

朱传娴

客户顾问

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如何使用SciFinder获取医药信息

--物质部分

中国药科大学

2018.06.07



提纲

- SciFinder中的物质检索
- SciFinder中的Markush检索
- 物质检索疑难分析
- 物质检索上机练习

SciFinder检索选项——物质检索

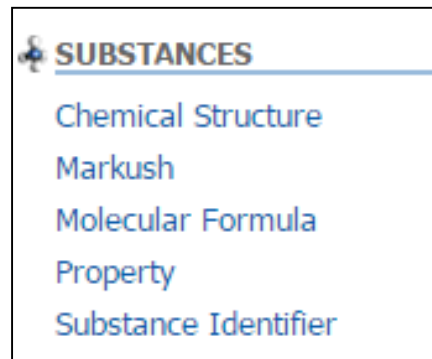
■ 物质检索方法

—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

物质检索——标识符检索

The screenshot displays the SciFinder web interface. At the top, there is a navigation bar with 'CAS Solutions' and the SciFinder logo. Below this, there are tabs for 'Explore', 'Saved Searches', and 'SciPlanner'. The main content area is divided into two sections. On the left, under 'REFERENCES', there is a list of search criteria: Research Topic, Author Name, Company Name, Document Identifier, Journal, Patent, and Tags. Below this, under 'SUBSTANCES', there is a list of search methods: Chemical Structure, Markush, Molecular Formula, Property, and Substance Identifier. The 'SUBSTANCES: SUBSTANCE IDENTIFIER' section is active, showing a search input field with the text 'qinghaosu'. Below the input field, there is a prompt 'Enter one per line.' and examples: '50-00-0', '999815', and 'Acetaminophen'. A blue 'Search' button is located at the bottom of this section.

提示:

1. 一次最多可输入25个物质。
2. 每行一个物质标识符。

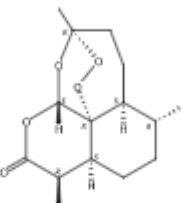
物质标识符包括CAS RN和化学名称，化学名称可以是通用名称、商品名、俗名。

SciFinder中的物质记录

点击CAS RN 获得物质详细信息

1. **63968-64-9** 🔍

~4864 📄 ~131 🧪



Absolute stereochemistry.

C₁₅ H₂₂ O₅
3,12-Epoxy-12H-pyrano[4,3-f]-1,2-benzodioxepin-10(3H)-one, octahydro-3,6,9-trimethyl-, (3R,5aS,6R,8aS,9R,12S,12aR)-

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

CAS Registry Number: 63968-64-9

- View Substance Detail
- Explore by Structure ▶
- Synthesize this...
- Get Reactions where Substance is a ▶
- Get Commercial Sources
- Get Regulatory Information
- Get References
- Export as Image
- Export as molfile
- Send to SciPlanner

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

SciFinder中的物质记录

SUBSTANCE DETAIL ?

Get References Get Reactions Get Commercial Sources

Return

CAS Registry Number 63968-64

~4,864 ~131

C₁₅ H₂₂ O₅
3,12-Epoxy-12*H*-pyrano[4,3-*j*]-1,2-benzodioxepin-10(3*H*)-one, octahydro-3,6,9-trimethyl-, (3*R*,5*a*,5,6*R*,8*a*,5,9*R*,12*S*,12*a*)-

Molecular Weight
282.33

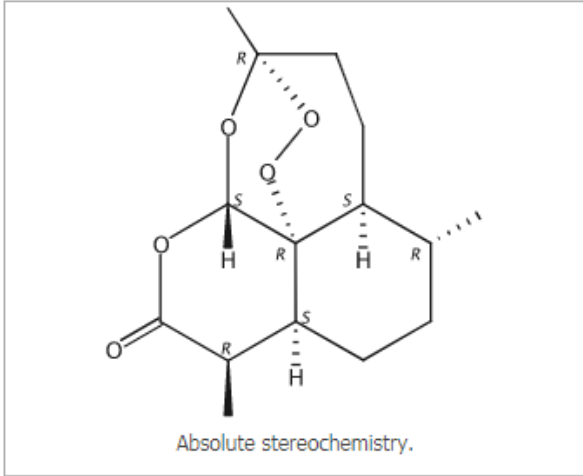
Melting Point (Experimental)
Value: 156-157 °C

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*-(3*α*,5*α*β,6β,8*α*β,9*α*,12β,12*a**R*^{*})]-(3*R*,5*a*,5,6*R*,8*a*,5,9*R*,12*S*,12*a*)-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...

由物质获得文献, 反应, 供应商等信息



Absolute stereochemistry.

物质详情

EXPERIMENTAL PROPERTIES

EXPERIMENTAL SPECTRA

实验数据与实验谱图

- ¹H NMR**
- ¹³C NMR**
- Hetero NMR
- IR
- Mass
- Raman
- UV and Visible
- Additional Spectra

¹³ C NMR Properties	Value	Condition	Note
Carbon-13 NMR Spectrum	See spectrum		(3)ACD
Carbon-13 NMR Spectrum	See spectrum		(4)ACD
Carbon-13 NMR Spectrum	See full text	1 of 8	(5)CAS

Notes

- (3) ACD: Spectral data were obtained from Advanced Chemistry Development, Inc.
- (4) Han, Jaehong; Journal of Natural Products 2001, V64(9), P1201-1205 CAPLUS
- (5) Yadav, J. S.; Tetrahedron 2010, V66(11), P2005-2009 CAPLUS

预测数据与预测谱图

PREDICTED PROPERTIES

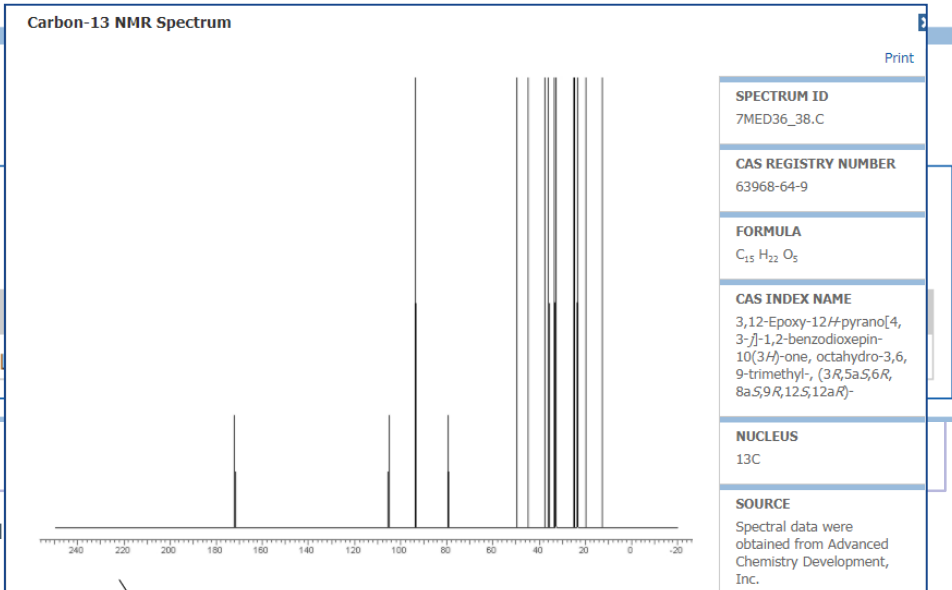
PREDICTED SPECTRA

- ¹H NMR**
- ¹³C NMR**

¹ H NMR Properties	Value
Proton NMR Spectrum	See spectrum

Notes

- (28) Predicted NMR data calculated using Advanced Chemistry Development, Inc. (ACD/



物质检索——Property explore

https://scifinder.cas

CAS Solutions

SCIFINDER[®]
A CAS SOLUTION

Explore Saved Searches

REFERENCES

- Research Topic
- Author Name
- Company Name
- Document Identifier
- Journal
- Patent
- Tags

SUBSTANCES

- Chemical Structure
- Markush
- Molecular Formula
- Property
- Substance Identifier

SUBSTANCE

Select Property...

- Bioconcentration Factor
- Boiling Point (°C)
- Density (g/cm³)
- Enthalpy of Vaporization (kJ/mol)
- Flash Point (°C)
- Freely Rotatable Bonds
- H Donor/Acceptor sum
- H Acceptors
- H Donors
- Koc
- logD
- logP
- Mass Intrinsic Solubility (g/L)
- Mass Solubility (g/L)
- Molar Intrinsic Solubility (mol/L)
- Molar Solubility (mol/L)
- Molar Volume (cm³/mol)
- Molecular Weight**
- pKa

Molecular Weight

250-400

Examples: 44, 25-35, >125

Search

寻找分子量在250-400之间的物质

物质结果集的筛选——Refine

SUBSTANCES ?

Get References Get Reactions Get Commercial Sources Tools ▾

Analyze **Refine**

Sort by: CAS Registry Number ▾

0 of 45142315 Substances Selected

Refine by: ?

- Chemical Structure
- Isotope-Containing
- Metal-Containing
- Commercial Availability
- Property Availability
- Property Value
- Reference Availability
- Atom Attachment

Structure Editor:

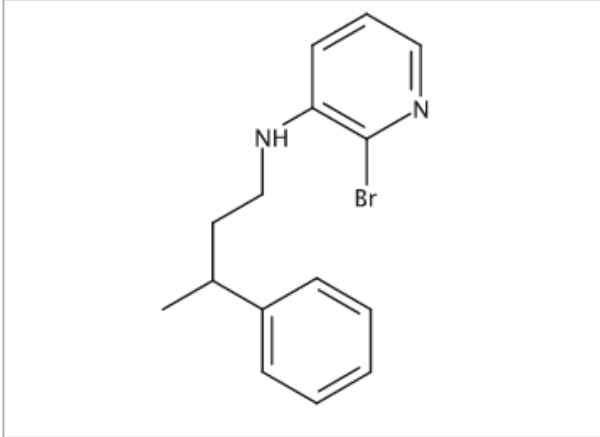
Java **Non-Java**

Click to Edit

Search type: **Exact Structure**

Only retrieve substances

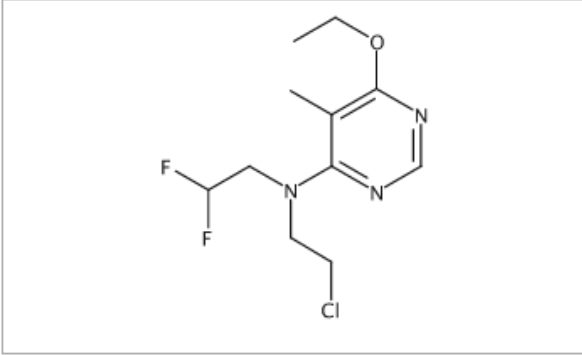
1. 1986293-22-4



C₁₅ H₁₇ Br N₂
3-Pyridinamine, 2-bromo-*N*-(3-phenylbutyl)-

▶ Key Physical Properties

2. 1986293-21-3



C₁₁ H₁₆ Cl F₂ N₃ O
4-Pyrimidinamine, *N*-(2-chloroethyl)-*N*-(2,2-difluoroethyl)-6-ethoxy-5-methyl-

▶ Key Physical Properties

4. 1986293-16-6

5. 1986293-14-4

4500多万个结构,
如何筛选黄酮类物质?

物质结果集的筛选——Refine

Structure Editor

Draw or change atoms or bonds.

Shortcut Keys

100%

Atom Short

Lock

C1=CC=C2C(=C1)OC(=C2)C3=CC=CC=C3

Get substances that match your query using:

- Exact search
- Substructure search

OK

Cancel

$C_{15}H_{10}O_2$ 222.24

锁环工具：避免在被锁定的环结构上出现新的环结构

SUBSTANCES ?

Analyze Refine

Refine by: ?

- Chemical Structure
- Isotope-Containing
- Metal-Containing
- Commercial Availability
- Property Availability
- Property Value
- Reference Availability
- Atom Attachment

Structure Editor:

Java Non-Java

Click image to change structure or view detail.

Search type: **Substructure**

Only retrieve substances that:

- Have references
- Are commercially available
- Are a single component
- Are in specific substance classes
- Are in specific types of studies

Refine

物质检索结果集

Explore ▾ Saved Searches ▾ SciPlanner

Property "Predicted - Molecular Weight, ..." > substances (45142315) > refine "substructure" (16901)

SUBSTANCES ⓘ

Get References Get Reactions Get Commercial Sources Tools ▾

Analyze Refine

Sort by: Relevance ▾

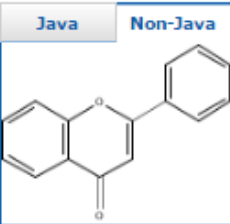
0 of 16901 Substances Selected

Refine by: ⓘ

- Chemical Structure
- Isotope-Containing
- Metal-Containing
- Commercial Availability
- Property Availability
- Property Value
- Reference Availability
- Atom Attachment

Structure Editor:

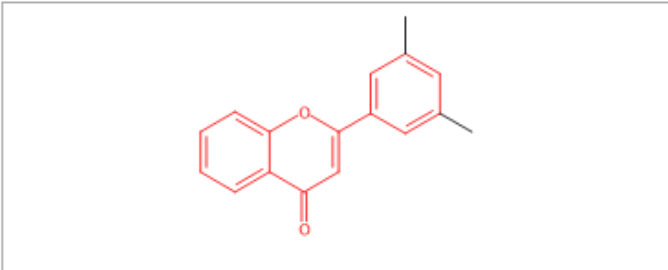
Java Non-Java



Click image to change structure or view detail.
Search type: **Substructure**

1. 1373355-19-1

~3

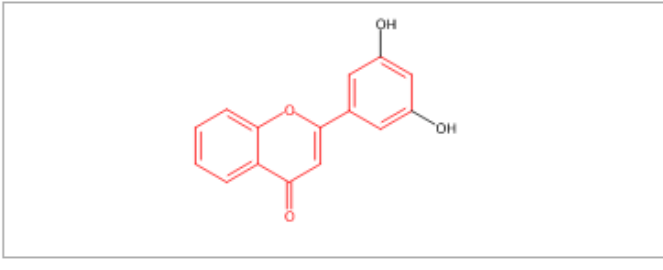


$C_{17}H_{14}O_2$
4,7-Dimethylflavone

▶ Key Physical Properties

2. 912915-64-1

~6 ~3

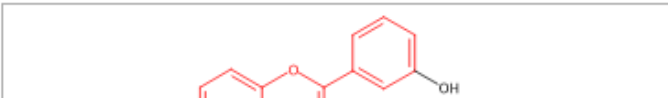


$C_{15}H_{10}O_4$
4,7-Dihydroxyflavone

▶ Key Physical Properties

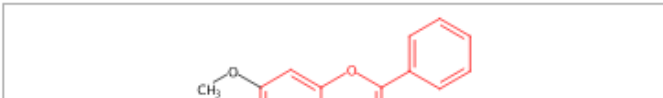
4. 6665-68-5

~38 ~7



5. 22395-22-8

~269 ~67



从4500多万个结构中
筛选出16901个黄酮类物质

物质检索——分子式

REFERENCES

- Research Topic
- Author Name
- Company Name
- Document Identifier
- Journal
- Patent
- Tags

SUBSTANCES

- Chemical Structure
- Markush
- Molecular Formula
- Property
- Substance Identifier

REACTIONS

- Reaction Structure

SUBSTANCES: MOLECULAR FORMULA

Examples:
H4SiO4
(C3H6O.C2H4O)x

Search

无机金属盐：金属离子和阴离子间用点 (.) 分开

1. 151-21-3
(Component: 151-41-7)
~84904 ~276

C₁₂H₂₆O₄S.Na
Sulfuric acid monododecyl ester sodium salt (1:1)

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

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

物质检索——结构

REFERENCES

- Research Topic
- Author Name
- Company Name
- Document Identifier
- Journal
- Patent
- Tags

SUBSTANCES

- Chemical Structure**
- Markush
- Molecular Formula
- Property
- Substance Identifier

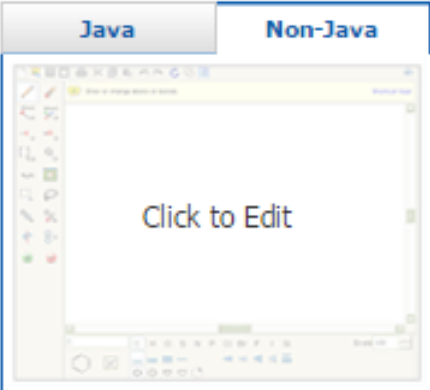
REACTIONS

- Reaction Structure

SUBSTANCES: CHEMICAL STRUCTURE

Structure Editor:

Java Non-Java



Click to Edit

Search Type:

- Exact Structure
- Substructure
- Similarity

Show precision analysis

ChemDraw
Launch a SciFinder substance or reaction

Import CXF

Search

[Advanced Search](#) Always Show

物质检索——结构

The image shows a screenshot of the 'Structure Editor' software interface. The interface includes a toolbar on the left with various drawing and editing tools, a central workspace for drawing chemical structures, and a 'Drawing Editor' panel on the right. The 'Drawing Editor' panel has radio buttons for 'Structure', 'Reaction', and 'Markush', and search options for 'Exact search', 'Substructure search', and 'Similarity search'. The interface also features a command line at the bottom with the text '(query)' and a list of elements: C, H, O, S, N, P, Cl, Br, F, I, Si. The interface is annotated with numerous Chinese labels pointing to specific tools and features.

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

负电子

C原子和单键恢复工具

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

单双键, RS构型, 不确定键定义工具

结构检索选择

常见环, 多元环工具

物质检索——精确结构检索

The screenshot displays the Structure Editor software interface. At the top, a toolbar contains various icons, with a callout box pointing to the 'I' icon (representing CAS RN input) and containing the text: "通过CAS RN转换结构: CAS RN: 50-36-2". The main workspace shows a chemical structure of a complex molecule, specifically a bicyclic amine derivative with a benzoyl group and a methoxy group. On the right side, the 'Drawing Editor' panel is visible, with 'Structure' selected. Below it, a search panel titled 'Get substances that match your query using:' has 'Exact search' selected, with a callout box around it containing the text: "精确结构检索". At the bottom of the interface, the molecular formula $C_{17}H_{21}NO_4$ and the molecular weight 303.36 are displayed.

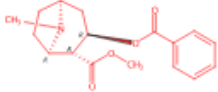
精确结构检索结果

Get References | Get Reactions | Get Commercial Sources | Tools | Create Posted

Sort by: Relevance

0 of 6 Substances Selected

1. **668-19-9**



Absolute stereochemistry.

C₁₇H₂₁N O₄
8-Azabicyclo[3.2.1]octane-2-carboxylic acid, 3-(benzoyloxy)-8-methyl-, methyl ester, (1*R*, 2*R*, 3*R*, 5*S*)-

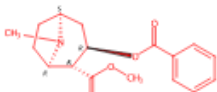
▶ Key Physical Properties
Spectra

可卡因

2. **114599-38-1**

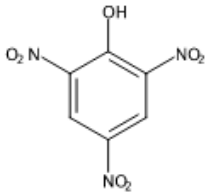
可卡因组合物

668-19-9
C₁₇H₂₁N O₄



Absolute stereochemistry.

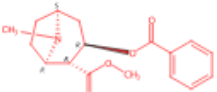
88-89-1
C₆H₃N₃O₇



C₁₇H₂₁N O₄ · C₆H₃N₃O₇
Alcocaine, picrate (6CI)

3. **109496-04-0**

(Component: 668-19-9)



* HCl

Absolute stereochemistry.

C₁₇H₂₁N O₄ · Cl H
Alcocaine, hydrochloride (6CI)

盐酸可卡因

物质检索——精确结构检索

精确结构检索：

获得被检索结构的盐，混合物，配合物，聚合物等，被检结构不能被取代

物质检索——亚结构检索

The screenshot displays the 'Structure Editor' window. The central workspace shows a chemical structure of a benzodioxane derivative with a phenyl group. The interface includes a toolbar on the left with various drawing tools, a top toolbar with file operations, and a right-hand panel with search settings. The search settings panel has 'Substructure search' selected and highlighted with a purple box. The bottom status bar shows the molecular formula $C_{15}H_{12}O_2$ and a numerical value 224.26.

Structure Editor

Select and draw structures with templates.

Drawing Editor:

- Structure
- Reaction
- Markush

Get substances that match your query using:

- Exact search
- Substructure search
- Similarity search

OK

Cancel

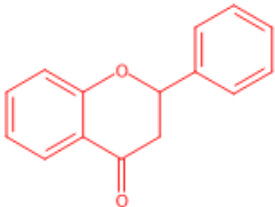
$C_{15}H_{12}O_2$ 224.26

物质检索——亚结构检索

0 of 23824 Substances Selected

1. 487-26-3

~2093

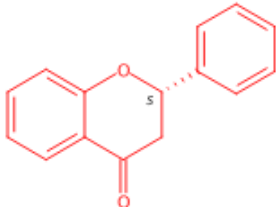


$C_{15}H_{12}O_2$
4-phenyl-4H-1-benzopyran-4-one, 2,3-dihydro-2-phenyl-

▶ Key Physical Properties
Regulatory Information
Spectra
Experimental Properties

2. 17002-31-2

~244



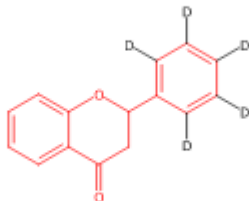
Absolute stereochemistry...Rotation (-).

$C_{15}H_{12}O_2$
4-phenyl-4H-1-benzopyran-4-one, 2,3-dihydro-

▶ Key Physical Properties
Experimental Properties

10. 146196-91-0

~1 ~5



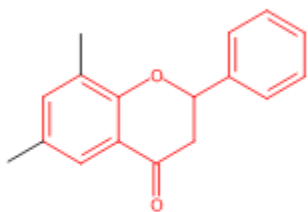
$C_{15}H_7D_5O_2$
4-(phenyl-d₅)-4H-1-benzopyran-4-one, 2,3-dihydro-2-(phenyl-d₅)- (9CI)

Spectra

同位素

亚结构检索结果

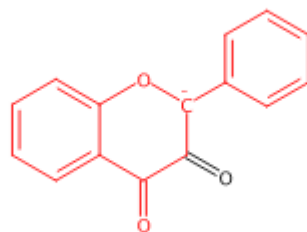
取代物



$C_{17}H_{16}O_2$
4H-1-Benzopyran-4-one, 2,3-dihydro-6,8-dimethyl-

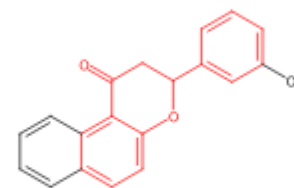
▶ Key Physical Properties
Experimental Properties

离子



$C_{15}H_9O_3$
2H-1-Benzopyran-3,4-dione, 2-phenyl-, ion(1-)

稠环物质



$C_{19}H_{14}O_3$
1H-Naphtho[2,1-b]pyran-1-one, 2,3-dihydro-3-(3-hydroxyphenyl)-

▶ Key Physical Properties

亚结构检索结果的限定

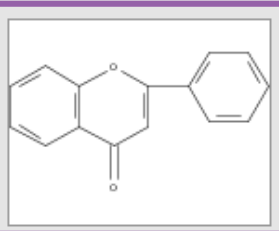
化学结构的再次限定

Analysis Refine

Refine by: ⓘ

- Chemical Structure
- Isotope-Containing
- Metal-Containing
- Commercial Availability
- Property Availability
- Property Value
- Reference Availability
- Atom Attachment

Chemical Structure:

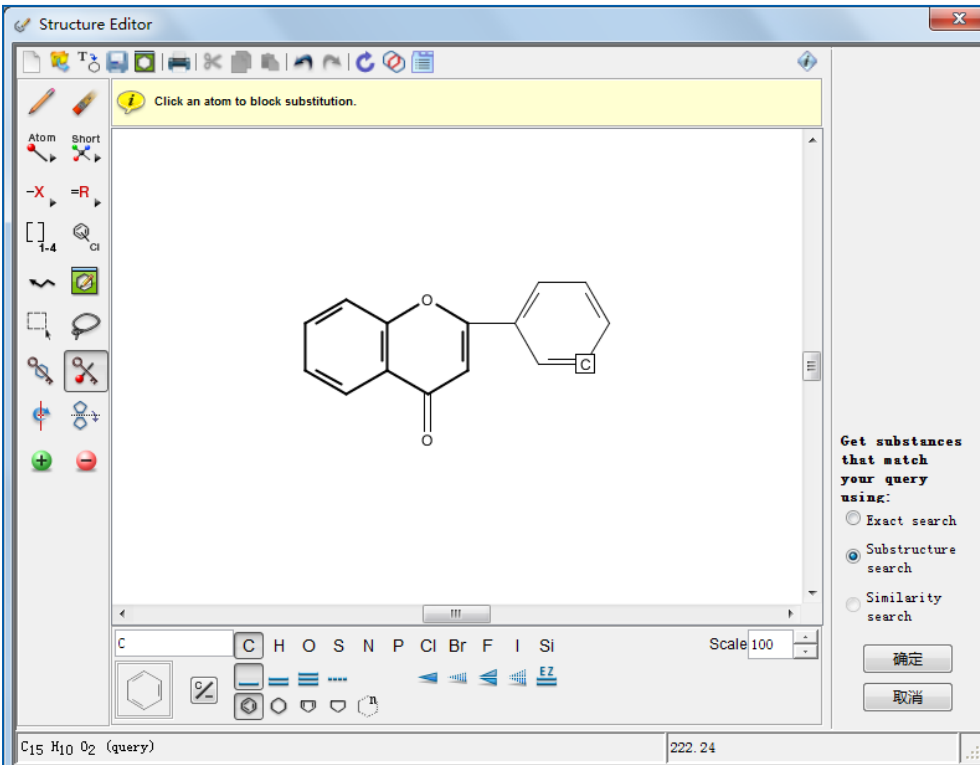


Click image to change structure or view detail

Search type: **Substructure**

Structure Editor

Click an atom to block substitution.



Get substances that match your query using:

- Exact search
- Substructure search
- Similarity search

确定 取消

C₁₅ H₁₀ O₂ (query) 222.24



环锁定

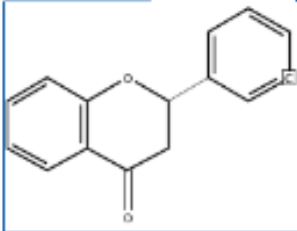


原子锁定

亚结构检索结果的限定

Structure Editor:

Java Non-Java



Click image to change structure or view detail.
Search type: **Substructure**

Only retrieve substances that:

- Have references
- Are commercially available
- Are a single component
- Are in specific substance classes
- Are in specific types of studies

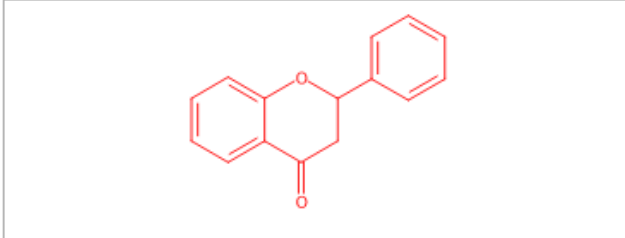
Refine

Get References Get Reactions Get Commercial Sources Tools

Sort by: Relevance

0 of 13826 Substances Selected

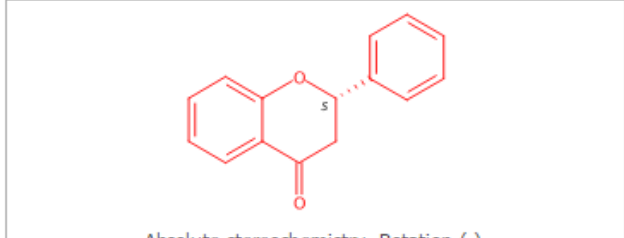
1. 487-26-3
~2093



$C_{15}H_{12}O_2$
4*H*-1-Benzopyran-4-one, 2,3-dihydro-2-phenyl-

Key Physical Properties
Regulatory Information
Spectra
Experimental Properties

2. 17002-31-2
~244



Absolute stereochemistry., Rotation (-).

$C_{15}H_{12}O_2$
4*H*-1-Benzopyran-4-one, 2,3-dihydro-2-phenyl-, (2*S*)-

Key Physical Properties
Experimental Properties

4. 104550-32-5
~3

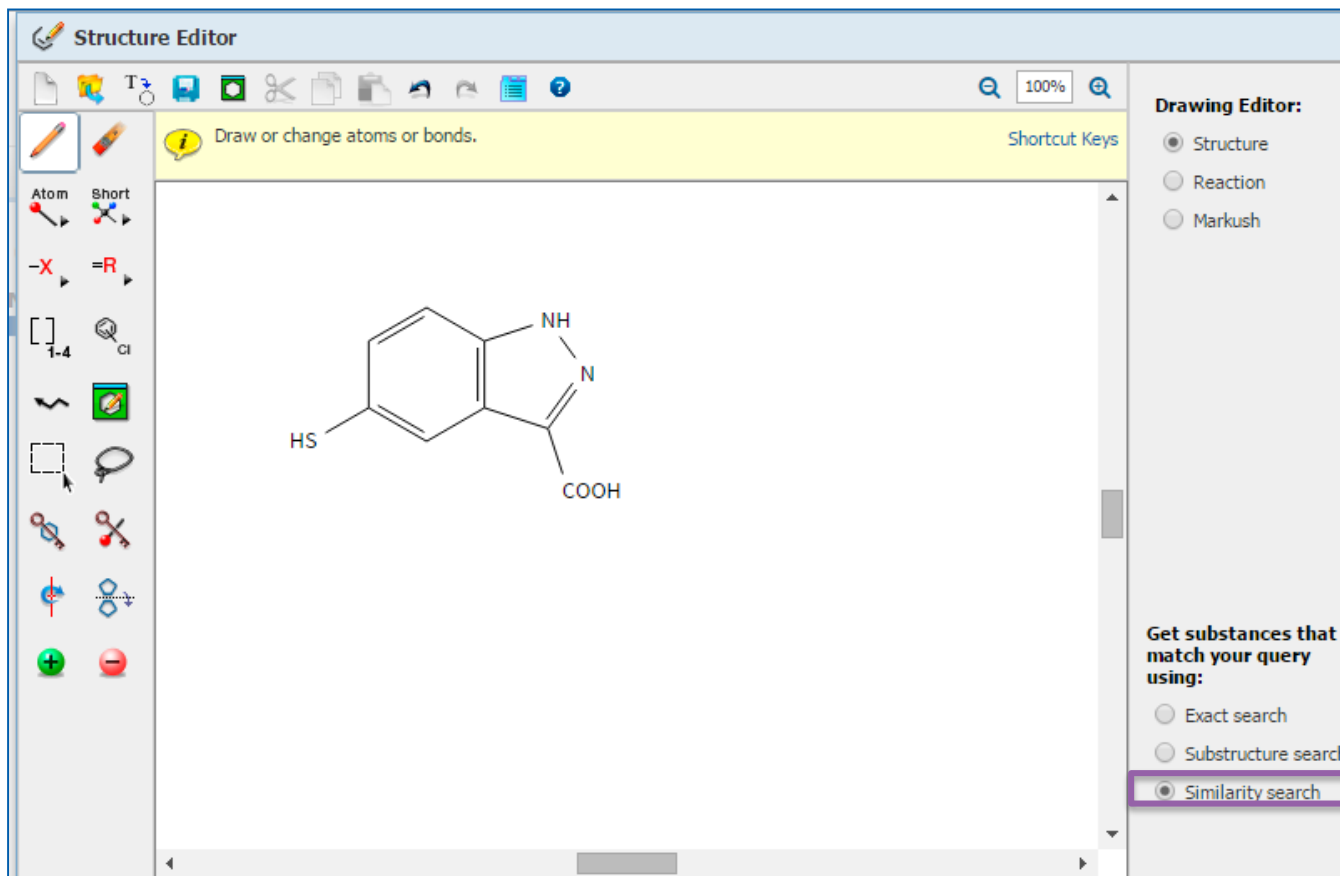
5. 75524-43-5
~2

物质检索——亚结构检索

- 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



相似结构检索结果

Select All Deselect All

0 of 6 Similarity Candidates Selected

	Substances
<input type="checkbox"/> ≥ 99 (most similar)	0
<input type="checkbox"/> 95-98	0
<input type="checkbox"/> 90-94	0
<input type="checkbox"/> 85-89	11
<input type="checkbox"/> 80-84	34
<input type="checkbox"/> 75-79	84
<input type="checkbox"/> 70-74	267
<input type="checkbox"/> 65-69	696
<input type="checkbox"/> 0-64 (least similar)	1818

Get Substances

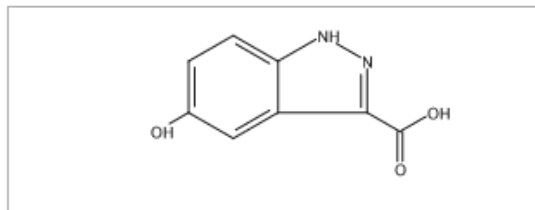
相似度越高，结构越相似

Score: 88

1. 885518-94-5

取代基变化

~1 ~35



$C_8H_6N_2O_3$

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

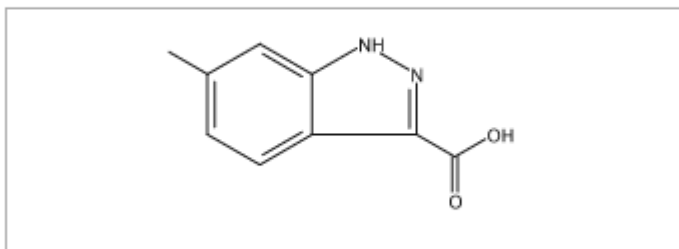
▶ Key Physical Properties

Score: 86

5. 858227-12-0

取代基位置变化

~7 ~41



$C_9H_8N_2O_2$

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

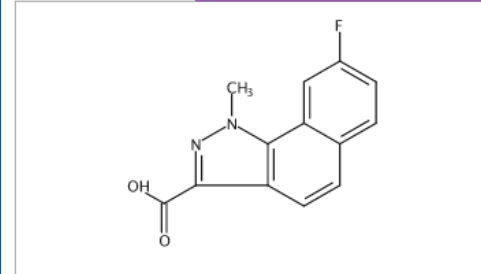
▶ Key Physical Properties

Score: 65

541. 1100422-

母体结构变化

~1



$C_{13}H_9FN_2O_2$

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

▶ Key Physical Properties



SCIFINDER®
A CAS SOLUTION

物质检索——相似结构检索

- 相似结构检索：

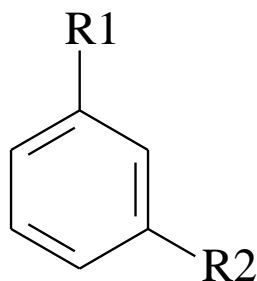
获得片段或整体结构与被检索结构相似的结果，母体结构可以被取代，也可以被改变

提纲

- SciFinder中的物质检索
- SciFinder中的Markush检索
- 物质检索疑难分析
- 物质检索上机练习

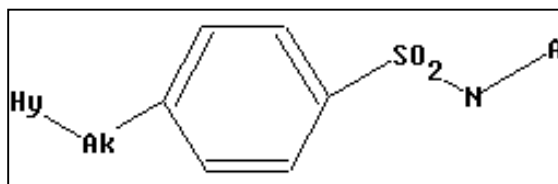
Markush检索

- 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 interface showing the chemical structure and the Markush search options.

Structure Editor

Draw or change atoms or bonds. Shortcut Keys

100%

Structure Editor:

- Structure
- Reaction
- Markush

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

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

REFERENCES ⓘ

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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

提纲

- SciFinder中的物质检索
- SciFinder中的Markush检索
- 物质检索疑难分析
- 物质检索上机练习

查看物质的生物活性和靶点信息

1. 111470-99-6

~1823 ~108

88150-42-9
C₂₀ H₂₅ Cl N₂ O₅

98-11-3
C₆ H₆ O₃ S

C₂₀ H₂₅ Cl N₂ O₅ · C₆ H₆ O₃ S
3,5-Pyridinedicarboxylic acid, 2-[(2-aminoethoxy)methyl]-4-(2-chlorophenyl)-1,4-dihydro-6-methyl-, 3-ethyl 5-methyl ester, benzenesulfonate (1:1)

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

Analyze Refine

Analyze by:

Bioactivity Indicators ▼

Cardiovascular agents (all) 1

Hypolipemic agents (all) 1

Ion channel blockers (all) 1

Receptor antagonists (all) 1

Renal agents 1

Show More

Analyze Refine

Analyze by:

Target Indicators ▼

C-reactive protein 1

Enzymes (all) 1

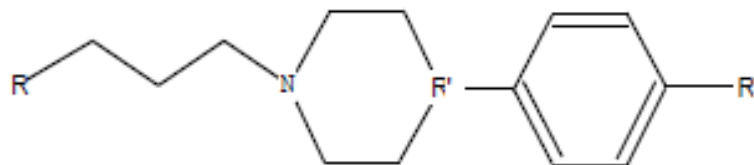
Lipoproteins (all) 1

Transport proteins (all) 1

Show More

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 interface includes a toolbar on the left with various drawing tools, a 'Drawing Editor' panel on the right with radio buttons for 'Structure', 'Reaction', and 'Markush', and a search panel at the bottom right with radio buttons for 'Exact search', 'Substructure search', and 'Similarity search'. The 'Substructure search' option is selected. At the bottom of the window, there is a status bar that reads 'Formula not available'.

检索具有相同结构特征的物质

CAS Solutions

SciFinder®

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Chemical Structure substructure > substances (3048)

SUBSTANCES

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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

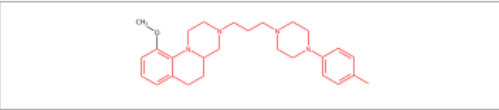
Prophetic in Patents 41

Combinatorial Study 22

Process 3

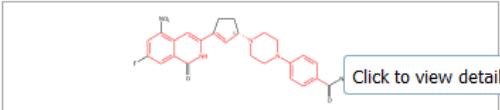
Show More

1. 1873376-11-4



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

2. 1868051-25-5

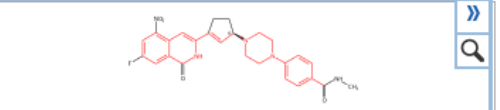


Absolute stereochemistry.

$C_{26}H_{26}FN_5O_4$
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

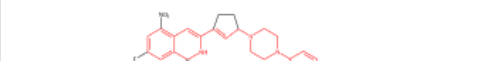


Absolute stereochemistry.

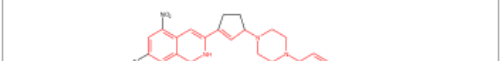
$C_{26}H_{26}FN_5O_4$
Benzamide, 4-[4-[(1*R*)-3-(7-fluoro-1,2-dihydro-5-nitro-1-oxo-3-isoquinolinyl)-2-cyclopenten-1-yl]-1-piperazinyl]-*N*-methyl-

Key Physical Properties

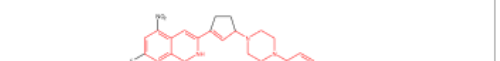
4. 1868051-23-3



5. 1868051-22-2



6. 1868051-02-8



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

HO₂C CO₂H

Et

Drawing 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

HOOC OOOH

Et

Drawing Editor:

Structure

Reaction

Markush

Get Markush patents that match your query using:

SciFinder®

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

REFERENCES ⓘ

Get Substances Get Reactions

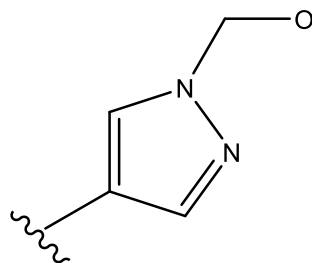
Analyze Refine Categorize Sort by: Accession Number ↓

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

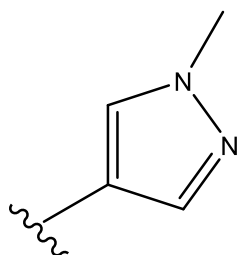
⚠ Explore References resulted in 0 references [Return](#)

Markush substructure > references (0)

REFERENCES

Analyze Refine

Analyze by:
No references available



Explore ▾ Saved Searches ▾ SciPlanner Save Print Export

Markush substructure > references (1)

REFERENCES ⓘ

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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

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

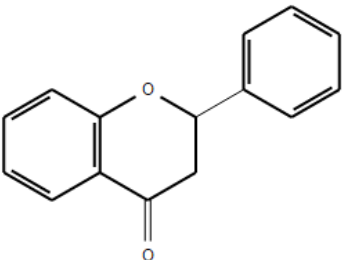
The invention relates to imidazo[5,1-a]isoindole derivs. of formula I, method for their prepn. and their use for the treatment of diseases related to IDO-mediated tryptophan metabolic pathways. Comps. of formula I.bul.M., wherein A is cycloalkyl, heterocycle and (hetero)aryl; R¹ is H, alkyl, cycloalkyl, (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、 $-R^a$ 、 $-OR^7$ 、 $-C(O)R^7$ 、 $-C(O)OR^7$ 、 $-S(O)_mR^7$ 、

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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Chemical Structure substructure with limiters > substances (17184)

SUBSTANCES

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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(c2ccccc2)C(=O)c3ccccc13
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(c2ccccc2)C(=O)c3ccccc13
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(c2ccccc2)C(=O)c3ccccc13
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(c2ccccc2)C(=O)c3ccccc13
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

Create Keep Me Posted Alert | Send to SciPlanner

Analyze | Refine | Sort by: Relevance | Display Options

0 of 1816 Substances Selected | Page: 1 of 37

Analyze by: Substance Role

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

1. 487-26-3
~2171 | ~65
O=C1OC(c2ccccc2)C(=O)c3ccccc13

2. 2545-13-3
~37 | ~2
Absolute stereochemistry, Rotation (-).

3. 6515-36-2
~262 | ~34
O=C1OC(c2ccccc2)C(=O)c3ccc(O)cc31

4. 6515-37-3
~200 | ~26
O=C1OC(c2ccc(O)cc2)C(=O)c3ccccc13

5. 4250-77-5

6. 17348-76-4

7. 21785-09-1


8. 480-39-7

两次分析功能组合:




Analyze — Substance Role — Biological Study & Occurrence

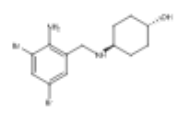
相同药效组份的物质

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

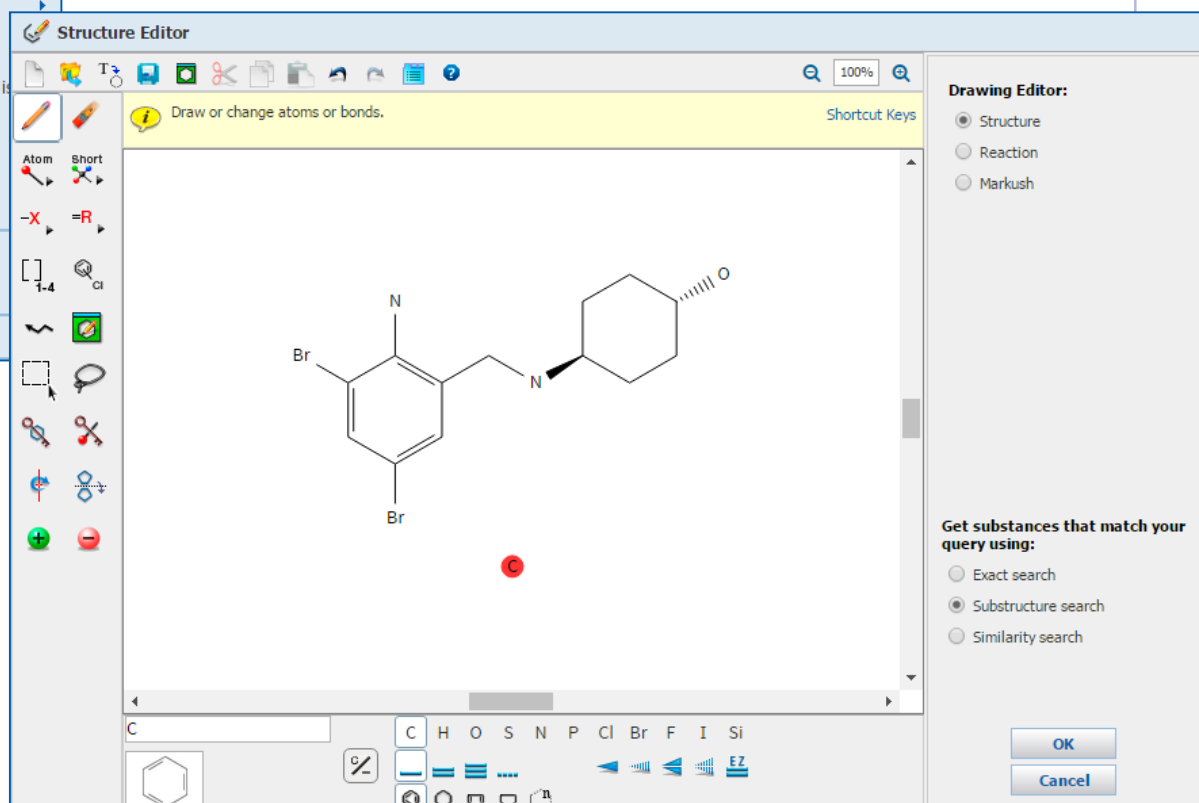
Export as Image

Export as molfile

Send to SciPlanner

Structure Editor

Draw or change atoms or bonds. Shortcut Keys



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

(Component: 18683-91-5)

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

18683-91-5
C₁₃ H₁₈ Br₂ N₂ O

Relative stereochemistry.

652-37-9
C₉ H₁₀ N₄ O₄

4. **1001052-99-8** ~5

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

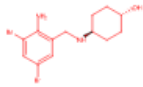
23828-92-4 (Component: 18683-91-5)
C₁₃ H₁₈ Br₂ N₂ O · Cl H

相同药效组份的物质

3. 96989-76-3

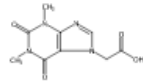
~54 ~13

18683-91-5
C₁₃ H₁₈ Br₂ N₂ O



Relative stereochemistry.

652-37-9
C₉ H₁₀ N₄ O₄

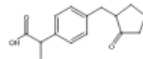


C₁₃ H₁₈ Br₂ N₂ O · C₉ H₁₀ N₄ O₄
7H-Purine-7-acetic acid, 1,2,3,6-tetrahydro-1,3-dimethyl-2,6-dioxo-, compd. with *trans*-4-[[2-amino-3,5-dibromophenyl)methyl]amino]cyclohexanol (1:1)
[Regulatory Information](#)

4. 1001052-99-8

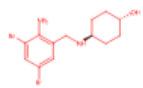
~5

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

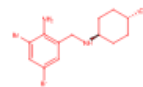
Relative stereochemistry.

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

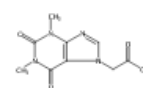
~2

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

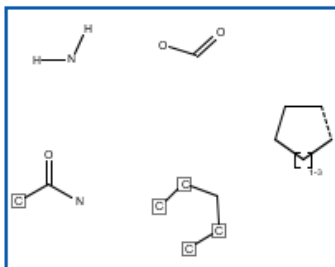
根据构效关系寻找潜药

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

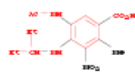
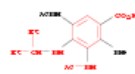
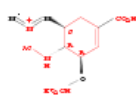
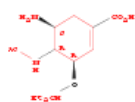
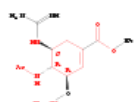
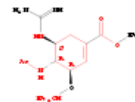
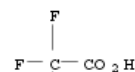
单组分物质

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

有机物质

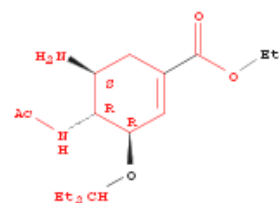
根据构效关系寻找潜药

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.</p> <p>C₁₄ H₂₂ N₄ O₄ 1-Cyclohexene-1-carboxylic acid, 4-(acetylamino)-5-azido-3-(1-ethylpropoxy)-, (3a,4β,5a)- (9CI)</p>
<p>5. Substance Detail 182367-71-1</p>  <p>Relative stereochemistry.</p> <p>C₁₄ H₂₄ N₂ O₄ 1-Cyclohexene-1-carboxylic acid, 4-(acetylamino)-5-amino-3-(1-ethylpropoxy)-, (3R,4R,5S)-rel</p>	<p>6. Substance Detail 182367-73-3</p>  <p>Relative stereochemistry.</p> <p>C₁₇ H₃₀ N₄ O₄ 1-Cyclohexene-1-carboxylic acid, 4-(acetylamino)-5-[(aminoiminomethyl)amino]-3-(1-ethylpropoxy)-, ethyl ester, (3R,4R,5S)-rel</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 1158"> <p>76-05-1 C₂ H F₃ O₂</p>  </div>

4. Substance Detail
182367-47-1

达菲核心成分

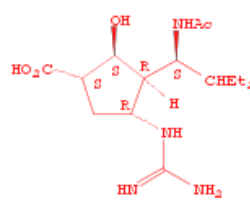


C₁₆ H₂₈ N₂ O₄
1-Cyclohexene-1-carboxylic acid, 4-(acetylamino)-5-amino-3-(1-ethylpropoxy)-, ethyl ester, (3a,4β,5a)- (9CI)

182368-47-4

1. Substance Detail
330600-85-6

帕拉米韦



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

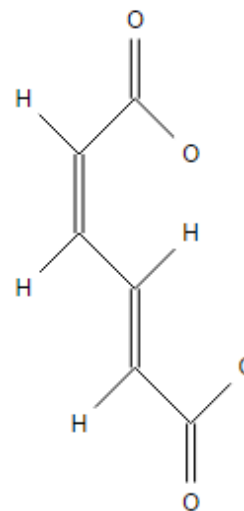
提纲

- SciFinder中的物质检索
- SciFinder中的Markush检索
- 物质检索疑难分析
- 物质检索上机练习

物质检索练习

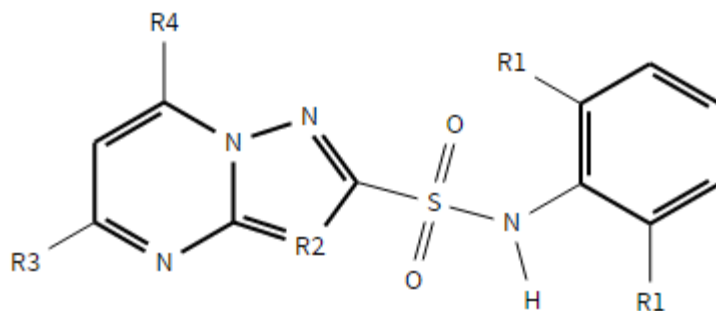
- 检索二茂铁
- 沐舒坦（Mucosolvan）的化学名是什么？主要药效是什么？

- 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

