



ELSEVIER

Reaxys<sup>®</sup>

快速搜索指南

June 2022



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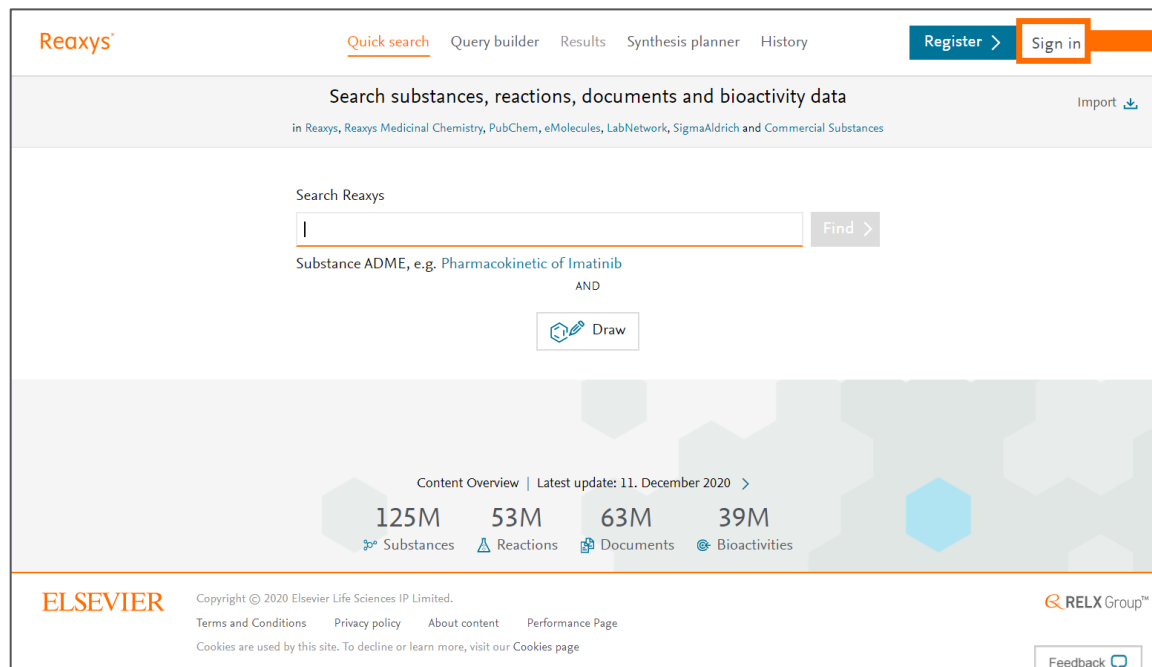
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# Reaxys的取得

連結: <https://www.reaxys.com>

登入畫面

連結: <https://www.reaxys.com/#/login>



Reaxys® Quick search Query builder Results Synthesis planner History Register > Sign in

Search substances, reactions, documents and bioactivity data  
in Reaxys, Reaxys Medicinal Chemistry, PubChem, eMolecules, LabNetwork, SigmaAldrich and Commercial Substances

Search Reaxys  
| Find >

Substance ADME, e.g. Pharmacokinetic of Imatinib  
AND

Draw

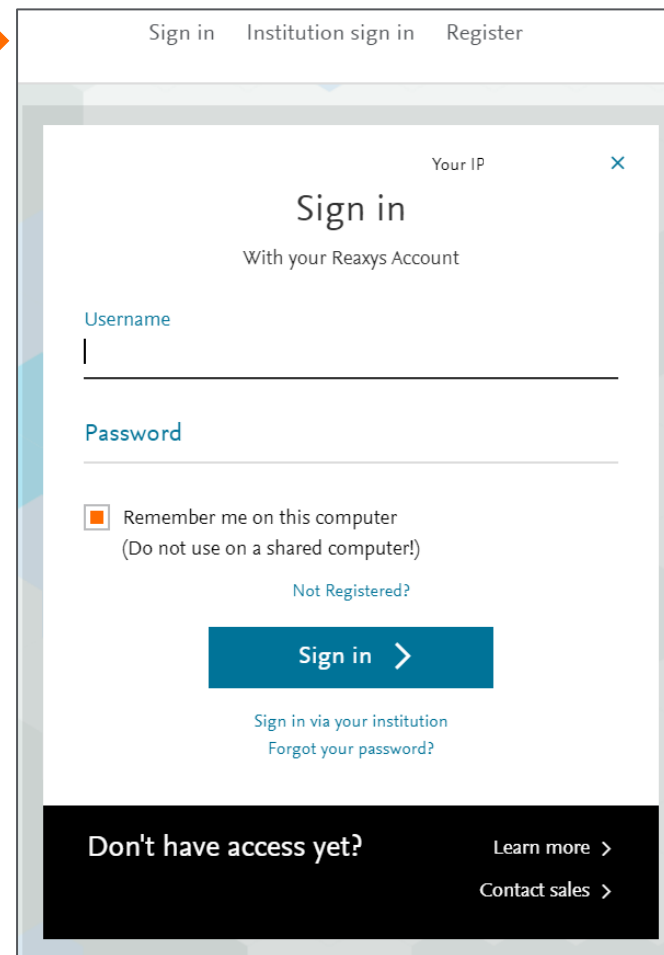
Content Overview | Latest update: 11. December 2020 >

125M 53M 63M 39M  
Substances Reactions Documents Bioactivities

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Feedback



Sign in Institution sign in Register

Your IP X

## Sign in

With your Reaxys Account

Username  
|

Password  
|

Remember me on this computer  
(Do not use on a shared computer!)

Not Registered?

Sign in >

Sign in via your institution  
Forgot your password?

Don't have access yet? Learn more >  
Contact sales >



# Reaxys 首頁畫面

Reaxys<sup>®</sup> TotalPatent One<sup>™</sup> **Quick search** Query builder Results Synthesis planner History Alerts

Search substances, reactions and documents  
in Reaxys, PubChem, eMolecules, LabNetwork, SigmaAldrich and Commercial Substances

Search Reaxys  Find >

Substance Properties, e.g. solubility of vitamin D3  
AND

Draw

Import

文字輸入

結構式和反應式輸入

批次導入結構

使用者檔案的設置與註銷

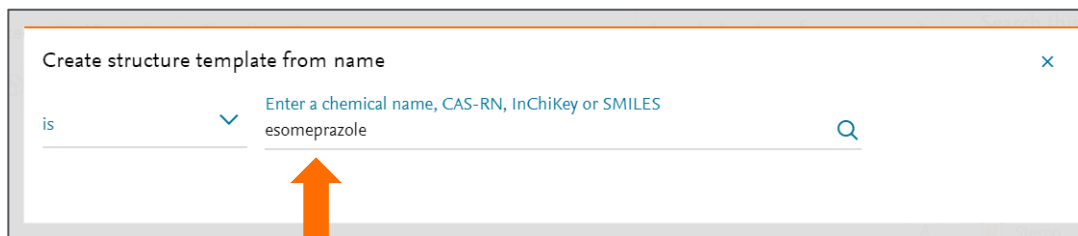
問題、使用者指南、輔助材料和常見問題

- ① **Quick search**: 結構搜索, 關鍵字搜索。
- ② **Query builder**: 結構式、物理性質等方面的乘法搜索。對搜索歷史進行乘法搜索。
- ③ **Results**: 搜索結果。對使用者需要的資訊進行優先排序。
- ④ **Synthesis planner**: 逆向合成路線搜索。
- ⑤ **History**: 搜索歷史。
- ⑥ **Alerts**: 瀏覽提示的搜索內容。

# 介面

可以用“ctrl+alt+C”複製ChemDraw中繪製的結構黏貼到Marvin JS上。

可以從化合物的名稱中調出結構。



Structure editor selected:  MarvinJS  ChemDrawJS

Insert structure from name >

Search this structure as:

- As drawn
- As substructure
  - On all atoms
  - On heteroatoms
- Similar
- Tautomers
- Stereo
- Additional ring closures
- Related Markush
- Salts
- Mixtures
- Isotopes
- Charges
- Radicals
- + More options

Clear Cancel **Transfer to query** >

點擊「Transfer to query」，進入搜索介面。

# 結構式和反應式繪製的搜索選項

## 搜索選項

Search this structure as:

As drawn

As substructure

On all atoms

On heteroatoms

Similar

### ① 結構搜索選項

- As drawn : 按照繪製的結構
- As substructure : 部分結構
  - On all atoms : 搜索所有原子的子結構
  - On heteroatoms : 只在雜原子上進行結構搜索
- Similar : 類似的化合物與反應

Tautomers

Stereo

Additional ring closures

Related Markush

Salts

Mixtures

Isotopes

Charges

Radicals

### ② 其他搜索選項

- Tautomers: 同分異構體
- Stereo: 立體異構體
- Additional ring closures: 額外的環形閉合
- Related Markush: 相關的Markush資料
- Salts : 鹽類
- Mixtures: 混合物
- Isotopes: 同位素
- Charges : 帶電分子
- Radicals : 自由基

# Quick Search 搜索預覽介面


Search for preparation of vitamin D3

Search Reaxys

preparation of vitamin D3 × **Find >**






Substance Effect, e.g. anticoagulant

AND

 Draw

修改和編輯搜索公式

Results for preparation of vitamin D3 New Edit

	158	Reactions	Reaction Query :  as drawn <small>Edit in Query Builder</small> <small>Create Alert</small>	<span>Preview Results</span> <span>View Results &gt;</span>
	18,507	Documents	Titles, Abstracts, Keywords : "preparation", "vitamin D3" <small>Edit in Query Builder</small> <small>Create Alert</small>	<span>Preview Results</span> <span>View Results &gt;</span>
	10,144,068	Documents	Titles, Abstracts, Keywords : "preparation" <small>Edit in Query Builder</small> <small>Create Alert</small>	<span>Preview Results</span> <span>View Results &gt;</span>
	115,575	Documents	Titles, Abstracts, Keywords : "vitamin D3" <small>Edit in Query Builder</small> <small>Create Alert</small>	<span>Preview Results</span> <span>View Results &gt;</span>

「View Results」進入搜索結果介面

快速搜尋會分析輸入的關鍵字，提供物質、反應式、文件或商業物質的選擇。

# Query Builder

靈活組合>100種搜索方式來減少雜訊

輸入關鍵字以查找特定搜索器。  
例如：輸入“Boil”來尋找“boiling point”搜索器。

Reaxys® TotalPatent One® Quick search Query builder Results Synthesis planner History Alerts

Search in: Reactions > Substances > Documents >

Import Save Reset form Delete all

Structure Molecular Formula CAS RN TI, AB & KW

結構式繪圖畫面 分子式輸入

Drag & Drop to build a new query

Search fields

Fields Forms History

Topics and Keywords

Identification

Physical Properties

Spectra

Pharmacological Data

Ecotoxicology

Other

Reactions

Bibliography

PubChem

搜索歷史也可用於搜索公式中。

調用你自己創造的搜索公式和我們為您建立的搜索公式範本。

超過100搜索器，供您挑選。

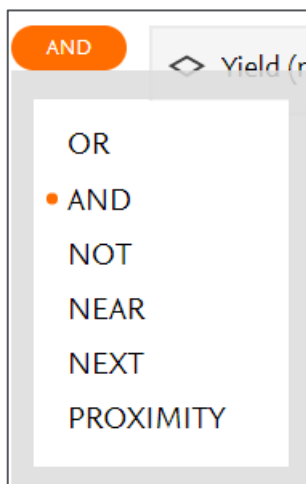


# Query Builder

選擇反應搜索、物質搜索和文獻搜索。

你所選擇的搜索專案會被顯示出來。

你可以保存你所創建的搜索公式。



點擊或按下Drug&Drop來調用一個項目。

- OR : 或
- AND : 和
- NOT : 不包括
- NEAR : 雙方必須靠近對方
- NEXT : 雙方必須靠在一起
- PROXIMITY : 雙方都很接近

# 反應搜索結果介面

## Reaxys Ranking:

按認為有用的順序排列，而非依年份或產量排列。

### <項目>

- ① 瀏覽搜索結果的軌跡
- ② 過濾功能
- ③ 匯出按鈕 (參考 P. 22)
- ④ 反應數據的來源文獻
- ⑤ 搜索結果的反應功能
- ⑥ 實驗式表示
- ⑦ 商業試劑資訊
- ⑧ 紀錄的詳細資訊連結

The screenshot shows the Reaxys search results page for 'TotalPatent One'. The interface includes a top navigation bar with 'Quick search', 'Query builder', 'Results', 'Synthesis planner', 'History', and 'Alerts'. A left sidebar contains a 'Filters' panel with various criteria like 'By Structure', 'Yield', 'Reagent/Catalyst', etc., and a 'Query' section. The main content area displays '225 Reactions' with an 'Export' button and a 'Reaxys Ranking' dropdown menu. A detailed view of a reaction is shown, including its chemical structure, conditions, yield (93.5%), and reference information. A table below the reaction details lists conditions, yield, and references for multiple entries.

Conditions	Yield	Reference
With $C_{68}H_{72}N_4O_{10}Ti_2$ ; dihydrogen peroxide In water; ethyl acetate at 0°C; for 24h; Reagent/catalyst; enantioselective reaction;	93.5%	Talsi, Evgenii P.; Bryliakov, Konstantin P. [Catalysis Today, 2017, vol. 279, p. 84 - 89]
Experimental Procedure ^		Full Text ↗ Cited 5 times ↗ Details > Abstract >
2.2. Standard procedure for small-scale catalytic sulfoxidation		
General procedure: Sulfide (OMS or LPS, 100 mol) and the Ti-salalen catalyst(1.1 mol) were dissolved in the solvent (typically: EtOAc, 6.0 mL),the mixture was thermostatted at desired temperature (typically 0 °C, or -20 to +20 °C for variable-temperature measurements),and 30% aqueous hydrogen peroxide (0.105 mmol of $H_2O_2$ ) was then introduced in one portion. Stirring (500 rpm) was continued at that temperature (typically 24 h). For low-temperature experiments, the reaction times were about 30 h at -10 °C and up to 10 days at -20 °C. To analyze the reaction outcome, 20 L aliquots of the reaction mixture were taken to a vial and immediately carefully evaporated to dryness with a stream of compressed air during ca. 15-20 s. The remaining solid was dissolved in 0.20 mL of 1% $Et_3N$ solution in isopropyl alcohol, and the contents of residual sulfide, (R)- and(S)-sulfoxide, and sulfone, were analyzed by chiral HPLC as noted above.		
With N-methyl-6-aza-5β,6β-epoxy-cholestane-3β-tert-butylidiphenylsilyloxy tetrafluoroborate In dichloromethane at -70 - 20°C; for 3h; Inert atmosphere;	86%	Zhou, Guobin; Guan, Yueqing [Heterocyclic Communications, 2016, vol. 2]

# 反應搜索結果中的篩選

**Filters**

Limit to > Exclude >

- By Structure
- Yield
- Reagent/Catalyst
- Solvent
- Catalyst Classes
- Solvent Classes
- Product Availability
- Reactant Availability
- Reaction Classes
- Document Type
- Publication Year
- Single step reactions only
- Experimental procedure only

- ← 結構
- ← 產率
- ← 試劑、催化劑
- ← 溶劑
- ← 催化劑類別
- ← 溶劑類別
- ← 產物的可能性
- ← 反應物的可能性
- ← 反應類別
- ← 來源的種類(文獻、專利)
- ← 出版年份
- ← 縮小到只有一步反應
- ← 縮小到只包含實驗性術語的名單

例如：溶劑的過濾

**Solvent**

- water 131
- dichloromethane 61
- ethanol 59
- methanol 54
- toluene 43
- isopropyl alcohol 34
- acetonitrile 28

Filter by value  [View more](#)

- 每個專案的細目可以通過點擊打開。
- 這些專案按照案件數量的順序進行排序。
- 可以通過輸入數位或單詞來過濾專案。

**Solvent 2** Clear selected  Sort by Occurrence

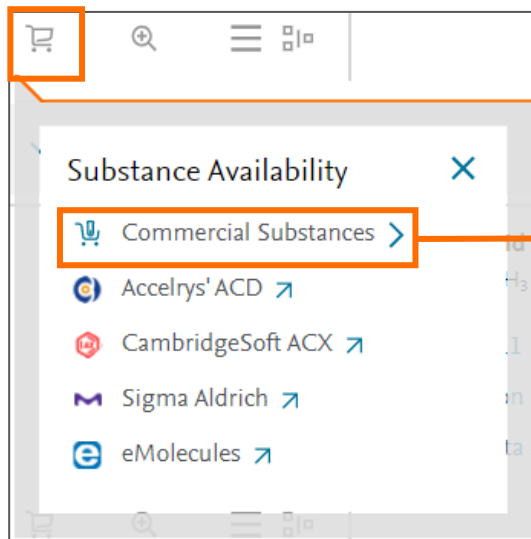
- water 131
- dichloromethane 61
- ethanol 59
- methanol 54
- toluene 43
- isopropyl alcohol 34
- acetonitrile 28
- ethyl acetate 24
- acetone 24
- tetrahydrofuran 22
- tert-butyl methyl ether 11

1 2 >

Limit to > Exclude >

# 商業試劑目錄資訊

點擊查看目錄資料庫，並通過點選連結到相應網站。



\*Accelrys ACD, CambridgeSoft ACX為付費資料庫，欲使用需單獨簽訂合同。

A screenshot of a product page for 'H-Gly-DL-Nva-OH'. The page includes a chemical structure, the chemical formula  $C_7H_{14}N_2O_3$ , and molecular weight 174.2. Below this, there are sections for 'Identification' and 'Supplier Information - 47'. The 'Supplier Information' section contains a table with the following data:

Supplier	Product	Purity	Package size & price	Availability
1Pluschem LLC USA	GLYCYL-DL-NORVALINE 2189-27-7 1P003R9C	>97.0percent(T)	1 g 229 USD	Shipment time: 2 weeks Tier Time: not specified Last updated: 2020-06-24
AA Blocks LLC USA	2-(2-Aminoacetamido);pentanoic acid 2189-27-7	>97.0percent(T); reagent grade	1 g 252 USD	Shipment time: 1 week Tier Time: Tier 1

可以檢查供應商、零件編號、純度、容量、價格和交貨日期。  
篩選功能使您將搜索範圍縮小到日本供應商。

# 詳細的來源文獻連結

**Full Text** : 您可以移動到期刊的文章頁面。

**Cited X times** : 來自 Scopus 的引用數量(點擊查看引用該文章的參考文獻列表)。

**Details** : 文章的細節(包括文章中的索引詞、物質和反應的細節)。

**Abstract** : 查看文章的摘要。

Reference

[Talsi, Evgenii P.; Bryliakov, Konstantin P.](#)  
[*Catalysis Today*, 2017, vol. 279, p. 84 - 89]

[Full Text](#) ↗ [Cited 4 times](#) ↗ [Details](#) > [Abstract](#) >

**Ti-Salan catalyzed asymmetric sulfoxidation of pyridylmethylthiobenzimidazoles to optically pure proton pump inhibitors**

1

[Talsi, Evgenii P.; Bryliakov, Konstantin P.](#) [*Catalysis Today*, 2017, vol. 279, p. 84 - 89]

[Abstract](#) ▾ [Index Terms](#) ▾ [Substances](#) 35 ▾ [Reactions](#) 19 ▾ [Full Text](#) ↗

※對於專利，也有權利要求的部分

Abstract

The asymmetric sulfoxidation of two pyridylmethylthiobenzimidazoles to anti-ulcer drugs of the PPI family (S)-omeprazole and a series of chiral titanium(IV) salen (>95percent) and enantioselectivities introduction of electron-withdrawing enantioselective catalysts. Like for the sulfoxidations, the temperature dependence of Ti-salen complexes is not with decreasing temperature. The active (presumably peroxotitanium) substrate.

Index terms

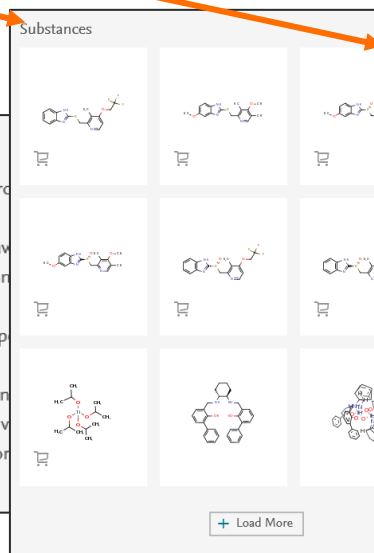
**Author keyword:** Asymmetric oxidation, Esomeprazole, Hydrogen peroxide, Mechanism, Salan, Titanium

**Compendex Terms:** Asymmetric oxidation, Electron-withdrawing groups, Enantioselective catalysts, Esomeprazole, Isoinversion, Proton pump inhibitors, Temperature dependence

**Compendex Terms:** Catalysis, Enantioselectivity, Hydrogen peroxide, Peroxides, Temperature distribution, Titanium

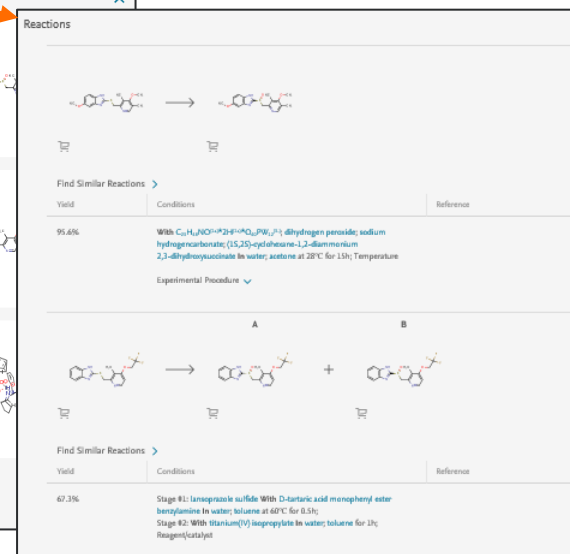
**Reaxys Index Terms:** Kagan-Modena oxidation, Oxidation kinetics, Oxidation reaction, catalyst, electron acceptor, enantiomer excess, enantioselective reaction, proton pump inhibitor, reaction kinetics, reaction optimization, separation method

Substances



+ Load More

Reactions

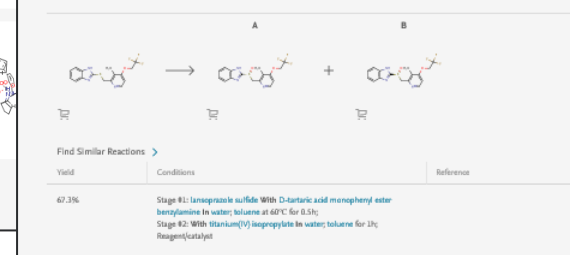


Find Similar Reactions >

Yield	Conditions	Reference
95.6%	With C <sub>10</sub> H <sub>14</sub> N <sub>2</sub> O <sub>2</sub> S <sub>2</sub> ·2H <sub>2</sub> O·2H <sub>2</sub> O; dithyrogen peroxide; sodium hydrogencarbonate; (1S,2S)-pylthiouracil-1,2-diammonium 2,3-dihydroxyacetate in water; acetone at 28°C for 15h; Temperature	

Experimental Procedure ▾

A B



Find Similar Reactions >

Yield	Conditions	Reference
67.3%	Stage 01: lomeprazole sulfide With D-tartaric acid monophenyl ester benzylamine in water; toluene at 60°C for 0.5h; Stage 02: With titanium(IV) isopropylate in water; toluene for 2h; Reagent(Catalyst)	

# 文獻中的作者和引用資料

點擊一個作者的名字將顯示該作者的Scopus搜索結果。

\*不需要訂閱Scopus就可以查看預覽介面

1 Ti-Salan catalyzed asymmetric sulfoxidation of pyridylmethylthiobenzimidazoles to optically pure proton pump inhibitors  
[Talsi, Evgenii P.](#) [Bryliakov, Konstantin P.](#) [Catalysis Today, 2017, vol. 279, p. 84 - 89]  
Abstract ▾ Index Terms ▾ Substances 35 ▾ Reactions 19 ▾ Full Text ▶

Cited 5 times

文獻タイトル	著者名	出版年	出版物名	被引用数
<input type="checkbox"/> 1 Zirconium-Salan Catalyzed Enantioselective $\alpha$ -Hydroxylation of $\beta$ -Keto Esters	Chen, J., Gu, H., Zhu, X., Nam, W., Wang, B.	2020	Advanced Synthesis and Catalysis 36(24), pp. 2976-2983	1
<input type="checkbox"/> 2 Modern Stereoselective Synthesis of Chiral Sulfinyl Compounds: Open Access	Wojaczyńska, E., Wojaczyński, J.	2020	Chemical Reviews 120(2), pp. 4578-4611	7
<input type="checkbox"/> 3 Salan vs. salen metal complexes in catalysis and medicinal applications: Virtues and pitfalls	Pessoa, J.C., Correia, I.	2019	Coordination Chemistry Reviews 388, pp. 227-247	31

Scopus 検索 収録誌 リスト SciVal Quick Link Test アカウントを作成 サインイン

## Bryliakov, Konstantin

Novosibirsk State University, Novosibirsk, Russian Federation 著者情報をすべて表示  
6701739175 <https://orcid.org/0000-0002-7009-8950> Is this you? Connect to Mendeley account

プロフィールを編集 アラートを設定 一致する可能性がある著者候補 SciValにエクスポート

### 指標の概要

144 文献数  
5043 2952 件の文献による被引用  
39 h-index: h-graph

### 文献数と被引用数のトレンド

13 文献数 481 被引用数

### 最も文献数が多いトピック 2015-2019

- Ferriyl Iron; Epoxidation; Dioxygenases 21 件の文献
- Dichloroethylaluminum; Copolymerization; Ethylenes 9 件の文献
- Epoxidation; Dioxirane; Enantioselectivity 3 件の文献

すべてのトピックを表示

144 件の文献 2952 件の文献による被引用 0 プレプリント 97 人の共著者 トピック

すべてをエクスポート すべてをリストに追加 並び替え: 出版日(新しい順)

Review • Open Access  
Post-metallocene catalysts for the synthesis of ultrahigh molecular weight polyethylene: Recent advances 0 被引用数

リストを検索結果の形式で表示  
4412 件の参考文献を表示

Cited X times以查看引用該文章的參考文獻列表。

## 什麼是Scopus?

Scopus 是Elsevier提供的世界上最大的摘要和引用資料資料庫。

不僅可以追蹤引用與被引用的關係，還可以高效地搜索文獻，利用文獻信息搜索共同研究者、分析趨勢。



ELSEVIER

# 通過Retrosynthesis制定合成途徑 ①

～如何繪製目標化合物的結構並進行路徑分析～

Retrosynthesis是一個根據Reaxys中包含的反應資料為目標化合物創建合成途徑的功能。

結構繪圖與普通的Reaxys繪圖相同。

Clear  Cancel  Synthesize  Feedback

- 生成的路線的最大數目
- 線上的最大分支數量
- 最大的步驟數
- 當歸因於一種商業化的化合物時將停止分析  
→ 建議不要使用（因為大分子有販售）
- 設定各反應的允許產量

## 通過Retrosynthesis制定合成途徑 ②

～如何分析化合物搜索結果中感興趣的化合物的途徑～

18

Synthesize

- > Find preparations
- > Create synthesis plans

Druglikeness Bioactivity

Physical Data - 19 Other Data

Parameters

Published ⓘ

Create upto 5 full routes.

Branches per step: 3

Max. number of steps: 5

Stop searching if building block is commercially available  Yes  No

Assumed yield for reactions without a given yield

0% 100%

Always show screen before creating plan

Create Plans >

解析



# 通過Retrosynthesis制定合成途徑 ③

~合成途徑開發的專案管理介面~

Reaxys<sup>®</sup> Quick search Query builder Results Retrosynthesis History Alerts

No.	Date/Time	Project name		No. of routes
9850	06 Oct 2021 05:09	Project #9850		Published <span>5</span> 

Draw new structure

Chemical structure: CN1C(=O)N(C1)c2ccc(cc2)c3ccc(cc3)C#N

Edit

確認生成路徑

刪除

如果您想繪製並分析一個新的結構

這個結構是以這個結構為基礎的  
如果您想編輯和分析

> Parameters

- 5 full routes (up to)
- 5 steps per route (up to)
- 3 branches per step (up to)
- Don't Stop at commercial building blocks
- 40% yield per step (assumed, if not published)



ELSEVIER

# 通過Retrosynthesis制定合成途徑 ④

~生成的合成路線的清單界面~

Project #424634  
0 selected  
Limit to Delete

My Synthesis Projects  
Draw

No Building blocks to target

No. of steps

Route topology

Get to routes

Custom Route #6  
6 steps

74 20 46 9

Published Route #1  
11 steps

74 57 3 39 22

該途徑的起始底物被標示出

因為可以監測路徑的步驟和分支數量，易於與其他路徑進行比較

Tree view >

Table view >

Preview

可以根據每條路線的步數進行排序

詳細的路徑  
「Tree View」：以枝狀的形式展示

# 通過Retrosynthesis制定合成途徑 ⑤

~合成途徑的樹狀圖畫面~

切換到另一條路線

顯示切換路徑中每個步驟的參考資料

改變反應資訊的顯示方式

輸出路徑

返回項目管理畫面等

The screenshot displays a retrosynthesis software interface. At the top, a toolbar contains icons for 'Export', 'Legend', and a series of icons for switching between different reaction pathways. Below the toolbar, a search bar is present, followed by 'Rotate', 'Fit view', and 'Copy route' buttons. The main area shows a reaction pathway tree with steps labeled Step 1 through Step 5. A table on the right provides detailed information for each step, including conditions, yield, and references.

Conditions	Yield	Reference
With $C_{68}H_{72}N_4O_{10}Ti_2$ ; dihydrogen peroxide In water; ethyl acetate at $0^{\circ}C$ ; for 24h; Reagent/catalyst; enantioselective reaction; Experimental Procedure $\nabla$	93.5%	Talsi, Evgenii P.; Bryliakov, Konstantin P. [Catalysis Today, 2017, vol. 279, p. 84 - 89] Full Text $\rightrightarrows$ Cited 9 times $\rightrightarrows$ Details $\rightrightarrows$
With N-methyl-6-aza-5 $\beta$ ,6 $\beta$ -epoxy-cholestane-3 $\beta$ -tert-butylidiphenylsilyloxy tetrafluoroborate In dichloromethane at $-70 - 20^{\circ}C$ ; for 3h; Inert atmosphere; enantioselective reaction;	86%	Zhou, Guobin; Guan, Yueqing [Heterocyclic Communications, 2016, vol. 22 19] Full Text $\rightrightarrows$ Cited 1 times $\rightrightarrows$ Details $\rightrightarrows$
With tert.-butylhydroperoxide In water; toluene at $-20^{\circ}C$ ; for 12h; Experimental Procedure $\nabla$	93 % ee	Current Patent Assignee: TEVA PHARMACEU INDUSTRIES LTD. - US2008/319195, 2008, A Location in patent: Page/Page column 5 Full Text $\rightrightarrows$ Details $\rightrightarrows$ Abstract $\rightrightarrows$

延長路徑

刪除部分路徑



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# 通過Retrosynthesis制定合成途徑 ⑥

～當無法獲得合成途徑時～

①如果該途徑可以由與被分析化合物結構相似的化合物產物

Published Route #1	No.	Date/Time	Project name	No. of routes
Project #9877				
My Synthesis Projects	10137	06 Oct 2021 07:43	Project #10137 <a href="#">Delete</a>	

Please select a substance for synthesis planning

Structure (1)	% Similarity	Chemical Name	No of Ref	No of preparations
	88.7	2-(((4-methoxy-3,5-dimethylpyridin-2-yl)methyl)sulfinyl)benzo[d]oxazole	1	3

[Submit >](#)

檢查相似程度，如果您對這種替代化合物感到滿意，請點擊「Submit」

②如果無法進行相似結構的分析時

→「No Results」

在這種情況下，您可以利用相似性進行複合搜索、建議從搜索結果中找到與您的目標相近的化合物，並用第4頁的方法對其進行分析。

# 化合物檢索結果畫面

## <項目>

- ① 瀏覽搜索結果的軌跡
- ② 過濾功能
- ③ 顯示合成熱門化合物的反應
- ④ 搜索結果的排序功能
- ⑤ 切換數據庫
- ⑥ 切換到網格顯示
- ⑦ 商業試劑資訊
- ⑧ 化合物的合成規劃
- ⑨ 連結到各化合物的合成方法和測量的物理性質

Reaxys TotalPatent One\* Quick search Query builder Results Synthesis planner History Alerts

1,268 Substances out of 16,699 Documents, containing 1,468 Reactions

① 1.27 K Preview

② Filters

Limit to > Exclude >

- By Structure
- Substances Classes
- Molecular Weight
- Number of Fragments
- Availability
- Availability in other databases
- Available Data
- Document Type
- Publication Year

③ Limit To Exclude Export Preparations

④ Sort search results

- No of References
- No of Fragments
- Molweight (g/mol)
- Molecular Formula
- Publication Year
- Comm. Availability
- Reaxys Registry Number

⑤ Reaxys - 1,268

No of References

Grid

⑦ Shopping cart icon

⑧ Grid view icon

⑨

**simvastatin**  
 $C_{25}H_{38}O_5$  418.574 4768037 123049-81-0, 79902-63-9

Identification Bioactivity - 2,165  
 Physical Data - 94 Other Data - 3,15  
 Spectra - 96

**lovastatin**  
 $C_{24}H_{36}O_5$  404.547 4720754 75330-75-5

Identification Bioactivity - 1,298 Preparations - 27  
 Physical Data - 249 Other Data - 3,113 Reactions - 263  
 Spectra - 50 Documents - 5,563

**mevastatin**  
 $C_{23}H_{34}O_5$  390.52 3630717 73573-88-3

Identification Bioactivity - 198 Preparations - 115  
 Physical Data - 19 Other Data - 1,197 Reactions - 10

# 詳細的化合物數據

The image shows a screenshot of a chemical database entry for simvastatin. The entry includes a chemical structure (1), the name 'simvastatin' (2), its molecular formula  $C_{25}H_{38}O_5$  and other identifiers (2), and a list of data categories: Identification, Physical Data - 90 (3), Spectra - 91 (3), Bioactivity - 1,823, and Other Data - 2,896 (3). On the right, there are links for Preparations - 49 (4), Reactions - 152 (5), and Documents - 8,583 (6). Below the main entry, three expanded panels show details for 'Physical Data - 90', 'Spectra - 95', and 'Other Data - 3067'. The 'Physical Data' panel lists Melting Point - 11, Density - 5, Association (MCS) - 10, Chromatographic Data - 8, and Circular Dichroism - 1. The 'Spectra' panel lists NMR Spectroscopy - 35, IR Spectroscopy - 16, Mass Spectrometry - 22, UV/VIS Spectroscopy - 1, and Raman Spectroscopy - 1. The 'Other Data' panel lists Use - 3064, Isolated from Natural Source - 1, and Quantum Chemical Calculations - 2.

① 結構式

② simvastatin  
 $C_{25}H_{38}O_5$  418.574 4768037 123049-81-0, 79902-63-9

Identification

Physical Data - 90

Spectra - 91

Bioactivity - 1,823

Other Data - 2,896

④ Preparations - 49 >

⑤ Reactions - 152 >

⑥ Documents - 8,583 >

simvastatin

Identification

Physical Data - 90

Melting Point - 11

Density - 5

Association (MCS) - 10

Chromatographic Data - 8

Circular Dichroism - 1

Spectra - 95

NMR Spectroscopy - 35

IR Spectroscopy - 16

Mass Spectrometry - 22

UV/VIS Spectroscopy - 1

Raman Spectroscopy - 1

Other Data - 3067

Use - 3064

Isolated from Natural Source - 1

Quantum Chemical Calculations - 2

## 顯示第一條記錄的細節

- ① 結構式
- ② 化學名
- ③ 記錄中包含的資料
- ④ 該化合物作為產物的反應
- ⑤ 包含此化合物的反應
- ⑥ 參考文獻

# 複合搜索結果的過濾

**Filters**

Limit to > Exclude >

- By Structure ▾ ← 構造
- Substances Classes ▾ ← 化合物分類
- Molecular Weight ▾ ← 分子量
- Number of Fragments ▾ ← 分支數
- Availability ▾ ← 取得的可能性
- Availability in other databases ▾ ← 包括在其他資料庫中
- Available Data ▾ ← 可供查看的資料（如反應、物理特性等）
- Document Type ▾ ← 文獻的種類（文獻、專利等）
- Publication Year ▾ ← 出版年份

例如：分子量的過濾

Molecular Weight	Count
<input type="checkbox"/> >348 - 360	1
<input type="checkbox"/> >360 - 372	3
<input type="checkbox"/> >372 - 384	6
<input type="checkbox"/> >384 - 396	31
<input type="checkbox"/> >396 - 408	85
<input type="checkbox"/> >408 - 420	144
<input type="checkbox"/> >420 - 432	43

Filter by value ▾ [View more](#)

- 每個專案的細目可以通過點擊打開。
- 這些專案按照案件數量的順序進行排序。
- 可以通過輸入數位或單詞來過濾專案。

Molecular Weight 2 Clear selected X ↓ ↑ Sort by Occurrence ▾ X

<input type="checkbox"/> >408 - 420	144
<input type="checkbox"/> >396 - 408	85
<input checked="" type="checkbox"/> >432 - 444	60
<input checked="" type="checkbox"/> >444 - 456	48
<input type="checkbox"/> >456 - 468	43
<input type="checkbox"/> >420 - 432	43
<input type="checkbox"/> >384 - 396	31
<input type="checkbox"/> >516 - 528	27
<input type="checkbox"/> >492 - 504	25
<input type="checkbox"/> >468 - 480	22
<input type="checkbox"/> >480 - 492	20

1 2 3 >

Limit to > Exclude >

# 搜索結果的匯出

以PDF格式或XML/Word/Excel等檔案格式匯出搜索結果

3,193 Reactions 585 Documents, 2,799 Substances

Limit To Excludes Export Save Plan Hide Conditions

1

Chemical reaction scheme showing a transformation of a complex organic molecule.

任何記錄或欄位都可以從搜索結果中選擇並匯出

Export reactions Reaxys

Choose a format: PDF/Print

Range: Range (e.g. 1-2, 1-10)

From: 1 To: 8

Export:

- All available data
- Identification data only
- Hit data only

Additional options:

- Include structures
- Include experimental procedure
- Include a description in the document

Export >

在搜索結果界面上，點擊「Export」

## 輸出設定界面：

輸出形式、輸出範圍、輸出內容  
選擇一個選項，然後點擊輸出按鈕  
每次輸出最多5000個項目  
24小時內最多10次

\*如果您未登錄通過IP身份驗證，則無法導出。

Exports

Your export is ready

Download > Cancel >

on Suk; Ho, Kam-Piu;  
enyang;  
1472, p. 160 - 166]  
Abstract >

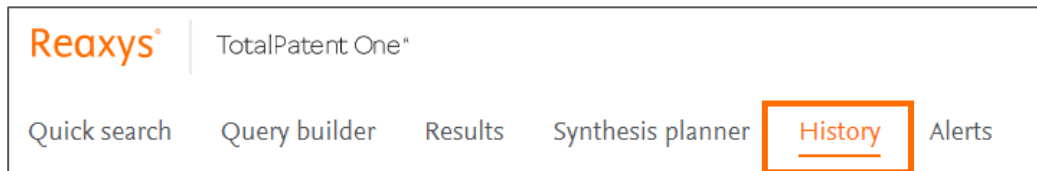
Exports Feedback



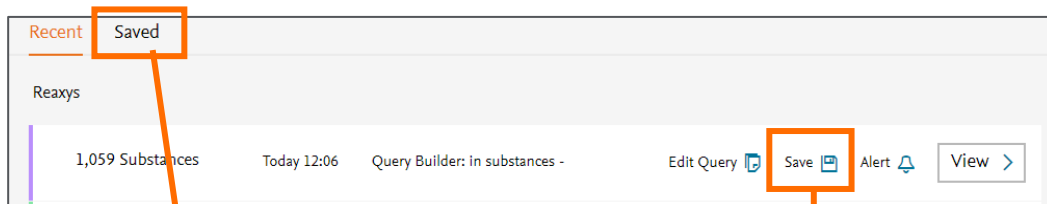
# 搜索結果的保存

可以存儲搜索結果中的任意記錄


- 保存的記錄可以在“History”介面上查看(如果使用者登錄個人帳號，在關閉視窗後將不會被刪除。)



打開畫面最上面的“History”標籤

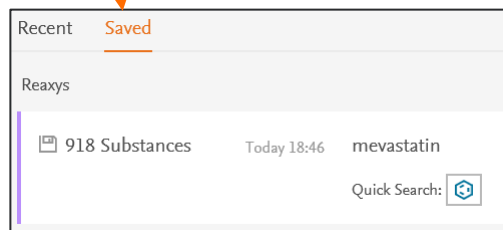


點擊你想保存的記錄的「Save」圖示

點擊 Save 

為結果輸入一個名稱，然後點擊「Save」

\*您也可以使用日文輸入名稱



點擊“Saved”選項

出現存儲資料的管理介面

註冊數據以列表形式顯示



# Alert的設定與管理①

Alert會儲存你的搜索指令，資料庫會定期自動提供符合標準的搜索結果。

- 有助於當您想要在相同條件下檢查相關反應、物質和物理性質的資訊。
- Alert結果將被發送到註冊的電子郵寄地址，同樣地Alert結果也可以發送給其他用戶並分享。
  - \* 使用Alert需要登入

## Alert的設定：

- ① 在執行了您設置的Alert搜索後，打開歷史記錄。
- ② 在“History”介面上，選擇要設置Alert的搜索歷史記錄。  
搜索歷史中會顯示各種選項，點擊”Alert”。

The screenshot displays the Reaxys interface. On the left, the 'Results' page shows 42,232 documents with various filters and a list of search results. An orange arrow points from the 'History' tab in the top navigation bar to the 'History' page. The 'History' page shows a list of search results with an 'Alert' button highlighted in an orange box at the bottom right.

# Alert的設定與管理②

## Alert的設定：

Alert configuration form showing fields for Query, Alert name, Send alerts to, Frequency, and Send alert. The 'Send alert' dropdown is highlighted, and an arrow points to the 'Alerts' management view. The 'ADVANCED ALERT CONTENT' section is also visible, with 'Hit details' selected. The 'Save' button is highlighted.

- Alert name: Alert名稱
- Send alerts to: 設定送達的電子郵件地址(可複數輸入)
- Frequency: 通知頻率(可以指定星期和日期。)
- Alert Content: 所需的資訊內容

設置上述內容並點擊「Save」

## Alert的管理：

Alerts management page showing a list of alerts. The 'New' link is highlighted, and an arrow points to the 'Alerts' management view. The 'Edit' and 'Delete' buttons for a specific alert are also highlighted. The text '顯示Alert的管理畫面' and '您可以在列表中查看已登錄的Alert' are overlaid on the page.

Alert設定的編輯與刪除

Send alert dropdown menu showing options: After any update, Upon first appearance in the database, and After any update (selected).

※若選擇「Send alert:」，建議同時選擇「After any update」。每次當Alert目標進行屬性、反應或文獻更新時，Alert都會通過電子郵件發送給使用者。

若選擇「Upon first appearance in the database」，僅在包括新化合物等情況下才會傳送資訊。因此，不會傳遞持續更新資訊。



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# 操作環境/聯繫細節

## 操作環境：

- Firefox (版本49以上)
- Chrome (版本53以上)
- Edge (版本14以上)
- Safari (版本9)
- Internet Explorer (版本11)

-Reaxys可以在無Java的環境中使用  
-可用於Windows和Macintosh

## 如需進一步訊息，請聯繫：

如果您在使用Reaxys方面有任何問題，請聯繫Elsevier Japan

- ◆ 聯絡資訊：<https://jp.service.elsevier.com/app/contact/supporthub/reaxys/>
- ◆ 電話號碼：03-5561-5035

有關Reaxys的資訊可以在以下連結中找到

- ◆ <https://www.elsevier.com/ja-jp/solutions/reaxys/reaxys-for-user>



# Thank you

如果您在使用Reaxys方面有任何問題，請聯繫Elsevier

- ◆ 聯絡資訊: [r.huang@elsevier.com](mailto:r.huang@elsevier.com)
- ◆ 電話號碼: +886-2-2522-5937

有關Reaxys的資訊可以在以下連結中找到

- ◆ <https://www.elsevier.com/zh-tw/solutions/reaxys>

