

新版 Reaxys 化學資料庫

收錄內容更多、操作更直覺

www.reaxys.com
new.reaxys.com

Elsevier 生命科學解決方案經理 梁成芝

2017

Reaxys 化學資料庫使用權限

- **Reaxys 化學資料庫**
 - IP 開放，免帳號密碼，無同時上線人數限制
 - www.reaxys.com
 - 新介面 <https://new.reaxys.com>
- 可使用 proxy 或 VPN 遠端連線，詳情請洽各校圖書館

Reaxys 中文線上學習資源



Reaxys 中文學習平台
taiwan.elsevier.com/reaxyshelp

學習影片 Learning Video

利用學習影片自我學習如何有效使用Reaxys，一步一步教學，讓資訊檢索變得更簡單。



文件下載 Document Download

快速上手Reaxys，並用實例介紹如何使用Reaxys功能，您可快速找到答案，讓學習變得更有興趣。



線上研討會 Webinar

邀請專家分享使用Reaxys技巧和實例演練操作，讓您從學習中了解如何與資訊互動。



連線問題 Connection Issues

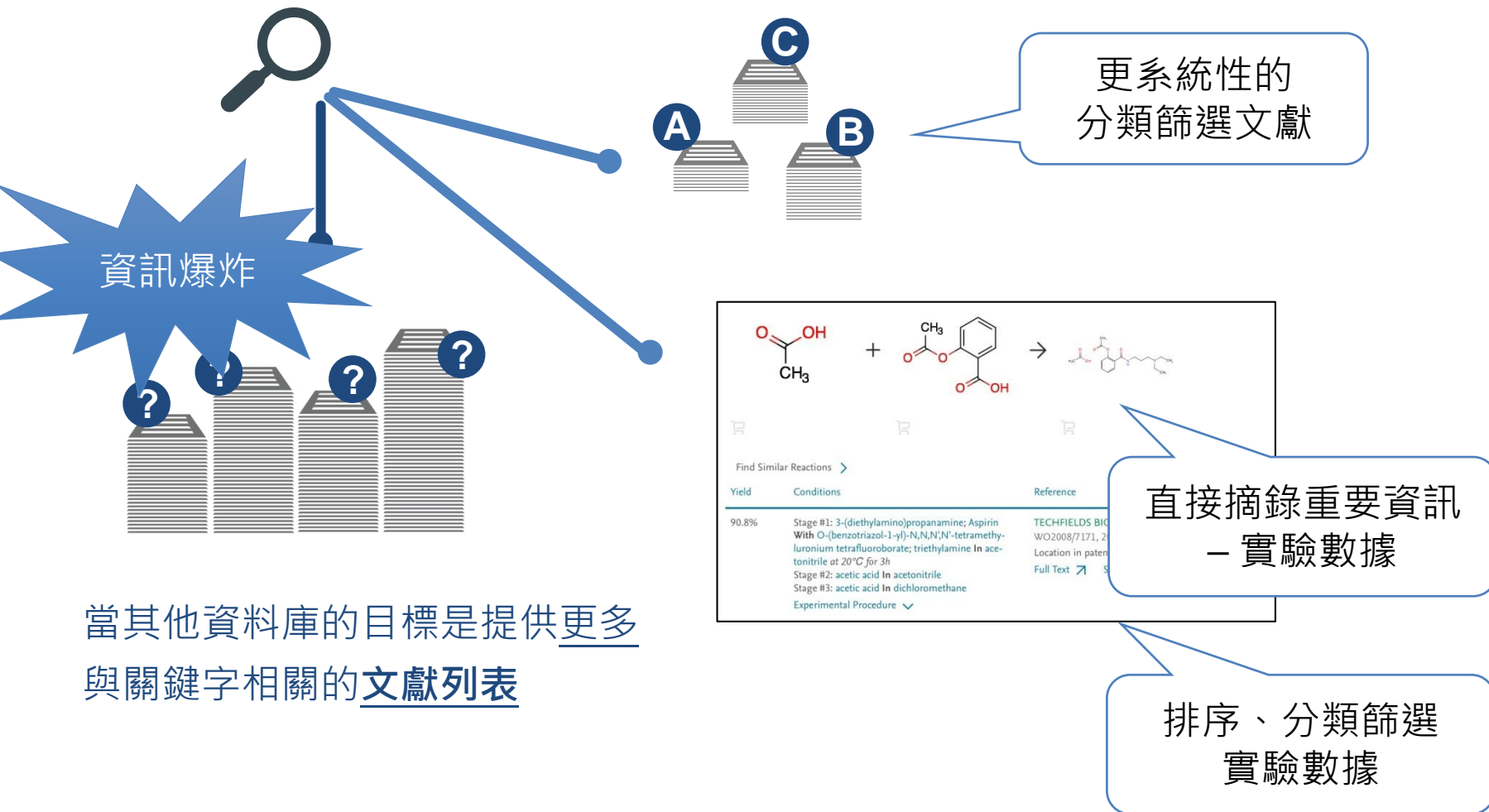
了解常見連線問題，並提供解決之道與聯絡方式。



本平台支援手機及
平板使用

Elsevier R&D Solution 致力於更快找到答案

提供多種搜尋邏輯，除了關鍵字，可整合結構、分子式、數據等資料逆向搜尋

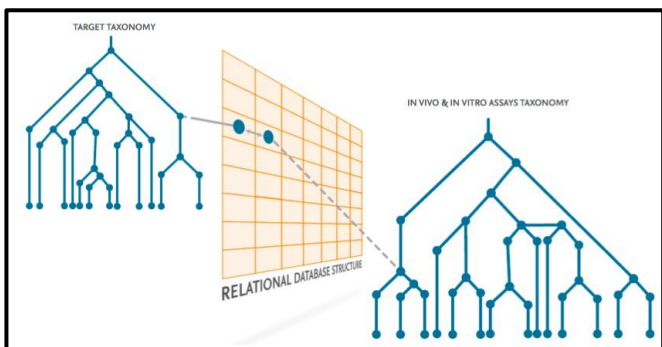


新版 Reaxys 三大變化



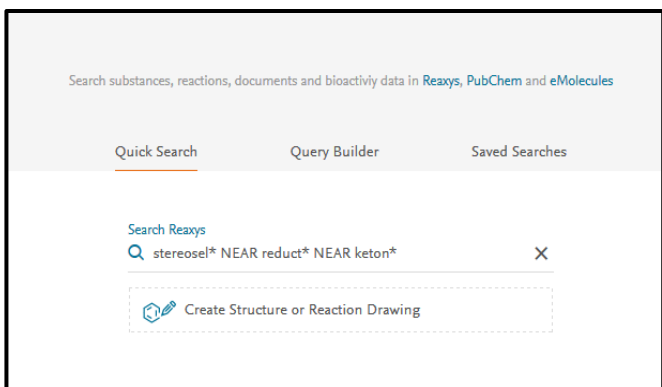
擴充收錄內容

- 16,000種期刊與主要專利局
- 5億筆實驗數據摘錄
- 281本期刊及專利**化學反應**全文材料方法摘錄



自動索引技術與資料庫架構

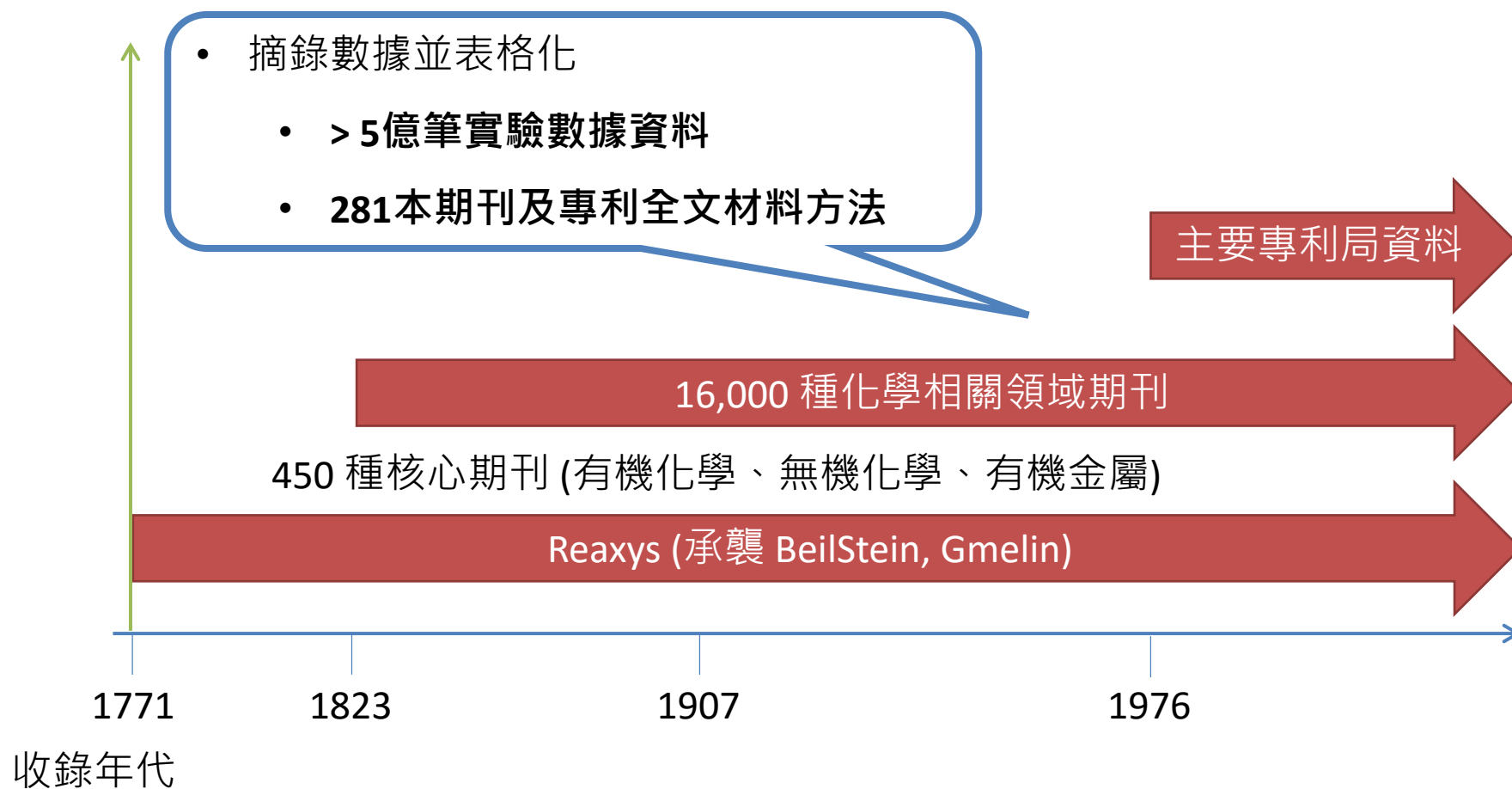
- 先進的全文自動索引技術
- 多元搜尋工具，如結構、實驗數值....更多
- 表格化整理與超連結串連



使用者介面

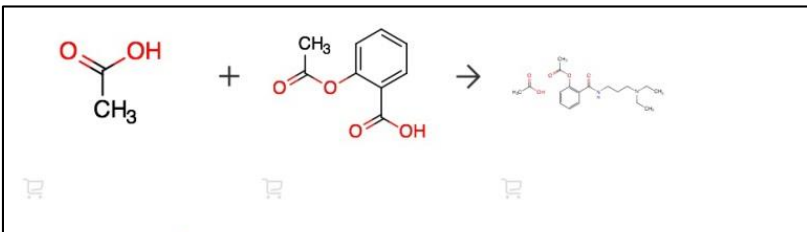
依據實際使用頻率設計
常用功能一目了然

Reaxys 收錄內容



自動索引技術 -- 資料表格化

直接比較數據資料，節省全文閱讀的時間與經費



Find Similar Reactions

Yield	Condition
90.8%	Stage #1: With O-(b)lurionium tonitrile at Stage #2: Stage #3: Experiment

Physical Data - 532

Dissociation Exponent - 27

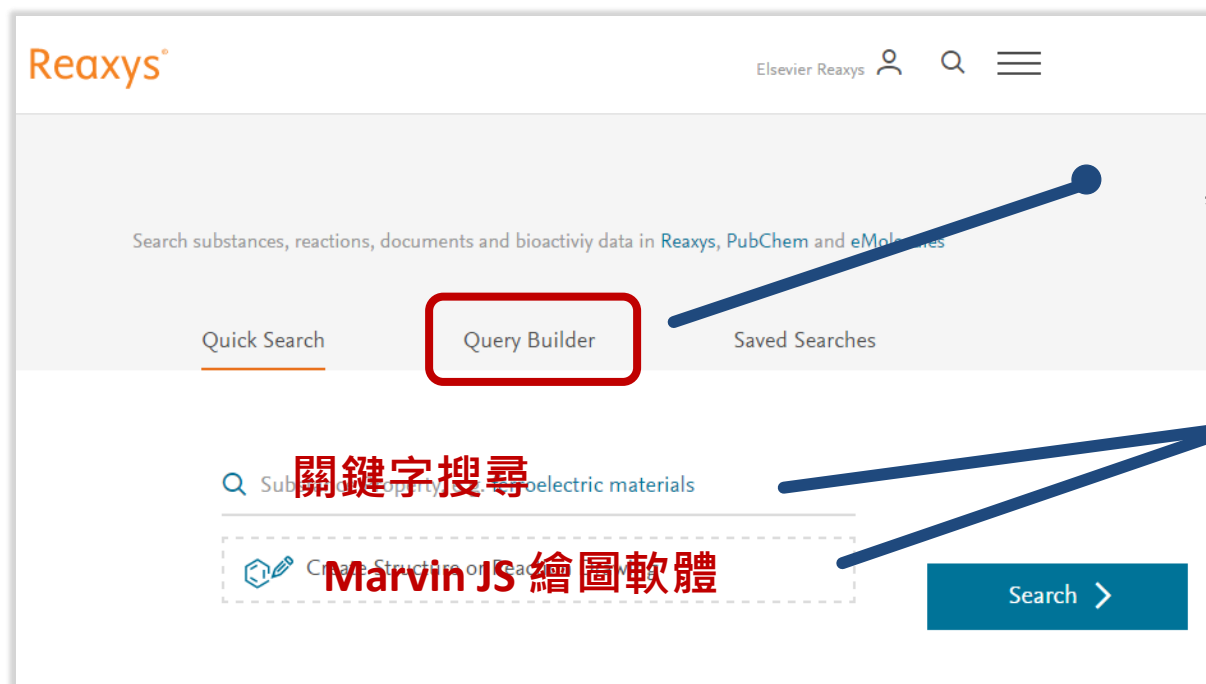
Dissociation Exponent (pK)	Dissociation Group	Temperature (Dissociation Exponent), °C	Solvent (Dissociation Exponent)	Method (Dissociation Exponent)	Type (Dissociation Exponent)	Reference
3.48	RCOO-H	25	dimethylsulfoxide, H2O	spectrophotometric	a1/apparent	Article, 2003 Citation Journals: Analytical Chemistry, 4, 75, 2003, 883 - 892
3.47		25	dimethylsulfoxide, H2O		a1/thermodynamic	Article, 2002 Citation Journals: Journal of Pharmaceutical Sciences, 4, 91, 2002, 933 - 942
3.55	COOH	37	H2O		a1/apparent	Article, 1995 Citation Journals: Biological and Pharmaceutical Bulletin, 2, 18, 1995, 310 - 314
3.6	COOH	25			a1/apparent	Article, 1993 Citation Journals: Chemical and Pharmaceutical Bulletin, 6, 41, 1993, 1137 - 1143

- 表格中的文字皆可篩選
- 沒有購買全文也可以獲得
 - 5 億筆實驗數據資料
 - 281 種期刊及專利的合成材料方法

450 → 12,000 本期刊

使用者介面

依據實際使用頻率設計，常用功能一目了然



進階搜尋

彙整 > 400 種搜尋欄位

> 95% 使用者

最常使用

關鍵字 + 結構搜尋

智慧辨識與預覽功能

自動辨識關鍵字，推薦相關結果，供您預覽及挑選

Search Reaxys

Q ZrO2 refractive index



關鍵字搜尋

支援 AND OR NOT * 等指令

4 Substances

Molecular formula : ZrO2 AND Property : refractive index

View Results >

Preview Results ▾

555 Documents

Titles, Abstract, Keywords : ZrO2, refractive index

Preview Results ▾

125471 Documents

Titles, Abstract, Keywords : refractive index

Preview Results ▾

38096 Documents

Titles, Abstract, Keywords : ZrO2

Preview Results ▾

自動辨識提供
化合物及物化特性搜尋
結果

自動推薦其他相關結果

預覽搜尋結果
是否符合需求

進入Query Builder
修改條件

View Result
使用 Filter 篩選

多元搜尋工具 – Query Builder

自由結合超過 400種欄位、歷史搜尋紀錄、搜尋指定數值的實驗數據

The screenshot shows the Reaxys Query Builder interface. At the top, there are navigation tabs: Quick search, **Query builder**, Results, Synthesis planner, and History. A 'Sign in' button is in the top right. Below the navigation bar, there's a search bar with a 'Search Substances' button and a dropdown arrow. To the left of the search bar are icons for Import, Save, Reset form, and Delete. Below the search bar, there are four tabs: Structure, Molecular Formula, CAS RN, and Doc. Index. The main area is a large canvas with the text 'Drag & Drop to build a new query'. On the right side, there's a 'Search properties' section with a search icon and three tabs: Fields, Forms, and History. Below these tabs is a list of available fields: Reaxys, PubChem, eMolecules, LabNetwork, and Structure. At the bottom right, there's a 'Feedback' button.

搜尋

超過 400 種欄位

常用欄位：

- 結構
- 分子式
- CAS 編號
- 關鍵字

Drag & Drop to build a new query

將要用的欄位拖到畫布上

Fields: 所有欄位

Forms: 預設常用欄位

History: 歷史紀錄

開始使用 Reaxys

- ✓ 找到**答案**而非堆積如山的待唸文獻
- ✓ 摘錄更多數據資料、合成方法
- ✓ 搜尋方法更多元彈性



Chemical reaction scheme showing the synthesis of aspirin (acetylsalicylic acid) from salicylic acid and acetic anhydride.

Find Similar Reactions >

Yield	Conditions
90.8%	Stage #1: 3-(diethylamino) With O-(benzotriazol-1-yl)uronium tetrafluoroborate nitrile at 20°C for 3h Stage #2: acetic acid In ac Stage #3: acetic acid In di Experimental Procedure

Physical Data - 532

Dissociation Exponent - 27

Dissociation Exponent (pK)	Dissociation Group	Tri (Diss Exponent)
3.48	RCOO-H	25
3.47		25
3.55	COOH	37
3.6	COOH	25

Lyophilized aspirin with trehalose may decrease the incidence of gastric injuries in healthy dogs Cited 1 times
Lin, Lee-Shuan; Kayasuga, Yuko; Shimohata, Nobuyuki; +6 others - Journal of Veterinary Medical Science, 2012, vol. 74, # 11, p. 1511 - 1516
Abstract Index Terms Full Text

Incidence of aspirin resistance in the patient group of a university hospital in Korea Cited 6 times
Lee, Young Kyung; Kim, Han-Sung; Park, Ji-Young; +1 other - Korean Journal of Laboratory Medicine, 2008, vol. 28, # 4, p. 251 - 257
Abstract Index Terms Full Text

Increased platelet expression of glycoprotein IIIa following aspirin treatment in aspirin-resistant but not aspirin-sensitive subjects Cited 3 times
Floyd, Christopher N.; Goodman, Timothy; Becker, Silke; +7 others - British Journal of Clinical Pharmacology, 2014, vol. 78, # 2, p. 320 - 328
Abstract Index Terms Full Text

Reaxys 搜尋實例與技巧

不同領域適用不同搜尋範例：

有機化學、分析方法、複合材料 (合金、陶瓷)與特性、高分子、藥物生物活性數據

Presented By

Date

大綱

- **Quick Search 關鍵字自動辨識**
 - 自動辨識 – 化合物、數據名稱
 - 自動辨識 – 關鍵字
 - 自動辨識 – 反應類型
- **搜尋結果**
 - 合成路徑規劃 (進階)
 - 包裝價格查詢
 - 查詢合成與分析材料方法「全文」 (進階)
 - 文獻匯出到 EndNote
- **Marvin JS 繪圖軟體**
 - 基本操作
 - 反應搜尋功能 (進階)
 - 衍生物相關功能 (進階)
- **Query Builder 進階搜尋**
 - 數據數值範圍搜尋
 - 搜尋結果關鍵字限縮 (進階)
 - 分子式衍生物搜尋功能 (進階)


自動辨識 – 化合物 Acrylonitrile

Acrylonitrile Mechanical Property










Search Reaxys


 Acrylonitrile










Reaxys[®] Quick search Query builder Results Synthesis planner History Sign in 

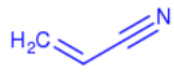
2 Filters and Analysis

- By Structure 
- Measurement pX 
- Highest Clinical Phases 
- Targets 
- Parameters 
- Substance Classes 
- Molecular Weight 
- Availability 
- Availability in other databases 

2 Substances out of 11,520 Documents, containing 14,725 Reactions, 3 Targets Reaxys - 2 


 0    No of References  


 1





acrylonitrile
C₃H₃N 53.0635 605310 107-13-1


- Identification
- Druglikeness
- Bioactivity (All)
- Physical Data - 458
- Spectra - 129
- Other Data - 80



Preparations - 294 


Reactions - 14,725 

Targets - 3 

Documents - 11,520 

 2

 Options  **cyanovinylidene**
cyanovinylidene, cyanovinylidene, cyanovinylidene, cyanovinylidene
C₃H₃N 51.0476 6796746

Feedback 

自動辨識 – 化合物 Bisphenol A

EPICHLOROHYDRIN

Search Reaxys

 bisphenol A HPLC NMR



Reaxys[®]


Quick search

Query builder

Results


Synthesis planner


History


Sign in 

1


Filters and Analysis


By Structure 


Substances Classes 

Molecular Weight 


Availability 

Available Data 

Document Type 
















Publication Year 

[Back to Results Preview](#)

Database: Reaxys - 1 

1 Substances out of 4,203 Documents containing 1,208 Reactions

☐ 0 selected: [Limit To](#)  [Exclude](#)  [Export](#) 

自動辨識 – 關鍵字 Cyanoacrylate Adhesive, UV curing,

文獻列表

2,458

Filters and Analysis

Index Terms (List)

- ☐ adhesive agent 1,113
- ☐ tissue adhesive 769
- ☐ drug efficacy parameter 112
- ☐ cosmetic 111
- ☐ toxicity 86
- ☐ dissociation energy 85
- ☐ glue 83

Document Type

- ☐ article 1,945
- ☐ review 167
- ☐ conference paper 112
- ☐ patent 98
- 67

Back to Results Preview

2,458 Documents with 699 Substances, 444 Reactions

0 selected: Limit To Exclude Export

Relevance

可依年代、
文獻種類排序

瀏覽/篩選
相關關鍵字

篩選文獻種類
如專利

☐ Cyanoacrylate adhesives: A critical review
1 Rajesh Raja - Reviews of Adhesion and Adhesives, 2016, vol. 4, # 4, p. 398 - 416
Abstract Index Terms Substances Full Text

☐ Current status of cyanoacrylate and fibrin tissue adhesives
2 Forseth; O'Grady; Toriumi - Journal of Long-Term Effects of Medical Implants, 1992, vol. 2, # 4, p. 221 - 233
Abstract Index Terms Full Text Cited 21 times

☐ CYANOACRYLATE ADHESIVES - AN OVERVIEW.
3 Millet - Meeting - American Chemical Society, Rubber Division, 1981, p. 41
Index Terms Full Text

☐ The current status of cyanoacrylate and fibrin tissue adhesives.
4 Forseth; O'Grady; Toriumi - Journal of long-term effects of medical implants, 1992, vol. 2, # 4, p. 221 - 233
Abstract Index Terms Full Text

☐ RECENT DEVELOPMENTS IN CYANOACRYLATE ADHESIVE TECHNOLOGY.
5 Melody - 1985, vol. 1, p. 49 - 61
Abstract Index Terms Full Text

Feedback

自動辨識 – 關鍵字 Lubricant Additives

13,013

Filters and Analysis

Index Terms (List)

☐ lubricating agent

10,327

☐ viscosity

2,062

☐ oxidation reaction

1,100

☐ electrooxidation

664

☐ antioxidant agent

643

☐ nanoparticle

564

☐ coefficient of friction

532

+ More

Document Type

☐ article

9,330

☐ conference paper

1,971

☐ patent

579

☐

310

☐

204

☐

189

< Back to Results Preview

13,013 Documents with 3,010 Substances, 1,503 Reactions

☐ 0 selected:

Limit To

Exclude

Export

Relevance

↑

↓

☐ Lubricating agents and their influence on their environment

1

Marat - Przegląd Włokienniczy, 2001, # 3, p. 27 - 29

Abstract

Index Terms

Full Text

☐ Corrosion and corrosion prevention in lubricant systems.

2

Smith - 1982, vol. 28, # 328, Apr. 1982, p. 136 - 139

Abstract

Index Terms

Full Text

☐ Significance of solid lubricants as lubricant additives.

3

Holinski - In: 5th Int. Colloquium on Additives for Lubricants and Operational Fluids, (Ostfildern, Fed. Rep. Germany: Jan. 14-16, 1986), W.J. Bartz (ed.), vol.II, Ostfildern, Fed. Rep Germany, Esslingen Tech. Akad., 1986, Session 6, Paper 6.6, p.6.6-1-6.6-11. (ISBN 3-924813-07-8), 1986, vol. II, Ostfildern, Fed. Rep Germany, Esslingen Tech. Akad., 1986, Session 6, Paper 6.6, p.6.6-1-6.6-11.

Abstract

Index Terms

Full Text

☐ Lubricant and additive effects on spur gear fatigue life

4

Townsend; Zaretsky - Journal of Synthetic Lubrication, 1989, vol. 6, # 2, p. 83 - 106

Abstract

Index Terms

Full Text

Cited 7 times

☐ Ionic liquids as tribological performance improving additive for in-service and



Feedback


瀏覽/篩選
相關關鍵字篩選文獻種類
如專利可依年代、
文獻種類排序

關鍵字自動辨識 -- 反應類型

RING-OPENING POLYMERIZATION

Reaxys®

[Quick search](#) [Query builder](#) [Results](#) [Synthesis planner](#) [History](#) Olivia Liang  

14 Reactions Condition : ring-opening polymerization [Preview Results](#) ▾ [View Results](#) >
[Edit in Query Builder](#) 

14,263 Abstract, Keywords : ring-opening polym [results](#) ▾

編輯搜尋條件

自動辨識提供相關反應

預覽搜尋結果
是否符合需求

使用 Filter
篩選

關鍵字自動辨識 -- 反應類型

EPOXIDATION

自動辨識提供 epoxidation
相關反應

38,377	Reactions	Condition : epoxidation	Preview Results ▾	View Results >
20,772	Documents	Titles, Abstract, Keywords : epoxidation	Preview Results ▾	View Results >

預覽搜尋結果
是否符合需求

使用 Filter
篩選

編輯搜尋條件

搜尋結果 – 包裝價格查詢

2

Options ▾

+

→

1 Synthesize ▾

Show All Details ▾ Find Similar

Yield	Conditions	Reference
90%	Stage #1: 6,7-dihydro carbonate In water at Stage #2: methyl 2-b 20°C; for 12h; Stage #3: With sulfur Experimental Proced	Mahmoodi, Nosrat O.; Ghavidast, Atefeh; Ashkan, Mitra; Mamaghani, Manouchehr; Zanjanchi, Mohammad Ali; Tabatabaeian, Khalil; Arabanian, Armin - Synthesis and Reactivity in Inorganic, Metal-Organic and Nano-Metal Chemistry, 2016, vol. 46, # 10, p. 1552 - 1557 Full Text ➤ Cited 2 times ➤ Show details ➤

Substance Availability

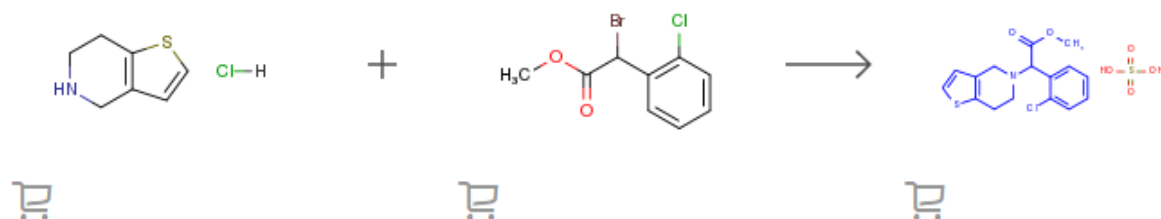
- Accelrys' ACD
- eMolecules
- CambridgeSoft ACX
- Sigma Aldrich
- Labnetwork

免費供應商網站：

- eMolecules
- Sigma Aldrich
- Labnetwork

搜尋結果 – 合成方法全文內容 Experimental Procedure

Clopidogrel Synthesis



Show All Details Find Similar Reactions

Yield	Conditions	Reference
-------	------------	-----------

90%

Stage #1: 6,7-dihydro-4H-thien

With sodium carbonate In water

Stage #2: methyl 2-bromo-2-(2

water; toluene at 20°C for 12 h

Stage #3: With sulfuric acid In

; Reagent/catalyst Solvent

[Experimental Procedure](#)

[Experimental Procedure](#)

One-Pot Procedure for the Synthesis of Racemic Clopidogrel Bisulfate (2)

To a vessel equipped with Dean-Stark assembly, 2-(thiophen-2-yl)ethanamine **5** (0.48 g, 4 mmol), PFA (0.13 g, 4.3 mmol), and toluene (6 mL) were added and the reaction mixture was refluxed for 2 h to obtain a yellow solution contain imine. After cooling to 20°C, a solution of 6N HCl (0.7 mL) in DMF was added into the reaction mixture and continued to heat at 50°C for 1 h to produce **4a** as a white precipitate. The reaction was cooled to 25°C and aqueous solution of 10 percent Na₂CO₃ was added and stirred for 30 min. Then a solution of methyl-2-bromo-2-(2-chlorophenyl)acetate **3** (1.04 g, 4 mmol) in toluene (7 mL) was added to the reaction mixture. The reaction mixture stirred at room temperature for 12 h. The aqueous layer is discarded and the organic layer was washed with water. The organic phase was evaporated, to afford viscose oil. To this oil, conc. H₂SO₄ (0.42 mL) and EtOAc (8 mL) was added. The mixture was stirred for 1 h. The precipitated crystals filtered off and washed with cool acetone. The pure racemic clopidogrel bisulfate **2** was dried in oven at 50°C (1.35 g, 90 percent yield). White powder; mp 220–222°C; IR: ν (KBr, cm⁻¹) 3434 (OH stretch), 3100, 2989, 2953, 1755 (C=O stretch), 1239, 1222 (C-O stretch), 1063.

搜尋結果 – 分析方法全文內容 Supporting information

分析材料方法若放在 Supporting Information 中，可以直接下載

HPLC (High
performance liquid
chromatography)

supporting
information

[Zhu, Yaoqiu; Zhou, Jiang; Jiao, Bo](#) - ACS Medicinal Chemistry Letters, 2013, vol. 4, # 3, p. 349 - 352

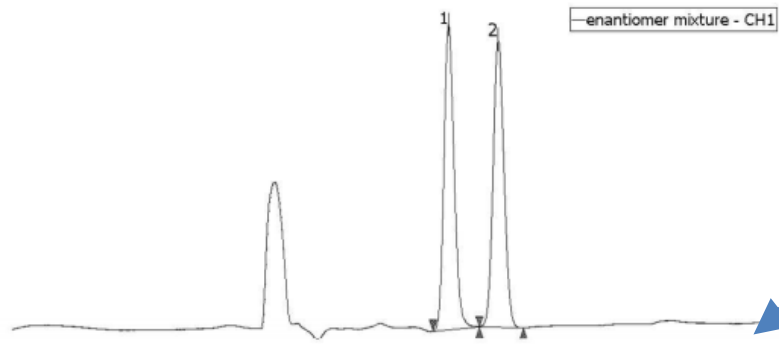
Full Text ↗

Cited 6 times ↗

Show details >

Chiral HPLC Chromatogram

Racemic Mixture Reference



點選 Full Text

打開 supporting information

Supporting information link

http://pubs.acs.org/doi/suppl/10.1021/ml300460t/suppl_file/ml300460t_si_001.pdf

獲得重要資訊

Chiral Analysis.

The synthesized clopidogrel (CPG) hydrochloride salts were subjected to chiral analysis on an LC-2000Plus HPLC system (Jasco, Tokyo, Japan) with a Chiralpak AD-H column (Daicel, Osaka, Japan) using a standard isocratic program for CPG analysis (10-15% i-propanol in n-hexane, 10 min, 1.0 mL/min). 1 Racemic CPG (with 50% of each enantiomer) was used as reference.

搜尋結果 -- 合成路徑規劃

Clopidogrel Synthesis

Reaxys

Quick search

Query builder

Results

Synthesis planner

History

Olivia Liang



Synthesis Planner

Edit

Autoplan 1 1

1 Plan 1

+ Create new

Plan 1

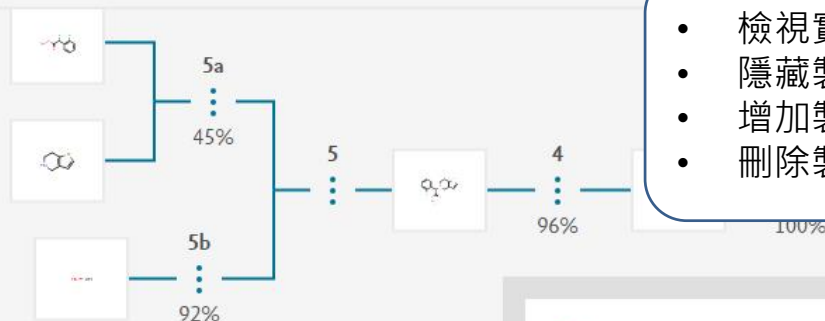
Import

Save

Export

Undo

Redo



- 檢視實驗條件
- 隱藏製備方法
- 增加製備方法 (手動/自動)
- 刪除製備方法

- Show conditions
- Hide preparation
- Add preparations
- Remove preparation

Feedback

搜尋結果 – 文獻匯出到EndNote

由文獻列表點選 Export，設定檔案格式與輸出範圍

Reaxys Quick search Query builder Results Synthesis planner

936 Documents with 4,238 Substances, 3,239 Reactions, 295 Targets

0 selected Limit To Exclude **Export**

Filters and Analysis
Index Terms (List)
Index Terms (ReaxysTree)

Export documents

Choose a format: Literature Management Systems

Range: All results - 936

Additional options: ☒ Include abstracts

Literature Management Systems

- PDF/Print
- XML
- Microsoft Word
- Microsoft Excel
- Literature Management Systems
- Electronic Lab Notebook
- RD File

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

- All results - 936
- Selected - 0
- Range (e.g. 1-2, 1-10)

Export >

Marvin JS 繪圖軟體 – 基本功能

The screenshot shows the Marvin JS web application interface in a Google Chrome browser window. The URL is https://www.reaxys.com/reaxys/js/sre_5_3_1_03/child_marvin_js.html. The interface includes a top toolbar with icons for file operations (open, save, delete, copy, paste), zooming, and 2D/3D toggles. A left sidebar contains drawing tools like eraser, bond types, and charge modification. A right sidebar displays a periodic table of elements. The central workspace shows a chemical structure with annotations for 2D/3D conversion and zooming. A bottom toolbar features common chemical structures like alkanes and rings. At the bottom, there are buttons for 'Transfer Query' and 'Cancel & Return', along with a footer note: 'Reaxys supports various structure editors. Please check "My Settings" for more.'

Annotations on the interface include:

- 選擇 (Select)
- 橡皮擦 (Eraser)
- 各種鍵結及畫筆 (Various bonds and drawing tools)
- 長碳鍵 (Long carbon bond)
- 改變元素電荷 (Change element charge)
- 開啟舊檔 (Open old file)
- 剪下複製貼上 (Cut, copy, paste)
- 週期表 (Periodic table)
- 展開/收起氫原子 (Expand/collapse hydrogen atoms)
- 3D 立體旋轉視圖 (3D isometric rotation view)
- 結構 3D 立體化 (Structure 3D isomerization)
- 結構 2D 平面化 (Structure 2D planarization)
- 放大、縮小、全部符合視窗大小、選擇範圍符合視窗大小 (Zoom in, zoom out, fit all to window, fit selection to window)
- 元素列表也可用鍵盤輸入 (Element list can also be entered via keyboard)
- 加入 → 或 + 等符號，或使用 atom mapping 功能 (Add → or + symbols, or use atom mapping function)
- 搜尋特定官能基 (Search for specific functional groups)
- 加入 Generic group (Add generic group)
- 常用結構模板 (Common structure templates)
- Generic 元素代號 (Generic element symbols)

- 無須 JAVA
- 可從 ChemDraw 複製貼上
- 輸出成透明背景高解析圖檔
- 基本功能
 - 模板、鍵結、元素與週期表
 - 選擇、旋轉、移動、縮放
 - 2D/3D 轉換、氫原子展開

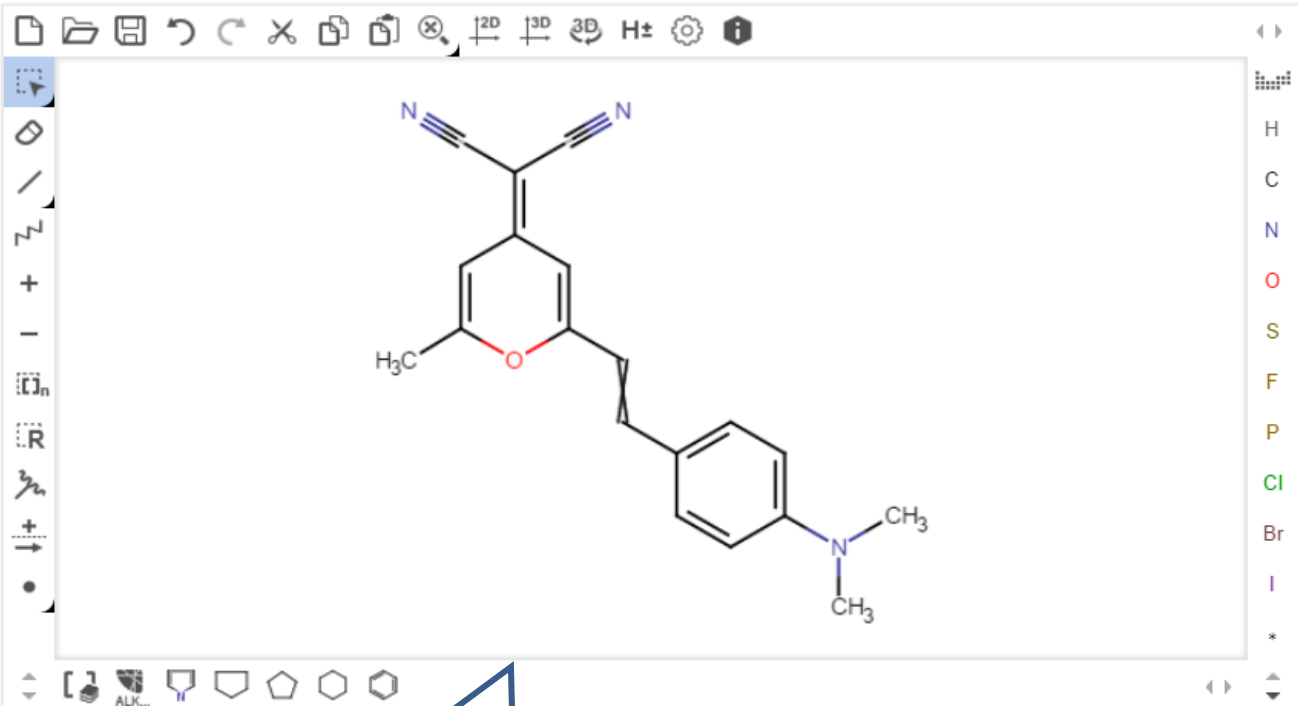
Marvin JS 繪圖軟體 – 基本功能

DCM, OLED 材質由名稱匯入結構

由名稱、CAS編號匯入結構

Structure editor

Create structure template from name >



Search this structure as:

- ☒ As drawn
- ☐ As substructure
- ☐ Similar



Include:

- ☐ T
- ☒ S
- ☒ A
- ☐ Related Markush
- ☒ Salts
- ☒ Mixtures
- ☒ Isotopes
- ☒ Charges
- ☒ Radicals

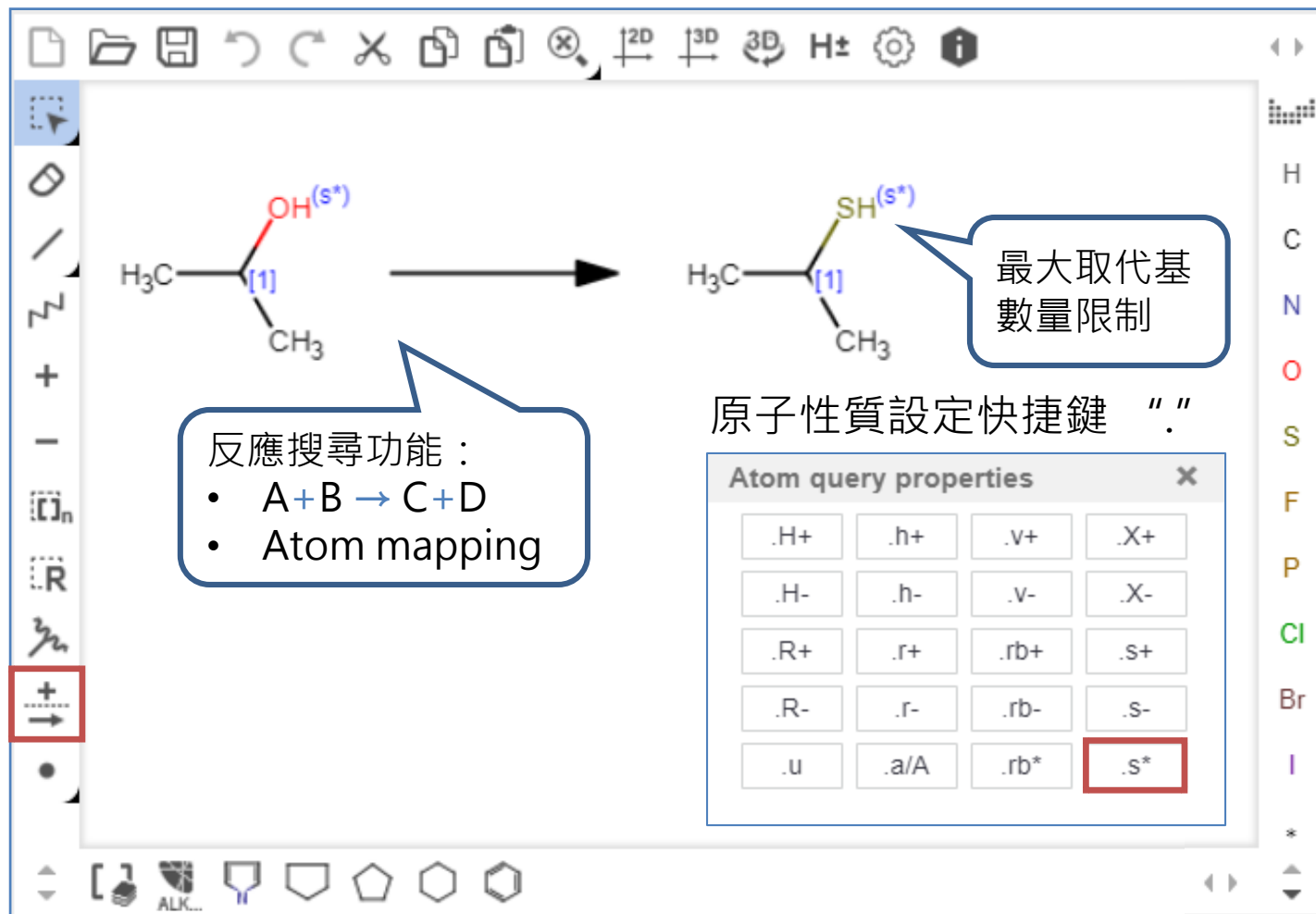
+ More options

Feedback

可再修改

Clear  Cancel  Transfer to query >

Marvin JS 繪圖軟體 – 反應搜尋功能



Search this structure as:

- ☐ As drawn
- ☒ As substructure
 - ☒ On all atoms
 - ☐ On heteroatoms
- ☐ Similar

Include

- ☐ Tautomers
- ☒ Stereo
- ☒ Additional ring closures
- ☐ Related Markush
- ☒ Salts
- ☒ Mixtures
- ☒ Isotopes
- ☒ Charges
- ☒ Radicals

+ More options

Reaction 搜尋結果

找到 1,235 筆反應

1,235 Reactions 495 Documents 1,970 Substances, 64 Targets



0



Limit To



Exclude



Export



Reaxys Ranking ↓



1



Show All Details ✓ Find Similar Reactions >

Yield

Conditions

Reference

94%

With Lawessons reagent In toluene for 0.5h; Heating;

Nishio, Takehiko - Journal of the Chemical Society, Perkin Transactions 1: Organic and Bio-Organic Chemistry (1972-1999), 1993, # 10, p. 1113 - 1118

Full Text ↗

Cited 24 times ↗

Show details >

若不使用 atom mapping

找到 3,239 個反應，但官能基的位置可能不同

3,239 Reactions out of 936 Documents containing 4,238 Substances, 295 Targets

☐ 0 selected [Limit To](#) [Exclude](#) [Export](#) [Sort by Reaxys Ranking](#) ↓

☐ 1 [Options](#) ▼

7(S)-7-acetylthio-7-deoxylincomycin

[1](#) [Synthesize](#) ▼

[Show All Details](#) ▼ [Find Similar Reactions](#) >

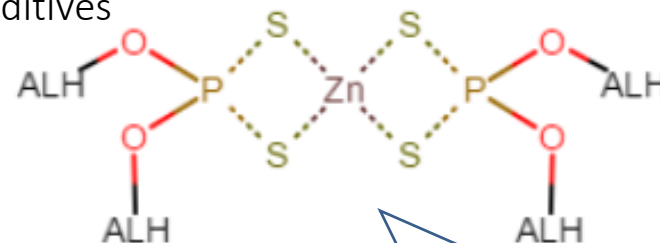
Yield	Conditions	Reference
94%	With methanol; sodium methylate at 20°C; for 0.333333h;	Meiji Seika Kaisha, Ltd. - EP1970377, 2008, A1 Location in patent: Page/Page column 48 Full Text Show details >

[Experimental Procedure](#) ▼

[Feedback](#)

Marvin JS 繪圖軟體 – 結構衍生物搜尋

ZDDP Zinc Dithiophosphate 潤滑油抗磨添加劑 Anti Wear Additives



完備的衍生物搜尋設定

自動辨識提供不同相似程度
化合物搜尋結果

自動推薦其他相關結果

Query Builder 搜尋指定波長範圍高折射率材料

REFRACTIVE INDEX

指定折射率範圍

Refractive Index ☐ Find any Hide fields ^ X

>=	▼	Refractive Index 2	Eq
=	▼	Wavelength (Refractive Index), nm 1530-1560	Eq
=	▼	Temperature (Refractive Index), °C	Eq

可自由輸入波長範圍

例如：短波紅外線常用遠距通訊區段
1530-1560 nm
近紅外光
750-1400nm

QueryBuilder -- 實驗數據搜尋

CdSe 的 XRD 數據 -- 原子間距離與角度、空間群、結晶相、晶體體系

Molecular Formula

is

Molecular Formula
CdSe

AND

Group

Interatomic Distances and Angles ☐ Find any Show fields

OR

Space Group ☐ Find any Show fields

OR

Crystal Phase ☐ Find any Show fields

OR

Crystal System ☐ Find any Show fields

QueryBuilder -- 實驗數據搜尋

CdSe 的 XRD 數據-搜尋結果

 1 **cadmium(II) selenide**
CdSe 191.37 11323271

CdSe

Hit Data - 91

Spectra - 226

Preparations - 174 >

Identification

Bioactivity - 72

Reactions - 468 >

Physical Data - 605

Other Data - 140

Documents - 1371 >



^ Hit Data - 91

- ✓ Crystal Phase - 27 hits out of 27
- ✓ Crystal System - 4 hits out of 4
- ✓ Interatomic Distances and Angles - 2 hits out of 2
- ✓ Space Group - 58 hits out of 58

QueryBuilder -- 實驗數據搜尋

CdSe 的 XRD 數據-搜尋結果

^ Space Group - 58 hits out of 58

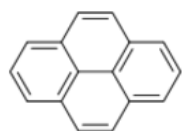
Location	Comment (Space Group)	Reference
	Method = Powder X-ray diffraction	<p>Han, Guoping; Wang, Lin; Pei, Cuijin; +5 others - Journal of Alloys and Compounds, 2014, vol. 610, p. 62 - 68 Full Text ↗ Cited 4 times ↗ Show details ></p> <p>Jin, Feng; Zheng, Mei-Ling; Zhang, Mei-Lin; +2 others - RSC Advances, 2014, vol. 4, # 63, p. 33206 - 33214 Full Text ↗ Cited 5 times ↗ Show details ></p> <p>Oyetunde, Temidayo; Afzaal, Mohammad; Vincent, Mark A.; +1 other - Dalton Transactions, 2016, vol. 45, # 46, p. 18603 - 18609 Full Text ↗ Show details ></p>

^ Crystal Phase - 6 hits out of 27

Description (Crystal Phase)	Reference
Zinc blende (ZnS), Powder X-ray Diffraction	<p>Mastai; Polsky; Koltypin; +2 others - Journal of the American Chemical Society, 1999, vol. 121, # 43, p. 10047 - 10052 Full Text ↗ Cited 69 times ↗ Show details ></p> <p>Manna; Scher; Alivisatos - Journal of the American Chemical Society, 2000, vol. 122, # 51, p. 12700 - 12706 Full Text ↗ Cited 1,440 times ↗ Show details ></p> <p>Kumar; Sharma - Journal of Physics and Chemistry of Solids, 1998, vol. 59, # 8, p. 1321 - 1325 Full Text ↗ Cited 18 times ↗ Show details ></p>

搜尋單重態與三重態電子轉移數據

磷光與螢光光譜資料

**pyrene**C₁₆H₁₀ 202.255 1307225 129-00-0

Hit Data - 2

Identification



Hit Data - 2

Fluorescence Spectroscopy - 1 hits out of 537

Description (Fluorescence Spectroscopy)	Reference
Energy transfer from singlet state	Ehli, Christian; Aminur Rahman; Jux, Norbert; +9 others - Journal of the American Chemical Society, 2006, vol. 128, # 34, p. 11222 - 11231 Full Text ↗ Cited 212 times ↗ Show details >

也可搜尋 delayed fluorescence

Phosphorescence Spectroscopy - 1 hits out of 43

Description (Phosphorescence Spectroscopy)	Reference
Energy transfer from triplet state	Borisevich, N. A.; Kazakov, S. M.; Kolesnik, E. E.; +4 others - Journal of Applied Spectroscopy, 2001, vol. 68, # 3, p. 447 - 454, Zhurnal Prikladnoi Spektroskopii, 2001, vol. 68, # 3, p. 343 - 348 Full Text ↗ Show details >

Phosphorescence Spectroscopy

☐ Find anyHide fields [^](#) [×](#)

is

Description (Phosphorescence Spectroscopy)
energy transfer from triplet state

is



Solvent (Phosphorescence Spectroscopy)



=



Temperature (Phosphorescence Spectroscopy), °C



AND

Fluorescence Spectroscopy

☐ Find anyHide fields [^](#) [×](#)

is

Description (Fluorescence Spectroscopy)
energy transfer from singlet state

is



Solvent (Fluorescence Spectroscopy)



=



Temperature (Fluorescence Spectroscopy), °C



Query Builder – 反應搜尋結果關鍵字限縮 Reaction Basic Index

66 個反應中，工業級大量生產的方法，只有 1 種

Reaxys[®]

Quick search

Query builder

Results

Synthesis planner

History

Sign in

?

1

Filters and Analysis

By Structure

Yield

Reagent/Catalyst

Solvent

Catalyst Classes

Solvent Classes

Product Availability

Reactant Availability

Reaction Classes

1

Reaction scheme showing the hydrogenation of cyclohexane-1,4-dicarboxylic acid to cis-1,4-bis(hydroxymethyl)cyclohexane.

Options

Hide Hit Details

Show All Details

Find Similar Reactions

Yield	Conditions	Reference
	With hydrogen in ethyl acetate at 180°C; under 60006 Torr; for 6h; Industrial scale;	Chen, Jiali; Guo, Li; Zhang, Fazhi - Catalysis Communications, 2014, vol. 55, p. 19 - 23 Full Text Cited 2 times Show details

Feedback

QueryBuilder – 分子式衍生物搜尋

未知物鑑定 -- 由天然物純化出、包含34個碳，旋光度=18.2的所有化合物

Molecular Formula

is



Molecular Formula
C34*

搭配分子式搜尋
C34* 表示此分子含有34個碳，其餘未知

AND

Isolation from Natural Product



Find any

Show fields



化合物來源為天然物

AND

Optical Rotatory Power



Find any

Hide fields



is



Type (Optical Rotatory Power)

is



Solvent (Optical Rotatory Power)

=



Optical Rotatory Power, deg
18.2

選擇旋光度
optical rotatory power (deg)
選擇 = 輸入 18.2

QueryBuilder --分子式衍生物搜尋

搜尋結晶外觀/顏色

Reaxys®

Quick search

Query builder

Results

Synthesis planner

History

Sign in



Search Substances > ▼



Import



Save



Reset form



Delete



Structure



Molecular Formula



CAS RN



Doc. Index

Crystal Property Description

☐ Find any

Hide fields ^ ×

is



Colour & Other Properties

brown



is



Point group



AND

Molecular Formula



is



Molecular Formula

Ag*



Search properties

Q crystal



crystal

Reaxys ^

Crystal Phase



Crystal Property Description



Crystal System



Decomposition



Transition Point(s) of Crystalline Modification(s)



Feedback

QueryBuilder --分子式衍生物搜尋

未知物鑑定 -- 搜尋含銀的咖啡色結晶，找到 236 種可能化合物

236

Filters and Analysis

By Structure ▾

Substances Classes ▾

Molecular Weight ▾

Availability ▾

Available Data ▾

Document Type ▾

Publication Year ▾

5

AgHO

Hit Data - 2

Crystal Property Description - 2 hits out of 12

silver hydroxide

AgHO 124.876 8128142

Hit Data - 2

Physical Data - 17

Spectra - 1

Other Data - 2

Preparations - 11 >


Reactions - 28 >

Documents - 82 >

Hit Data - 2

Crystal Property Description - 2 hits out of 3

Colour & Other Properties	Reference
brown	Rouch, Anne; Castellan, Tessa; Fabing, Isabelle; +5 others - RSC Advances, 2013, vol. 3, # 2, p. 413 - 426 Full Text ↗ Cited 9 times ↗ Show details >
brown	Fisher, Aaron S.; Khalid, Mian B.; Widstrom, Matthew; +1 other - Journal of the Electrochemical Society, 2012, vol. 159, # 5, p. A592-A597 Full Text ↗ Cited 9 times ↗ Show details >

Feedback 

活用分子式搜尋與分子量排序

搜尋指定碳數區間的石墨烯 (135種 → 14 種)

The screenshot displays the Reaxys search interface. At the top right is a 'Search Substances' button. Below it is a toolbar with icons for Import, Save, Reset form, and Delete, followed by search filters for Structure, Molecular Formula, CAS RN, and Doc. Index. The main search area contains two criteria:

- Chemical Name:** The dropdown menu is set to 'is', and the search term is 'graphene'. A callout bubble points to this term with the text: '化合物名稱為 graphene 石墨烯'.
- Molecular Formula:** The dropdown menu is set to 'is', and the search term is 'C[1-60]'. A callout bubble points to this term with the text: 'C[1-60] 表示 碳數範圍必須介於 1-60 之間'.

An 'AND' button is located between the two criteria. On the right side of the search area, there are icons for clearing the search (X) and viewing results (🔍).

Query Builder 搜尋未知比例合金

Ti?Al?V?* 表示此分子含有
未知數量的鈦Ti, 鋁 Al, 鈮 V ,
並含有其他未知成份

Molecular Formula

is



Molecular Formula
Ti?Al?V?*



AND

Mechanical Properties ☒ Find any

Show fields



必須含有 Mechanical Properties 數據

例如：拉伸強度 Tensile strength、降
伏點 (彈性極限) yield point

搜尋陶瓷複合材料

活用 LINEAR STRUCTURE FORMULA 欄位

Y?O? 表示氧化鈮種類未限定
*表示混合物比例未知
分子式最後加上 * 表示可能包含未知成份

Linear Structure Formula

is



Linear Structure Formula

Y?O?*ZrO2*



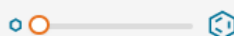
[Back to Query Builder](#)

Database: [Reaxys - 15](#)



15 Substances out of 219 Documents containing 76 Reactions

☐ 0 selected: [Options](#)



No of References



1

yttria stabilized zirconia
11385211

Y2O3#dotZrO2

Identification

Physical Data - 188

Spectra - 17

Bioactivity - 12

Other Data - 3

Preparations - 40

Reactions - 68

Documents - 208

Reaxys 中文線上學習資源



Reaxys 中文學習平台
taiwan.elsevier.com/reaxyshelp

學習影片 Learning Video

利用學習影片自我學習如何有效使用Reaxys，一步一步教學，讓資訊檢索變得更簡單。



文件下載 Document Download

快速上手Reaxys，並用實例介紹如何使用Reaxys功能，您可快速找到答案，讓學習變得更有興趣。



線上研討會 Webinar

邀請專家分享使用Reaxys技巧和實例演練操作，讓您從學習中了解如何與資訊互動。



連線問題 Connection Issues

了解常見連線問題，並提供解決之道與聯絡方式。



本平台支援手機及
平板使用



Thank You!

附錄

Marvin JS 搜尋小技巧

由 ChemDraw 複製結構到 MarvinJS

Reaxys 結構搜尋 – 匯入與匯出 – 1



Edit → Copy as → SMILES

Ctrl + V 貼上

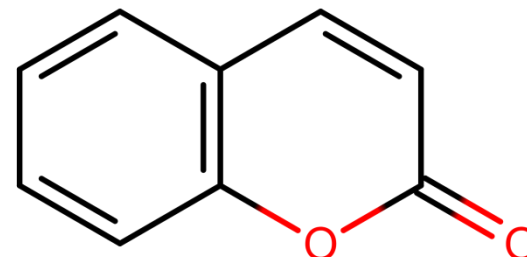
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由化合物名稱產生結構

Reaxys 結構搜尋 – 匯入與匯出 – 2

化合物名稱
Coumarin



Create structure template from name >

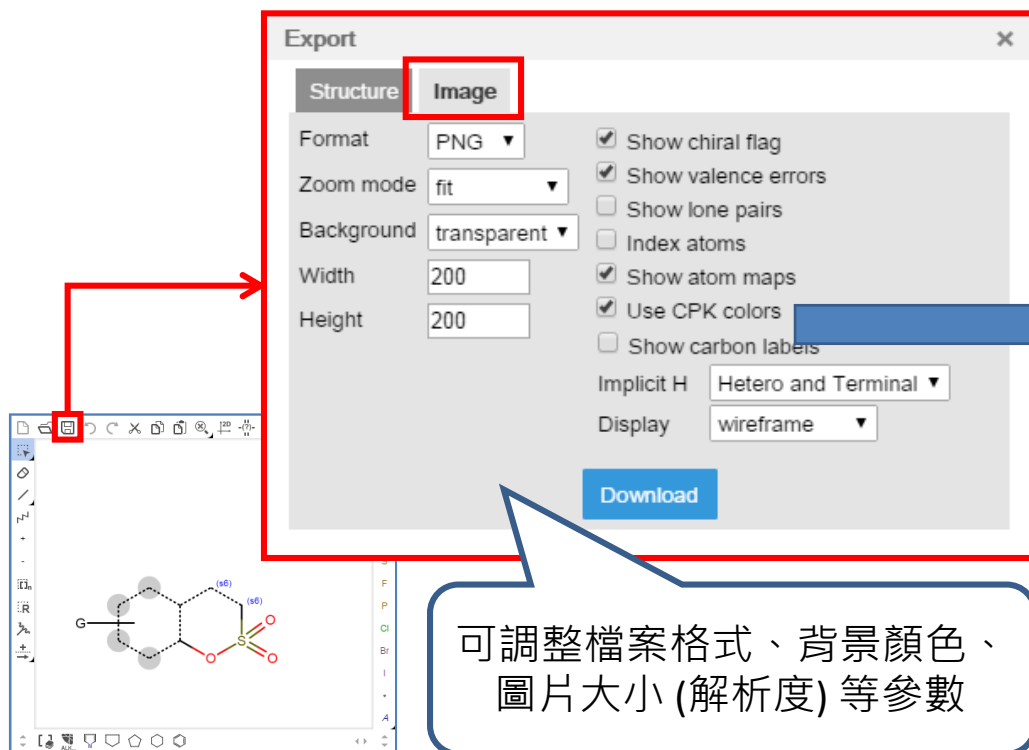
NewReaxys new.reaxys.com

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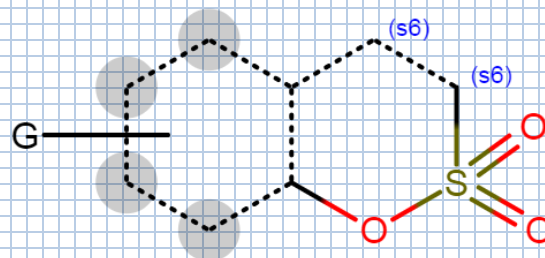
<https://youtu.be/Y2sBPt4o>

將化學結構存成透明背景的圖檔

Reaxys 結構搜尋 – 匯入與匯出 – 3



背景透明的結構圖檔
可在 ppt 或海報使用



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儲存可編輯的結構檔 .mrv

Reaxys 結構搜尋 – 匯入與匯出 – 4

The diagram illustrates the workflow for saving and loading chemical structure files in Reaxys. It features three main windows and several callouts:

- Export Window:** A window titled "Export" with tabs for "Structure" and "Image". The "Structure" tab is selected, showing the "ChemAxon Marvin Document (MRV)" format. The content area displays XML code for a chemical structure. A red box highlights the "Structure" tab and the XML code. A callout "儲存檔案" (Save File) points to the "Structure" tab.
- Marvin JS Window:** A window titled "Marvin JS" showing a chemical structure. A callout "讀取檔案" (Load File) points to the "File" menu.
- Chemical Structure Window:** A window showing a chemical structure. A callout "匯入舊檔" (Load Old File) points to the "File" menu.
- Text Box:** A callout "支援多種檔案格式，也可匯入其他繪圖軟體的檔案" (Supports multiple file formats, can also import files from other drawing software) points to the "Chemical Structure" window.

The XML code in the "Export" window is as follows:

```
<?xml version="1.0" encoding="UTF-8" ?>
<cmf>
  <queryType="Any"/><bond atomRefs2="a6 a1" order="1"
  <queryType="Any"/><bond atomRefs2="a9 a10" order="1"
  <queryType="Any"/><bond atomRefs2="a10 a6" order="1"
  <queryType="Any"/><bond atomRefs2="a8 a9" order="1"/><bond
  atomRefs2="a8 a12" order="2"/><bond atomRefs2="a5 a7" order="1"/>
  <bond atomRefs2="a7 a8" order="1"/><bond atomRefs2="a8 a11"
  order="2"/><bond atomRefs2="a14 a13" order="1"/></bondArray>
  <molecule id="sg1" molID="m2" role="MulticenterSgroup" atomRefs="a1
  a4 a2 a3" center="a14"/></molecule></MChemicalStruct>
</MDocument></cmf>
```

Use Ctrl+C to copy the selected source above.

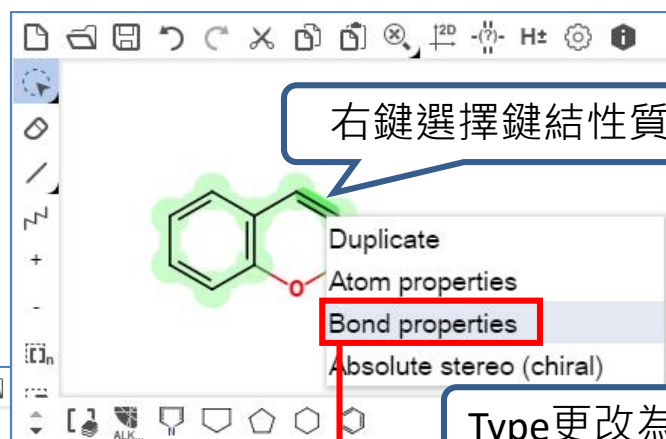
Download

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不確定鍵結種類，該如何搜尋？

Reaxys 結構搜尋 – 衍生物搜尋 – bond property



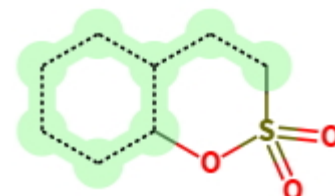
不確定鍵結種類時，可以用虛線表示任意鍵結 (如單鍵、雙鍵、其他)，可以一次找到所有符合條件的化合物

任意形狀選取

Bond properties

Type	any
Topology	undefined
Reacting center	undefined

Ok

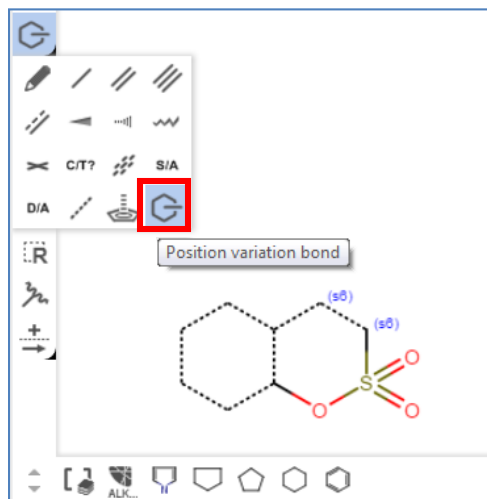


NewReaxys new.reaxys.com

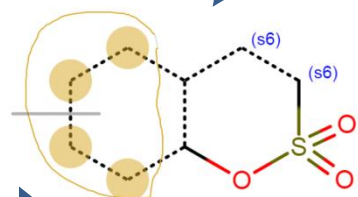
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不確定鍵結位置，該如何搜尋？

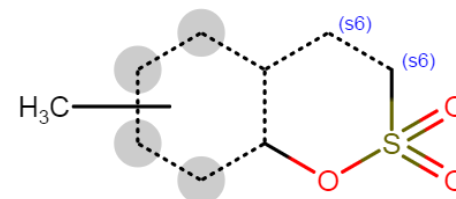
Reaxys 結構搜尋 – 衍生物搜尋 – position variation bond



圈選可能接上
取代基的原子



鍵結與官能基種類
可以再調整



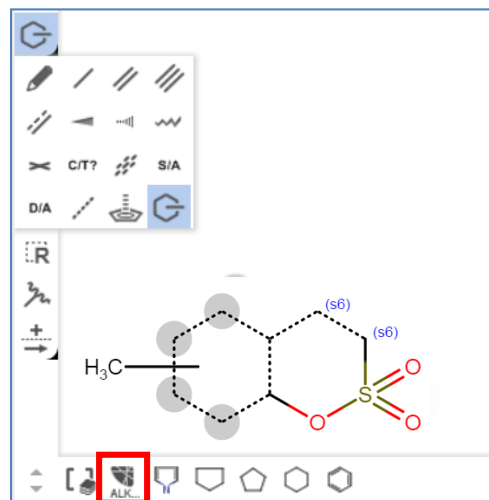
4 個灰色標記的原子
任 1 個接上甲基
就會被搜尋到

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在指定位置，搜尋任意官能基

Reaxys 結構搜尋 – 衍生物搜尋 – G 代表 any functional group



Search this structure as:

- ☒ As drawn
- ☐ As substructure
- ☐ Similar

選擇精準搜尋
As drawn

Reaxys Group Generics

Acyclic Cyclic

ACY ACH

Carb Hetero

ABC ABH AHC AHH

Alkynyl Alkoxy

AYL AYH AOX AOH

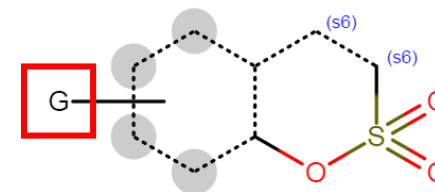
Alkyl

ALK ALH

Alkenyl

AEL AEH

G GH G* GH* Pol



搜尋結果中 G 的位置
可能接上任意官能基

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允許取代基

Reaxys 結構搜尋 – 衍生物搜尋 – Substitution 最高數量

在綠色原子上
按右鍵

設定取代基最高數量
最大 = 6

Atom properties

Atom properties	
Change to: Element	
Basic	Advanced
Total H (H)	
Implicit H (h)	
Bond orders (v)	
Connections (X)	
Ring count (R)	<not set>
Smallest ring size (r)	
Ring bond (rb)	<not set>
Substitutions (s)	exactly 6
Unsaturated (u)	<not set>
Aromaticity (a/A)	as drawn

Ok

搭配精準搜尋 As drawn
可以在指定位置，
指定取代基的最高數量

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