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SciFinder物质检索难点解析

中国药科大学

SCIFINDER®
A CAS SOLUTION

提纲

- 快速获得物质的生物活性及靶点信息
- 检索具有相同结构特征物质
- Markush检索
- 如何判断物质的新颖性
- 筛选天然产物
- 查找具有相同药效组份的物质
- 根据构效关系寻找潜药
- 如何检索有同位素标记的物质

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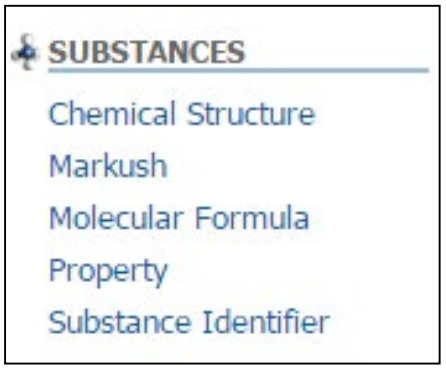
SciFinder检索选项——物质检索

- 物质检索方法
  - —结构式检索
  - —分子式检索
  - —理化性质检索
  - —物质标识符检索：化学名称，CAS RN



- 物质检索策略推荐
  - —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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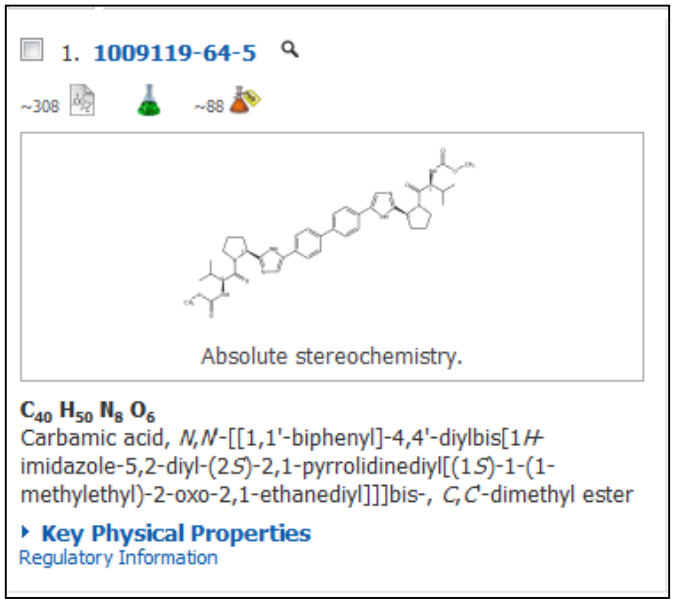
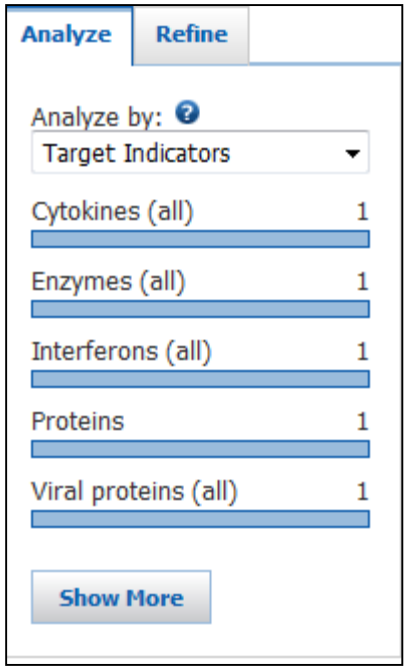
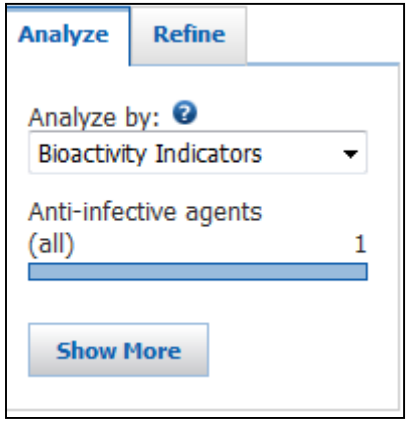
快速获得物质的生物活性及靶点信息





作用靶点



生物活性

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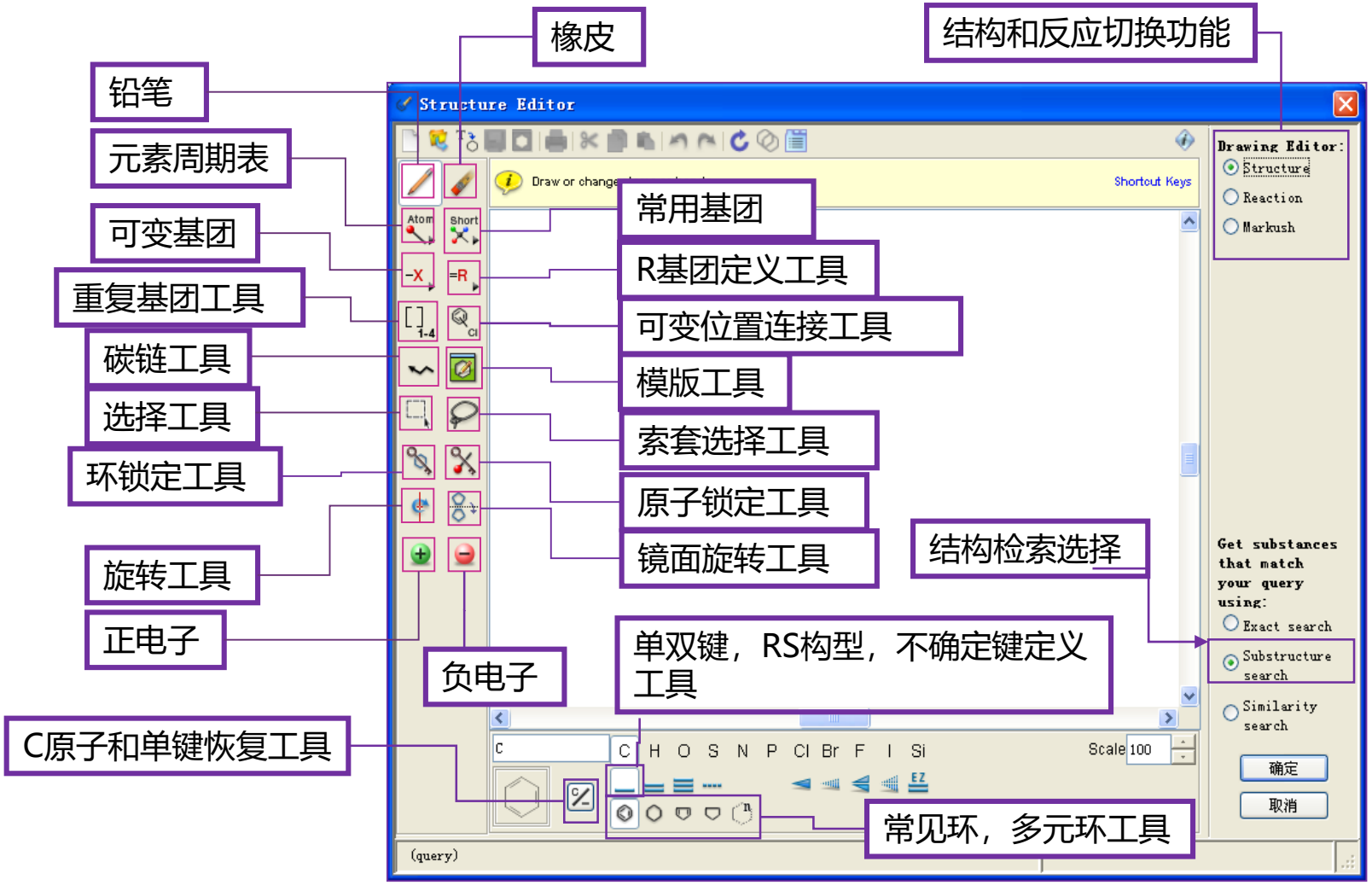
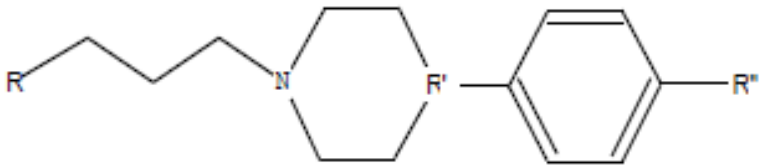
绘图面板


橡皮
结构和反应切换功能
铅笔
元素周期表
可变基团
重复基团工具
碳链工具
选择工具
环锁定工具
旋转工具
正电子
C原子和单键恢复工具
负电子
常用基团
R基团定义工具
可变位置连接工具
模版工具
索套选择工具
原子锁定工具
镜面旋转工具
结构检索选择
单双键，RS构型，不确定键定义工具
常见环，多元环工具
Structure Editor
Drawing Editor:
Structure
Reaction
Markush
Shortcut Keys
Get substances that match your query using:
Exact search
Substructure search
Similarity search
确定
取消
Scale 100
(query)

检索具有相同结构特征的物质

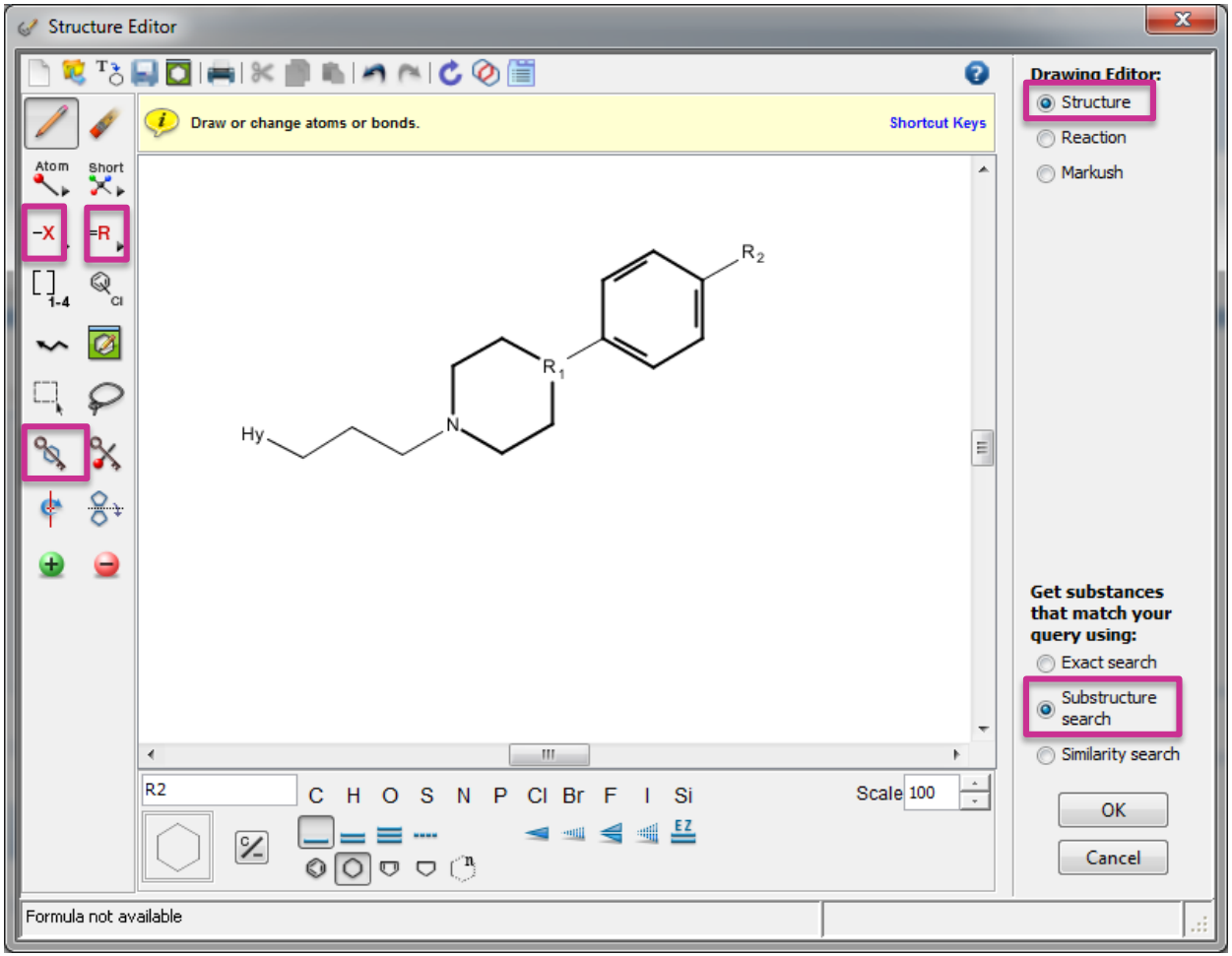
查询报道具有如下结构特征专利文献:



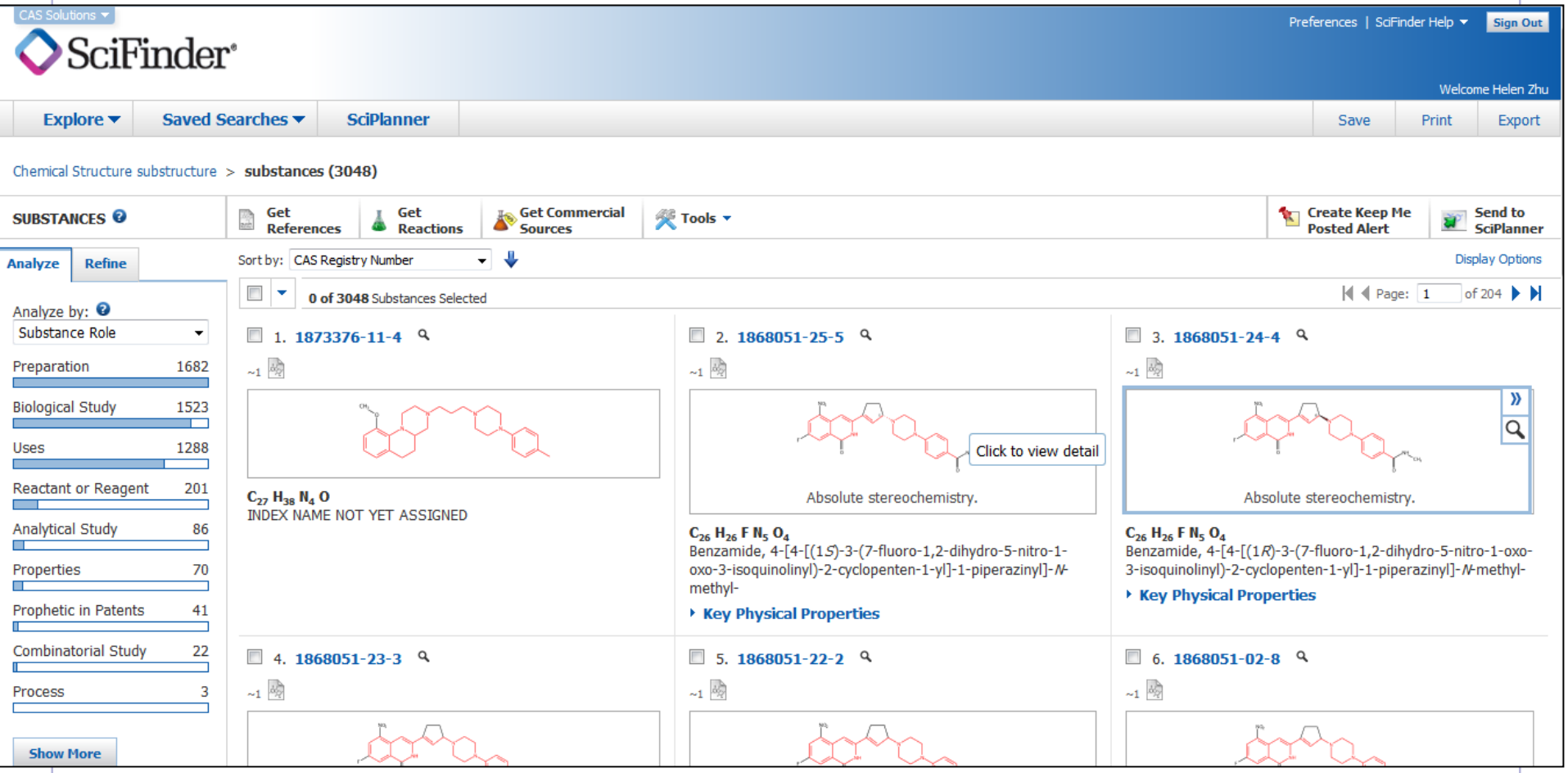
要求:

- R = 任意杂环
- R' = C, N, P
- R" = C,N
- 6 圆环均为单环
- 价键不饱和的地方均允许有取代

检索具有相同结构特征的物质



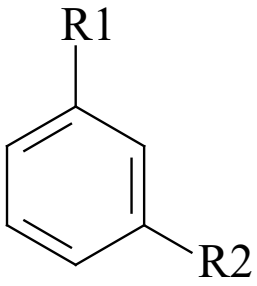
检索具有相同结构特征的物质



Markush检索

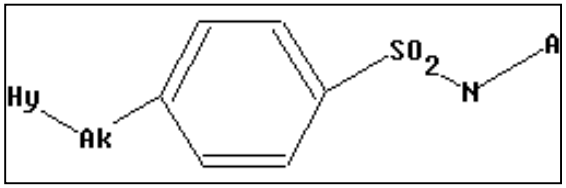
- 具体物质[Specific Substance]：
  — 以具体化学结构陈述的特定物质，会被分配CAS RN

- 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
  — 专利中所陈述的预测物质，不会被分配CAS RN
  — Markush检索，能检索到通过结构检索检不到的专利

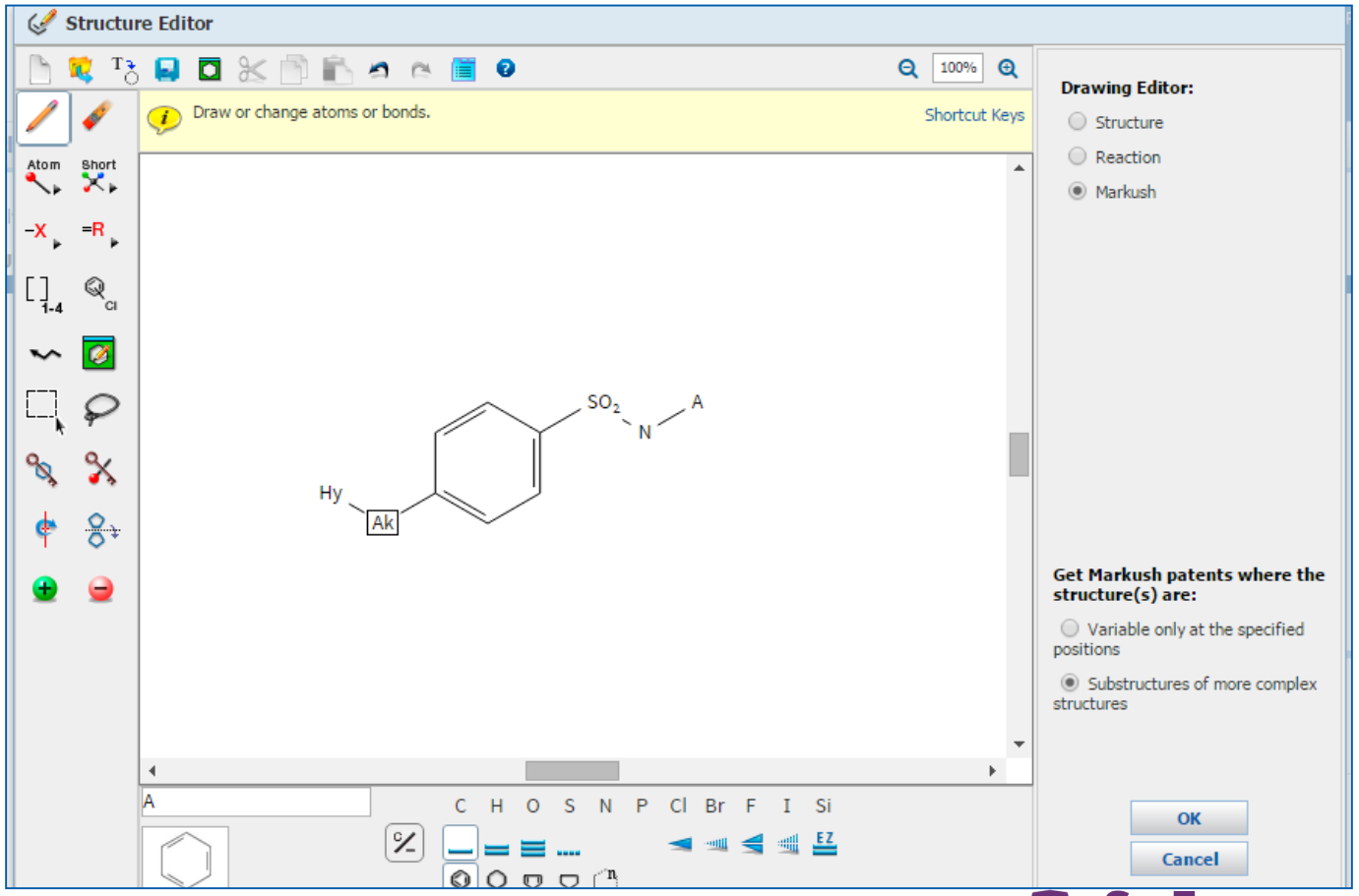


R1 = H, Br, Cl, I

R2 = Br, Cl, I, —CH_2–halogen, —CH(–CH_3)–halogen,



可用SciFinder中的Markush检索查看专利中化合物结构保护范围。



Markush检索

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Welcome Helen Zhu

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Markush substructure > **references (1969)** > Compounds and methods for anti...

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Patent 1969

Journal 1

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0 of 1969 References Selected Page: 1 of 99

1. **Compounds and methods for anticoagulation therapy**

Quick View PATENTPAK ▾

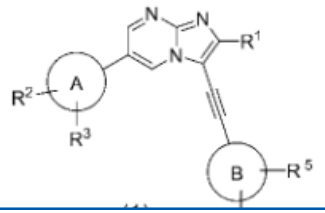
By Allende Rodriguez, Mikel; Hermida Santos, Jose; Montes Diaz, Ramon; Oyarzabal Santamarina, Julen
From PCT Int. Appl. (2016), WO 2016120432 A1 20160804. | Language: English, Database: CAPLUS

The invention relates to certain compds. that are inducers of Heat shock 70 kDa protein 1A/1B (HSPA1A/B) and their use for anticoagulation therapy; and to a method for anticoagulation therapy that comprises the administration of one of these inducer compds. It has been here proved that induction of Heat shock 70 kDa protein 1A/1B by administration of one of these inducer compds. has antithrombotic effects without accelerating or altering bleeding time.

2. **Preparation of new imidazopyrimidine derivatives as negative allosteric modulators of metabotropic glutamate receptor subtype 2 (mGlu2 receptor)**

Quick View PATENTPAK ▾

By Urashima, Kuniko; Tojo, Kengo; Koike, Shoko; Masumoto, Shuji
From Jpn. Kokai Tokkyo Koho (2016), JP 2016132660 A 20160725. | Language: Japanese, Database: CAPLUS



The title imidazo[1,2-a]pyrimidine derivs. I [R^1 = H or halogen; ring A Ph or pyridyl; R^2, R^3 (same or different) = hydrogen, halogen, C_{1-4} alkyl or C_{1-4} alkoxy each optionally substituted with 1-5 halogen atoms; or in case where R^2 and R^3 are at the adjacent substitution position, R^2 and R^3 together with ring A form C_{5-8} carbocyclic ring (optionally substituted with 1-5 halogen or 1-2 hydroxy group) or 5- or 6-membered satd. heterocyclic ring; ring B = Ph or pyridyl; R^4, R^5 (same or different) = H, halogen, hydroxy, amino, -C(O)OR^a, -C(O)NR^aR^b, SO_3H, $SO_2NR^aR^b$, SO_2R^b, or $NR^aSO_2R^b$; R^a, R^b (same...

全部是专利

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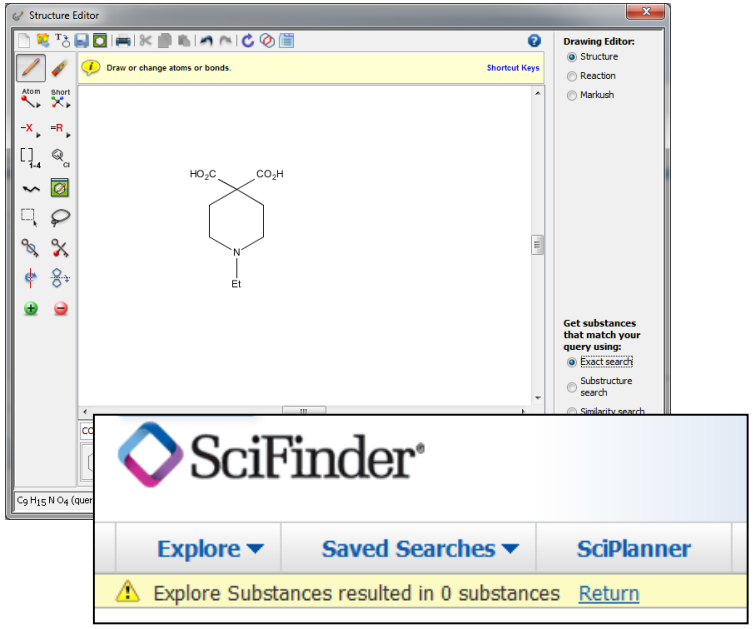
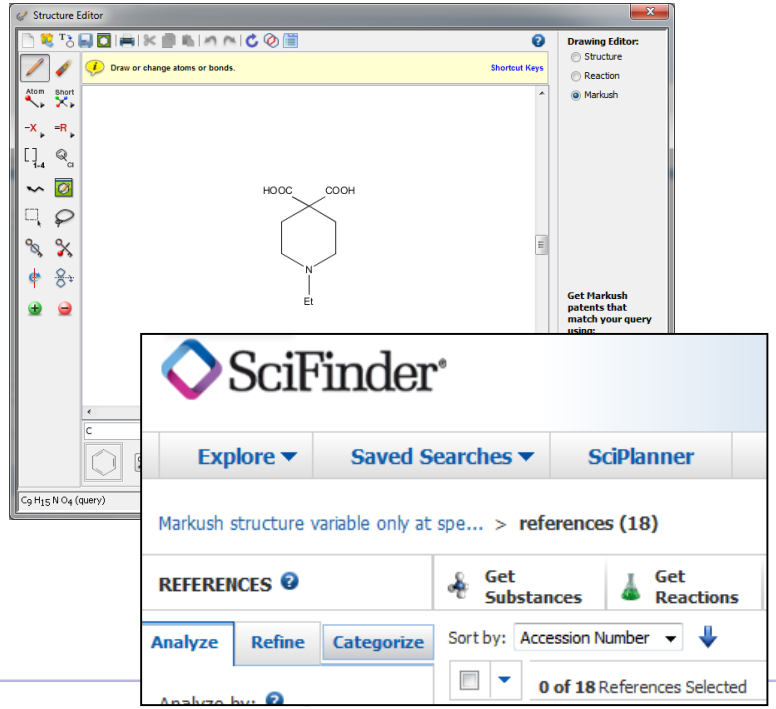
如何判断结构的新颖型

新颖性：是否存在？是否能申请专利？

SciFinder相关物质库：Registry和Marpat

检索方法：物质检索？Markush检索？





如何判断结构的新颖型

- SciFinder中的Markush检索仅仅只做初步的专利评估
- 尽量不要画具体结构进行检索
- 如果Markush检索结果为零，请对结构进行适当的扩展后再检索。
- 检索结果仍然为零，不代表一定没有被其他专利保护

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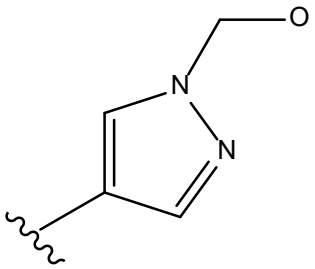
如何判断结构的新颖型



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Markush substructure > **references (0)**

REFERENCES

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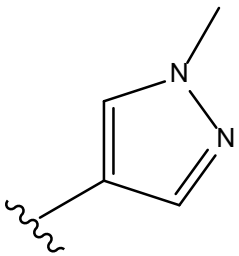
No references available



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Analyze by: Author Name ▾

Chi Jiangtao 1
Dong Qing 1
Tu Wangyang 1
Xu Guoji 1
Zhang Haitang 1

0 of 1 Reference Selected

1. **Preparation of imidazo[5,1-α]isoindole derivatives useful for the treatment of diseasess related to IDO-mediated tryptophan metabolic pathways**

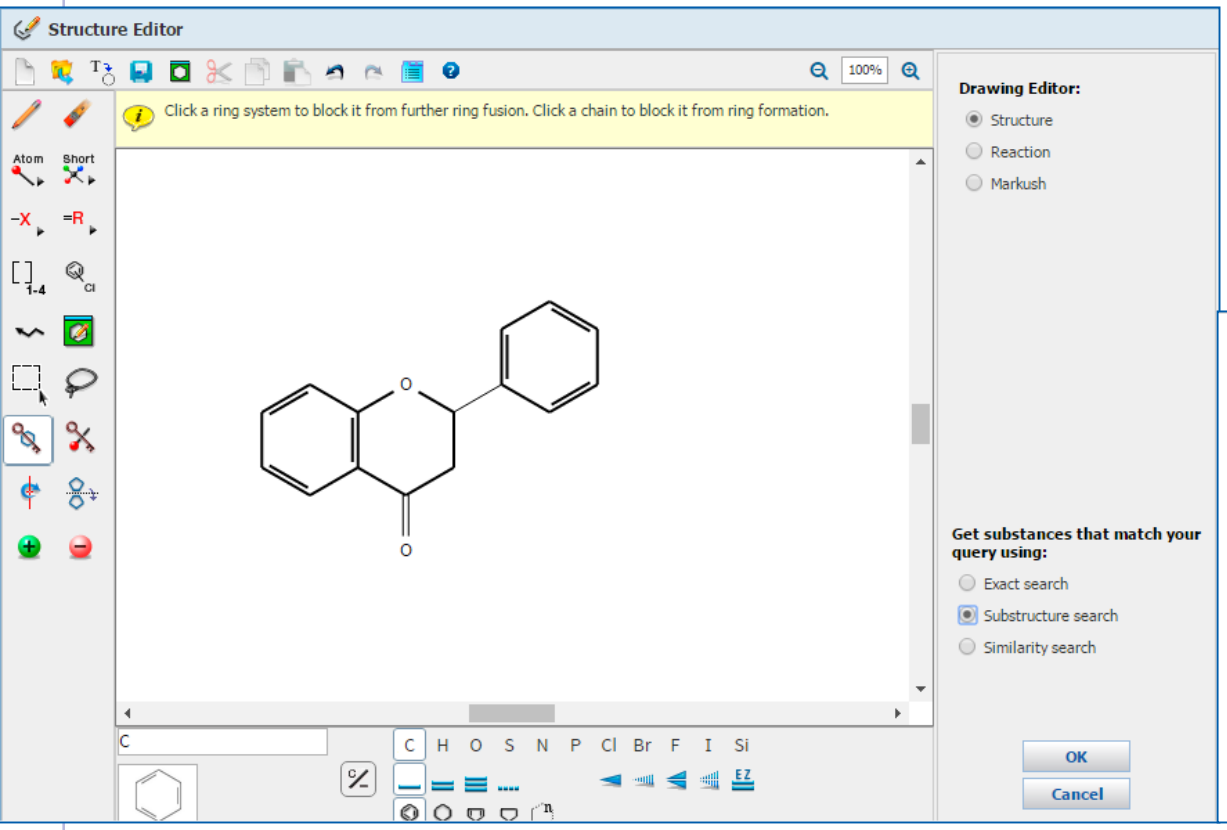
Quick View PATENTPAK

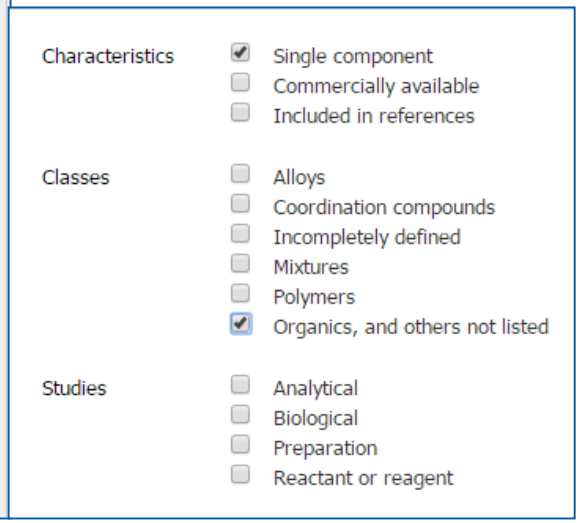
By Tu, Wangyang; Xu, Guoji; Zhang, Haitang; Chi, Jiangtao; Dong, Qing
From PCT Int. Appl. (2016), WO 2016169421 A1 20161027. | Language: Chinese, Database: CAPLUS

The invention relates to imidazo[5,1-α]isoindole derivs. of formula I, method for their prepn. and their use for the treatment of diseasess related to IDO-mediated tryptophan metabolic pathways. Compds. of formula I.bul.M$_y$, wherein A is cycloalkyl, heterocycle and (hetero)aryl; R^1 is H, alkyl, cycloalkyl, (hetero)aryl, etc.; each R^2 is independently H, alkyl, alkoxy, halo, NO_2, etc.; each R^3 is independently H, alkyl, cycloalkyl, CN, etc.; M is inorg. acid or org. acid, preferably TFA; p is 0

其中所述的烷基、卤代烷基、环烷基、杂环基、芳基和杂芳基任选进一步被选自烷基、卤代烷基、卤素、氨基、硝基、氰基、羟基、烷氧基、卤代烷氧基、羟烷基、环烷基、杂环基、芳基、杂芳基、$-R^a$、$-OR^7$、$-C(O)R^7$、$-C(O)OR^7$、$-S(O)_mR^7$、

筛选天然产物





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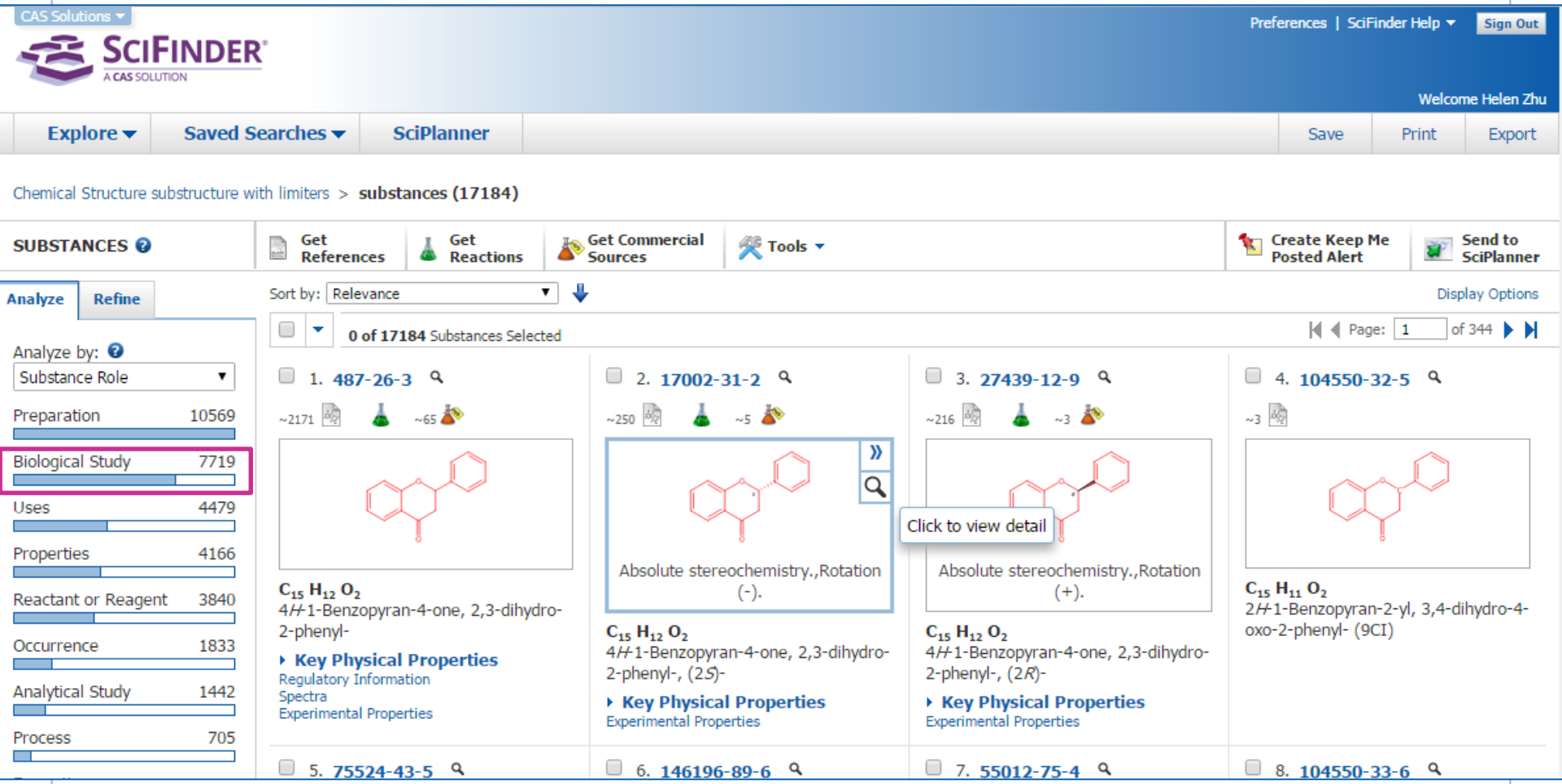
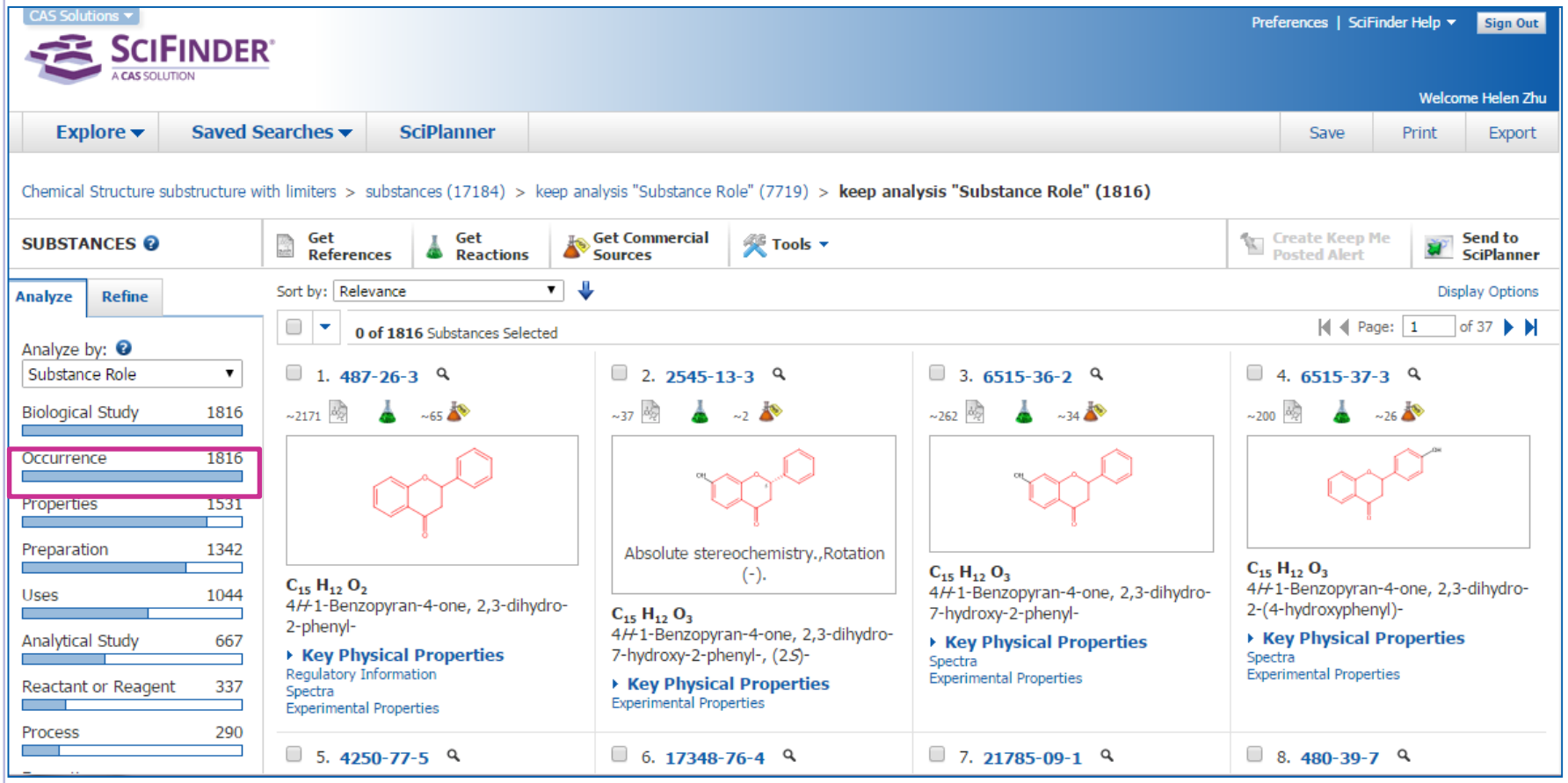
筛选天然产物



哪些黄酮类物质是天然存在的呢？

筛选天然产物



两次分析功能组合：

Analyze — Substance Role — Biological Study & Occurrence

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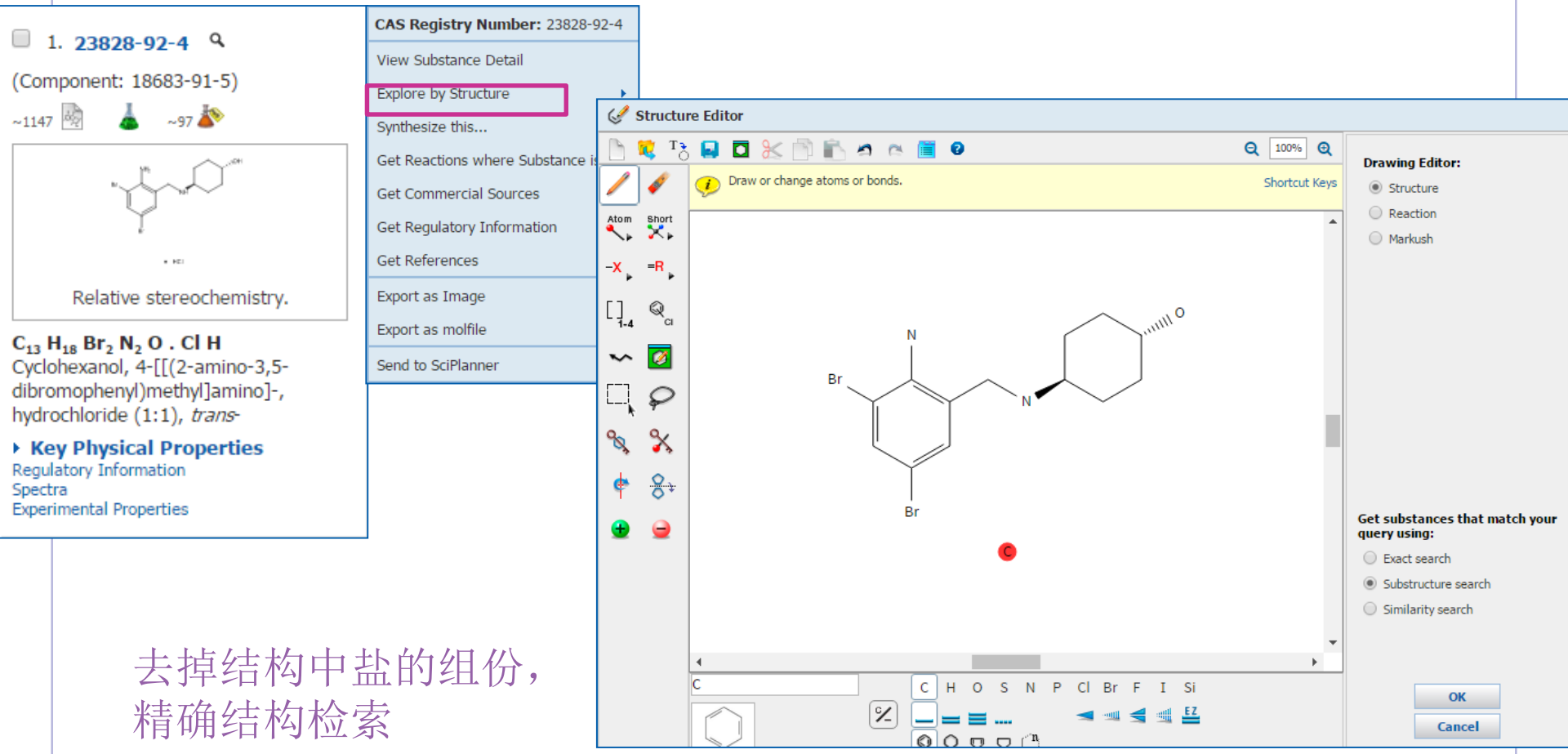
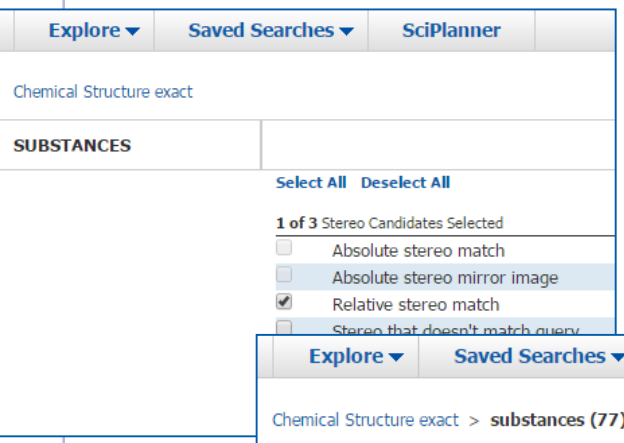
相同药效组份的物质

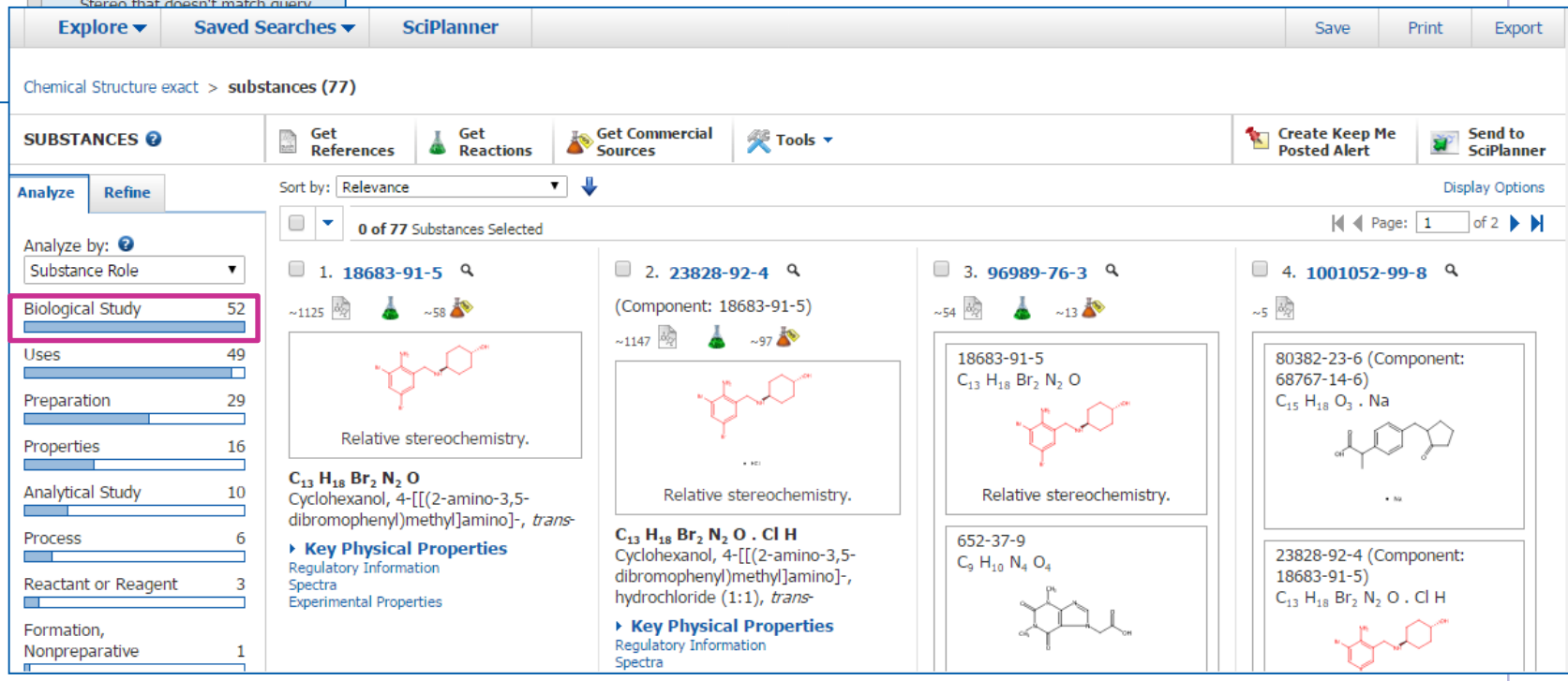
寻找与沐舒坦有相同药效组分的药物？



去掉结构中盐的组份，
精确结构检索

相同药效组份的物质





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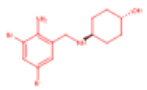
相同药效组份的物质

3. **96989-76-3**

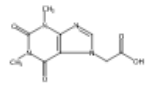
~54 ~13

18683-91-5
$C_{13}H_{18}Br_2N_2O$



Relative stereochemistry.

652-37-9
$C_9H_{10}N_4O_4$



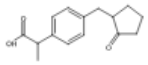
$C_{13}H_{18}Br_2N_2O \cdot C_9H_{10}N_4O_4$
7*H*-Purine-7-acetic acid, 1,2,3,6-tetrahydro-1,3-dimethyl-2,6-dioxo-, compd. with *trans*-4-[[(2-amino-3,5-dibromophenyl)methyl]amino] cyclohexanol (1:1)

Regulatory Information

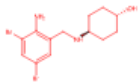
4. **1001052-99-8**

~5

80382-23-6 (Component: 68767-14-6)
$C_{15}H_{18}O_3 \cdot Na$



23828-92-4 (Component: 18683-91-5)
$C_{13}H_{18}Br_2N_2O \cdot ClH$



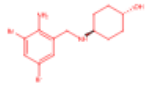
Relative stereochemistry.

$C_{15}H_{18}O_3 \cdot C_{13}H_{18}Br_2N_2O \cdot ClH \cdot Na$
Benzeneacetic acid, α-methyl-4-[(2-oxocyclopentyl)methyl]-, sodium salt (1:1), mixt. with *trans*-4-[[(2-amino-3,5-dibromophenyl)methyl]amino] cyclohexanol hydrochloride (1:1)

7. **204714-60-3**

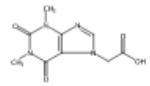
~2

18683-91-5
$C_{13}H_{18}Br_2N_2O$



Relative stereochemistry.

652-37-9
$C_9H_{10}N_4O_4$



$C_{13}H_{18}Br_2N_2O \cdot C_9H_{10}N_4O_4 \cdot H_2O$
7*H*-Purine-7-acetic acid, 1,2,3,6-tetrahydro-1,3-dimethyl-2,6-dioxo-, compd. with *trans*-4-[[(2-amino-3,5-dibromophenyl)methyl]amino] cyclohexanol, hydrate (1:1:1)

都有生物活性研究

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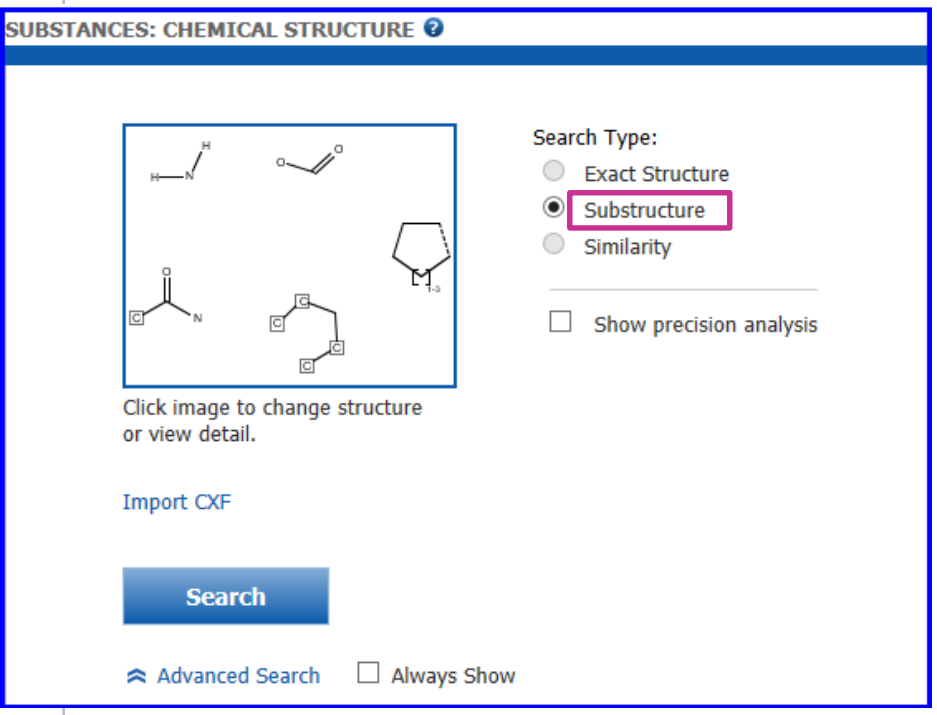
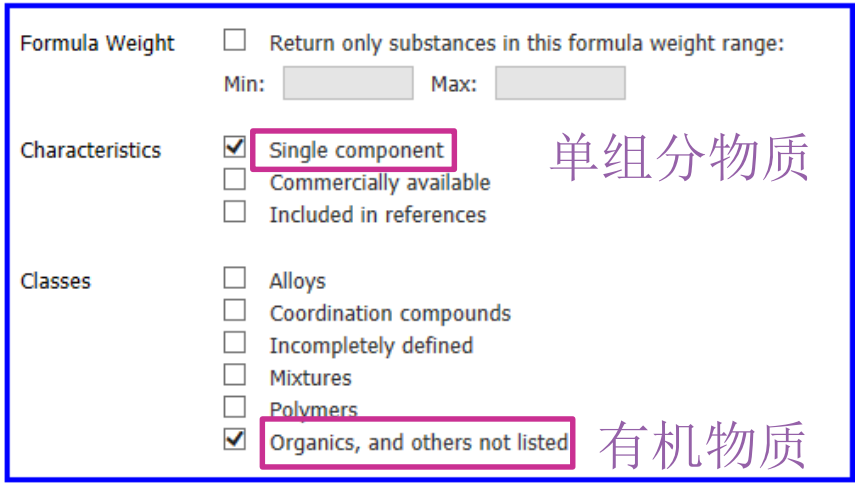
根据构效关系寻找潜药

作用机理 编辑本段

帕拉米韦是Babu等在分析唾液酸、扎那米韦、奥司他韦与NA的互相作用机制及构效关系的基础上设计并合成的环戊烷衍生物，与环连接的基团有亲水的羧基和胍基以及疏水的异戊基和乙酰氨基，4个极性不同的基团分别作用于流感病毒NA结构中不同的活性位点区域。羧基部分与NA活性位点的3个精氨酸残基Arg118，Arg292，





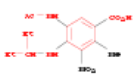
SciFinder® A CAS SOLUTION

根据构效关系寻找潜药

0 of 704 Substances Selected

1. **Substance Detail**
127971-59-9

~1

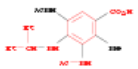


C15 H21 N3 O5
Benzoic acid, 5-(acetylamino)-4-[(1-ethylpropyl)amino]-2-methyl-3-nitro-

Experimental Properties

2. **Substance Detail**
127971-80-6

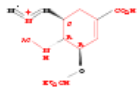
~1



C17 H25 N3 O4
Benzoic acid, 3,5-bis(acetylamino)-4-[(1-ethylpropyl)amino]-2-methyl-

3. **Substance Detail**
182367-45-9

~1

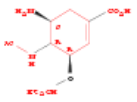


Relative stereochemistry.

C14 H22 N4 O4
1-Cyclohexene-1-carboxylic acid, 4-(acetylamino)-5-azido-3-(1-ethylpropoxy)-, (3α,4β,5α)-(9CI)

5. **Substance Detail**
182367-71-1

~2

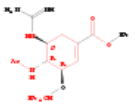


Relative stereochemistry.

C14 H24 N2 O4
1-Cyclohexene-1-carboxylic acid, 4-(acetylamino)-5-amino-3-(1-ethylpropoxy)-, (3*R*,4*R*,5*S*)-*rel*-

6. **Substance Detail**
182367-73-3

~1



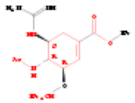
Relative stereochemistry.

C17 H30 N4 O4
1-Cyclohexene-1-carboxylic acid, 4-(acetylamino)-5-[(aminoiminomethyl)amino]-3-(1-ethylpropoxy)-, ethyl ester, (3*R*,4*R*,5*S*)-*rel*-

7. **Substance Detail**
182367-74-4

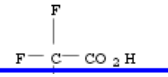
~1

182367-73-3
C17 H30 N4 O4



Relative stereochemistry.

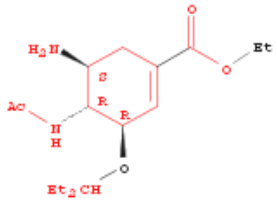
76-05-1
C2 H F3 O2



4. **Substance Detail**
182367-47-1

达菲核心成分

~1



C16 H28 N2 O4
1-Cyclohexene-1-carboxylic acid, 4-(acetylamino)-5-amino-3-(1-ethylpropoxy)-, ethyl ester, (3α,4β,5α)-(9CI)

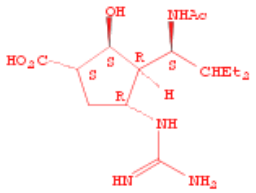
182368-47-4

~1

1. **Substance Detail**
330600-85-6

帕拉米韦

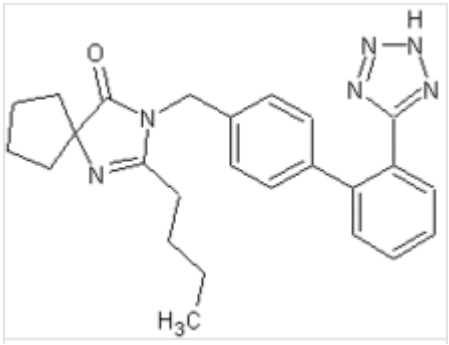
~286



C15 H28 N4 O4
Cyclopentanecarboxylic acid, 3-[(1*S*)-1-(acetylamino)-2-ethylbutyl]-4-[(aminoiminomethyl)amino]-2-hydroxy-, (1*S*,2*S*,3*R*,4*R*)-

SciFinder® A CAS SOLUTION

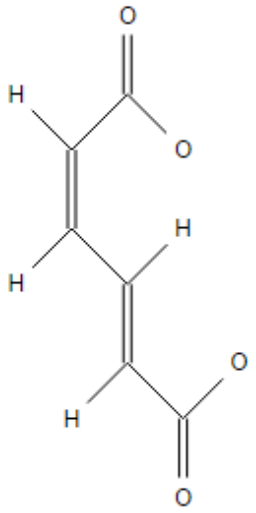
检索有同位素标记的物质



检索厄贝沙坦的氘代化合物

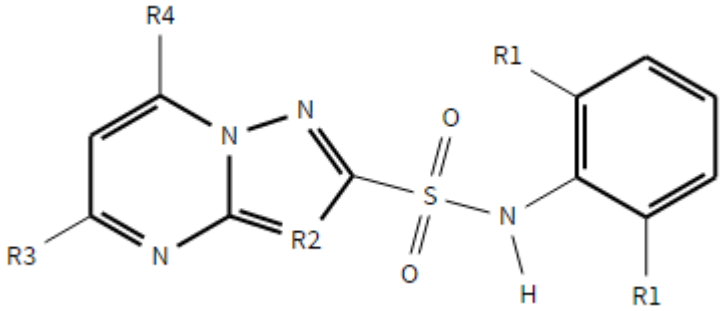
物质检索练习

- 检索Na2HPO4
- 检索异氰酸酯类化合物（Isocyanates）的分析测定方法
- 检索环上有以下结构特征的天然化合物



物质检索练习

- 找到包含如下物质的**所有**相关文献:



要求:

- R1 = X, H, -NO2, -CF3
- R2 = C 或 N
- R3 = 任意非氢原子
- R4 = 2-5个碳的碳链
- 结构中的环不发生稠环

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