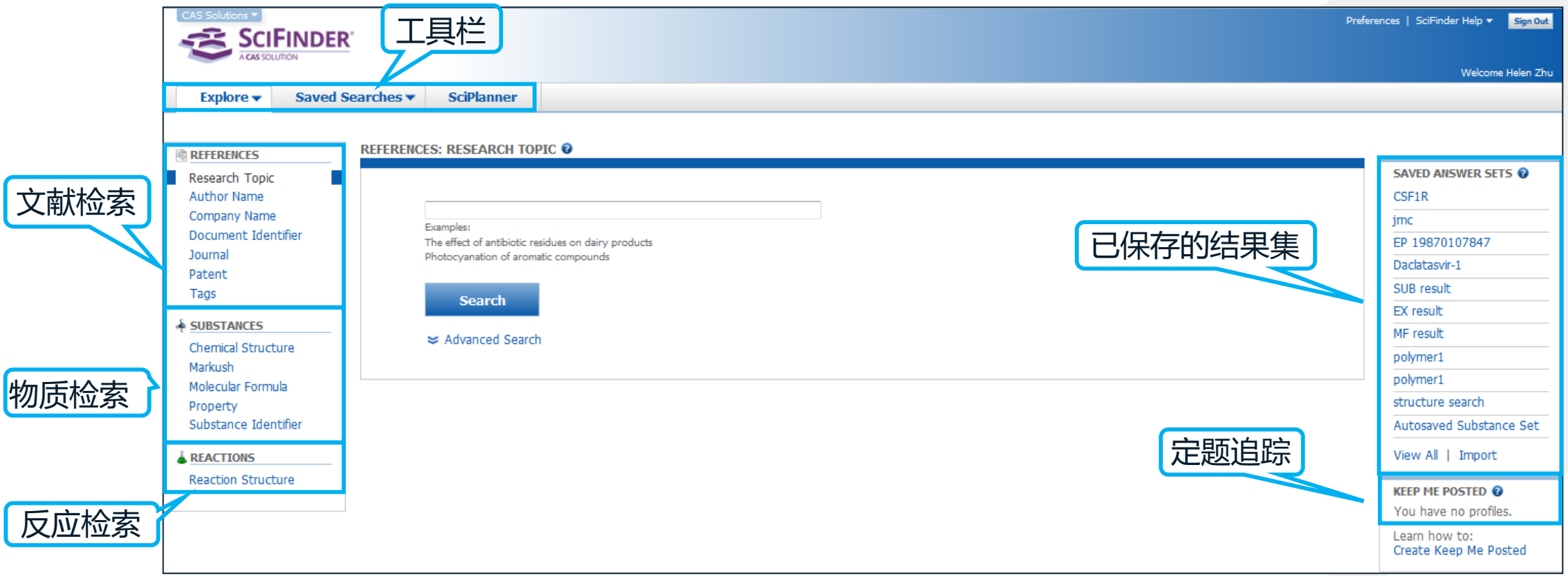
CAS SciFinder登录网址

https://SciFinder.cas.org



每个用户必须注册后才能使用

CAS SciFinder主界面



大纲

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  - 如何高效获取反应详情（Synthetic Methods）
- **分析相关信息的获取 (CAS Analytical Methods)**

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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文献检索--主题

主题检索： 老药新用治疗COVID-19

检索式：drug repurposing in COVID-19

关键词之间用介词连接：in, with, of…

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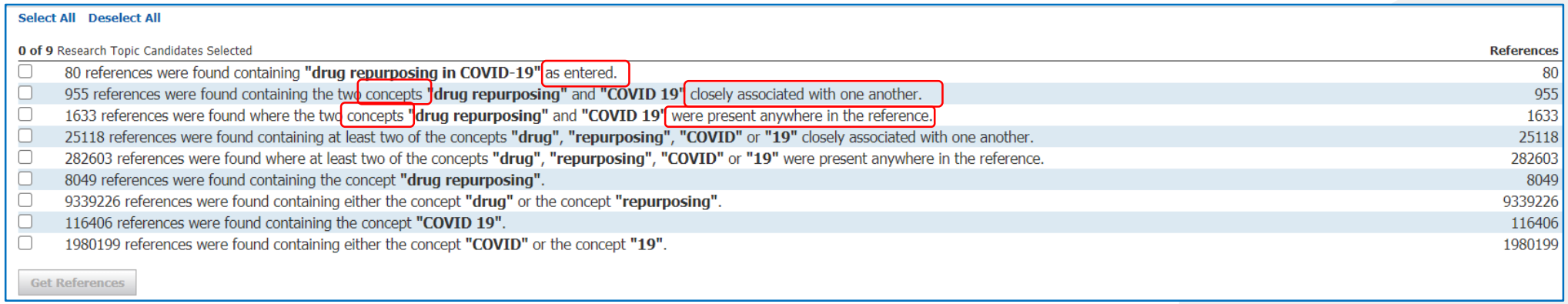
主题检索的候选项



Select All Deselect All

0 of 9 Research Topic Candidates Selected — **References**

☐	80 references were found containing **"drug repurposing in COVID-19"** as entered.	80
☐	955 references were found containing the two concepts **"drug repurposing"** and **"COVID 19"** closely associated with one another.	955
☐	1633 references were found where the two concepts **"drug repurposing"** and **"COVID 19"** were present anywhere in the reference.	1633
☐	25118 references were found containing at least two of the concepts **"drug"**, **"repurposing"**, **"COVID"** or **"19"** closely associated with one another.	25118
☐	282603 references were found where at least two of the concepts **"drug"**, **"repurposing"**, **"COVID"** or **"19"** were present anywhere in the reference.	282603
☐	8049 references were found containing the concept **"drug repurposing"**.	8049
☐	9339226 references were found containing either the concept **"drug"** or the concept **"repurposing"**.	9339226
☐	116406 references were found containing the concept **"COVID 19"**.	116406
☐	1980199 references were found containing either the concept **"COVID"** or the concept **"19"**.	1980199

Get References

"Concepts"表示对主题词做了同义词的扩展;

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

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

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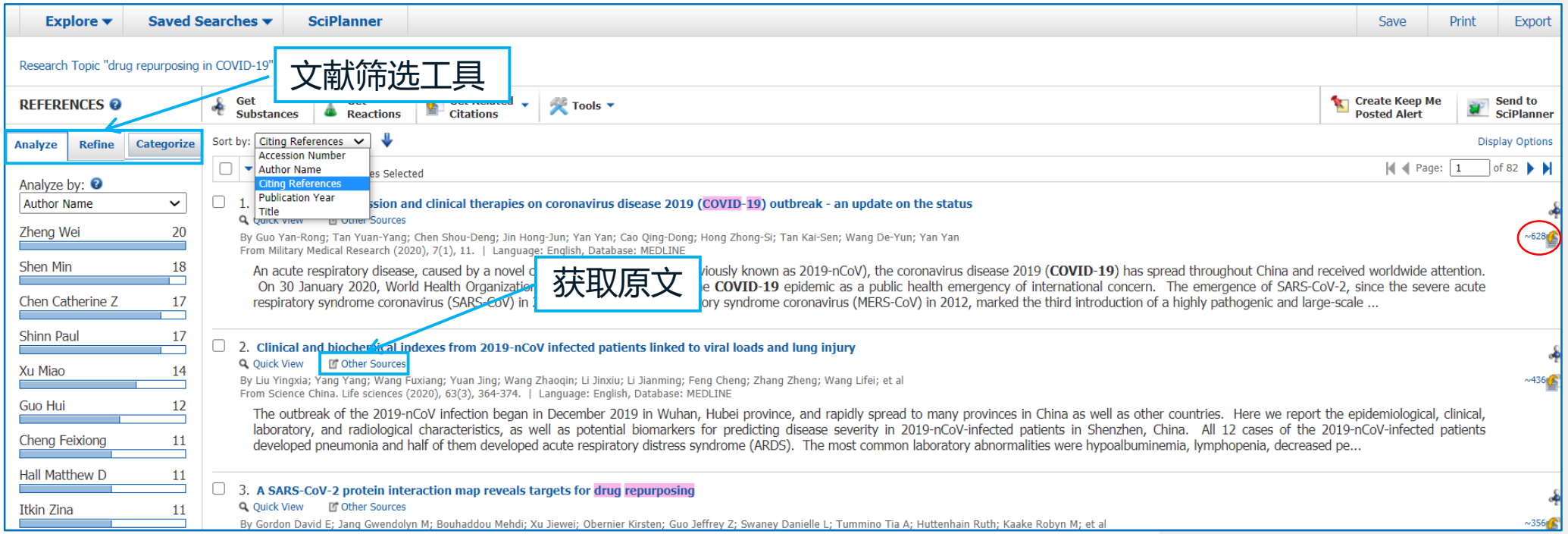
文献结果集的排序--Citing Reference



Citing Reference: 帮助找到最重要的文献

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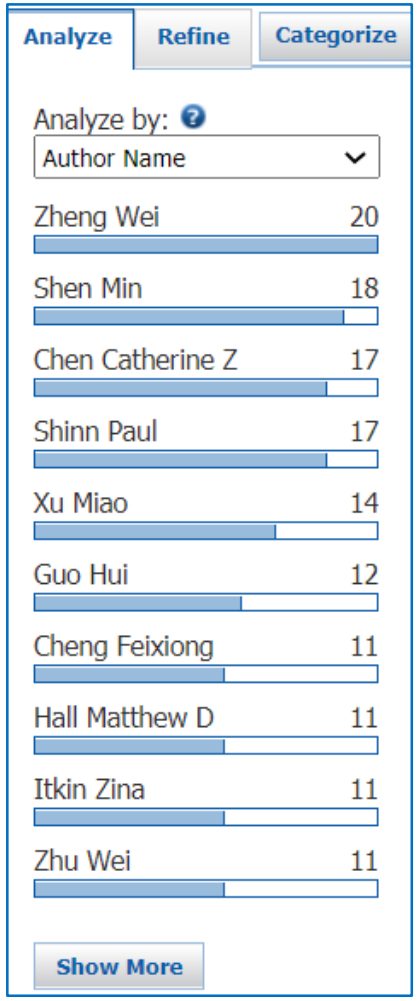
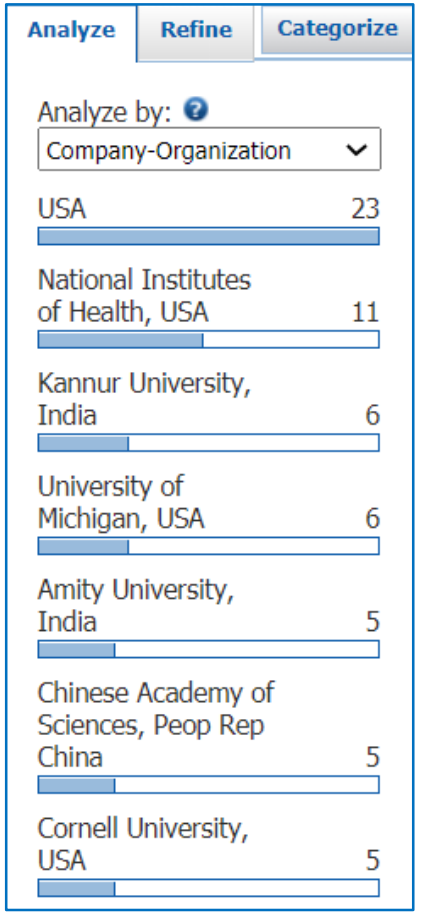
文献结果集的筛选--Analyze

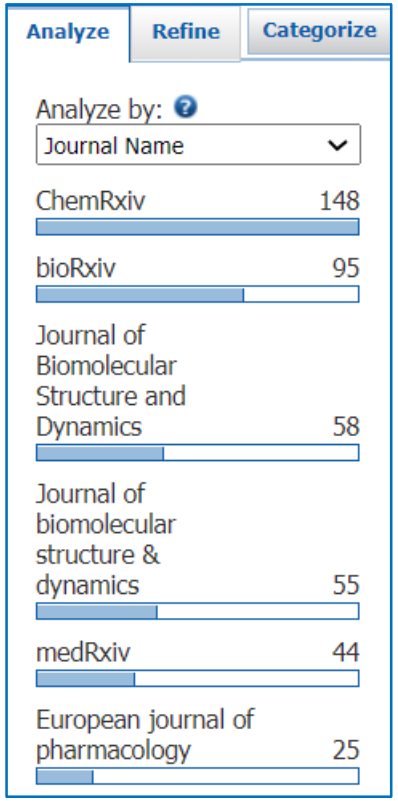
本领域研究人员



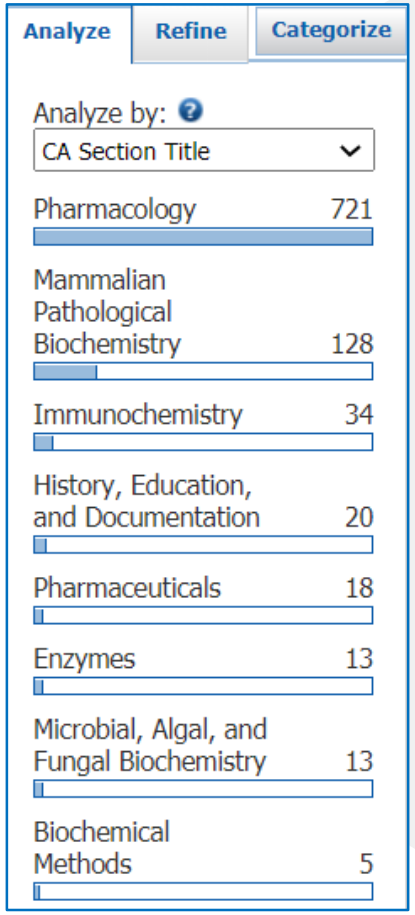
本领域研究机构、
合作伙伴、竞争对手



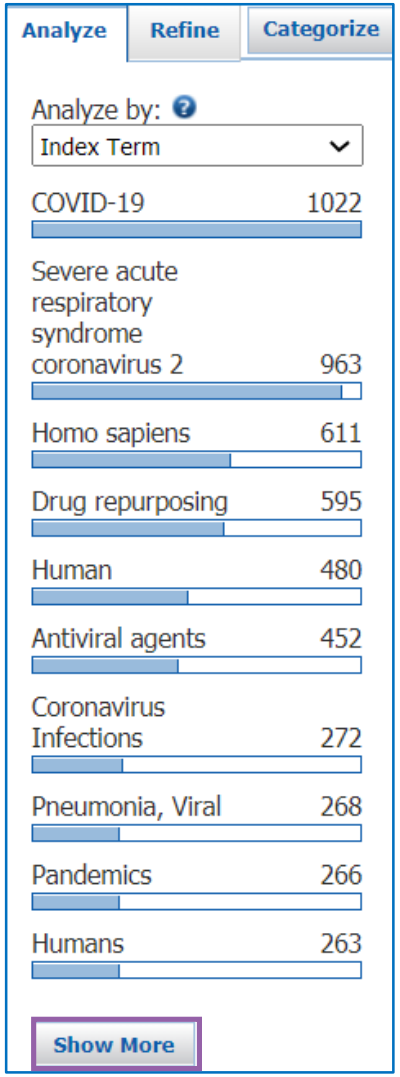
期刊



涉及学科领域

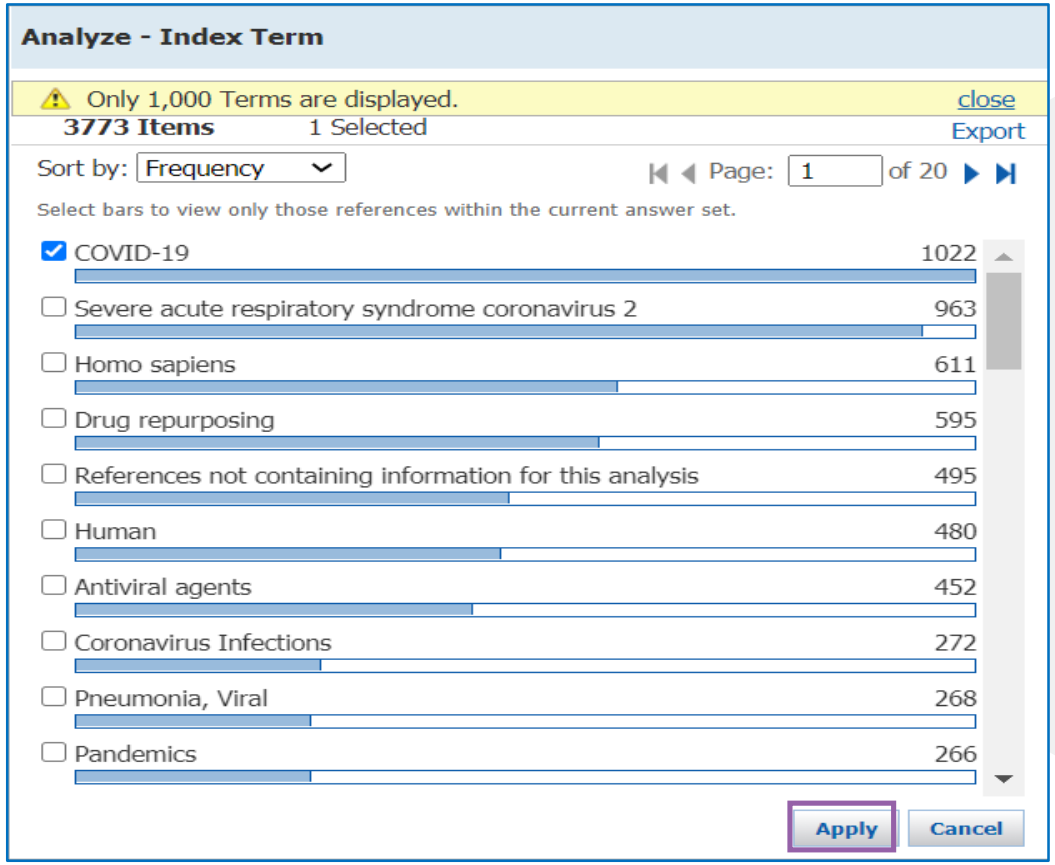


文献结果集的筛选--Analyze



Index Term：

帮助用户了解涉及到的重要技术术语，并修正检索词



选择感兴趣的内容，点击Apply

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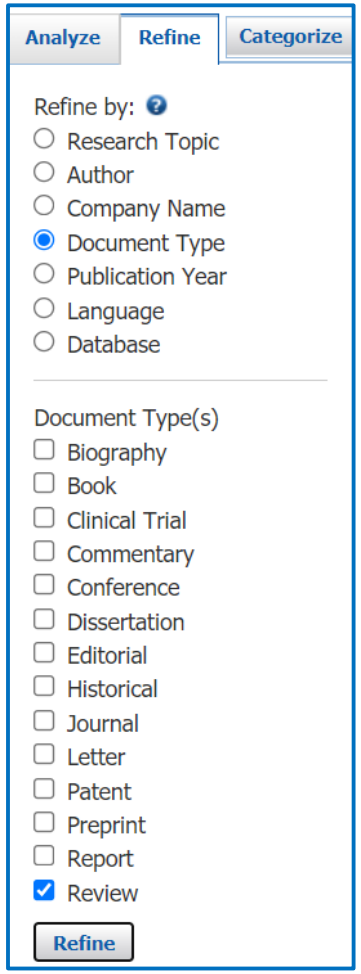
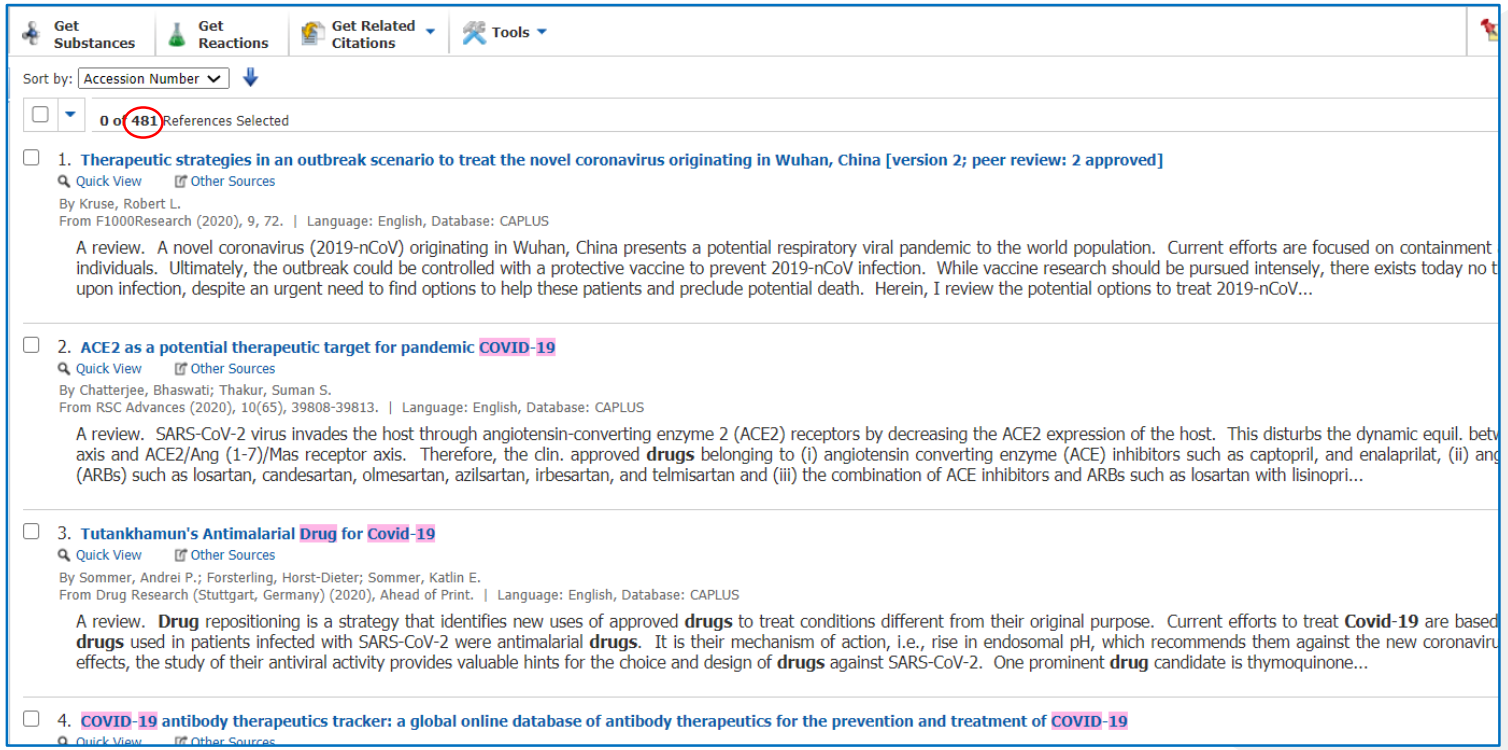
文献结果集的筛选--Refine

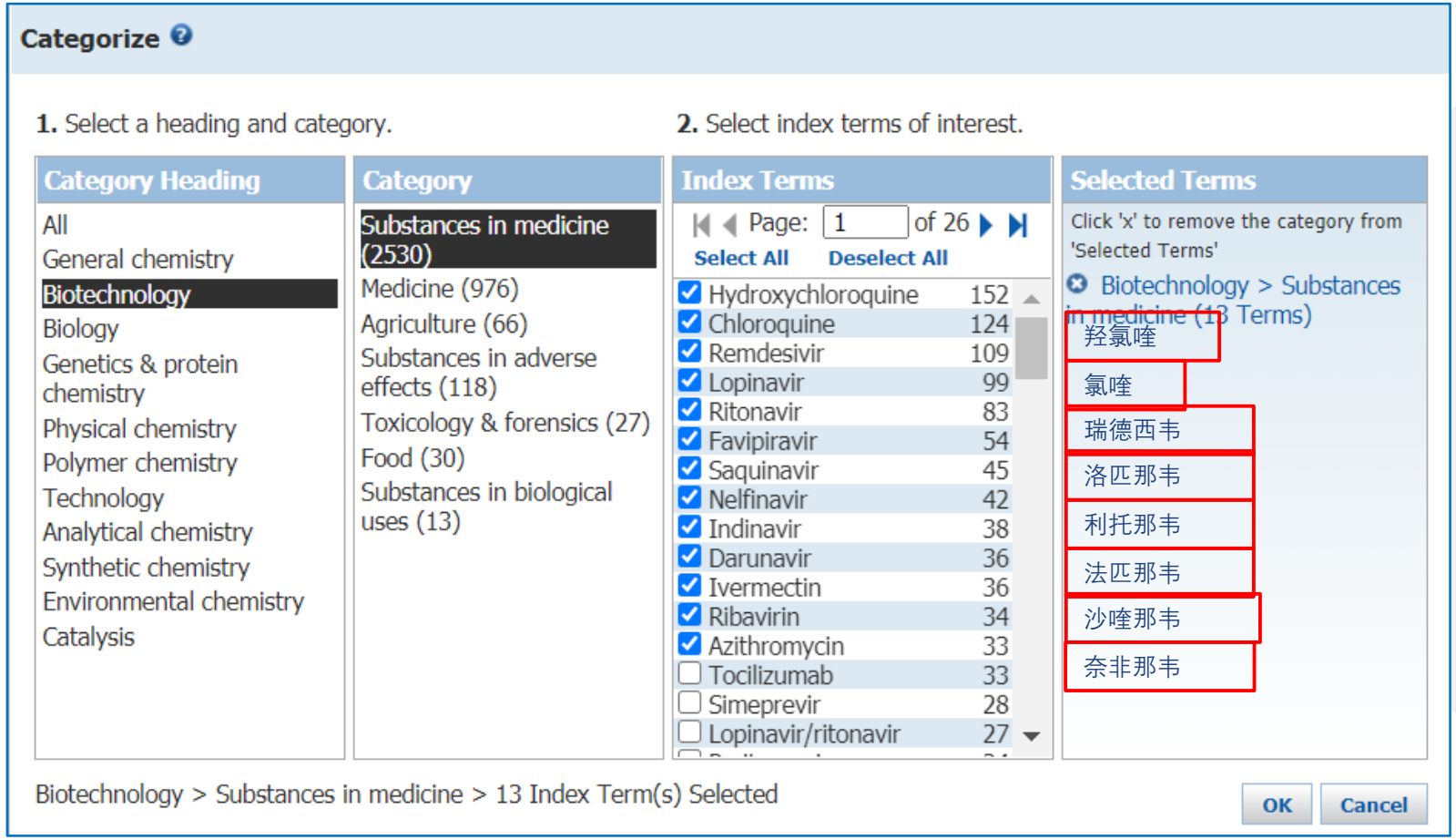




Refine： 帮助用户迅速获得需要的文献

文献结果集的筛选--Categorize

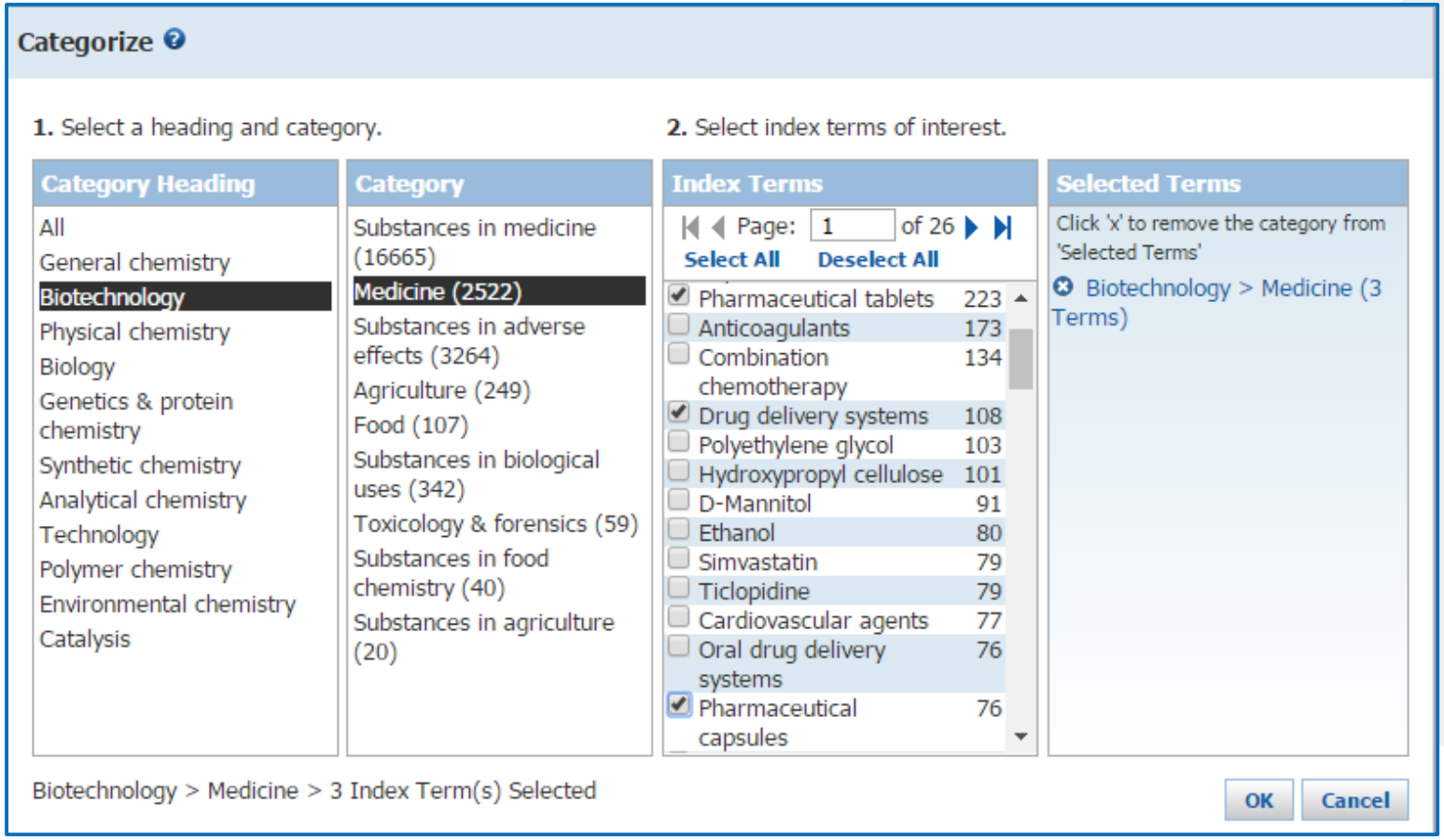
学科领域主分类　　学科领域副分类　　Index Term　　选中的Index Term



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

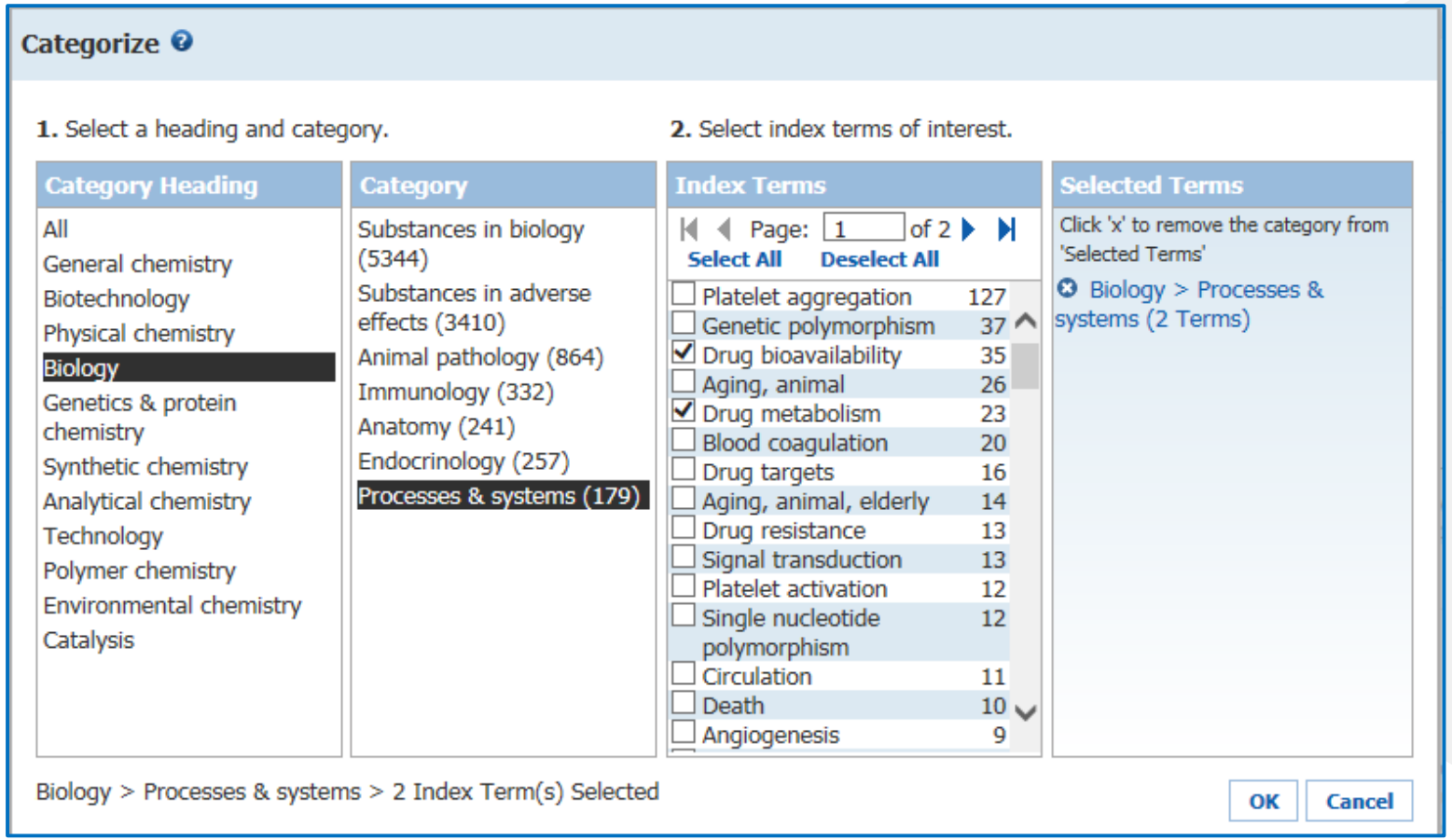
药剂学文献信息检索策略

- Step 1: 由结构信息获取文献
- Step 2: 通过Catagorize系统分类功能筛选药剂学文献



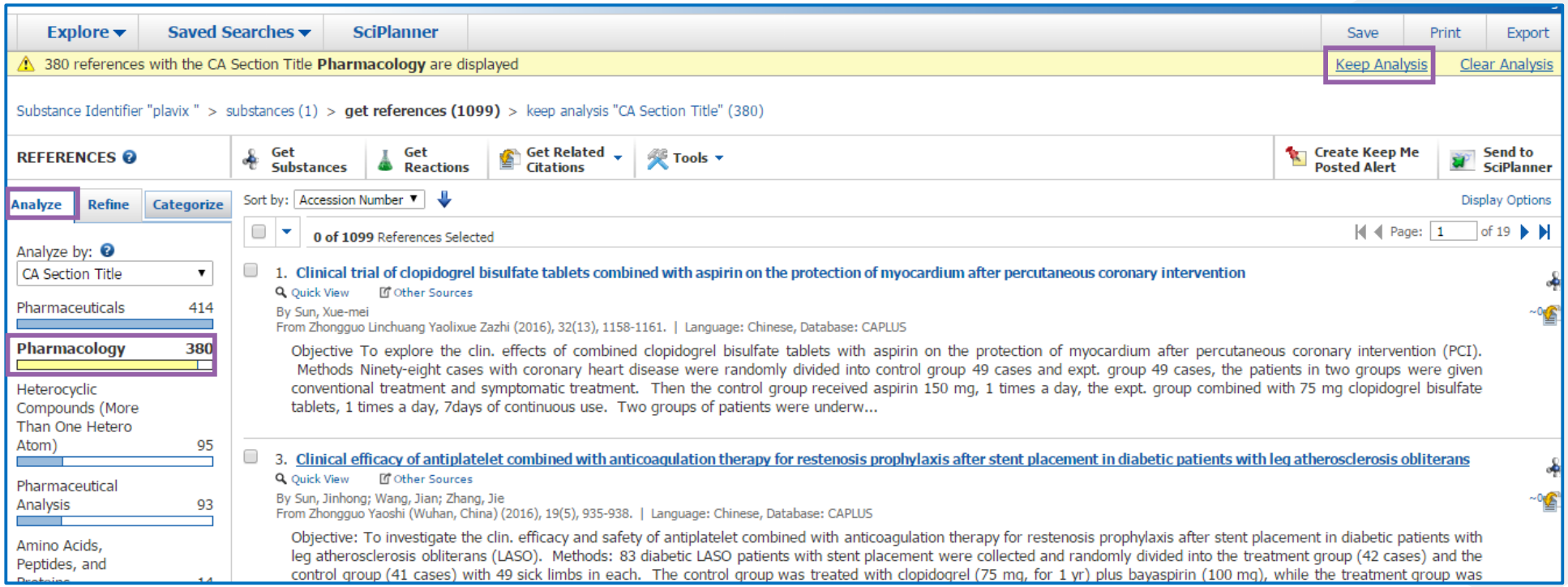
药代动力学文献信息检索策略

- Step 1: 由结构信息获取文献
- Step 2: 通过Catagorize系统分类功能筛选药代动力学文献



药理学文献信息检索策略

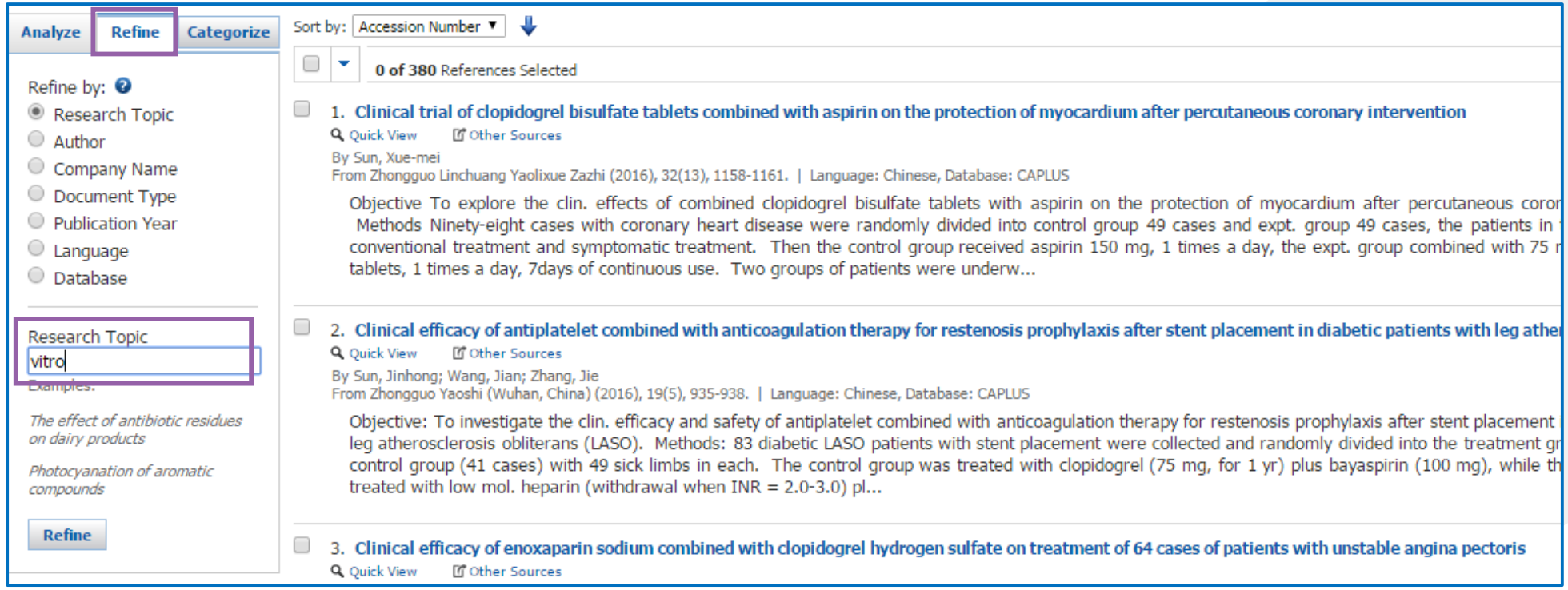
Step 1: 由结构信息获取文献
Step 2: 选择analyze， CA section title，Pharmacology，点击keep analysis



药理学文献信息检索策略

获得体外实验文献的检索方法

Step 3: 选择refine，research topic，输入vitro



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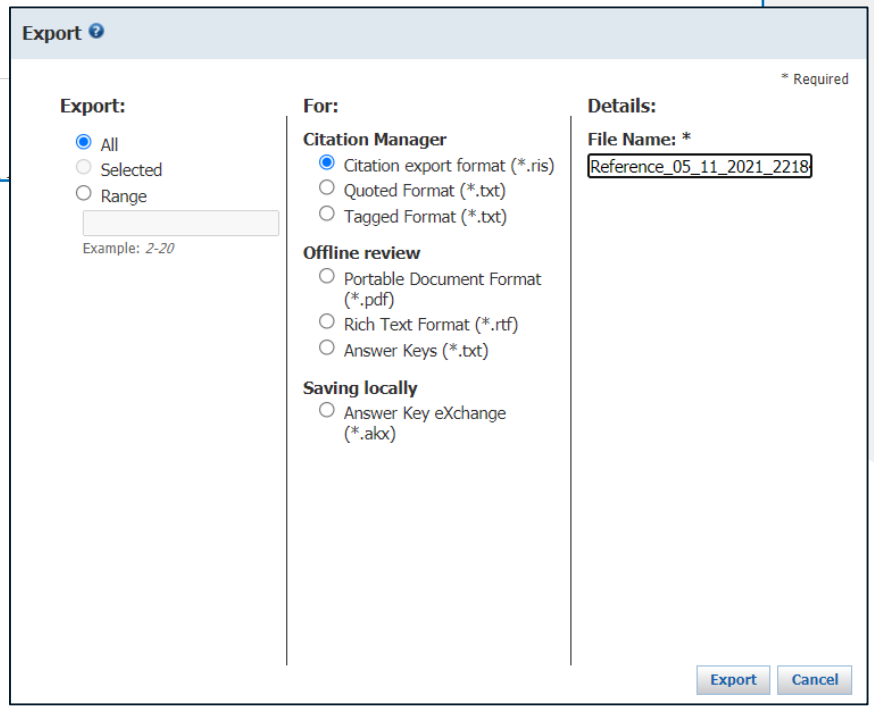
文献结果集的保存

查看文献详情



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Export：导出至本地电脑。

Print：打印成PDF格式

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

Offline Review：保存成PDF，RTF等格式，用于脱机浏览

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文献结果详情--题录、摘要、索引

2. Potential Therapeutic Options for COVID-19

By: Zheng, Xiaoqin; Li, Lanjuan

A review. The recently emerged coronavirus disease 2019 (COVID-19) has rapidly evolved into a pandemic with over 10 million infections and over 500 thousand deaths. There are currently no effective therapies or vaccines available to protect against this coronavirus infection. In this review, we discuss potential therapeutic options for COVID-19 based on the available information from previous research on severe acute respiratory syndrome (SARS) and Middle East respiratory syndrome (MERS). Substantial efforts are underway to discover new therapeutic agents for COVID-19, including the repurposing of existing agents and the development of novel agents that specifically target SARS-coronavirus 2 (SARS-CoV-2) or host factors. Through the screening of compd. libraries, various classes of drugs, such as ribavirin, remdesivir, lopinavir/ritonavir, and hydroxychloroquine have been identified as potential therapeutic candidates against COVID-19. Novel antiviral drugs for SARS-coronavirus 2 are being developed to target viral enzymes or functional proteins, as well as host factors or cell signaling pathways.

Indexing

Pharmacology (Section1-0)

Section cross-reference(s): 14

Concepts 重要概念

Anticoronaviral agents
Antiviral agents
COVID-19
Drug repurposing
Drug screening
Middle East respiratory syndrome
Severe acute respiratory syndrome
Severe acute respiratory syndrome coronavirus 2

potential therapeutic options for COVID-19

Substances 重要物质

118-42-3 Hydroxychloroquine
36791-04-5 Ribavirin
369372-47-4 Lopinavir/ritonavir
1809249-37-3 Remdesivir

potential therapeutic options for COVID-19

Therapeutic use; Biological study; Uses

Supplementary Terms

review SARS CoV2 coronavirus COVID19 antiviral agent

QUICK LINKS

0 Tags, 0 Comments

SOURCE

Infectious Microbes & Diseases
Volume2
Issue3
Pages89-95
Journal; General Review; Online Computer File
2020
CODEN:IMDNCQ
ISSN:2641-5917
DOI:10.1097/IM9.0000000000000033

COMPANY/ORGANIZATION

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

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专利工作流程解决方案

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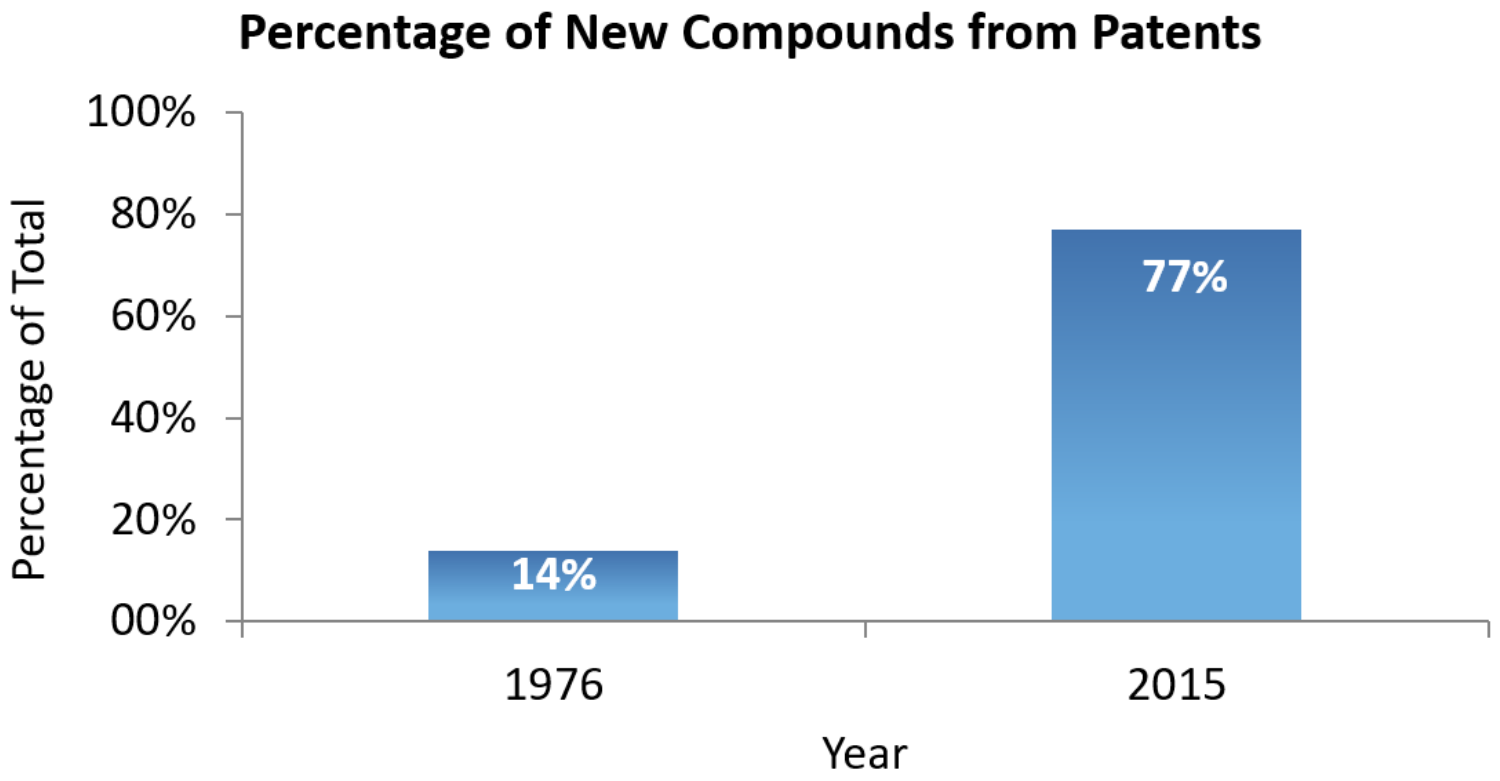
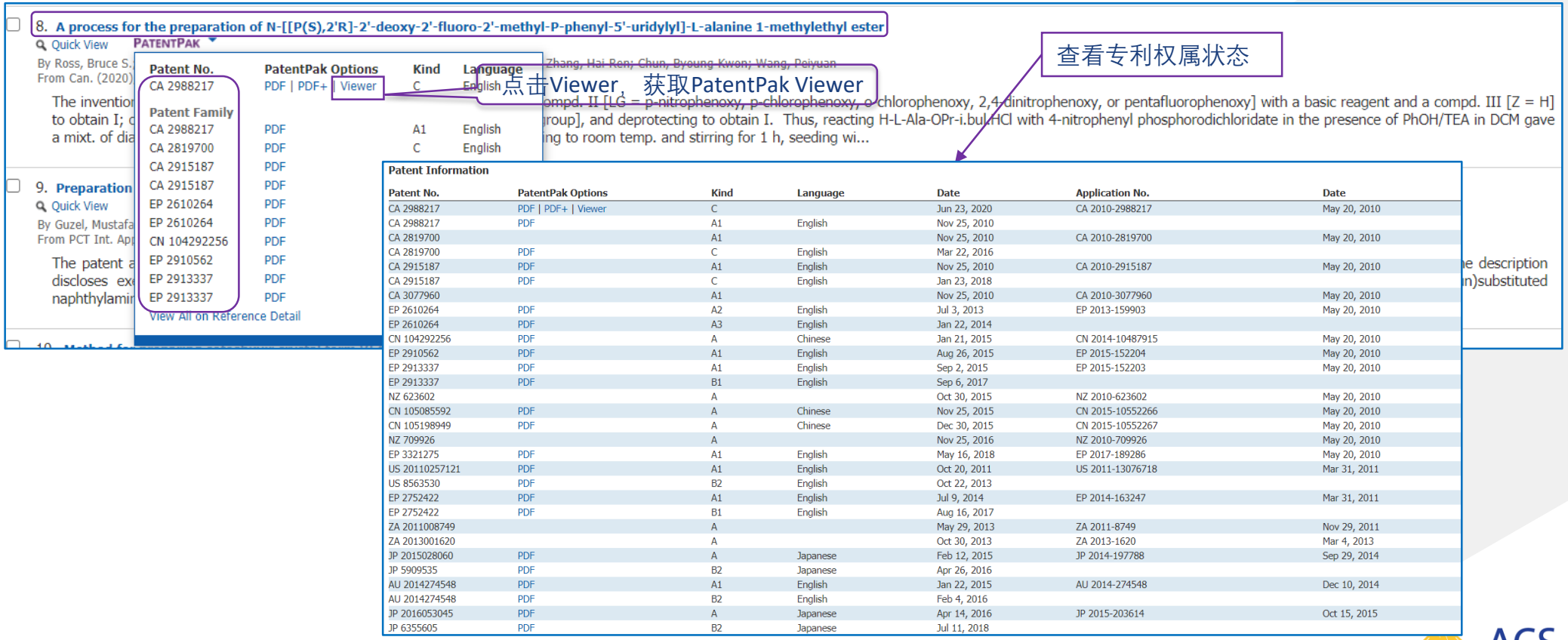
越来越多的新化合物倾向于首先通过专利公布



CAS PatentPak

——专利工作流程解决方案：



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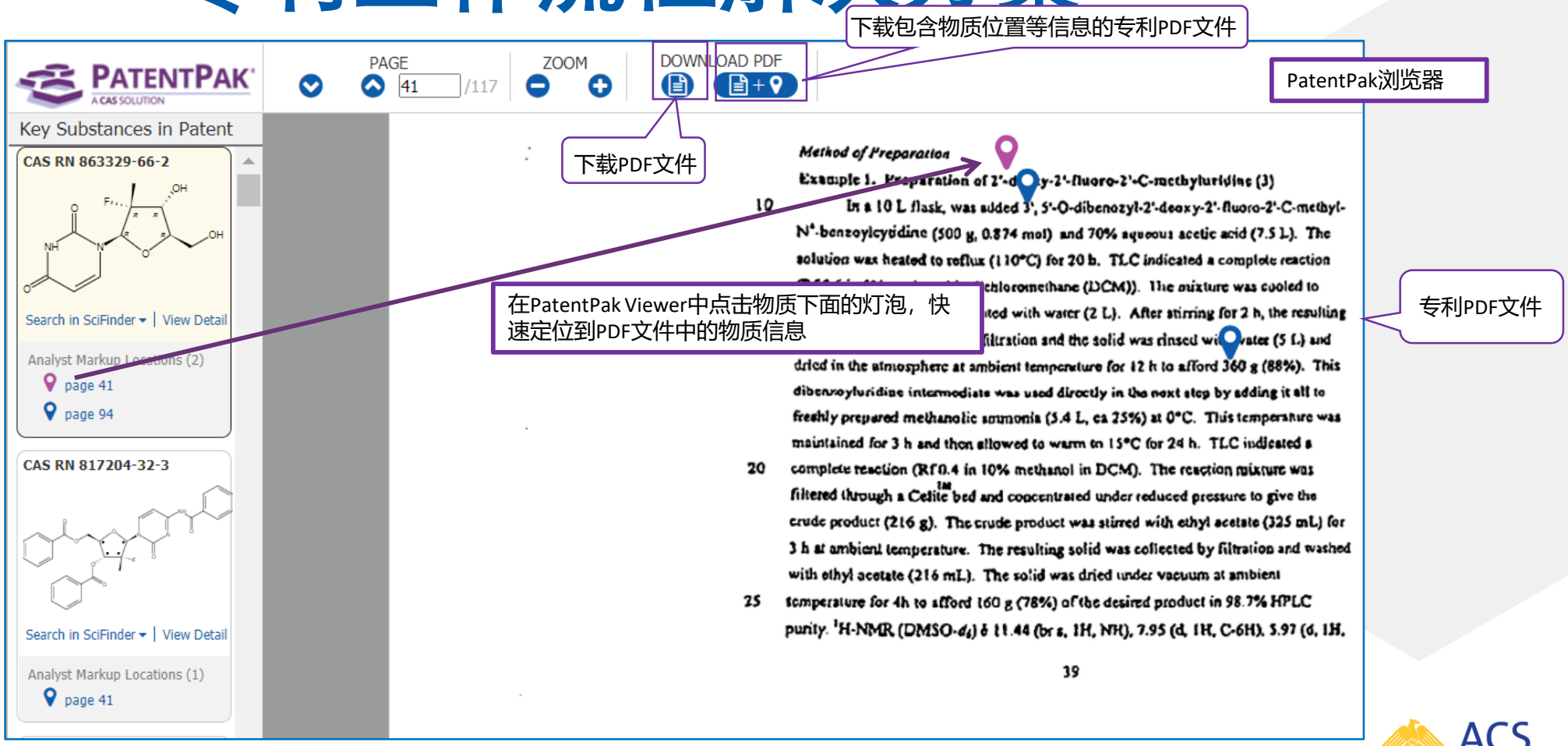
CAS PatentPak

——专利工作流程解决方案



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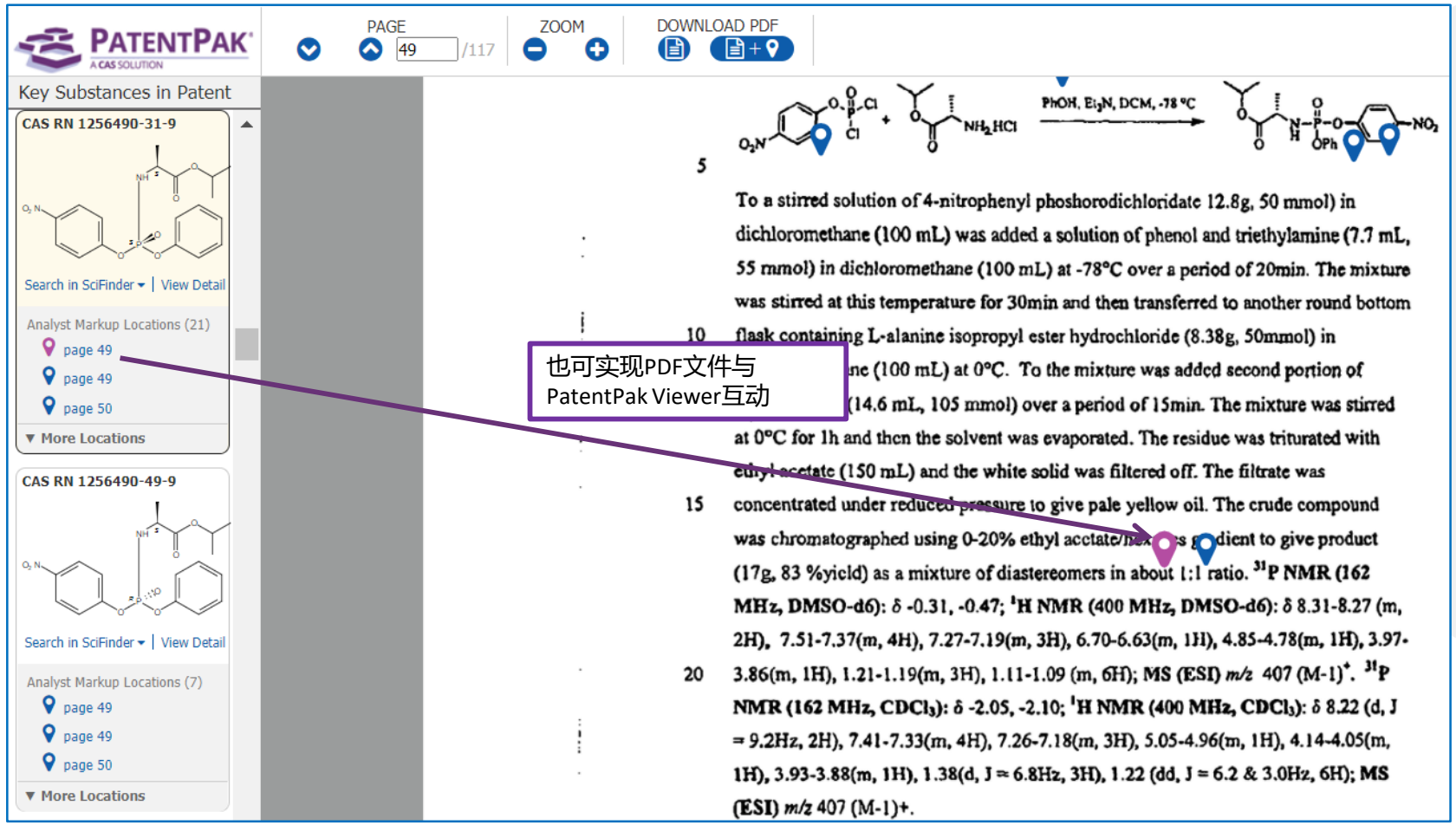
CAS PatentPak

——专利工作流程解决方案



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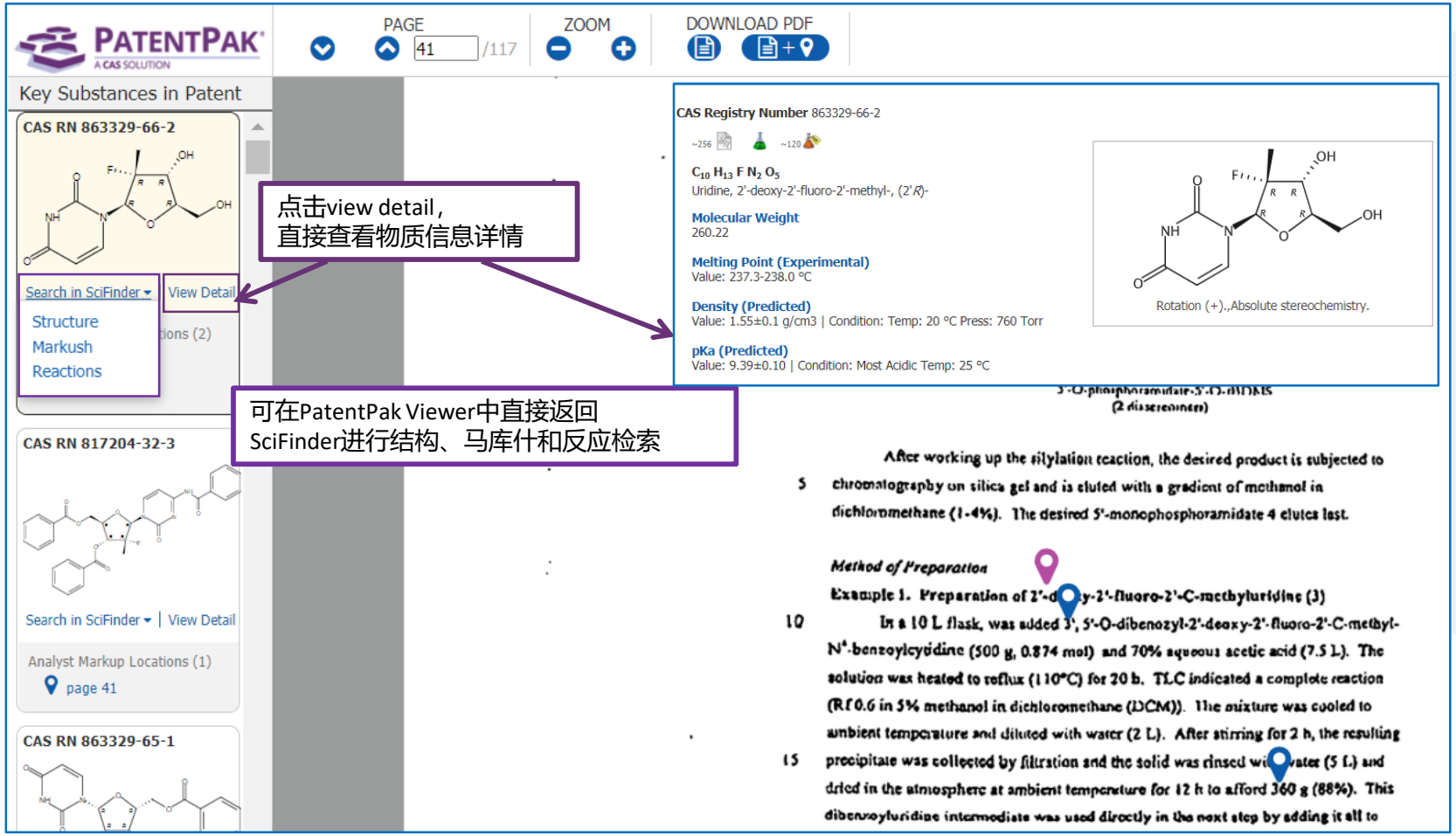

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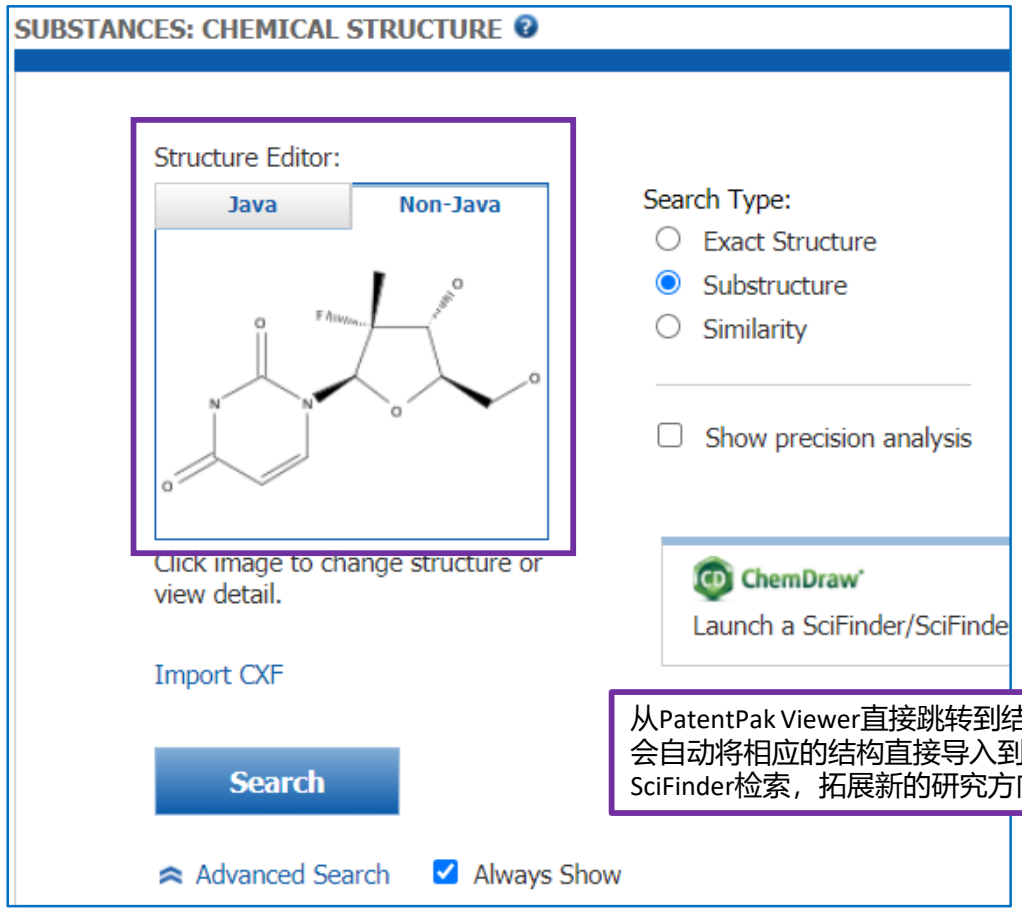
CAS PatentPak
——专利工作流程解决方案



从PatentPak Viewer直接跳转到结构检索界面，同时无需绘制，系统会自动将相应的结构直接导入到绘图面板，点击Search即开始SciFinder检索，拓展新的研究方向

节省您最宝贵的资源——时间

- 即时获得来自世界上46家专利授权机构的逾1800万份专利PDF文件，且数量持续增加
- 专利族涵盖了多种语言
- 通过CAS登记号获得物质在专利文献中的相关信息
- 专利研究安全保密
- 每日更新
- SciFinder检索功能中内置交互式浏览器
- 每日更新
- SciFinder检索功能中内置交互式浏览器

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文献检索小结

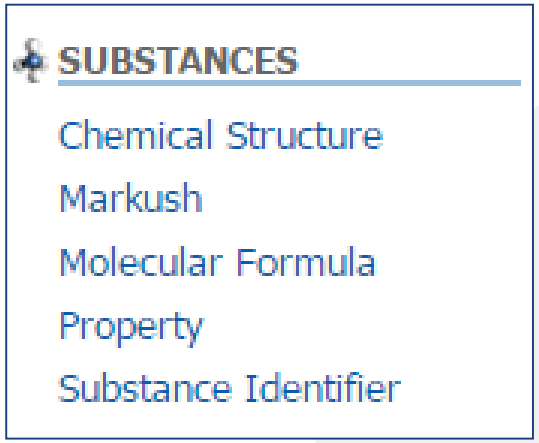
1. 主题检索时，使用介词 in, with, of 等作为连接词
2. 跟据检索要求选择合适的候选项
3. 通过SciFinder 的Analyze/Refine功能来缩小检索的范围
4. 尝试将不同的Analyze/Refine功能组合起来用，会有更多的收益
5. 使用Categorize可以让系统来实现自动分类

大纲

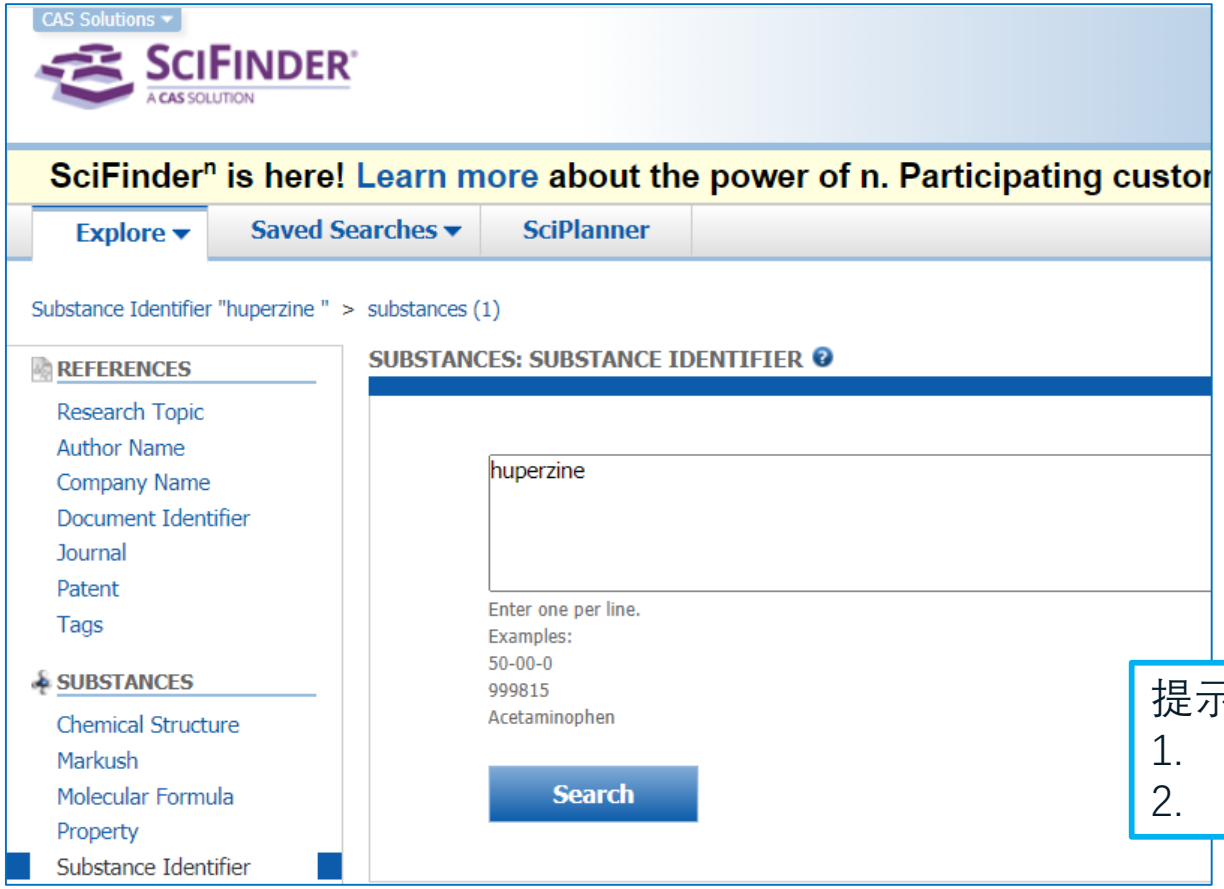
- CAS及CAS SciFinder介绍
- 文献相关信息的获取策略
  - 文献检索方法
  - 文献结果排序、筛选和详情
  - 如何高效阅读专利文献详情(CAS PatentPak)
- **物质相关信息的获取策略**
  - 常见的物质检索方法
  - 物质结果排序、筛选和详情
- 反应相关信息的获取策略
  - 反应的获取方法
  - 反应结果排序、筛选和详情
  - 如何高效获取反应详情（Synthetic Methods）
- 分析相关信息的获取 (CAS Analytical Methods)

CAS SciFinder检索--物质检索

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



物质检索--标识符检索

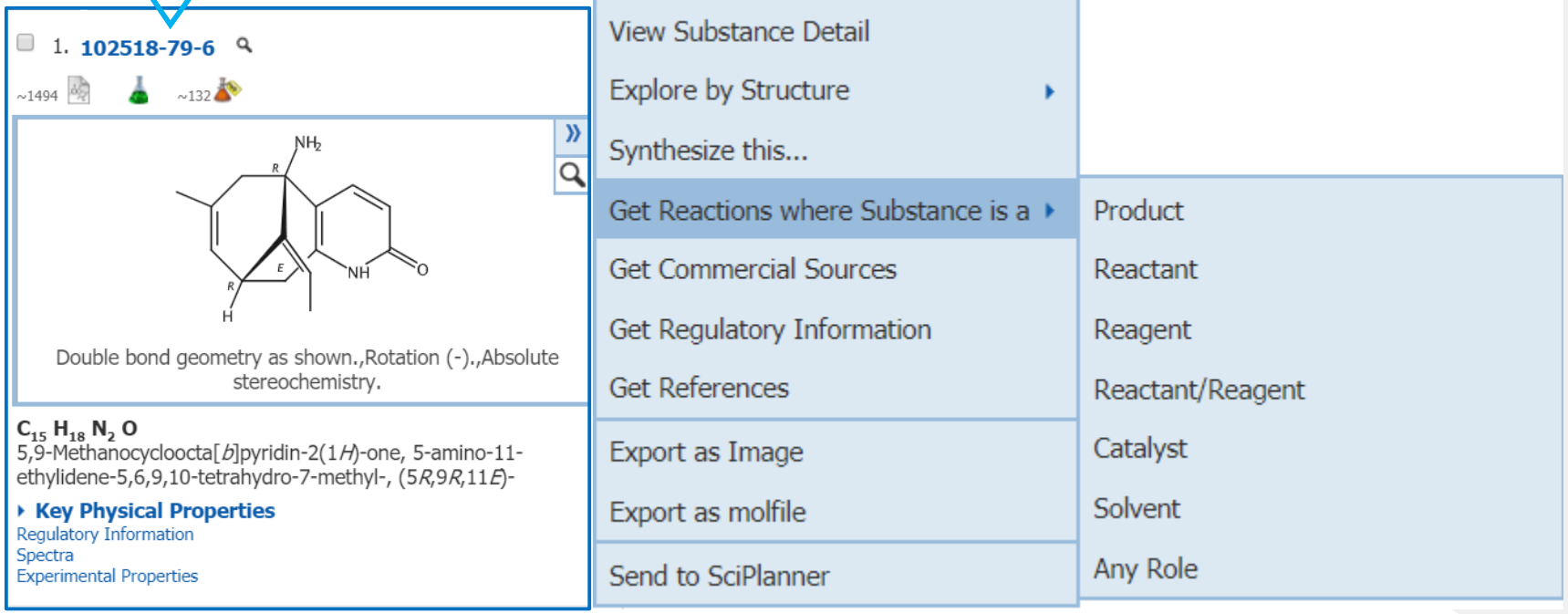


提示：
1. 一次最多可输入25个物质。
2. 每行一个物质标识符。

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

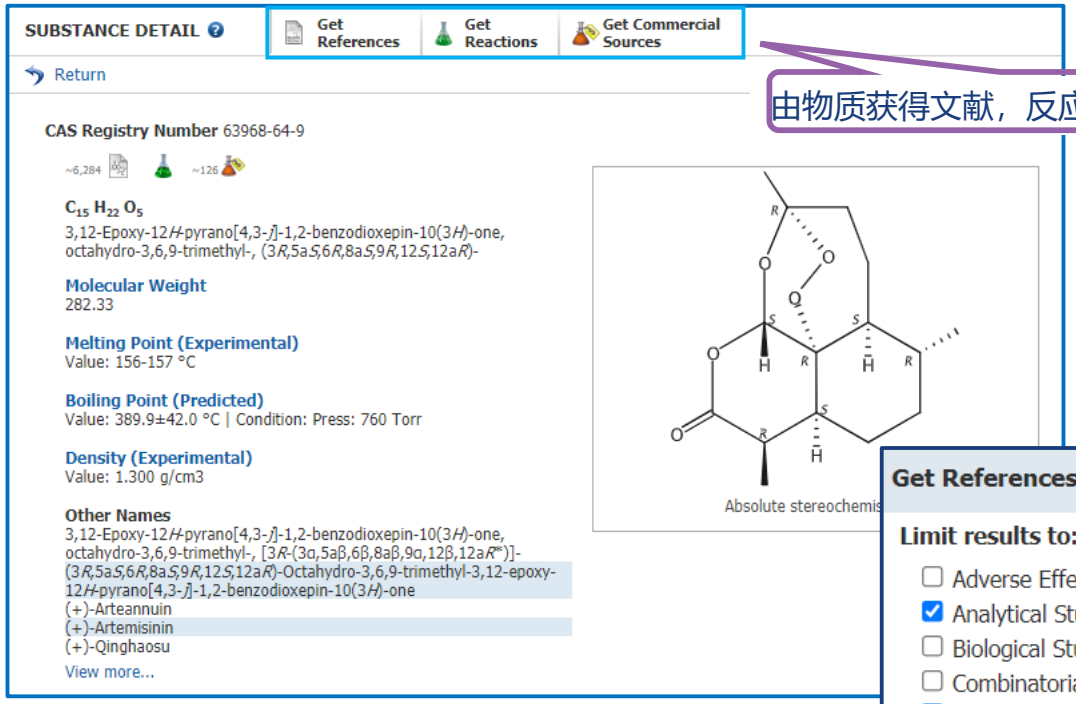
物质结果集

点击CAS RN 获得物质详细信息

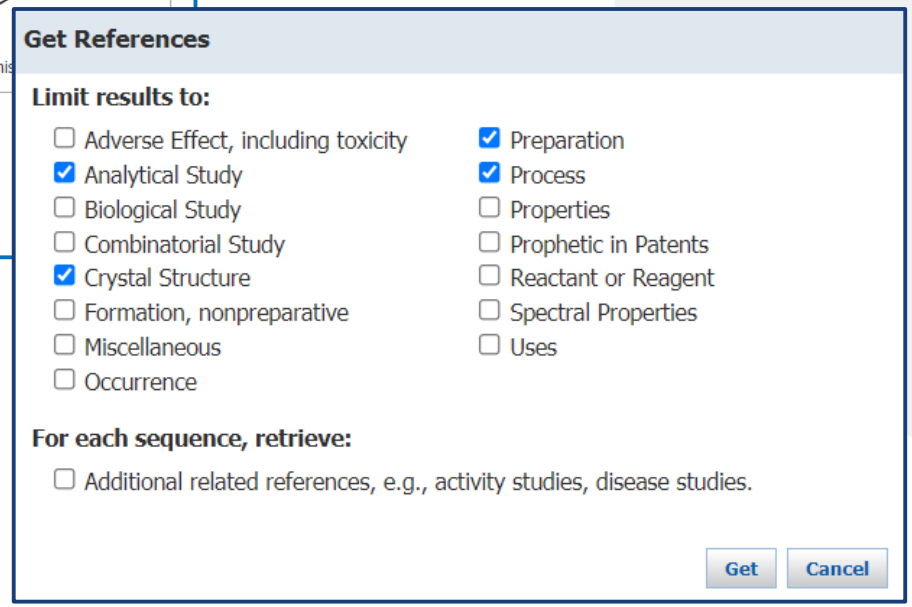


在SciFinder中，鼠标滑过物质，即可打开物质标准菜单，获得与物质相关的所有内容

物质结果详情



由物质获得文献，反应，供应商等信息



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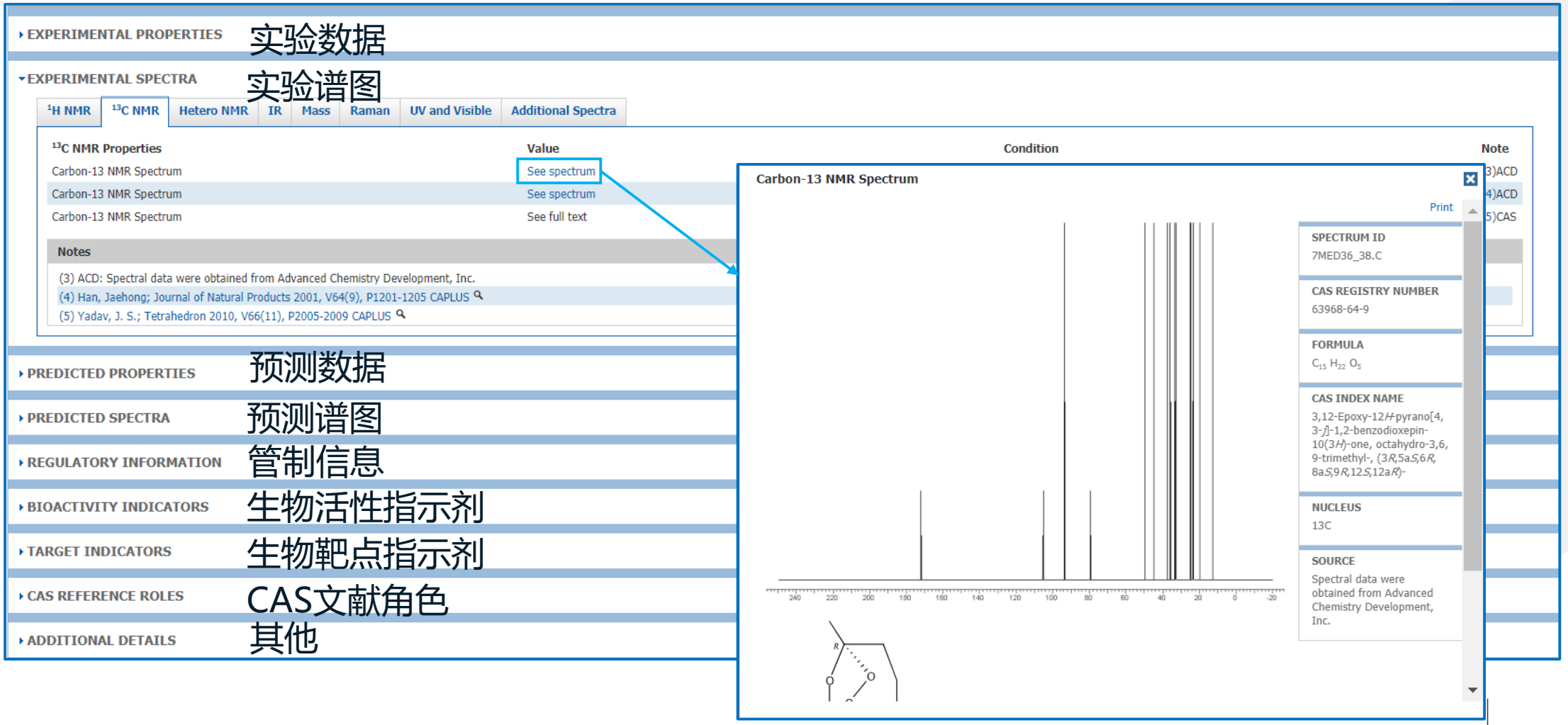
物质结果详情—实验数据实验谱图



物质结果详情—生物活性

BIOACTIVITY INDICATORS

Indicators	References
Cytoprotective agents (all) > Neuroprotective agents	134
Enzyme inhibitors (all) > Cholinesterase inhibitors	130
Natural products, pharmaceutical	140
Nervous system agents (all) > > Anti-Alzheimer agents	198
Nervous system agents (all) > > > Cognition enhancers	97
Nervous system agents (all) > Neuroprotective agents	134

神经保护剂

胆碱酯酶抑制剂

抗阿尔茨海默病

认知促进剂

TARGET INDICATORS

Indicators	References
Apoptosis-regulating proteins (all) > Bax proteins	10
Cytokines (all) > > > Interleukin 1β	12
Cytokines (all) > > > Interleukin 1β	12
Cytokines (all) > > Interleukin 6	10
Cytokines (all) > > Interleukin 6	10
Cytokines (all) > > Interleukin 6	10
Cytokines (all) > > Tumor necrosis factor α	15
Cytokines (all) > > Tumor necrosis factor α	15
Cytoskeletal proteins (all) > > > Tau proteins	12

Bax蛋白

白细胞介素-1β

白细胞介素 6

肿瘤坏死因子-α

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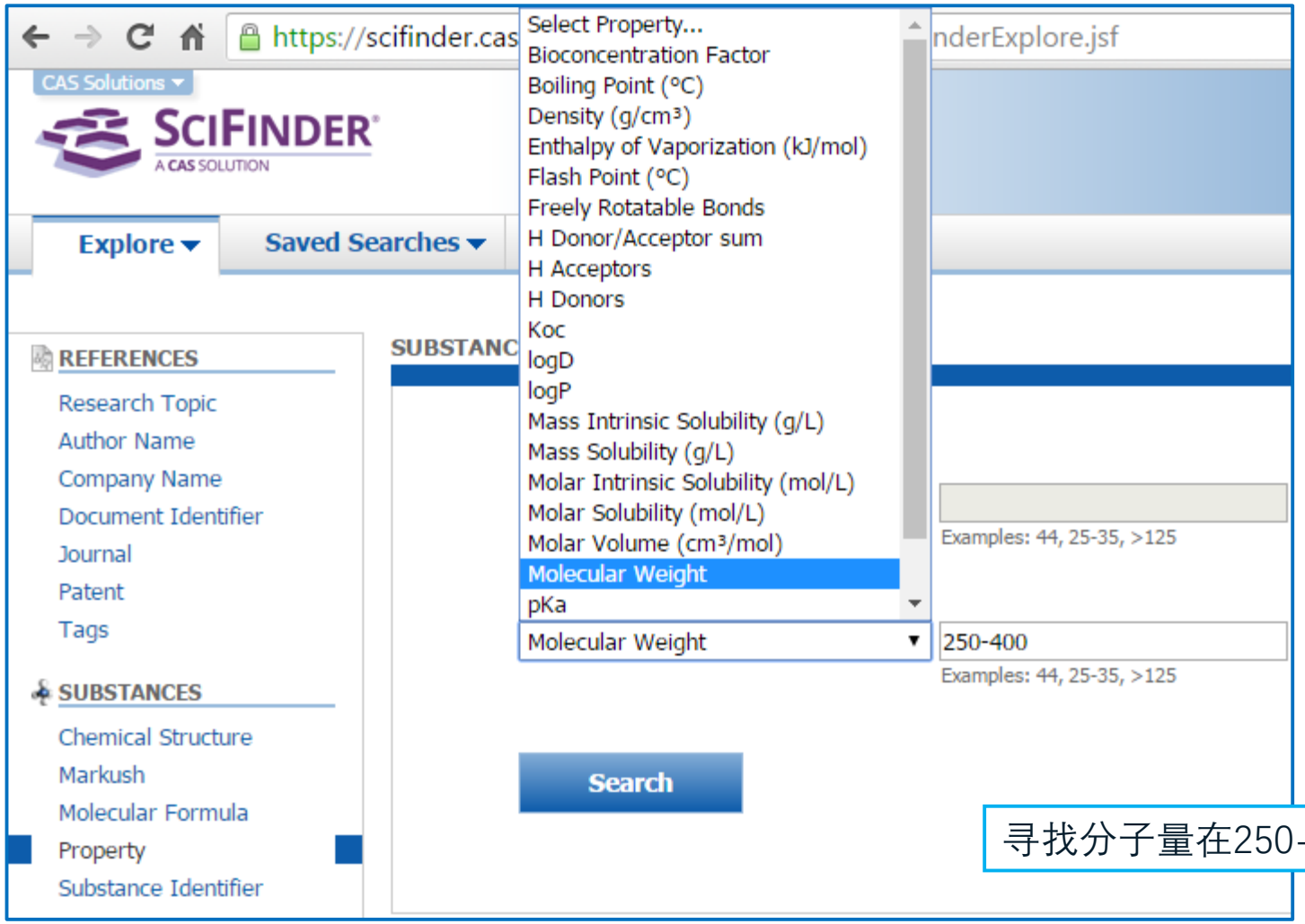
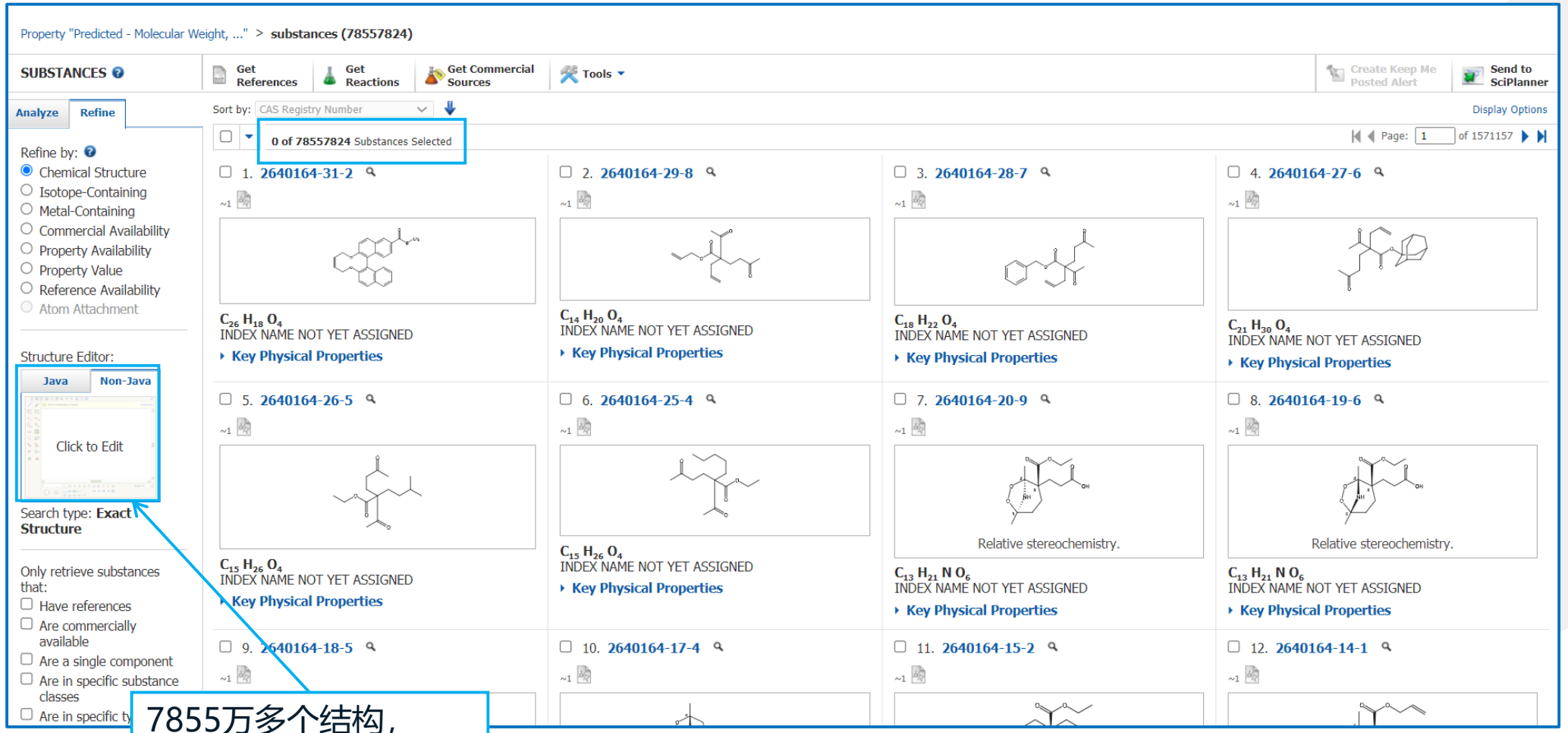
物质检索--Property Explorer



寻找分子量在250-400之间的物质

物质结果集的筛选--Refine



7855万多个结构，

如何筛选黄酮类物质?

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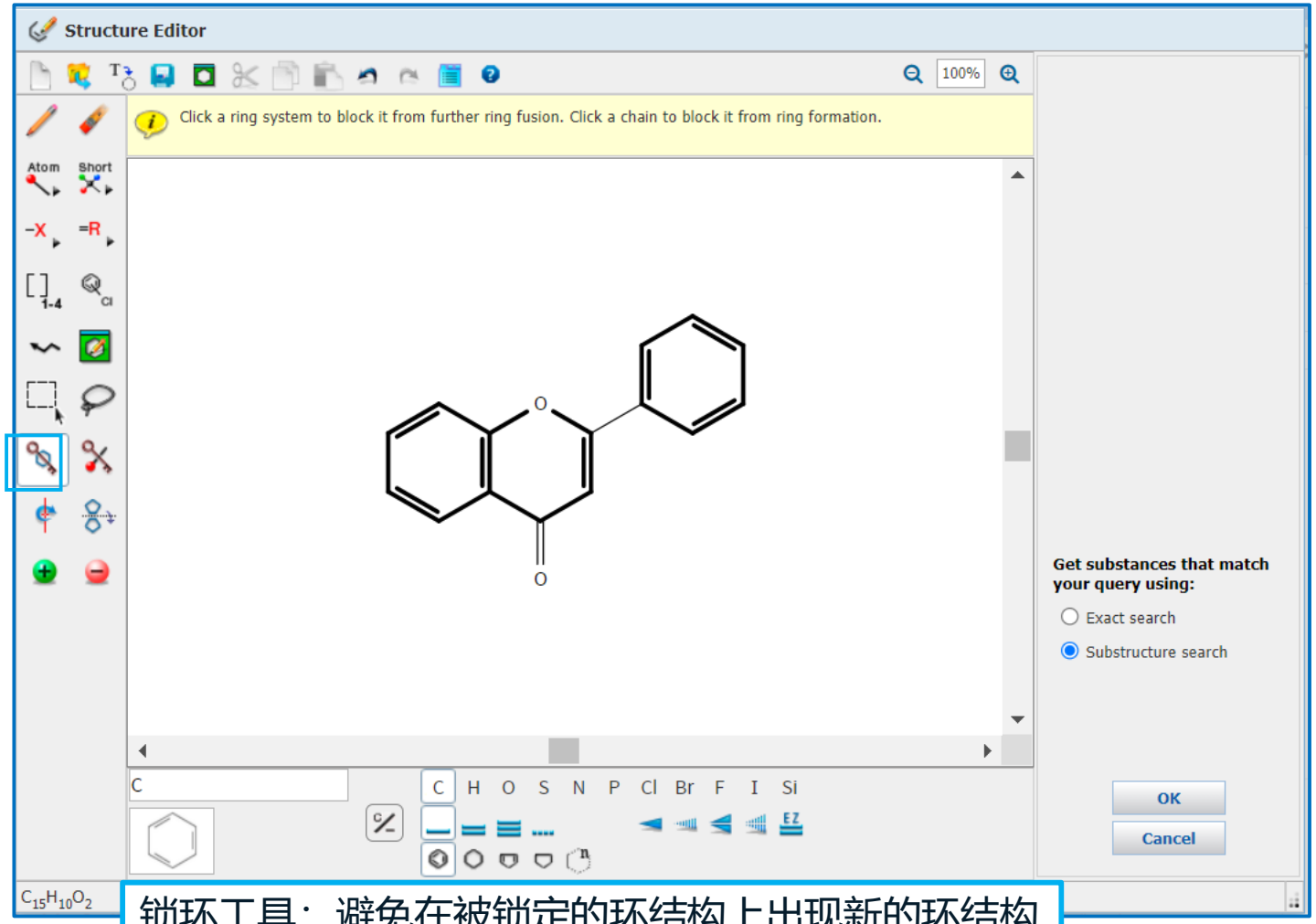
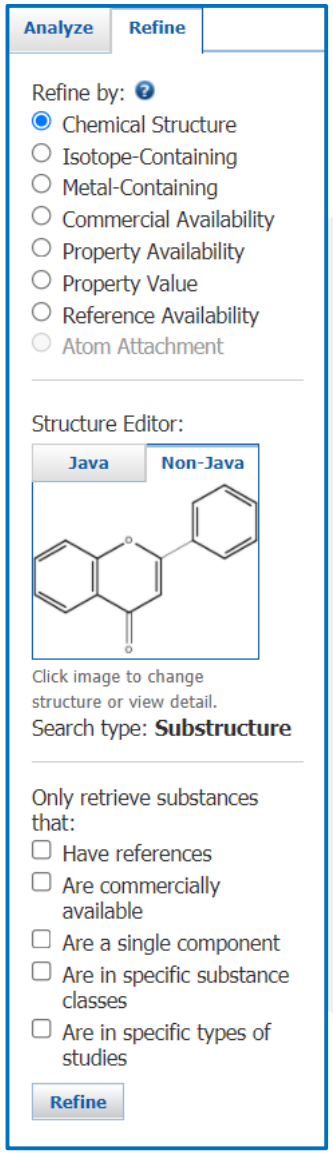
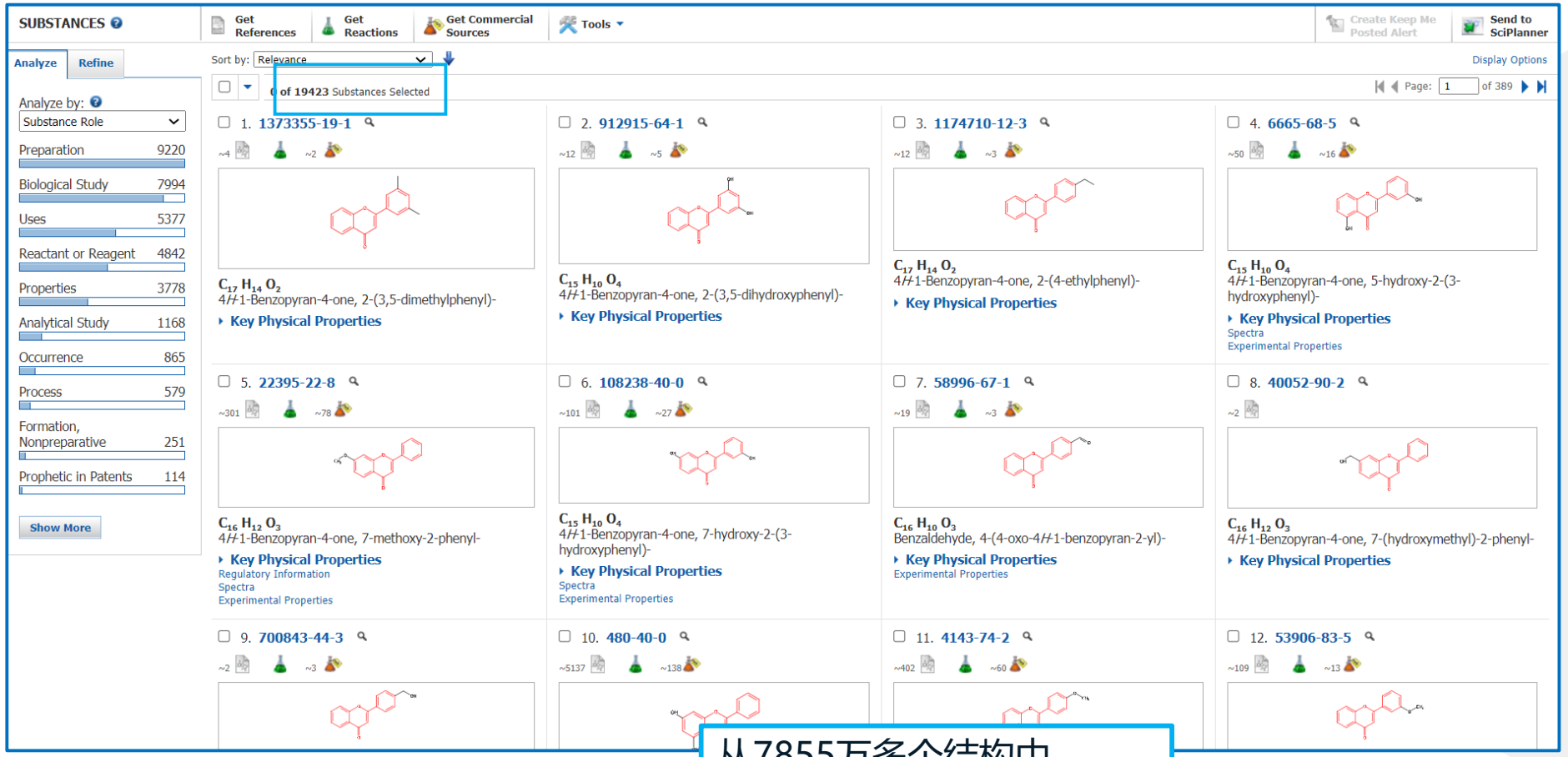
物质结果集的筛选--Refine



锁环工具：避免在被锁定的环结构上出现新的环结构



物质结果集的筛选--Refine



从7855万多个结构中

筛选出19423个黄酮类物质

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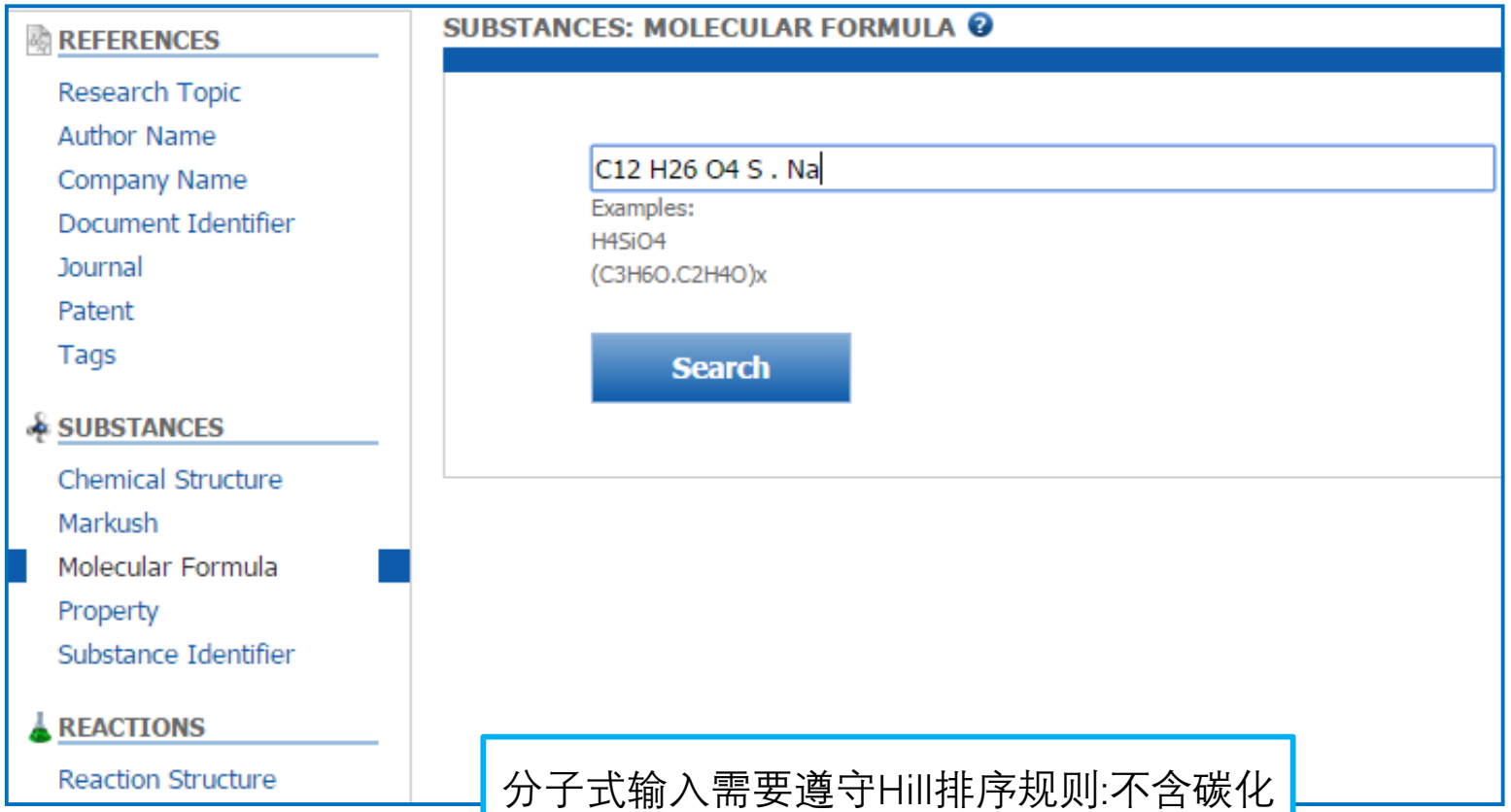
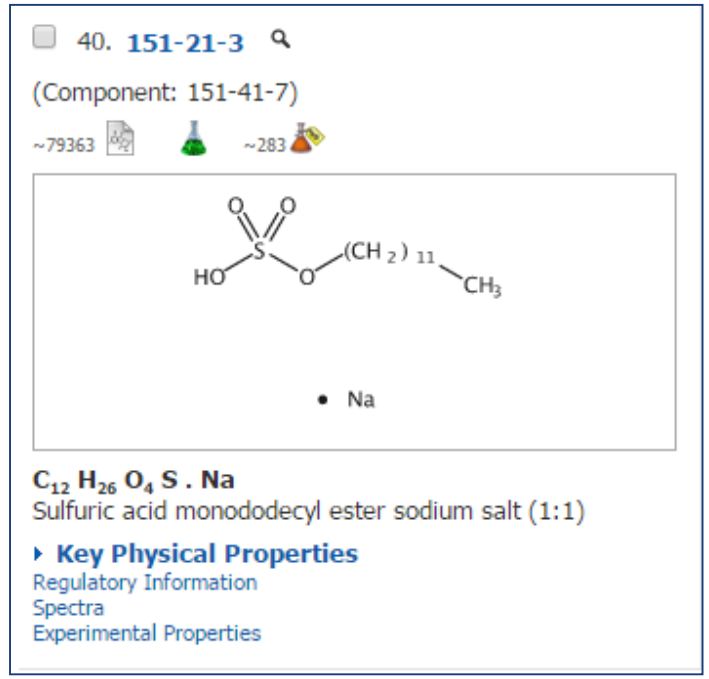
物质检索--分子式检索



无机金属盐：金属离子和阴离子间用点（.）分开



分子式输入需要遵守Hill排序规则:不含碳化合物,按元素符号的字母顺序排列;分子式为含碳化合物时,则“C”在前；如有氢则紧随其后,其它元素符号按字母顺序排在氢的后面

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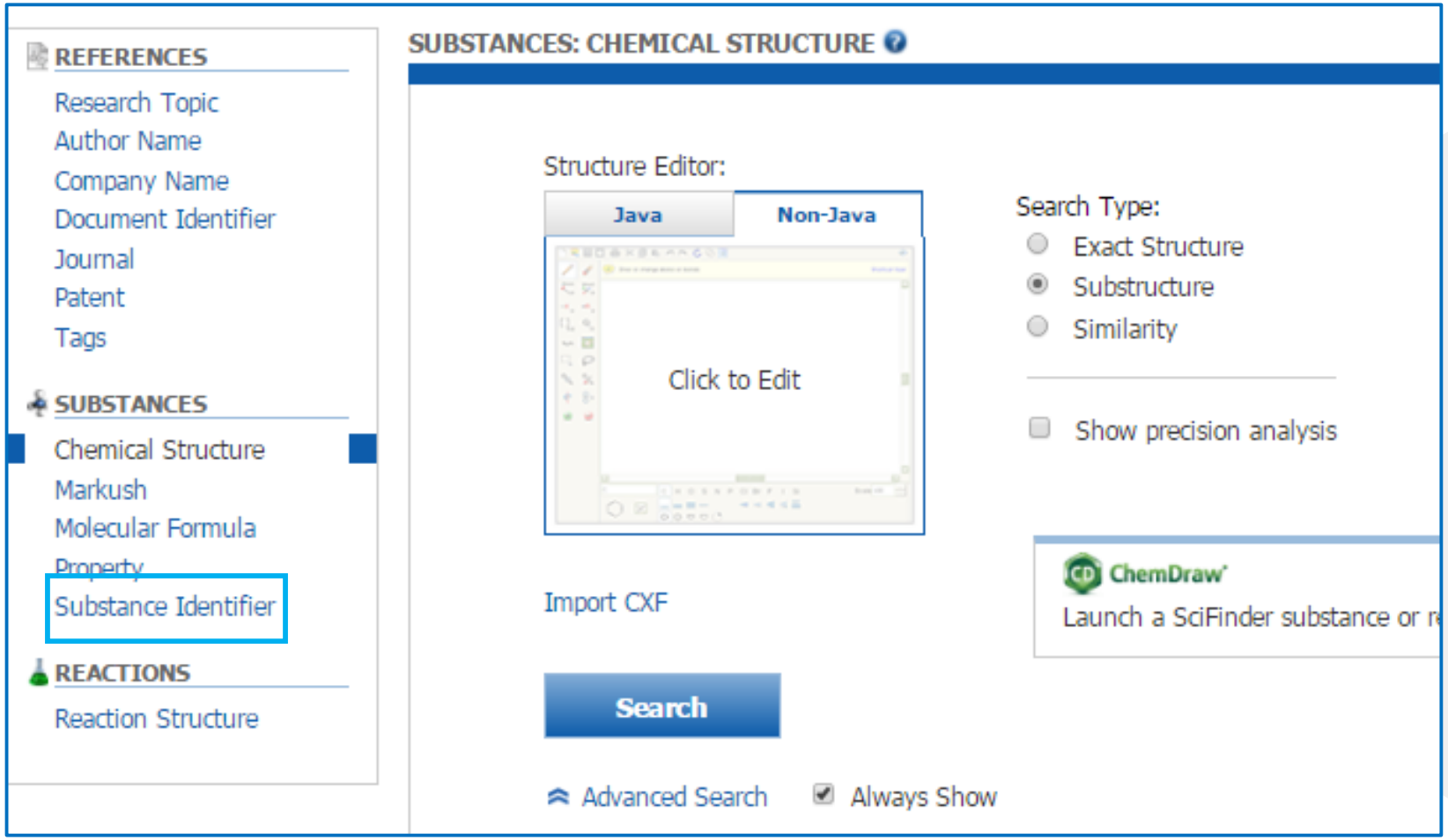
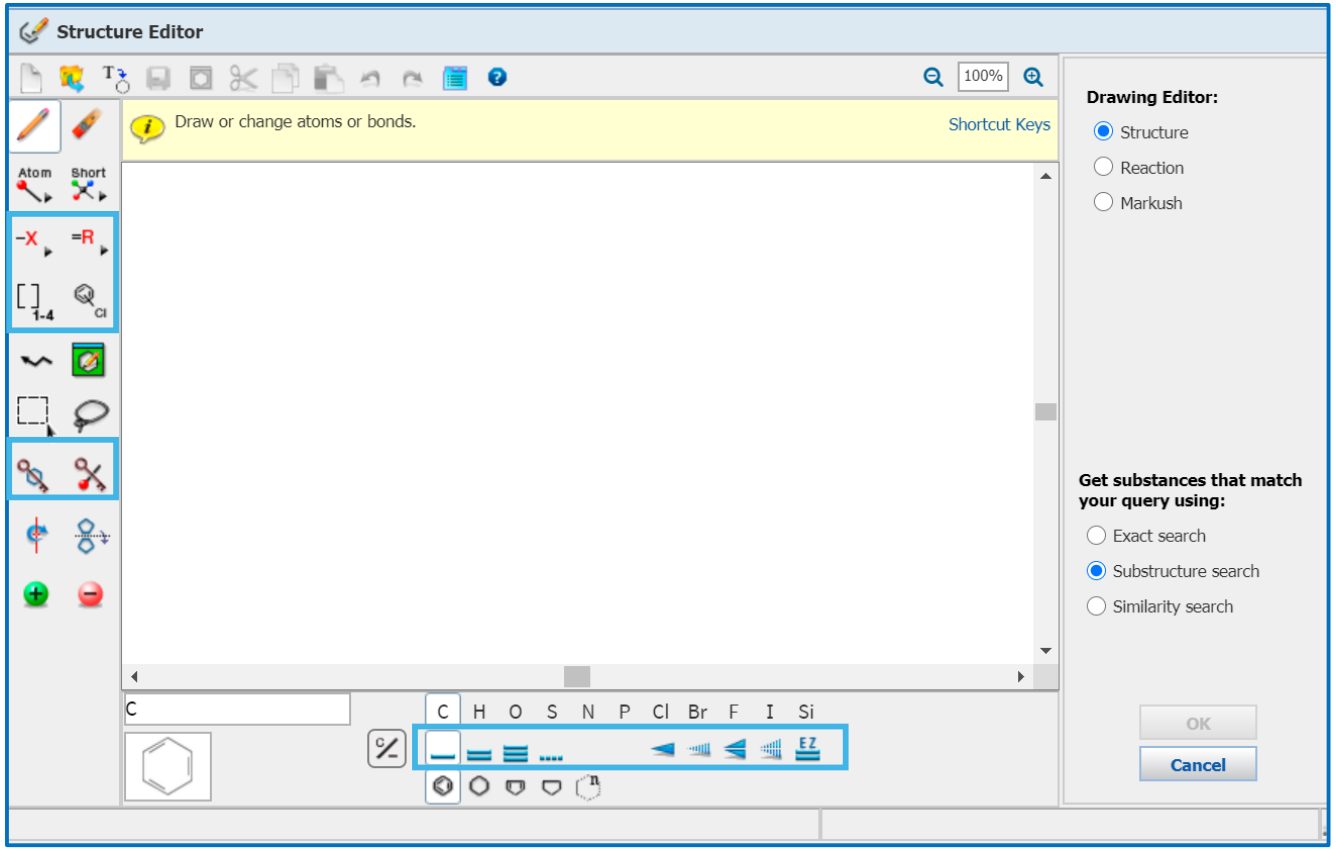
物质检索--结构式检索



物质检索--结构编辑器



重要绘制工具注释

选择可变基团

自定义R基团

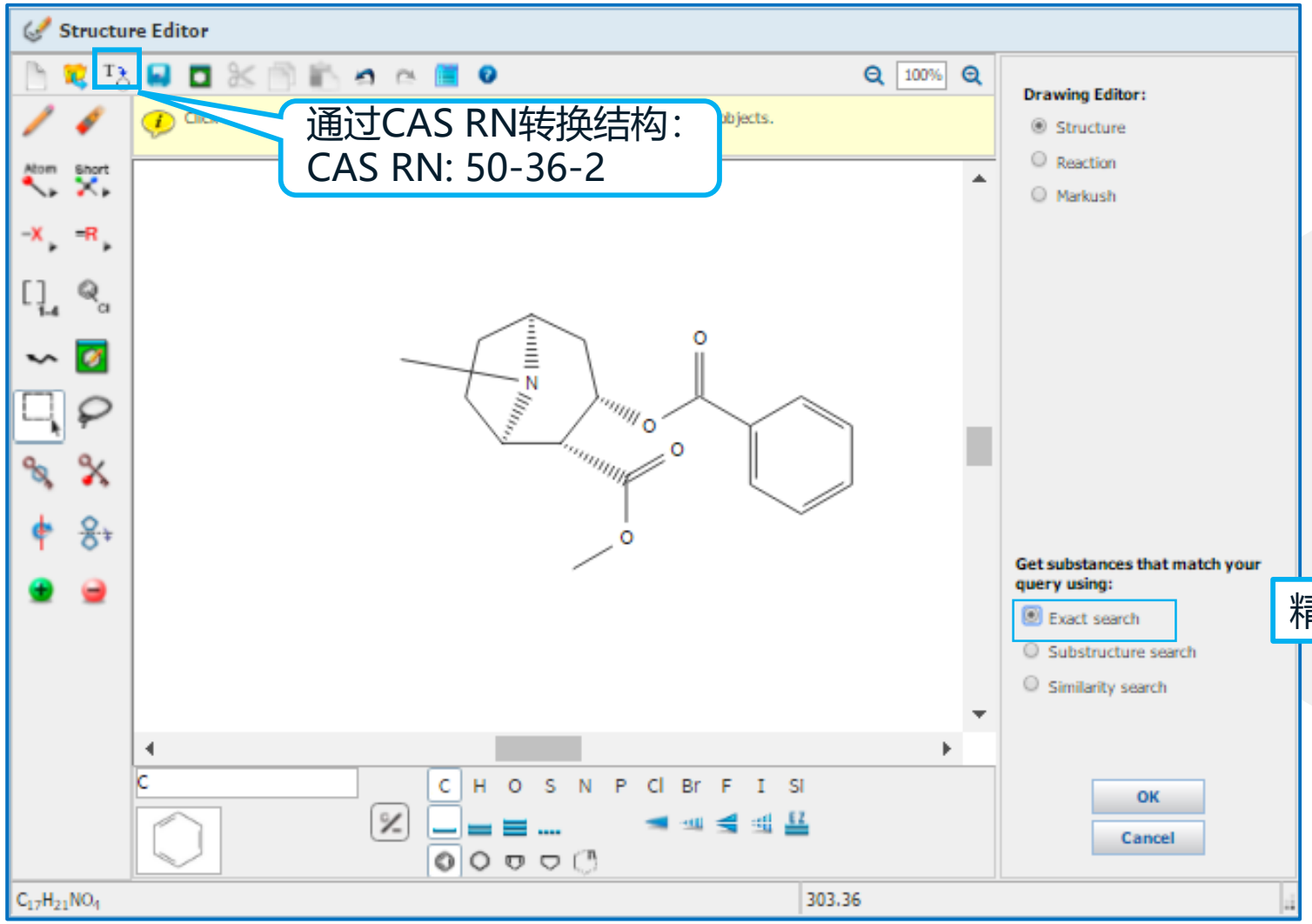
重复工具

取代位置可变

锁环工具

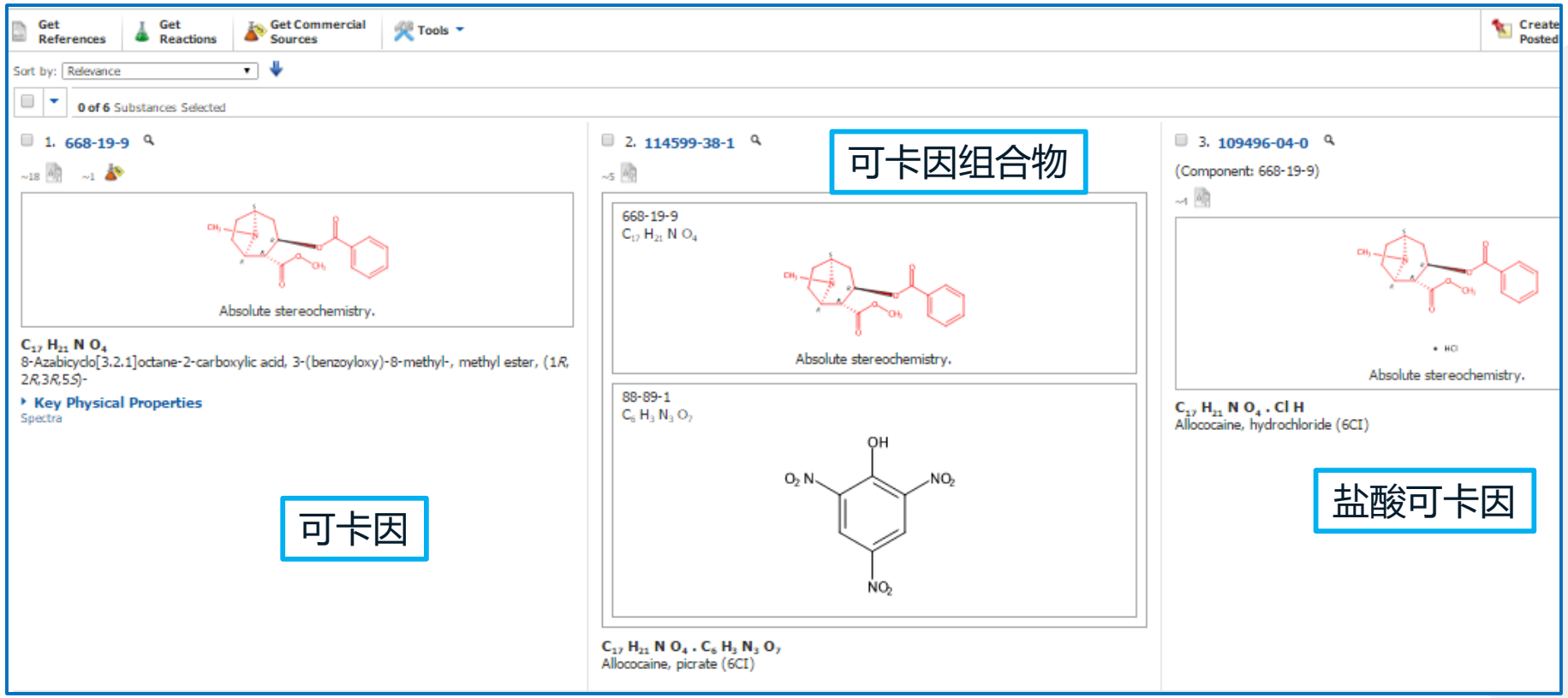
锁原子工具

物质检索--精确结构检索



精确结构检索

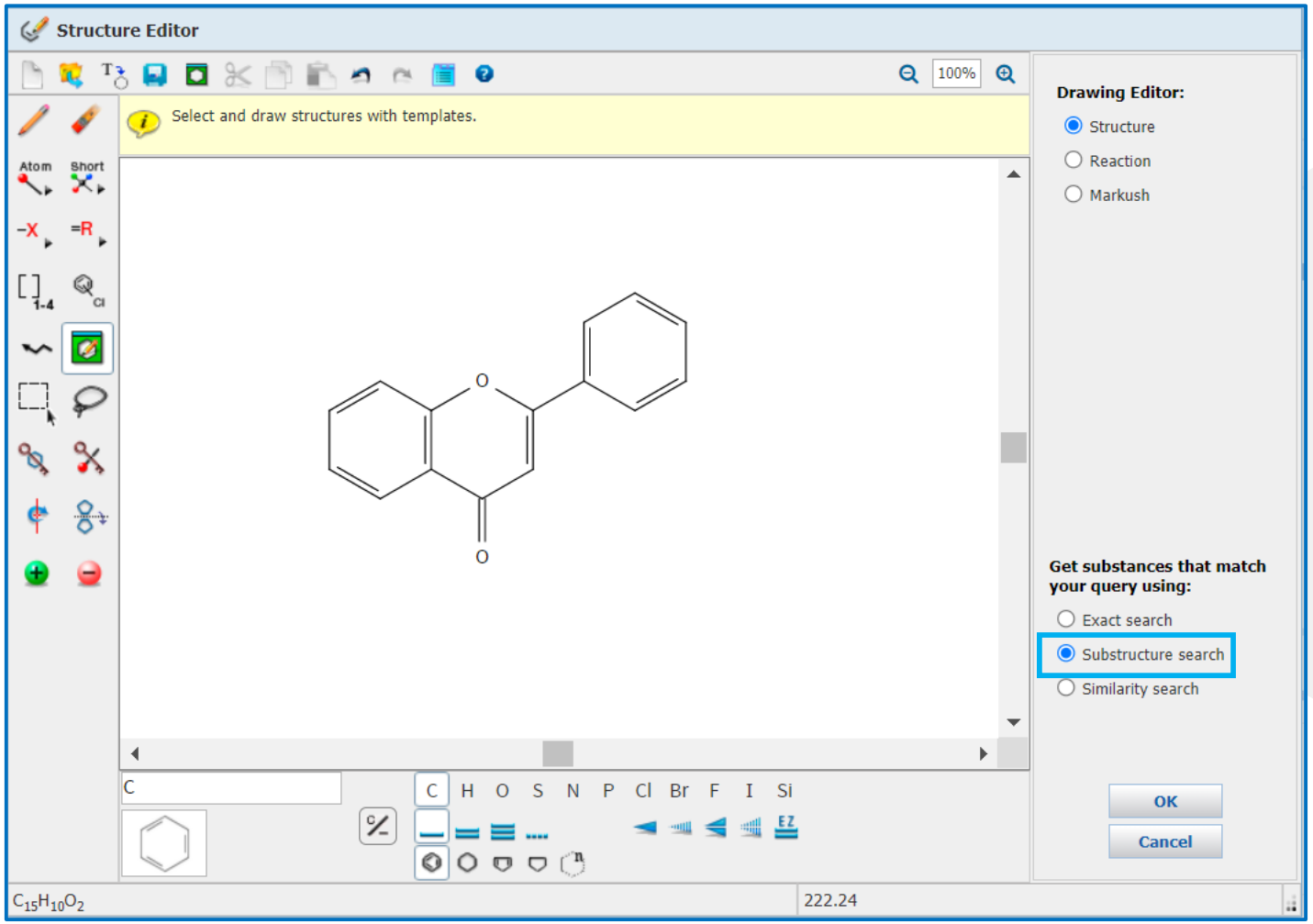
物质检索--精确结构检索



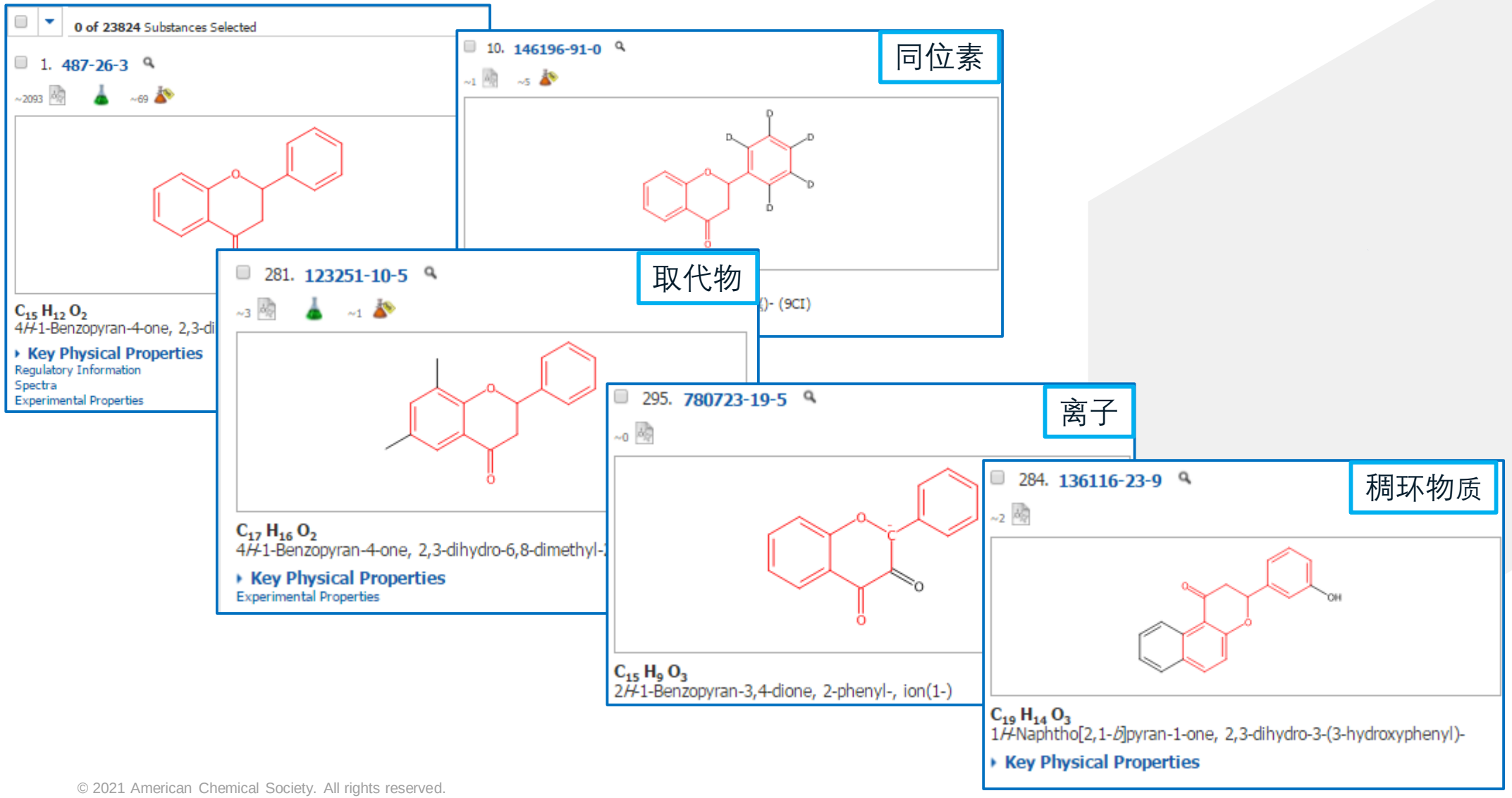
精确结构检索：

获得被检索结构的盐，混合物，配合物，聚合物等，被检结构不能被取代

物质检索--亚结构检索



物质检索--亚结构检索结果集



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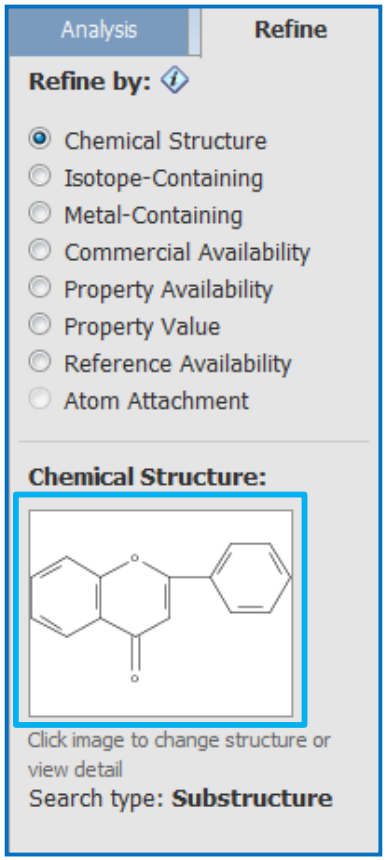
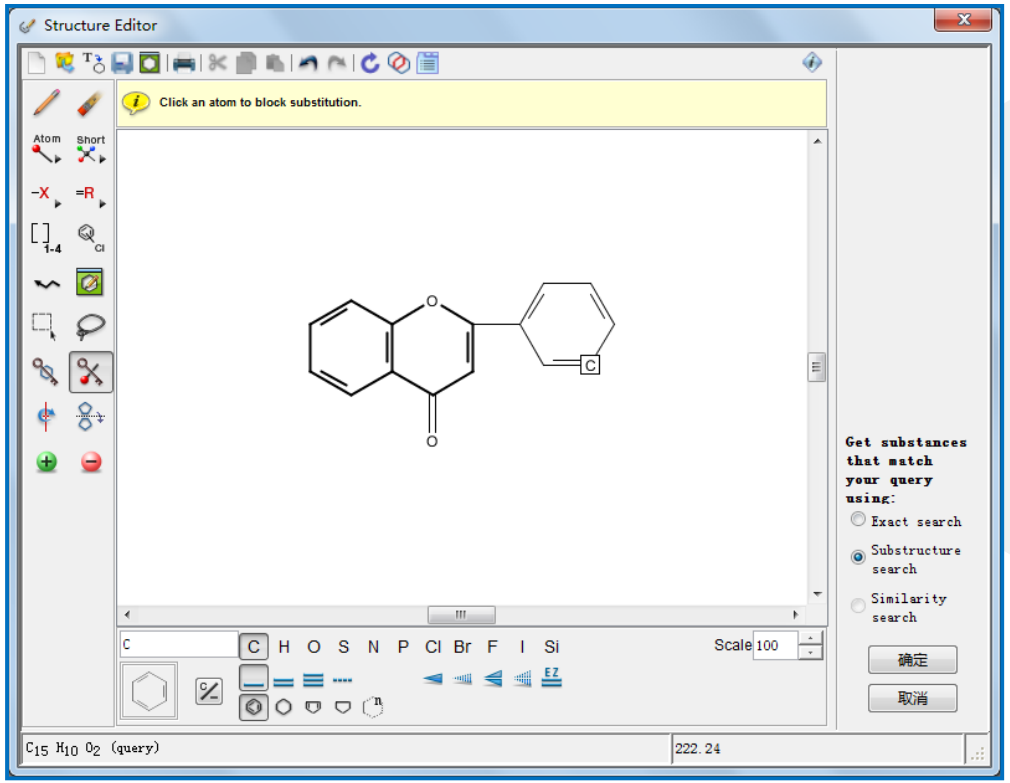
物质检索--亚结构检索结果集的限定



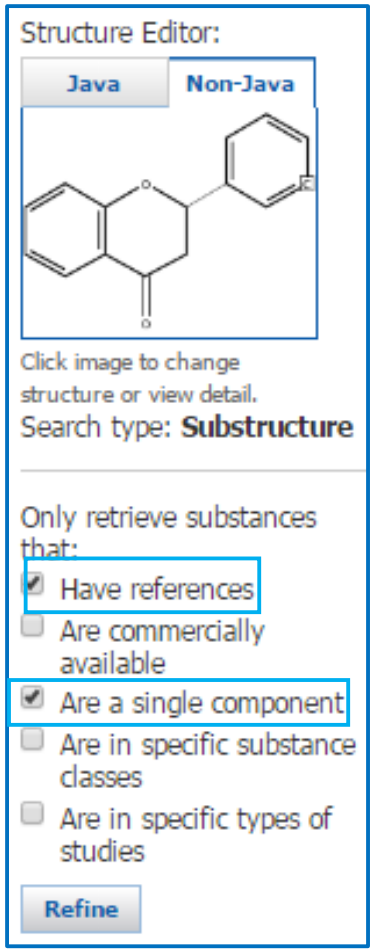
化学结构的再次限定

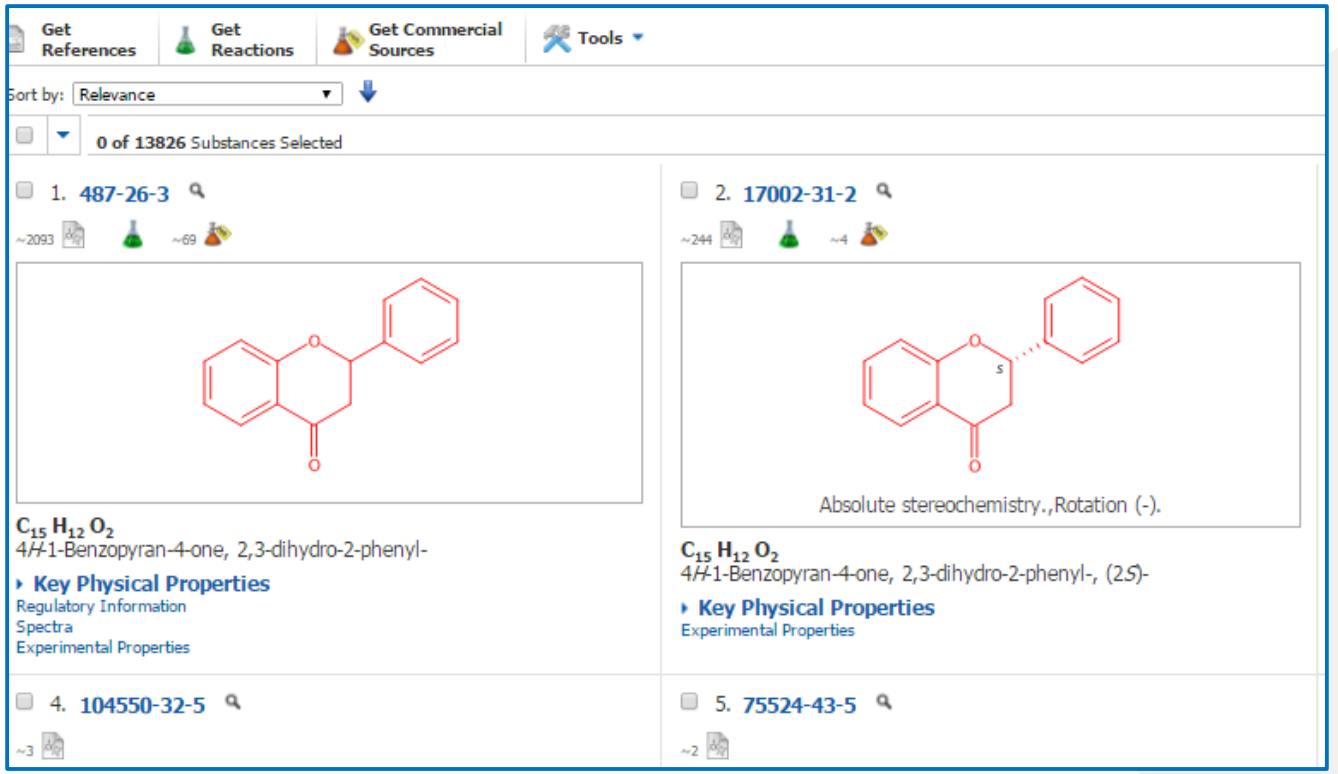


环锁定

原子锁定

物质检索--亚结构检索结果集的限定

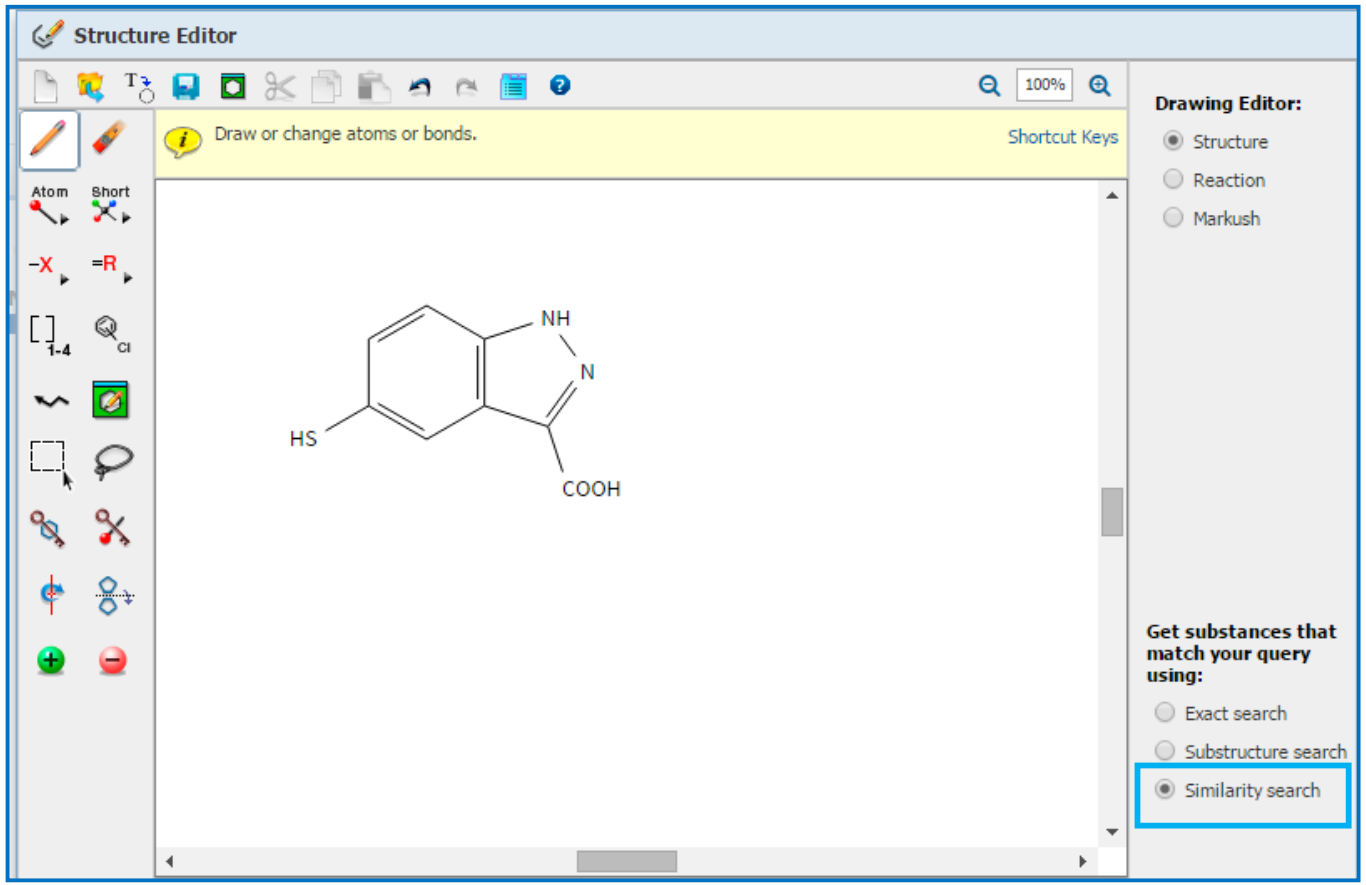




亚结构检索：

包括精确结构检索结果，及被检索结构的修饰结构

物质检索--相似结构检索



物质检索--相似结构检索结果

Select All Deselect All

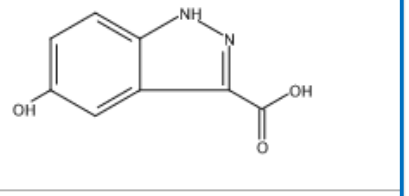
0 of 6 Similarity Candidates Selected	Substances
≥ 99 (most similar)	0
95-98	0
90-94	0
85-89	11
80-84	34
75-79	84
70-74	267
	696
	1818

相似度越高，结构越相似

Score: 88

1. 885518-94-5

取代基变化



$C_8H_6N_2O_3$

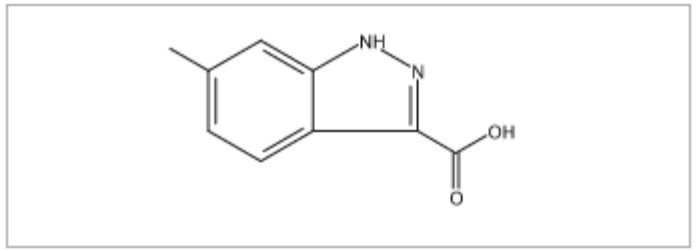
1*H*-Indazole-3-carboxylic acid, 5-hydroxy-

Key Physical Properties

Score: 86

5. 858227-12-0

取代基位置变化



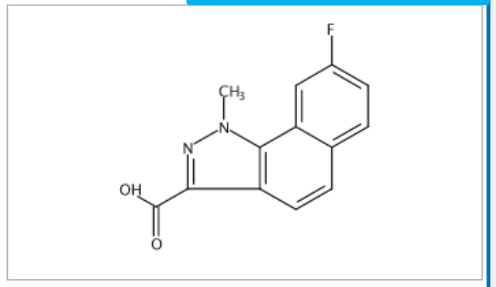
$C_9H_8N_2O_2$

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

Score: 65

541. 1100422-

母体结构变化



$C_{13}H_9FN_2O_2$

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

相似结构检索：

获得片段或整体结构与被检索结构相似的结果，母体结构可以被取代，也可以被改变

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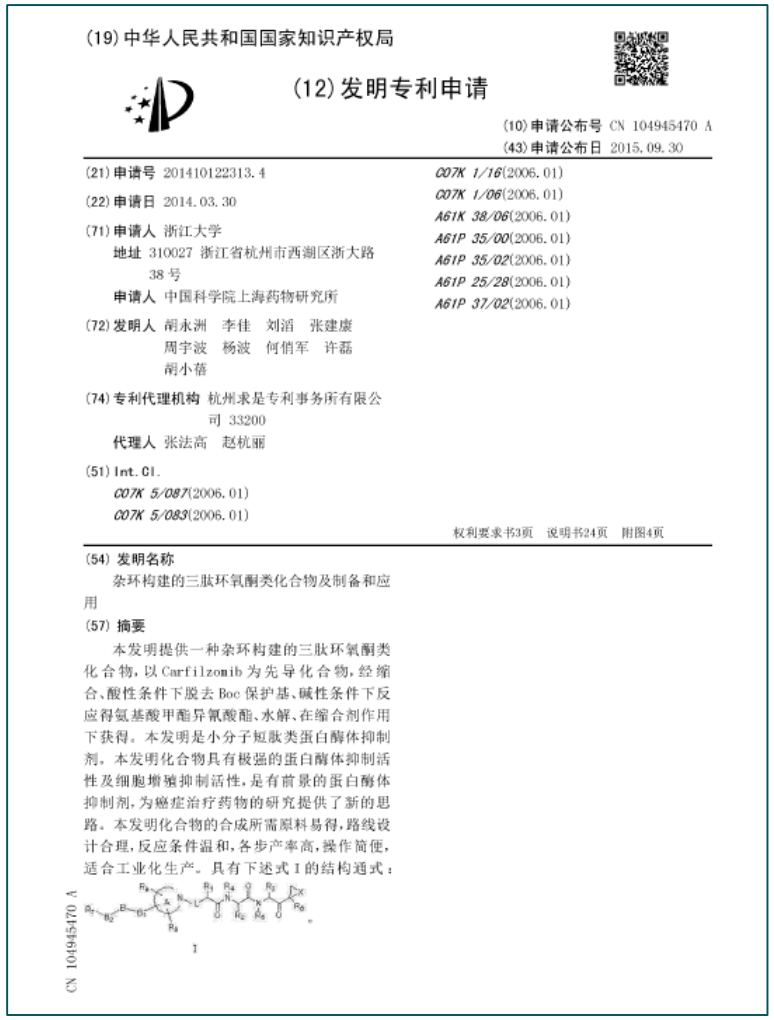
CAS Markush检索



(19)中华人民共和国国家知识产权局

(12)发明专利申请

(10)申请公布号 CN 104945470 A
(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.
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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℃；^1H 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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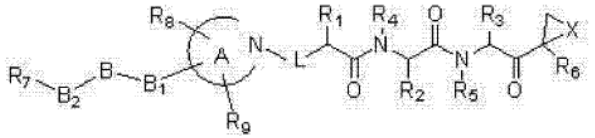
CAS Markush检索

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

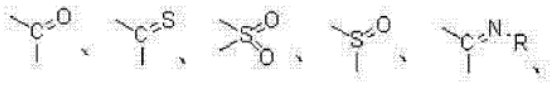
其中：

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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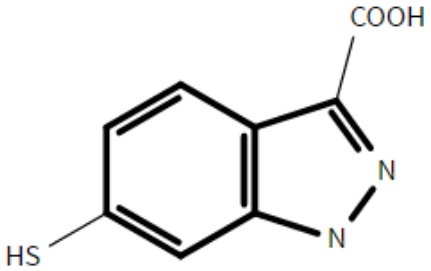
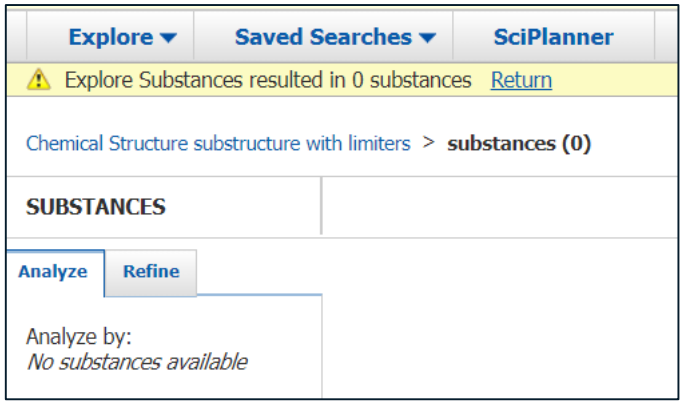
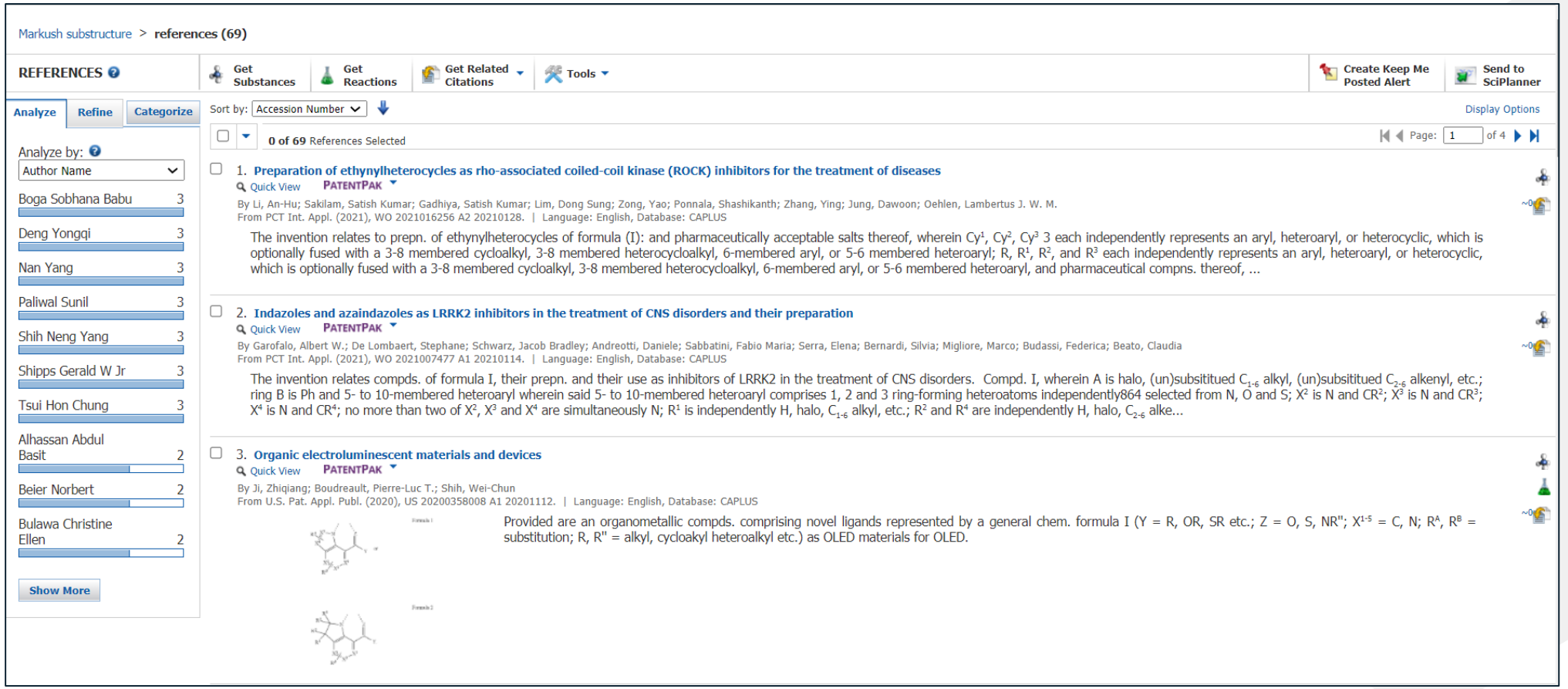
CAS Markush检索





Substance检索结果为0!

CAS Markush检索



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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物质检索小结

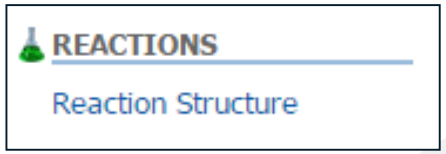
1. 选择合适的检索方式
2. 利用结构绘制工具合理扩大结构检索范围：R基团、可变基团、可变位置取代等
3. 利用结构绘制工具适当限定检索结构：环锁工具、原子锁工具、EZ构型限定等
4. 正确理解Exact、Substructure、Similarity检索结果集的意义和范围
5. 充分利用物质筛选项准确定位目标物质：Reaction Role、Reference Role等
6. 利用CAS Markush检索尽可能全面的获得结构的公开信息

大纲

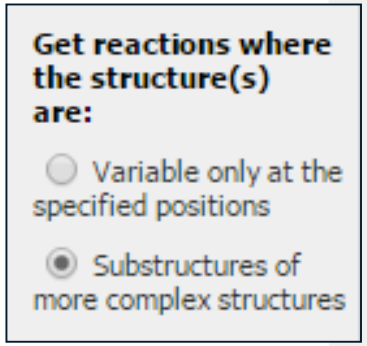
- CAS及CAS SciFinder介绍
- 文献相关信息的获取策略
  - 文献检索方法
  - 文献结果排序、筛选和详情
  - 如何高效阅读专利文献详情(CAS PatentPak)
- 物质相关信息的获取策略
  - 常见的物质检索方法
  - 物质结果排序、筛选和详情
- **反应相关信息的获取策略**
  - 反应的获取方法
  - 反应结果排序、筛选和详情
  - 如何高效获取反应详情（Synthetic Methods）
- 分析相关信息的获取 (CAS Analytical Methods)

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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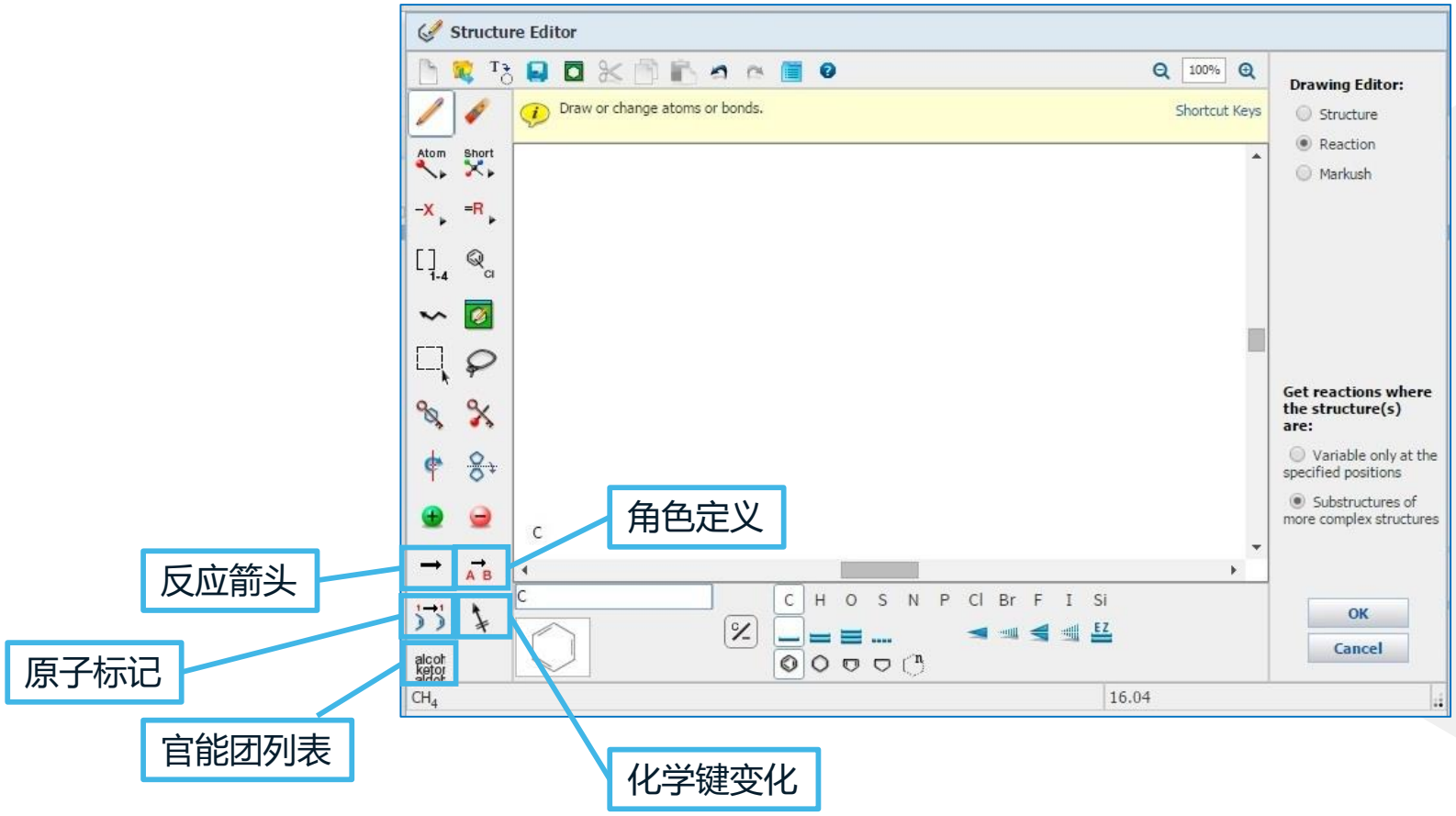
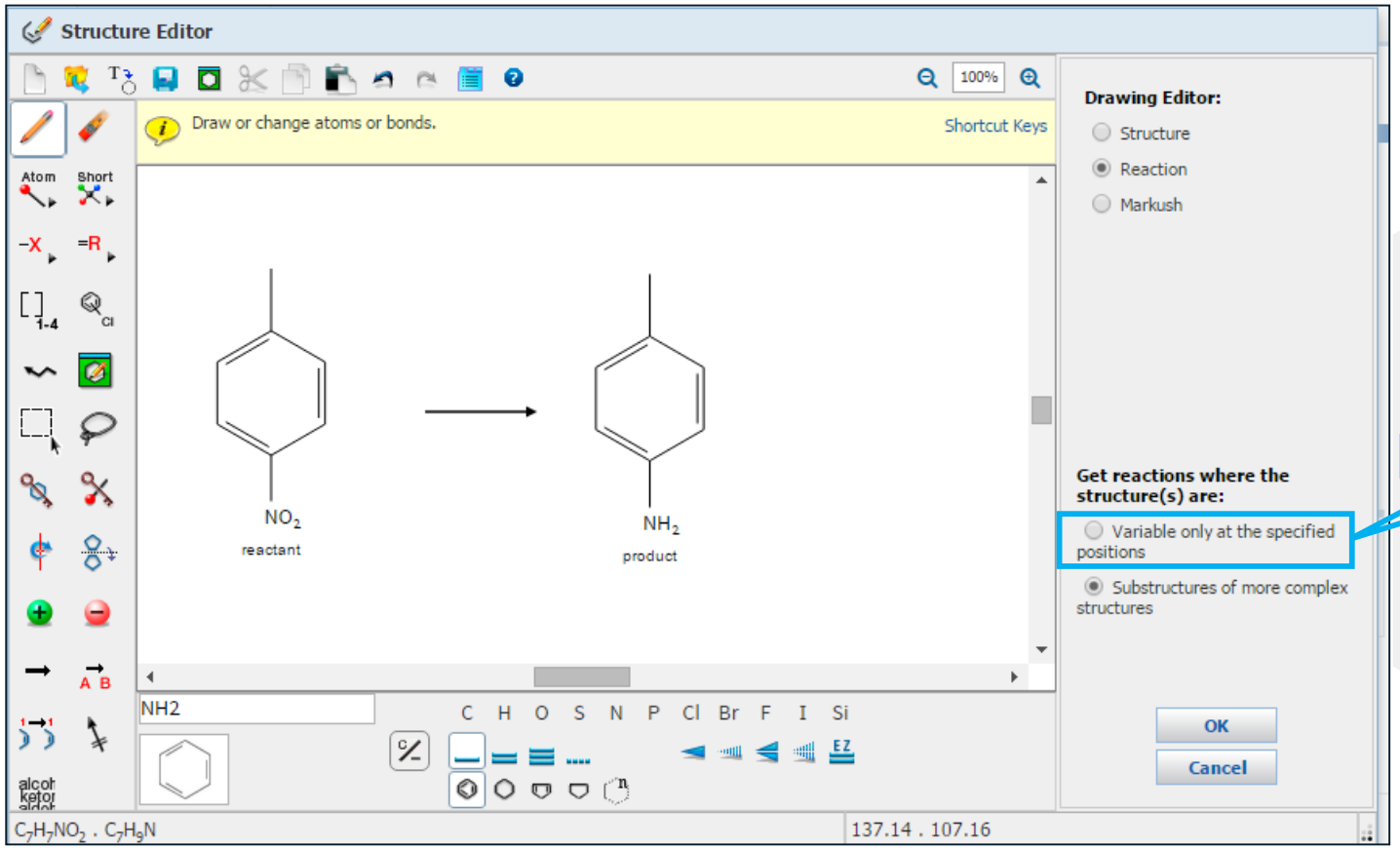
结构编辑器--绘制反应工具



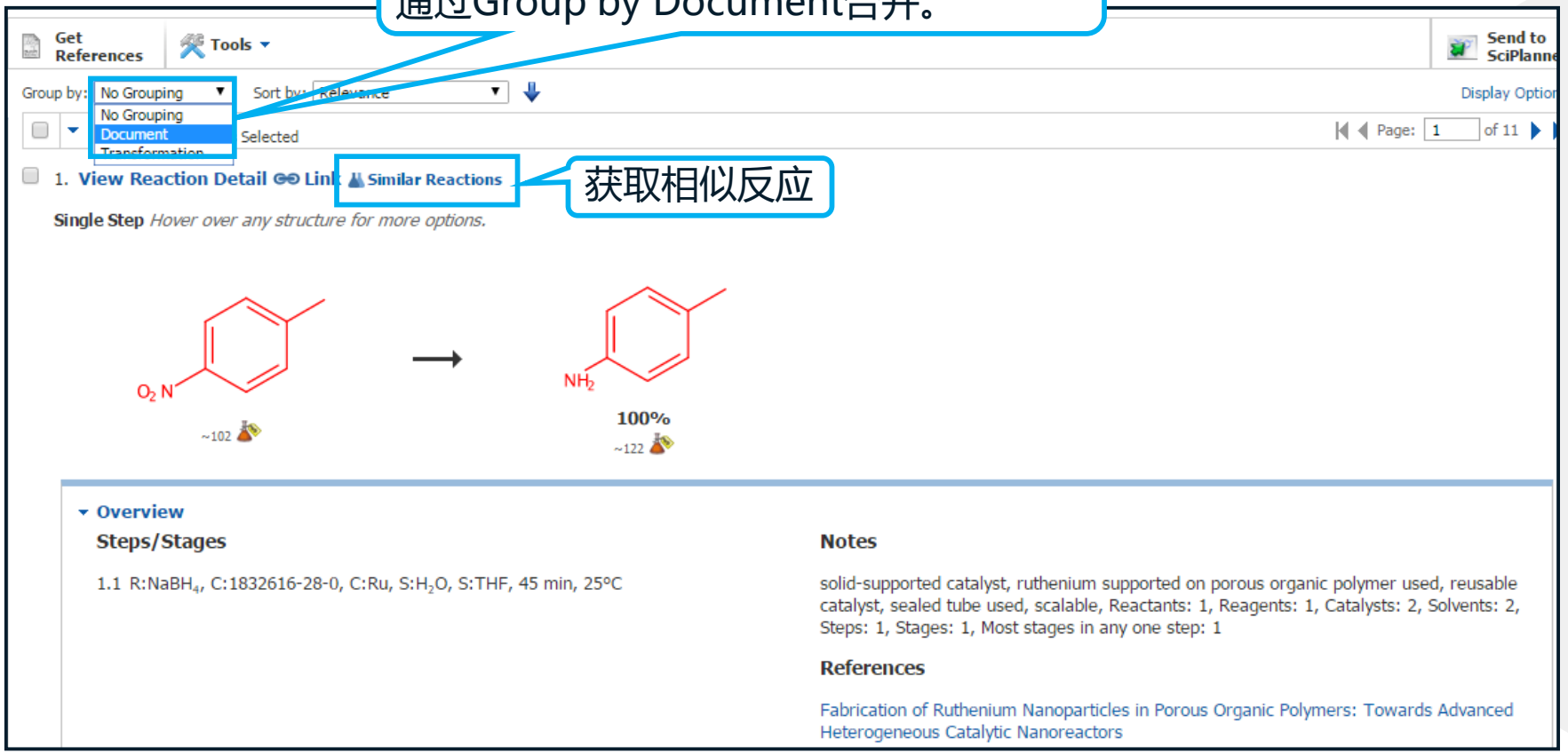
反应检索--精确反应检索



精确反应检索

反应检索结果集--排序

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



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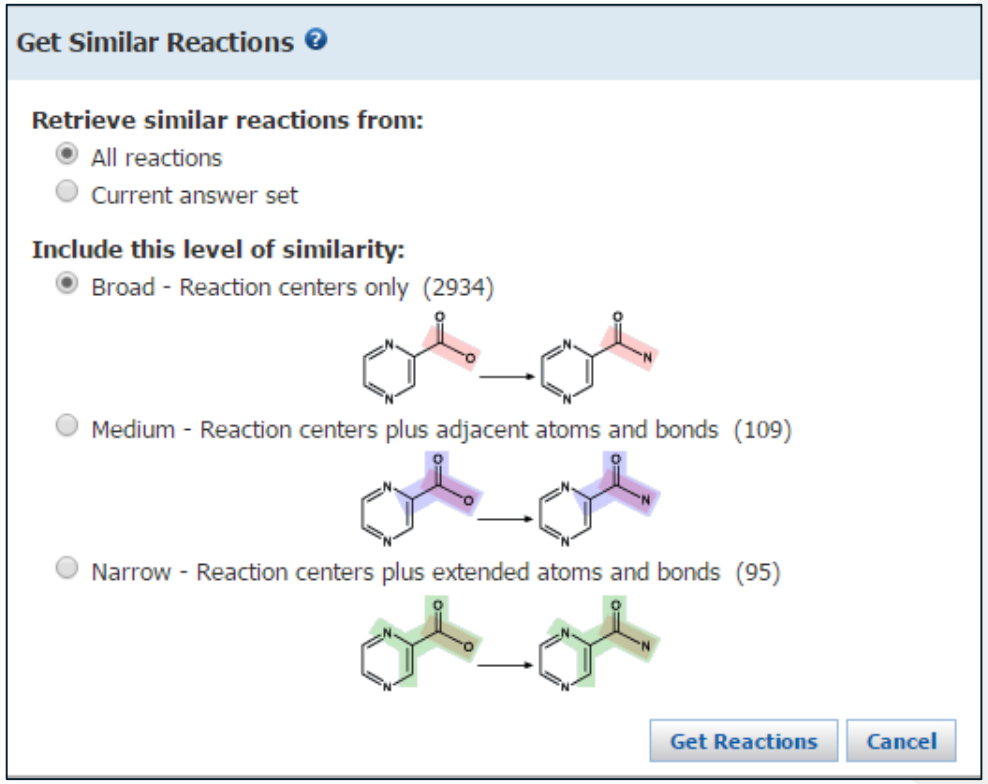
扩展反应检索--获取相似反应

选择相似反应的相似限制：

Broad：仅反应中心相似

Miedum：反应中心及附属原子和键

Narrow：反应中心及扩展的原子和键



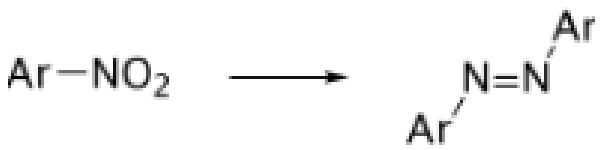
按照反应类型排序

Group by: Transformation ▾ Sort by: Frequency ▾

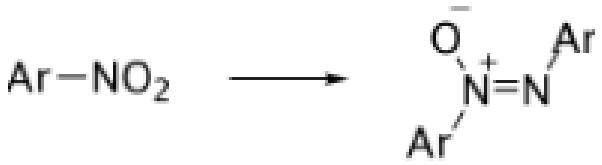
0 of 560 Reactions Selected

1. **Reduction of Nitro Compounds to Amines**
538 Reactions

2. **Reduction of Nitro to Azo Compounds**
11 Reactions



3. **Reduction of Nitro to Azoxy Compounds**
11 Reactions



更精确的查找需要的反应

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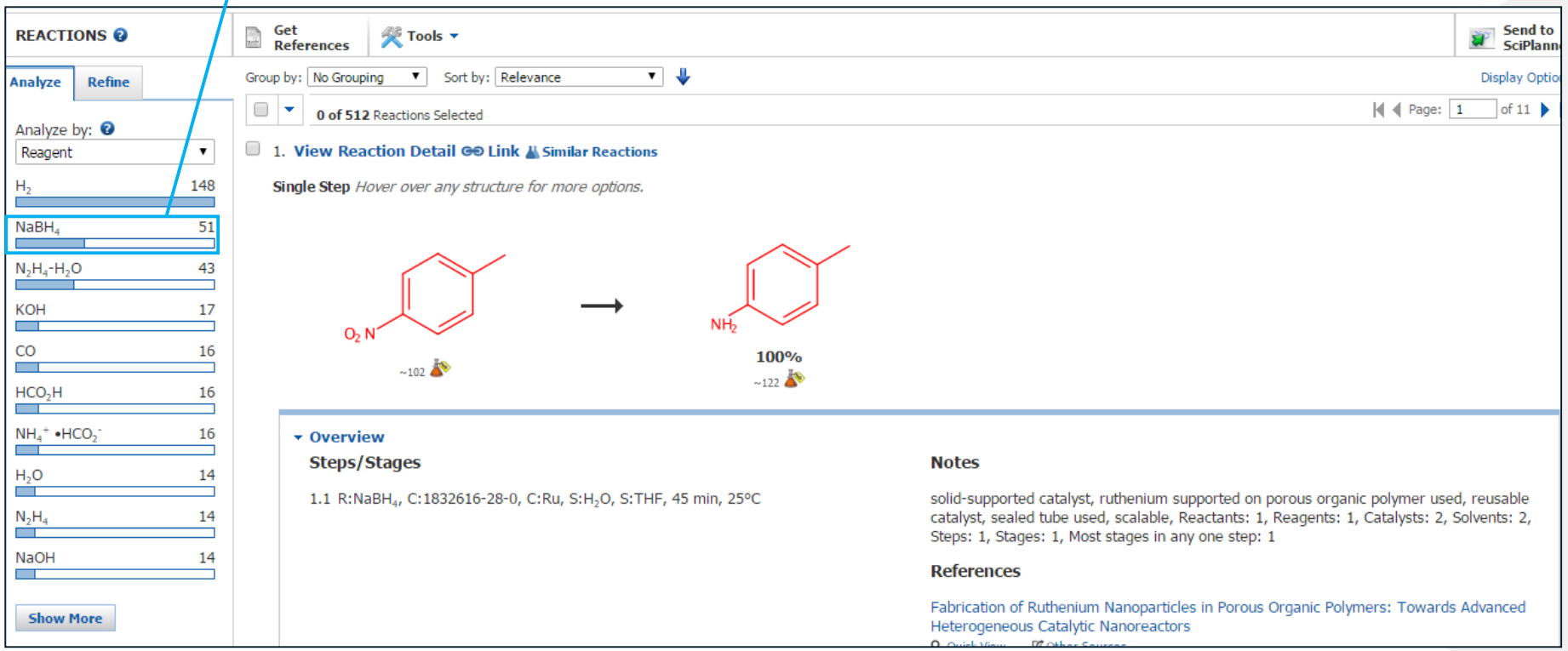
反应检索结果集--筛选

获得特定物质做还原剂的反应



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反应检索结果--Experimental Procedure

Single Step *Hover over any structure for more options.*

Overview

Steps/Stages

1.1 R:H_2, R:Cs_2CO_3, C:1610424-70-8, C:1034343-98-0 (oxide), S:PhMe, 2 h, 100°C, 1 atm

Notes

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

References

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

Quick View Other Sources

By Sabater, Sara et al

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

Experimental Procedure

ACS Catalysis

General/Typical Procedure: **General Procedure for Nitroarene Reductions.** Molecular hydrogen was added with a balloon filled with 1 atm of H_2 to a mixture of nitroarene (0.3 mmol), Cs_2CO_3 (0.3 mmol), anisole as internal standard (0.3 mmol), and NHC-Pd-rGO (6×10^{-3} mmol, based on metal) in toluene (5 mL). The system was then evacuated and backfilled with H_2 in cycles for three times before putting the reaction vessel in an oil bath at 100°C for 2h. Yields were determined by GC analyses using anisole (0.3 mmol) as internal standard. Products were identified according to spectroscopic data of the commercially available compounds. Entry: 4; Yield 100%.

不用阅读全文，直接获得包含实验过程的反应记录

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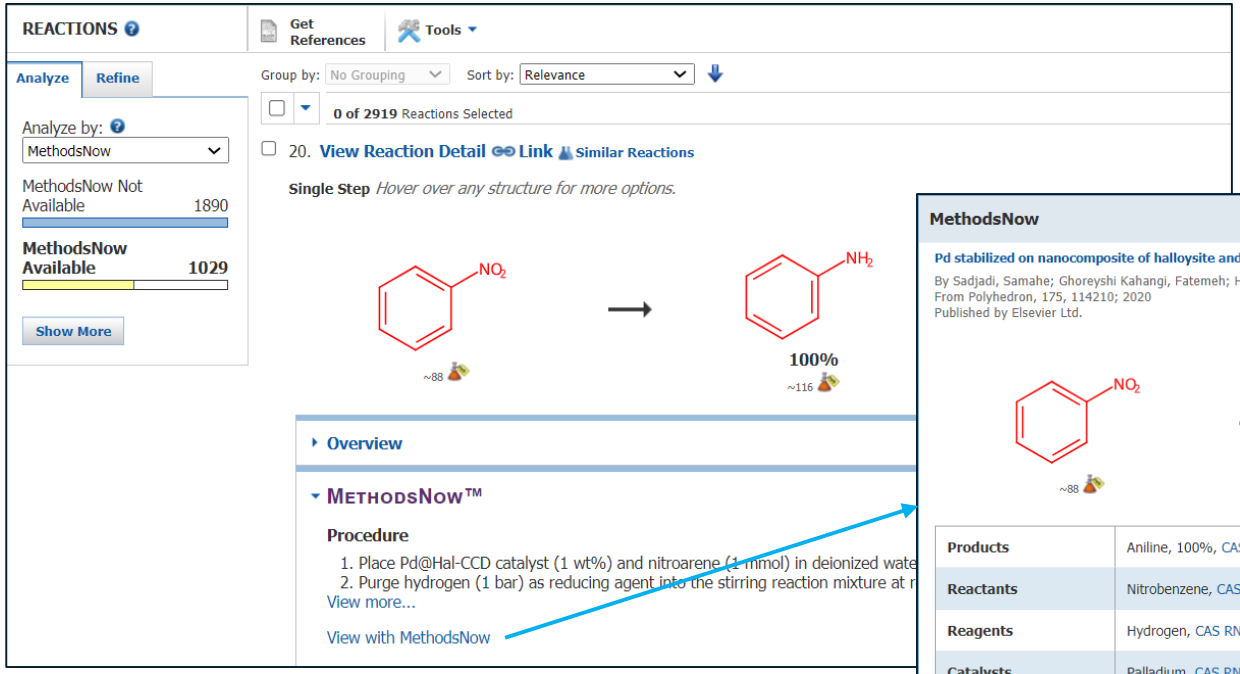
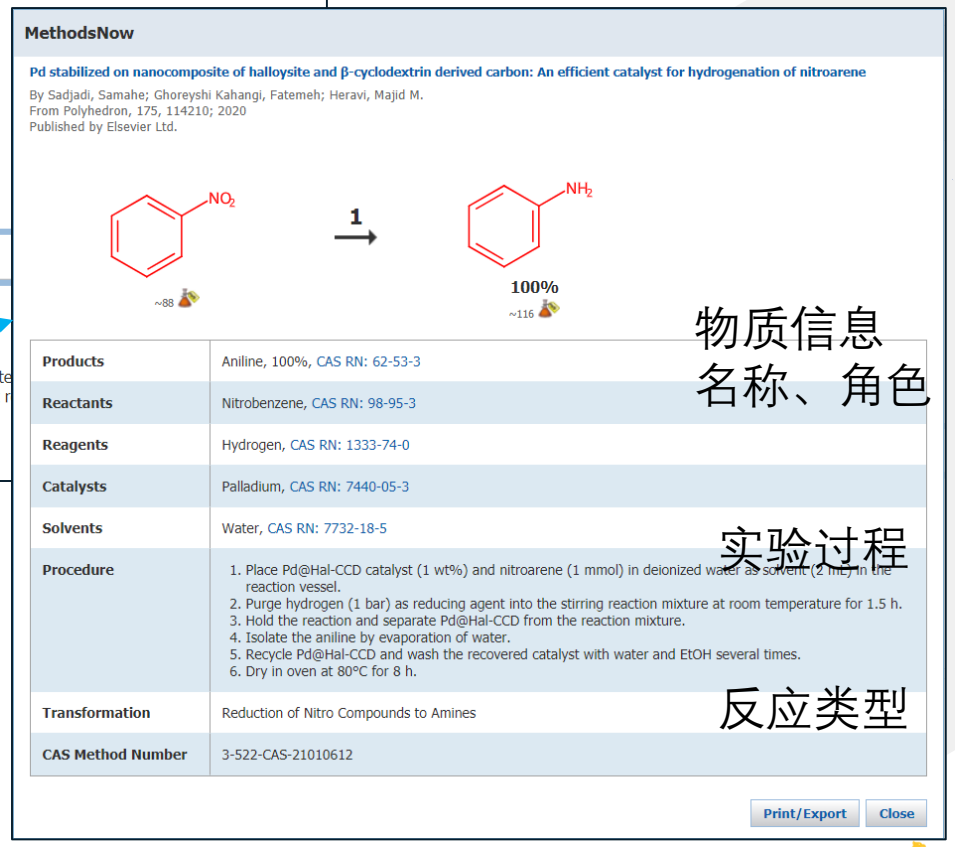
反应检索结果--MethodsNow





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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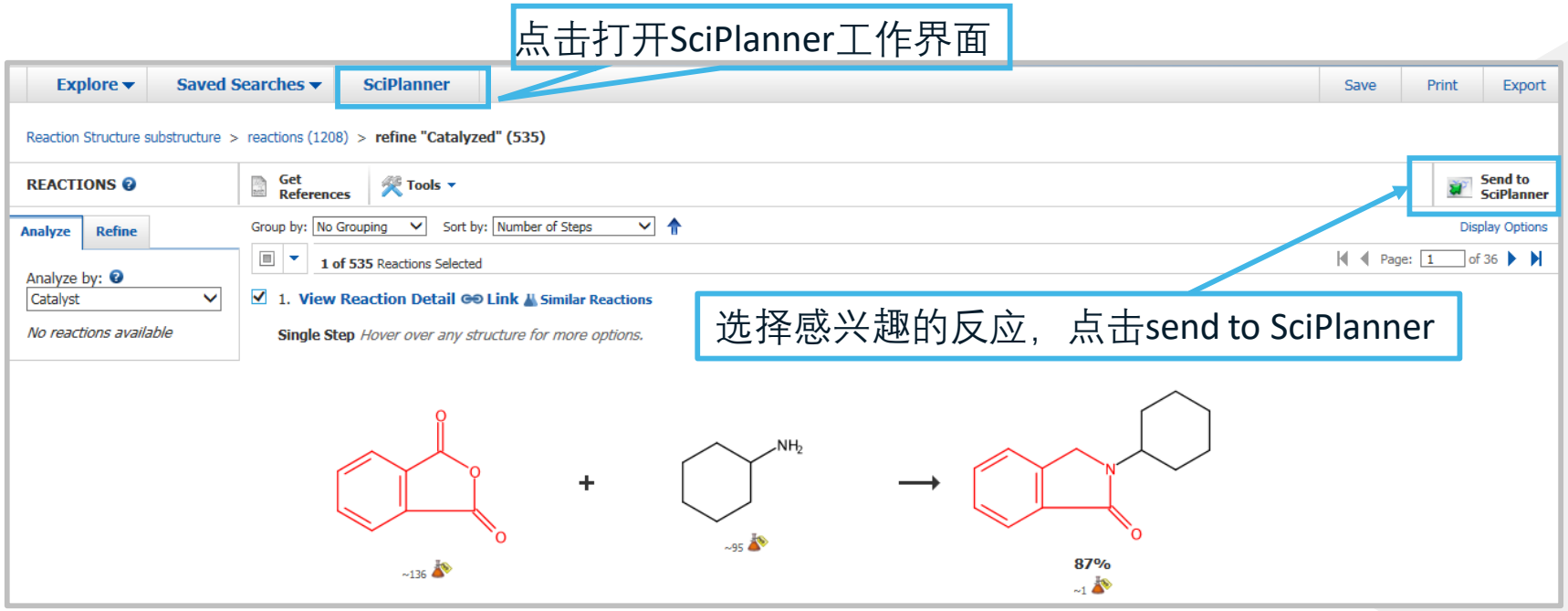
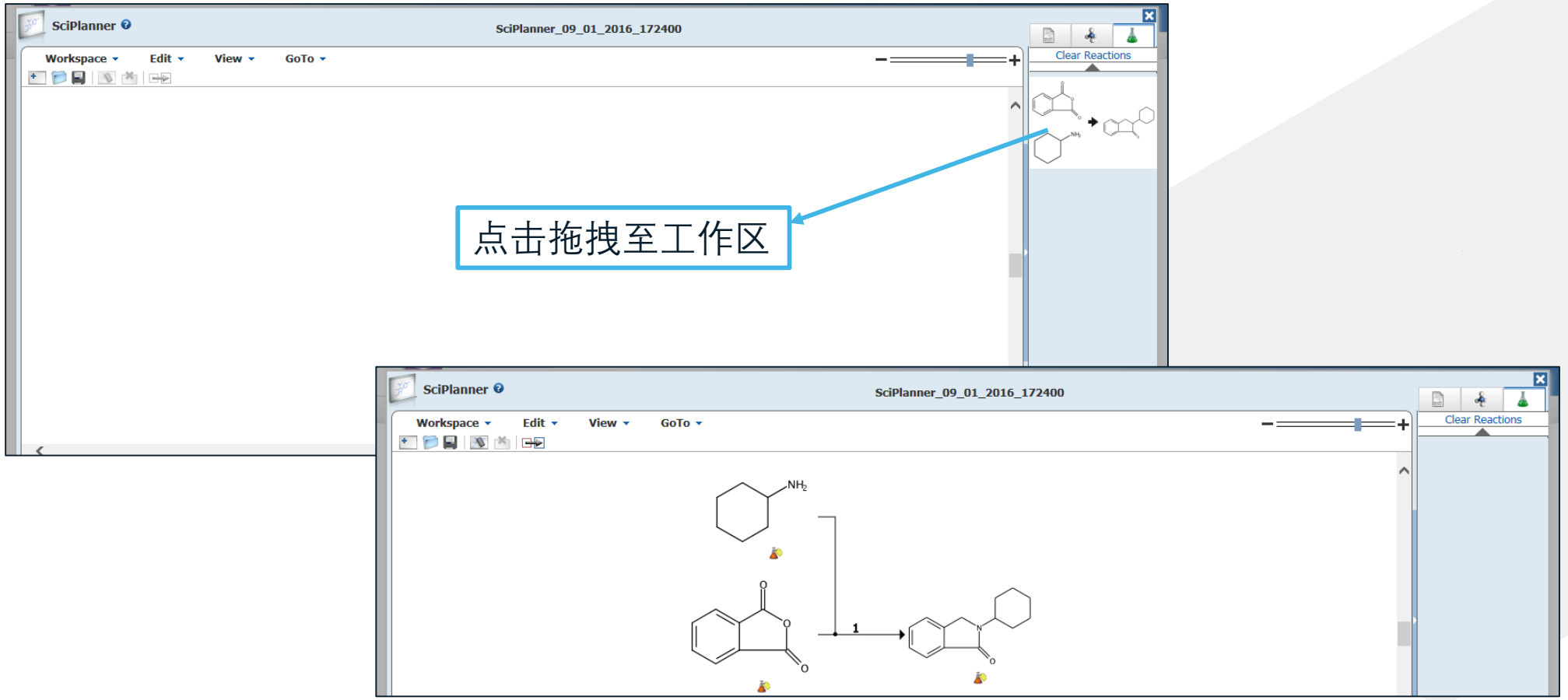
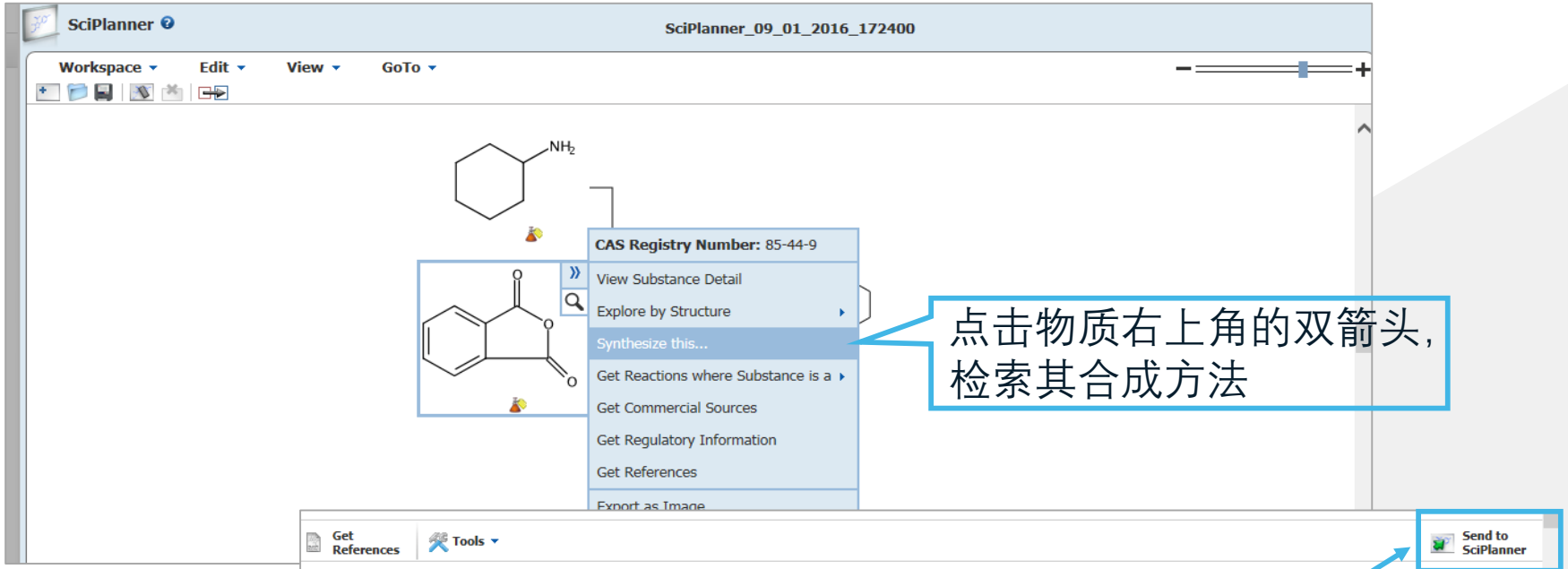
SciPlanner--设计合成反应路线

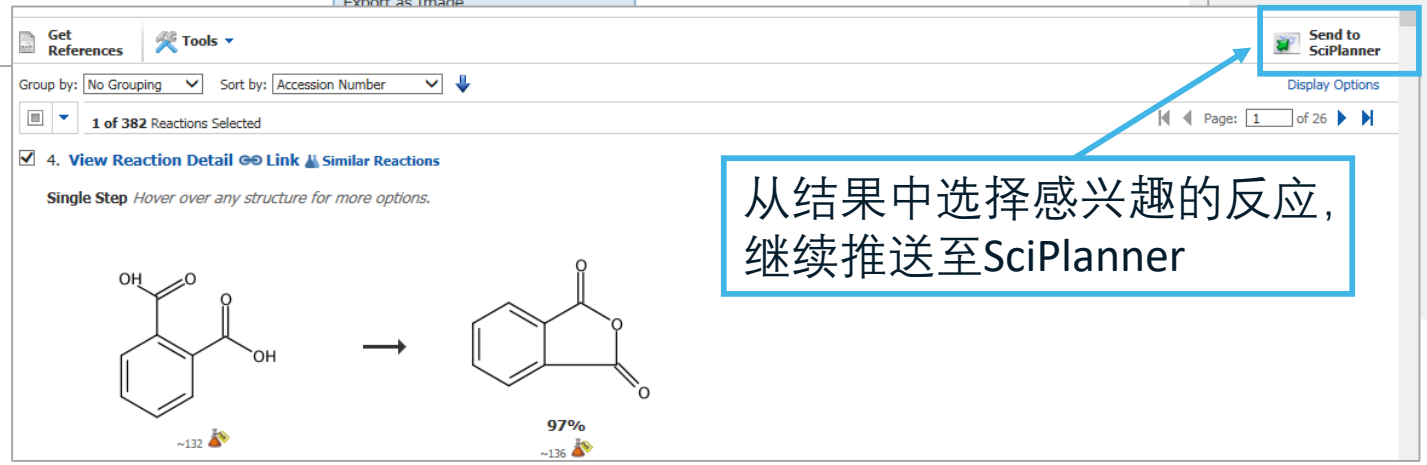


SciPlanner--工作界面

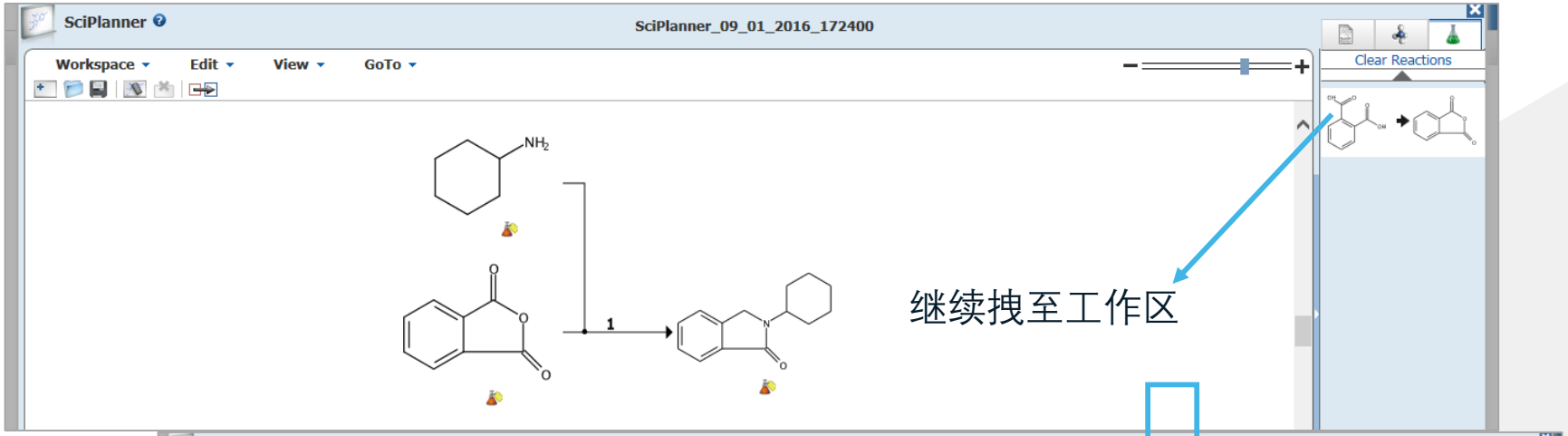


SciPlanner--工作界面

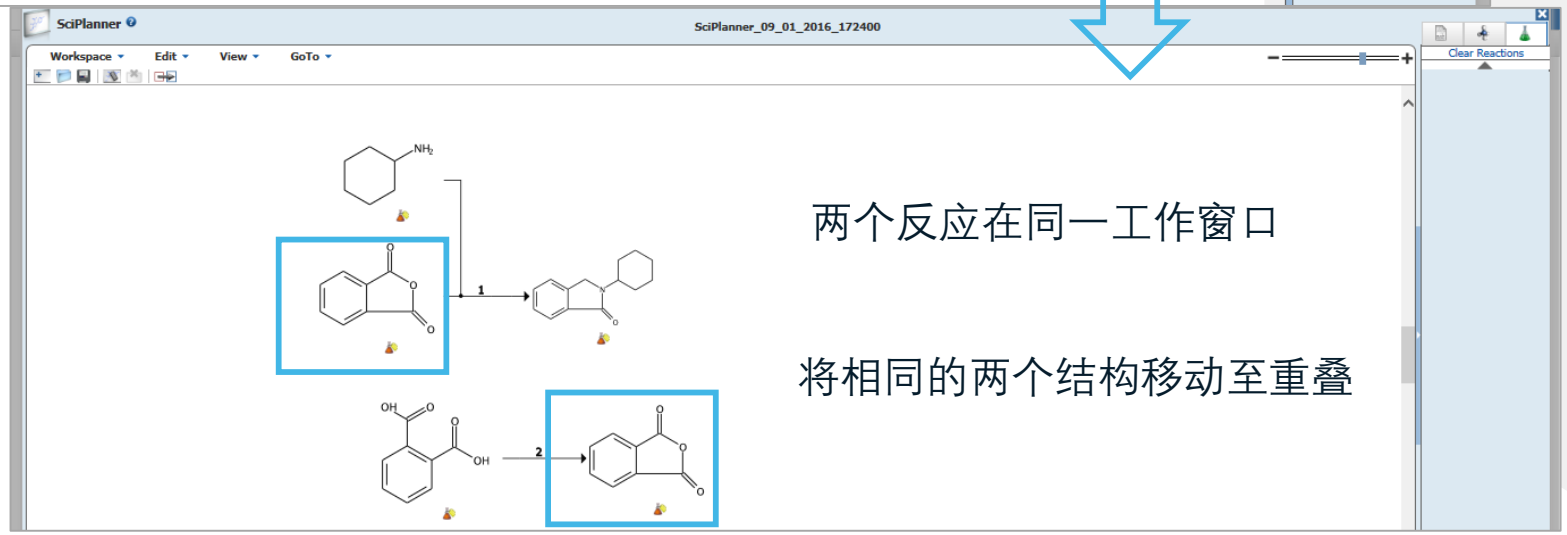




SciPlanner--工作界面



继续拽至工作区



两个反应在同一工作窗口

将相同的两个结构移动至重叠

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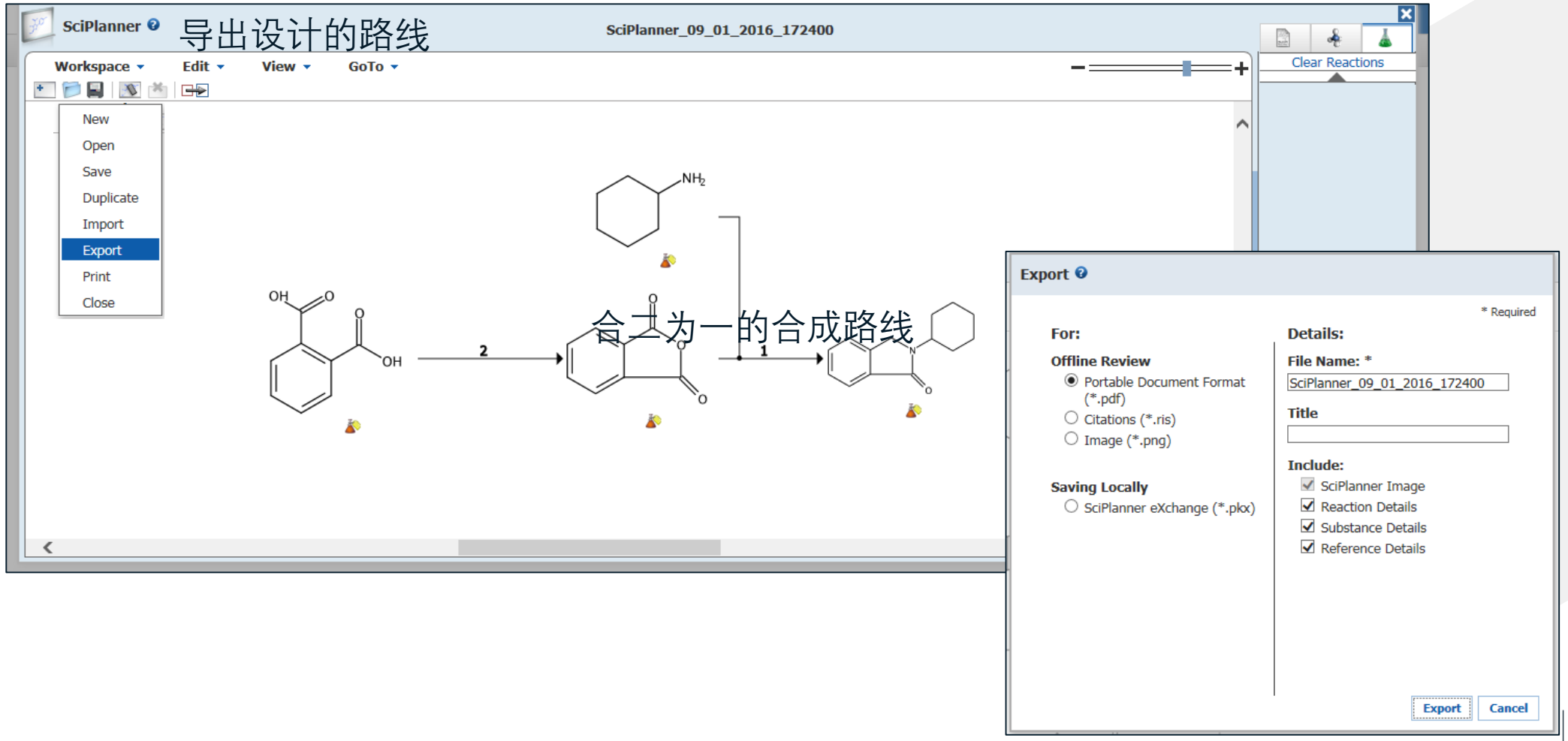
SciPlanner--设计拟合成的反应路线



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
- 文献相关信息的获取策略
  - 文献检索方法
  - 文献结果排序、筛选和详情
  - 如何高效阅读专利文献详情(CAS PatentPak)
- 物质相关信息的获取策略
  - 常见的物质检索方法
  - 物质结果排序、筛选和详情
- 反应相关信息的获取策略
  - 反应的获取方法
  - 反应结果排序、筛选和详情
  - 如何高效获取反应详情（Synthetic Methods）
- **分析相关信息的获取 (CAS Analytical Methods)**

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MethodsNow – CAS Analytical Methods (www.methodsnow.com)

- 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…

目前有13个大类，45个小类。某些子项目属于多种方法分类

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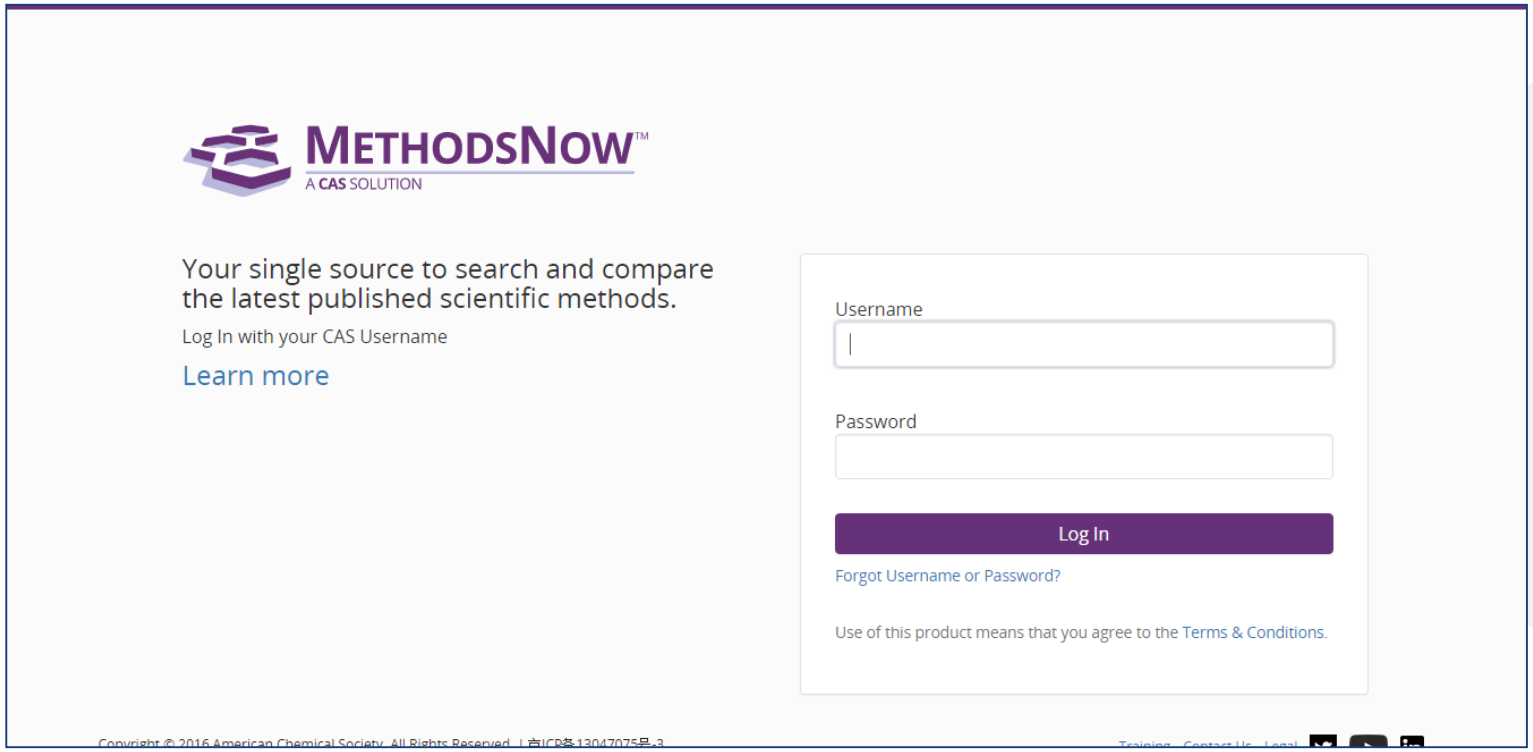
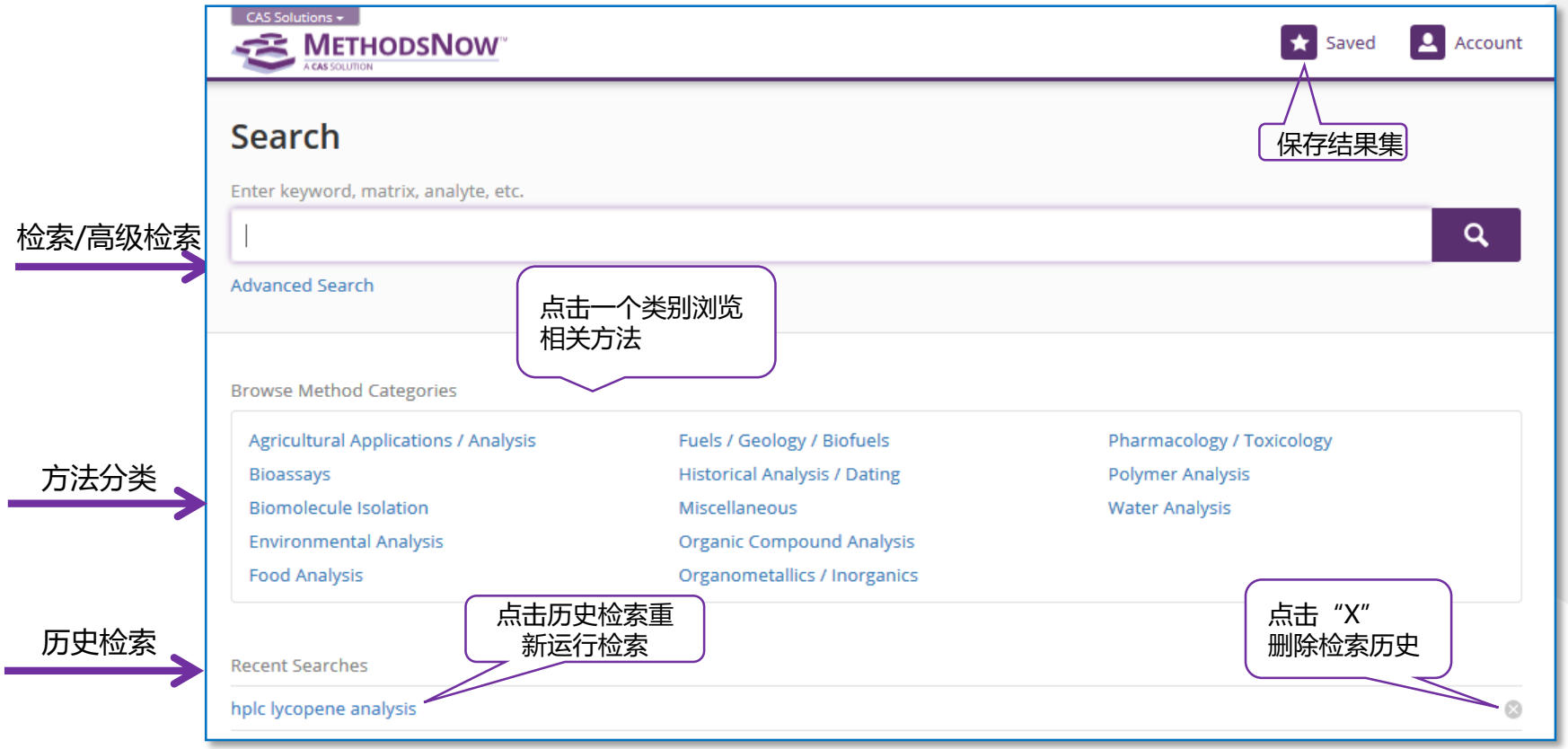
MethodsNow – CAS Analytical Methods (www.methodsnow.com)



登陆www.methodsnow.com
输入SciFinder的账号密码

MethodsNow – CAS Analytical Methods (www.methodsnow.com)



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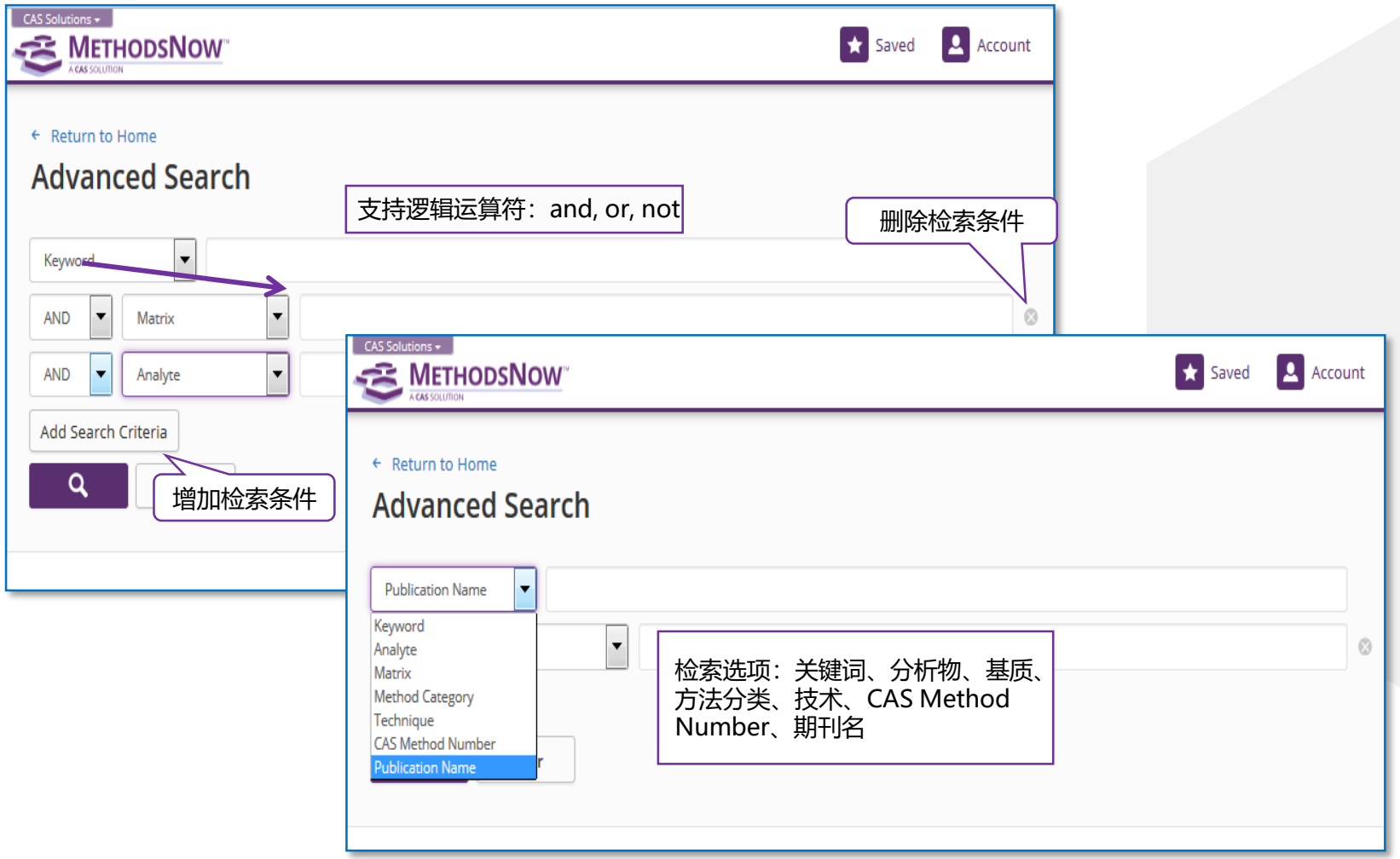
MethodsNow – CAS Analytical Methods (www.methodsnow.com)



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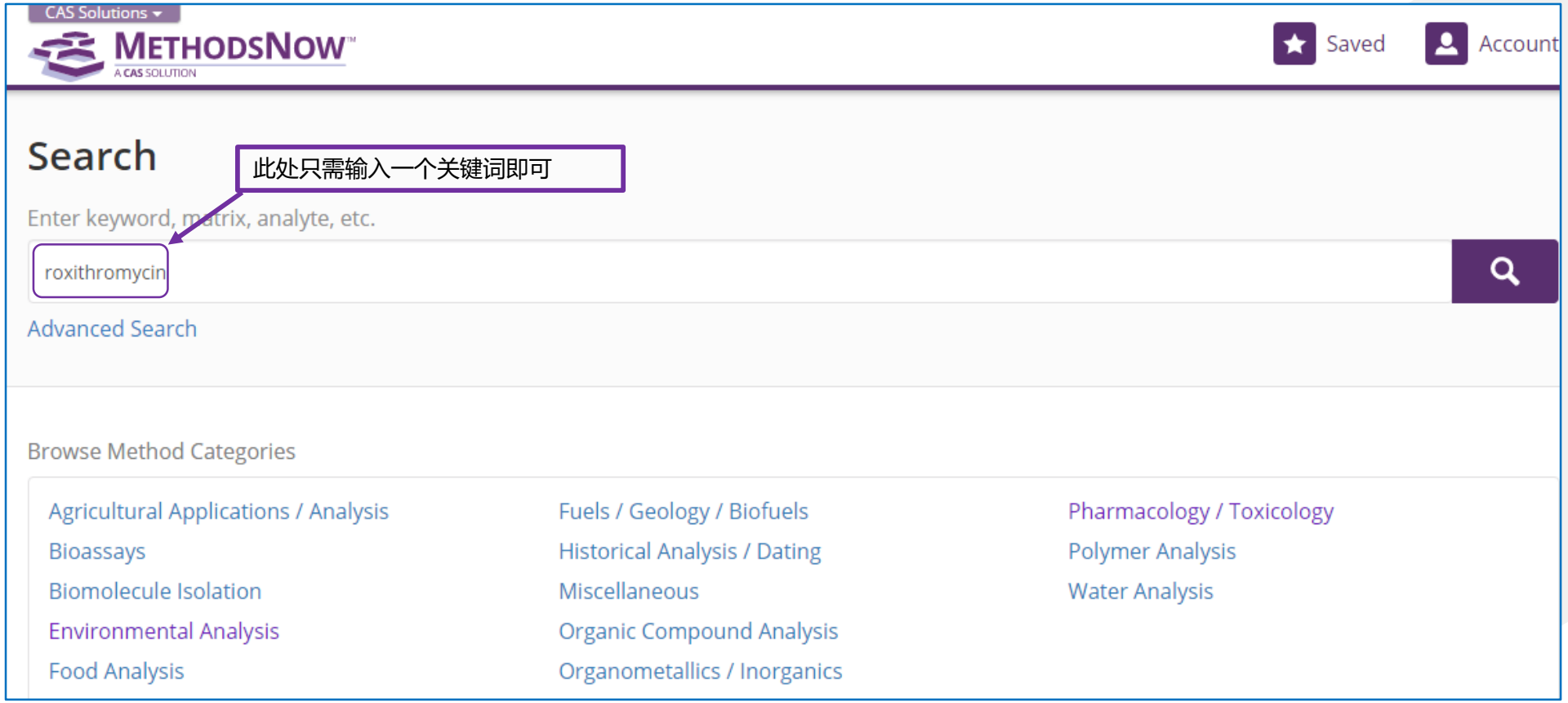
案例：高效液相色谱法测定血液中罗红霉素的含量



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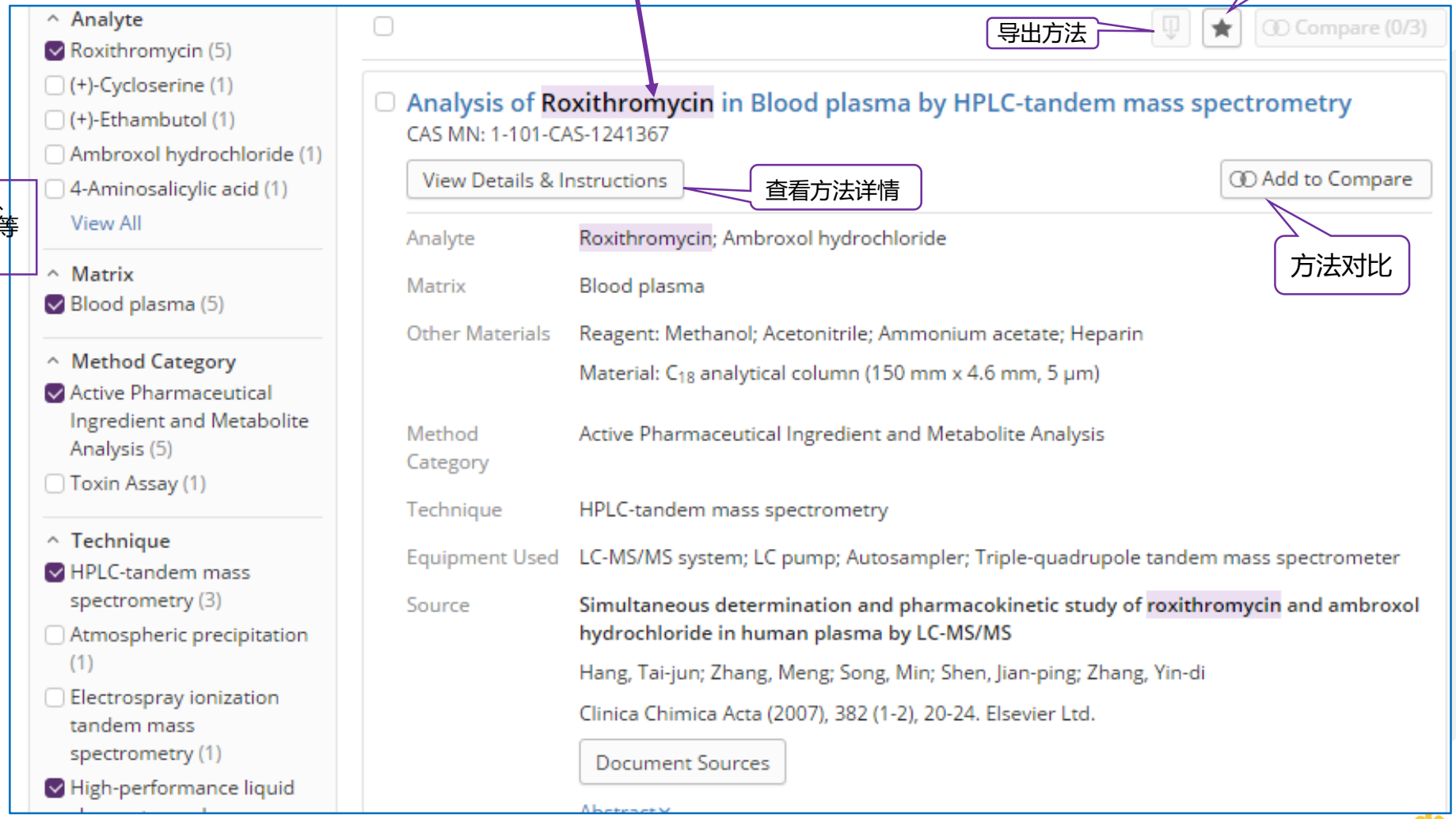
结果显示

典型分析方法标题格式：通过某技术手段在某基质中分析某物质

保存方法

导出方法

限定分析物、基质、方法等条件



结果显示

Method Detail (2 of 5)

实验材料

Analysis of Roxithromycin in Blood plasma b

CAS MN: 1-101-CAS-67878

Method Category: Active Pharmaceutical Ingredient and Metabolite Analysis
Technique: Fluorescence; HPLC

Materials	Role
Roxithromycin	analyte
Blood plasma	matrix
Column, 125 x 4.6 mm i.d. LiChrospher RP-18e	materia
SPE Bakerbond cartridges, C18	material

文献信息

Source

Determination of roxithromycin in human plasma by HPLC with fluorescence and UV absorbance detection: Application to a pharmacokinetic study

Glowka, Franciszek K.; Karazniewicz-Lada, Marta

Journal of Chromatography B: Analytical Technologies in the Biomedical and Life Sciences (2007), 852 (1-2), 669 - 673. Elsevier B.V.

CODEN: JCBAAI | ISSN: 15700232 | DOI: 10.1016/j.jchromb.2007.02.022

Document Sources

Abstract

A selective HPLC method with fluorescence detection for the determination of roxithromycin (ROX) in human plasma was described. After solid-phase extraction (SPE), ROX and erythromycin (internal standard, I.S.) were derivatized by treatment with 9-fluorenylmethyl chloroformate (FMOC-Cl). Optimal resolution of fluorescence derivatives of ROX and I.S. was obtained during one anal. run using reversed phase, C_{18} column. The mobile phase was composed of potassium dihydrogenphosphate solution, pH 7.5 and acetonitrile. Fluorescence of the compounds was measured at the maximum excitation, 255 nm and emission, 313 nm, of ROX derivatives Validation parameters of the method were also established. After SPE, differences in recoveries of ROX and erythromycin from human plasma were observed The linear range of the standard curve of ROX in plasma was 0.5-10.0 mg/l. The validated method was successfully applied for pharmacokinetic studies of ROX after administration of a single tablet of ROX.

设备条件

Equipment Used

HPLC system, HP 1100, Hewlett-Packard, Waldbronn, Germany

Autosampler, G1313A

Conditions

Chromatographic

HPLC : mobile phase : 700 ml of acetonitrile + 300 ml of a 0.05 mol/L
column oven : at 40 °C, fluorescence detector excitation wavelength

Instructions

实验步骤

Standards Preparation

1. Prepare stock solutions of roxithromycin (ROX) and erythromycin (I.S.) with 1 g/L each in methanol.
2. Prepare standard solutions: 5.0, 7.5,15.0, 20.0, 50.0, 75.0 and 100.0 mg/L of ROX and 20.0 mg/l of I.S. in methanol.
3. Transfer the volume of 50 µL aliquots of the sample to a glass vial containing 0.5 ml blank human plasma.

Solid phase extraction procedure

1. Process the resulting plasma samples containing: 0.5, 0.75, 1.5, 2.0, 5.0, 7.5 and 10.0 mg/l of ROX and 20.0 mg/l of I.S.according to the SPE.
2. Add the volume of 0.5 ml of a phosphate buffer, pH 7.5 (prepared as a mixture of 85.2 ml of 1/15 M Na_2HP0_4 and 14.8 ml 1/15 M KH_2PO_4).
3. Transfer the samples into C18 SPE Bakerbond cartridges (J.T. Baker Mallinckrodt Deventer, Holland).
4. Wash the absorbed analytes with water and elute with methanol.
5. Evaporate the organic liquid to dryness at 40 °C.

Derivatization

1. Dissolve the residue in 200 µL aliquots of acetonitrile and transfer the sample to a glass reaction vial.
2. Add a 100 µL aliquots of a 2.5 mg/L 9-fluorenylmethyl chloroformate (FMOC-Cl) in acetonitrile and 100 µL aliquots of a phosphate buffer, pH 7.5.
3. Incubate the sample at 40 °C for 40 min.
4. Inject an aliquot 100 µL after derivatization, onto the chromatographic system.

HPLC

1. Prepare the mobile phase by mixing 700 mL of acetonitrile with 300 ml of a 0.05 mol/L solution of potassium dihydrogenphosphate in water, adjust to pH 7.5 with a 10% sodium hydroxide solution.
2. Determine ROX and I.S. in human plasma in a chromatograph model HP 1100 (Hewlett-Packard, Waldbronn, Germany).
3. Set at a flow rate of quaternary pump at 2 mL/min, a column oven at 40 °C and a fluorescence detector model HP 1046A and G13 21 A-1100, at an excitation wavelength (Ex) of 255 nm and emission wavelength (Em) of 315 nm.
4. Inject the samples (100 µL) using autosampler model G1313A.
5. Perform the separation on a 125 x 4.6 mm i.d. LiChrospher RP-18e column packed with 5 µm particles, with a guard column (LiChrospher RP-18e), both from Merck.

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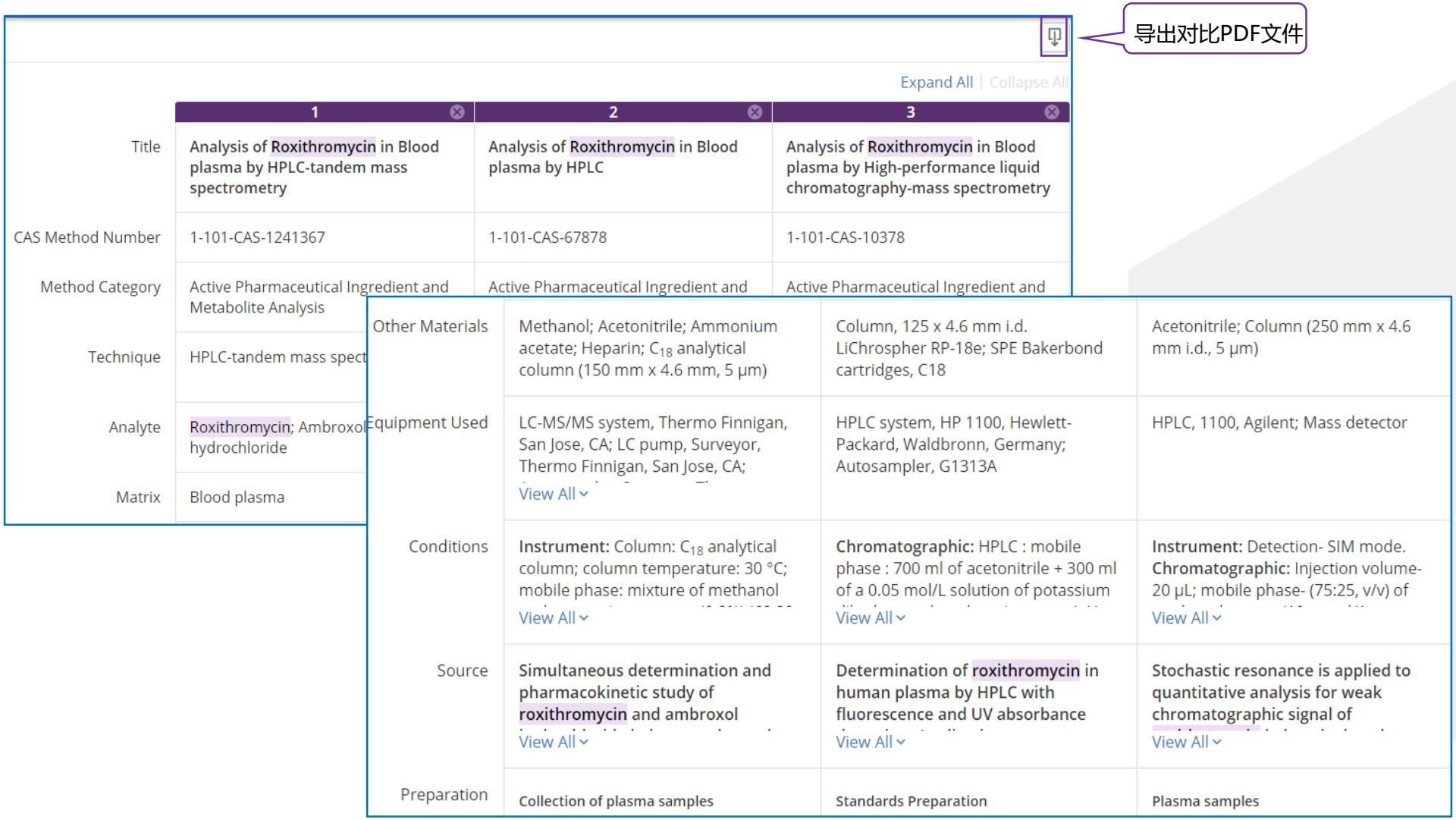
结果显示



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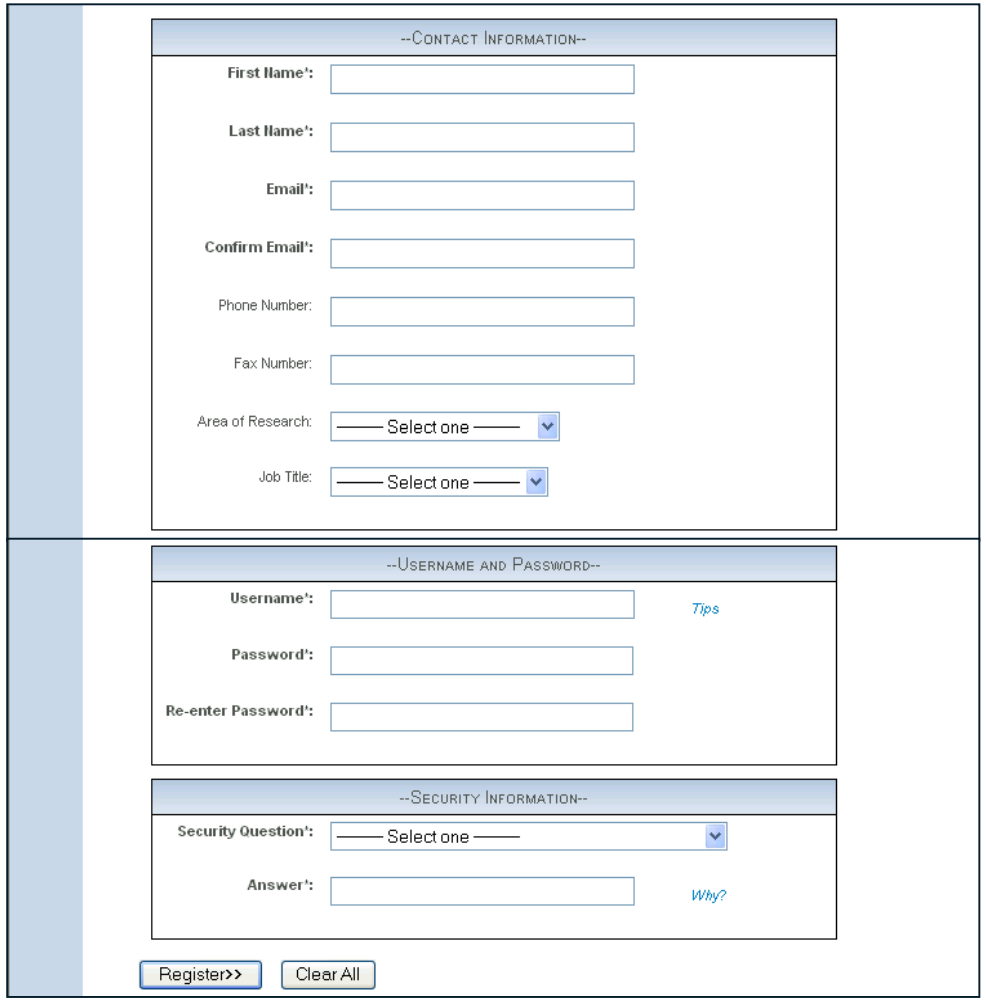

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- _（下划线）
- .（句点）
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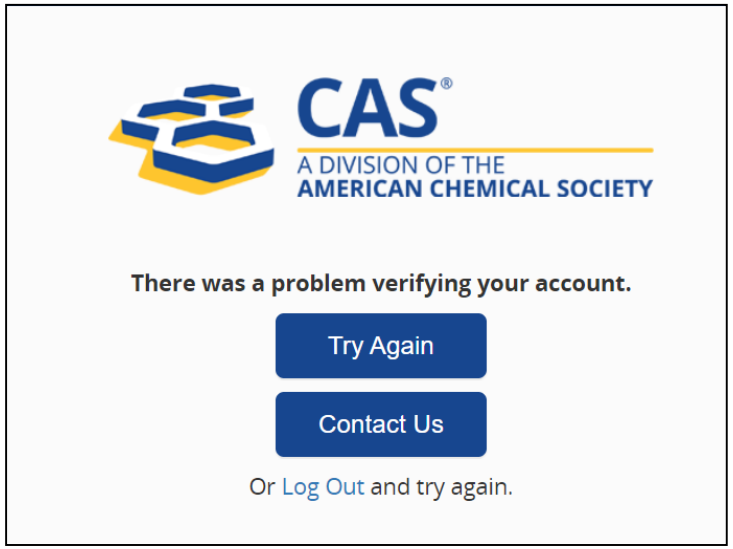

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