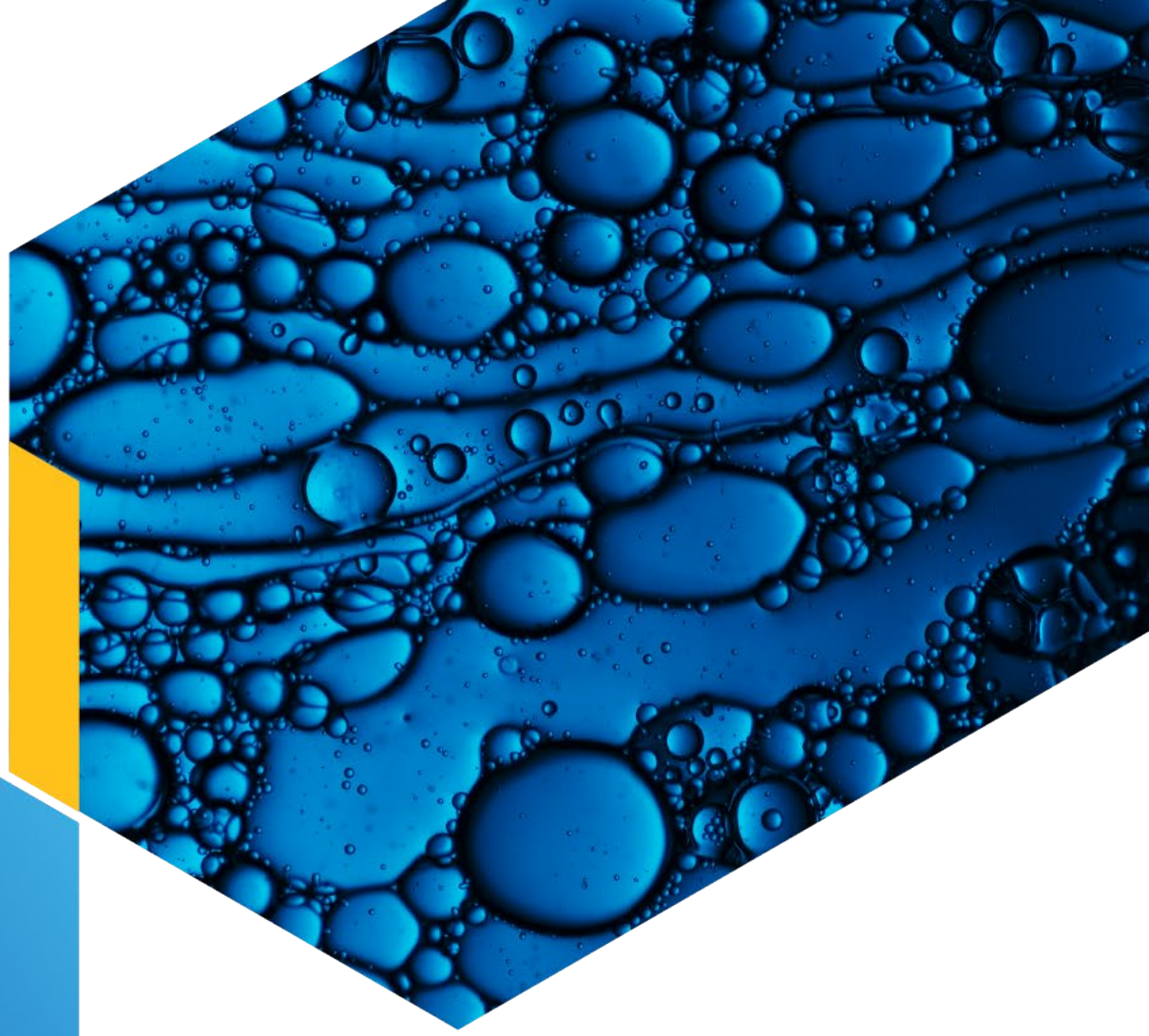

利用CAS SciFinder获取科技信息

2021.6

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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
- **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

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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

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FORESIGHT

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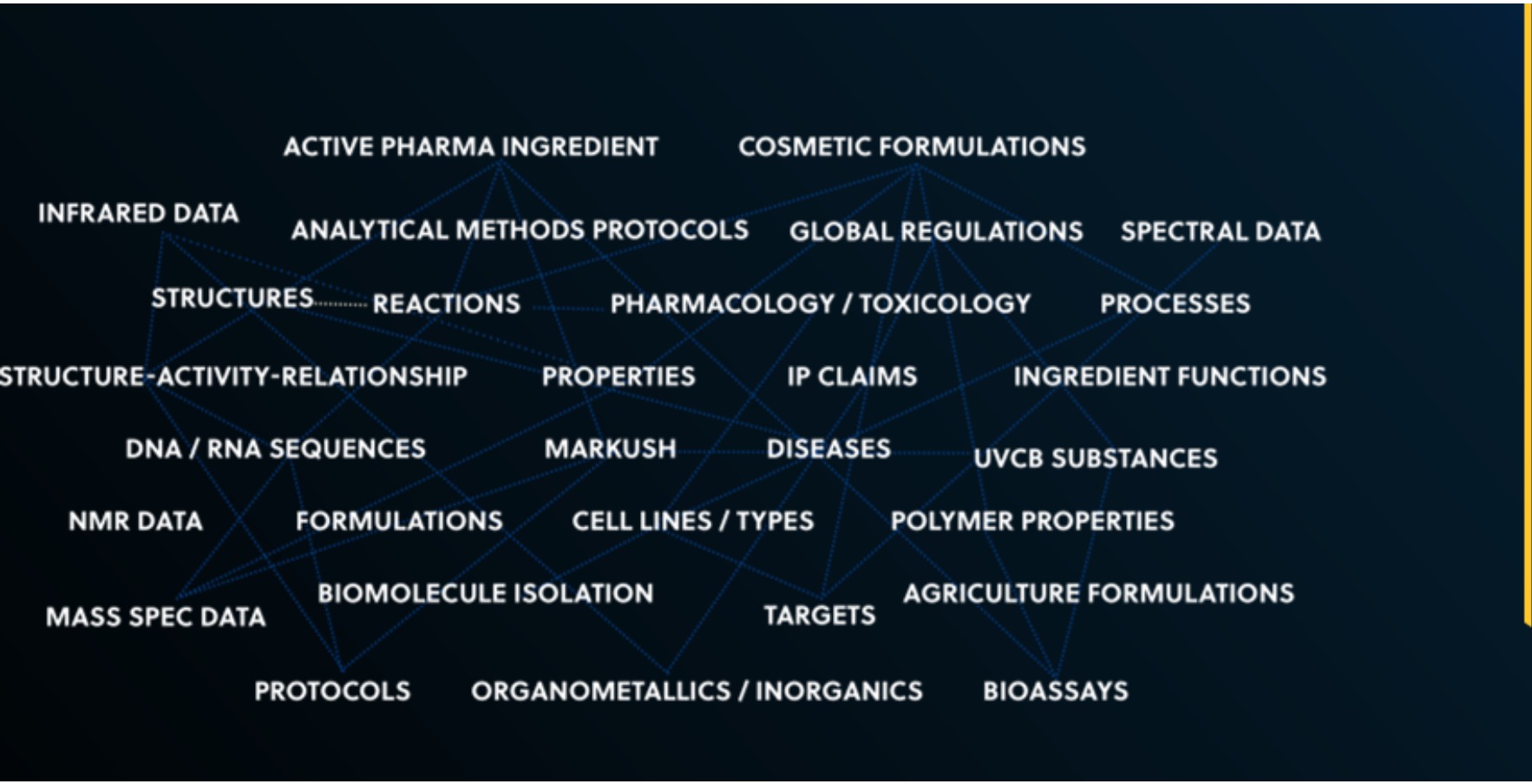

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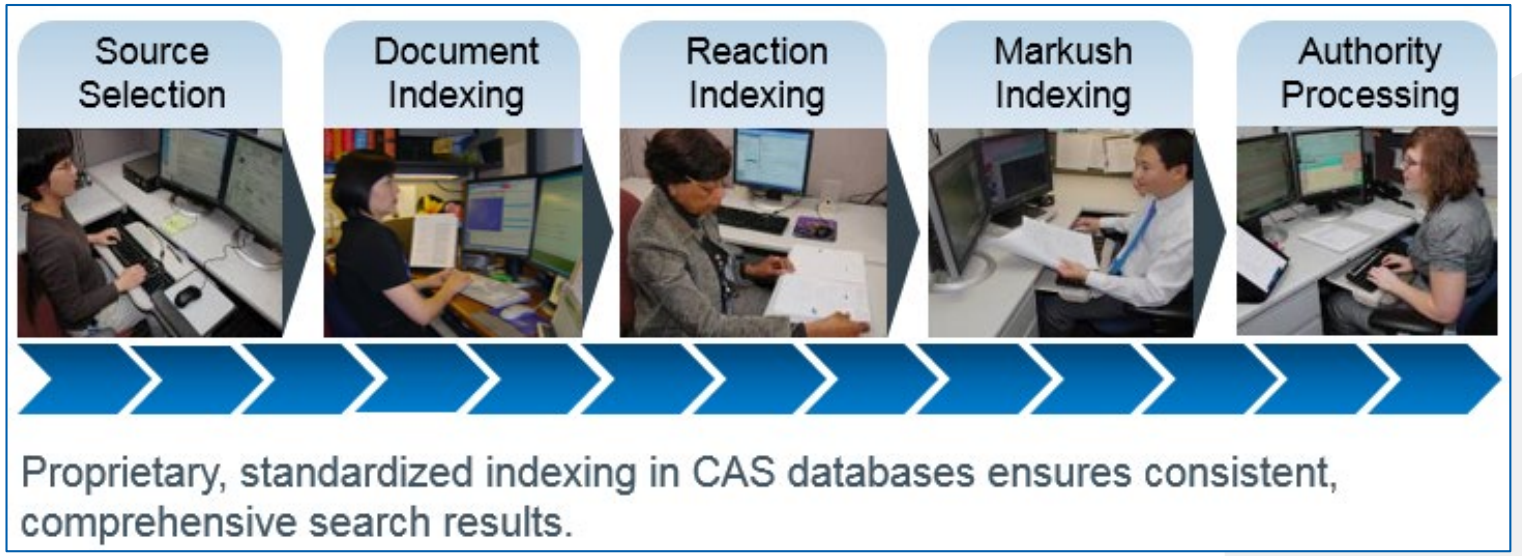
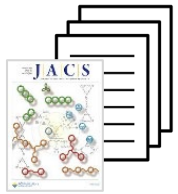
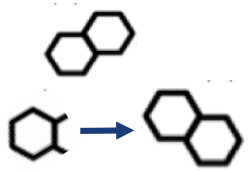
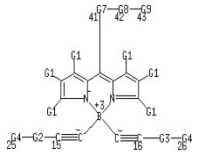


Data pre-repository



1990
Smith, M.
anthracene





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

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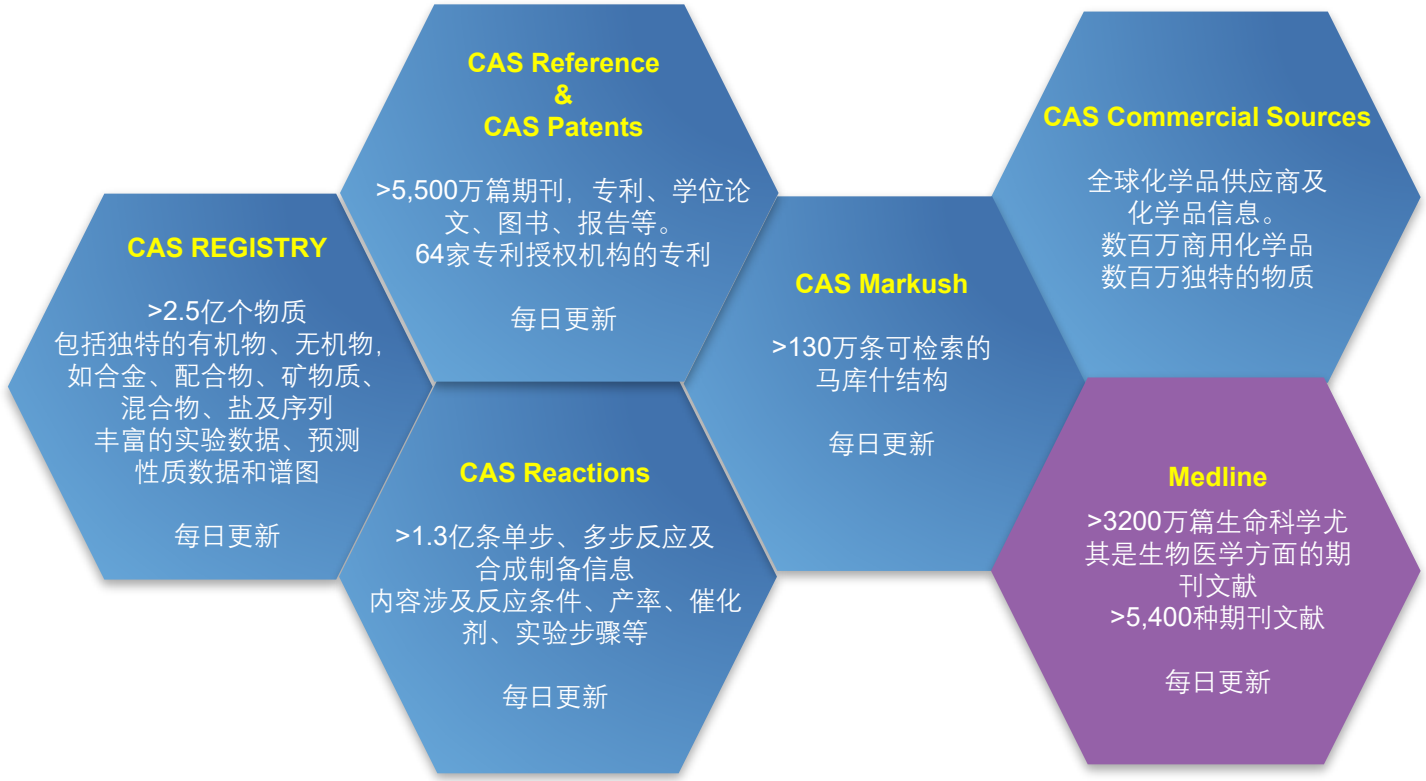

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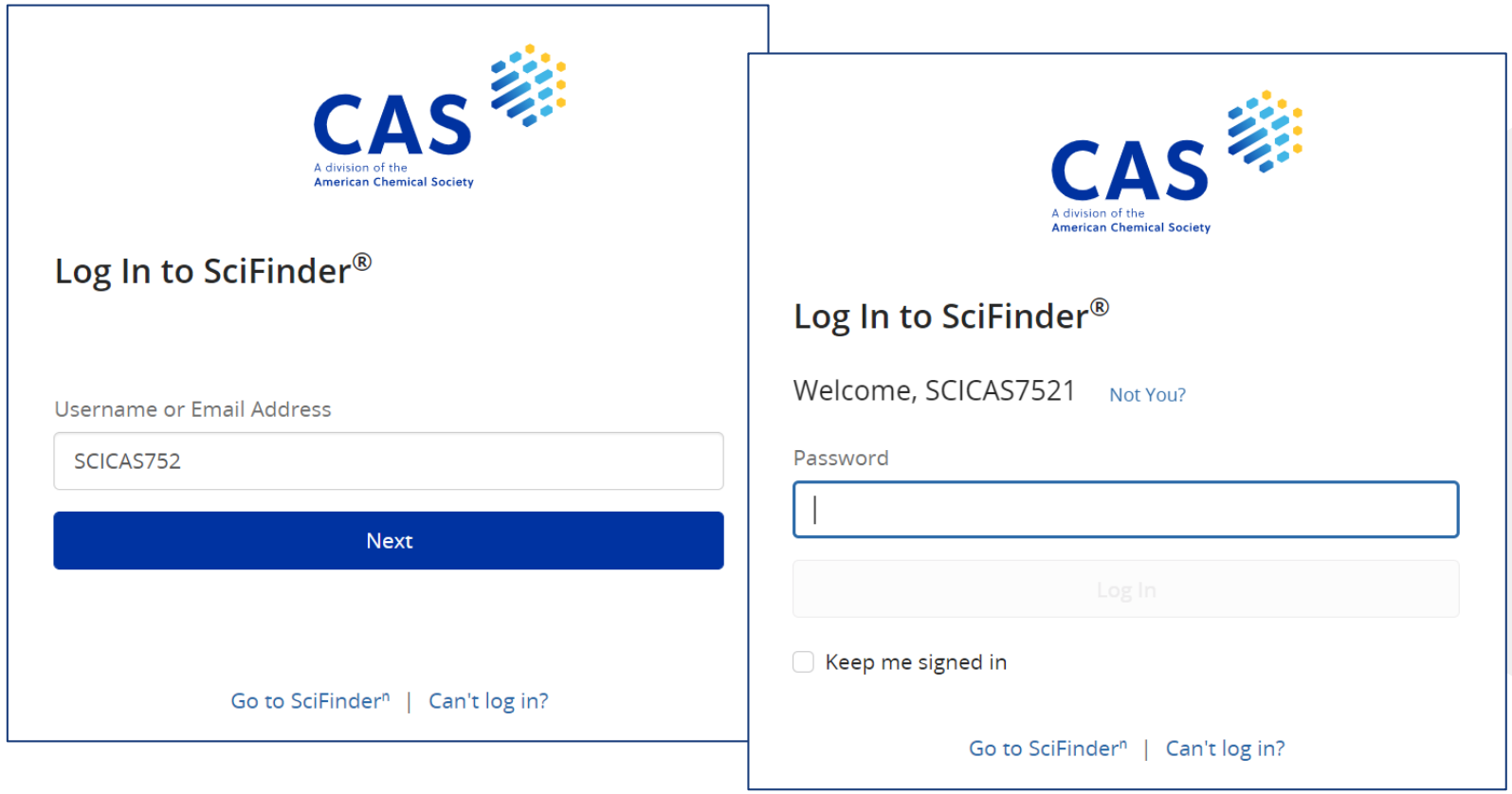

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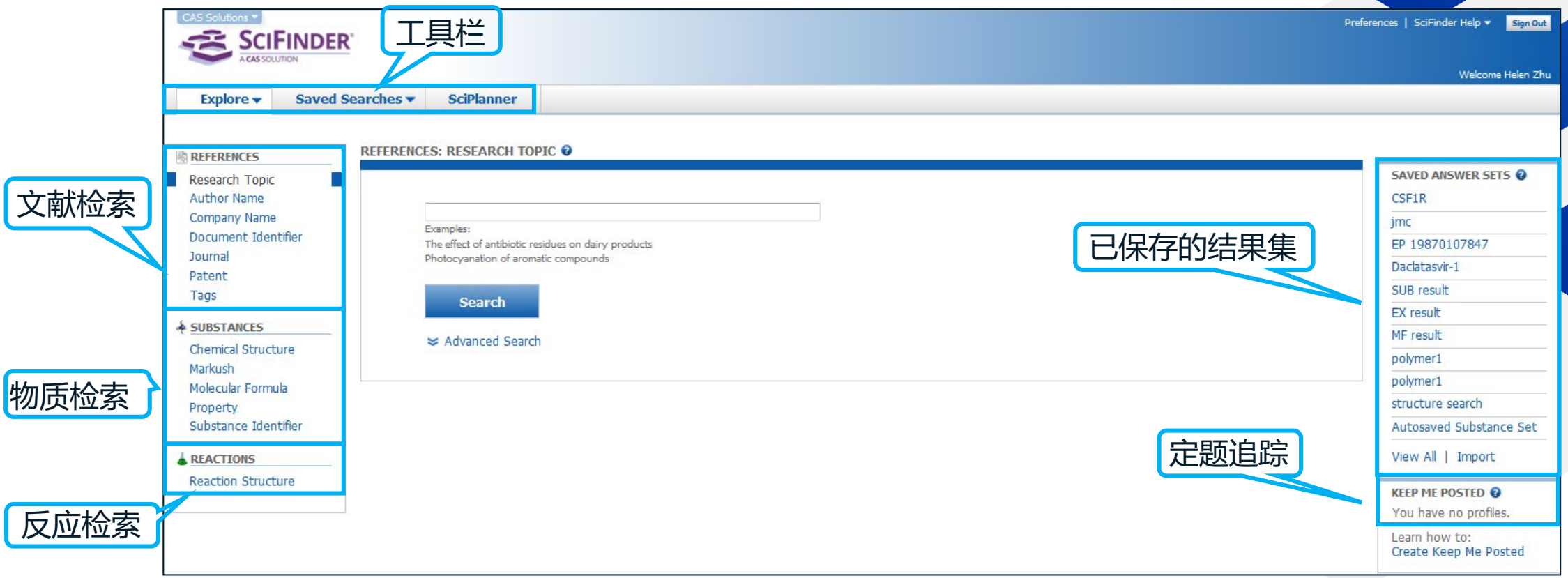

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  - 文献检索方法
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- 物质相关信息的获取策略
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- 反应相关信息的获取策略
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  - 反应结果排序、筛选和详情

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  - 作者名检索
  - 机构名检索
  - 文献标识符检索
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  - 从物质，反应获得文献
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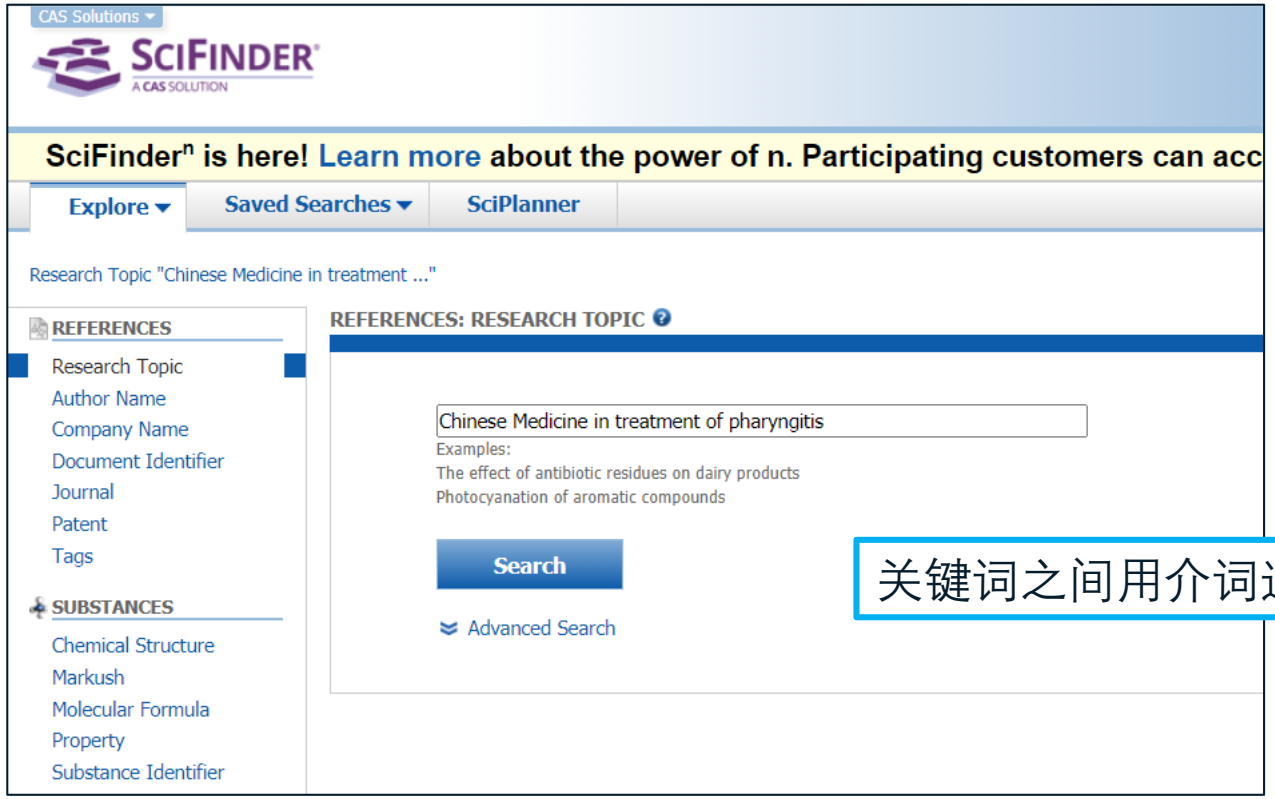
  - 关注物质有关的文献：先获得物质，再获得文献
  - 关注某科研人员的文献：作者名检索
  - 关注某机构科研进展：机构名检索

文献检索--主题

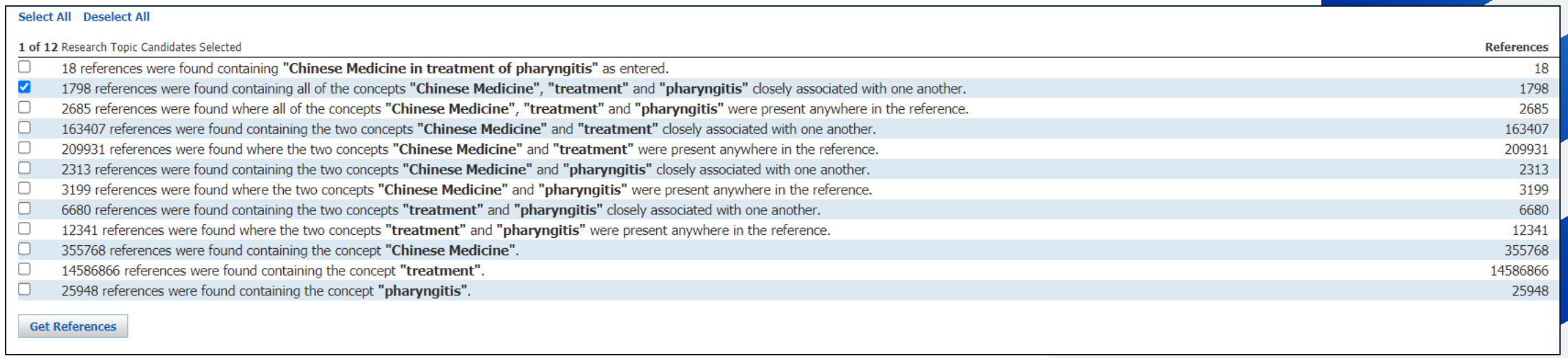
主题检索：中药在咽炎治疗中的应用

检索式： Chinese Medicine **in** treatment **of** pharyngitis



关键词之间用介词连接：in, with, of...

主题检索的候选项



Select All Deselect All

1 of 12 Research Topic Candidates Selected

		References
☐	18 references were found containing **"Chinese Medicine in treatment of pharyngitis"** as entered.	18
☑	1798 references were found containing all of the concepts **"Chinese Medicine"**, **"treatment"** and **"pharyngitis"** closely associated with one another.	1798
☐	2685 references were found where all of the concepts **"Chinese Medicine"**, **"treatment"** and **"pharyngitis"** were present anywhere in the reference.	2685
☐	163407 references were found containing the two concepts **"Chinese Medicine"** and **"treatment"** closely associated with one another.	163407
☐	209931 references were found where the two concepts **"Chinese Medicine"** and **"treatment"** were present anywhere in the reference.	209931
☐	2313 references were found containing the two concepts **"Chinese Medicine"** and **"pharyngitis"** closely associated with one another.	2313
☐	3199 references were found where the two concepts **"Chinese Medicine"** and **"pharyngitis"** were present anywhere in the reference.	3199
☐	6680 references were found containing the two concepts **"treatment"** and **"pharyngitis"** closely associated with one another.	6680
☐	12341 references were found where the two concepts **"treatment"** and **"pharyngitis"** were present anywhere in the reference.	12341
☐	355768 references were found containing the concept **"Chinese Medicine"**.	355768
☐	14586866 references were found containing the concept **"treatment"**.	14586866
☐	25948 references were found containing the concept **"pharyngitis"**.	25948

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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Research Topic "Chinese Medicine in treatment ..." > r

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- Accession Number
- Author Name
- Citing References
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Display Options

Page: 1 of 89

Analyze by: Author Name

Name Not Translated	26
Xu Jun	15
Wang Yajun	10
Zhang Jianjun	10
Chen Zhijin	9
Jiang Guochao	8
Qu Yunzhi	7
Shen Juanyan	7
Wang Wei	7
Yang Gaolin	7

Show More

1. **f flavonoids and organic acid from Trollius chinensis Bunge**
Quick View | Other Sources
By Li, Yao-Lan; Ma, Shuang-Cheng; Yang, Yi-Ting; Ye, Shao-Ming; But, Paul Pui-Hay
From Journal of Ethnopharmacology (2002), 79(3), 365-368. | Language: English, Database: CAPLUS

The flower of Trollius chinensis Bunge is used for **trea**...ctions, **pharyngitis**, tonsillitis, and bronchitis in **Chinese** folk **medicine**. The antiviral activities of the crude ext., total flavonoids, orientin, vitexin and proglobeflowery acid isolated from the flowers of T. c... a type 3 (Para 3) virus were investigated. The results showed that the crude ext. and total flavonoids exhibited a weak antiviral activity against Para 3. Orientin and vitexin demonstrated potent or moderate... a 3. Proglobeflowery acid showed w...

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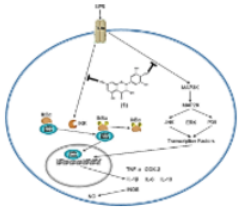
2. **Suppression of Inflammatory Responses by Dihydromyricetin, a Flavonoid from Ampelopsis grossedentata, via Inhibiting the Activation of NF-κB and MAPK Signaling Pathways**
Quick View | Other Sources
By Hou, X. L.; Tong, Q.; Wang, W. Q.; Shi, C. Y.; Xiong, W.; Chen, J.; Liu, X.; Fang, J. G.
From Journal of Natural Products (2015), 78(7), 1689-1696. | Language: English, Database: CAPLUS



Ampelopsis grossedentata, an indigenous plant in southern China, has been used for **treating pharyngitis** in traditional **Chinese medicine** for hundreds of years. In this study, the authors explored the anti-inflammatory activity of dihydromyricetin, its major bioactive component, and the underlying mechanism of this action. The authors demonstrated that dihydromyricetin suppressed the levels of pro-inflammatory cytokines such as tumor necrosis factor-α (TNF-α), interleukin-1β (IL-1β), and interleukin-6 (IL-6) as well as increased the level of the anti-inflammatory cytokine interleukin-10 (IL-10...

3. **Physalin A induces apoptosis via p53-Noxa-mediated ROS generation, and autophagy plays a protective role against apoptosis through p38-NF-κB survival pathway in A375-S2 cells**
Quick View | Other Sources
By He, Hao; Zang, Ling-He; Feng, Yong-Sheng; Chen, Li-Xia; Kang, Ning; Tashiro, Shin-ichi; Onodera, Satoshi; Qiu, Feng; Ikejima, Takashi
From Journal of Ethnopharmacology (2013), 148(2), 544-555. | Language: English, Database: CAPLUS

Physalin A is a bioactive withanolide isolated from natural plant Physalis alkekengi L. var. franchetii (Mast.) Makino, a traditional **Chinese** herbal **medicine** named Jindenglong which has long been used for the **treatment** of cough, **sore throat**, hepatitis, eczema, dysuria and tumors in China. Based on the previous study that physalin A induced cytotoxic effect in human melanoma A375-S2 cells, this study was designed to further illustrate the mol. mechanisms

Citing Reference: 帮助找到最重要的文献

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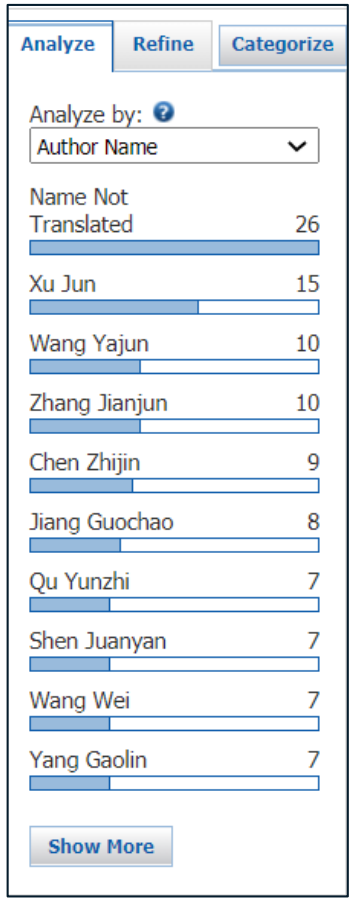
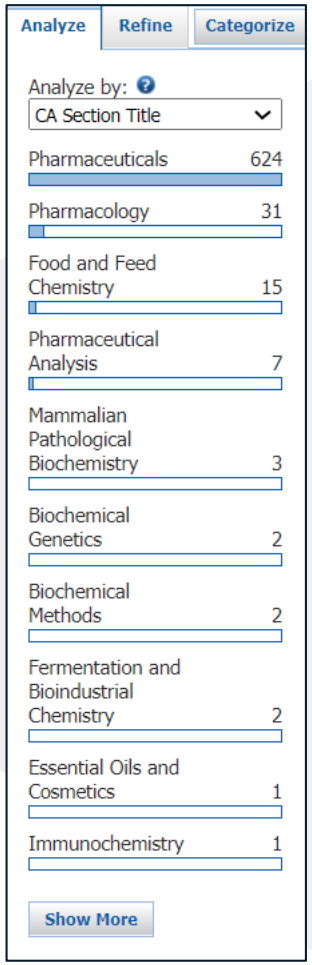
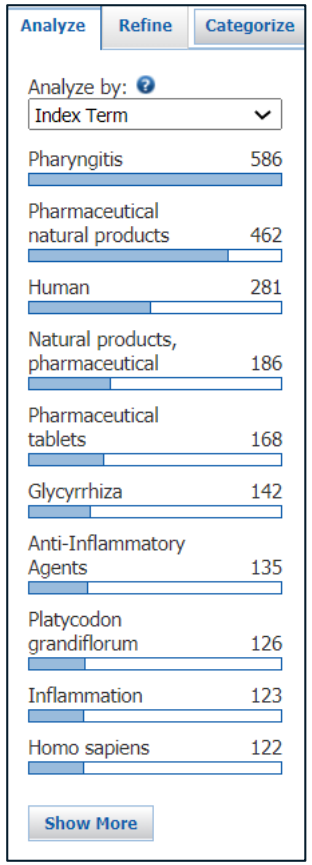
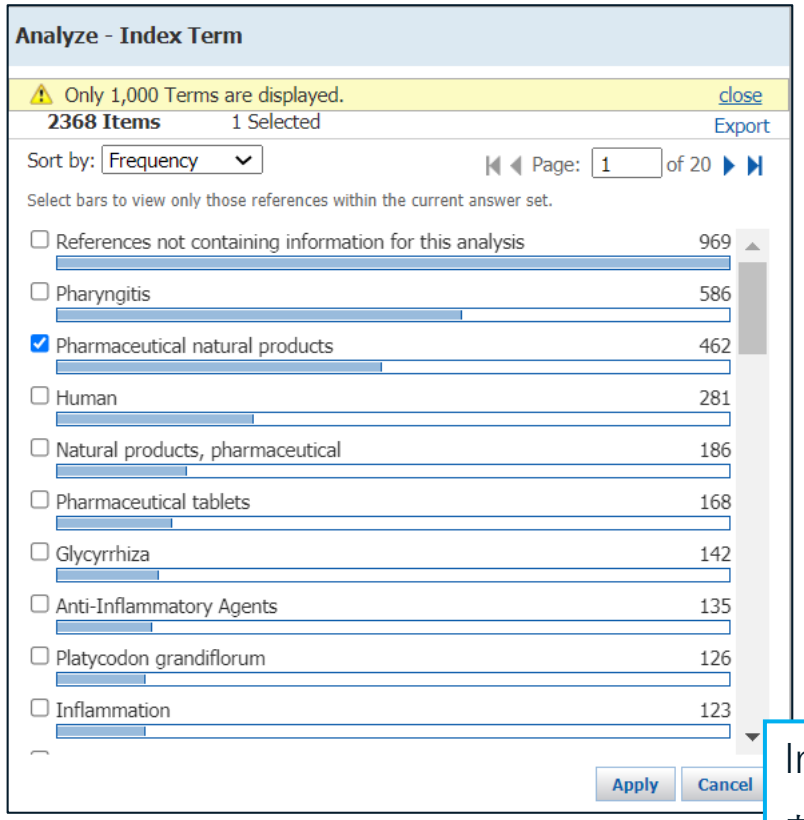
文献结果集的筛选--Analyze





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

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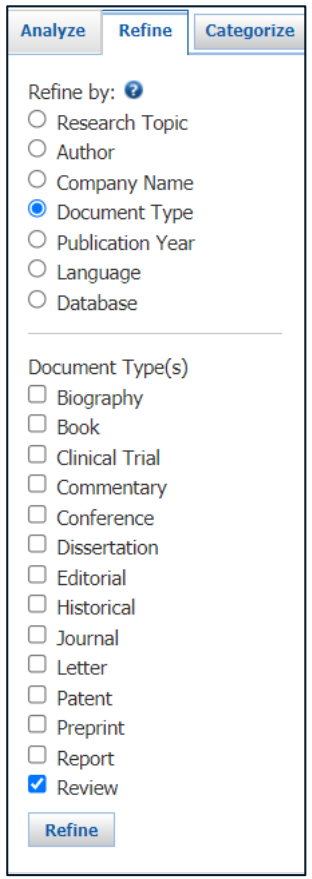

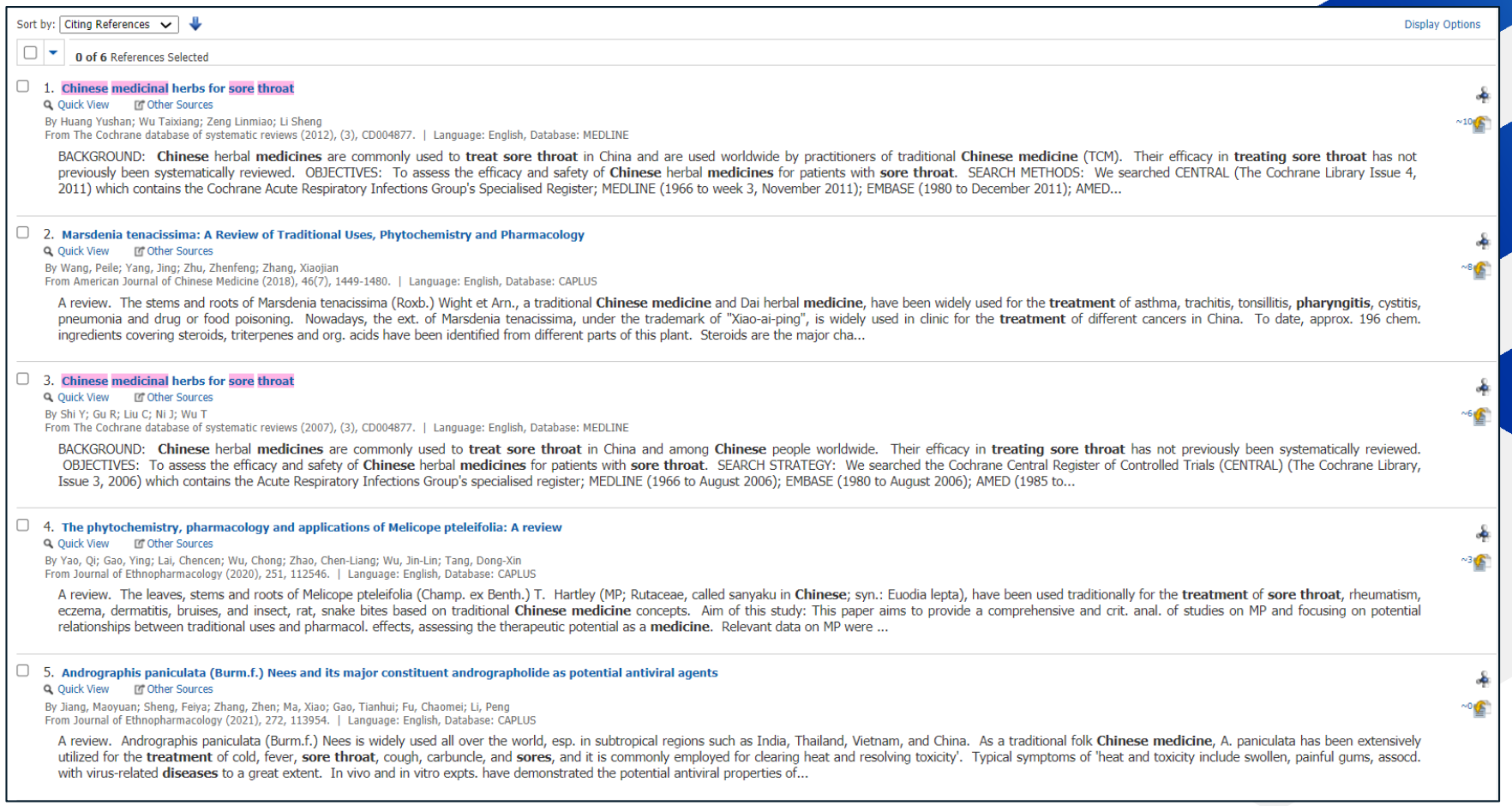

Refine： 帮助用户迅速获得需要的文献

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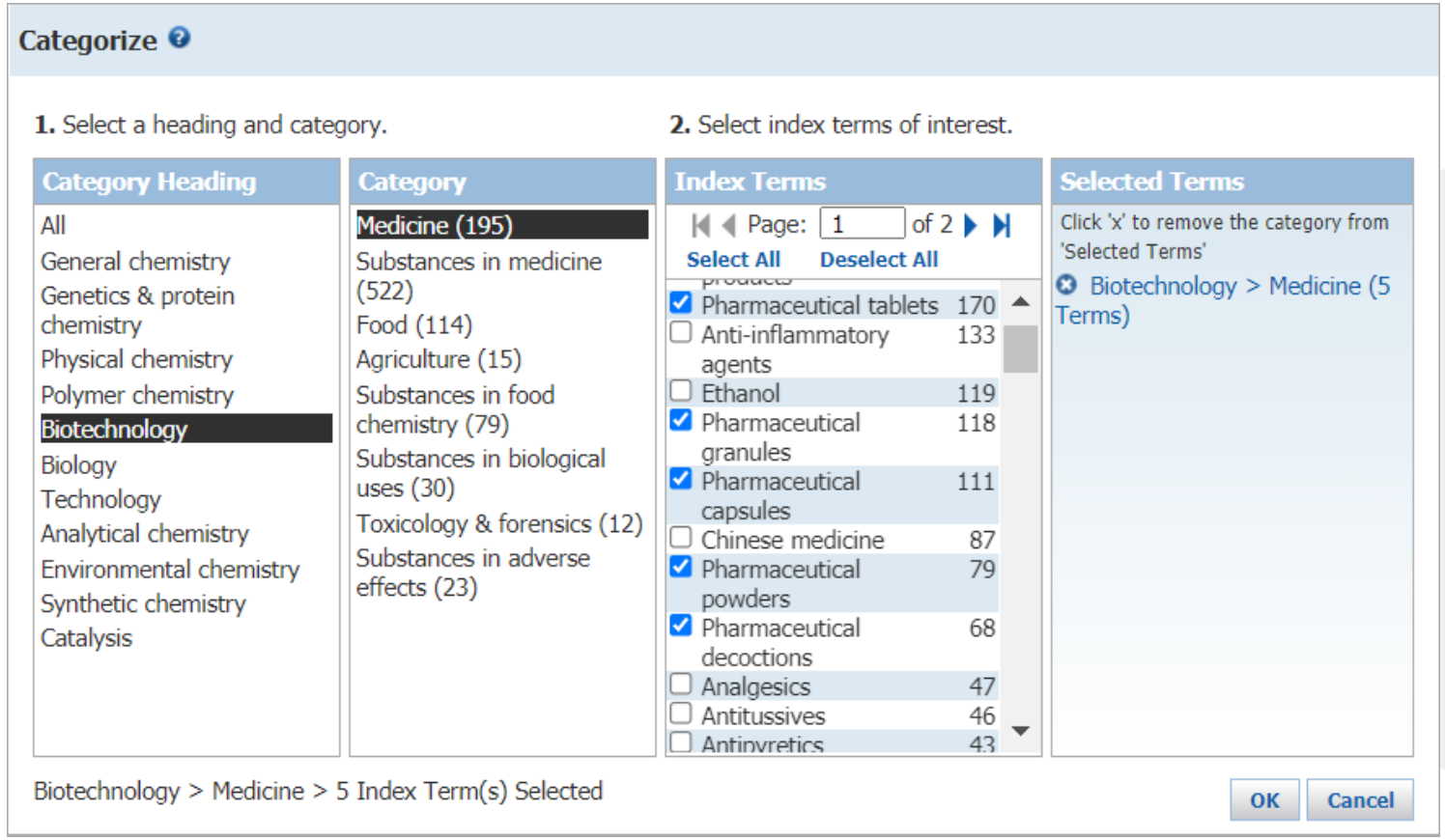

Categorize学科分类功能，基于Index Term，根据大学科方向对文献进行自动分类。

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Save：保存在服务器上，方便以后登陆查看，每次可存1万条记录。

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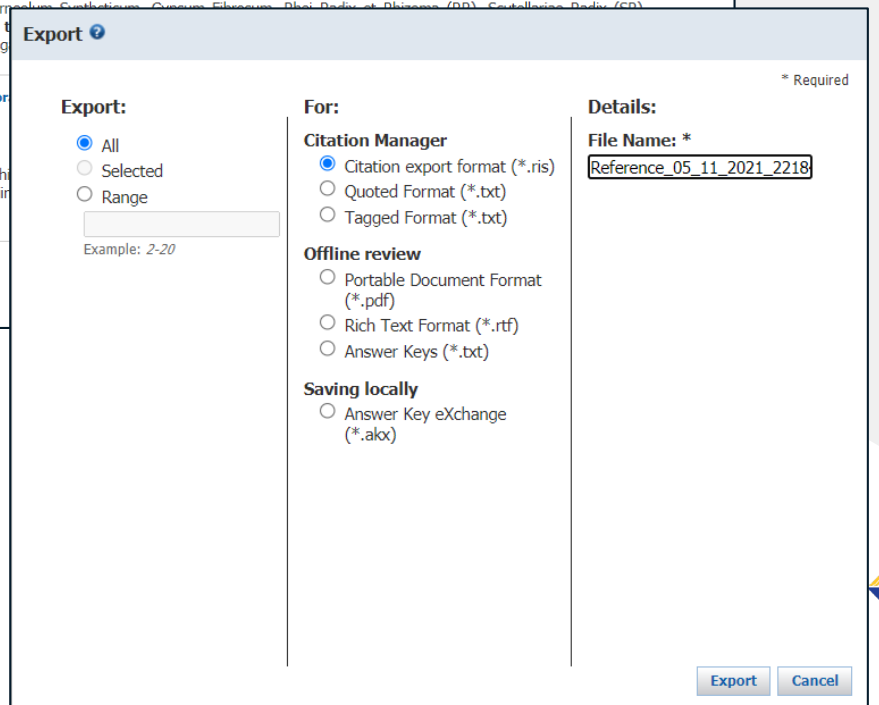

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文献结果详情--题录、摘要、索引

1. Development and validation of a UPLC-DAD-MS method for characterization and quantification of alkaloids in Menispermi Rhizoma and its preparations

By: Liu, Yanan; Song, Xiao; Yan, Ruiqing; Li, Tianxiang; Chai, Xin; Qi, Aidi; Wang, Yuefei; Jiang, Zhenzuo

Menispermi Rhizoma (MR), a well known traditional Chinese medicine, is widely used to prevent and treat sore throat, enteritis, dysentery, and rheumatoid arthralgia clin. However, many rhizomes of Chinese herbal medicines are mistaken as MR due to their similar appearance, which could affect MR quality and cause serious consequences for patients. To guarantee the quality of MR products, an ultra-high-performance liq. chromatog.-diode array detector-tandem mass spectrometry (UPLC-DAD-MS) method was established for the characterization of major active ingredients in MR and its prepns. By comparing their retention times and characteristic fragmentations with those of authentic compds., 9 alkaloids in MR were unequivocally identified as acutumidine, acutumine, magnoflorine, menisperine, dauricine, menisporphine, N-demethyl-N-formyldehydronuciferine, 6-O-demethylmenisporphine, and dauriporphine. Quant. anal. of the 9 alkaloids in MR and its prepns. was accomplished by UPLC-DAD. A UPLC C18 column was employed for the chromatog. sepn. which was effected by a gradient elution with acetonitrile and 0.1% aq. formic acid soln. contg. 5 mM ammonium acetate at a flow rate of 0.3 mL/min. This quant. method was validated with good linearity ($R^2 \geq 0.9991$), desirable intra- and inter-day precisions (RSD ≤ 3.32%), and acceptable recoveries (97.90-106.8%). The method was also successfully applied to quantify 9 alkaloids in 8 batches of MR, 6 batches of MR capsules and 2 batches of MR pills. A counterfeit MR sample from Henan province was identified by the validated method, followed by further verification by appearance and microscopic identification. The developed UPLC-DAD-MS method overcame the shortcomings of other quality control methods, such as scant chem. marker, long anal. time, consumption of large amts. of org. solvents and limitation to MR or its single dosage form.

Indexing

Pharmaceutical Analysis (Section64-2)

Section cross-

Concepts 重要概念

Pharmaceutical natural products

Menispermi Rhizoma; RP-UPLC-DAD-MS method for characterization and detn. of alkaloids in Menispermi Rhizoma

Mass spectrometry

RP-UPLC, combined with; RP-UPLC-DAD-MS method for characterization and detn. of alkaloids in Menispermi Rhizoma

Counterfeiting
Pharmaceutical capsules
Quality control
Menispermum dauricum
Pharmaceutical tablets

RP-UPLC-DAD-MS method for characterization and detn. of alkaloids in Menispermi Rhizoma

Alkaloids

RP-UPLC-DAD-MS method for characterization and detn. of alkaloids in Menispermi Rhizoma

Analyte; Analytical study

Substances 重要物质

111017-06-2

RP-UPLC-DAD-MS method for characterization and detn. of alkaloids in Menispermi Rhizoma

Analyte; Natural product occurrence; Properties; Analytical study; Biological study; Occurrence

524-17-4 Dauricine
2141-09-5 Magnoflorine
17088-50-5 Acutumine
18145-26-1 Acutumidine
25342-82-9 Menisperine
83287-02-9 Menisporphine
83287-03-0 6-O-Demethylmenisporphine
88142-60-3 Dauriporphine

RP-UPLC-DAD-MS method for characterization and detn

Analyte; Properties; Analytical study

QUICK LINKS

0 Tags, 0 Comments

SOURCE

Journal of Food and Drug Analysis
Volume21
Issue2
Pages206-218
Journal; Online Computer File
2013
CODEN:JFDAAF
ISSN:1021-9498
DOI:10.1016/j.jfda.2013.05.012

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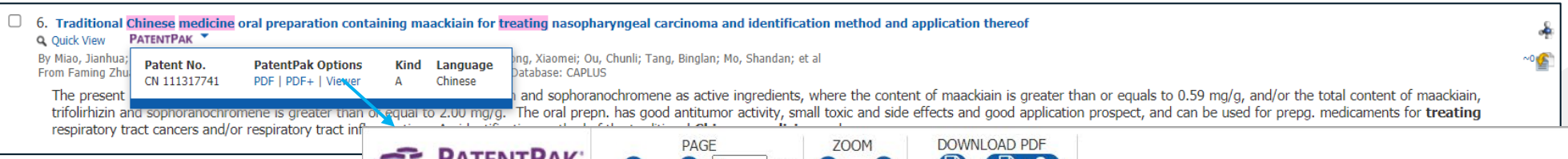

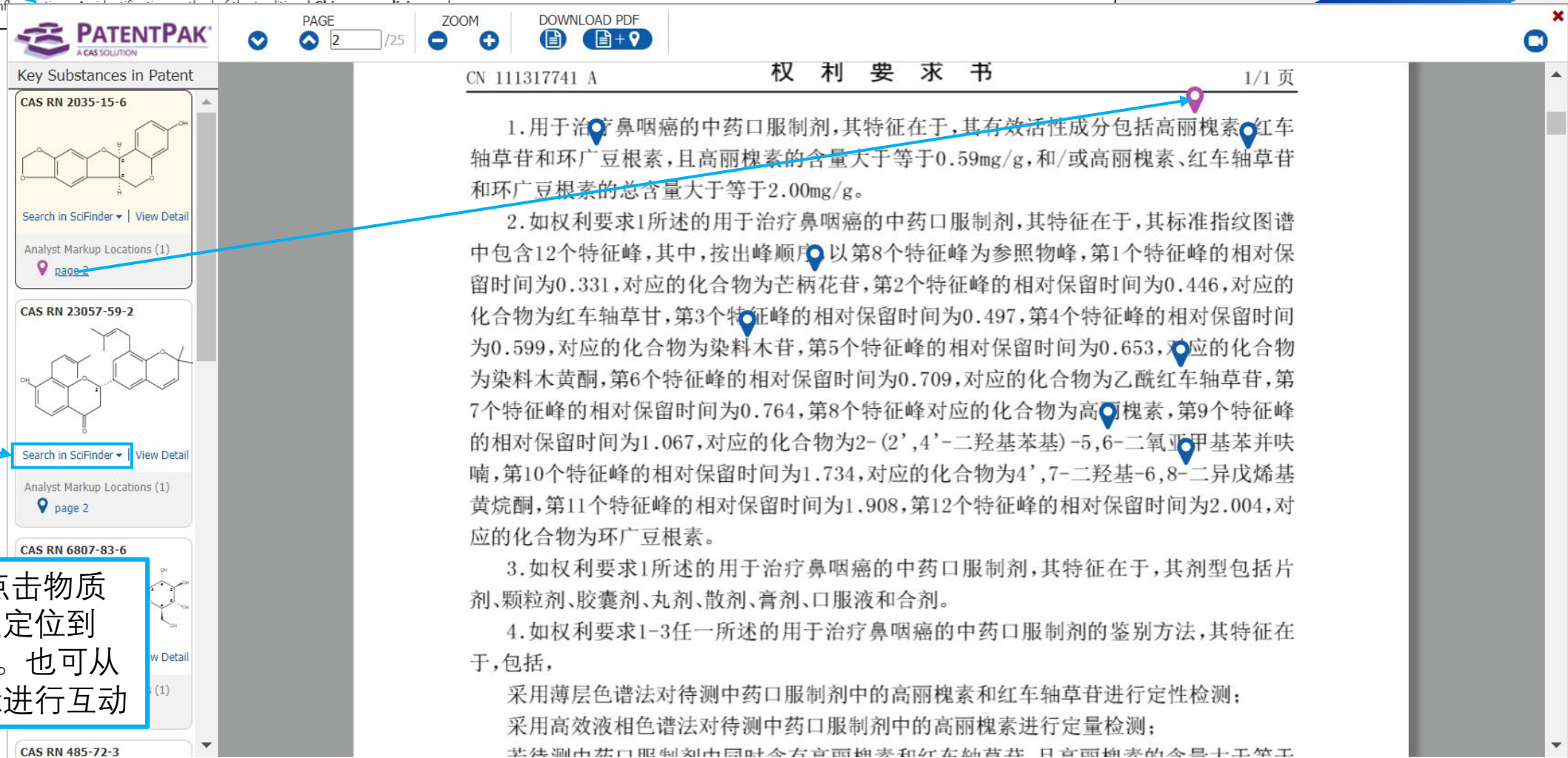

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1. 主题检索时，使用介词 in, with, of 等作为连接词
2. 跟据检索要求选择合适的候选项
3. 通过SciFinder 的Analyze/Refine功能来缩小检索的范围
4. 尝试将不同的Analyze/Refine功能组合起来用，会有更多的收益
5. 使用Categorize可以让系统来实现自动分类

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  - 文献检索方法
  - 文献结果排序、筛选和详情
- **物质相关信息的获取策略**
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  - 分子式检索
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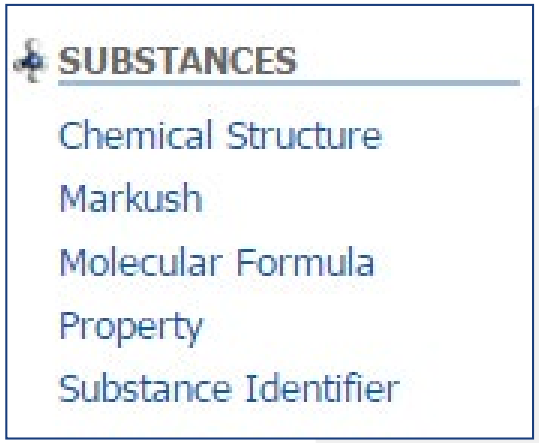
  - 物质标识符检索：化学名称、CAS RN
  - 从文献或反应结果获得
- 检索策略推荐
  - 有机化合物，天然产物：结构检索
  - 无机物，合金：分子式检索
  - 高分子化合物：分子式检索和结构检索



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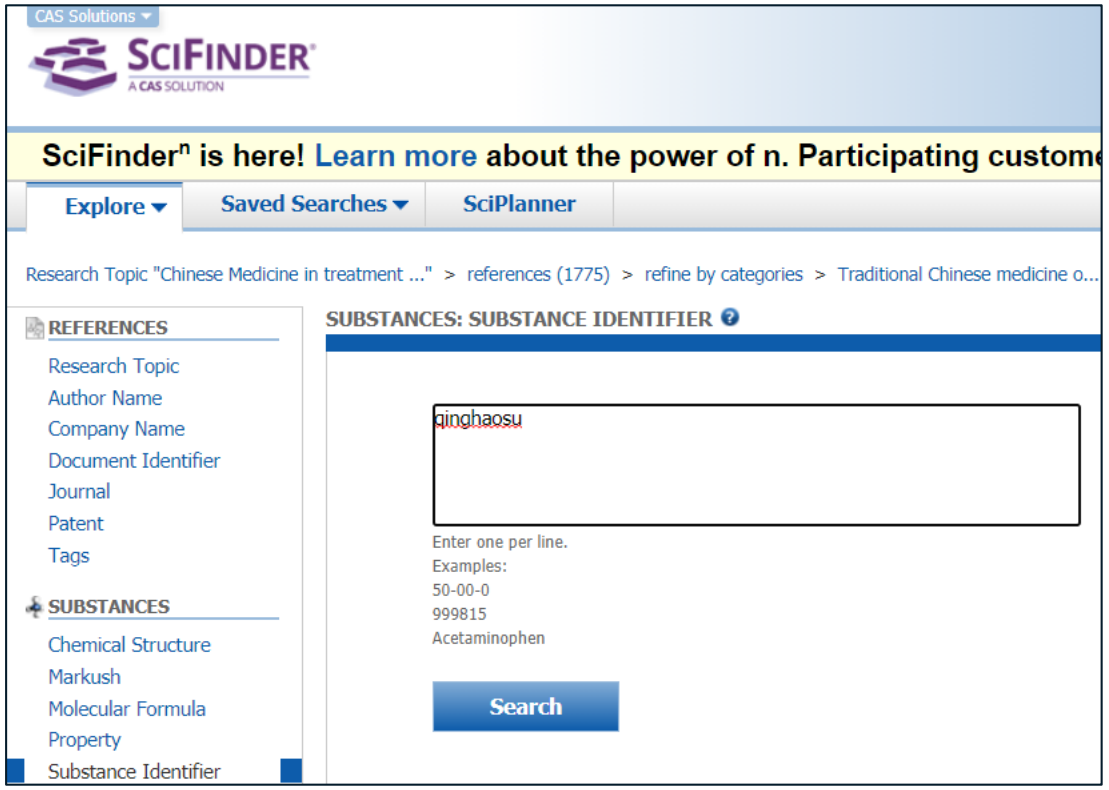
物质检索--标识符检索

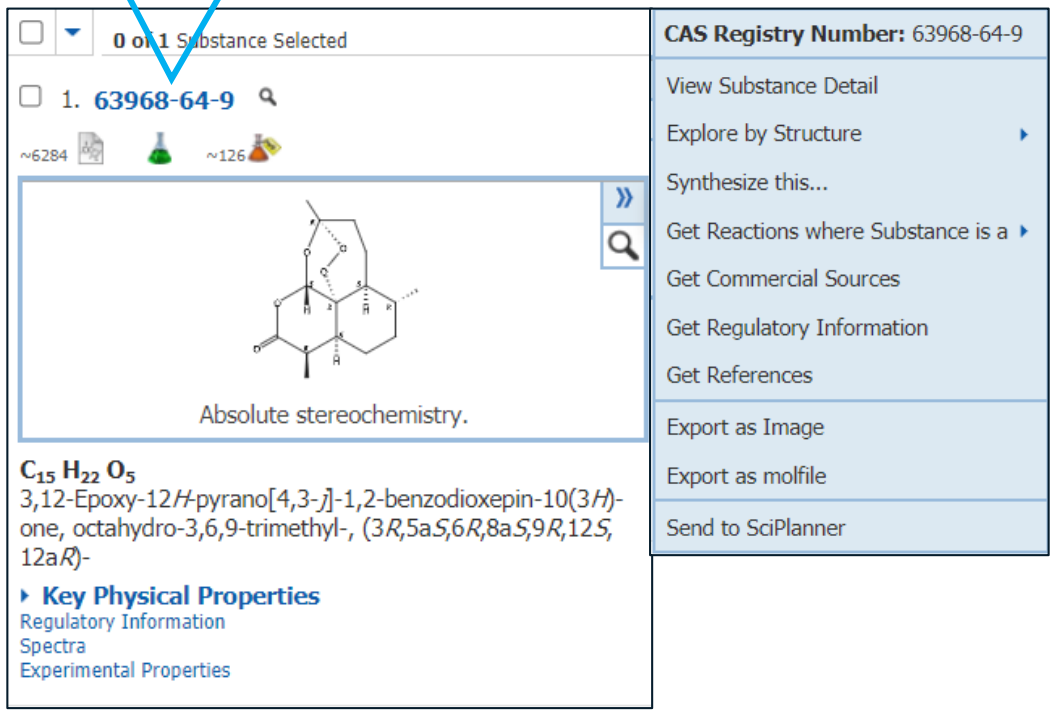


提示：
1. 一次最多可输入25个物质。
2. 每行一个物质标识符。

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

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物质结果详情

SUBSTANCE DETAIL | Get References | Get Reactions | Get Commercial Sources

Return

CAS Registry Number 63968-64-9

~6,284 ~126

$C_{15}H_{22}O_5$

3,12-Epoxy-12*H*-pyrano[4,3-*j*]-1,2-benzodioxepin-10(3*H*)-one, octahydro-3,6,9-trimethyl-, (3*R*,5a*S*,6*R*,8a*S*,9*R*,12*S*,12a*R*)-

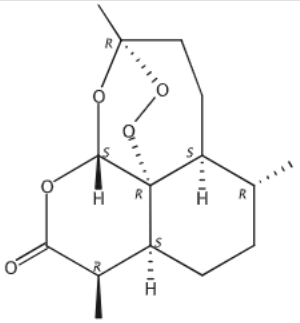
Molecular Weight
282.33

Melting Point (Experimental)
Value: 156-157 °C

Boiling Point (Predicted)
Value: 389.9±42.0 °C | Condition: Press: 760 Torr

Density (Experimental)
Value: 1.300 g/cm3

Other Names
3,12-Epoxy-12*H*-pyrano[4,3-*j*]-1,2-benzodioxepin-10(3*H*)-one, octahydro-3,6,9-trimethyl-, [3*R*-(3α,5aβ,6β,8aβ,9α,12β,12a*R**)]-
(3*R*,5a*S*,6*R*,8a*S*,9*R*,12*S*,12a*R*)-Octahydro-3,6,9-trimethyl-3,12-epoxy-12*H*-pyrano[4,3-*j*]-1,2-benzodioxepin-10(3*H*)-one
(+)-Arteannuin
(+)-Artemisinin
(+)-Qinghaosu
View more...



Absolute stereochemistry.

Get References

Limit results to:

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

For each sequence, retrieve:

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

Get | Cancel

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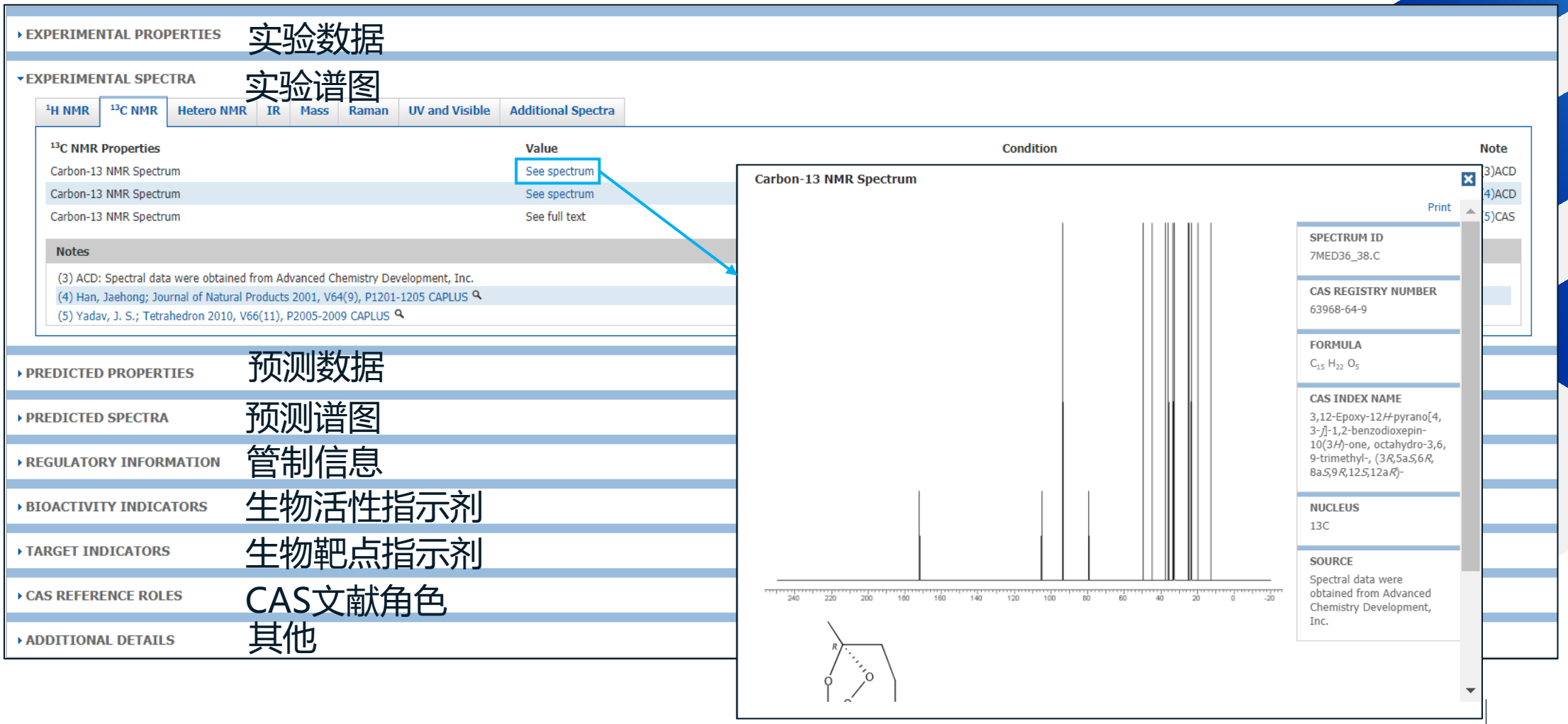
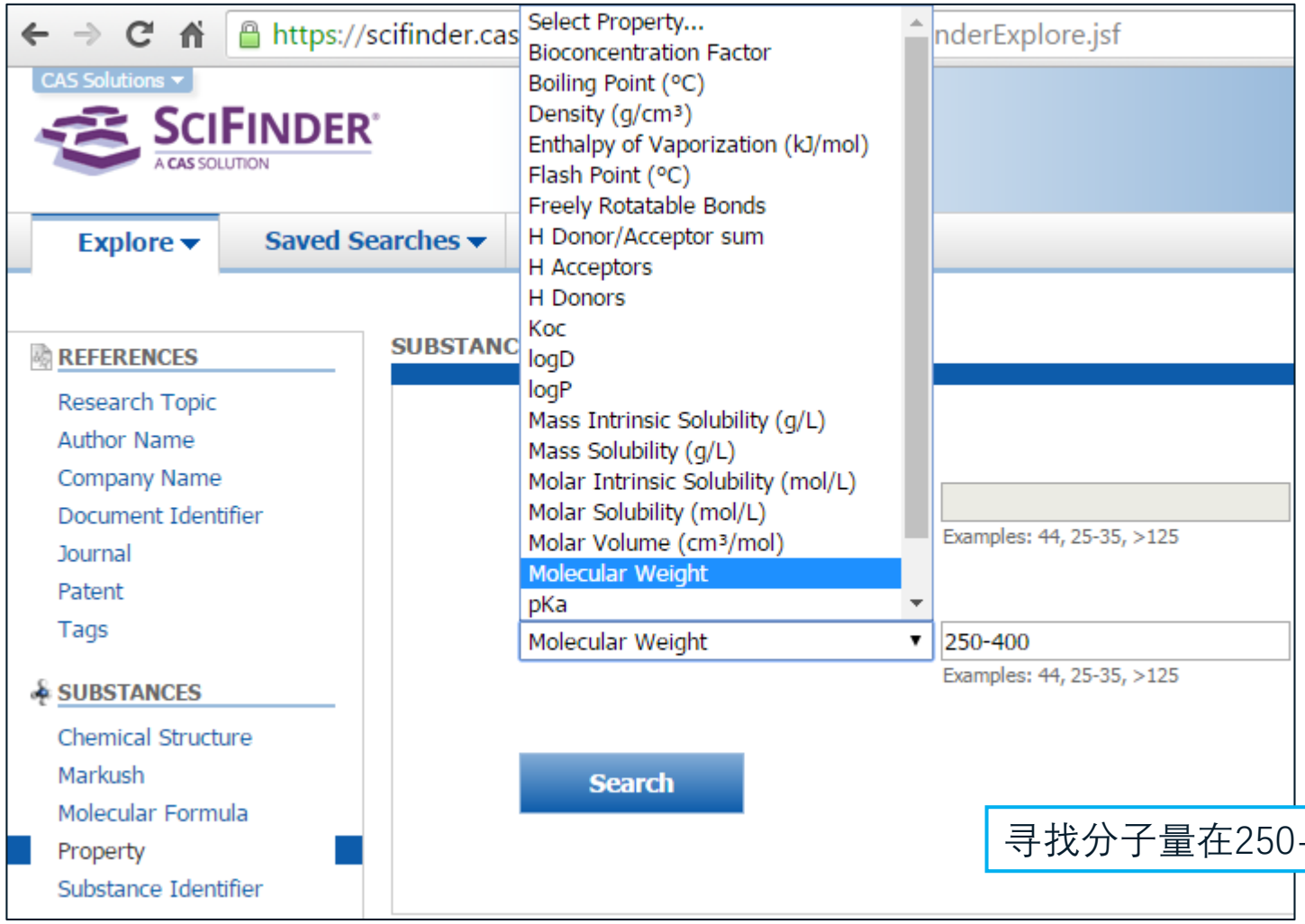
物质结果详情

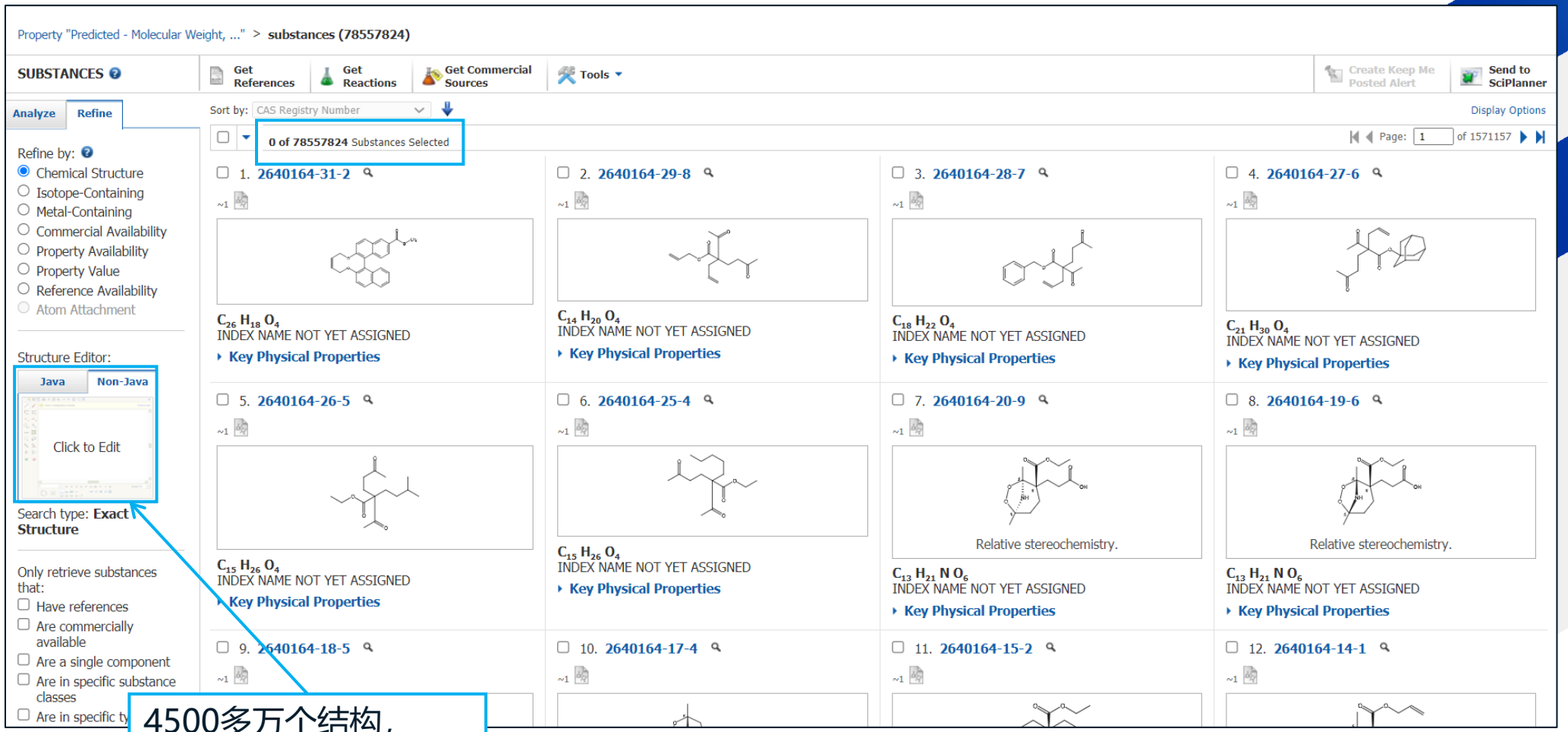


物质检索--Property Explorer



寻找分子量在250-400之间的物质

物质结果集的筛选--Refine



4500多万个结构，

如何筛选黄酮类物质?

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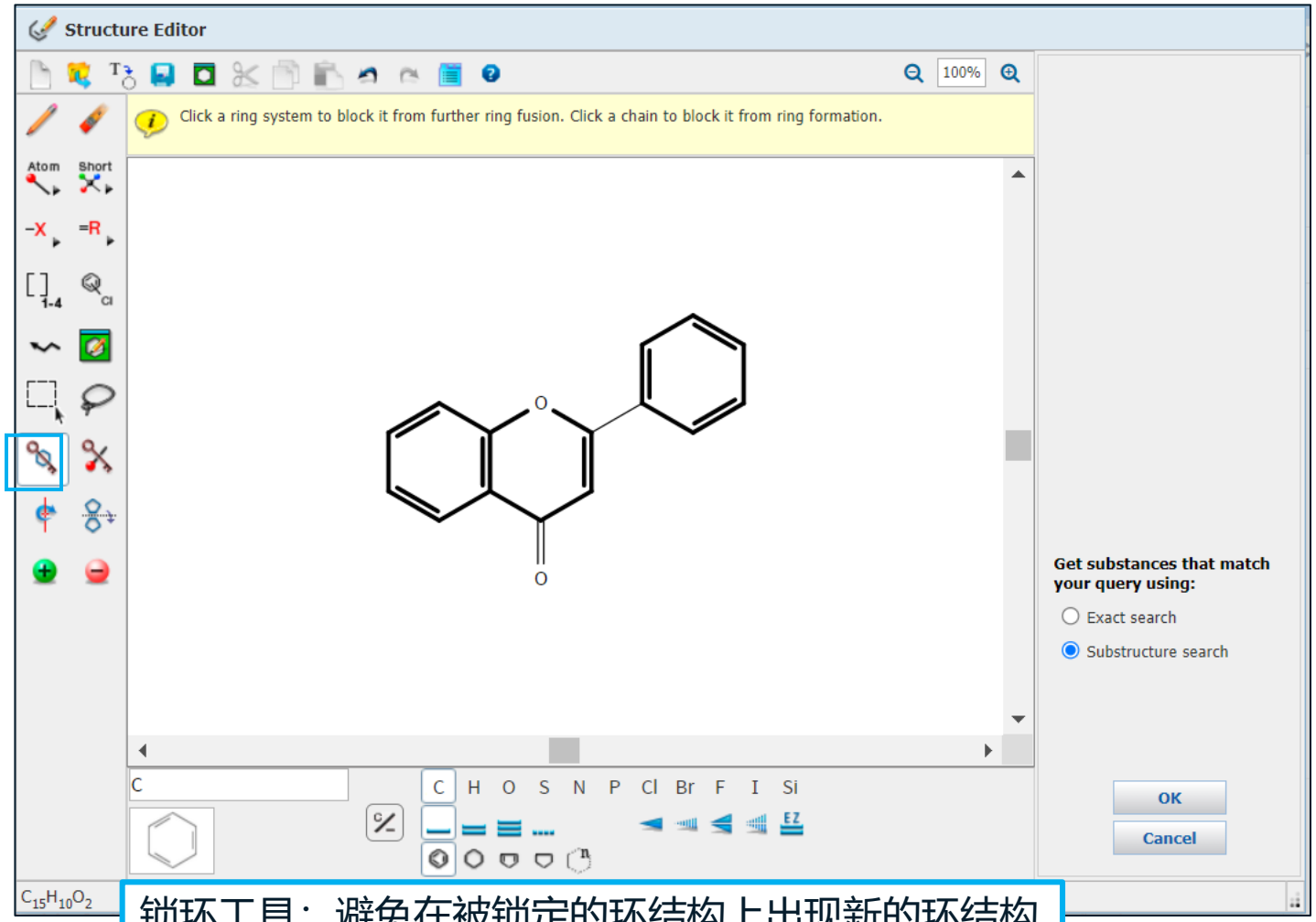
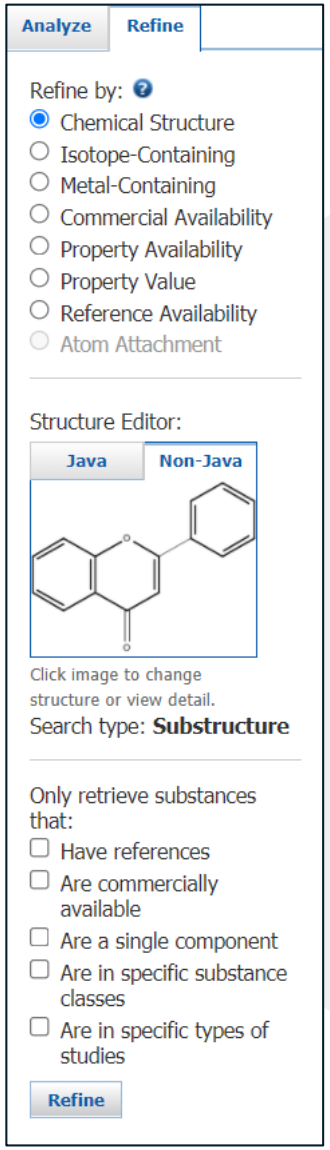
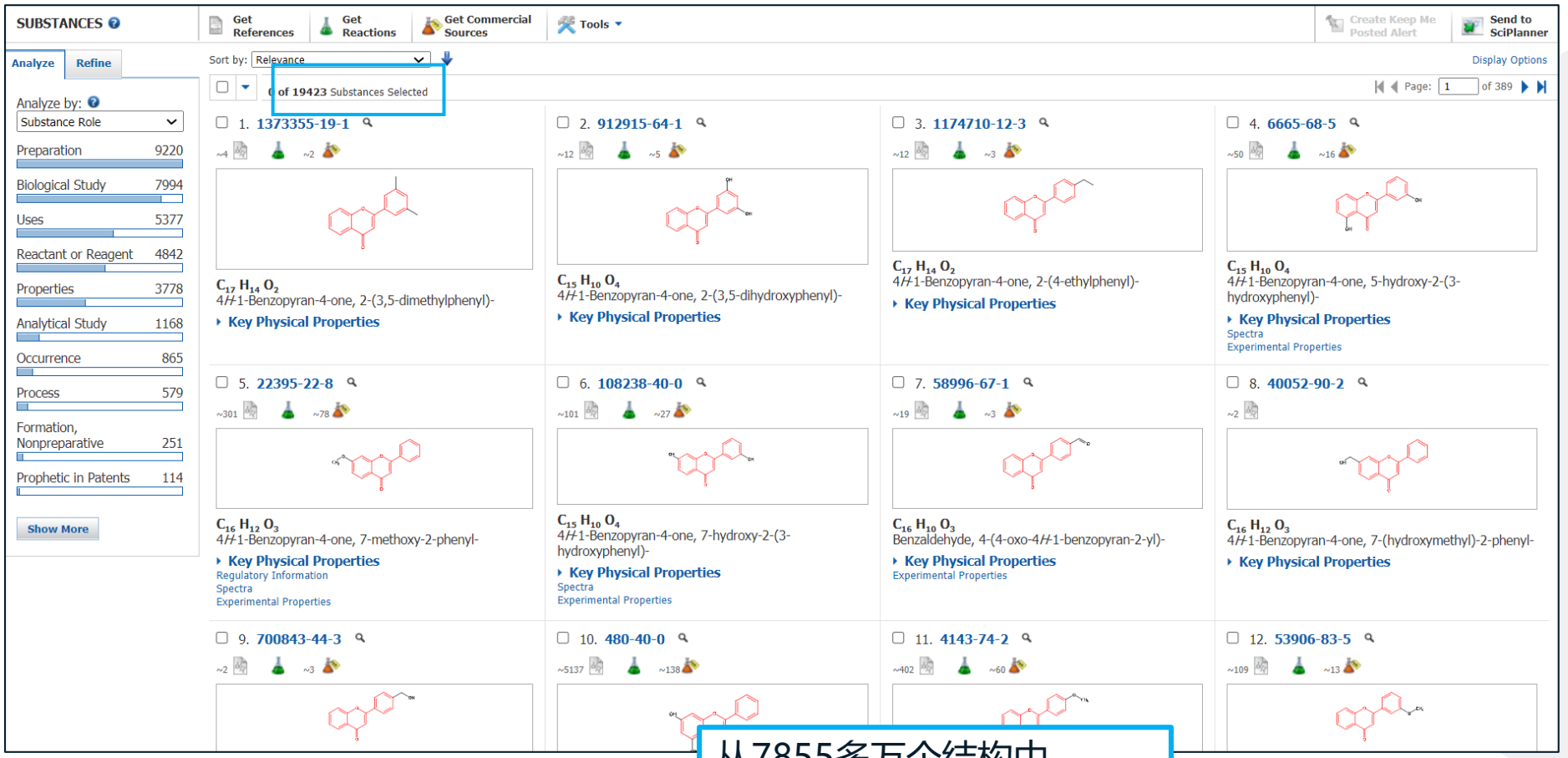
物质结果集的筛选--Refine



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多万个结构中

筛选出19423个黄酮类物质

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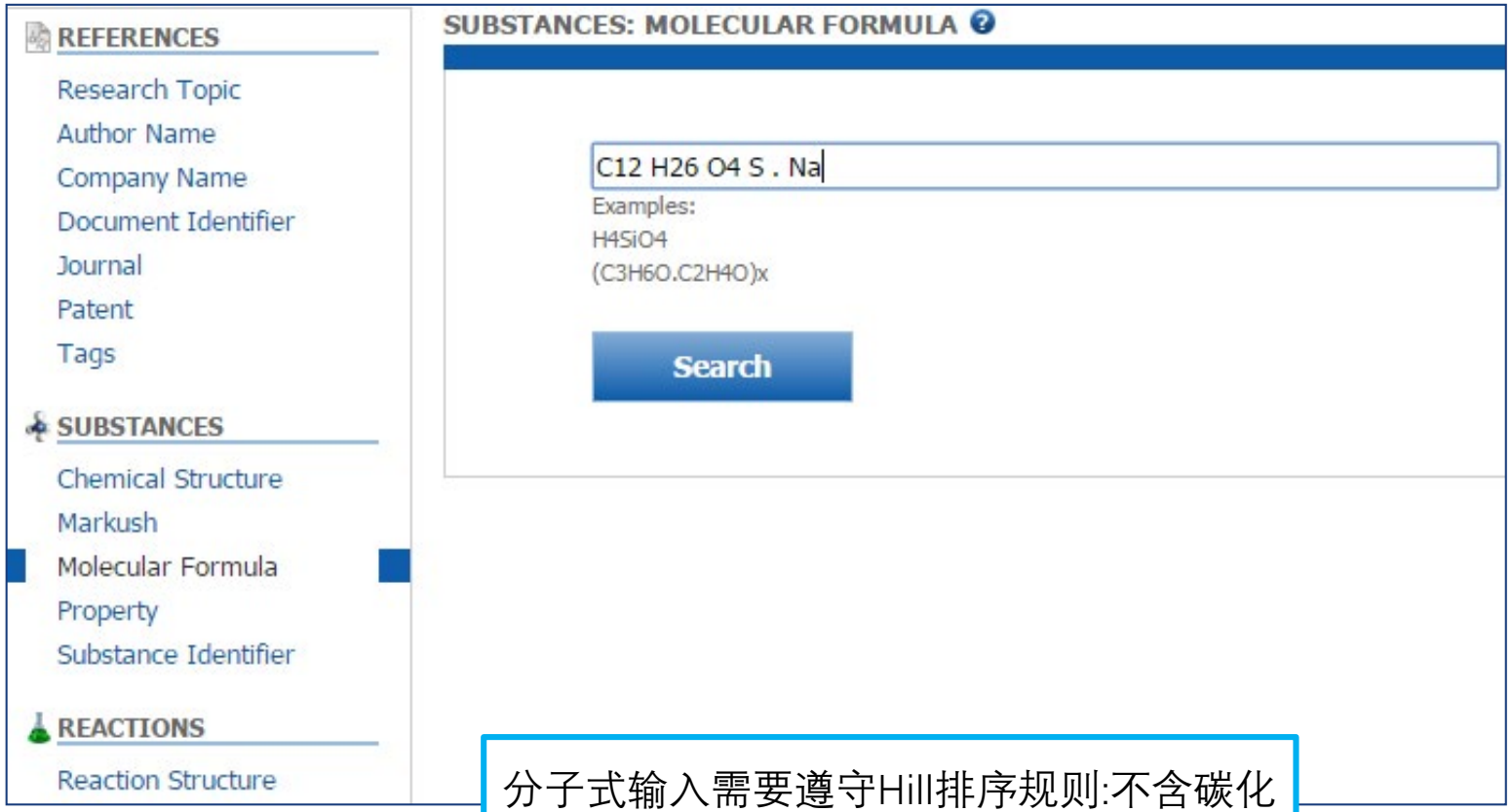
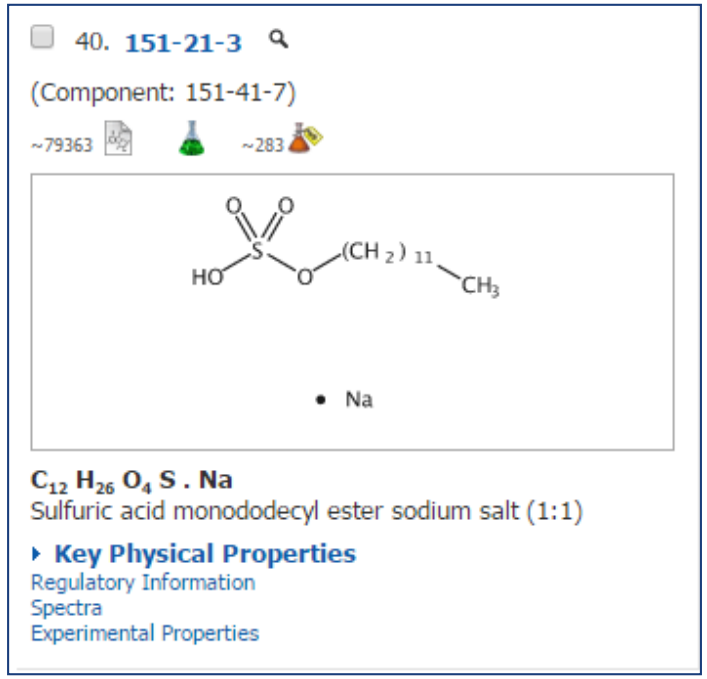
物质检索--分子式检索



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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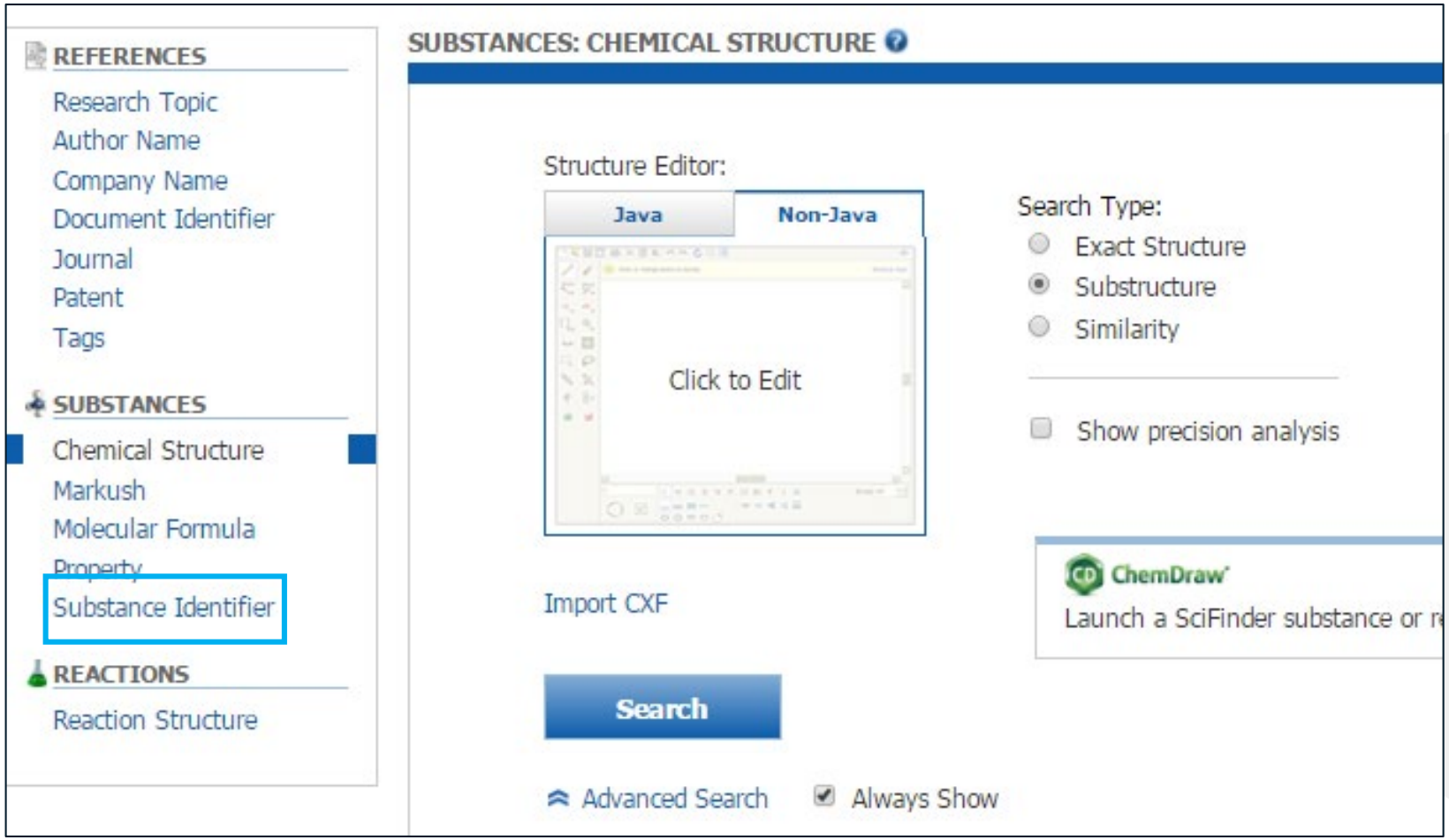
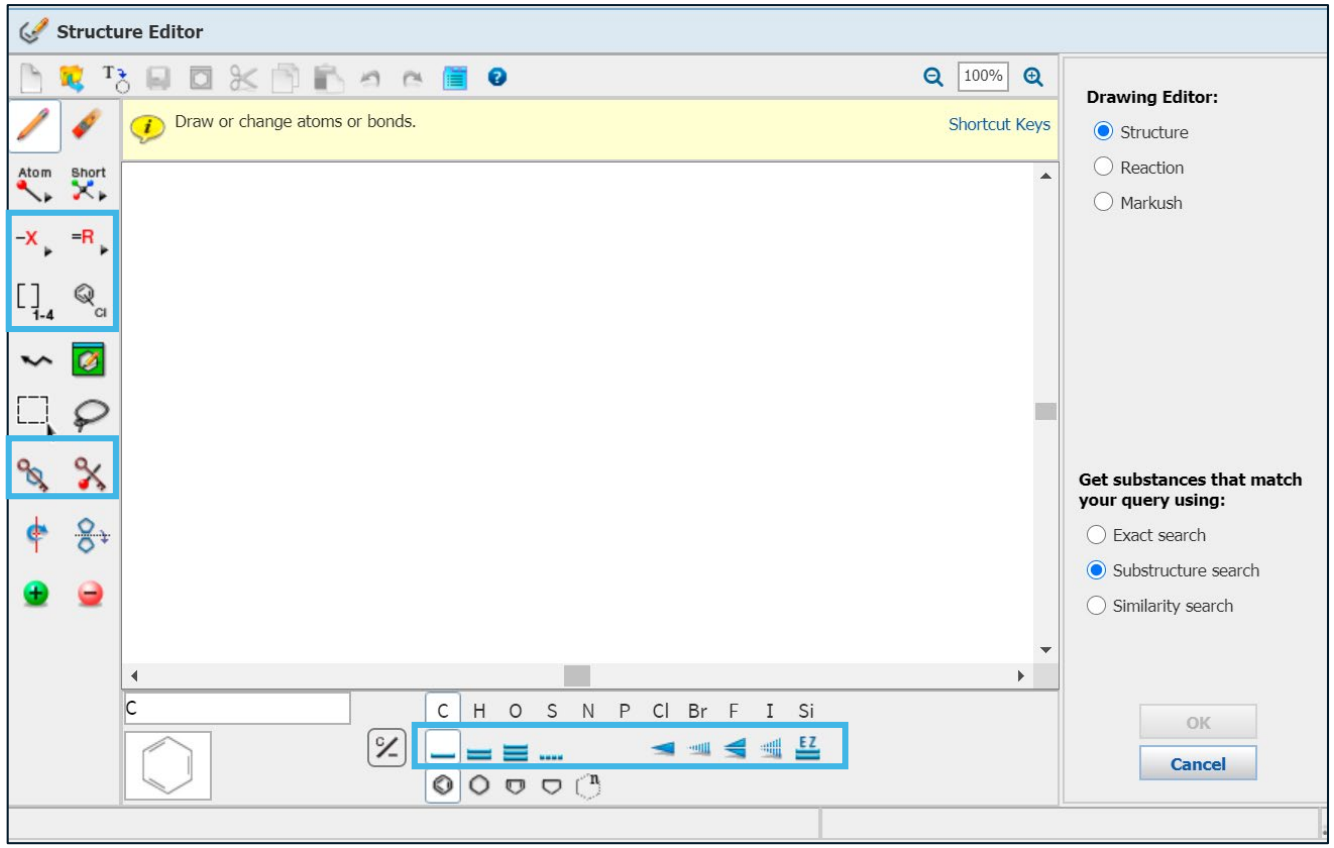
物质检索--结构式检索



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

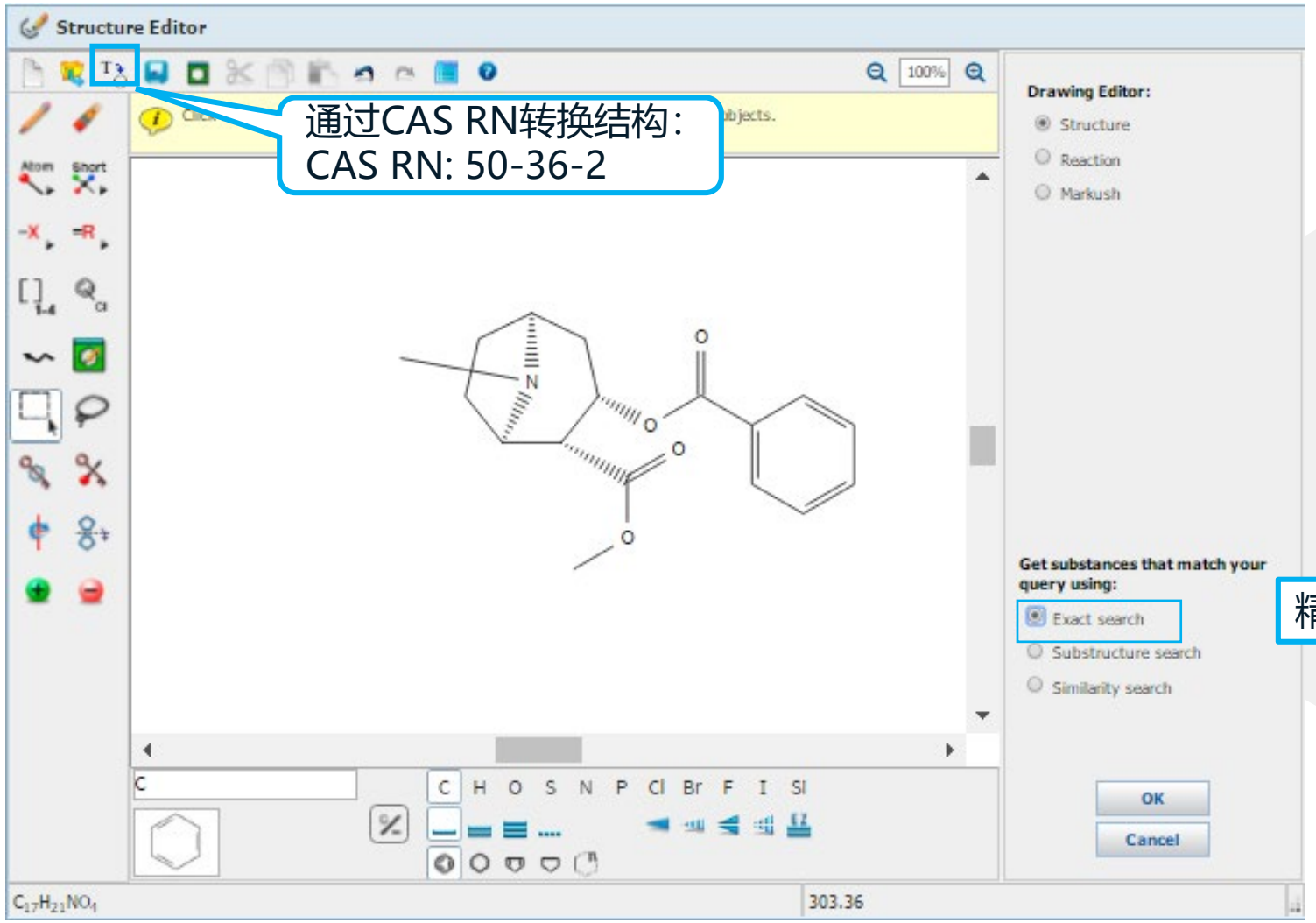
重复工具

取代位置可变

锁环工具

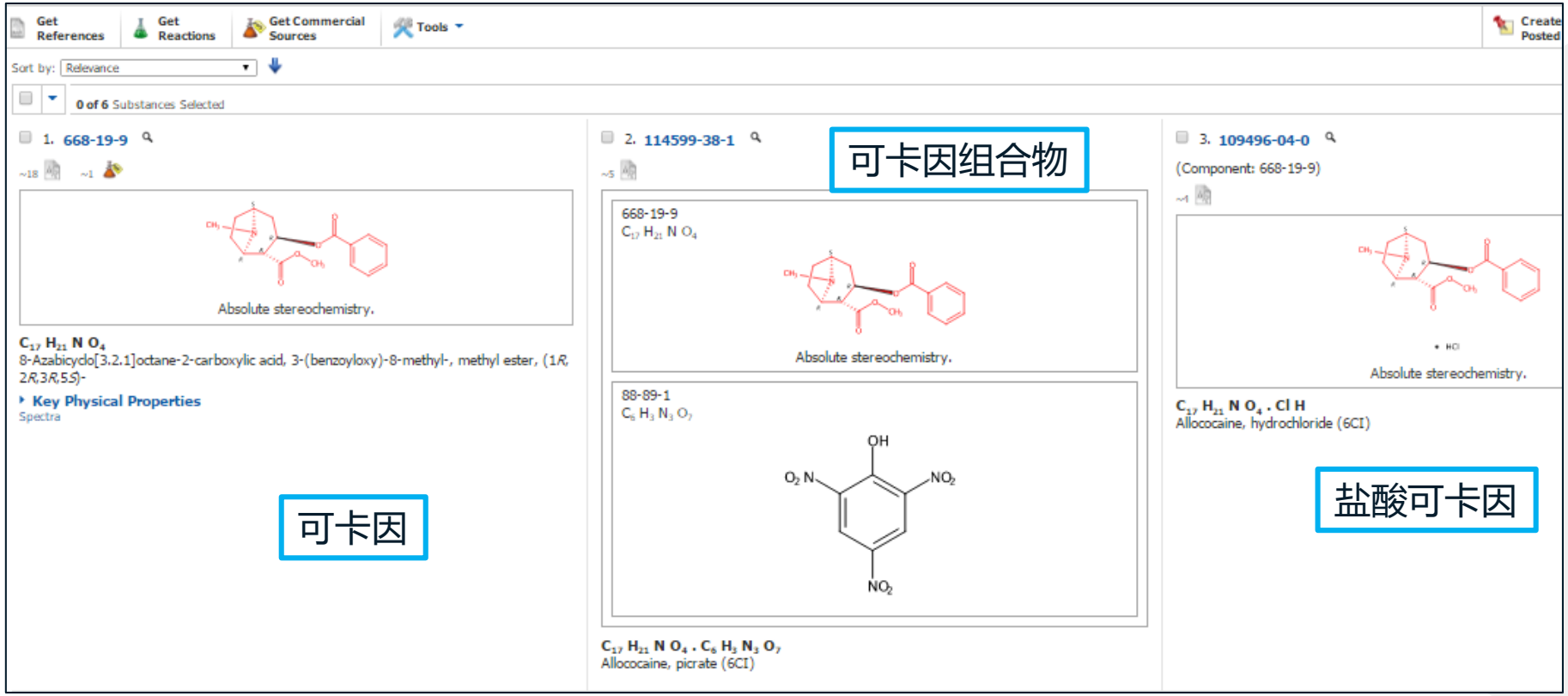
锁原子工具

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

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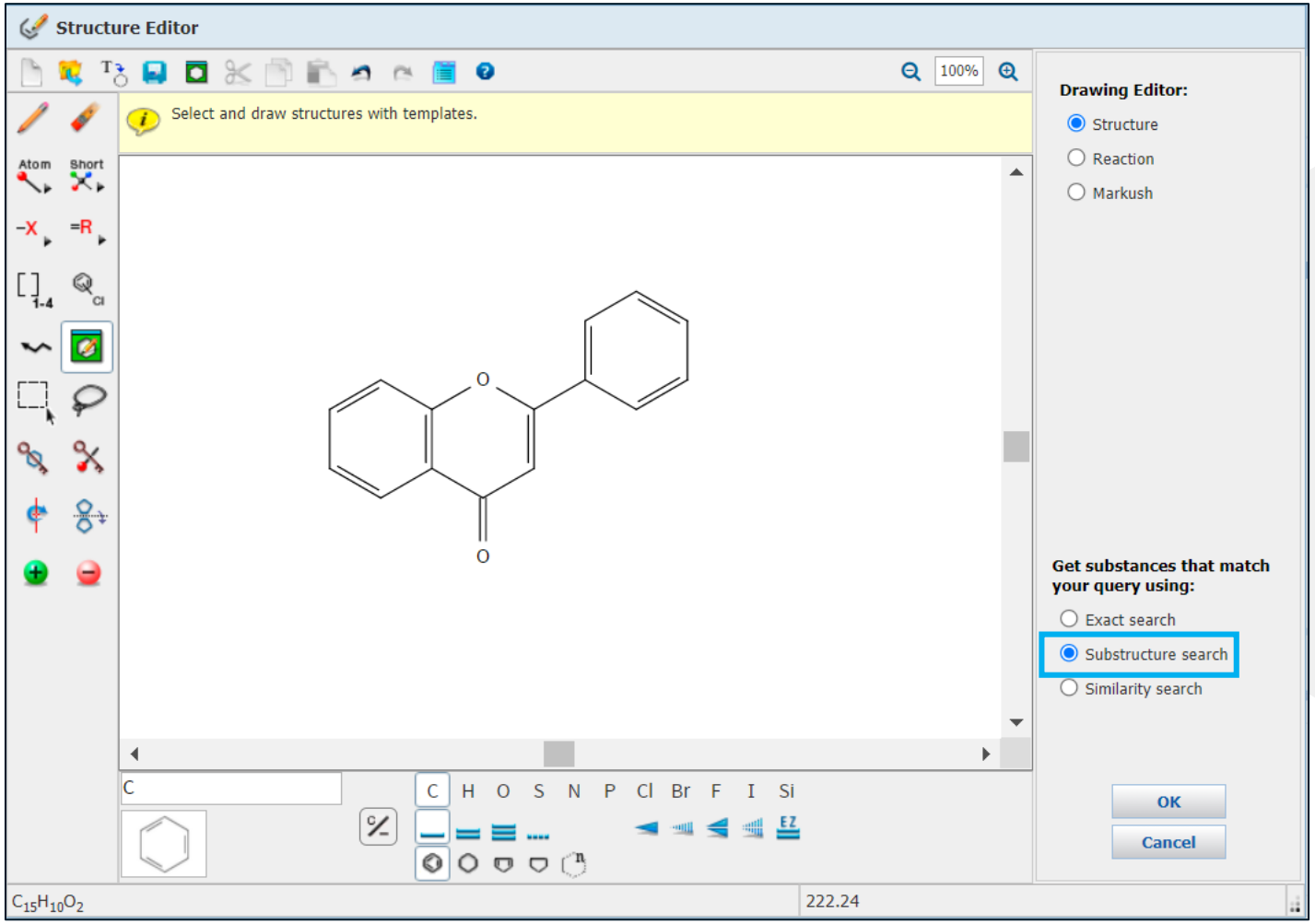
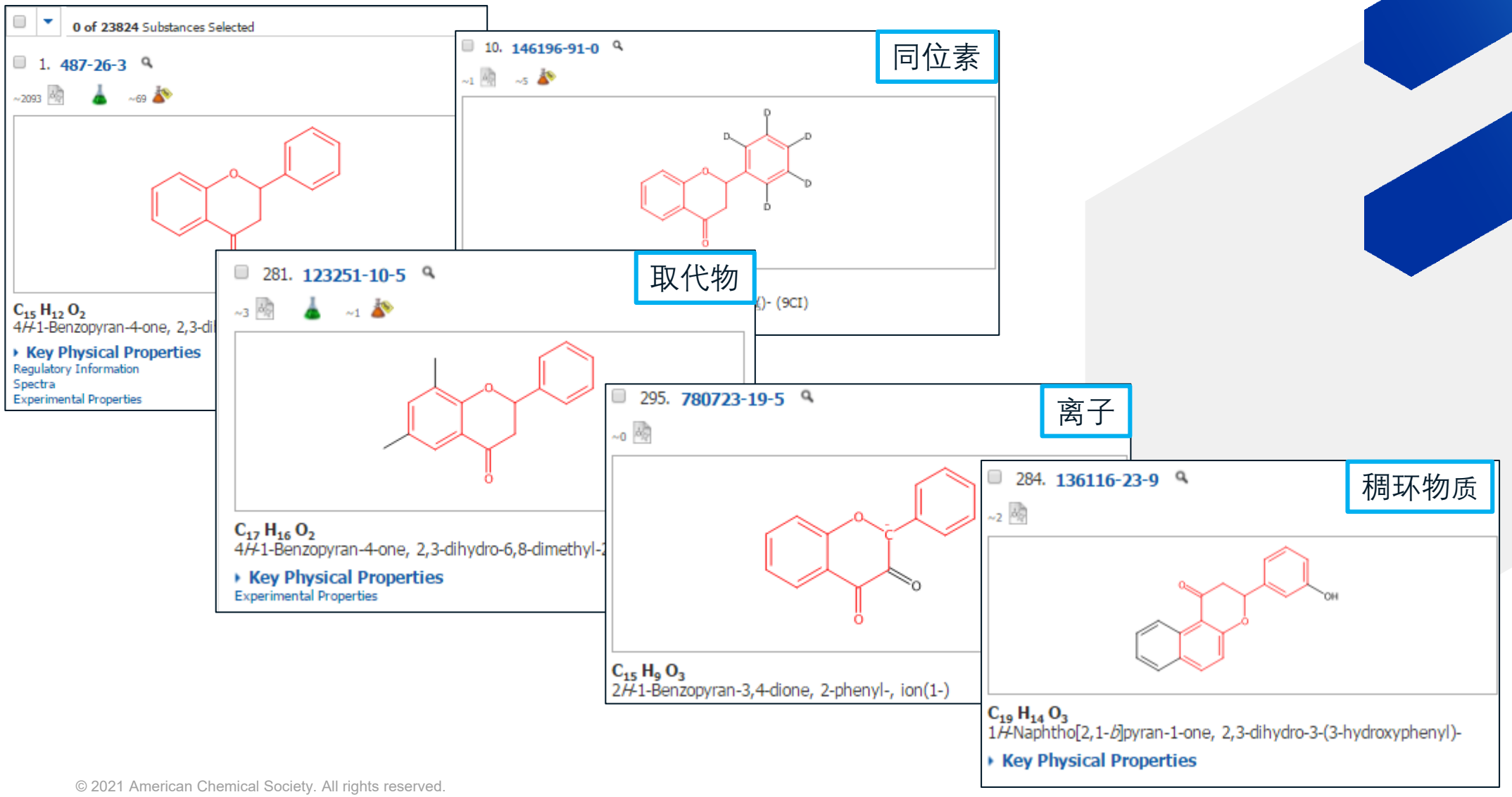
物质检索--亚结构检索



物质检索--亚结构检索结果集



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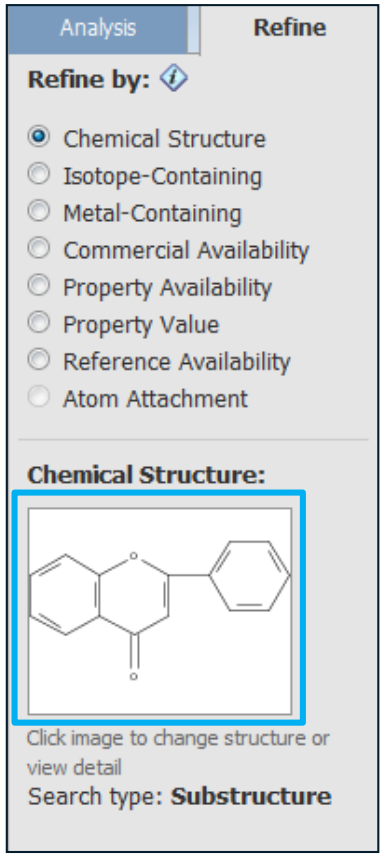
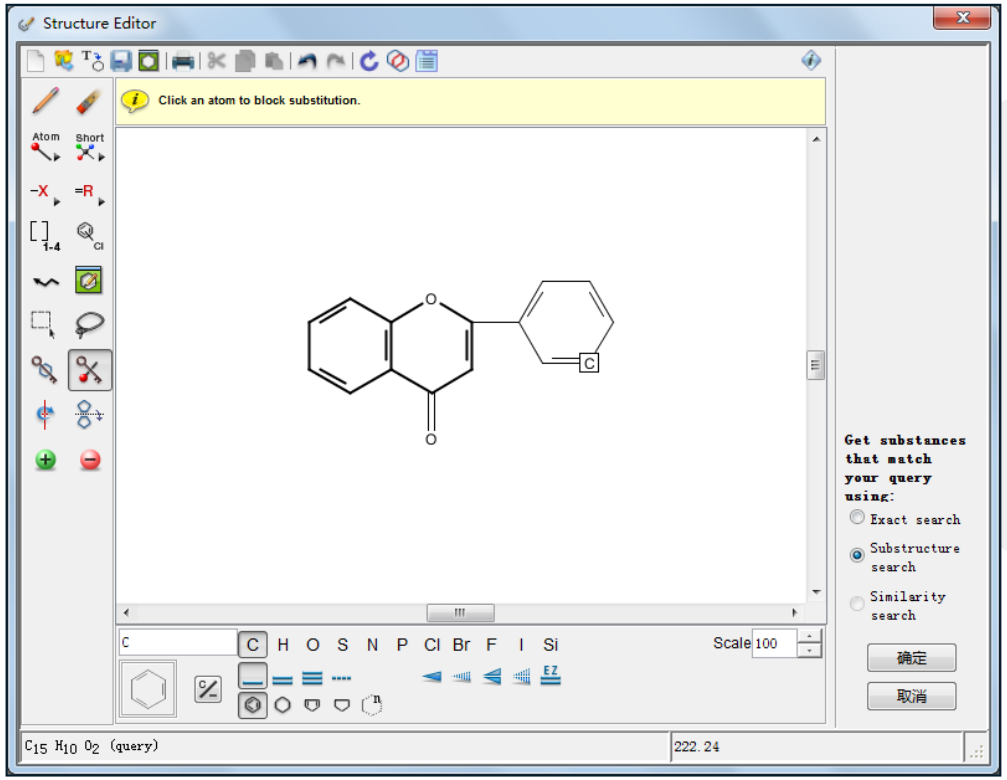
物质检索--亚结构检索结果集的限定



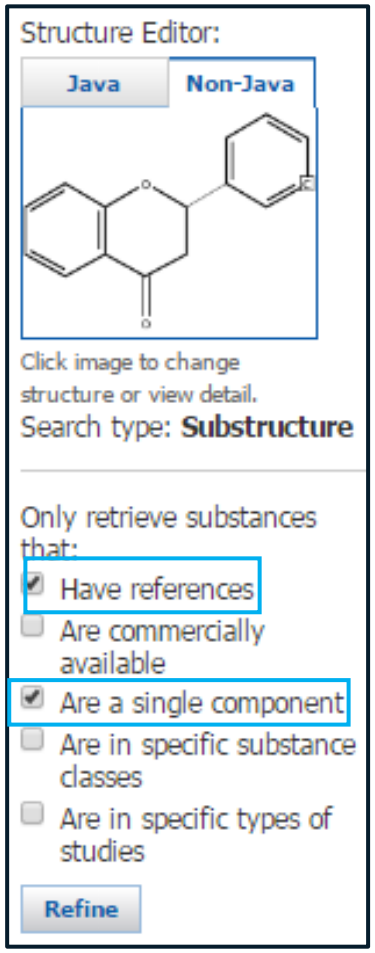
化学结构的再次限定

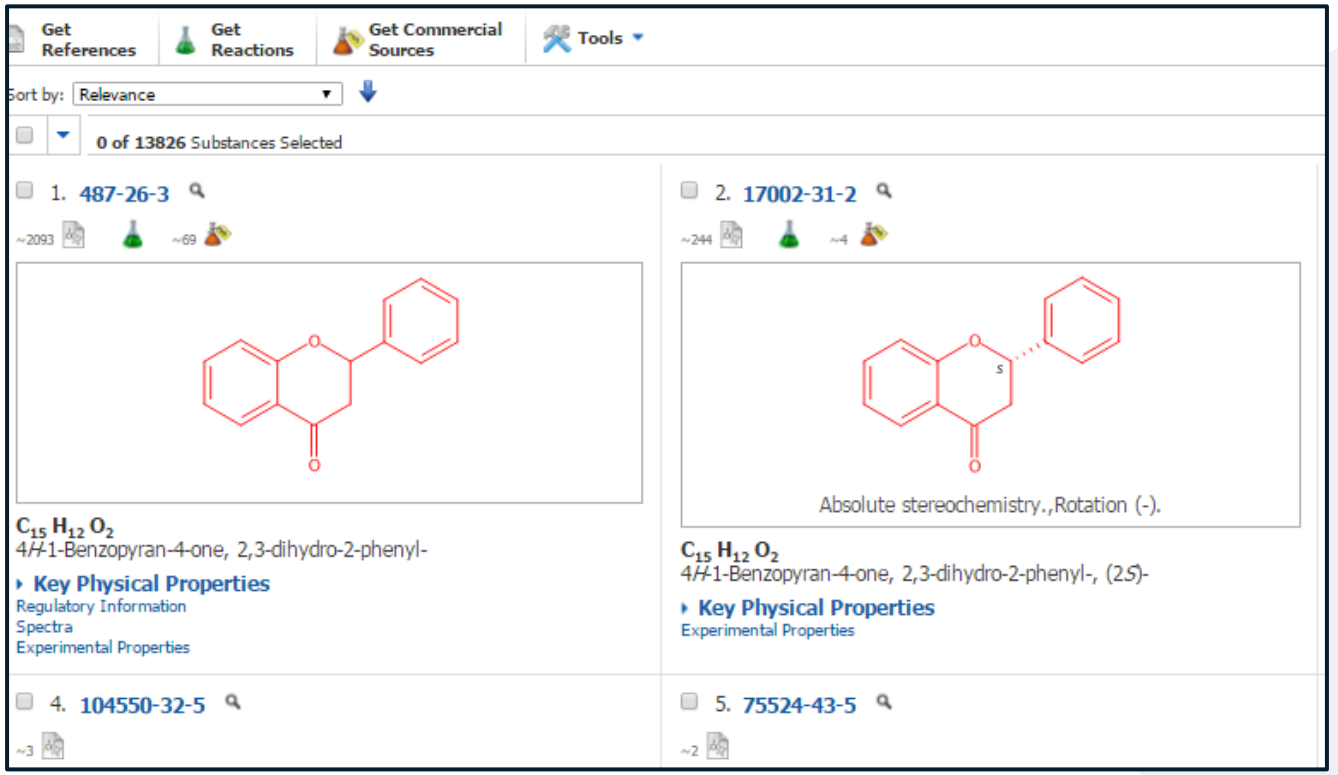


环锁定

原子锁定

物质检索--亚结构检索结果集的限定

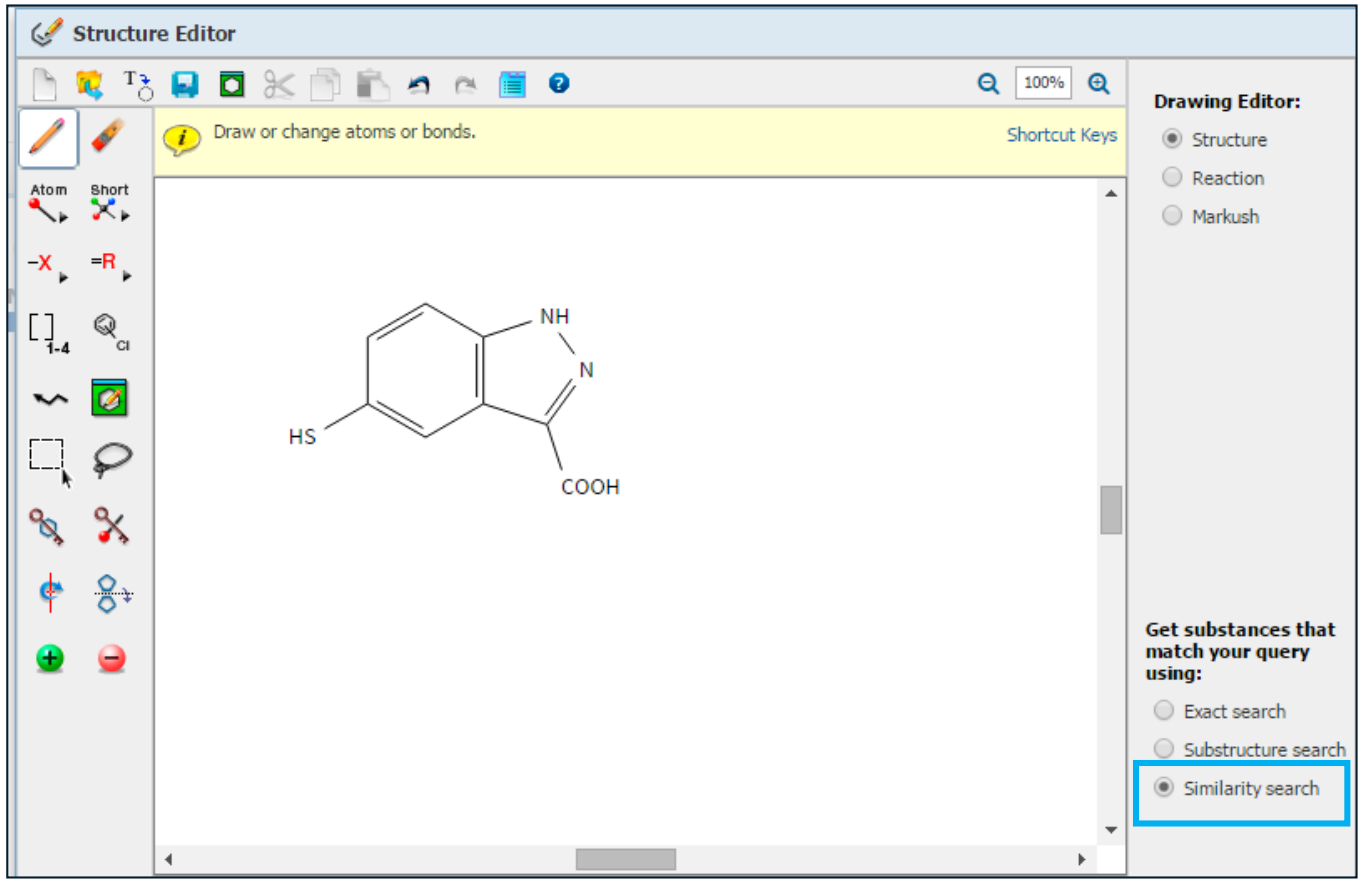




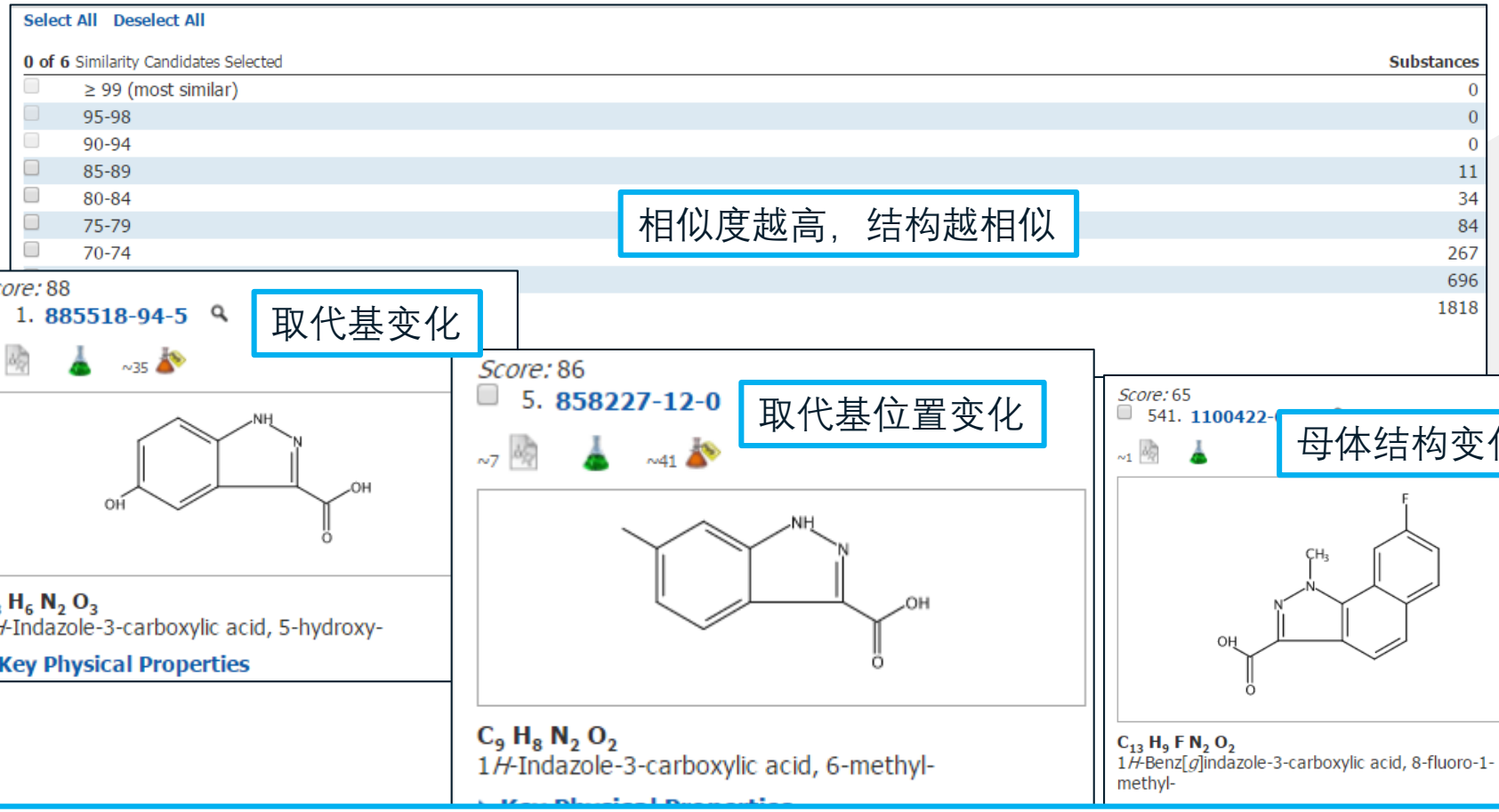
亚结构检索：

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



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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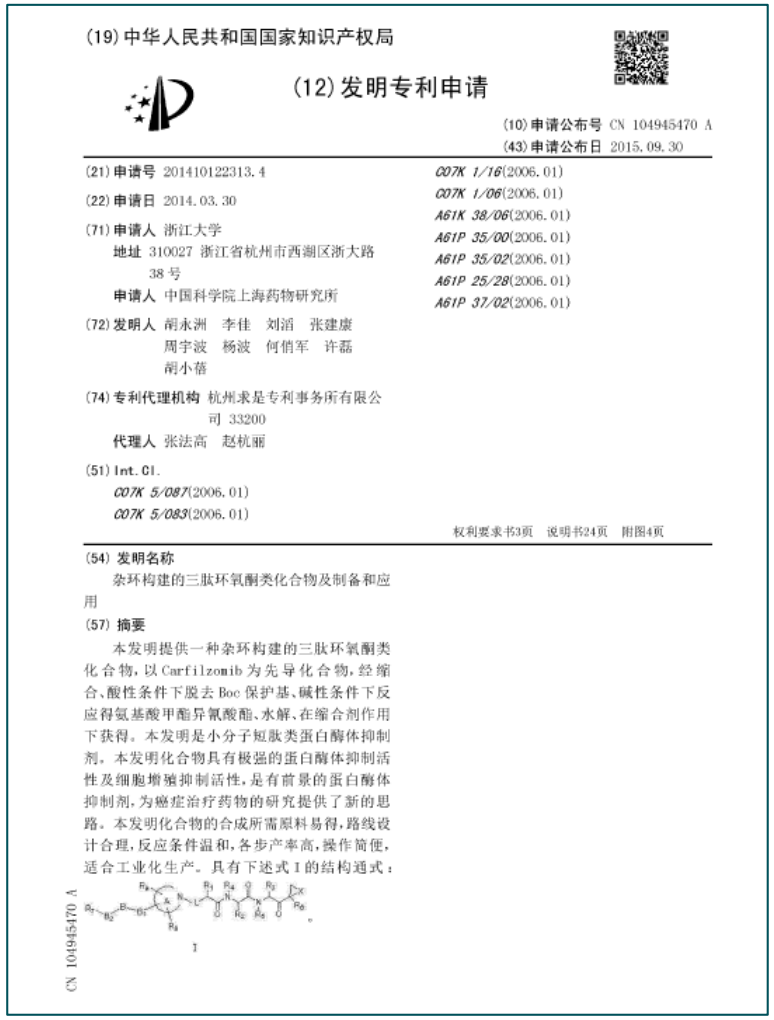
CAS Markush检索



(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.
C07K 5/087(2006.01)
C07K 5/083(2006.01)
C07K 1/16(2006.01)
C07K 1/06(2006.01)
A61K 38/06(2006.01)
A61P 35/00(2006.01)
A61P 35/02(2006.01)
A61P 25/28(2006.01)
A61P 37/02(2006.01)

权利要求书3页 说明书24页 附图4页

(54)发明名称

杂环构建的三肽环氧酮类化合物及制备和应用

(57)摘要

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

I

CN 104945470 A

具体实施方式

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

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

将1-(叔丁氧羰基)哌啶-4-甲酸(2.75g,12mmol)置于50mL三颈瓶中，N_2保护下加入25mL无水CH_2Cl_2，然后缓缓滴入吡啶(2.5mL,30mmol)和二氯亚砜(1.1mL,14mmol)，该反应液置于室温反应半小时。随后，2-氨基吡嗪(0.95g,10mmol)和三乙胺(5.7mL,40mmol)溶于15mL CH_2Cl_2后缓缓滴入上述反应液，室温反应6小时。反应液加30mL饱和食盐水稀释，分出有机层，水层CH_2Cl_2提取(15mL×3)，合并有机层，无水硫酸钠干燥后减压除去溶剂，柱层析分离得白色固体2.3g，收率74%。m.p.：134-136℃；^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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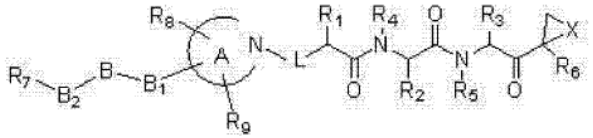
CAS Markush检索

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

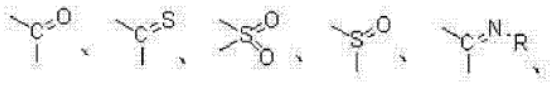
其中：

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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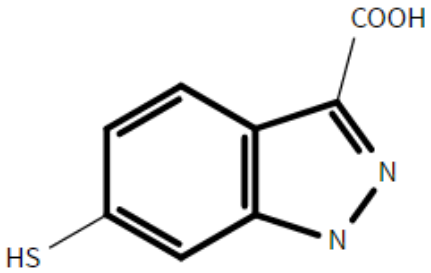
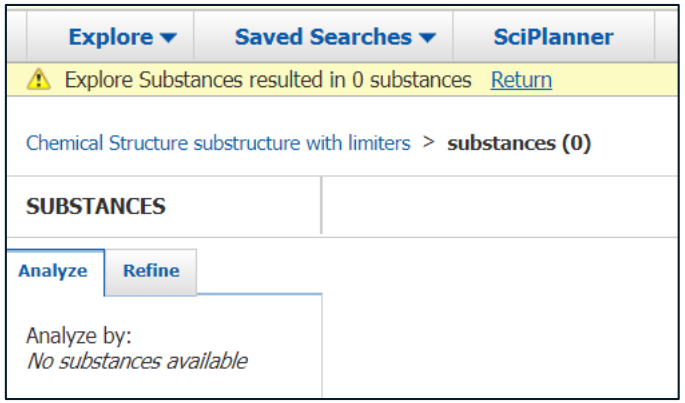
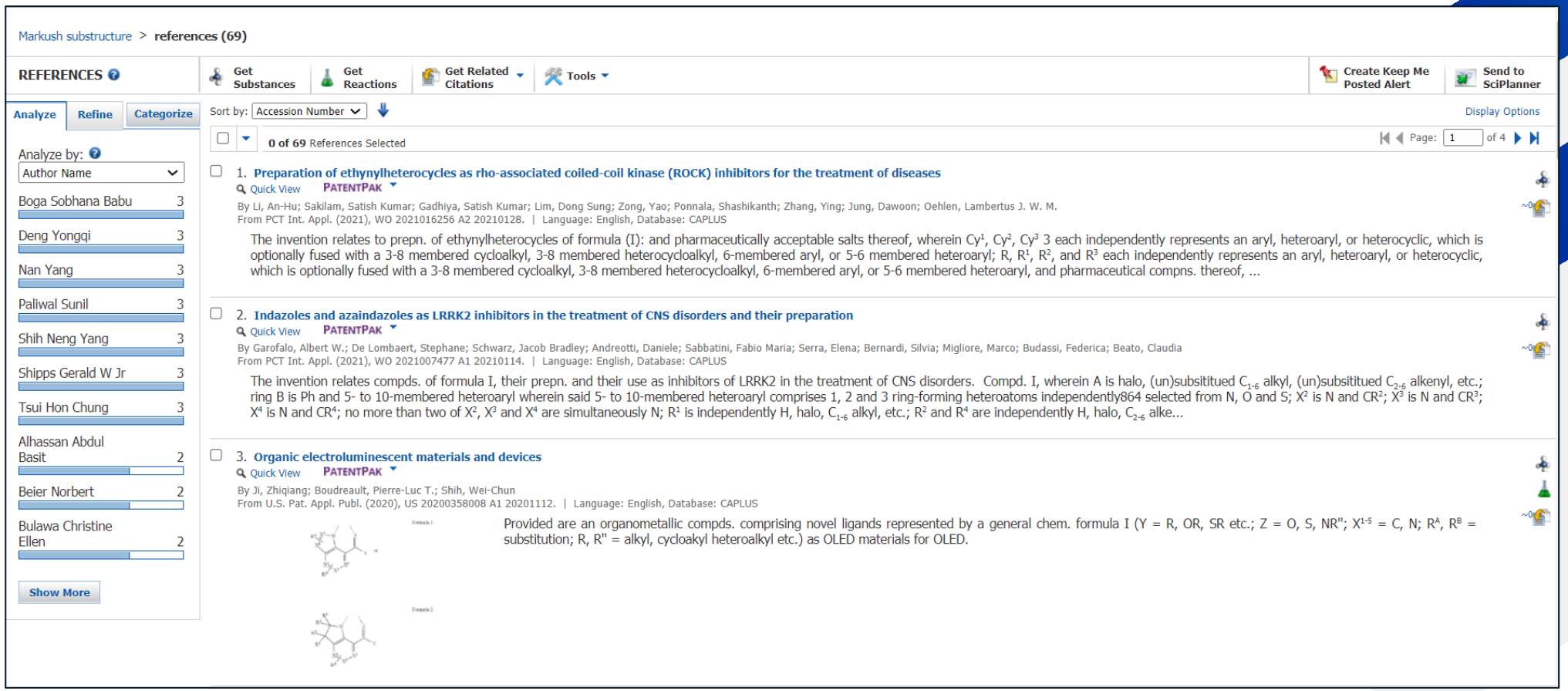
CAS Markush检索





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

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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
- 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、筛选及详情

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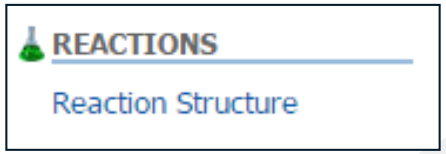
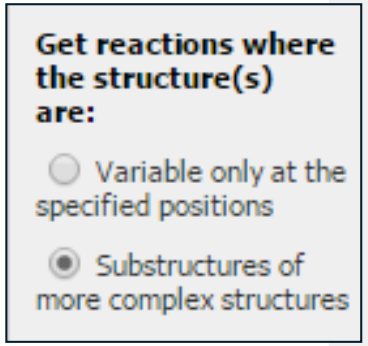
CAS SciFinder检索--反应检索

- 反应检索方法
  - 结构式



- 常用获取方法
  - 已知物质：由物质获取反应
  - 已知文献：从文献中获取反应
  - 精确结构反应检索
  - 亚结构反应检索



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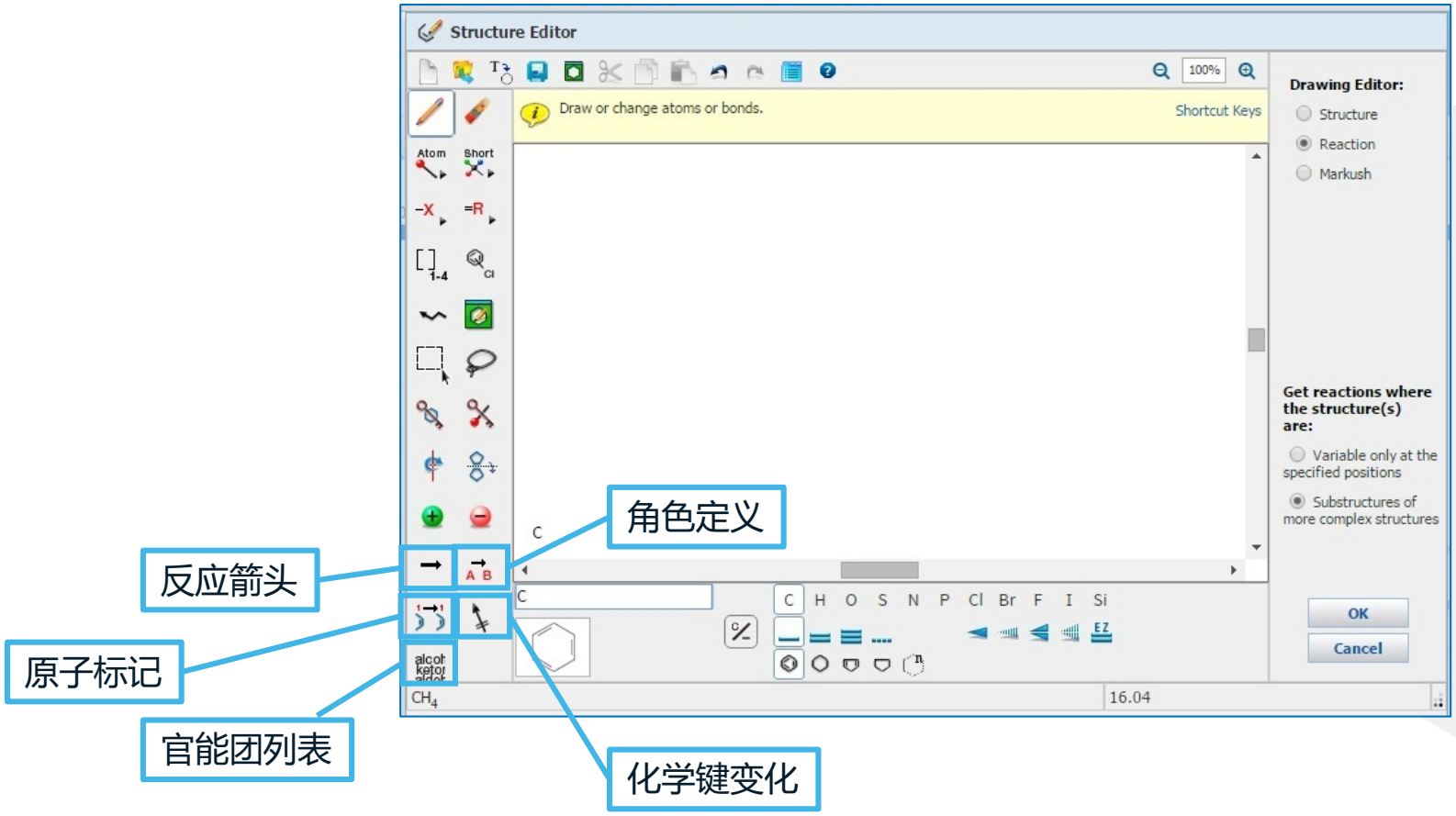
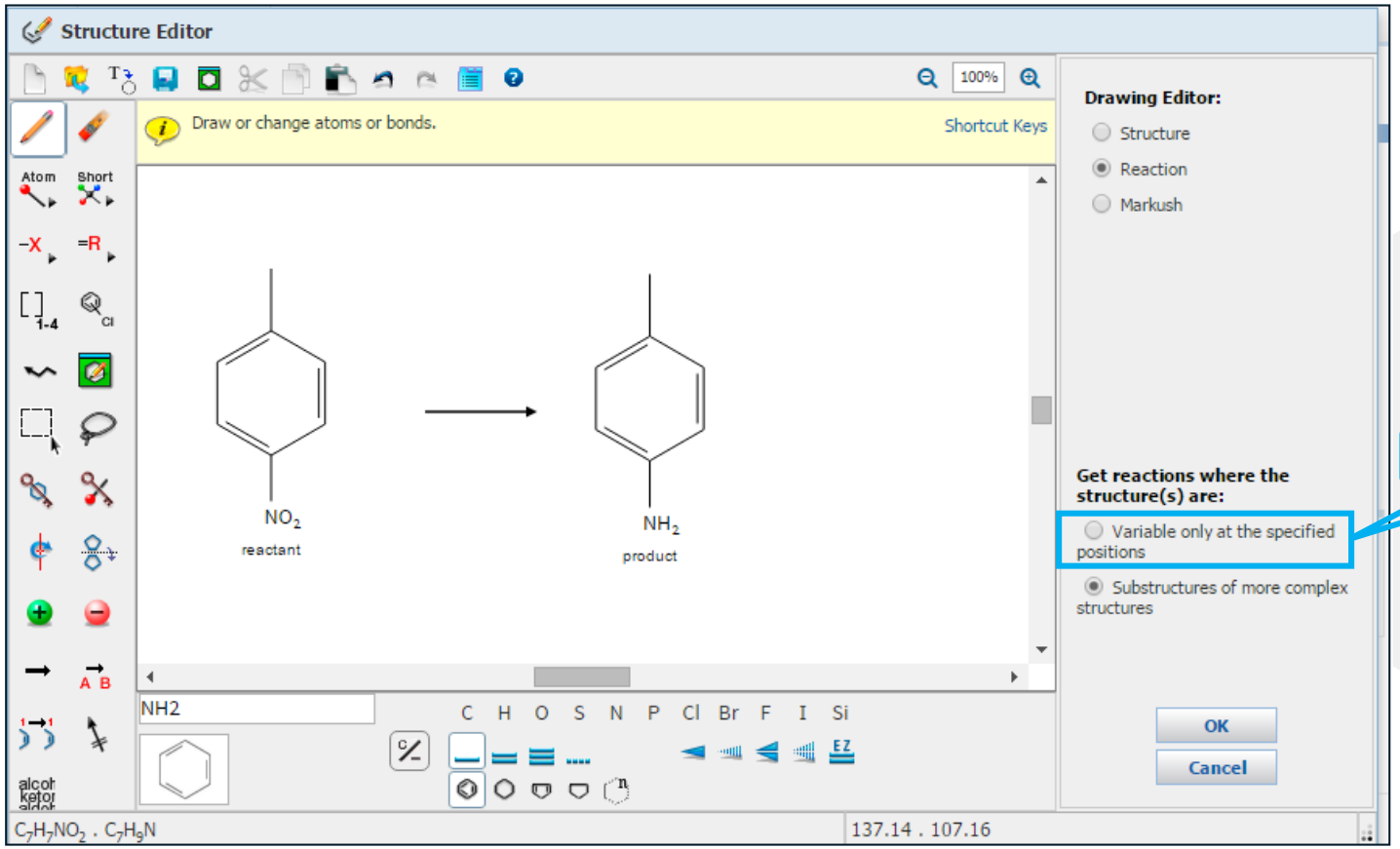
结构编辑器--绘制反应工具



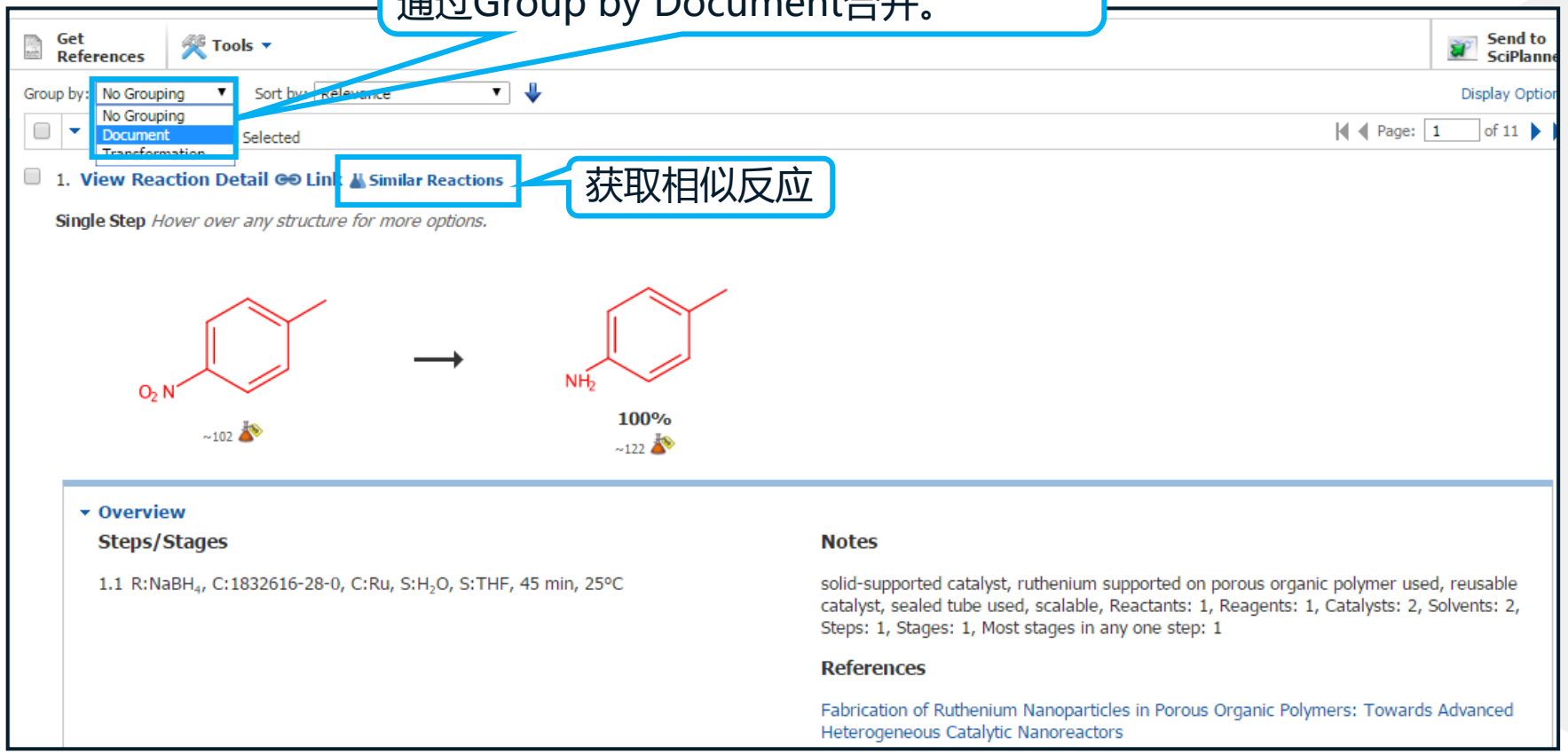
反应检索--精确反应检索



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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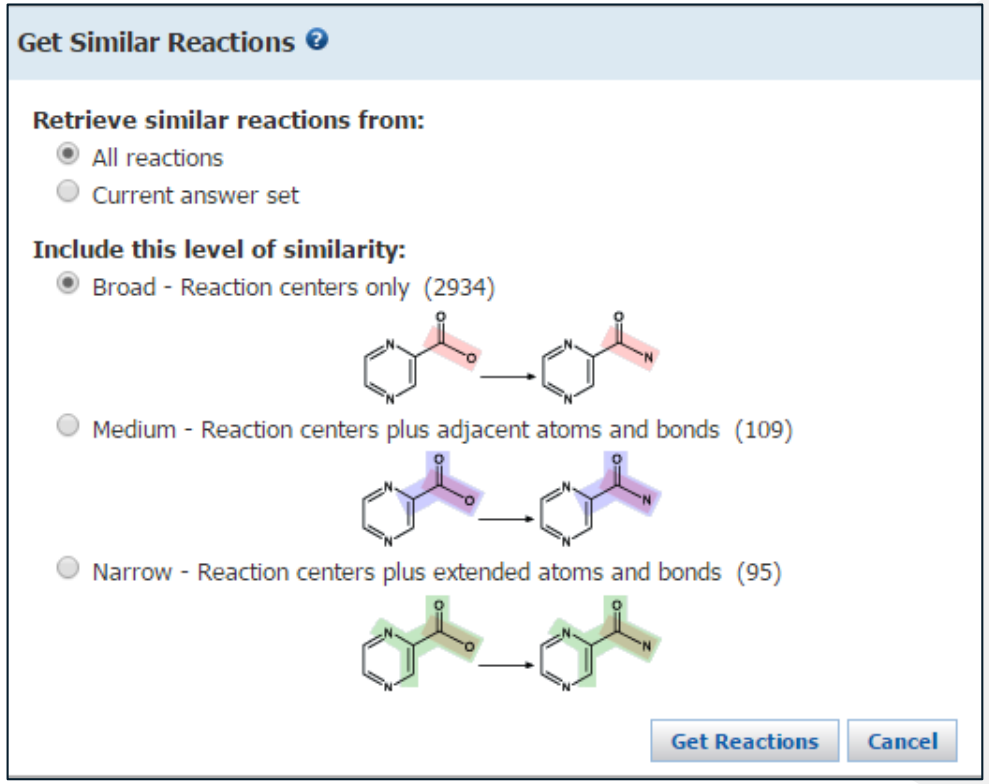
扩展反应检索--获取相似反应

选择相似反应的相似限制：

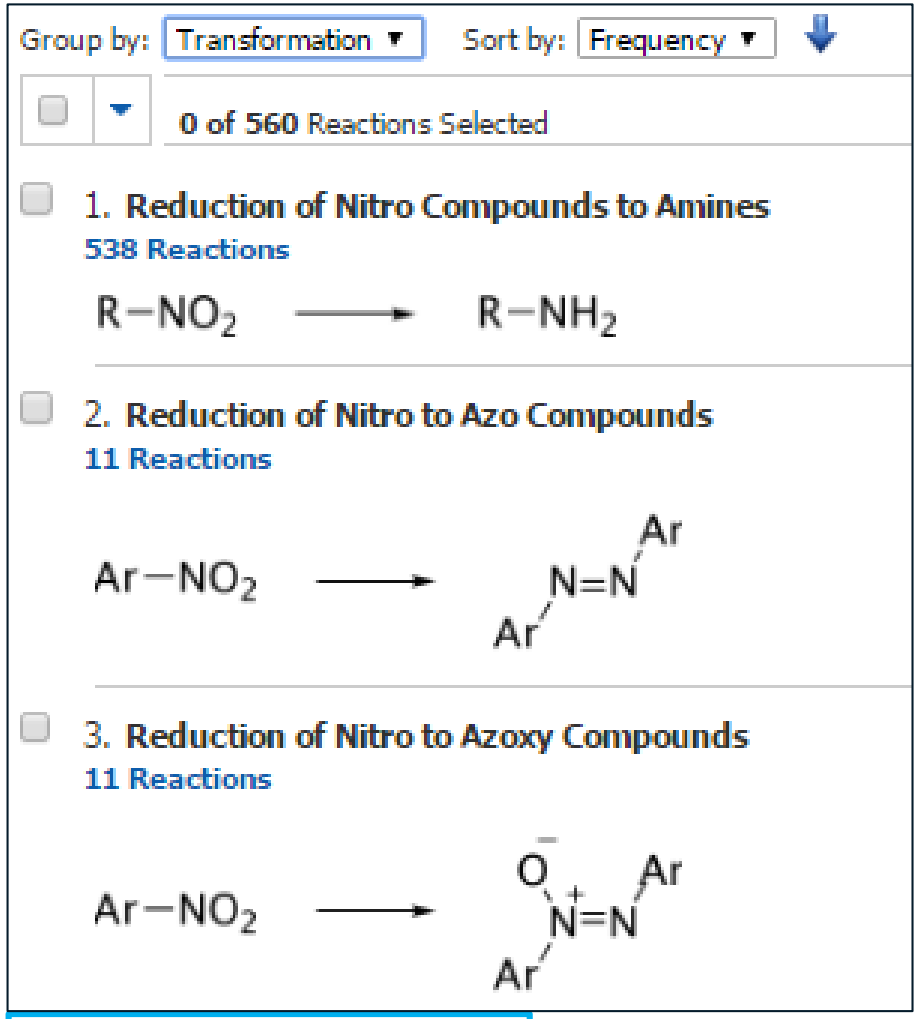
Broad：仅反应中心相似

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



更精确的查找需要的反应

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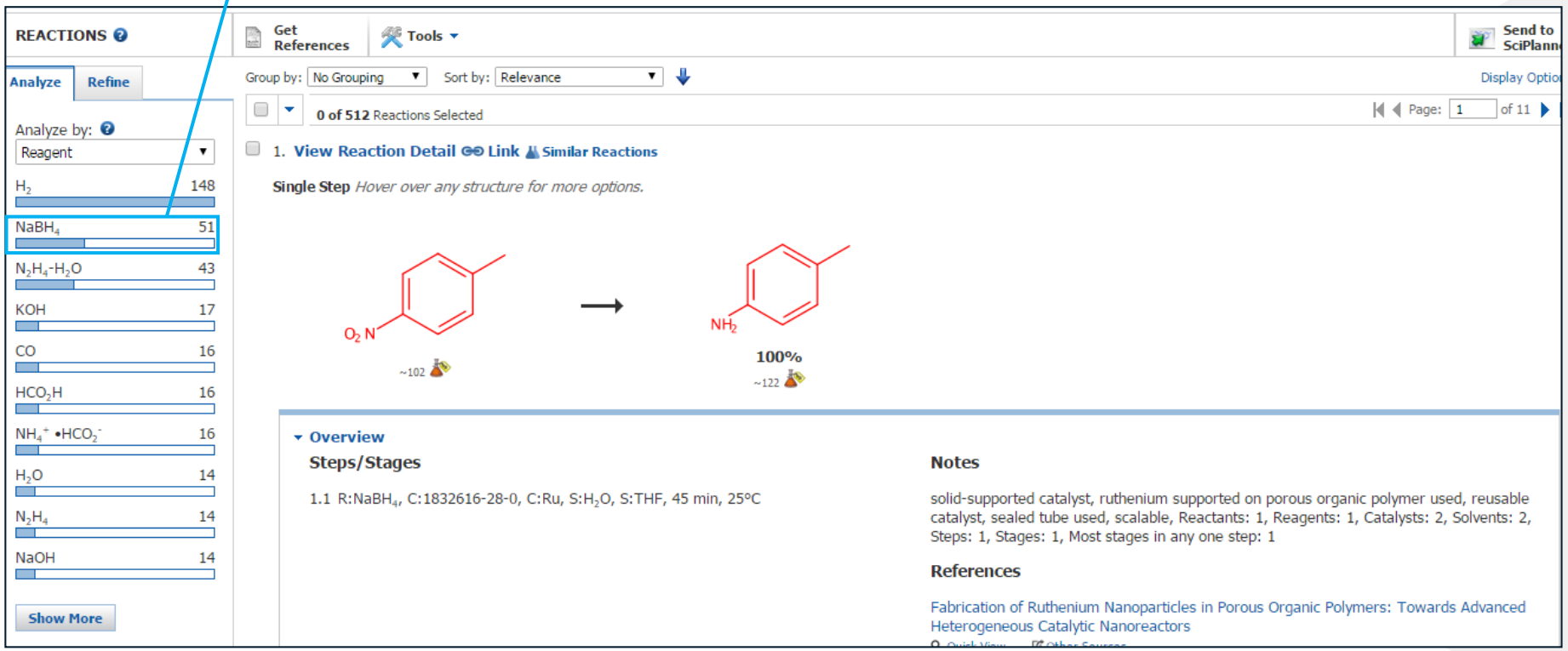
反应检索结果集--筛选

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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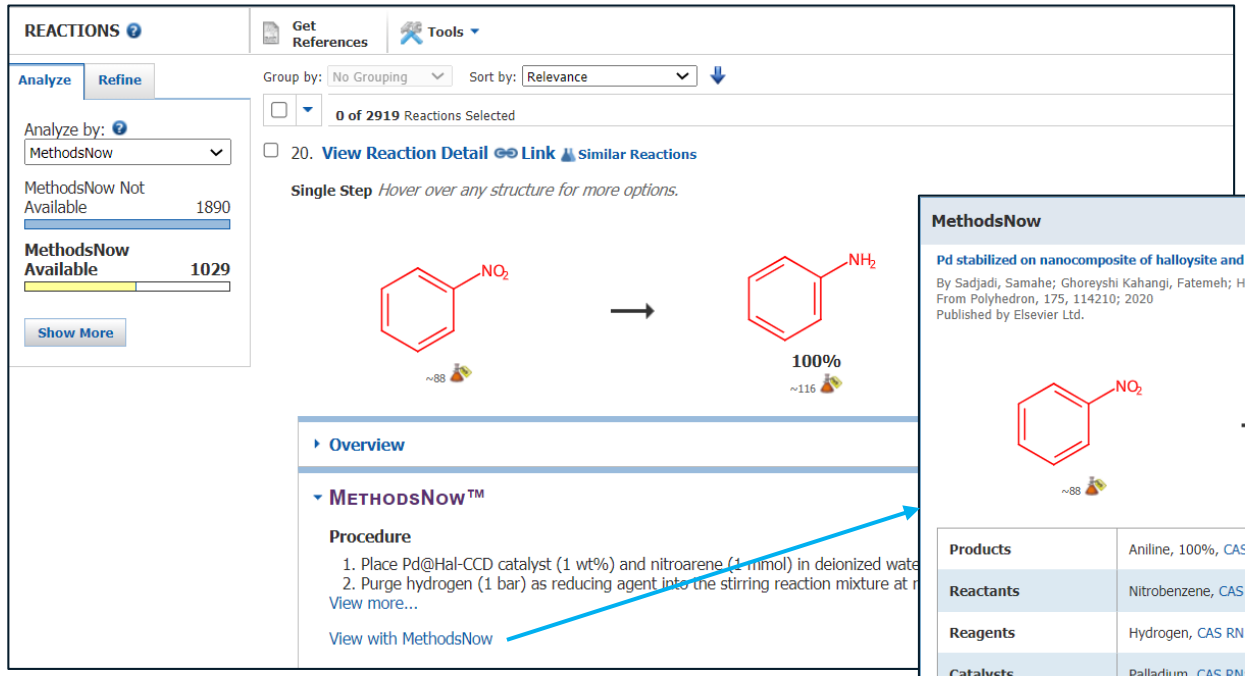
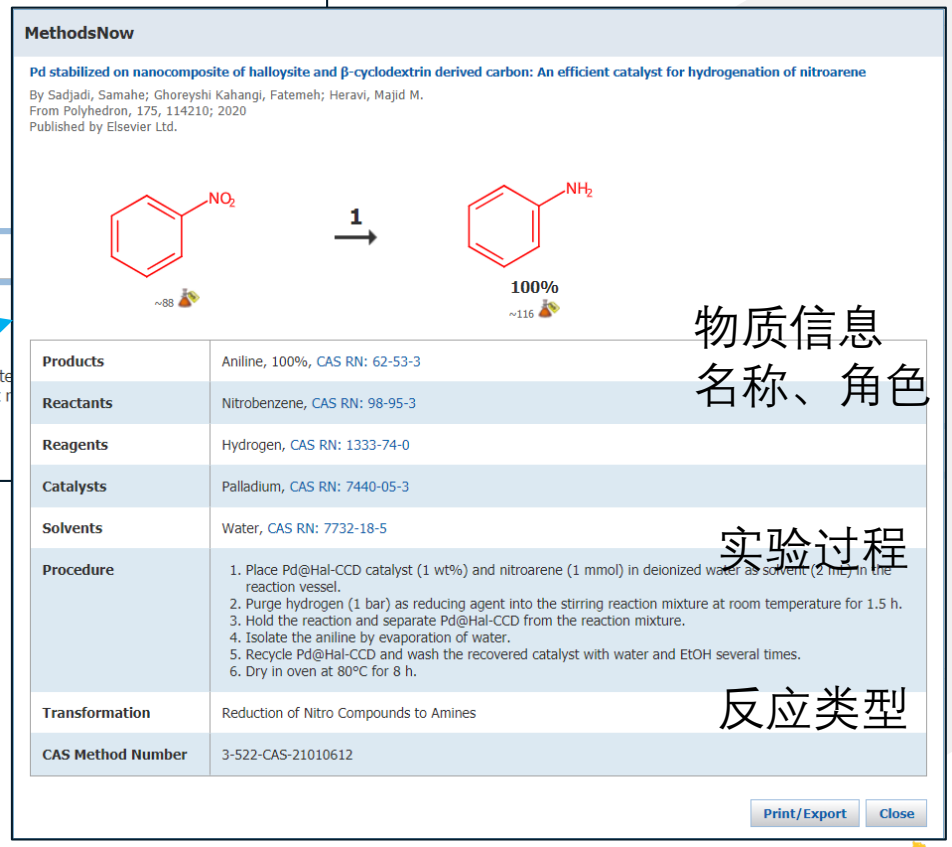
反应检索结果--MethodsNow





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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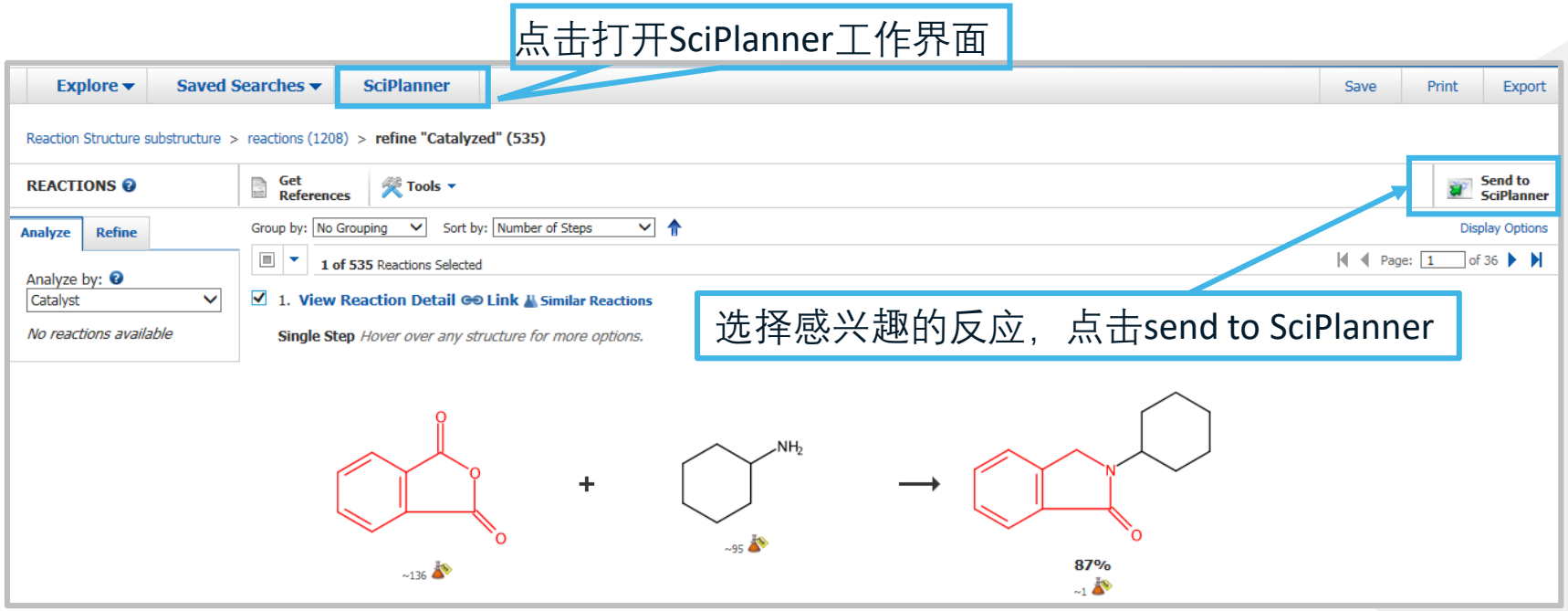
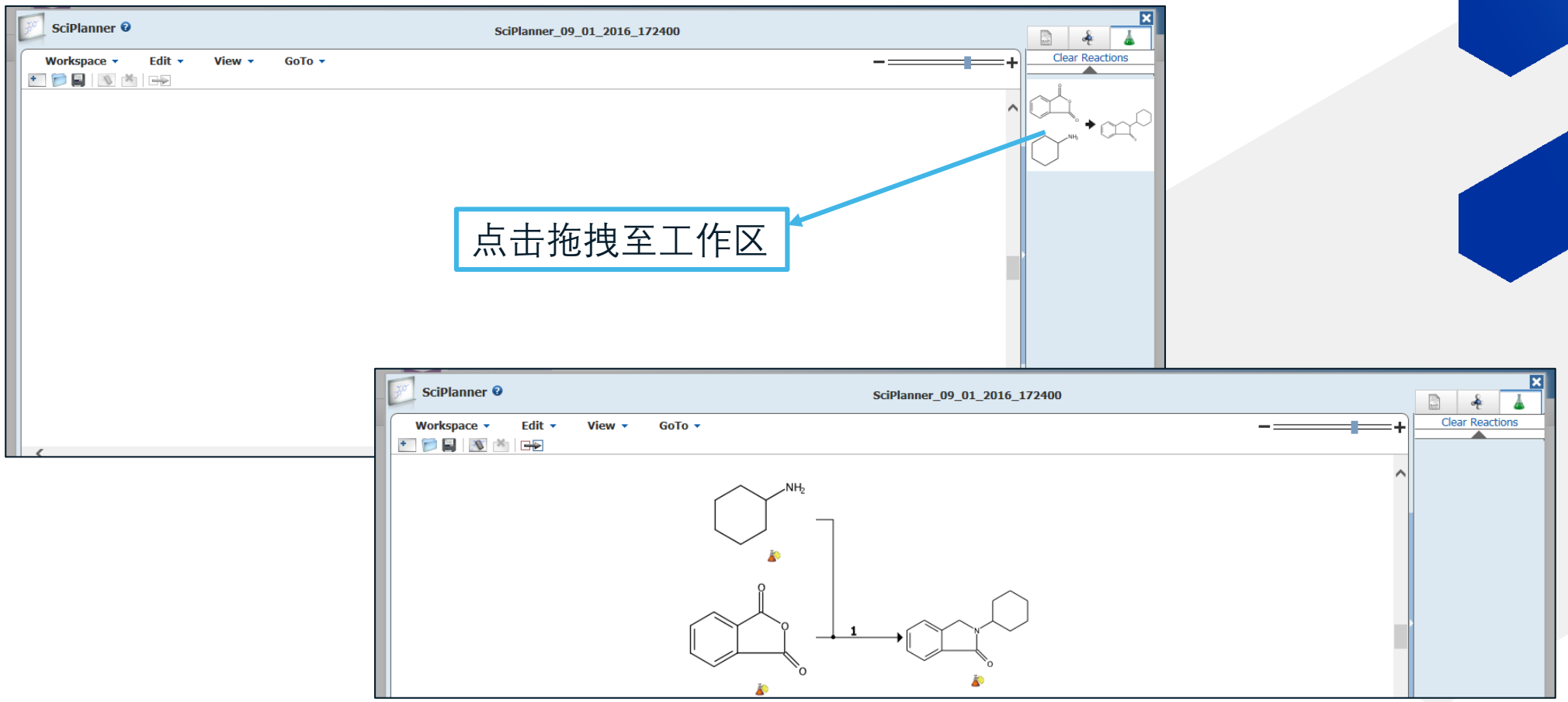
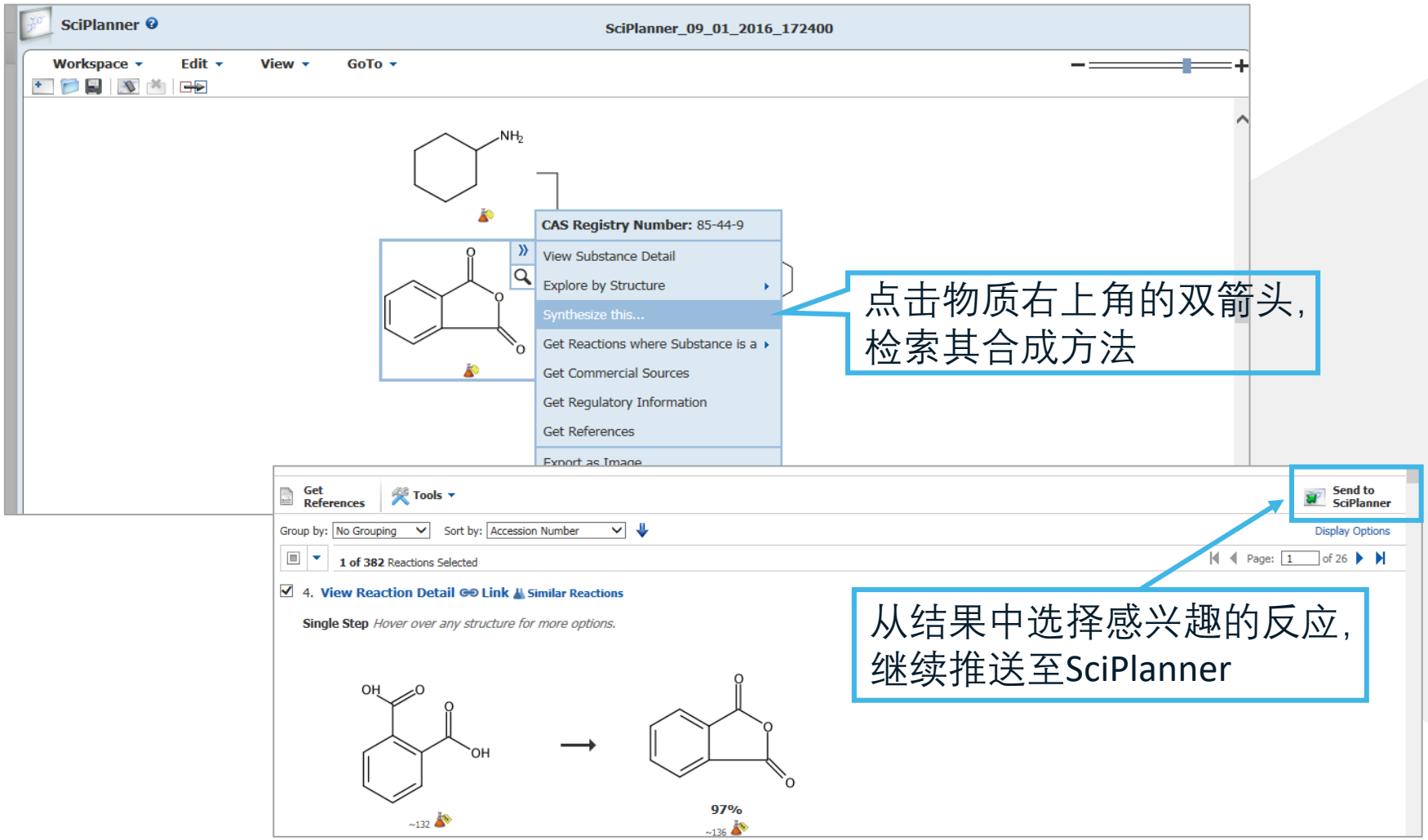
SciPlanner--设计合成反应路线



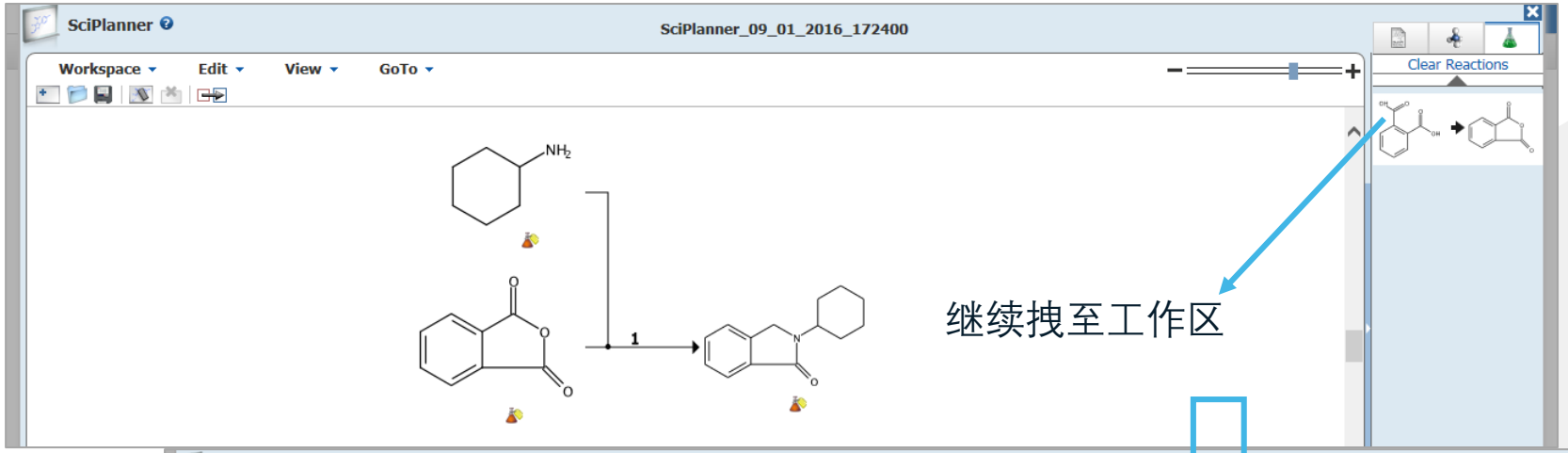
SciPlanner--工作界面



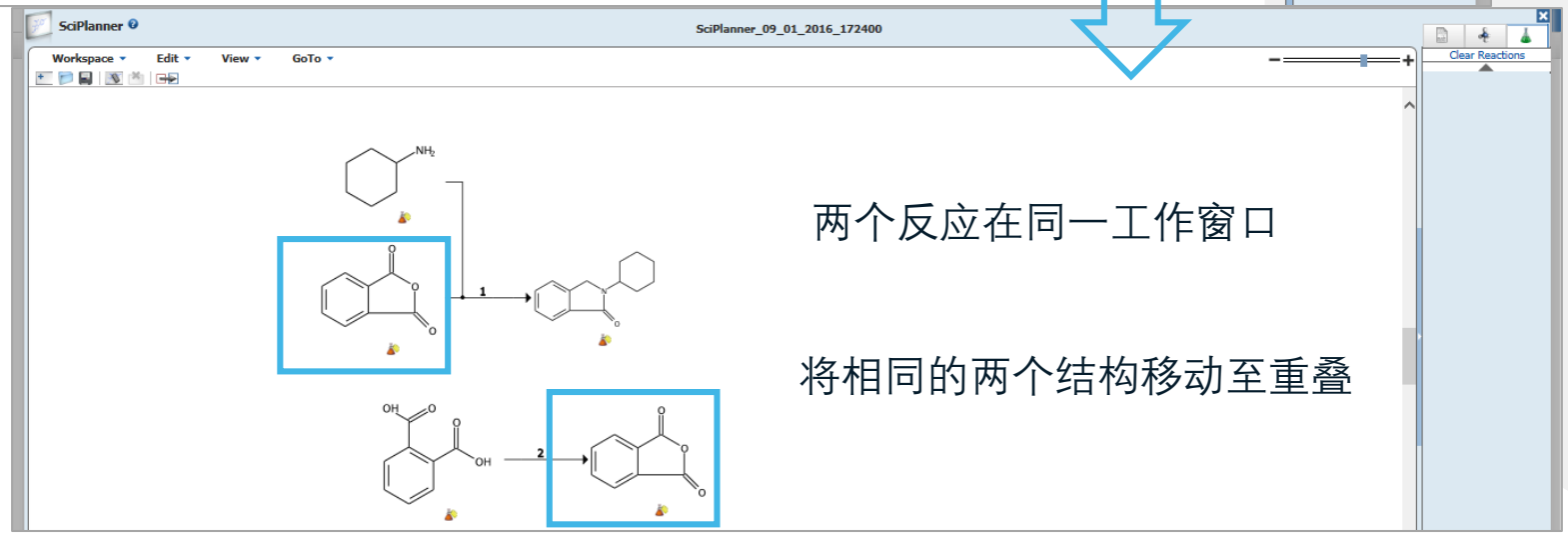
SciPlanner--工作界面



SciPlanner--工作界面



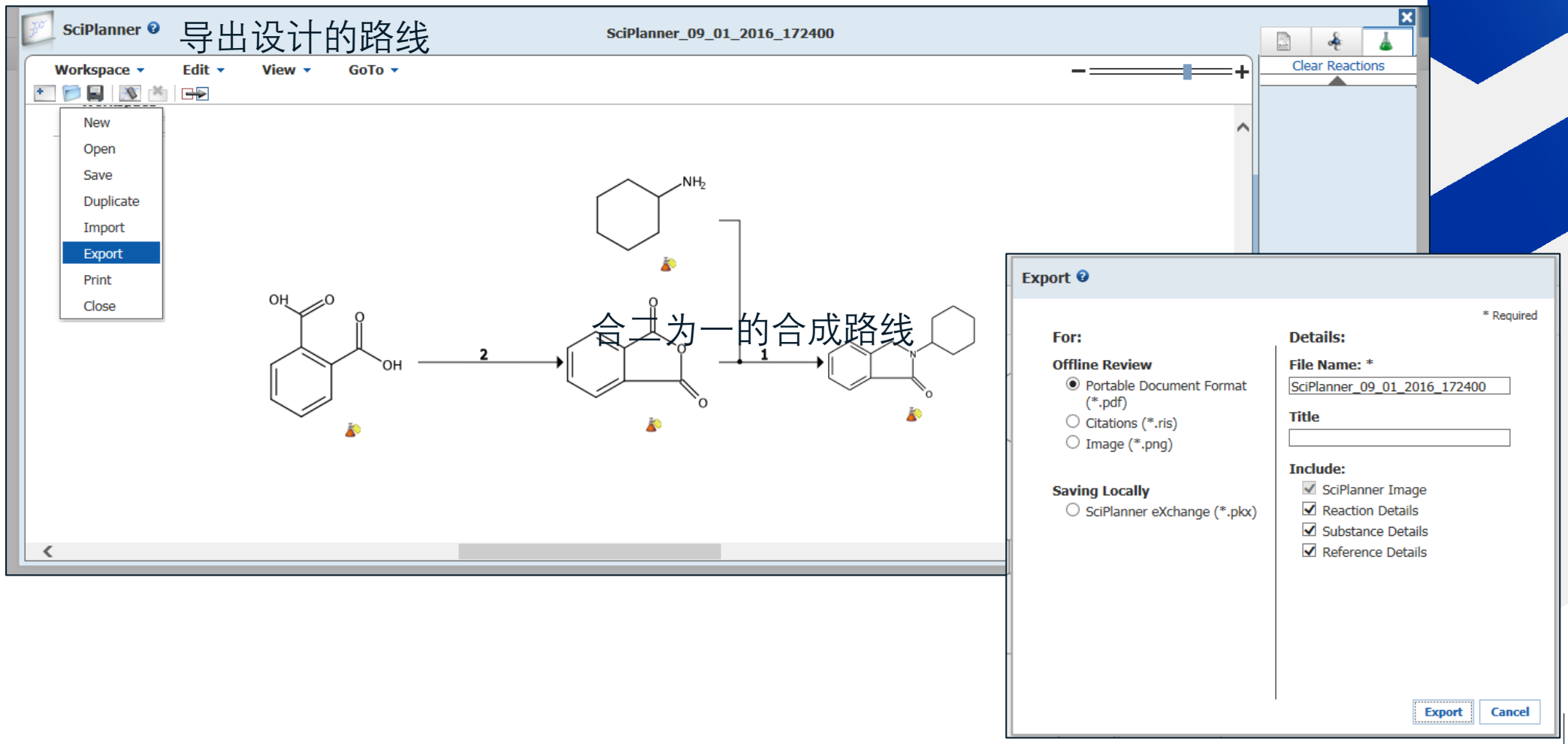
继续拽至工作区



两个反应在同一工作窗口

将相同的两个结构移动至重叠

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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浏览器选择建议

- Windows 7以上用户建议升级IE到10以上，不支持IE7、IE8
- Chrome和FireFox浏览器在所有系统上的表现都优于IE浏览器
- 不建议使用360浏览器检索SciFinder，会被自动拦截相关功能或插件

如何获取CAS SciFinder账号

填写注册申请表（如下）、提交证件照片（学生证的个人信息页和学籍注册页或是工作证的个人信息页照片，放在附件中），用申请注册的邮箱发送至china@acs-i.org

SciFinder 注册信息确认

个人信息(Personal Information)

学校名称(University):

院系(College):

专业(Major):

中文名(Name):

电话(Tel):

身份（Identity）：□ 教师

□ 博士 年级(Grade):

□ 硕士 年级(Grade):

□ 本科 年级(Grade):

联系信息(Contact Information)

院系办公室联系电话（School/Dept. Contact Tel）：

院系办公室联系人（School/Dept. Contact Person）：

Email Address:

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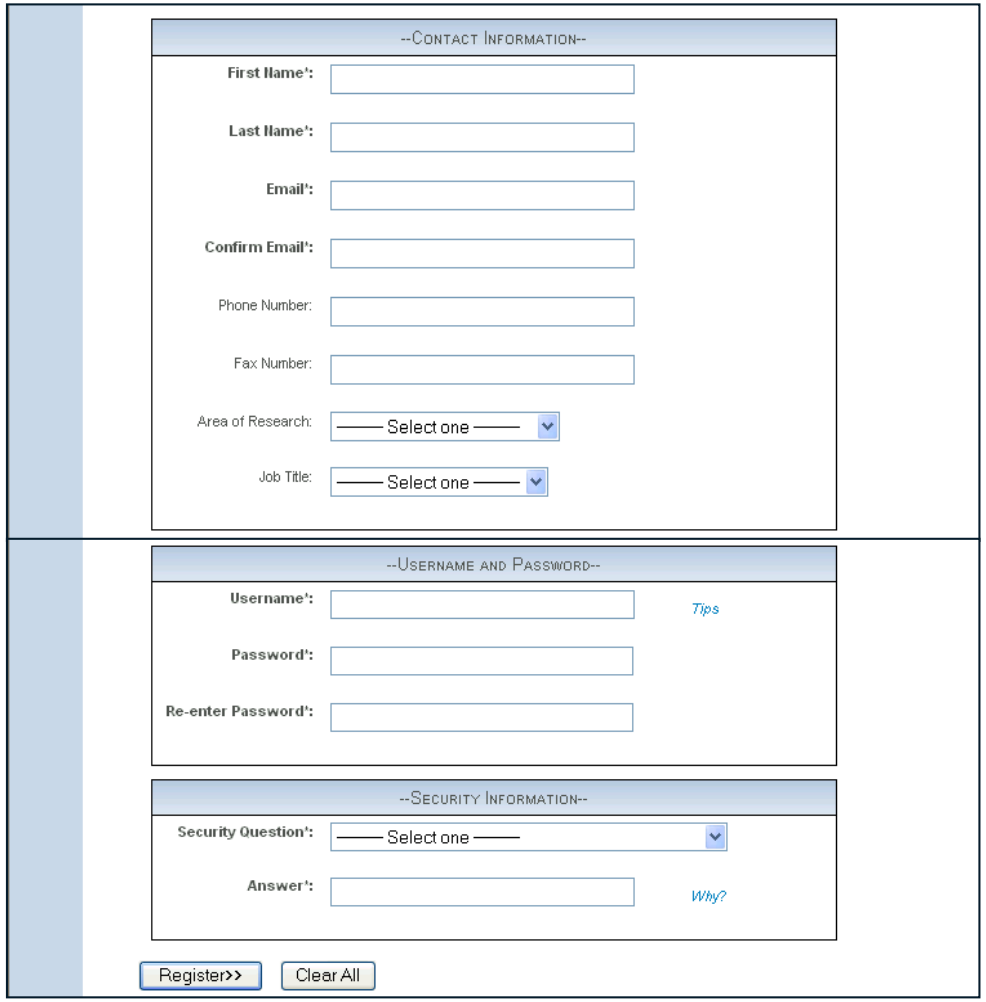
如何获取CAS SciFinder账号



请注意：
1.必须输入真实姓名和邮箱。
2.用户名必须是唯一的，且包含 5-15 个字符。它可以只包含字母或字母组合、数字和/或以下特殊字符：

- -（破折号）
- _（下划线）
- .（句点）
- @（表示“at”的符号）

3.密码必须包含 7-15 个字符，并且至少包含三种以下字符：

- 字母
- 混合的大小写字母
- 数字
- 非字母数字的字符（例如 @、#、%、&、*）

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

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如何获取CAS SciFinder账号

所有信息提交后注册成功。

之后直接点击https://SciFinder.cas.org即可访问SciFinder数据库

使用注意事项

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

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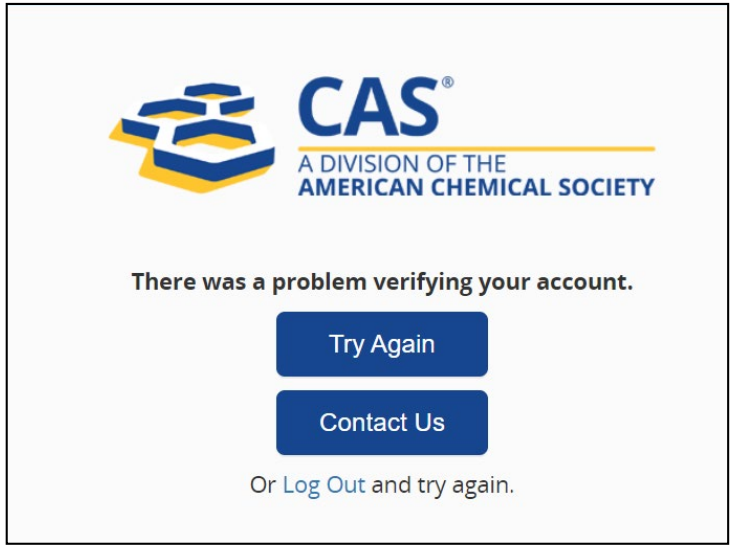
常见问题



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

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