

朱传娴

客户顾问

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SciFinder物质检索难点解析

中国药科大学



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

SciFinder检索选项——物质检索

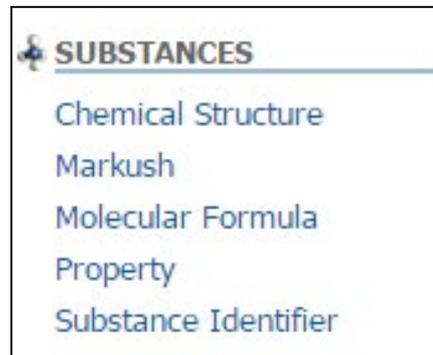
■ 物质检索方法

—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

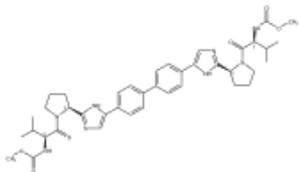
—无机物，合金：分子式检索

—高分子化合物：分子式检索和结构检索

快速获得物质的生物活性及靶点信息

1. 1009119-64-5

~308 ~88



Absolute stereochemistry.

C₄₀ H₅₀ N₈ O₆
Carbamic acid, *N,N*-[[[1,1'-biphenyl]-4,4'-diylbis[1*H*-imidazole-5,2-diyl-(2*S*)-2,1-pyrrolidinediyl][(1*S*)-1-(1-methylethyl)-2-oxo-2,1-ethanediy]]]bis-, *C,C'*-dimethyl ester

► **Key Physical Properties**
Regulatory Information

Analyze Refine

Analyze by:

Target Indicators

Cytokines (all)	1
Enzymes (all)	1
Interferons (all)	1
Proteins	1
Viral proteins (all)	1

Show More

作用靶点

Analyze Refine

Analyze by:

Bioactivity Indicators

Anti-infective agents (all)	1
-----------------------------	---

Show More

生物活性

绘图面板

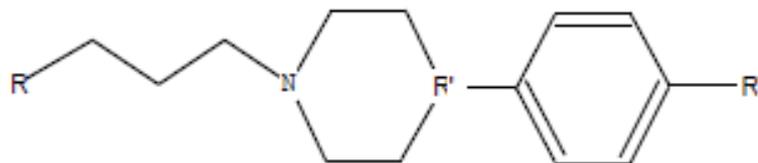
The image shows a screenshot of the 'Structure Editor' software interface. The interface includes a top toolbar, a central workspace, and a right-hand panel. Various tools and features are highlighted with purple boxes and Chinese labels:

- 橡皮** (Eraser)
- 结构和反应切换功能** (Structure and reaction switching function)
- 铅笔** (Pencil)
- 元素周期表** (Periodic table)
- 可变基团** (Variable group)
- 重复基团工具** (Repeat group tool)
- 碳链工具** (Carbon chain tool)
- 选择工具** (Selection tool)
- 环锁定工具** (Ring locking tool)
- 旋转工具** (Rotation tool)
- 正电子** (Positron)
- C原子和单键恢复工具** (C atom and single bond recovery tool)
- 常用基团** (Common group)
- R基团定义工具** (R group definition tool)
- 可变位置连接工具** (Variable position connection tool)
- 模版工具** (Template tool)
- 索套选择工具** (Loop selection tool)
- 原子锁定工具** (Atom locking tool)
- 镜面旋转工具** (Mirror rotation tool)
- 结构检索选择** (Structure search selection)
- 单双键, RS构型, 不确定键定义工具** (Single/double bond, RS configuration, uncertain bond definition tool)
- 负电子** (Negatrons)
- 常见环, 多元环工具** (Common rings, multi-ring tool)

The right-hand panel, titled 'Drawing Editor', shows options for 'Structure', 'Reaction', and 'Markush'. Below it, there is a section for 'Get substances that match your query using:' with radio buttons for 'Exact search', 'Substructure search', and 'Similarity search'. At the bottom of this panel are '确定' (OK) and '取消' (Cancel) buttons.

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

The screenshot displays the Structure Editor window. The central canvas shows a chemical structure consisting of a piperidine ring with a propyl chain attached to the nitrogen atom (labeled 'Hy') and a phenyl ring attached to the piperidine ring (labeled 'R₁'). The phenyl ring has a substituent 'R₂' at the para position. The left sidebar contains various drawing tools, with the 'Delete' (-X) and 'Add' (=R) tools highlighted in red boxes. The right sidebar, titled 'Drawing Editor', has the 'Structure' option selected. Below this, under 'Get substances that match your query using:', the 'Substructure search' option is selected. The bottom of the window features a toolbar with element selection buttons (C, H, O, S, N, P, Cl, Br, F, I, Si) and a 'Scale' field set to 100. A status bar at the bottom left indicates 'Formula not available'.

检索具有相同结构特征的物质

CAS Solutions

SciFinder®

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Save | Print | Export

Chemical Structure substructure > substances (3048)

SUBSTANCES

Get References | Get Reactions | Get Commercial Sources | Tools

Create Keep Me Posted Alert | Send to SciPlanner

Analyze | Refine

Sort by: CAS Registry Number

0 of 3048 Substances Selected

Page: 1 of 204

Analyze by: Substance Role

Preparation 1682

Biological Study 1523

Uses 1288

Reactant or Reagent 201

Analytical Study 86

Properties 70

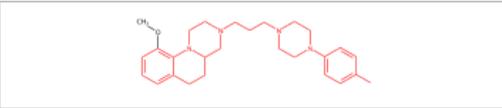
Prophetic in Patents 41

Combinatorial Study 22

Process 3

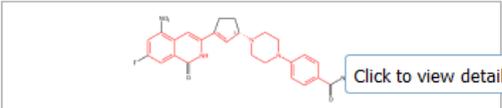
Show More

1. 1873376-11-4



$C_{27}H_{38}N_4O$
INDEX NAME NOT YET ASSIGNED

2. 1868051-25-5

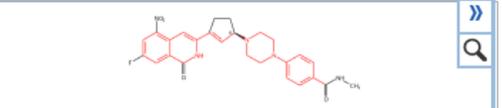


Absolute stereochemistry.

$C_{26}H_{26}FN_5O_4$
Benzamide, 4-[4-[(1*S*)-3-(7-fluoro-1,2-dihydro-5-nitro-1-oxo-3-isoquinolinyl)-2-cyclopenten-1-yl]-1-piperazinyl]-*N*-methyl-

Key Physical Properties

3. 1868051-24-4

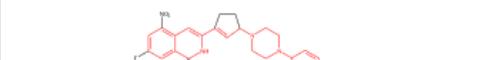


Absolute stereochemistry.

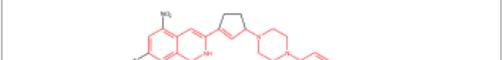
$C_{26}H_{26}FN_5O_4$
Benzamide, 4-[4-[(1*R*)-3-(7-fluoro-1,2-dihydro-5-nitro-1-oxo-3-isoquinolinyl)-2-cyclopenten-1-yl]-1-piperazinyl]-*N*-methyl-

Key Physical Properties

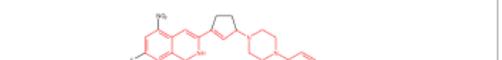
4. 1868051-23-3



5. 1868051-22-2

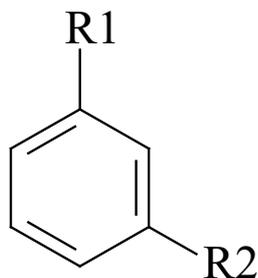


6. 1868051-02-8



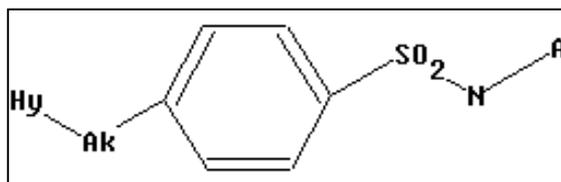
Markush检索

- 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, —CH₂—halogen, —CH—halogen,
|
CH₃



可用SciFinder中的Markush检索
查看专利中化合物结构保护范围。

Structure Editor

Draw or change atoms or bonds. Shortcut Keys

100%

Atom Short

-X =R

[] 1-4

Cl

Get Markush patents where the structure(s) are:

Variable only at the specified positions

Substructures of more complex structures

OK

Cancel

A C H O S N P Cl Br F I Si

Markush检索

SCIFINDER[®]
A CAS SOLUTION

Welcome Helen Zhu

Explore ▾ Saved Searches ▾ SciPlanner Save Print Export

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

REFERENCES ⓘ

Get Substances Get Reactions Get Related Citations Tools ▾ Create Keep Me Posted Alert Send to SciPlanner

Analyze Refine Categorize

Sort by: Accession Number ▾ ↓

0 of 1969 References Selected

Display Options

Analyze by: Document Type ▾

Patent	1969
Journal	1

Show More

1. **Compounds and methods for anticoagulation therapy**
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)**
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 [R¹ = H or halogen; ring A Ph or pyridyl; R², R³ (same or different) = hydrogen, halogen, C₁₋₄ alkyl or C₁₋₄ alkoxy each optionally substituted with 1-5 halogen atoms; or in case where R² and R³ are at the adjacent substitution position, R² and R³ together with ring A form C₅₋₈ 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; R⁴, R⁵ (same or different) = H, halogen, hydroxy, amino, -C(O)OR^a, -C(O)NR^b, SO₃H, SO₂NR^aR^b, SO₂R^b, or NR^aSO₂R^b; R^a, R^b (same...

全部是专利

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？

Structure Editor

Draw or change atoms or bonds.

Atom Short

Structure Editor:
 Structure
 Reaction
 Markush

Get substances that match your query using:
 Exact search
 Substructure search
 Similarity search

SciFinder®

Explore Saved Searches SciPlanner

Explore Substances resulted in 0 substances [Return](#)

Structure Editor

Draw or change atoms or bonds.

Atom Short

Structure Editor:
 Structure
 Reaction
 Markush

Get Markush patents that match your query using:

SciFinder®

Explore Saved Searches SciPlanner

Markush structure variable only at spe... > **references (18)**

REFERENCES ⓘ

Get Substances Get Reactions

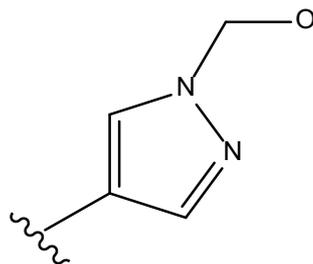
Analyze Refine Categorize Sort by: Accession Number

0 of 18 References Selected

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

如何判断结构的新颖型



Explore Saved Searches SciPlanner

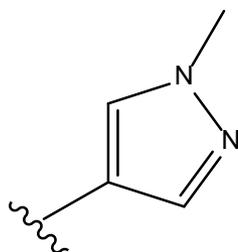
⚠ Explore References resulted in 0 references [Return](#)

Markush substructure > references (0)

REFERENCES

Analyze Refine

Analyze by:
No references available



Explore Saved Searches SciPlanner Save Print Export

Markush substructure > references (1)

REFERENCES ⓘ

Get Substances Get Reactions Get Related Citations Tools

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Analyze Refine Categorize

Analyze by: Author Name

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

Sort by: Accession Number

0 of 1 Reference Selected

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

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

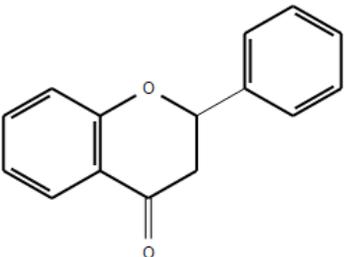
The invention relates to imidazo[5,1-a]isoindole derivs. of formula I, method for their prepn. and their use for the treatment of diseases related to IDO-mediated tryptophan metabolic pathways. Comps. of formula I.bul.M., wherein A is cycloalkyl, heterocycle and (hetero)aryl; R¹ is H, alkyl, cycloalkyl, (hetero)aryl, etc.; each R² is independently H, alkyl, alkoxy, halo, NO₂, etc.; each R³ is independently H, alkyl, cycloalkyl, CN, etc.; M is inorg. acid or org. acid, preferably TEA; n 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、-OR⁷、-C(O)R⁷、-C(O)OR⁷、-S(O)_mR⁷、

筛选天然产物

Structure Editor

Click a ring system to block it from further ring fusion. Click a chain to block it from ring formation.



Drawing Editor:

- Structure
- Reaction
- Markush

Get substances that match your query using:

- Exact search
- Substructure search
- Similarity search

Characteristics

- Single component
- Commercially available
- Included in references

Classes

- Alloys
- Coordination compounds
- Incompletely defined
- Mixtures
- Polymers
- Organics, and others not listed

Studies

- Analytical
- Biological
- Preparation
- Reactant or reagent

OK

Cancel

筛选天然产物

CAS Solutions

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WELCOME Helen Zhu

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Chemical Structure substructure with limiters > substances (17184)

SUBSTANCES

Get References | Get Reactions | Get Commercial Sources | Tools

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Analyze | Refine

Sort by: Relevance

0 of 17184 Substances Selected

Page: 1 of 344

Analyze by: Substance Role

Preparation: 10569

Biological Study: 7719

Uses: 4479

Properties: 4166

Reactant or Reagent: 3840

Occurrence: 1833

Analytical Study: 1442

Process: 705

1. 487-26-3
~2171 | ~65
O=C1OC(C2=CC=CC=C2)C3=CC=CC=C13
C₁₅ H₁₂ O₂
4*H*-1-Benzopyran-4-one, 2,3-dihydro-2-phenyl-
▶ **Key Physical Properties**
Regulatory Information
Spectra
Experimental Properties

2. 17002-31-2
~250 | ~5
O=C1OC(C2=CC=CC=C2)C3=CC=CC=C1[C@H]3
C₁₅ H₁₂ O₂
4*H*-1-Benzopyran-4-one, 2,3-dihydro-2-phenyl-, (2*S*)-
▶ **Key Physical Properties**
Experimental Properties

3. 27439-12-9
~216 | ~3
O=C1OC(C2=CC=CC=C2)C3=CC=CC=C1[C@@H]3
C₁₅ H₁₂ O₂
4*H*-1-Benzopyran-4-one, 2,3-dihydro-2-phenyl-, (2*R*)-
▶ **Key Physical Properties**
Experimental Properties

4. 104550-32-5
~3
O=C1OC(C2=CC=CC=C2)C3=CC=CC=C13
C₁₅ H₁₁ O₂
2*H*-1-Benzopyran-2-yl, 3,4-dihydro-4-oxo-2-phenyl- (9CI)

5. 75524-43-5

6. 146196-89-6

7. 55012-75-4

8. 104550-33-6

哪些黄酮类物质是天然存在的呢？

筛选天然产物

CAS Solutions | Preferences | SciFinder Help | Sign Out

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Chemical Structure substructure with limiters > substances (17184) > keep analysis "Substance Role" (7719) > keep analysis "Substance Role" (1816)

SUBSTANCES | Get References | Get Reactions | Get Commercial Sources | Tools

Analyze | Refine | Sort by: Relevance | Display Options

Analyze by: Substance Role

Biological Study	1816
Occurrence	1816
Properties	1531
Preparation	1342
Uses	1044
Analytical Study	667
Reactant or Reagent	337
Process	290

0 of 1816 Substances Selected

<input type="checkbox"/> 1. 487-26-3 ~2171 C₁₅ H₁₂ O₂ 4 <i>H</i> -1-Benzopyran-4-one, 2,3-dihydro-2-phenyl- ▶ Key Physical Properties Regulatory Information Spectra Experimental Properties	<input type="checkbox"/> 2. 2545-13-3 ~37 Absolute stereochemistry.,Rotation (-). C₁₅ H₁₂ O₃ 4 <i>H</i> -1-Benzopyran-4-one, 2,3-dihydro-7-hydroxy-2-phenyl-, (2 <i>S</i>)- ▶ Key Physical Properties Experimental Properties	<input type="checkbox"/> 3. 6515-36-2 ~262 C₁₅ H₁₂ O₃ 4 <i>H</i> -1-Benzopyran-4-one, 2,3-dihydro-7-hydroxy-2-phenyl- ▶ Key Physical Properties Spectra Experimental Properties	<input type="checkbox"/> 4. 6515-37-3 ~200 C₁₅ H₁₂ O₃ 4 <i>H</i> -1-Benzopyran-4-one, 2,3-dihydro-2-(4-hydroxyphenyl)- ▶ Key Physical Properties Spectra Experimental Properties
<input type="checkbox"/> 5. 4250-77-5	<input type="checkbox"/> 6. 17348-76-4	<input type="checkbox"/> 7. 21785-09-1	<input type="checkbox"/> 8. 480-39-7

两次分析功能组合:

Analyze — Substance Role — Biological Study & Occurrence

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？

1. **23828-92-4**

(Component: 18683-91-5)

~1147 ~97

Relative stereochemistry.

C₁₃ H₁₈ Br₂ N₂ O · Cl H
Cyclohexanol, 4-[[[(2-amino-3,5-dibromophenyl)methyl]amino]-, hydrochloride (1:1), *trans*-

► **Key Physical Properties**
Regulatory Information
Spectra
Experimental Properties

CAS Registry Number: 23828-92-4

View Substance Detail

Explore by Structure

Synthesize this...

Get Reactions where Substance is

Get Commercial Sources

Get Regulatory Information

Get References

Export as Image

Export as molfile

Send to SciPlanner

Structure Editor

Draw or change atoms or bonds. Shortcut Keys

Drawing Editor:

- Structure
- Reaction
- Markush

Get substances that match your query using:

- Exact search
- Substructure search
- Similarity search

OK Cancel

去掉结构中盐的组份，
精确结构检索

相同药效组份的物质

Explore Saved Searches SciPlanner

Chemical Structure exact

SUBSTANCES

Select All Deselect All

1 of 3 Stereo Candidates Selected

- Absolute stereo match
- Absolute stereo mirror image
- Relative stereo match
- Stereo that doesn't match query

Explore Saved Searches SciPlanner Save Print Export

Chemical Structure exact > substances (77)

SUBSTANCES Get References Get Reactions Get Commercial Sources Tools

Create Keep Me Posted Alert Send to SciPlanner

Analyze Refine

Sort by: Relevance

0 of 77 Substances Selected

Page: 1 of 2

Analyze by: Substance Role

Biological Study	52
Uses	49
Preparation	29
Properties	16
Analytical Study	10
Process	6
Reactant or Reagent	3
Formation, Nonpreparative	1

1. **18683-91-5**

~1125 ~58

Relative stereochemistry.

C₁₃ H₁₈ Br₂ N₂ O
Cyclohexanol, 4-[[[(2-amino-3,5-dibromophenyl)methyl]amino]-, *trans*-

► **Key Physical Properties**
Regulatory Information
Spectra
Experimental Properties

2. **23828-92-4**

~1147 ~97

Relative stereochemistry.

C₁₃ H₁₈ Br₂ N₂ O · Cl H
Cyclohexanol, 4-[[[(2-amino-3,5-dibromophenyl)methyl]amino]-, hydrochloride (1:1), *trans*-

► **Key Physical Properties**
Regulatory Information
Spectra

3. **96989-76-3**

~54 ~13

Relative stereochemistry.

18683-91-5
C₁₃ H₁₈ Br₂ N₂ O

652-37-9
C₉ H₁₀ N₄ O₄

4. **1001052-99-8**

~5

Relative stereochemistry.

80382-23-6 (Component: 68767-14-6)
C₁₅ H₁₈ O₃ · Na

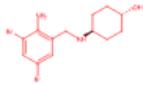
23828-92-4 (Component: 18683-91-5)
C₁₃ H₁₈ Br₂ N₂ O · Cl H

相同药效组份的物质

3. 96989-76-3

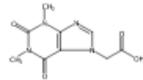
~54 ~13

18683-91-5
C₁₃ H₁₈ Br₂ N₂ O



Relative stereochemistry.

652-37-9
C₉ H₁₀ N₄ O₄

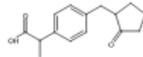


C₁₃ H₁₈ Br₂ N₂ O · C₉ H₁₀ N₄ O₄
7H-Purine-7-acetic acid, 1,2,3,6-tetrahydro-1,3-dimethyl-2,6-dioxo-, compd. with *trans*-4-[[[(2-amino-3,5-dibromophenyl)methyl]amino]cyclohexanol (1:1)
[Regulatory Information](#)

4. 1001052-99-8

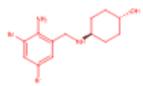
~5

80382-23-6 (Component: 68767-14-6)
C₁₅ H₁₈ O₃ · Na



· Na

23828-92-4 (Component: 18683-91-5)
C₁₃ H₁₈ Br₂ N₂ O · Cl H



· HCl

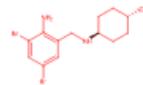
Relative stereochemistry.

C₁₅ H₁₈ O₃ · C₁₃ H₁₈ Br₂ N₂ O · Cl H · 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

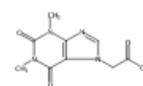
~2

18683-91-5
C₁₃ H₁₈ Br₂ N₂ O



Relative stereochemistry.

652-37-9
C₉ H₁₀ N₄ O₄



C₁₃ H₁₈ Br₂ N₂ O · C₉ H₁₀ N₄ O₄ · H₂ O
7H-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

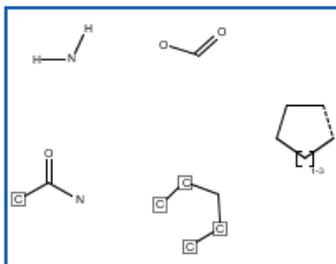
根据构效关系寻找潜药

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,

SUBSTANCES: CHEMICAL STRUCTURE ?



Search Type:

- Exact Structure
- Substructure
- Similarity

Show precision analysis

Click image to change structure or view detail.

Import CXF

Search

[Advanced Search](#) Always Show

Formula Weight Return only substances in this formula weight range:

Min: Max:

Characteristics Single component
 Commercially available
 Included in references

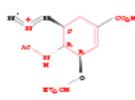
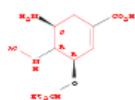
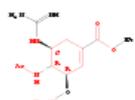
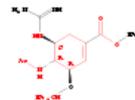
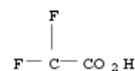
单组分物质

Classes Alloys
 Coordination compounds
 Incompletely defined
 Mixtures
 Polymers
 Organics, and others not listed

有机物质

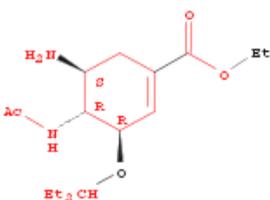
根据构效关系寻找潜药

0 of 704 Substances Selected

<p>1. Substance Detail 127971-59-9</p>  <p>C₁₅ H₂₁ N₃ O₅ Benzoic acid, 5-(acetylamino)-4-[(1-ethylpropyl)amino]-2-methyl-3-nitro-</p> <p>Experimental Properties</p>	<p>2. Substance Detail 127971-80-6</p>  <p>C₁₇ H₂₅ N₃ O₄ Benzoic acid, 3,5-bis(acetylamino)-4-[(1-ethylpropyl)amino]-2-methyl-</p>	<p>3. Substance Detail 182367-45-9</p>  <p>Relative stereochemistry. C₁₄ H₂₂ N₄ O₄ 1-Cyclohexene-1-carboxylic acid, 4-(acetylamino)-5-azido-3-(1-ethylpropoxy)-, (3α,4β,5α)-(9CI)</p>
<p>5. Substance Detail 182367-71-1</p>  <p>Relative stereochemistry. C₁₄ H₂₄ N₂ O₄ 1-Cyclohexene-1-carboxylic acid, 4-(acetylamino)-5-amino-3-(1-ethylpropoxy)-, (3<i>R</i>,4<i>R</i>,5<i>S</i>)-<i>rel</i></p>	<p>6. Substance Detail 182367-73-3</p>  <p>Relative stereochemistry. C₁₇ H₃₀ N₄ O₄ 1-Cyclohexene-1-carboxylic acid, 4-(acetylamino)-5-[(aminoiminomethyl)amino]-3-(1-ethylpropoxy)-, ethyl ester, (3<i>R</i>,4<i>R</i>,5<i>S</i>)-<i>rel</i></p>	<p>7. Substance Detail 182367-74-4</p> <div data-bbox="850 778 1188 1006"> <p>182367-73-3 C₁₇ H₃₀ N₄ O₄</p>  <p>Relative stereochemistry.</p> </div> <div data-bbox="850 1013 1188 1156"> <p>76-05-1 C₂ H F₃ O₂</p>  </div>

4. Substance Detail
182367-47-1

达菲核心成分

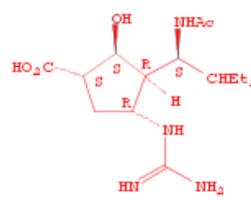


C₁₆ H₂₈ N₂ O₄
1-Cyclohexene-1-carboxylic acid, 4-(acetylamino)-5-amino-3-(1-ethylpropoxy)-, ethyl ester, (3 α ,4 β ,5 α)-(9CI)

182368-47-4

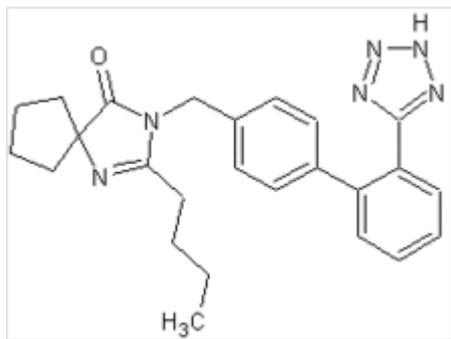
1. Substance Detail
330600-85-6

帕拉米韦



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*)-

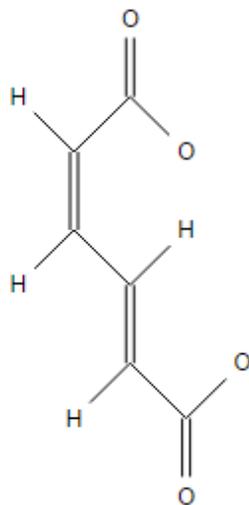
检索有同位素标记的物质



检索厄贝沙坦的氘代化合物

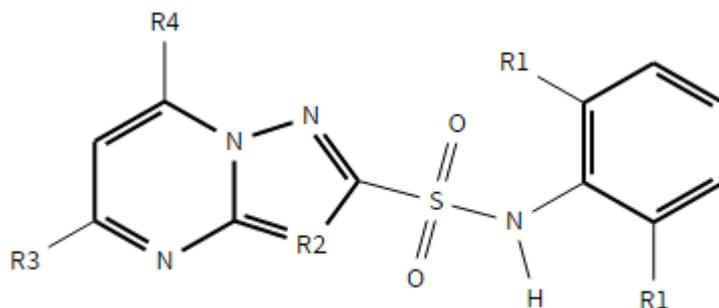
物质检索练习

- 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

美国化学文摘社北京代表处

010-62508026

china@acs-i.org

