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美国化学文摘社

SciFinder^{n}在天然药物化学研究方面的应用

CAS
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AMERICAN CHEMICAL SOCIETY

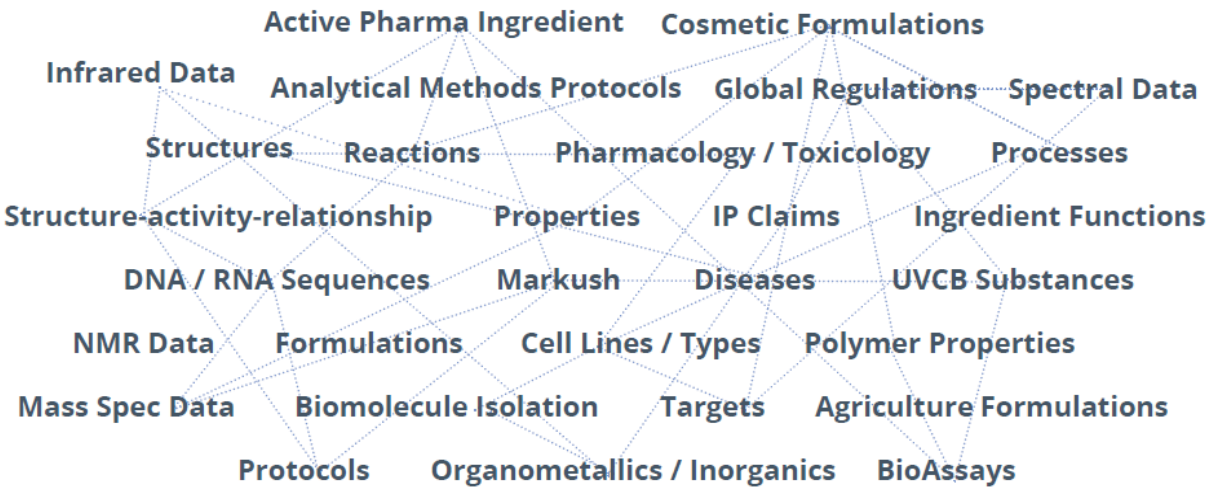
SciFinder^{n}涵盖内容的独特性

54 Million scientific journals and documents

64 PATENT OFFICES worldwide

179 MILLION substances

50 LANGUAGES translated



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SciFinder Discovery平台涵盖内容的独特性

- 化学物质数量全球领先。目前收录的化学物质数量已超过1.79亿个，是进行新化合物确认的唯一可用资源。
- 生物大分子数量全球领先。目前收录来自期刊和专利中的约5.8亿条序列（包括蛋白、核酸）
- 由CAS创建的CAS登记号是化学物质的黄金标准；是对物质进行确认的唯一身份识别号；是在进行化学品进出口交易时，必须向相关国家管控机构提供的身份识别号；是在申报课题项目时，需向评议组提供的身份识别号
- CAS几乎收录了从高分子聚合物到纳米颗粒的所有类别的物质，包括有机物、无机物、聚合物、合金、矿物质、配合物、混合物、生物序列等

Sources: https://www.cas.org/about/cas-content

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SciFinder Discovery平台涵盖内容的独特性

- CAS不但收录专利中报道的确定结构的物质，还收录专利中的通式结构（马库什结构），帮助用户在使用CAS的数据后能够最大程度的避免专利法律风险
- 化学反应数量全球领先，目前收录的化学反应数量超过1.34亿条，是确认新的化学反应、工艺和方法时必不可缺的资源
- 近千名科学家每天阅读来自全球的科技文献，并根据CAS制定的规则和标准、从信息专家和科学家的角度对原文中重要的信息进行改写和标引，从而节省CAS的用户花在阅读、理解、总结科技原文文献所需的时间，将更多的时间投入到其他的工作中

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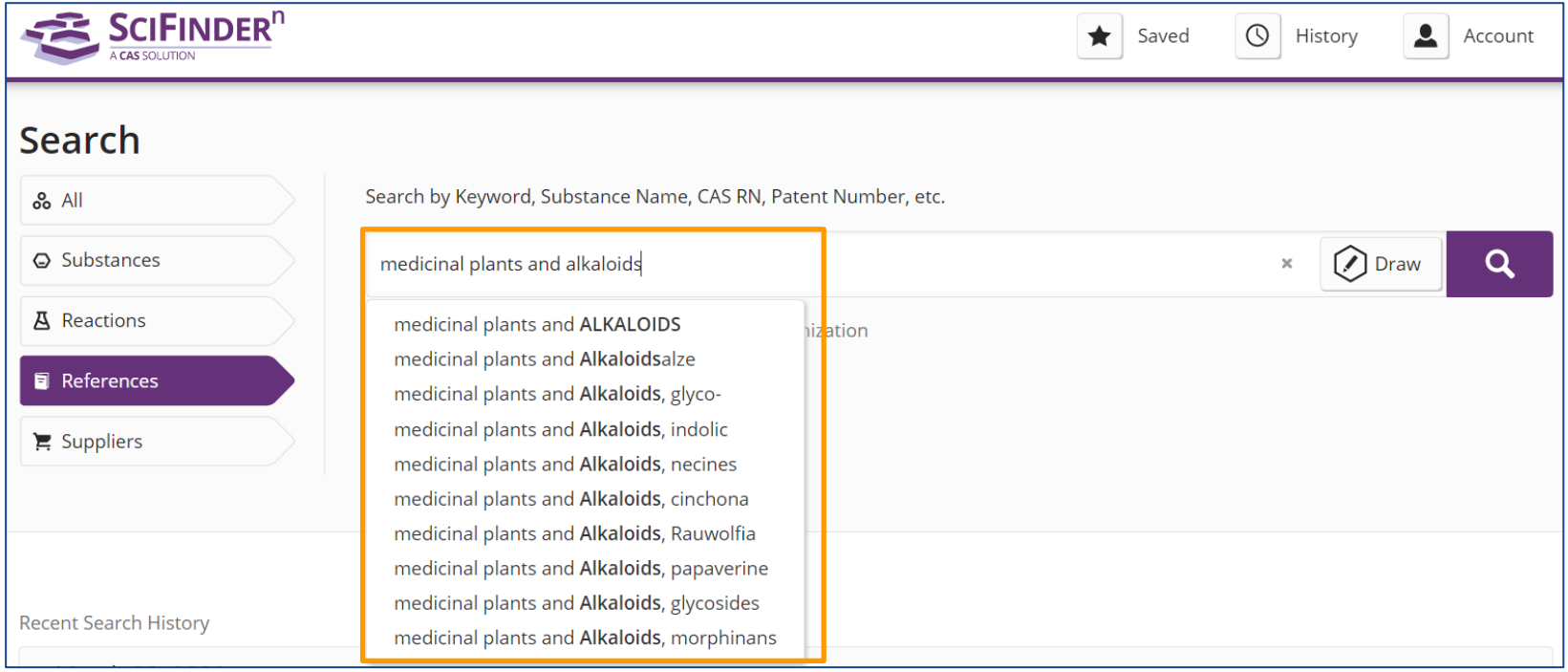
大纲

- 天然活性成分的提取分离和活性研究
- 根据谱图信息来分析物质结构
- 骨架结构新颖性的确定
- 具有生物活性的衍生化结构检索
- 结构改造与合成

优选布尔逻辑运算符支持的文献主题检索，充分利用提示词启发检索思路



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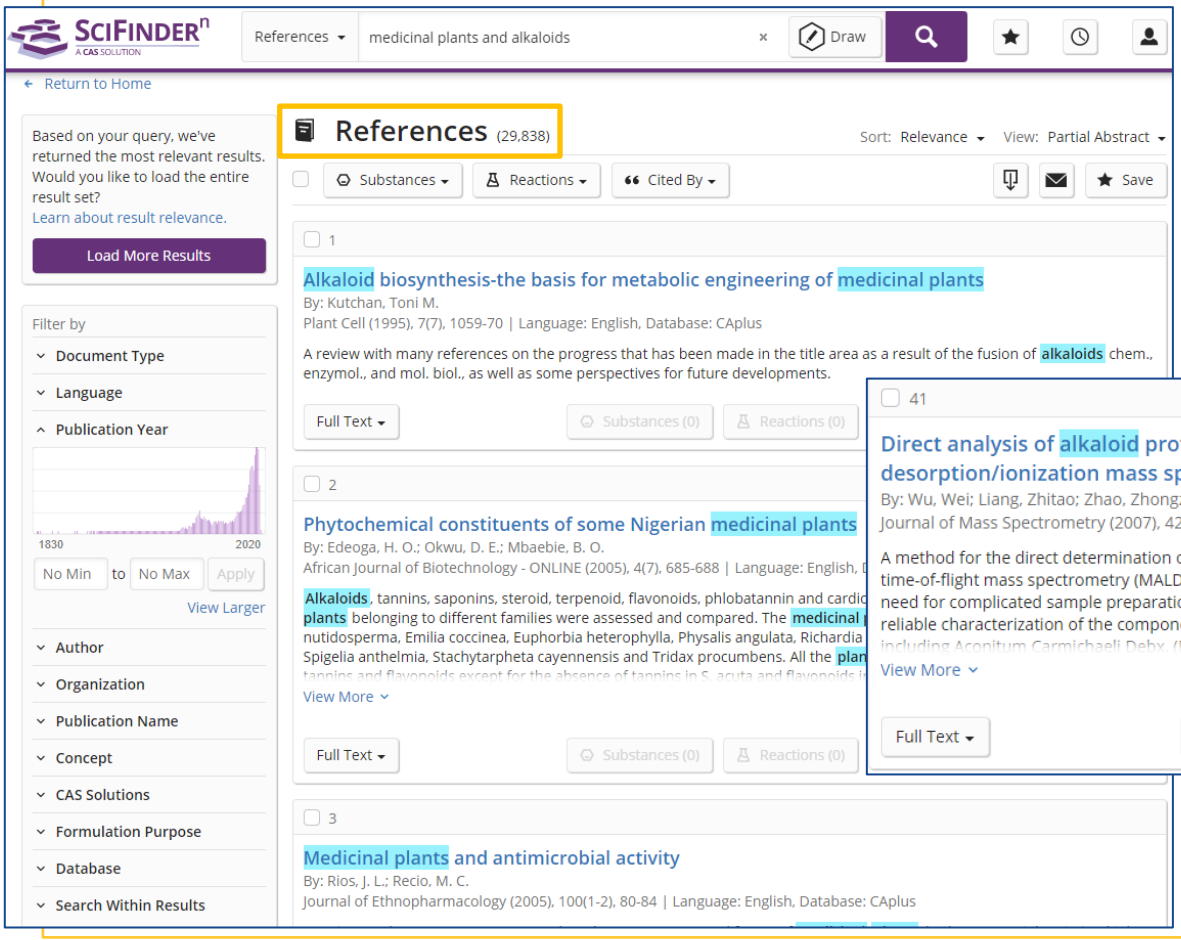

medicinal plants and alkaloids

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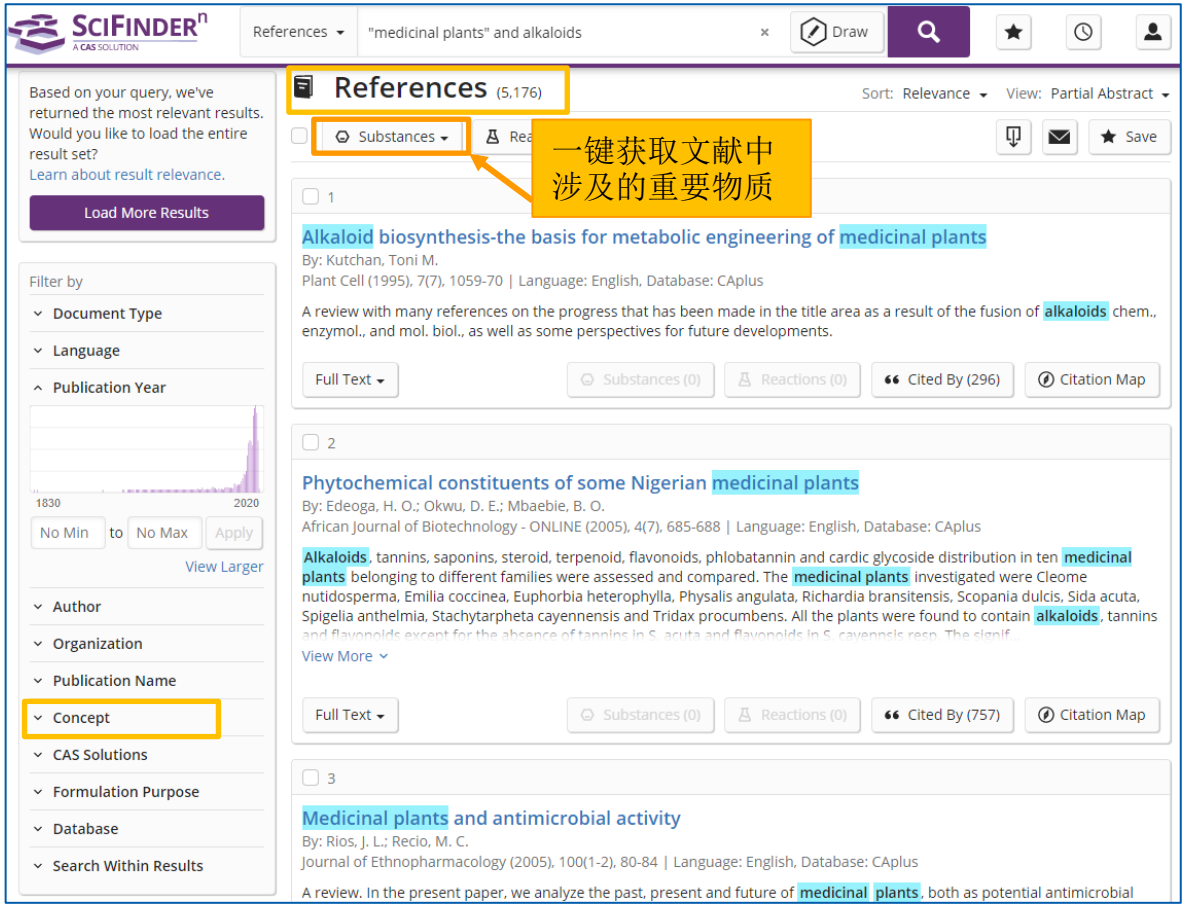
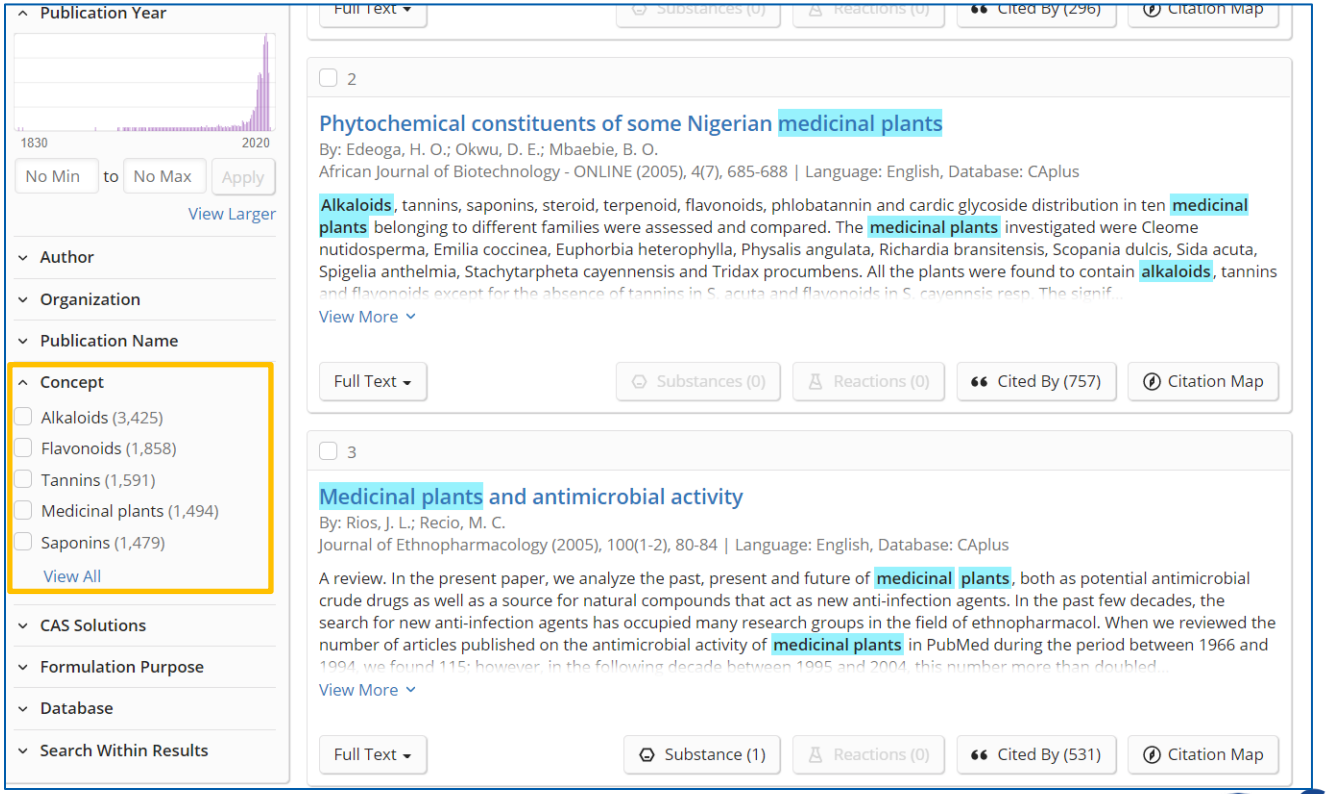


“medicinal plants” and alkaloids

通过Concept概念词库，进一步分析文献涉及的研究点



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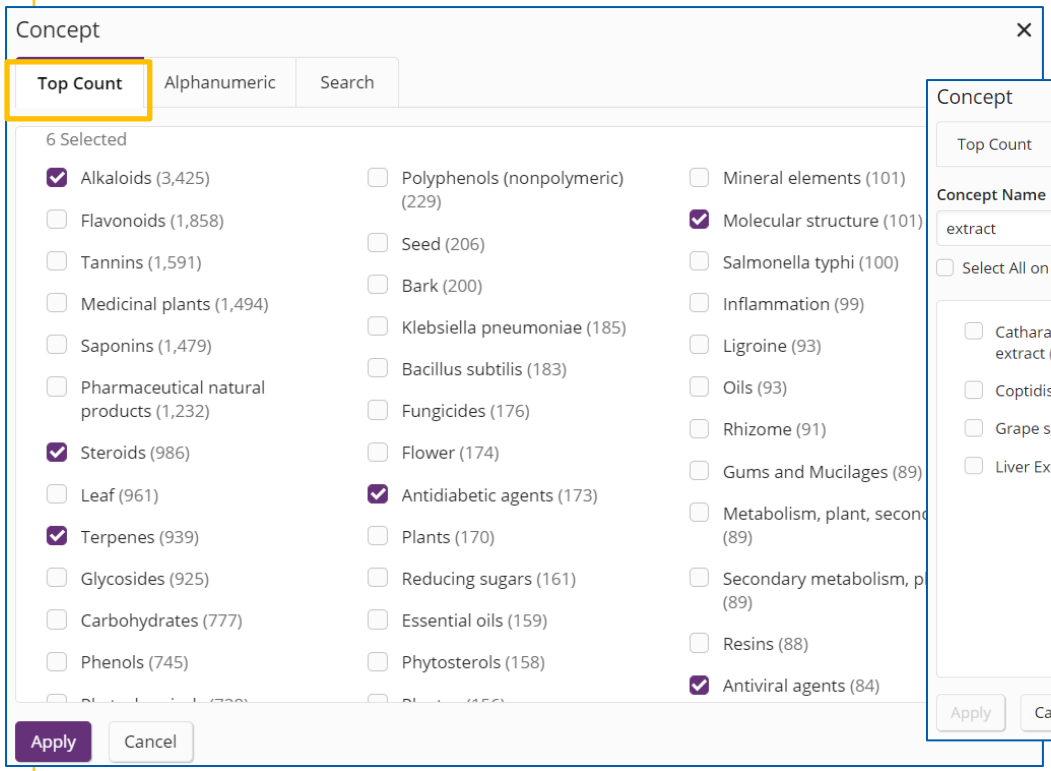
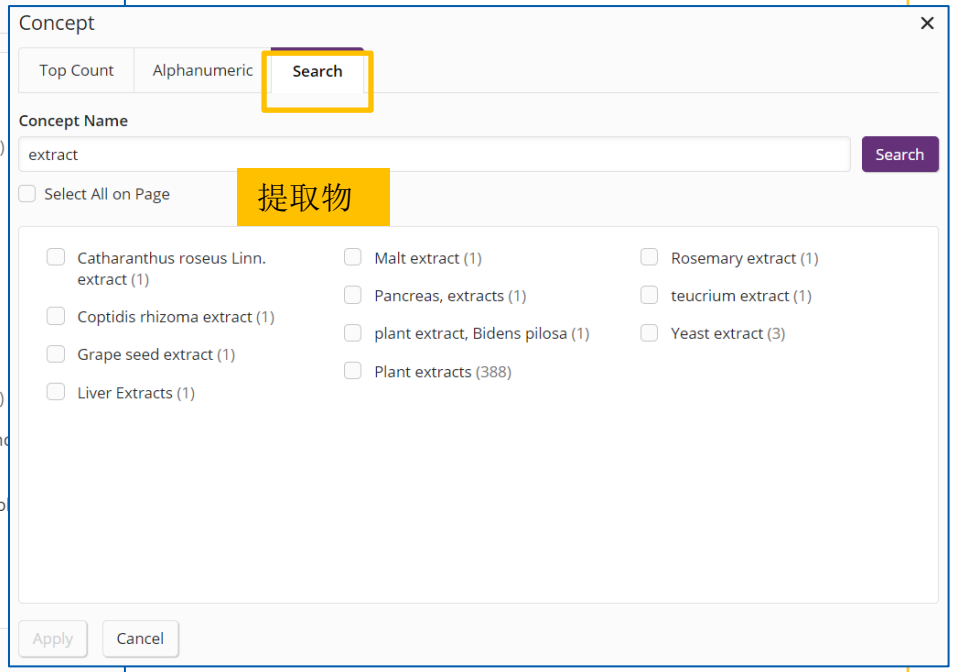
浏览涉及的研究点，并选择或再次检索自己密切关注的研究点





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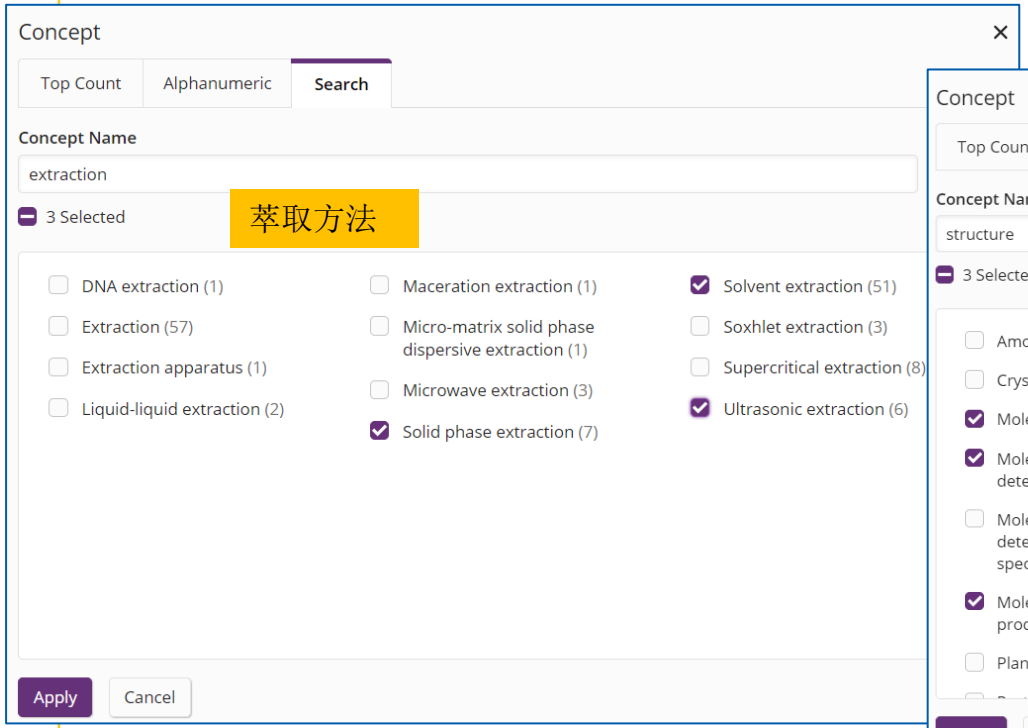

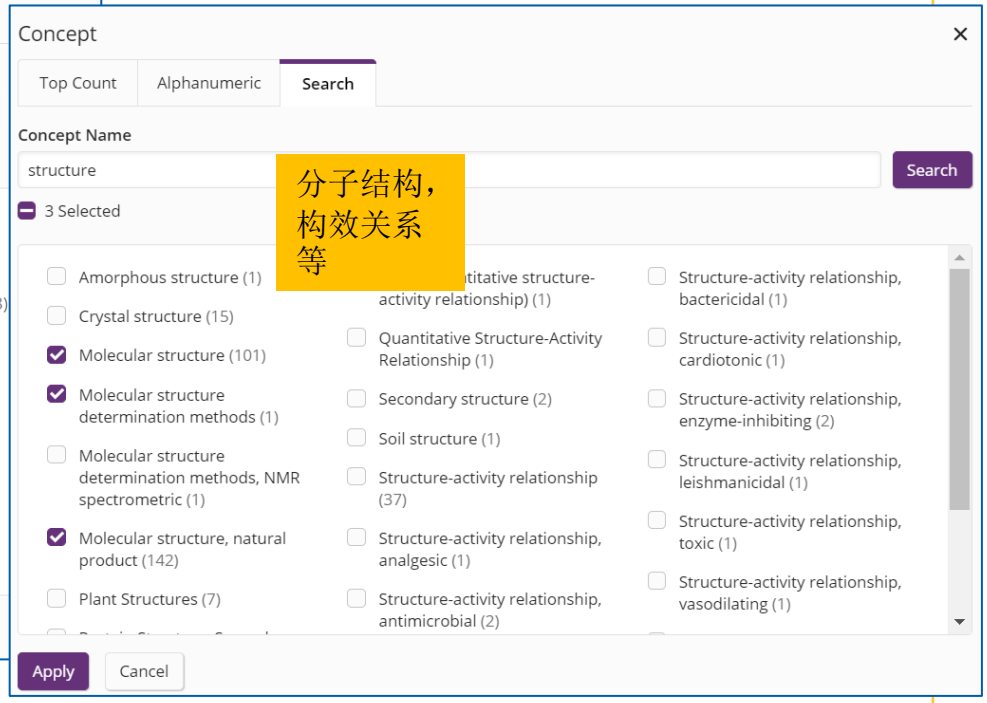

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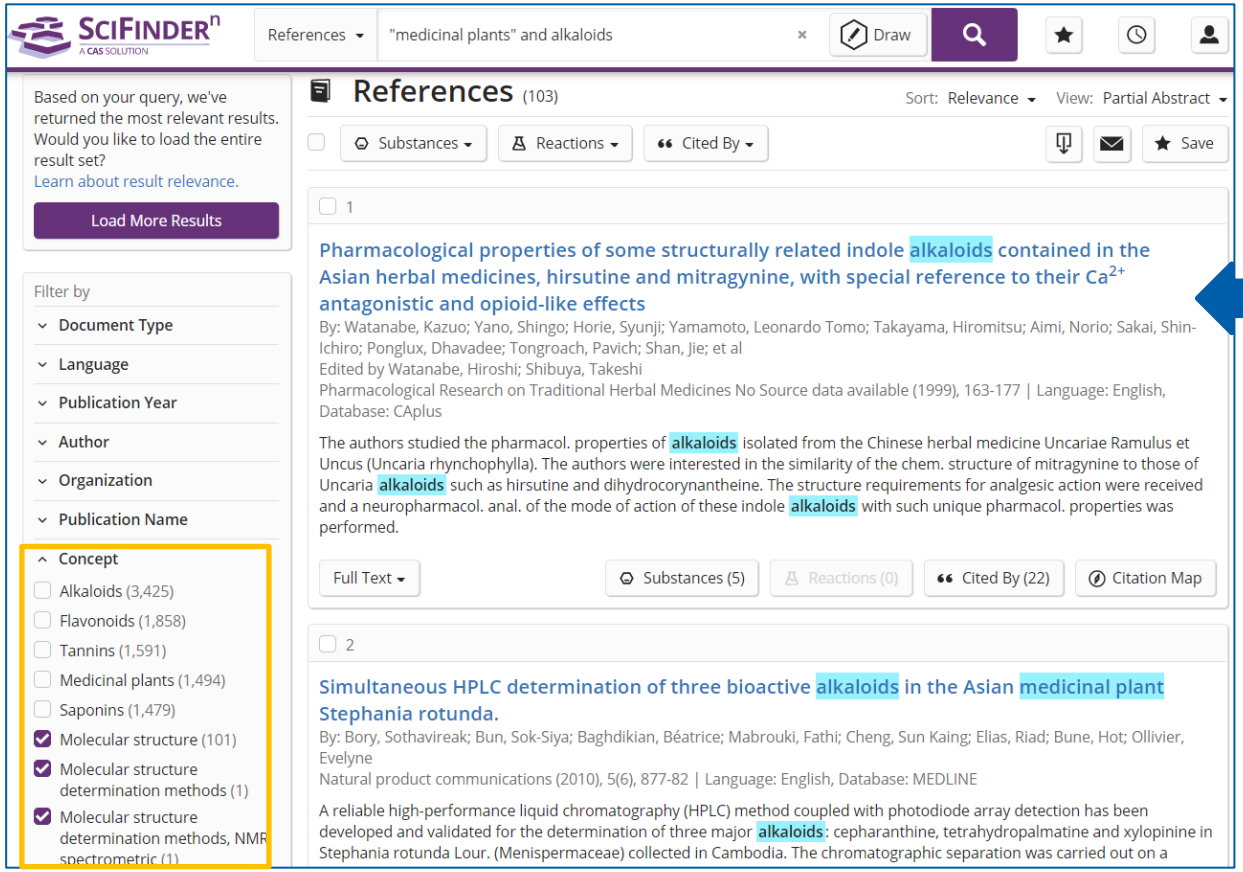

获得分子结构及测定方法相关的研究文献

点击文献标题，
查看文献详情

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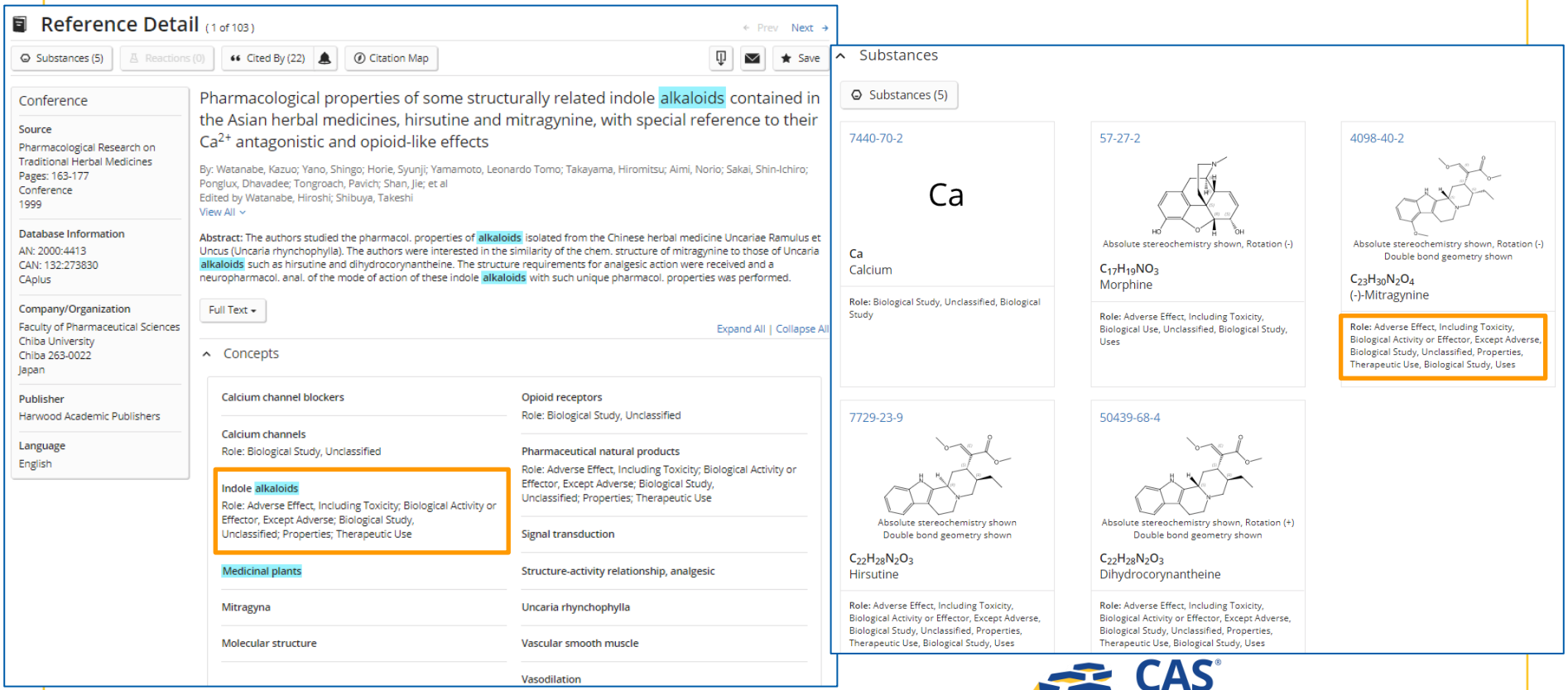
充分利用人工标引信息，快速了解文献详情



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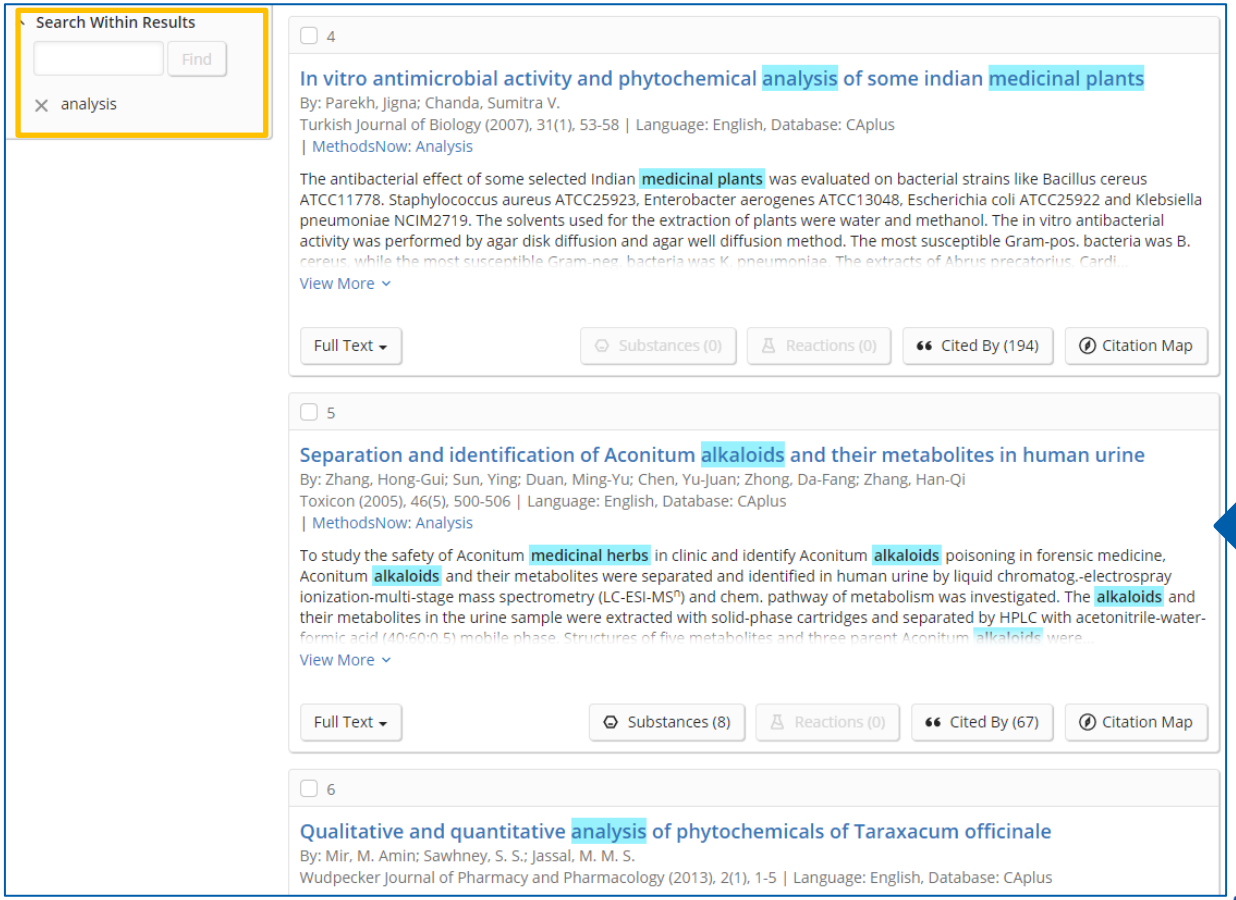

通过Search Within Results，输入感兴趣的检索词进行二次检索，如分析研究

点击文献标题，查看文献详情

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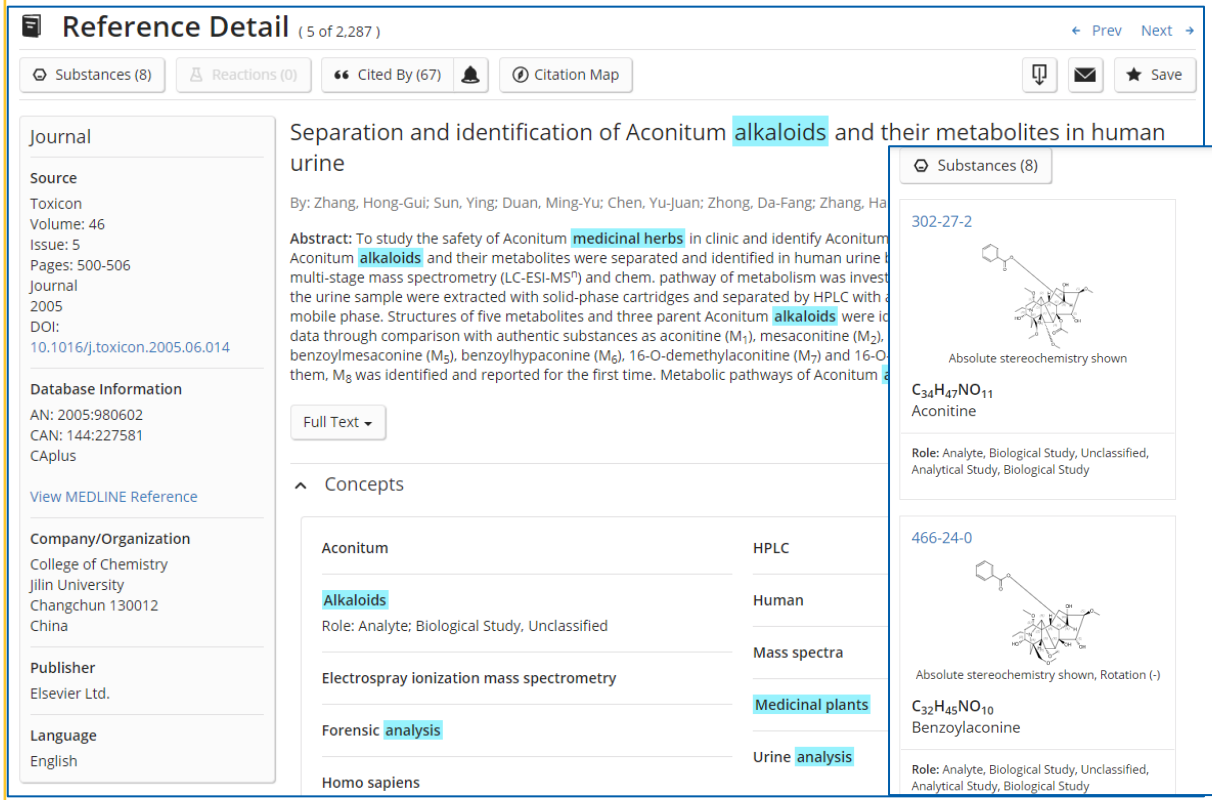
充分利用人工标引信息，快速了解文献详情



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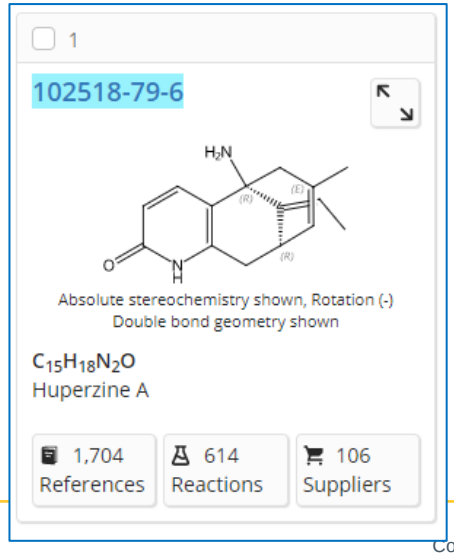
示例：查找有关天然药物提取，分析，剂型，药理等信息

- 以石杉碱甲为例：CAS No. 102518-79-6
- 执行相同检索策略：CAS号检索，由物质获得文献结果集
- 在文献结果集中通过筛选选项获取所需信息

SciFinder^{n} 结果



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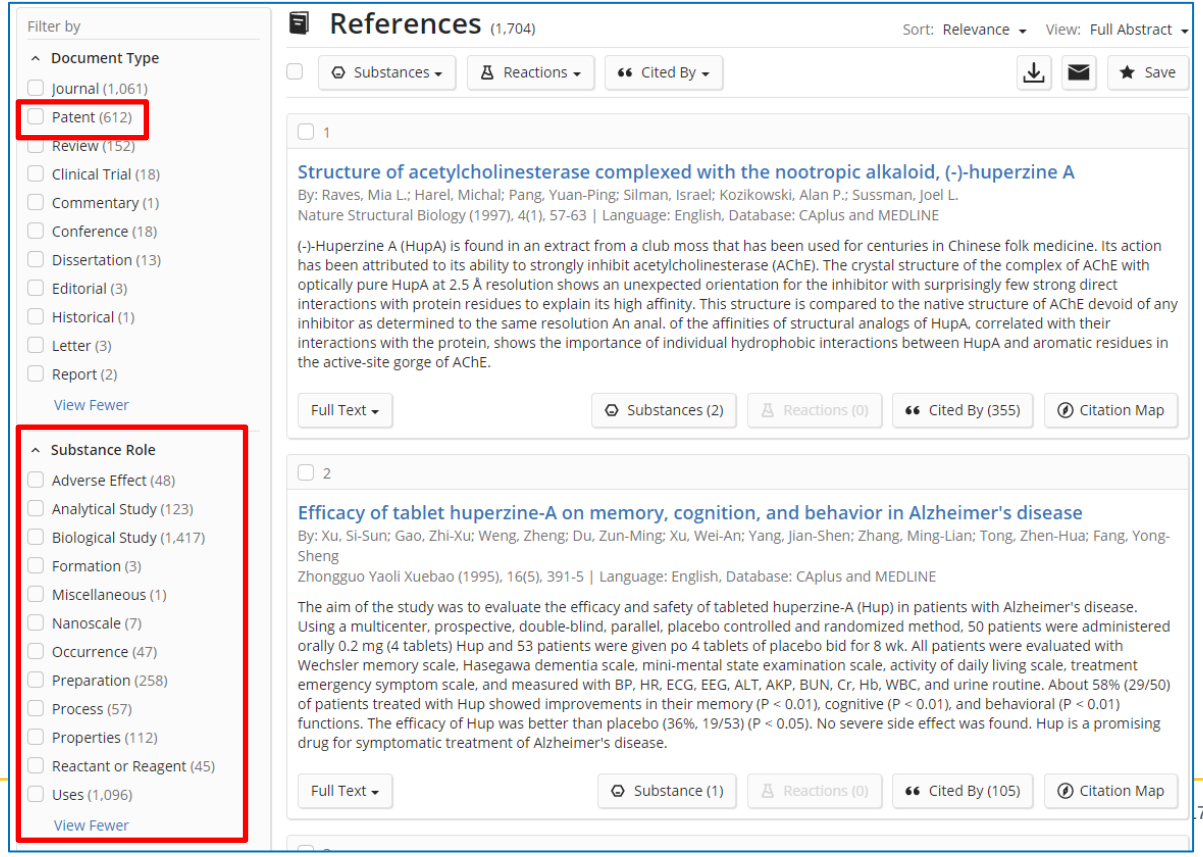
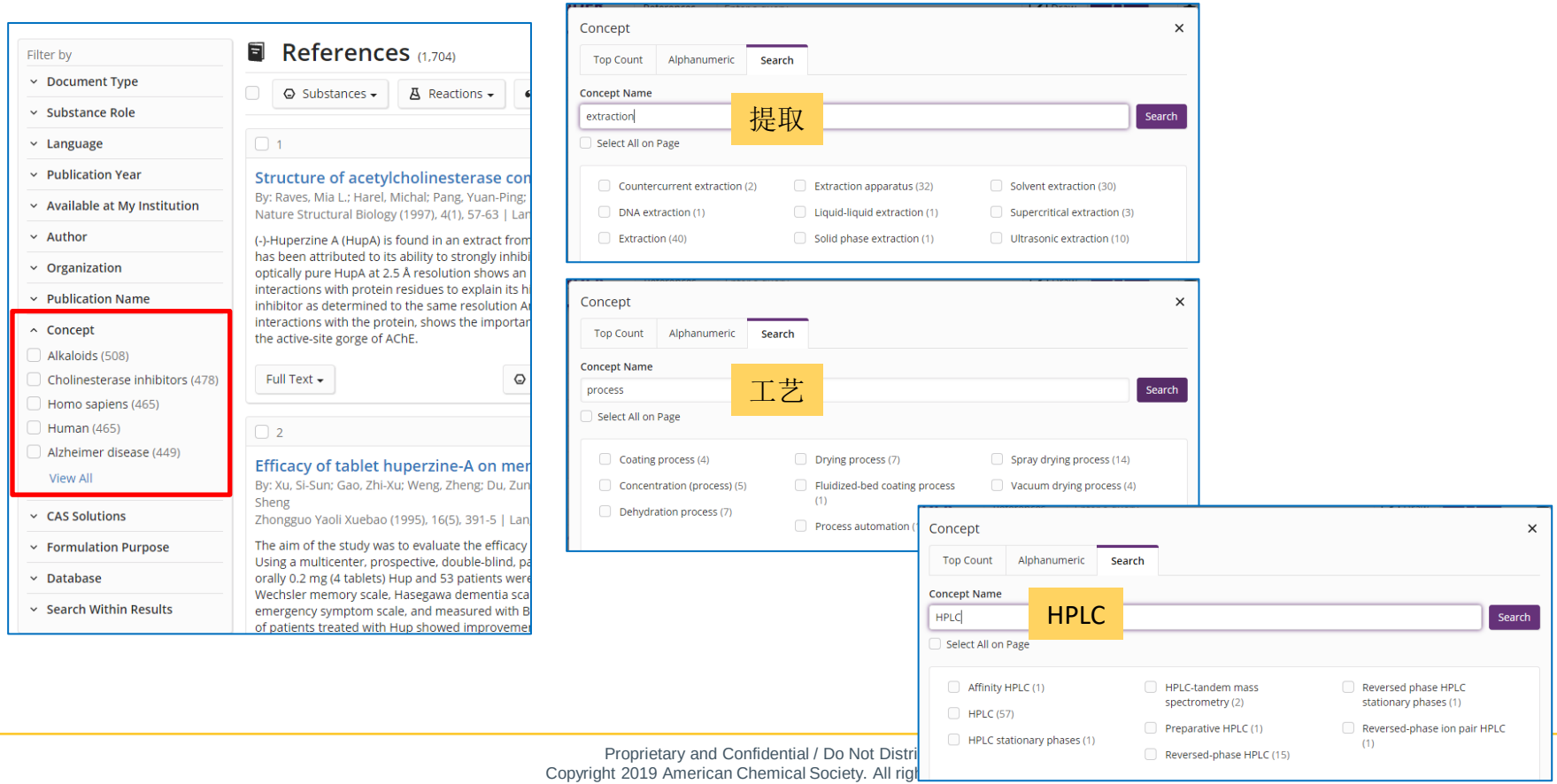
SciFinder^{n}文献结果

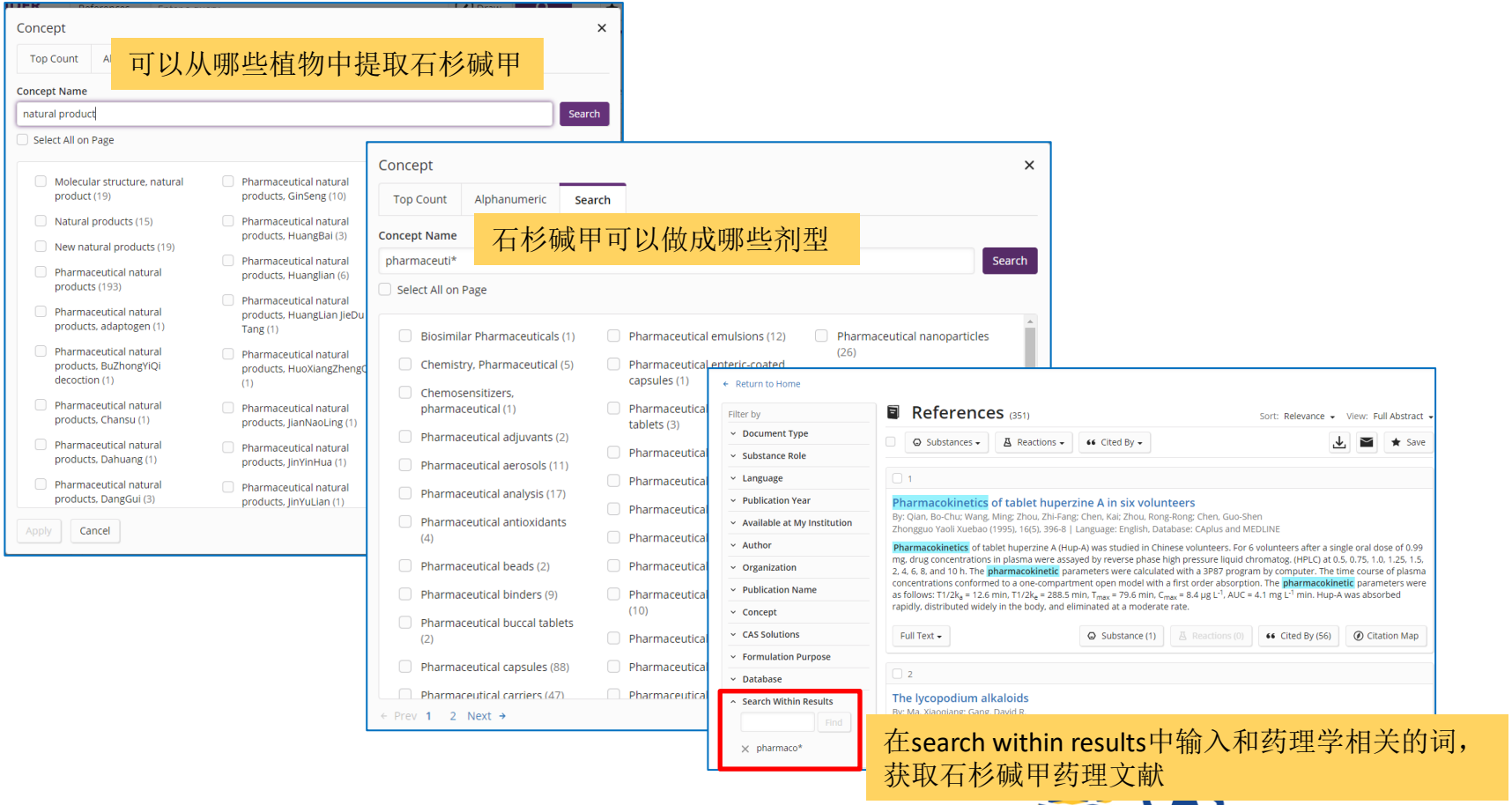
共计文献结果1704
其中专利612篇
收录期刊，专利，临床试验报告，
学位论文等丰富的文献类型

可以根据物质不同的研究领域
直接筛选文献：
如药物副作用，分析，生物，
制备，工艺，属性，用途等



通过Concept，快速聚焦关注的技术领域，获取所需信息





大纲

- 天然活性成分的提取分离和活性等研究
- 根据谱图信息来分析物质结构
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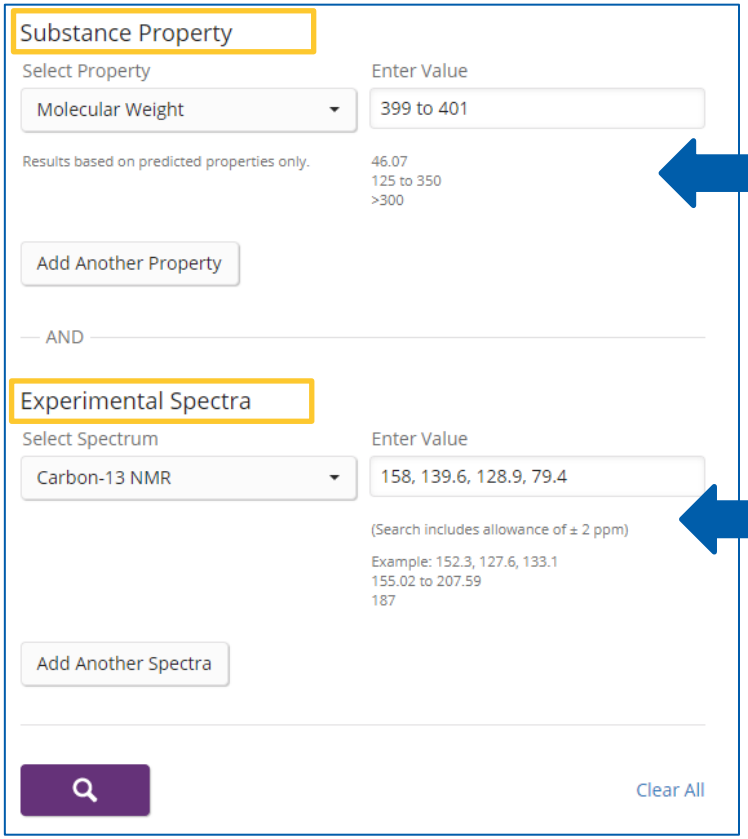
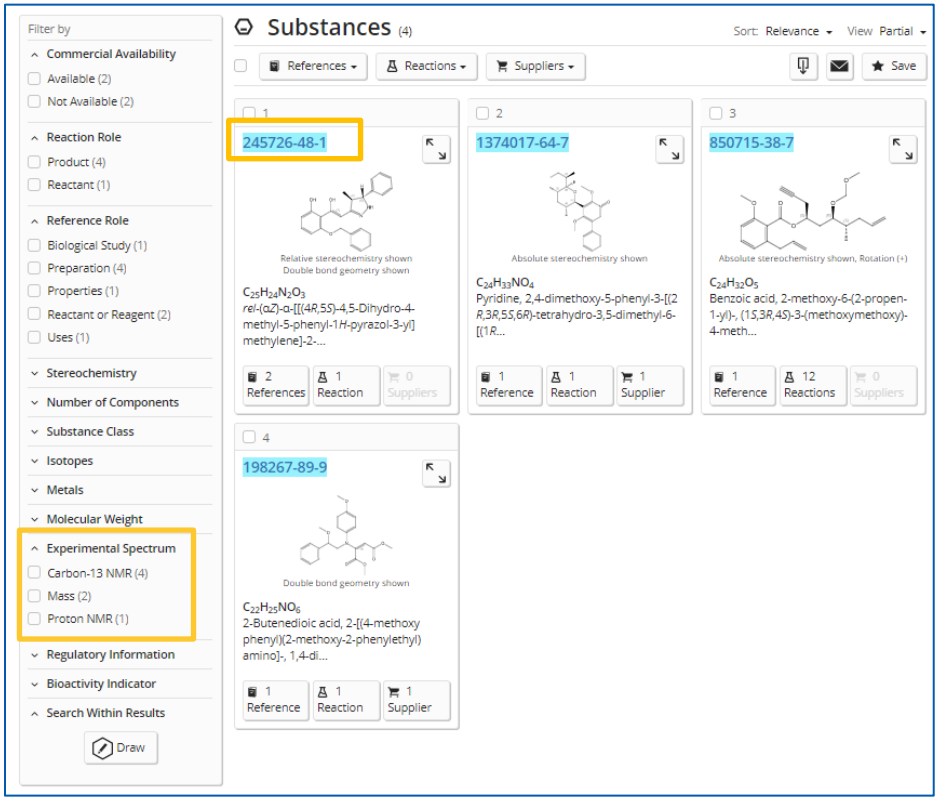
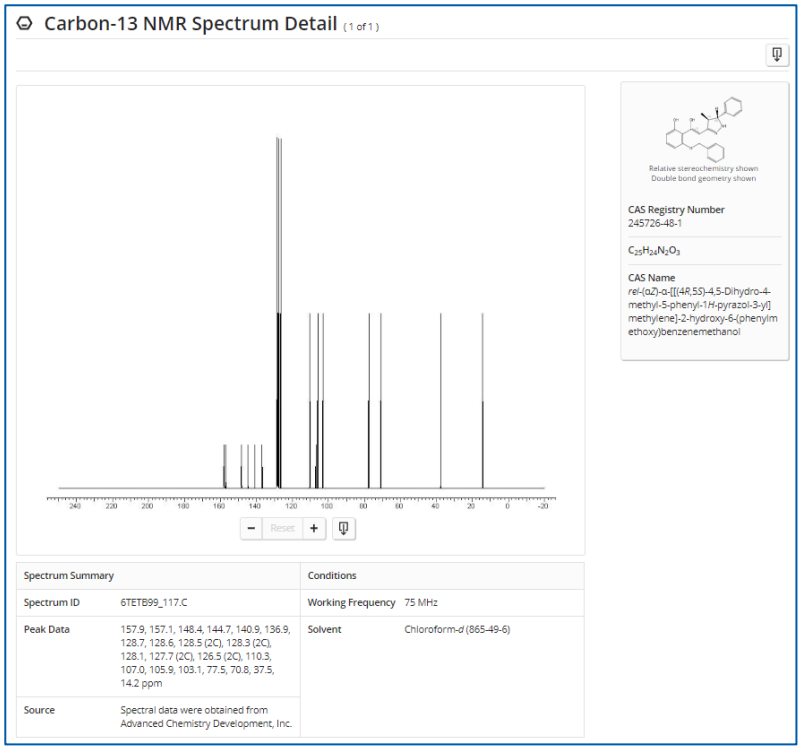
例1：已知质谱和核磁谱图信息，分析天然活性成分的结构



根据example中提供的格式，输入谱峰值或者数值范围。

点击CAS RN查看具体的谱图信息；根据Experimental Spectra查看其他谱图研究信息





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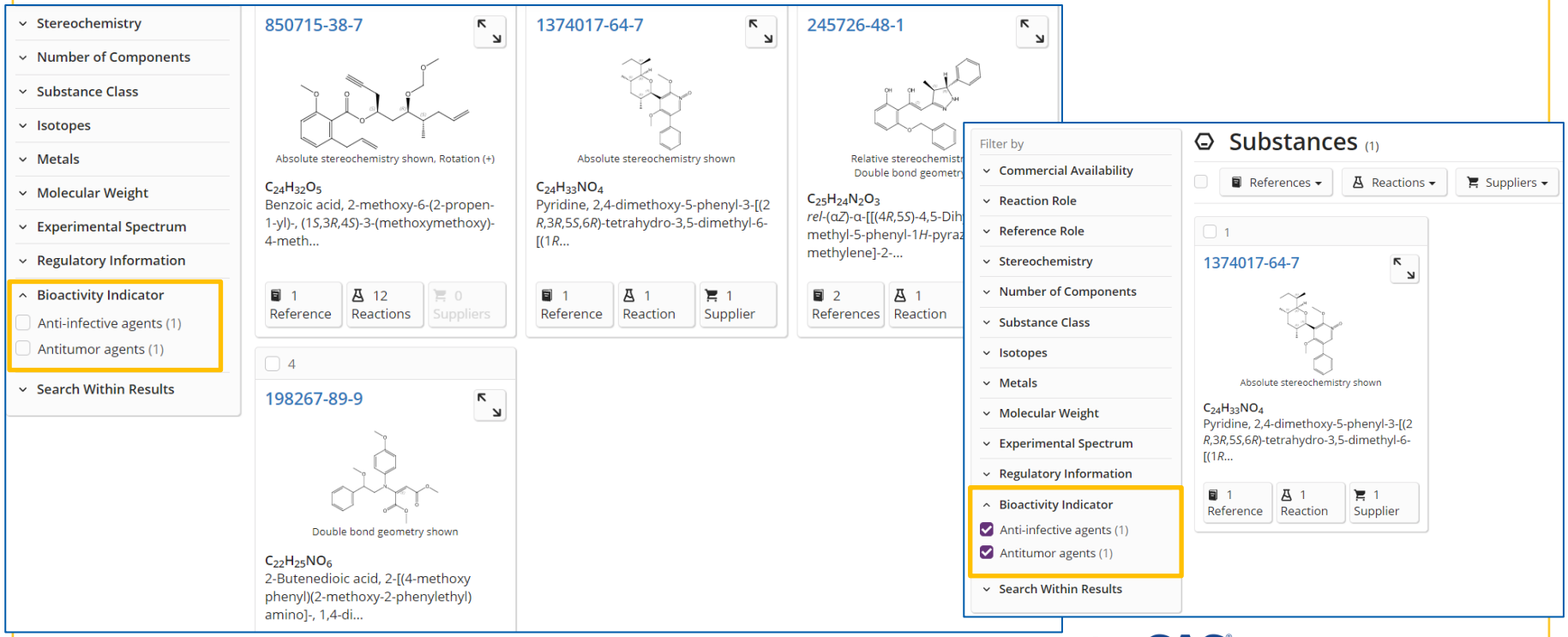
再通过Bioactivity Indicator，查看对应的活性研究信息



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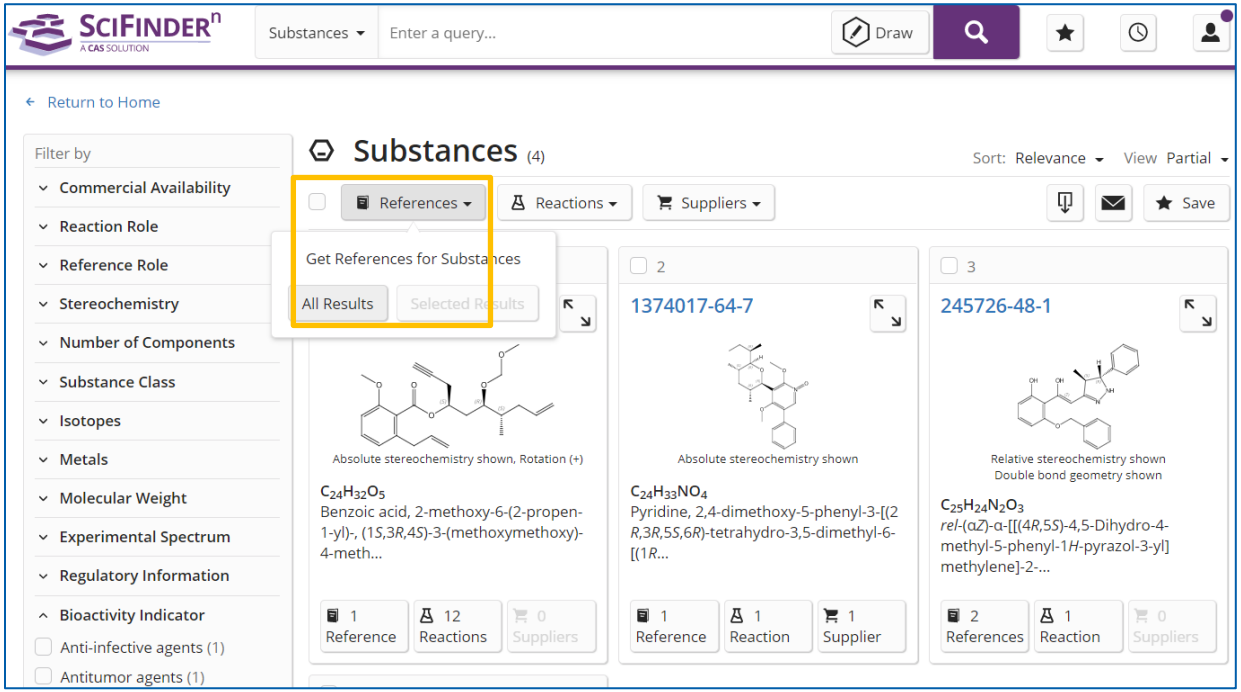
一键获得对应的研究文献



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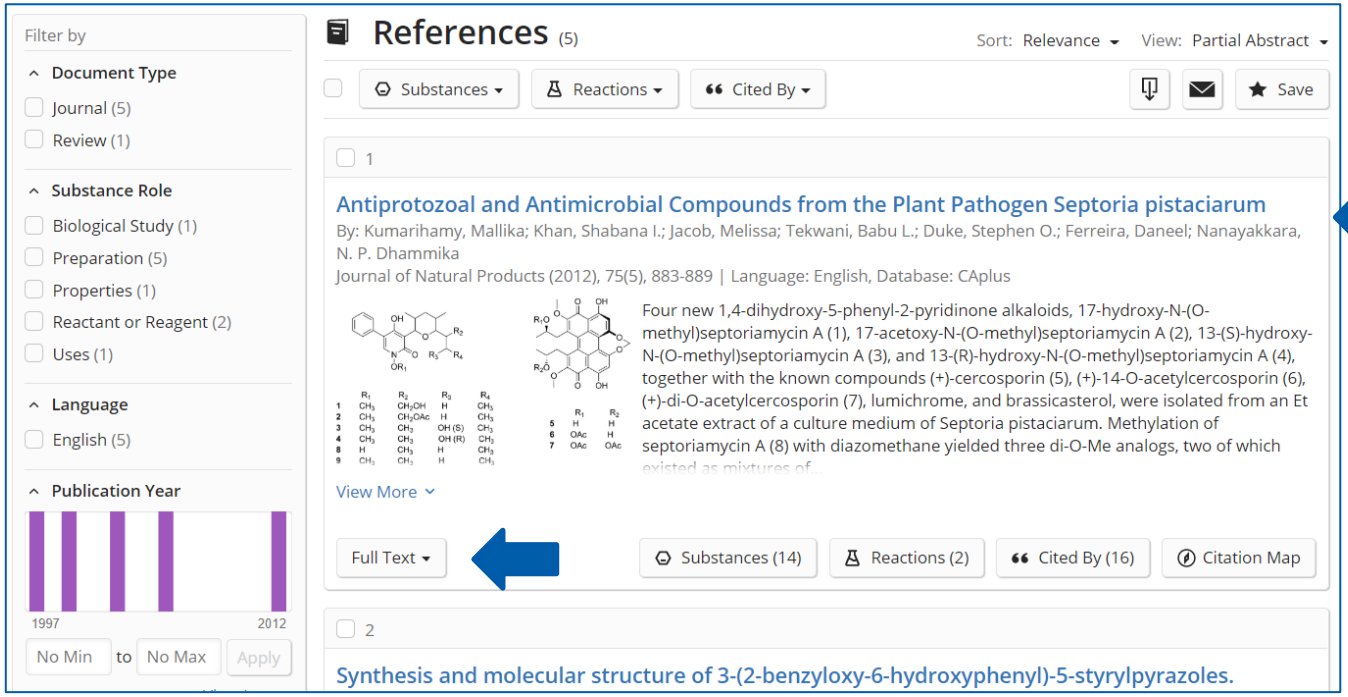
根据文献详情判断文献主旨



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文献详情

Reference Detail (1 of 5)

Prev Next

Substances (14) | Reactions (2) | Cited By (16) | Citation Map | Save

Journal

Source
Journal of Natural Products
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Issue: 5
Pages: 883-889
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2012
DOI:
10.1021/np200940b

Database Information
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CAN: 156:583096
CAplus

View MEDLINE Reference

Company/Organization
National Center for Natural Products Research, Research Institute of Pharmaceutical Sciences, and Department of Pharmacognosy, School of Pharmacy
The University of Mississippi
University, Mississippi 38677
United States

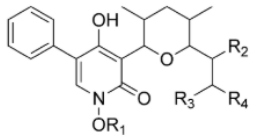
Publisher
American Chemical Society-American Society of Pharmacognosy

Language
English

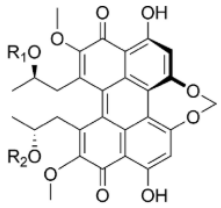
Antiprotozoal and Antimicrobial Compounds from the Plant Pathogen Septoria pistaciarum

By: Kumarihamy, Mallika; Khan, Shabana I.; Jacob, Melissa; Tekwani, Babu L.; Duke, Stephen O.; Ferreira, Daneel; Nanayakkara, N. P. Dhammika

Abstract: Four new 1,4-dihydroxy-5-phenyl-2-pyridinone alkaloids, 17-hydroxy-N-(O-methyl)septoriamycin A (1), 17-acetoxy-N-(O-methyl)septoriamycin A (2), 13-(S)-hydroxy-N-(O-methyl)septoriamycin A (3), and 13-(R)-hydroxy-N-(O-methyl)septoriamycin A (4), together with the known compounds (+)-cercosporin (5), (+)-14-O-acetylcercosporin (6), (+)-di-O-acetylcercosporin (7), lumichrome, and brassicasterol, were isolated from an Et acetate extract of a culture medium of Septoria pistaciarum. Methylation of septoriamycin A (8) with diazomethane yielded three di-O-Me analogs, two of which existed as mixtures of rotamers. We previously reported antimalarial activity of septoriamycin A. This compound also exhibited significant activity against Leishmania donovani promastigotes. Compounds 5-7 showed moderate in vitro activity against L. donovani promastigotes and chloroquine-sensitive (D6) and -resistant (W2) strains of Plasmodium falciparum, whereas compound 5 was fairly active against methicillin-sensitive and methicillin-resistant strains of Staphylococcus aureus. Compounds 5-7 also displayed moderate phytotoxic activity against both a dicot (lettuce, Lactuca sativa) and a monocot (bentgrass, Agrostis stolonifera) and cytotoxicity against a panel of cell lines.



	R_1	R_2	R_3	R_4
1	CH_3	CH_2OH	H	CH_3
2	CH_3	CH_2OAc	H	CH_3
3	CH_3	CH_3	OH (S)	CH_3
4	CH_3	CH_3	OH (R)	CH_3
8	H	CH_3	H	CH_3
9	CH_3	CH_3	H	CH_3



	R_1	R_2
5	H	H
6	OAc	H
7	OAc	OAc

Full Text

Expand All | Collapse All

- Concepts
- Substances
- Citations

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浏览概念词库和物质列表，获取文献中关键的研究点和物质对应的研究角色

Substances

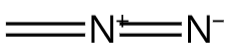
Substances (14)

74-88-4

CH_3I
Methyl iodide

Role: Reactant, Reactant or Reagent

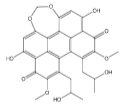
334-88-3



CH_2N_2
Diazomethane

Role: Reactant, Reactant or Reagent

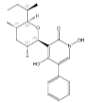
150132-90-4



$C_{29}H_{26}O_{10}$
(13b*R*)-5,12-Dihydroxy-8,9-bis[(2*R*)-2-hydroxypropyl]-7,10-dimethoxyperylo[1,12-*def*]-1,3-dioxepin-6,11-dione

Role: Pharmacological Activity, Properties, Purification or Recovery, Therapeutic Use, Biological Study, Preparation, Uses

1234619-27-2

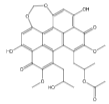


Absolute stereochemistry shown, Rotation (+)

$C_{22}H_{29}NO_4$
1,4-Dihydroxy-5-phenyl-3-[(2*R*,3*R*,5*S*,6*R*)-tetrahydro-3,5-dimethyl-6-[(1*R*)-1-methylpropyl]-2*H*-pyran-2-yl]-2(1*H*)-pyridinone

Role: Pharmacological Activity, Purification or Recovery, Reactant, Therapeutic Use, Biological Study, Preparation, Reactant or Reagent, Uses

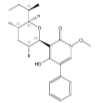
62574-07-6



$C_{31}H_{28}O_{11}$
(13b*R*)-8-[(8*R*)-2-(Acetyloxy)propyl]-5,12-dihydroxy-9-[(2*R*)-2-hydroxypropyl]-7,10-dimethoxyperylo[1,12-*def*]-1,3-dioxepin-6,11-dione

Role: Pharmacological Activity, Properties, Purification or Recovery, Therapeutic Use, Biological Study, Preparation, Uses

1234619-28-3



Absolute stereochemistry shown, Rotation (+)

$C_{23}H_{31}NO_4$
4-Hydroxy-1-methoxy-5-phenyl-3-[(2*R*,3*R*,5*S*,6*R*)-tetrahydro-3,5-dimethyl-6-[(1*R*)-1-methylpropyl]-2*H*-pyran-2-yl]-2(1*H*)-pyridinone

Role: Properties, Synthetic Preparation, Preparation

Concepts

天然产物、结构和活性

Agrostis stolonifera	Lettuce
Antimalarials	Methicillin-resistant Staphylococcus aureus
Antimicrobial agents	Molecular structure, natural product
Antitumor agents	Mycosphaerella pistaciarum
Cytotoxicity	Natural products
Lactuca sativa	Phytotoxicity
Leishmania donovani	Plasmodium falciparum
Leishmanicides	Staphylococcus aureus

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大纲

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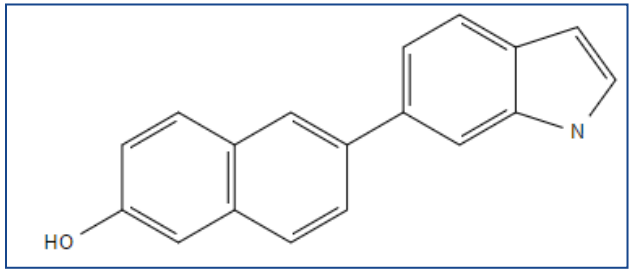
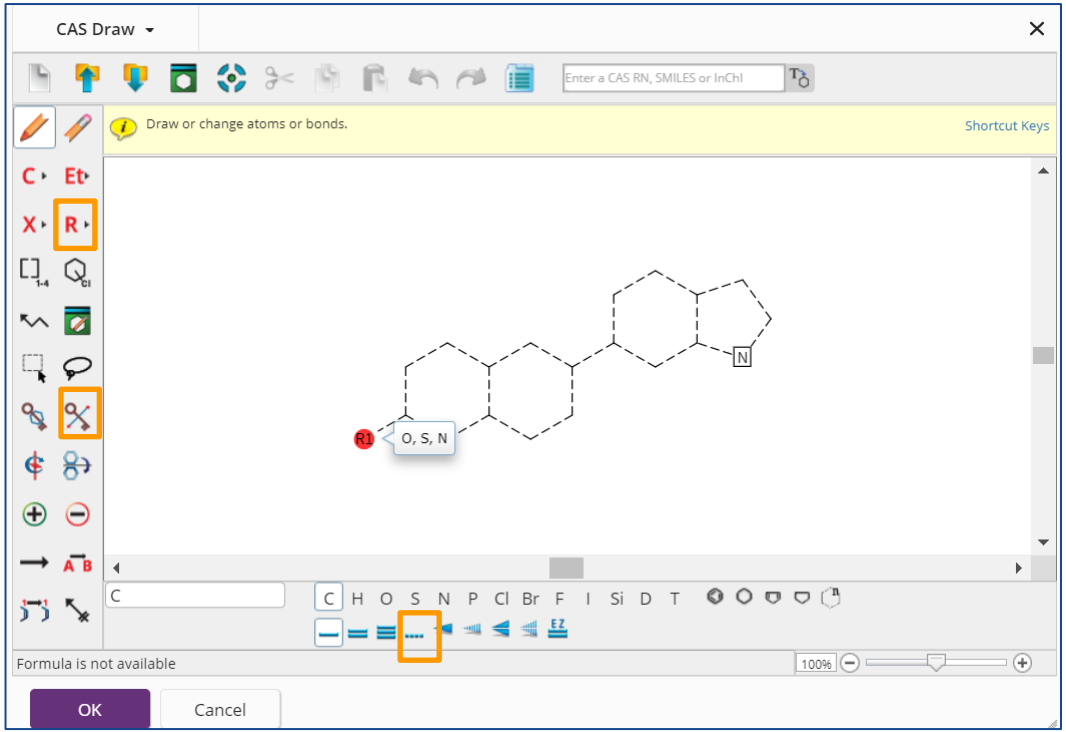
- 根据谱图信息来分析物质结构
- 骨架结构新颖性的确定
- 具有生物活性的衍生化结构检索
- 结构改造与合成

根据已知结构来绘制并检索同一环系骨架结构的物质





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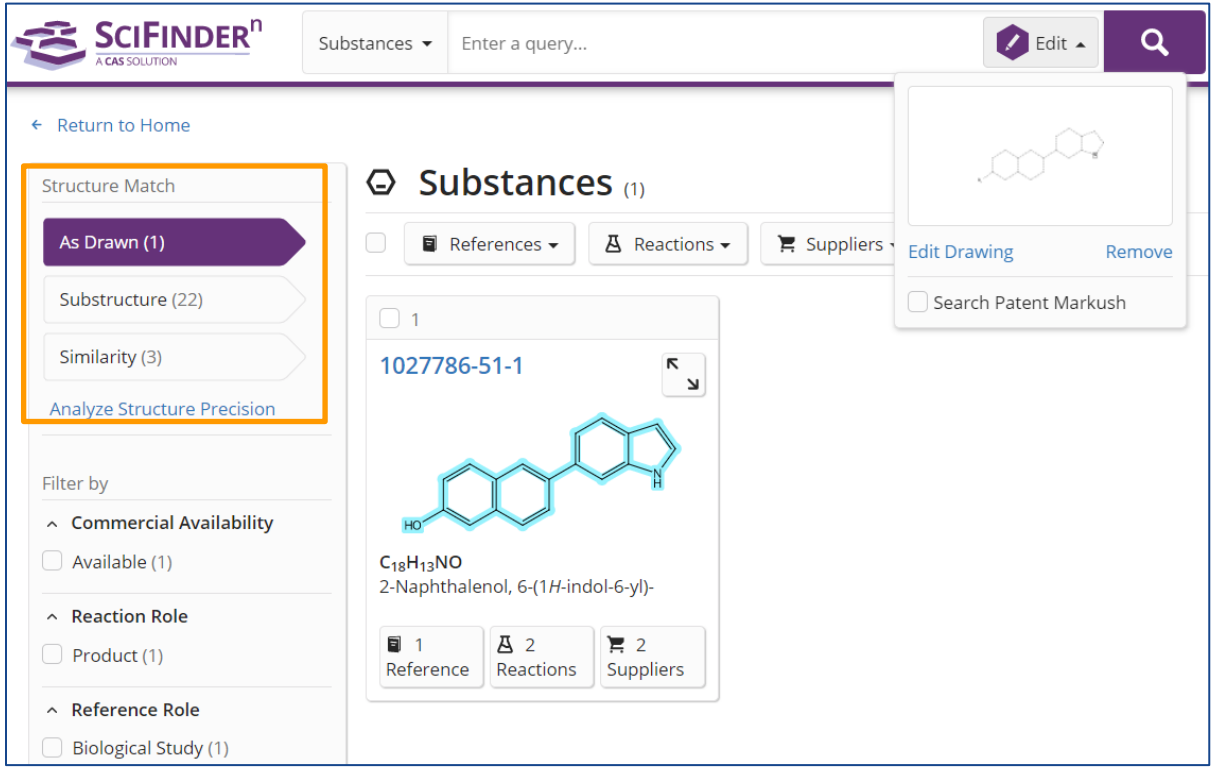
一次检索，同时获得精确结构、亚结构和相似结构结果



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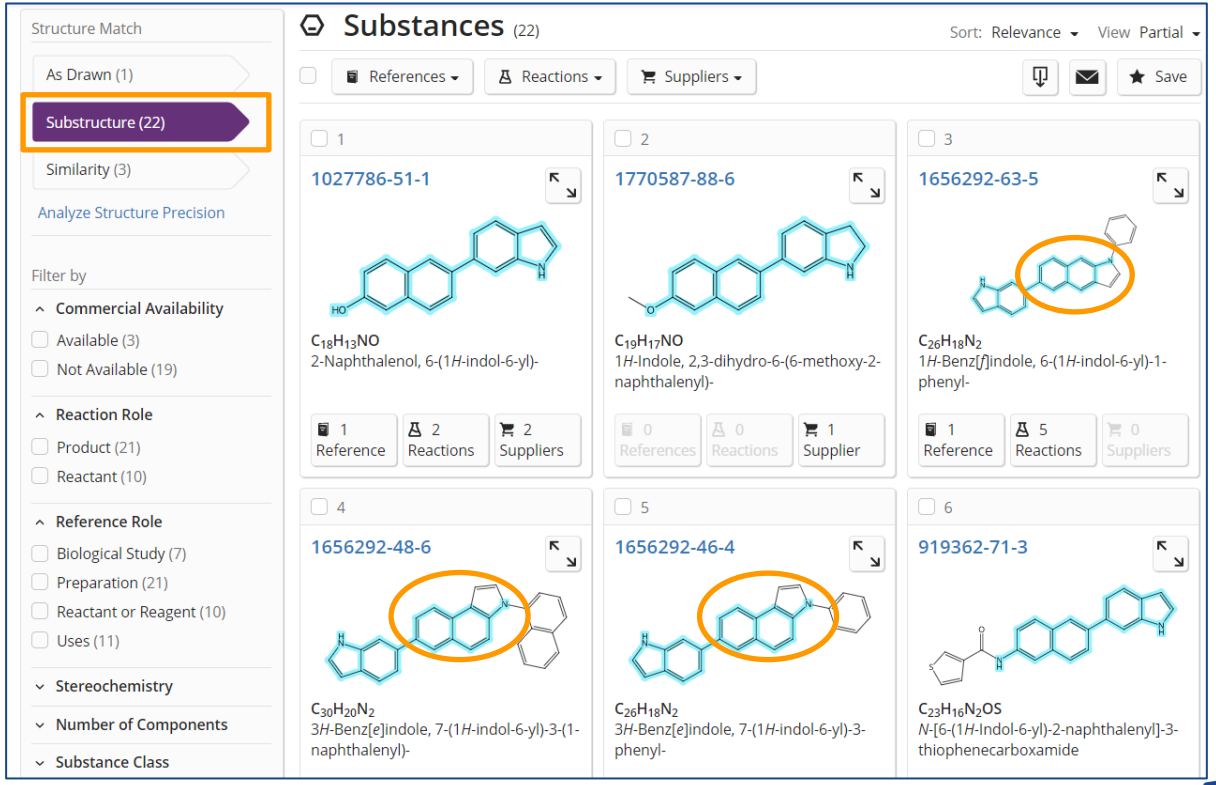
浏览亚结构检索结果，完善检索结构



如果不希望母核上出现并环，可使用环锁定工具修改检索结构

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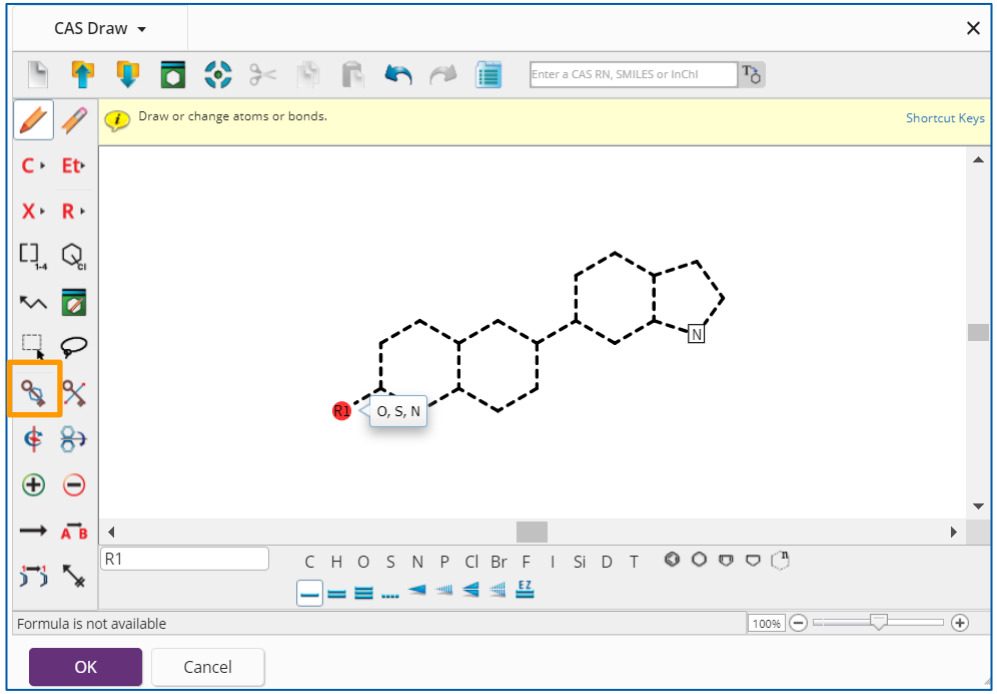
进一步修改检索结构式



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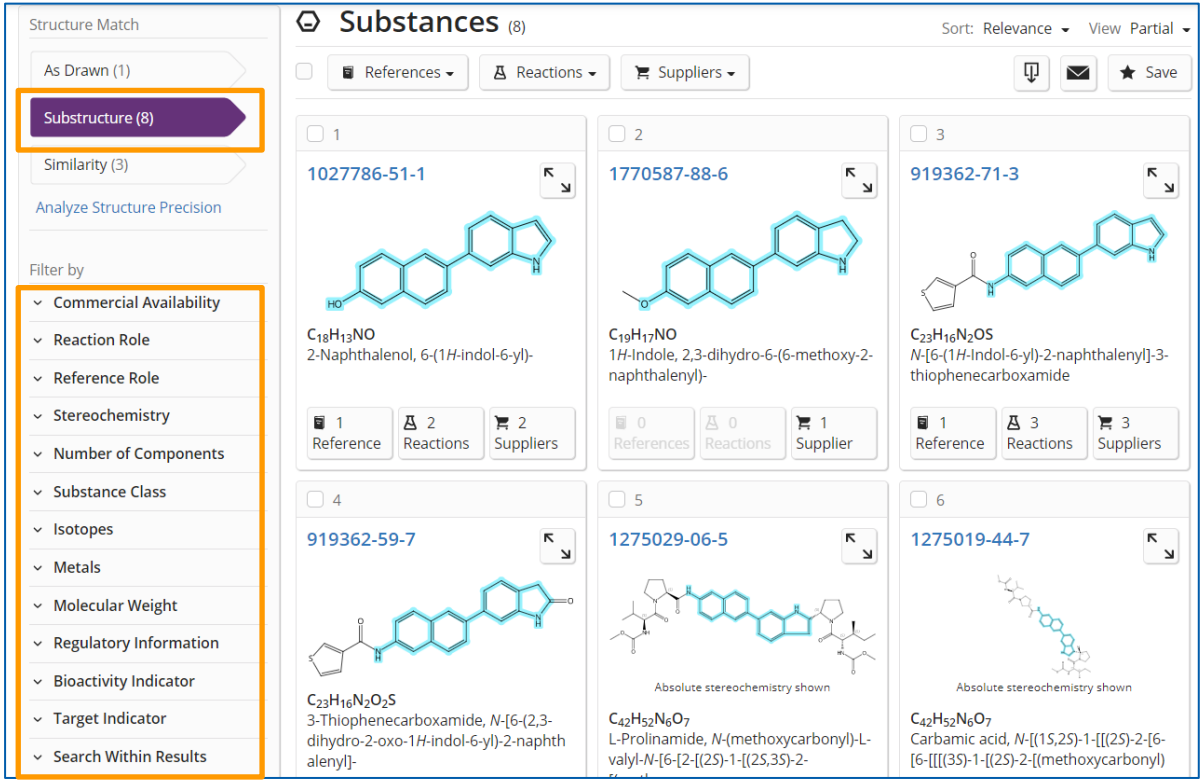
可进一步通过左侧聚类项，分析物质的理化属性、生物活性和研究角色等信息



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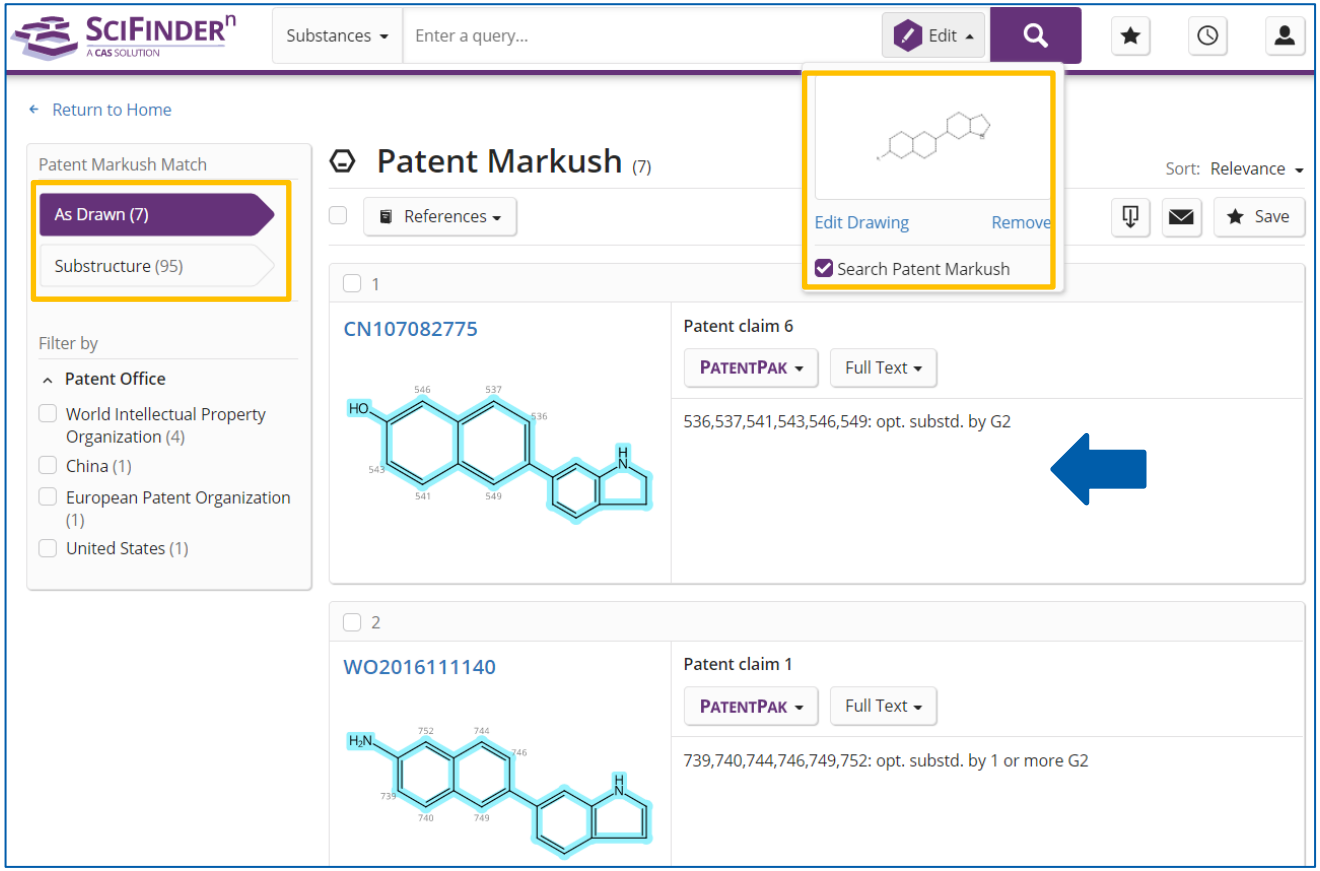

同时需要进行Markush结构检索，尽可能全面地获取公开的结构信息

根据匹配的结构结果、取代关系和原文匹配位置描述，再通过PatentPak进入原文定位处仔细分析专利风险。

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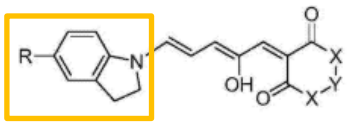
专利原文中匹配的结构展示

CN 107082775 A　　权　利　要　求　书　　1/2 页

1.一种光致变色化合物，其结构如式A所示，



A

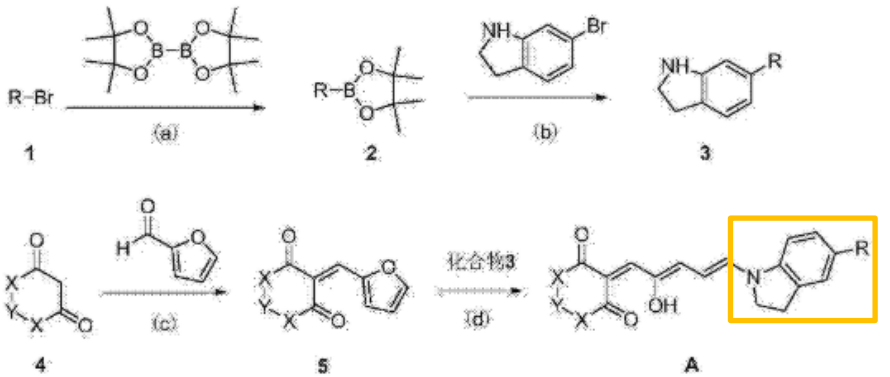
其中，R是荧光基团，为取代的或未取代的萘，蒽，芘，1,8-萘酰亚胺，氧杂蒽，吡啶，吡嗪，R上的取代基为$C_{1\sim4}$烷基、卤素、羟基、$C_{1\sim4}$烷氧基或$C_{1\sim4}$烷胺基；

X是氧，Y是$C(CH_3)_2$；或者

X是$N(CH_3)$，Y是C(O)。

CN 107082775 A　　权　利　要　求　书　　2

6.制备权利要求1或2所述的光致变色化合物的方法，合成路线如下：



其中，R、X和Y的定义如权利要求1或2所述；合成过程包括步骤：

(a)在钯催化和碱条件下化合物1与联硼酸频那醇酯反应得到化合物2；

(b)在钯催化和碱条件下化合物2与5-溴吲哚啉通过suzuki偶联反应得到化合物3；

(c)化合物4与糠醛反应得到化合物5；

(d)化合物5和化合物3反应得到目标产物A。

大纲

- 天然活性成分的提取分离和活性等研究
- 根据谱图信息来分析物质结构
- 骨架结构新颖性的确定
- 具有生物活性的衍生化结构检索
- 结构改造与合成

衍生化结构检索的目的

新颖性：天然产物提取物可能是全新的化合物，也有可能已被现有文献报道。

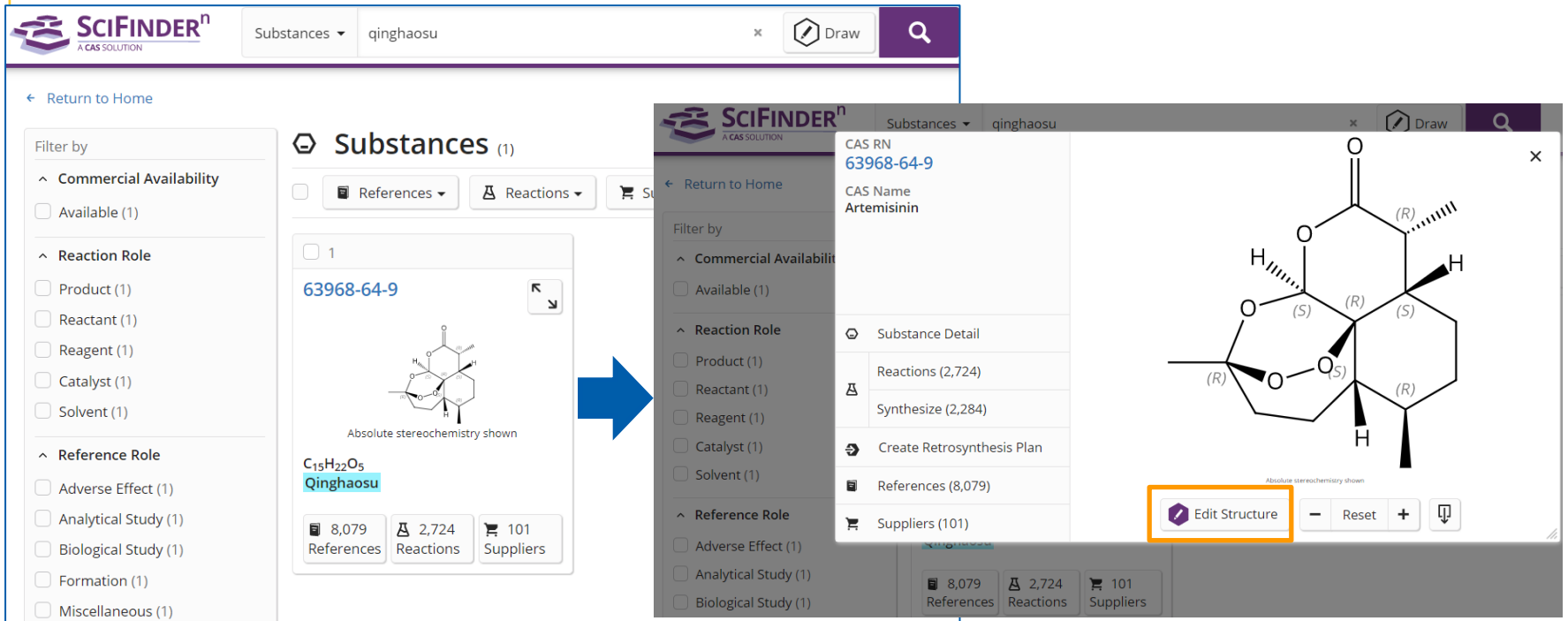
生物活性：提取物可能具有显著的生物活性，也有可能没有足够的生物活性特征。

稳定性：很多提取物稳定性并不理想。

还有**生物利用度**和**毒性**等各种直接成药的缺陷。

无论是为了提高天然提取物的生物活性、生物利用度、增强稳定性、降低毒性，还是为了创造新分子等，都可以尝试通过研究结构衍生化来实现。

例：青蒿素的生物利用度低，需要通过结构改造来研究其衍生化合物



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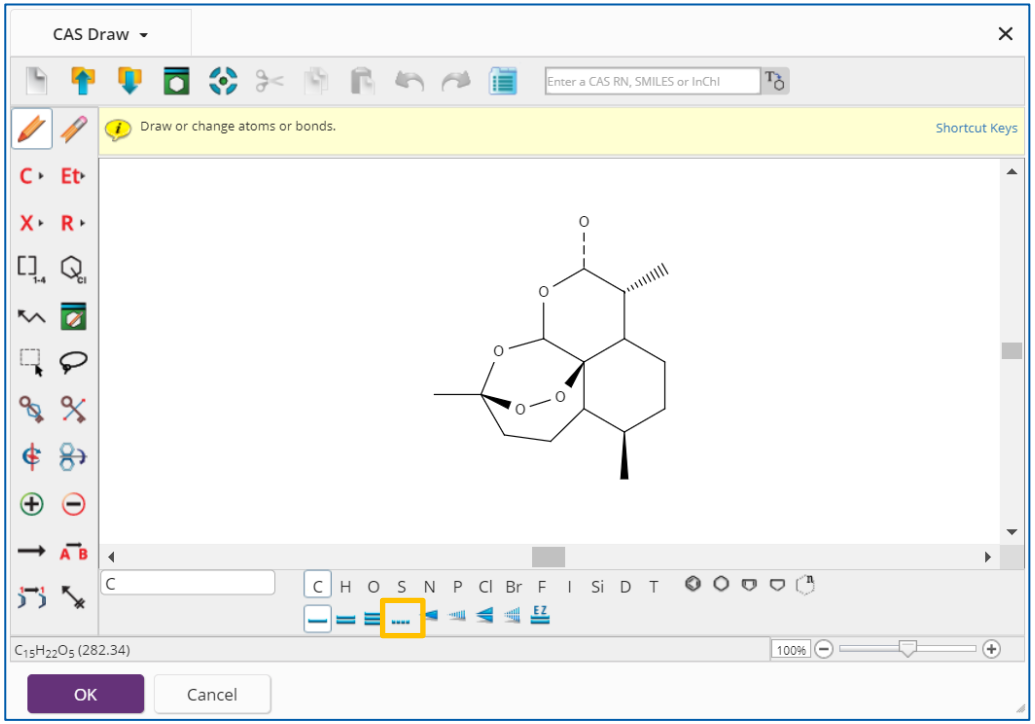

根据需要，通过CAS Draw中的绘图工具修改母核结构

考虑从何处着手衍生化，

然后限定结构检索式

结构编辑器使用指南
https://scifinder-n.cas.org/help/#t=Drawing_Search_Queries%2FDrawing_with_CAS_Draw.htm

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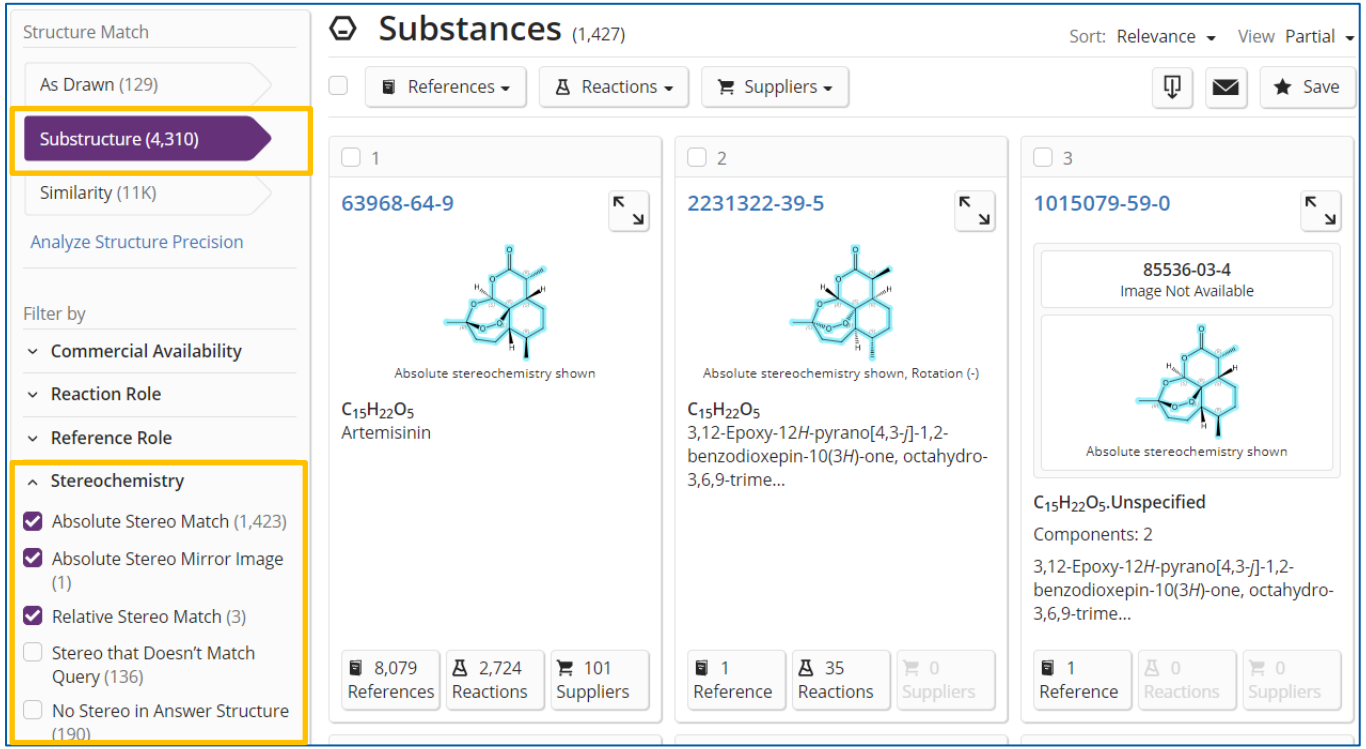
通过亚结构结果获取含有同一母核的结构



根据Stereochemistry获取各类相关手性的物质结果

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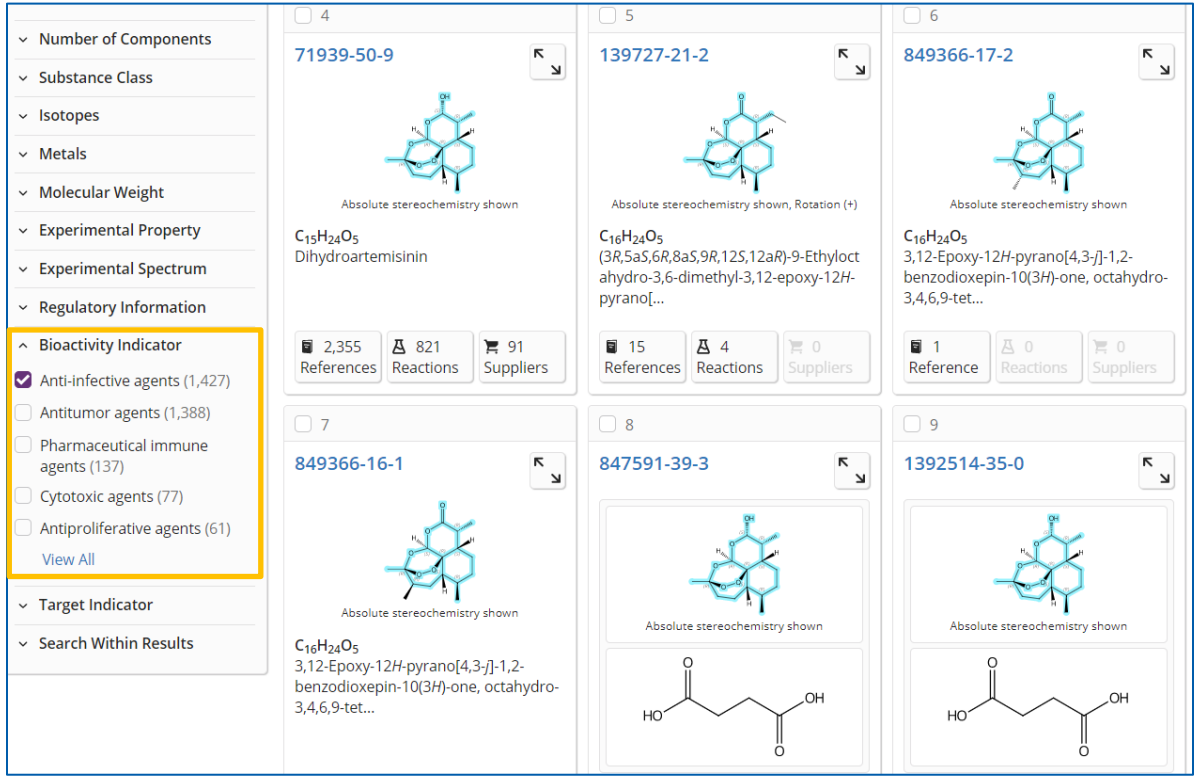
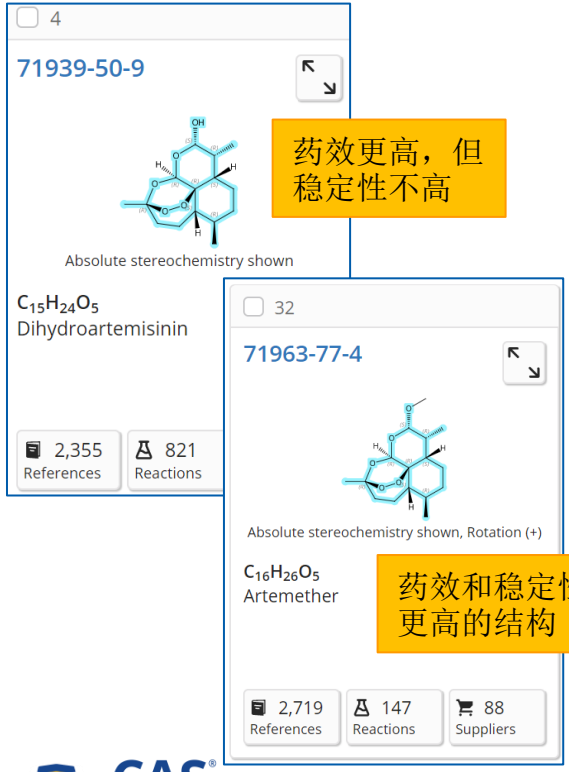
根据Bioactivity Indicator,筛选感兴趣的生物活性





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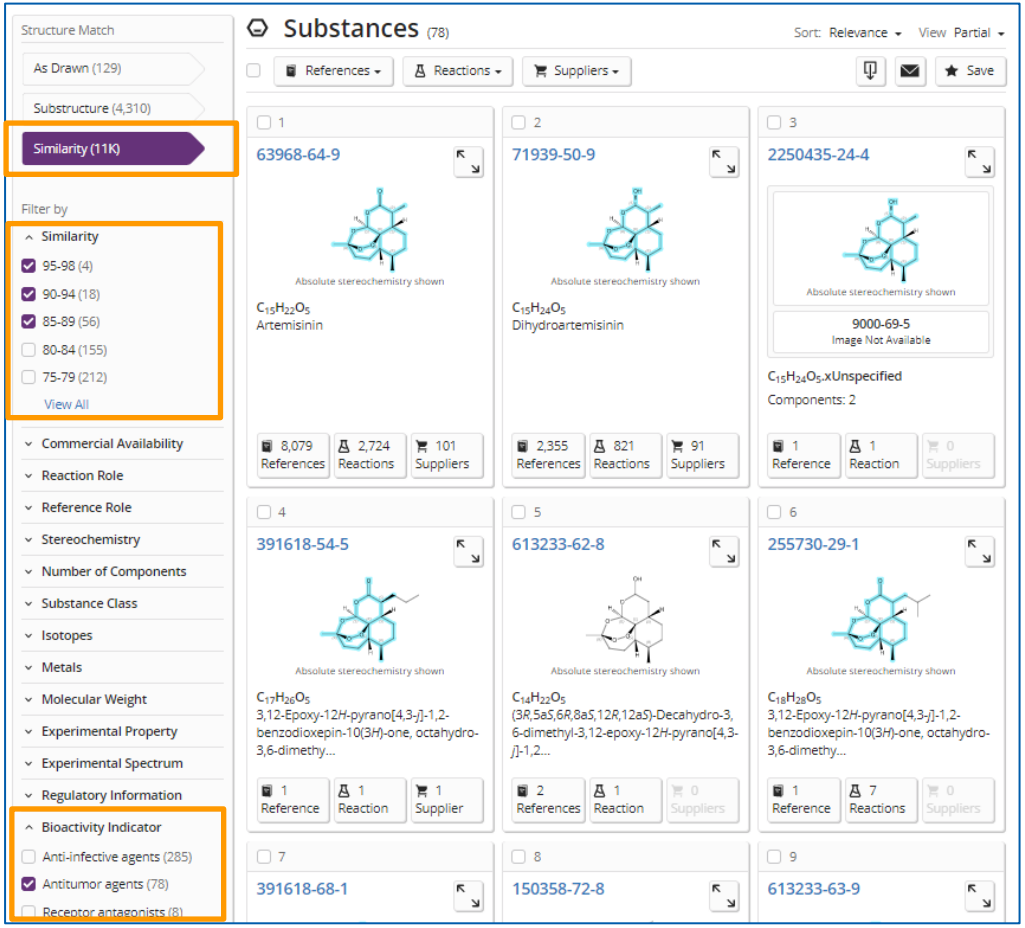

通过Similarity的结果，获取更广泛的相似骨架结构；并继续通过Bioactivity Indicator，发现其对应的潜在功效

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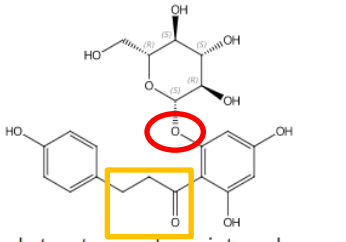
大纲

- 天然活性成分的提取分离和活性等研究
- 根据谱图信息来分析物质结构
- 骨架结构新颖性的确定
- 具有生物活性的衍生化结构检索
- 结构改造与合成

例1：提高稳定性的结构改造

60-81-1

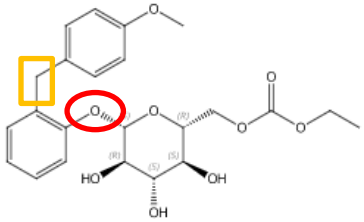


Absolute stereochemistry shown

$C_{21}H_{24}O_{10}$
Phloridzin

天然提取物根皮苷

408504-26-7

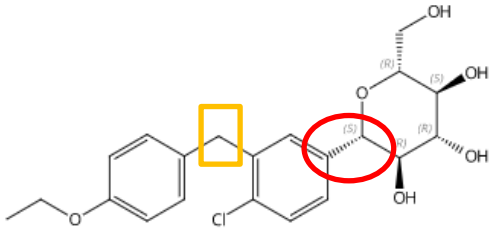


Absolute stereochemistry shown

$C_{23}H_{28}O_9$
Sergliflozin etabonate

结构改造物A

461432-26-8

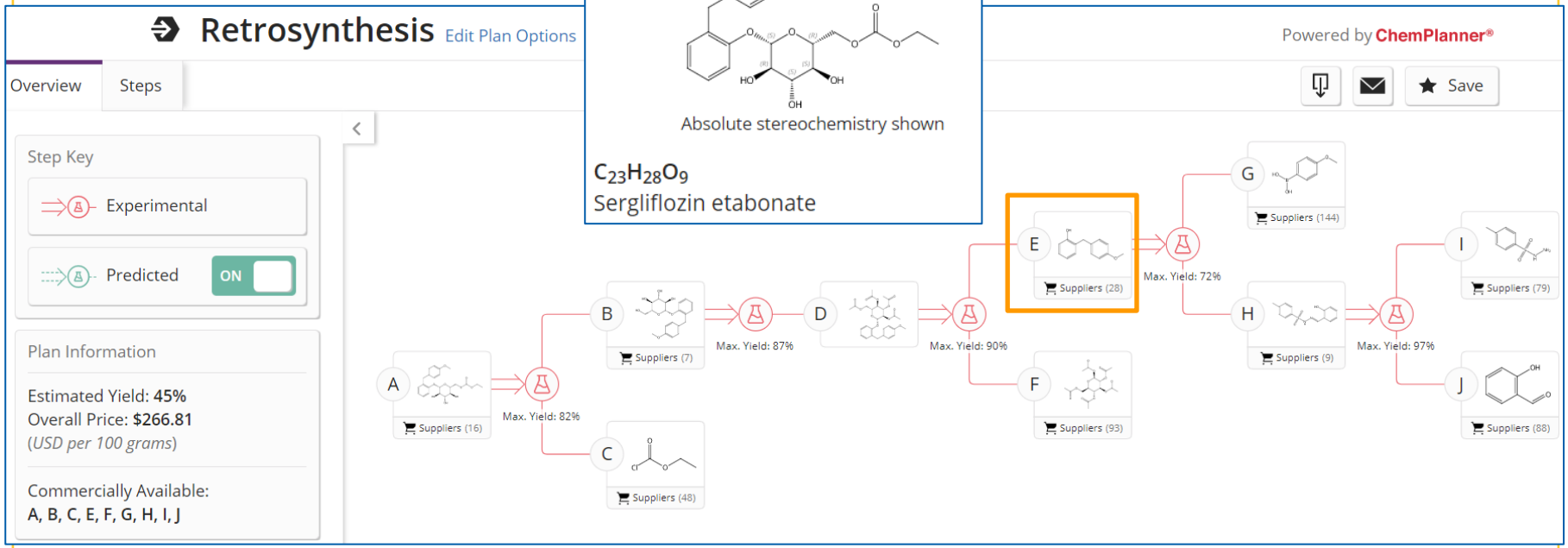


Absolute stereochemistry shown, Rotation (+)

$C_{21}H_{25}ClO_6$
Dapagliflozin

结构改造物B

快速纵览最优逆合成反应路线，并锁定关键起始原料和反应类型



点击每个试剂瓶查看实验条件等更为详细的合成信息

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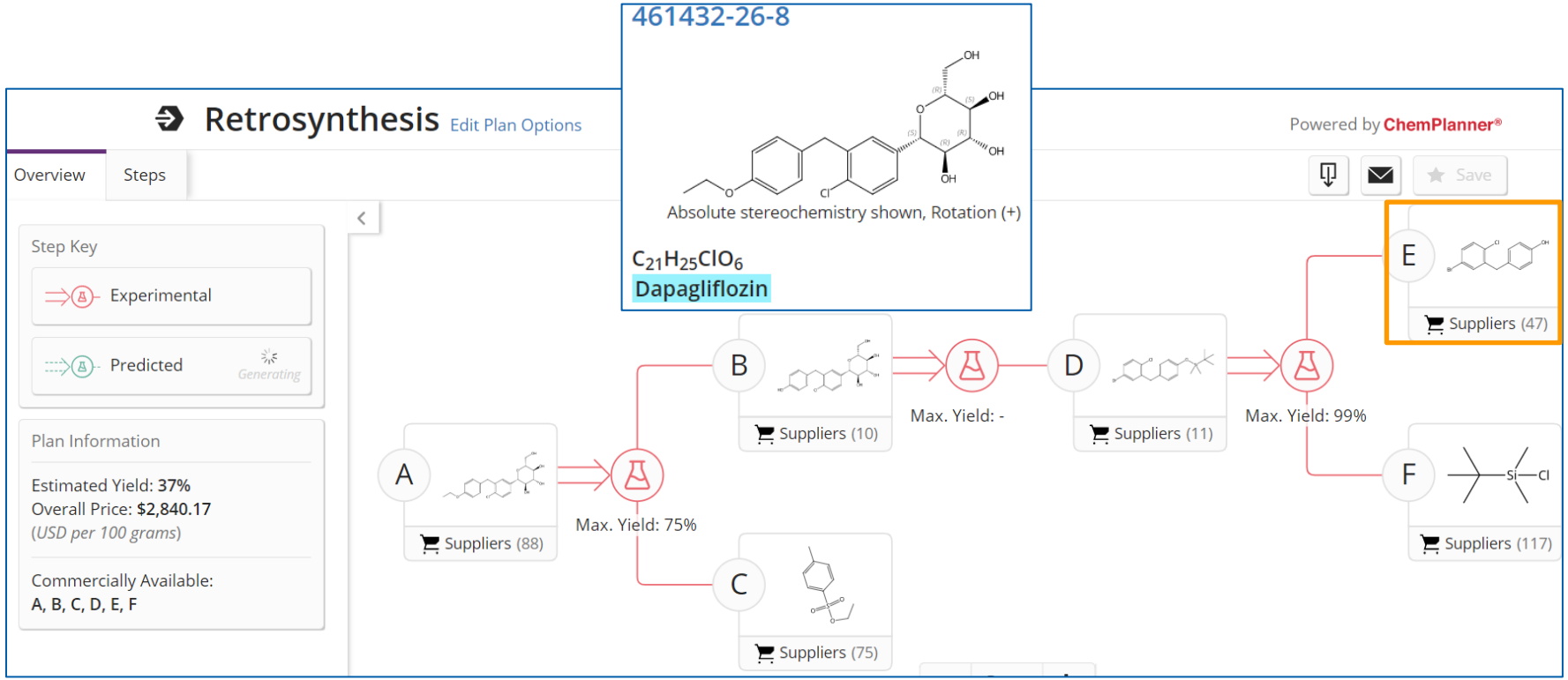
快速纵览最优逆合成反应路线，并锁定关键起始原料和反应类型



点击每个试剂瓶查看实验条件等更为详细的合成信息

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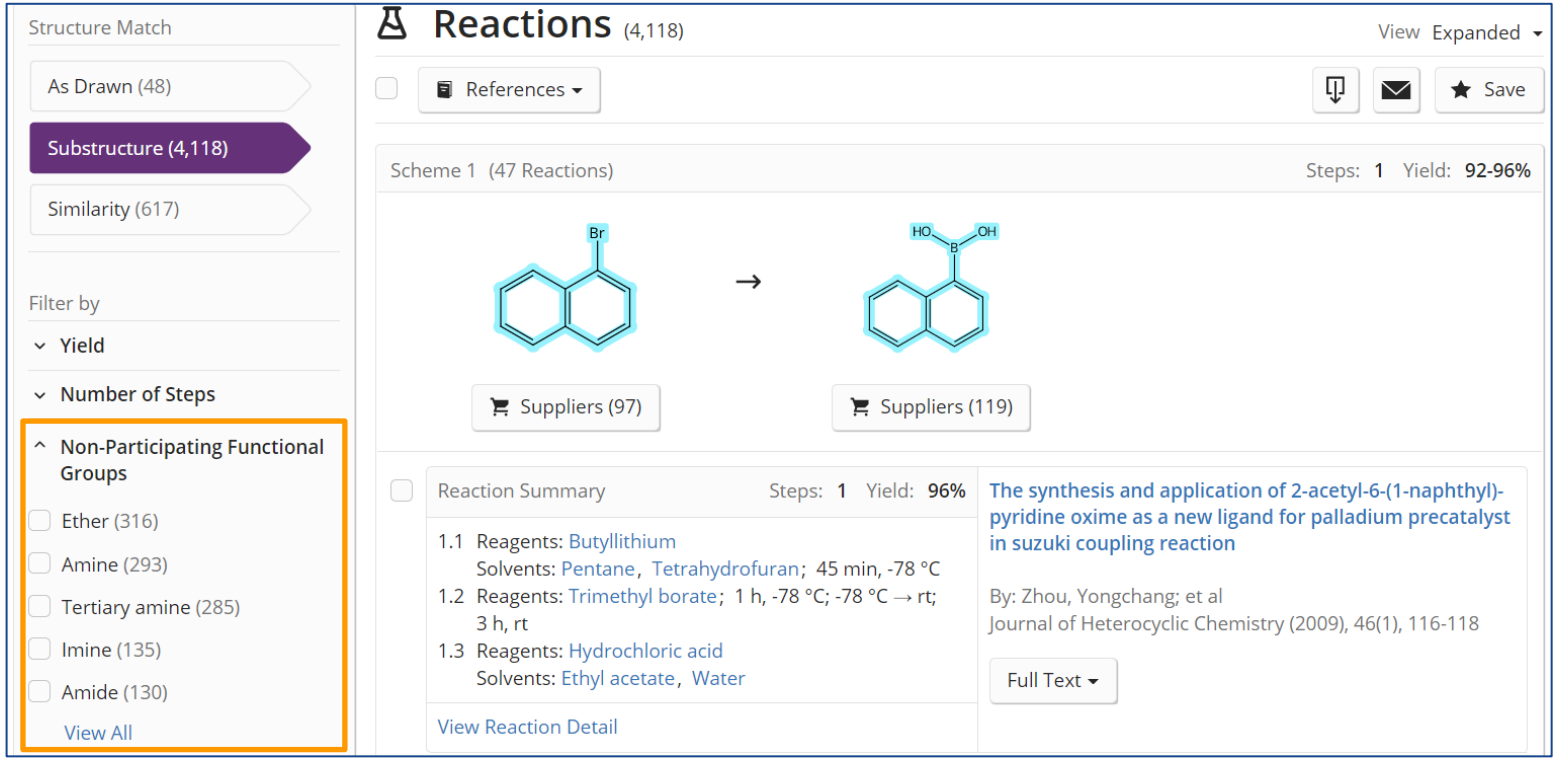
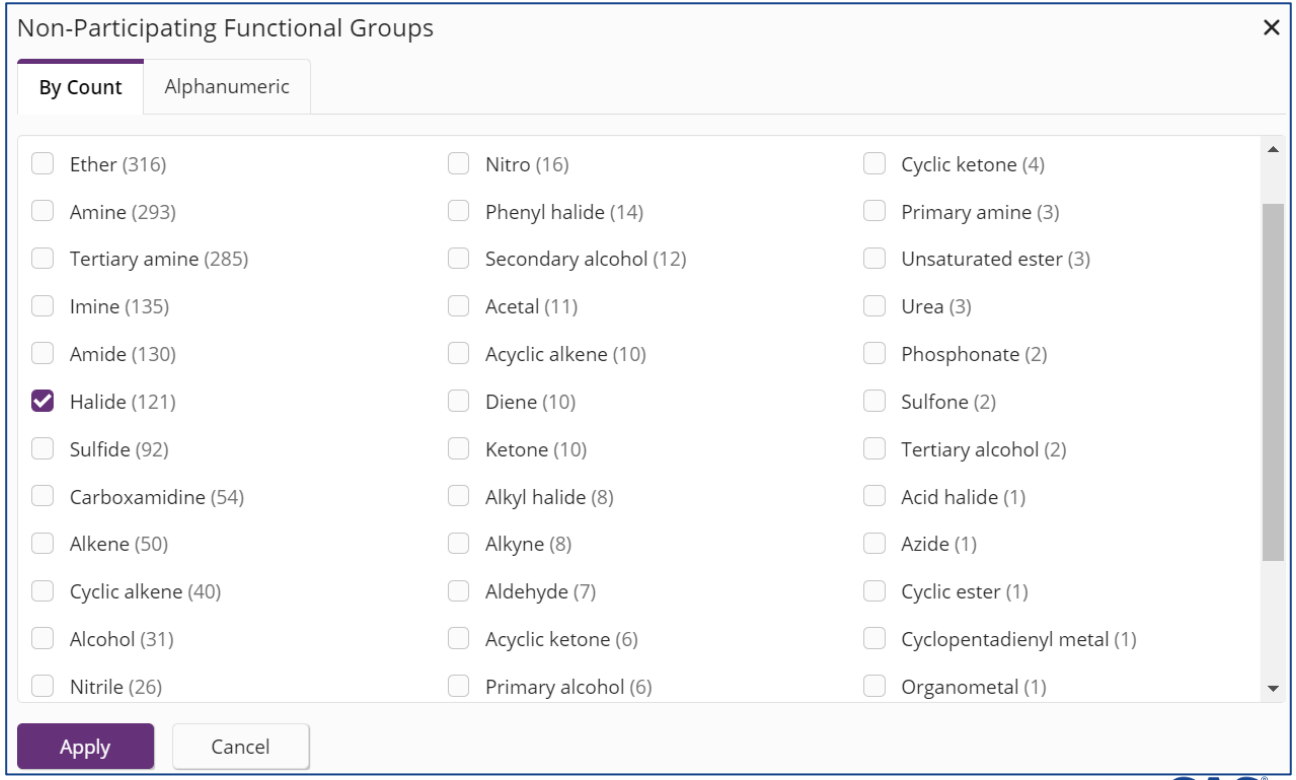
例2：通过Non-Participating Functional Groups，查看反应前后没有发生变化的官能团列表

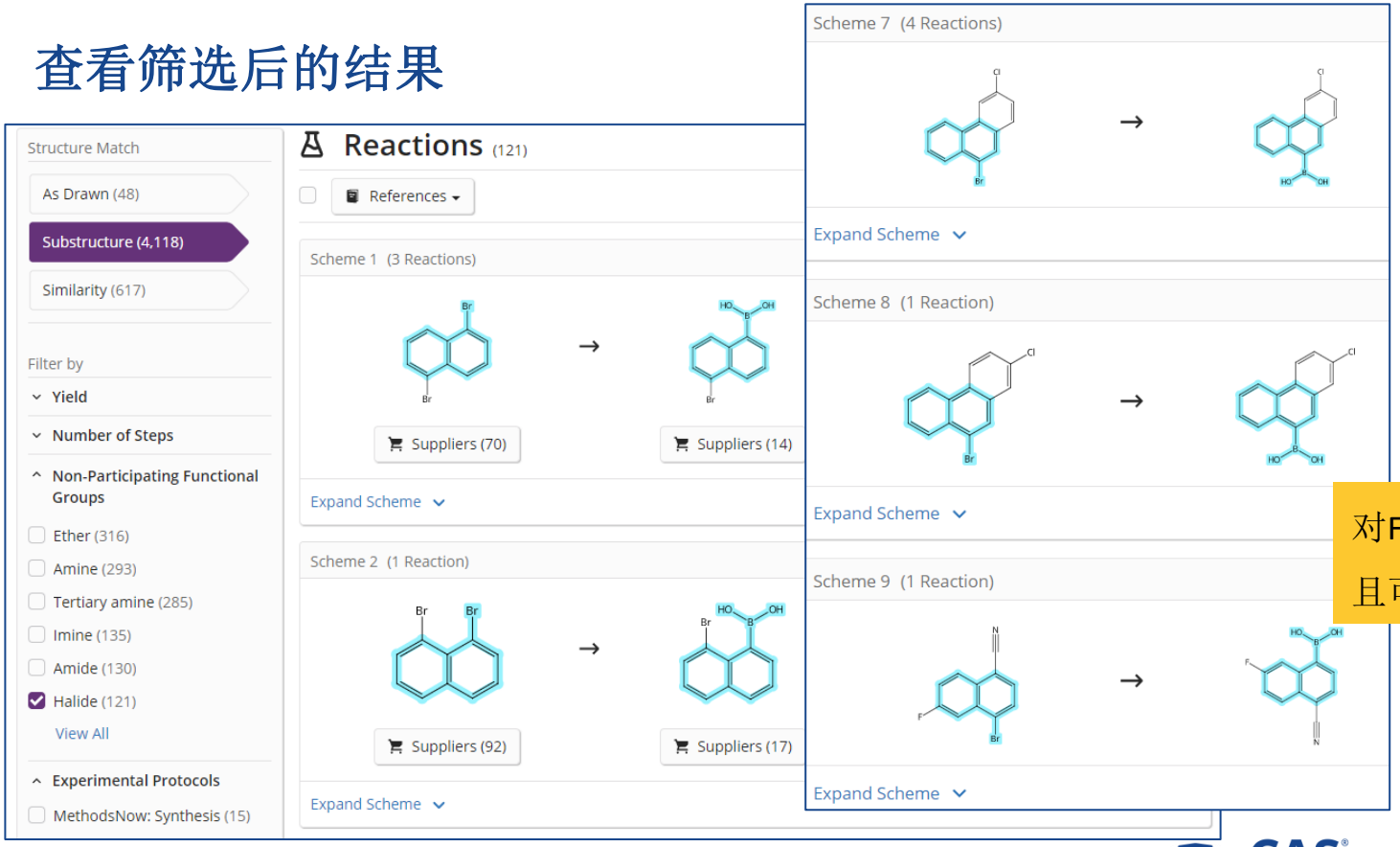


点击View All查看所有的Non-Participating Functional Groups

浏览同时共存的官能团，并根据拟采用的原料结构选择不参与反应的官能团



查看筛选后的结果



对F, Cl和Br有选择性，

且可控制Br的反应当量

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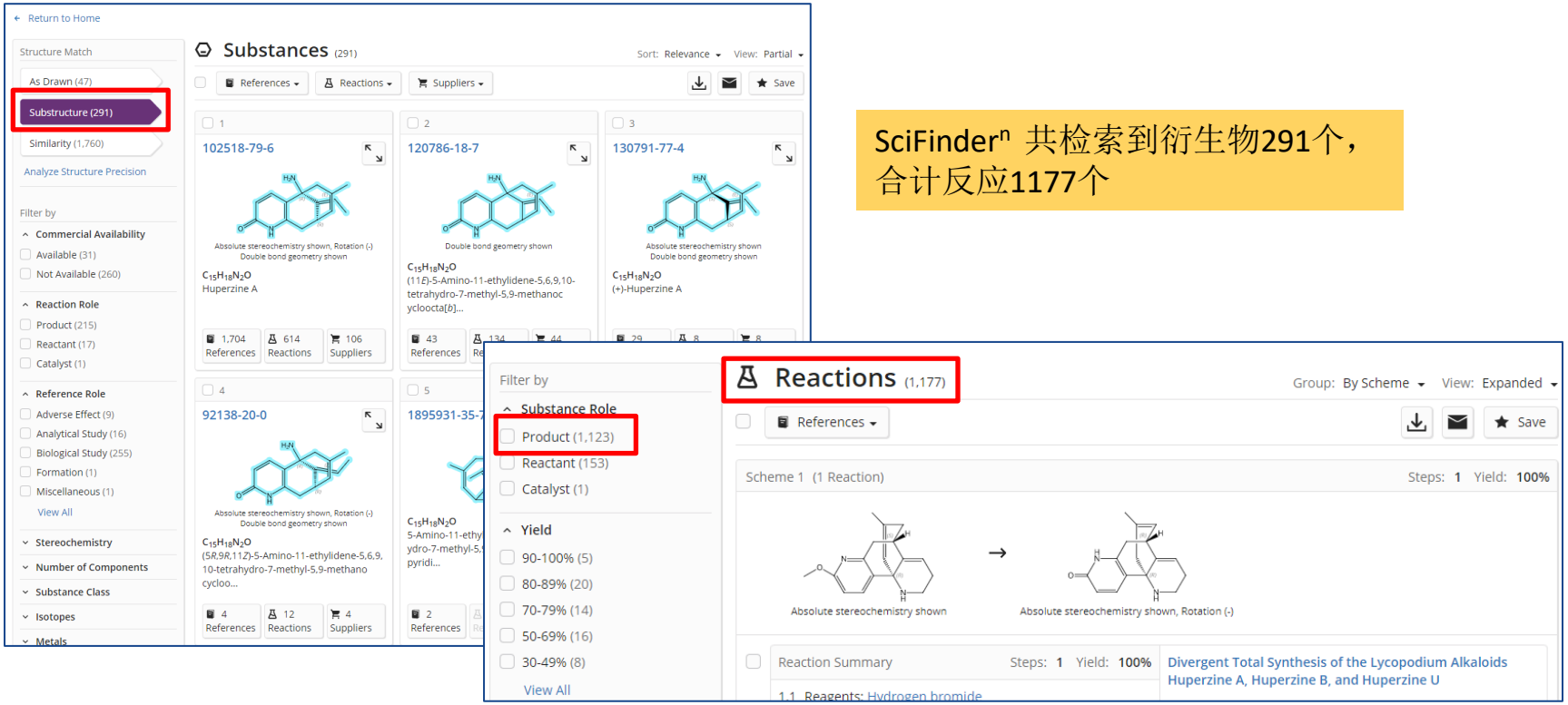
例3：已知天然产物结构，获取其衍生物及合成信息

- 以石杉碱甲为例：CAS No. 102518-79-6
- 执行相同检索策略：结构式检索

SciFinder^{n}结果



SciFinder^n 共检索到衍生物291个，合计反应1177个

在线学习资源

1.CAS官网上的培训资料
https://www.cas.org/support/training/scifinder-n

2.SciFinder-n Help使用指南
https://scifinder-n.cas.org/help/#t=Searching_in_SciFinder-n%2FIntroduction_to_searching.htm

3.SciFinder-n What's New功能更新动态
https://scifinder-n.cas.org/help/#t=About_SciFinder-n%2FSciFinderN_Release_Notes%2FSciFinderN_Release_Notes.htm

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