

Reaxys 全方位版與Reaxys基本版差異

創新研究與教學的綜合體驗，培養次世代科學家與AI工具協作的核心技能

Reaxys基本版

- 有機、無機、有機金屬物理化學特性、實驗量測數據，保留文獻出處。
- 反應式、產率、試劑與催化劑，保留詳細文獻出處。
- 化學研究、藥物開發最快、最詳盡的專利收集與專利空間中文譯本
- 獨家商用材料資料庫



Retrosynthesis (Reaxys Basic)

Reaxys[®] Quick search Query builder Results **Retrosynthesis** History Alerts Ryan Huang

Structure editor selected: MarvinJS ChemDrawJS

Insert structure from name >

Parameters

Published ⓘ

Length & depth of synthesis plans ⓘ

Full routes: 10 ▾

Last step only

Branches per step: 5 ▾

Max. number of steps: 10 ▾

Stop searching if building block is commercially available Yes No

Assumed yield for reactions without a given yield

0% 100%

Clear Cancel Synthesize

查詢已發表分子的已發表合成路徑

No.	Date	Project name	No. of routes
2255047	10 Sep 2024	Project #2255047	Published 3

View >

查詢已發表分子可以得到詳細的實驗步驟與條件

No.	Date	Project name	No. of routes
			No Results

查詢“創新的分子”會顯示沒有結果

The New Retrosynthesis feature with AI prediction

Reaxys[®] Quick search Query builder Results Retrosynthesis History Alerts Ryan Huang 5

Structure editor selected: MarvinJS ChemDrawJS

Insert structure from name >

My Synthesis Projects

Draw

Structure editor selected: MarvinJS ChemDrawJS

Marvin JS by Chemaxon

Use Ctrl + Scroll to zoom in/out.

Clear Cancel Synthesize >

Parameters

Predicted

15 steps per route (up to)
Regioselectivity **ignored**
RCS: delivery time **up to 10 days**
RCS: **no** price limit
Standard processing time
No intermediates defined
Stereochemistry supported

Powered by **iktos** [Edit](#)

Published

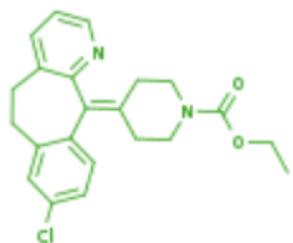
10 full routes (up to)
5 branches per step (up to)
10 steps per route (up to)
Stop at commercial building blocks
20% yield per step (assumed, if not published)

Feedback

利用神經網路訓練的AI工具預測「創新」分子的合成路徑

查詢已發表分子的已發表合成路徑

Bioactivity in Reaxys Academic Edition



loratadine
C₂₂H₂₃N₂O₂Cl 382.89 4273483 79794-75-5

Identification Physical Data - 64 Preparations - 22 >
Druglikeness Spectra - 37 Reactions - 294 >
Bioactivity (All) Other Data - 766 Targets - 146 >
Documents - 3,693 >

RAE生物活性數據會有詳盡的數值
實驗方法、細胞株、活性的靶點，
使用者能參考pX值(生物活性數值)。

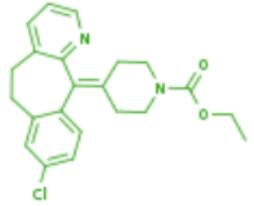
Bioactivity (All)

- In vitro: Efficacy - 614
- In vivo: Animal Model - 283
- Metabolism - 246
- Pharmacokinetic - 530
- Toxicity/Safety Pharmacology - 72

Quantitative Results Show/Hide columns ▾

pX	Parameter	Value (qual)	Unit	Action on target	Target	Cell	7...	Reference
8.52	IC50		nM	Inhibitor	Aldehyde oxidase:Wild			Current Patent Assignee: IDOGEN - WO2008/147283, 2 A1 Full Text Details Abstract >
8.27	IC50		nM	Antagonist	Histamine H1 receptor [human]:Wild	HeLa cell line		Cutrona, Kara J.; Miller, Scott J.; Stone, Elizabeth A. <i>Journal of the American Chemical Society</i> , 2020, vol. 142, # 29, 12690 - 12698 Full Text Cited 15 times Details Abstract >
8	mRNA expression	Active				heart fibroblast		Li, Jinshuang; Ding, Hao; Li, Yong; Zhou, Hao; Wang, Wanhong; Mei, Yong; Zhang, Rong <i>Journal of Amino Acids</i> , 2021, vol. 2021, # 1, 1-10 Full Text Details Abstract >

Drug targets in Reaxys Academic Edition



loratadine
C₂₂H₂₃N₂O₂Cl 382.89 4273483 79794-75-5

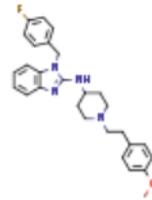
Identification Physical Data - 64 Preparations - 22 >
Druglikeness Spectra - 37 Reactions - 294 >
Bioactivity (All) Other Data - 766 **Targets - 146** >
Documents - 3,693 >

100    ...

146 Targets out of 294 Documents, 1 Substances, 22 Reactions

0      Sort alphabetically A-Z 

Single protein
1 5-hydroxytryptamine receptor 1A (rat, Wild) Substances - 6 >
Documents - 1 >
Synonyms: 5-ht-1a, 5-ht1a, 5-hydroxytryptamine receptor 1a, 5ht1a, htr1a, serotonin receptor 1a
Mutant/chimera Details: Wild
Uniprot: [p19327](#)
Show target details v

Most active substance:

63     ...
Ki (inhibition constant)=900nM

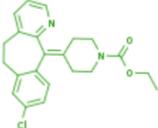
RAE Targets會整理已報導的蛋白靶點，使用者可以評估生物活性的專一性與有效性。

Bioactivity Visualization in Reaxys Academic Edition

Reaxys - 82 Commercial Substances - 10 PubChem - 122

82 Substances out of 3,712 Documents, containing 307 Reactions, 149 Targets

Limit To Exclude Export Preparations No of References Grid **Bioactivity Visualization**

1 

100 

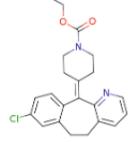
Filters

- Limit to >
- Exclude >
- By Structure >
- Measurement pX >
- Parameters >
- Targets >
- Target Species >
- Target Type >
- Substance action on target >
- Molecular Weight >
- Effect >
- Document Type >
- Publication Year >
- Current Patent Assignee >
- LogP >

Targets

Targets	5-Hydroxytrypt... receptor	5-Hydroxytrypt... receptor	5-Hydroxytrypt... receptor	Adenylate cyclase type 1	Adenylate cyclase type 2	Adenylate cyclase type 5	Alcohol oxidas... [mouse]	Aldehyde oxidase	Aldehyde oxidase 1	Aldehyde oxidase 3	Aldehyde oxidase 4	alpha1-adrene... receptor	Angiotensin-c... enzyme 2	ATP-binding c... member 2	ATP-dependen...se ABCB1	Beta-hexosami...ne nagZ)	beta-lactamase ... (linase)	bile acidreceptor	calcium channel	Carbonic anhydrase 1	Carbonic anhydrase 2	Carbonic anhydrase 4
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Substances

Substances	5-Hydroxytrypt... receptor	5-Hydroxytrypt... receptor	5-Hydroxytrypt... receptor	Adenylate cyclase type 1	Adenylate cyclase type 2	Adenylate cyclase type 5	Alcohol oxidas... [mouse]	Aldehyde oxidase	Aldehyde oxidase 1	Aldehyde oxidase 3	Aldehyde oxidase 4	alpha1-adrene... receptor	Angiotensin-c... enzyme 2	ATP-binding c... member 2	ATP-dependen...se ABCB1	Beta-hexosami...ne nagZ)	beta-lactamase ... (linase)	bile acidreceptor	calcium channel	Carbonic anhydrase 1	Carbonic anhydrase 2	Carbonic anhydrase 4
loratadine 	1	5.5	1	5.8	5.2	4.7		8.5	5.3		1	1		5.3								
11364466																						
11364466																						
isoloratadine																						

RAE Bioactivity Visualization
可以探索一個分子或一組分子的

Substances Exit Full Screen

Navigator

