



ELSEVIER

Reaxys資料庫教育訓練(臺大)
Smarter search in chemistry to save your
valuable time

Ryan Huang 黃恪涵

Life Science Solutions – Elsevier

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2021.10.1



Reaxys 全國學術授權版本



NAR Labs 財團法人國家實驗研究院

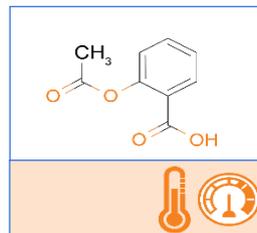
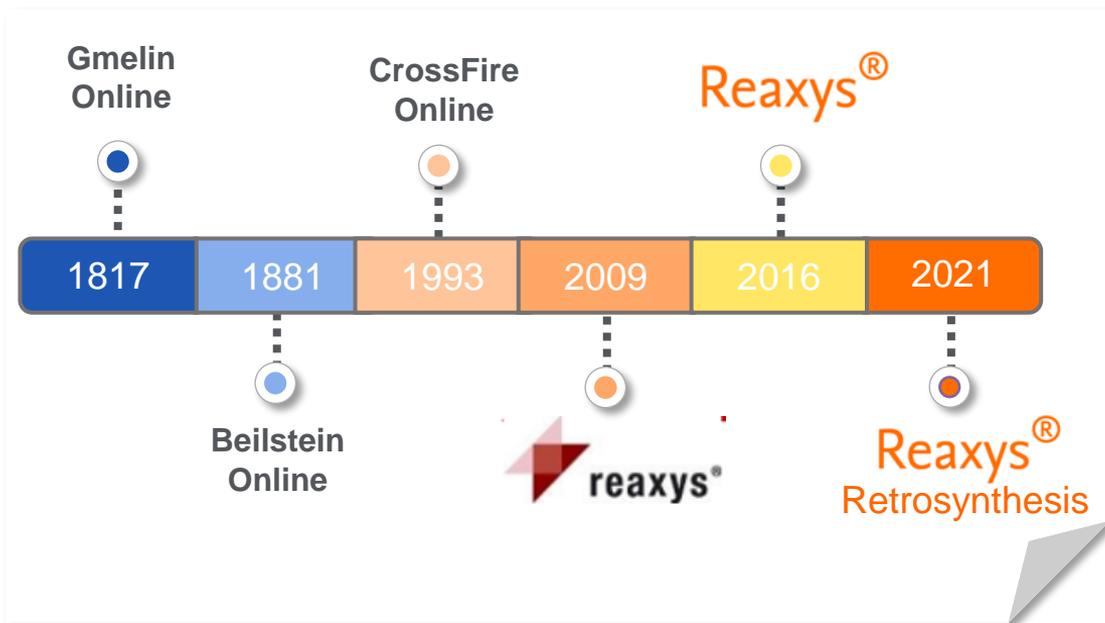
科技政策研究與資訊中心

Science & Technology Policy Research and Information Center

- 科技部科政中心贊助，授權設有化學、應化、藥學等大專院校**限研究用途**使用
- 免費教育推廣、技術支援、**網路自學資源**
- Webinars網路會議分享化學研究新知
- NTU PhD Prize (9月)



豐富的歷史與先進的內容



>118 Million
有機、無機及有
機金屬物質
>500 Million
公開實驗數據
(物性、光譜、
生物活性等)



>49 Million
化學反應(反應條件、
溶劑、催化劑及產
率等)



>54 M 文獻記錄
>16,000 期刊, 專利
涉及有機化學, 材料
化學, 生物醫藥, 地
球科學, 工程等多種
領域

Reaxys提供關鍵的實驗數據，讓研究人員回答重要的研究問題

Journals, patents,
conference
proceedings



人工閱讀、擷取重要的”實驗數據
結構、物理特性、光譜、製備反應、生物活性(藥物毒
性、藥物靶點蛋白、藥物活性、細胞、動物試驗)

回答關鍵的研究問題：

- 有沒有相似的物質被研究過？
- 我的題目有人發表過嗎？
- 相似的物質有哪些已知的特性？
- 這個結構適合拿來發展藥物嗎？
- 該用買的？還是用合成的？買要多少錢？合成有多少成功率？

Agenda

1. 基本介面導覽
2. Quick Search -關鍵字
3. Quick Search -結構搜尋
4. 物質資料編排
5. 反應式搜尋
6. Query Builder進階搜尋-反應式搜尋
7. Query Builder進階搜尋-天然物萃取與光譜查詢
8. Retrosynthes面板
9. 網路自我學習資源 Youtube
10. 化學供應商資料庫
11. 帳號&資料整理與匯出政策



如何連上Reaxys

在學校IP範圍內，打開瀏覽器鍵入 <http://www.reaxys.com>

Reaxys® Quick search History Alerts Ryan Huang Import

點擊X跳過註冊視窗

Welcome to Reaxys

Ready to take the shortest path from chemistry question to relevant answer? Reaxys gives you the best means to explore the world of chemistry.
To learn more visit our [support hub page](#).

Create your account or sign in to access all these features!

- Create alerts & save searches
- Reduce timeouts
- Customize structure editor settings and layout

No Thanks Sign-in Register

Content Overview | Latest update: 11. September 2019 >

118M 49M 59M 37M 1.5M
Substances

Reaxys使用瀏覽器Cookies來強化您的使用體驗



ELSEVIER

Reaxys 介面導覽

學習展示要點



快速搜尋

Reaxys®

Quick search

Query builder

Results

Retrosynthesis

History

Alerts

Ryan Huang



Search substances, reactions, documents and bioactivity data

Import

in Reaxys, Reaxys Medicinal Chemistry, PubChem, SigmaAldrich and Commercial Substances

Search Reaxys

Find >

Substance Effect, e.g. anticoagulant

AND



Draw

- 關鍵字查詢文獻
- 關鍵字查詢物質

結構編輯器

- 如何畫結構搜尋物質
- 如何搜尋核心骨架、相似結構 (Scaffold, Core structure)
- ChemDraw相容 (複製&貼上)

Content Overview | Latest update: 29. September

157M

56M

68M

Substances

Reactions

Documents

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RELX Group™

Feedback



ELSEVIER

預覽頁面

Reaxys®

[Quick search](#)

[Query builder](#)

[Results](#)

[Synthesis planner](#)

[History](#)

[Alerts](#)

Ryan Huang 



Results for Simvastatin

New  Edit 

實驗數據

	323	Substances	Structure :  as drawn Edit in Query Builder  Create Alert 	Preview Results ▾	View Results >
	37,538	Documents	Titles, Abstracts, Keywords : "Simvastatin" Edit in Query Builder  Create Alert 	Preview Results ▾	View Results >
	3	Commercial Substances	Structure :  as drawn Edit in Query Builder  Create Alert 	Preview Results ▾	View Results >
	22	Targets	Target(s) : hmg-coa reductase Edit in Query Builder  Create Alert 	Preview Results ▾	View Results >
	70	Reactions	Reaction Query :  as drawn Edit in Query Builder  Create Alert 	Preview Results ▾	View Results >

生物靶點

反應、合成方法



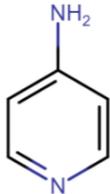
進階搜尋 Query Builder

- 天然萃取物搜尋
- NMR圖譜的搜尋
- 反應條件的進階搜尋

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

Search in: Reactions > Targets > Substances > Documents >

Import Save Reset form Delete all Patent Assignee Structure Molecular Formula CAS RN TI, AB & KW

◇ Structure  X

As drawn

AND

◇ NMR Spectroscopy Find any Show fields (Description...Original Text) X

Search fields

Fields Forms History

- Topics and Keywords
- Identification
- Physical Properties
- Spectra
- MedChem
- Other
- Reactions
- Bibliography

AND
OR
NOT

自行組合搜尋條件 (例如結合結構+NMR圖譜)

超過百種搜尋條件

逆合成面板 (規劃合成路徑、合成材料與反應條件)

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

New

Draw new structure

No.	Date/Time	Project name		No. of routes
5581	30 Sep 2021 11:22	Project #5581		Predicted In progress Published 1 View
5319	29 Sep 2021 05:43	Project #5319		View
5146	28 Sep 2021 00:01	Project #5146		Predicted 0 Published 4

Draw

找到文獻報導的合成計畫

- 如何查詢、比較合成計畫
- 儲存、資料匯出 (需登入個人帳號)

個人化儲存/郵件提醒

Reaxys[®]

Quick search

Query builder

Results

Retrosynthesis

History

Alerts

Ryan Huang 



History

Recent **Saved**

Reaxys

 72 Reactions

Jul 26 2021

test1

Edit Query 

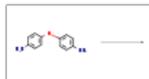
Delete 

Rename 

Alert 

View 

Query Builder: in reactions - AND Fulltext of reaction "NMR"



 1,213 Substances

Oct 13 2020

biotin project

Edit Query 

Delete 

Rename 

Alert 

View 

Quick Search:



- 儲存功能
- 資料匯出限制
(需登入個人帳號)



ELSEVIER

Quick Search

關鍵字查詢文獻



Quick Search 關鍵字查詢文獻

Reaxys

Quick search Query builder ^{New} Results Synthesis planner History Alerts

Ryan Huang

Search for 184475-35-2 Import

Search Reaxys

184475-35-2 Find >

Documents, e.g. published by Schrock

AND

Draw

鈣鈦礦太陽能電池
Perovskite Solar Cell

Content Overview | Latest update: 11. September 2019 >

118M	49M	59M	37M	1.5M
Substances	Reactions	Documents	Bioactivities	Targets

Quick Search 關鍵字查詢文獻

Reaxys®

Quick search

Query builder

Results

Retrosynthesis

History

Alerts

Ryan Huang  

Results for Perovskite solar cell

New  Edit 



14,952

Documents

Titles, Abstracts, Keywords : "Perovskite", "solar", "cell"

Edit in Query Builder  Create Alert 

Preview Results 

View Results 



27,489

Documents

Titles, Abstracts, Keywords : "Perovskite", "solar"

Edit in Query Builder  Create Alert 

Preview Results 

View

“Perovskite Solar Cell”
利用前後””限制搜尋範圍

Reaxys®

Quick search

Query builder

Results

Retrosynthesis

History

Alerts

Ryan Huang  

Results for "Perovskite solar cell"

New  Edit 



6,561

Documents

Titles, Abstracts, Keywords : "Perovskite solar cell"

Edit in Query Builder  Create Alert 

Preview Results 

View Results 



Quick Search 關鍵字查詢文獻

- 文章類型篩選

Reaxys®

Quick search

Query builder

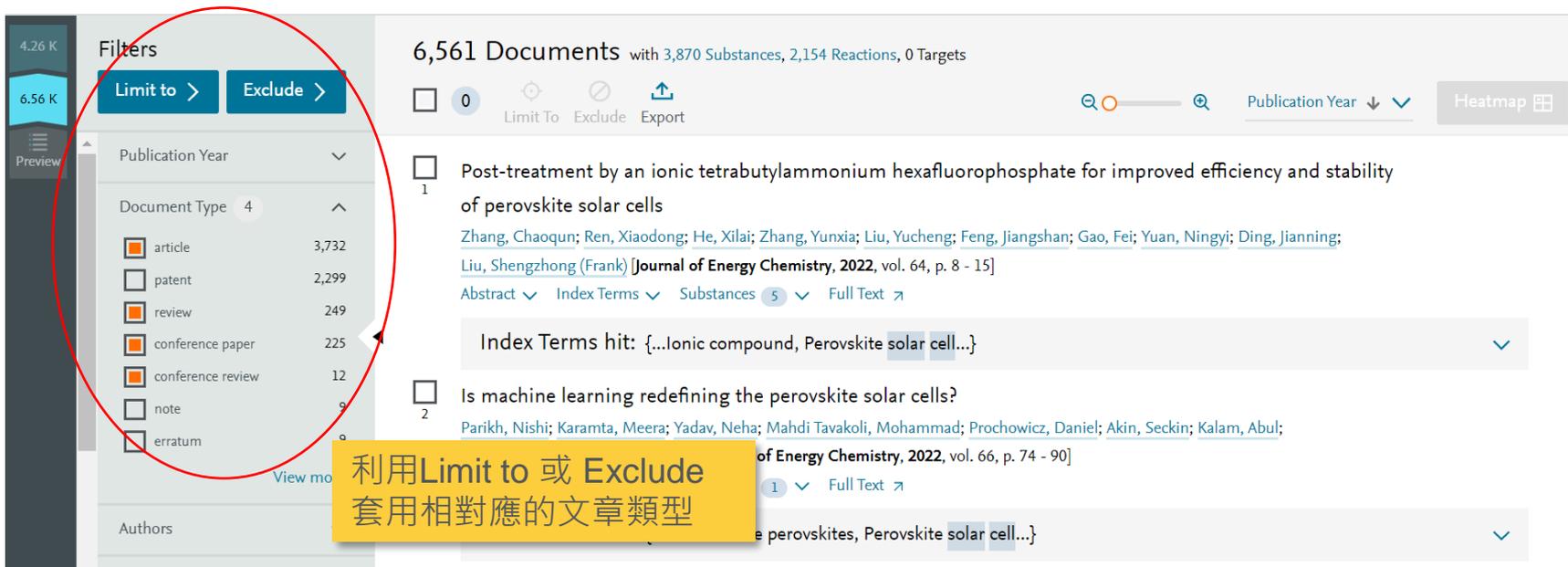
Results

Retrosynthesis

History

Alerts

Ryan Huang 



4.26 K
6.56 K
Preview

Filters

Limit to > Exclude >

Publication Year

Document Type 4

- article 3,732
- patent 2,299
- review 249
- conference paper 225
- conference review 12
- note 9
- erratum 0

View more

Authors

6,561 Documents with 3,870 Substances, 2,154 Reactions, 0 Targets

0 Limit To Exclude Export

Publication Year Heatmap

1 Post-treatment by an ionic tetrabutylammonium hexafluorophosphate for improved efficiency and stability of perovskite solar cells
[Zhang, Chaoqun](#); [Ren, Xiaodong](#); [He, Xilai](#); [Zhang, Yunxia](#); [Liu, Yucheng](#); [Feng, Jiangshan](#); [Gao, Fei](#); [Yuan, Ningyi](#); [Ding, Jianing](#); [Liu, Shengzhong \(Frank\)](#) *Journal of Energy Chemistry*, 2022, vol. 64, p. 8 - 15
Abstract Index Terms Substances 5 Full Text

Index Terms hit: {...Ionic compound, Perovskite solar cell...}

2 Is machine learning redefining the perovskite solar cells?
[Parikh, Nishi](#); [Karamta, Meera](#); [Yadav, Neha](#); [Mahdi Tavakoli, Mohammad](#); [Prochowicz, Daniel](#); [Akin, Seckin](#); [Kalam, Abul](#); *Journal of Energy Chemistry*, 2022, vol. 66, p. 74 - 90
1 Full Text

perovskites, Perovskite solar cell...

利用Limit to 或 Exclude 套用相對應的文章類型

Quick Search 關鍵字查詢文獻

- 文章類型篩選

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

6,561 Documents with 3,870 Substances, 2,154 Reactions, 0 Targets

4.26 K 6.56 K

不要忽略過濾器追蹤欄
隨時回到篩選前的搜尋結果

Document Type 4

- article 3,732
- patent 2,299
- review 249
- conference paper 225
- conference review 12
- note 9
- erratum 9

View more

Authors

1 Post-treatment by an ionic tetrabutylammonium hexafluorophosphate for improved efficiency and stability of perovskite solar cells
Zhang, Chaoqun; Ren, Xiaodong; He, Xilai; Zhang, Yunxia; Liu, Yucheng; Feng, Jiangshan; Gao, Fei; Yuan, Ningyi; Ding, Jianning; Liu, Shengzhong (Frank) *Journal of Energy Chemistry*, 2022, vol. 64, p. 8 - 15
Abstract Index Terms Substances 5 Full Text

Index Terms hit: {...Ionic compound, Perovskite solar cell...}

2 Is machine learning redefining the perovskite solar cells?
Parikh, Nishi; Karamta, Meera; Yadav, Neha; Mahdi Tavakoli, Mohammad; Prochowicz, Daniel; Akin, Seckin; Kalam, Abul; Satapathi, Soumitra; Yadav, Pankaj *Journal of Energy Chemistry*, 2022, vol. 66, p. 74 - 90
Abstract Index Terms Substances 1 Full Text

Index Terms hit: {...Metal halide perovskites, Perovskite solar cell...}

Quick Search 關鍵字查詢文獻

- 文章排序

Reaxys®

Quick search Query builder **Results** Retrosynthesis History Alerts

Ryan Huang  

4,26 K

6.56 K

Preview

Filters

Limit to > Exclude >

Publication Year 

Document Type 

- article 3,732
- review 249
- conference paper 225
- conference review 12
- note 9
- erratum 9
- short survey 7

[View more](#)

Authors 

Patent Assignee 

Patent Office 

4,262 Documents

with 2,105 Substances, 684 Reactions, 0 Targets

0   

Limit To Exclude Export

Publication Year  



Sort search results 

- Relevance
- Publication Year**  
- Document Type
- Cited By 

1 Post-treatment by an ionic tetrabutylammonium hexafluorophosphate for improvement of perovskite solar cells

[Zhang, Chaoqun; Ren, Xiaodong; He, Xilai; Zhang, Yunxia; Liu, Yucheng; Feng, Jiangshan; Gao, Fei; Yu, Liu, Shengzhong \(Frank\) \[Journal of Energy Chemistry, 2022, vol. 64, p. 8 - 15\]](#)

[Abstract](#) [Index Terms](#) [Substances](#) 5 [Full Text](#) [↗](#)

Index Terms hit: {...Ionic compound, Perovskite solar cell...}

2 Is machine learning redefining the perovskite solar cells?

[Parikh, Nishi; Karamta, Meera; Yadav, Neha; Mahdi Tavakoli, Mohammad; Prochowicz, Daniel; Akin, Seckin; Kalam, Abul; Satapathi, Soumitra; Yadav, Pankaj \[Journal of Energy Chemistry, 2022, vol. 66, p. 74 - 81\]](#)

[Abstract](#) [Index Terms](#) [Substances](#) 1 [Full Text](#) [↗](#)

Index Terms hit: {...Metal halide perovskites, Perovskite solar cell...}

3 High-performance perovskite solar cells based on dopant-free hole-transporting material fabricated by a thermal-assisted blade-coating method with efficiency exceeding 21%

[Lee, Kun-Mu; Chiu, Wei-Hao; Tei, Yu-Heian; Wang, Chao-Shan; Tao, Yu-Tai; Lin, Yan-Duo \[Chemical Engineering Journal, 2022, vol. 428, p. 132 - 141\]](#)

Feedback 

Relevance: 依關鍵字命中數目排序
Cited By: 依引用強度排序

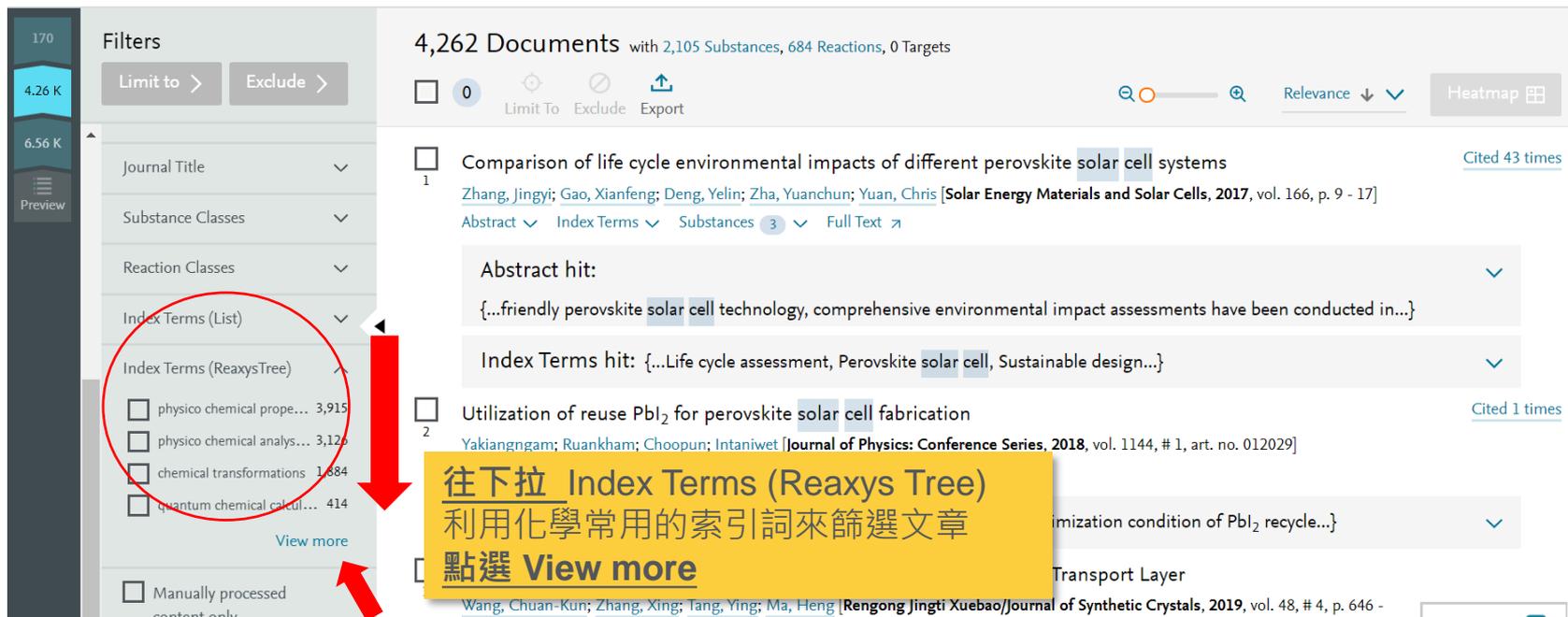
Quick Search 關鍵字查詢文獻

- 索引詞篩選 (Index Terms Reaxys Tree)

Reaxys®

Quick search Query builder **Results** Retrosynthesis History Alerts

Ryan Huang  



170
4.26 K
6.56 K
Preview

Filters

Limit to > Exclude >

Journal Title
Substance Classes
Reaction Classes
Index Terms (List)
Index Terms (ReaxysTree)
physico chemical prope... 3,915
physico chemical analys... 3,126
chemical transformations 1,884
quantum chemical calcul... 414
View more
Manually processed content only

4,262 Documents with 2,105 Substances, 684 Reactions, 0 Targets

Limit To Exclude Export

Relevance Heatmap

1 Comparison of life cycle environmental impacts of different perovskite solar cell systems [Cited 43 times](#)
[Zhang, Jingyi](#); [Gao, Xianfeng](#); [Deng, Yelin](#); [Zha, Yuanchun](#); [Yuan, Chris](#) [Solar Energy Materials and Solar Cells, 2017, vol. 166, p. 9 - 17]
Abstract Index Terms Substances (3) Full Text

Abstract hit: {...friendly perovskite solar cell technology, comprehensive environmental impact assessments have been conducted in...}

Index Terms hit: {...Life cycle assessment, Perovskite solar cell, Sustainable design...}

2 Utilization of reuse PbI_2 for perovskite solar cell fabrication [Cited 1 times](#)
[Yakiangngam](#); [Ruankham](#); [Choopun](#); [Intaniwet](#) [Journal of Physics: Conference Series, 2018, vol. 1144, # 1, art. no. 012029]
optimization condition of PbI_2 recycle...}

Transport Layer
[Wang, Chuan-Kun](#); [Zhang, Xing](#); [Tang, Ying](#); [Ma, Heng](#) [Rengong Jingti Xuebao/Journal of Synthetic Crystals, 2019, vol. 48, # 4, p. 646 -

往下拉 Index Terms (Reaxys Tree)
利用化學常用的索引詞來篩選文章
點選 View more

Quick Search 關鍵字查詢文獻

- 索引詞篩選 (Index Terms Reaxys Tree)

Index Terms (ReaxysTree) 3221

- Index Terms (ReaxysTree) 4,262
 - physico chemical properties 3,915
 - electrical property 3,461
 - permittivity 719
 - electrical conductivity 329
 - piezoelectricity 48
 - photovoltaic effect 3,221
 - photoelectricity 545
 - resistivity 252
 - ferroelectricity 202
 - photoconductivity 104
 - thermoelectricity 56

Selected search items:

photovoltaic effect

Index Terms (ReaxysTree) 170

- Index Terms (ReaxysTree) 4,262
 - physico chemical properties 3,915
 - physico chemical analysis methods 3,126
 - spectroscopical analysis 2,433
 - separation method 1,652
 - crystal structure determination 1,255
 - microscopy 946
 - scanning probe microscopy 796
 - electron microscopy 242
 - transmission electron microscopy 170
 - scanning electron microscopy 66
 - optical microscopy 31
 - electro analytical method 287

Selected search items:

transmission electr...



ELSEVIER

Quick Search

結構搜尋



Quick Search 結構搜尋

Reaxys®

Quick search

Query builder

Results

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Ryan Huang 



Search substances, reactions, documents and bioactivity data

Import 

in Reaxys, Reaxys Medicinal Chemistry, PubChem, SigmaAldrich and Commercial Substances

Search Reaxys

Find >

Substance Effect, e.g. [anticoagulant](#)

AND



Draw

Content Overview | Latest update: 29. September 2021 >

157M

 Substances

56M

 Reactions

68M

 Documents

41M

 Bioactivities



ELSEVIER

MarvinJS 結構編輯器

Reaxys[®]

Quick search Query builder Results Retrosynthesis History Alerts

Ryan Huang  

Structure editor selected: MarvinJS ChemDrawJS

Insert structure from name >



基本工具、鍵結工具



原子鎖、重複基團



常見的環、醣



元素週期表與
原子列表



原子屬性
定義工具



Search this structure as:

- As drawn
- As substructure
- Similar
- Tautomers
- Stereo
- Additional ring closures
- Related Markush
- Salts
- Mixtures
- Isotopes
- Charges
- Radicals

+ More options

Clear 

Cancel 

Transfer to query >

絕對結構搜尋 As drawn

Reaxys[®]

Quick search Query builder Results Retrosynthesis History Alerts

Ryan Huang  

Structure editor selected: MarvinJS ChemDrawJS

Insert structure from name >

Search this structure as:

As drawn

As substructure

Similar

Tautomers

Stereo

Additional ring closures

Related Markush

Salts

Mixtures

Isotopes

Charges

Radicals

+ More options

搜尋跟我畫的一模一樣

容許：
異構物
鹽
同位素
離子型態
混合物

Clear 

Cancel 

Transfer to query >



相似結構搜尋 As substructure

Reaxys®

Quick search Query builder Results Retrosynthesis History Alerts

Ryan Huang  

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

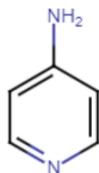
Salts

Mixtures

Isotopes

Charges

我畫的結構為核心結構
在“所有氫原子沒有畫出
來的地方”容許取代基



Clear 

Cancel 

Transfer to query >

相似結構搜尋 S^{lock} & S^{max}

Reaxys®

Quick search Query builder Results Retrosynthesis History Alerts

Ryan Huang  

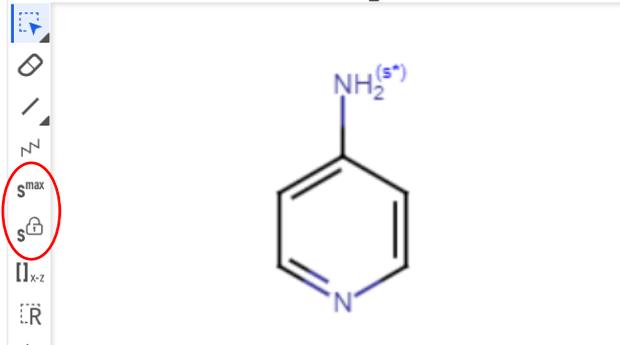
Structure editor selected: MarvinJS ChemDrawJS

Insert structure from name >

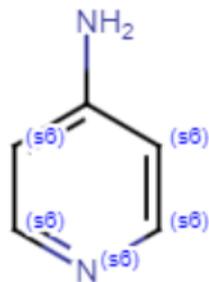
Search this structure as:

- As drawn
- As substructure
- On all atoms
- On heteroatoms
- Similar
- Tautomers
- Stereo
- Additional ring closures
- Related Markush
- Salts



用 As substructure 開放所有位置取代基
搭配 S^{lock} 把不要的地方鎖起來



用 As drawn
搭配 S^{max} 把發生取代的地方打開

Clear 

Cancel ×

Transfer to query >

Charges



不定位鍵的使用

Reaxys

Quick search Query builder Results Retrosynthesis History Alerts

Ryan Huang  

Structure editor selected: MarvinJS ChemDrawJS

Insert structure from name >

Search this structure as:

As drawn

As substructure

Similar

Tautomers

Stereo

Additional ring closures

Related Markush

Salts

Mixtures

Isotopes

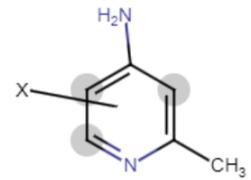
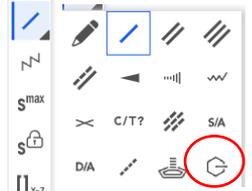
Charges

Radicals

+ More options

1

4



1. 點選選擇工具
2. 按住鍵盤Shift
3. 左鍵選擇不定位鍵可以出現的位置
4. 選擇不定位鍵

Clear  Cancel  Transfer to query >

[\(151\) Reaxys 結構編輯器 - 不定位鍵 - YouTube](#)



更多關於結構編輯器的進階技巧

[\(151\) Reaxys 結構編輯器 - 縮寫官能基團 - YouTube](#)

[\(151\) Reaxys 結構編輯器 - 原子屬性列表 - YouTube](#)

[\(151\) Reaxys 結構編輯器 - G 任意官能基工具定義 - YouTube](#)

[\(151\) Reaxys 結構編輯器 - R 基團與末端定義工具 - YouTube](#)

[\(151\) Reaxys 結構編輯器 - 原子列表與原子列表非 - YouTube](#)

[\(151\) Reaxys 結構編輯器 - 鹽類與同位素 - YouTube](#)



訂閱Elsevier Taiwan 自學線上資源

YouTube TW taiwan elsevier

Elsevier Taiwan 台灣愛思唯爾
782 位訂閱者 · 202 部影片
台灣愛思唯爾，旗下商品(包括系統)之活動、教學及宣傳影片。

訂閱

Elsevier Taiwan
416 位訂閱者 · 235 部影片
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已訂閱

Reaxys - 基本介紹
觀看次數：10次 · 1 週前
Elsevier Taiwan
本影片作者為Sam Yu - Elsevier 大中華區Reaxys 專業講師如您對Reaxys 的搜尋有任何問題，歡迎與我們...

YouTube TW taiwan elsevier

Reaxys 線上教育訓練
22 部影片 · 觀看次數：9次 · 昨天更新

全部播放

Reaxys - 基本介紹
Elsevier Taiwan
4:56

Reaxys - 快速搜尋
Elsevier Taiwan
11:38

Reaxys - 進階搜尋
Elsevier Taiwan
8:15

Reaxys - 註冊個人帳號
Elsevier Taiwan
14:46

Reaxys 結構編輯器 - 基本介紹
Elsevier Taiwan
2:42

Reaxys 結構編輯器 - 不定位鍵

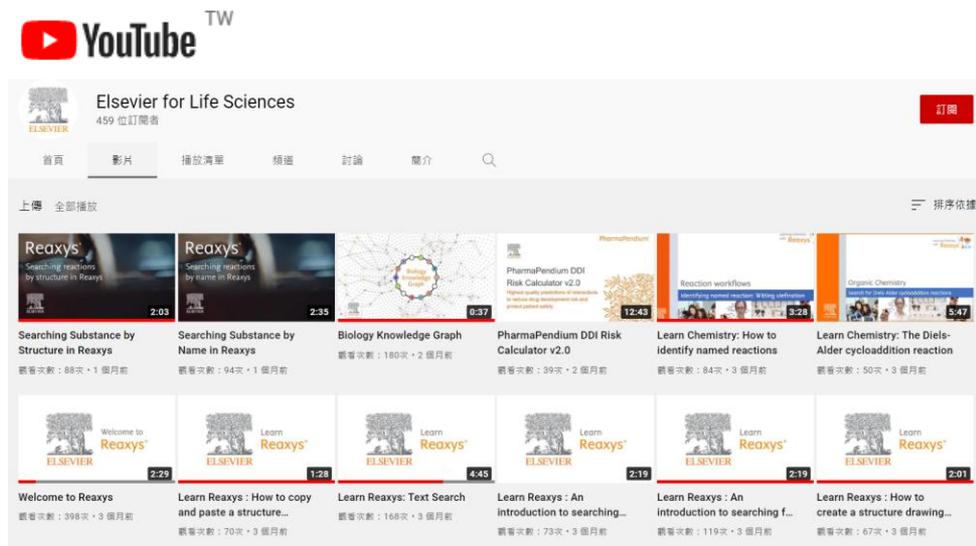
Elsevier Taiwan 已訂閱

無廣告、持續更新中

<https://www.youtube.com/playlist?list=PLBSTWuNnJA14laTo5zNkqaJ9va-LUtj0>



訂閱Elsevier Taiwan 自學線上資源



YouTube TW

Elsevier for Life Sciences
459 位訂閱者

訂閱

首頁 影片 播放清單 頻道 討論 簡介

上傳 全部播放 排序依據

Reaxys
Searching reactions by structure in Reaxys
2:03

Reaxys
Searching reactions by name in Reaxys
2:35

Biology Knowledge Graph
觀看次數：180次 · 2 個月前
0:37

PharmaPendium DDI Risk Calculator v2.0
觀看次數：39次 · 2 個月前
12:43

Learn Chemistry: How to identify named reactions
觀看次數：84次 · 3 個月前
3:28

Learn Chemistry: The Diels-Alder cycloaddition reaction
觀看次數：50次 · 3 個月前
5:47

Welcome to Reaxys
觀看次數：398次 · 3 個月前
2:29

Learn Reaxys : How to copy and paste a structure...
觀看次數：70次 · 3 個月前
1:28

Learn Reaxys: Text Search
觀看次數：168次 · 3 個月前
4:45

Learn Reaxys : An introduction to searching...
觀看次數：73次 · 3 個月前
2:19

Learn Reaxys : An introduction to searching f...
觀看次數：119次 · 3 個月前
2:19

Learn Reaxys : How to create a structure drawing...
觀看次數：67次 · 3 個月前
2:01

RxED Learning Chemistry with Reaxys (English)



[\(152\) RxED: Learning Chemistry with Reaxys - YouTube](#)

應用案例- 新穎性搜尋Novelty Search

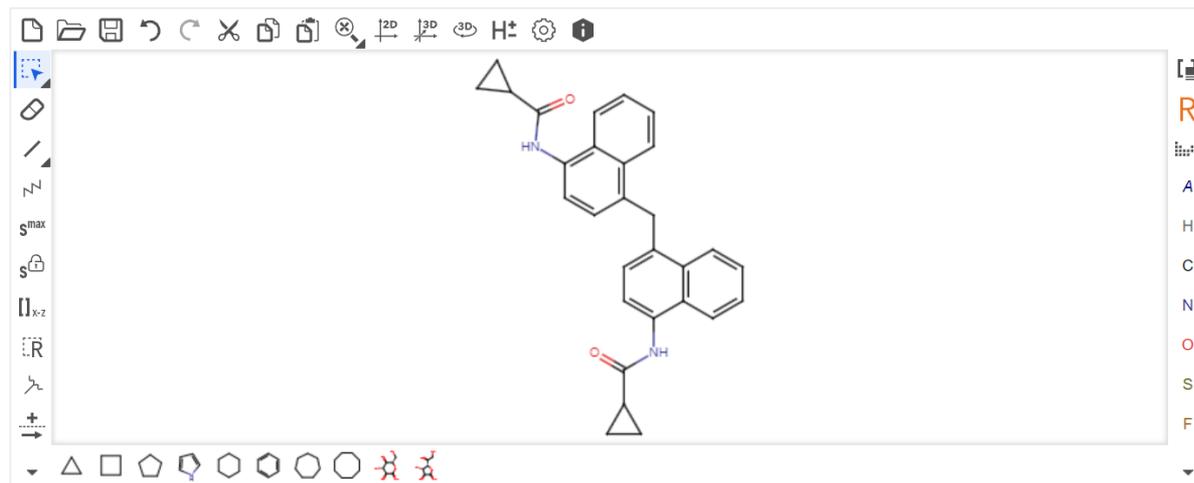
Reaxys

Quick search Query builder Results Retrosynthesis History Alerts

Ryan Huang  

Structure editor selected: MarvinJS ChemDrawJS

Insert structure from name >



Search this structure as:

- As drawn
- As substructure
- Similar
 - Tautomers
 - Stereo
 - Additional ring closures
 - Related Markush
 - Salts
 - Mixtures
 - Isotopes
 - Charges
 - Radicals



O=C(NC1=CC=C(CC2=C3C=CC=CC3=C(NC(=O)C3CC3)C=C2)C2=C1C=CC=C2)C1CC1



ELSEVIER

Substance Page

物質數據整理



預覽頁面選擇Substances

Results for Simvastatin

New Edit

	323	Substances	Structure : as drawn Edit in Query Builder Create Alert	Preview Results	View Results >
	37,538	Documents	Titles, Abstracts, Keywords : "Simvastatin" Edit in Query Builder Create Alert	Preview Results	View Results >
	3	Commercial Substances	Structure : as drawn Edit in Query Builder Create Alert	Preview Results	View Results >

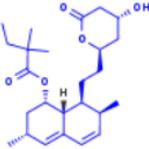
Reaxys人工擷取重要的實驗數據，並保留原始文獻出處

- 物理性質、光譜

323 Substances out of 12,342 Documents, containing 177 Reactions, 175 Targets Reaxys - 323

0 selected Limit To Exclude Export Preparations Search Sort by No of References Grid Heatmap

1



simvastatin
C₂₅H₃₈O₅ 418.574 4768037 123049-81-0, 79902-63-9

Identification

Druglikeness

Bioactivity (All)

Physical Data - 94

Spectra - 96

Other Data - 3,152

Preparations - 49 >

Reactions - 161 >

Targets - 165 >

Documents - 12,211 >

這個物質有哪些物理特性已經被報導過了？

Reaxys人工擷取重要的實驗數據，並保留原始文獻出處

- 物理性質、光譜

Solubility, g·l ⁻¹	Saturation	Temperature (Solubility (MCS)), °C	Solvent (Solubility (MCS))	Location	Comment (Solubility (MCS))	Reference
					water, soluble in organic solvents	[Macromolecular Bioscience, 2014, vol. 14, # 11, p. 1530 - 1500] Full Text ↗ Cited 27 times ↗ Details > Abstract >
6.73904	in pure solvent		aq. phosphate buffer	supporting information		Chung, Sanny S. W.; Cuellar, Rebecca A. D.; Wang, Xiangyuan; Reczek, Peter R.; Georg, Gunda I.; Wolgemuth, Debra J.[ACS Medicinal Chemistry Letters, 2013, vol. 4, # 5, p. 446 - 450] Full Text ↗ Cited 8 times ↗ Details > Abstract >
15	in solution	25	aq. phosphate buffer			Ambike, Anshuman A.; Mahapatra, Sankar K.; Mishra, Sushant K.; Mishra, Sushant K.; Mishra, Sushant K.; Mishra, Sushant K.[Journal of Pharmaceutical Sciences, 2005, vol. 22, # 6, p. 990 - 998] Full Text ↗ Cited 149 times ↗ Details > Abstract >
7.3E-05	in pure solvent	25	H2O			Matsuyama, Kenji; Nakagawa, Kimiko; Nakai, Aki; Konishi, Yuriko; Nishikata, Mayumi; Tanaka, Hiromi; Uchida, Takahiro[Biological and pharmaceutical bulletin, 2002, vol. 25, # 3, p. 346 - 350] Full Text ↗ Details > Abstract >
79.55	in pure solvent	25	propan-2-ol			Matsuyama, Kenji; Nakagawa, Kimiko; Nakai, Aki; Konishi, Yuriko; Nishikata, Mayumi; Tanaka, Hiromi; Uchida, Takahiro[Biological and pharmaceutical bulletin, 2002, vol. 25, # 3, p. 346 - 350] Full Text ↗ Details > Abstract >
19.09	in pure solvent	25	diethyl ether			Matsuyama, Kenji; Nakagawa, Kimiko; Nakai, Aki; Konishi, Yuriko; Nishikata, Mayumi; Tanaka, Hiromi; Uchida, Takahiro[Biological and pharmaceutical bulletin, 2002, vol. 25, # 3, p. 346 - 350] Full Text ↗ Details > Abstract >

提供原始文獻連結

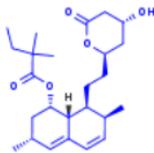
Reaxys以人工擷取重要的實驗數據，並保留原始文獻出處

- 專利出處、純化方法、專利名稱

323 Substances out of 12,342 Documents, containing 177 Reactions, 175 Targets Reaxys - 323

0 selected Limit To Exclude Export Preparations 🔍 🔍 Sort by No of References ↓ Grid Heatmap

1



[View related Markush](#)

simvastatin
C₂₅H₃₈O₅ 418.574 4768037 123049-81-0, 79902-63-9

Identification Bioactivity (All) Spectra - 96

Druglikeness Physical Data - 94 Other Data - 3,152

Preparations - 49 >

Reactions - 161 >

Targets - 165 >

Documents - 12,211 >

這個物質是否有相關的專利文件報導？

搜尋涵蓋此結構的專利結構式

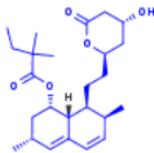
Reaxys以人工擷取重要的實驗數據，並保留原始文獻出處

- 合成反應 & 購物車

323 Substances out of 12,342 Documents, containing 177 Reactions, 175 Targets Reaxys - 323

0 selected Limit To Exclude Export Preparations Sort by No of References Grid Heatmap

1



simvastatin
C₂₅H₃₈O₅ 418.574 4768037 123049-81-0, 79902-63-9

Identification	Bioactivity (All)	Spectra - 96
Druglikeness	Physical Data - 94	Other Data - 3,152

- Preparations - 49
- Reactions - 161
- Targets - 165
- Documents - 12,211

這個物質哪裡買？
多少錢？

我該如何合成這個化合物？

Reaxys以人工擷取重要的實驗數據，並保留原始文獻出處

- 生物活性應用

熱圖分析

323 Substances out of 12,342 Documents, containing 177 Reactions, 175 Targets

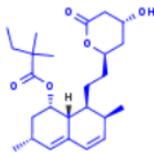
0 selected Limit To Exclude Export Preparations

Reaxys - 323

Sort by No of References ↓

Grid Heatmap

1



simvastatin
C₂₅H₃₈O₅ 418.574 4768037 123049-81-0, 79902-63-9

Identification
Druglikeness

Bioactivity (All)
Physical Data - 94

Spectra - 96
Other Data - 3,152

Preparations - 49
Reactions - 161
Targets - 165
Documents - 12,211

RMC模組提供：

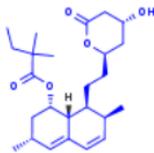
- 有哪些生物活性已經被報導過？
- 是否有毒性？有哪些實驗已經證實？
- 如果我要進行細胞試驗？有哪些細胞株已經測試過？從哪個濃度開始較為適當？
- 有哪些蛋白質被報導與此物質有作用？

Reaxys以人工擷取重要的實驗數據，並保留原始文獻出處

- 天然萃取物、應用

323 Substances out of 12,342 Documents, containing 177 Reactions, 175 Targets Reaxys - 323

0 selected Limit To Exclude Export Preparations Sort by No of References Grid Heatmap



simvastatin
C₂₅H₃₈O₅ 418.574 4768037 123049-81-0, 79902-63-9

Identification Bioactivity (All)
Druglikeness Physical Data - 94

Spectra - 96
Other Data - 3,152

Preparations - 49
Reactions - 161
Targets - 165
Documents - 12,211

Other Data - 3152

- Use - 3149
- Isolated from Natural Source - 1

化合物的用途？
從天然物萃取的證據？

動手練習

1. Gefitinib的溶解度Solubility是多少？
 2. Gefitinib的UV/VIS的吸收光譜是多少？
 3. 在Reaxys內找到一篇涵蓋Gefitinib高引用的文獻
 4. 能不能用Gefitinib的Core Scaffold去尋找更多相似的結構？
- Gefitinib是對表皮生長因子受體EGFR突變跟過度表達而產生的癌症的有效藥物，應用於肺癌的治療與研究



ELSEVIER

Reactions Search

反應式查詢

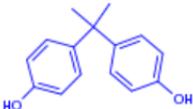


您可以用各種方式搜尋Reaction

1. 由物質資訊連結到製備方式
2. 由關鍵字搜尋反應式
3. 由結構搜尋反應式



由物質頁面連結到製備方式 Preparation

1 

BPA
HOC6H4C(CH3)2C6H4OH 228.291 1107700 80-05-7

Identification Physical Data - 346
Druglikeness Spectra - 139
Bioactivity (All) Other Data - 470

Preparations - 98 >
Reactions - 1,366 >
Targets - 157 >
Documents - 13,432 >

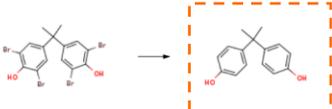


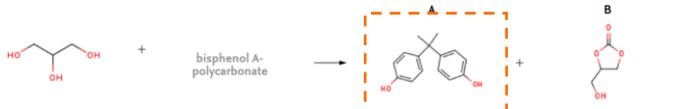
只出現在產物

可出現在產物或起始物

99 Reactions out of 236 Documents containing 132 Substances, 436 Targets

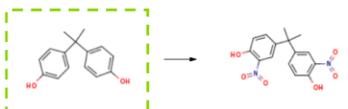
0 selected Limit To Exclude Export Syn-Plan Show Conditions Reaxys - 99 Sort by Reaxys Ranking

1 
4 Conditions Find Similar Reaction ID: 46083924

2 
1 Conditions Find Similar Reaction ID: 44100782

1,402 Reactions out of 1,138 Documents containing 1,923 Substances, 1,080 Targets

0 selected Limit To Exclude Export Syn-Plan Show Conditions Reaxys - 1,402 Sort by Reaxys Ranking

1 
8 Conditions Find Similar Reaction ID: 70732

2 
4 Conditions Find Similar Reaction ID: 46083924

由關鍵字搜尋反應式

Reaxys®

[Quick search](#)

[Query builder](#)

[Results](#)

[Synthesis planner](#)

[History](#)

[Alerts](#)

Ryan Huang 



Search for "radical cyclization"

Import 

Search Reaxys

"radical cyclization"



Find >

Reactions, e.g. [Suzuki coupling](#)

AND



Draw

[Content Overview](#) | Latest update: 31. August 2020 >

118M

 Substances

49M

 Reactions

59M

 Documents

37M

 Bioactivities

ELSEVIER

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30.09.2021

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由關鍵字搜尋反應式

Reaxys®

[Quick search](#)

[Query builder](#)

[Results](#)

[Synthesis planner](#)

[History](#)

[Alerts](#)

Ryan Huang



Results for "radical cyclization"

New Edit

	75	Reactions	Condition : radical cyclization Edit in Query Builder Create Alert	Preview Results	View Results >
	6,113	Documents	Titles, Abstracts, Keywords : "radical cyclization" Edit in Query Builder Create Alert	Preview Results	View Results >



30.09.2021

ELSEVIER

由關鍵字搜尋反應式

Reaxys®

Quick search Query builder **Results** Synthesis planner History Alerts

Ryan Huang  

75 **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

75 Reactions out of 86 Documents containing 232 Substances, 40 Targets

0 selected     

Limit To Exclude Export Syn-Plan Hide Conditions

  Sort by Reaxys Ranking 

1  



1 Hits  9 Conditions  Find Similar > Reaction ID: 8578406 

Conditions	Yield	Reference
With 2,2'-azobis(isobutyronitrile); tri-n-butyl-tin hydride In toluene for 4h; Cyclization; radical cyclization; Heating;	68%	Orito, Kazuhiko; Uchiito, Shiho; Satoh, Yoshitaka; Tatsuzawa, Takashi; Harada, Rika; Tokuda, Masao [Organic Letters, 2000, vol. 2, # 3, p. 307 - 310] Full Text Cited 62 times Details Abstract >

[+ Show all conditions](#) 1 hit out of 1

2  

[Feedback](#) 



30.09.2021

結構編輯器畫結構搜尋反應式

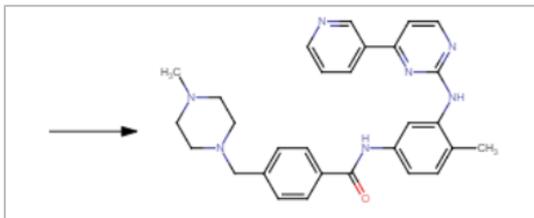
Reaxys® Quick search Query builder Results Synthesis planner History Alerts

Structure editor selected: MarvinJS ChemDrawJS Insert structure from name >

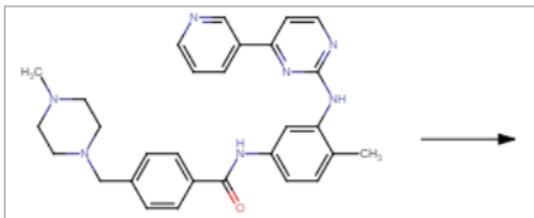
反應箭頭

Clear Cancel Transfer to query >

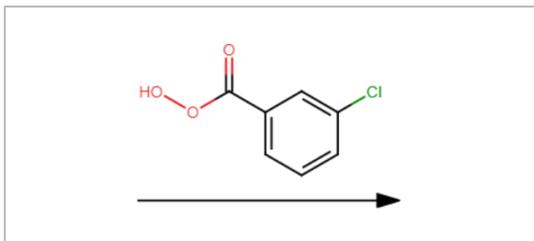
畫結構搜尋反應式



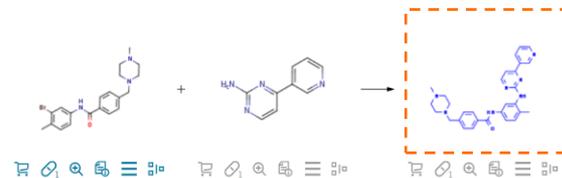
箭頭在左
產物



箭頭在右
起始物



箭頭在下
催化劑或溶劑



Conditions Find Similar Reaction ID: 29521413

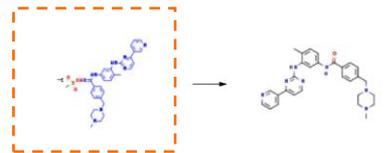
Conditions

With tris(dibenzylideneacetone)dipalladium⁰ chloroform complex; 2,2'-bis-(diphenylphosphino)-1,1'-binaphthyl; sodium t-butanol In 5,5-dimethyl-1,3-cyclohexadiene at 140°C; for 5h; Temperature;

Yield Reference

92% Kang, Julie; Lee, Jun Young; Park, Jeong-Hoon; Chang, Dong-Jo [Journal of labelled compounds and radiopharmaceuticals, 2020, vol. 63, # 4, p. 174 - 182]

Full Text Details Abstract



Conditions Find Similar Reaction ID: 32441176

Conditions

With ammonia In water; isopropyl alcohol at 20°C; for 4h; pH=7.6 - 8.5;

Experimental Procedure

Yield Reference

93% KRKA, D. D., NOVO MESTO; BENKIC Primož; TIHI Jaroslav; PECAVAR Anica; GERMAN Tamara; VREČER Franc; VAJS Anamarija; SKRABANJA Vida

WO2011/157450, 2011, A1
Location in patent: Page/Page column 19
Full Text Details Abstract

With dihydrogen peroxide; methyltrioxorhenium(VII) In dichloromethane; water at 15°C; for 5h; Experimental Procedure

100% METHYLGENE INC.
WO2005/92899, 2005, A1

Location in patent: Page/Page column 73
Full Text Details Abstract

With 3-chloro-benzenecarboxylic acid In dichloromethane at 20°C; Inert atmosphere;

100% Roudesly, Fares; Veiros, Luis F.; Obler, Julie; Poli, Giovanni [Organic Letters, 2018, vol. 20, # 8, p. 2346 - 2350]

Full Text Cited 19 times Details Abstract

反應式搜尋的基本工具

Reaxys®

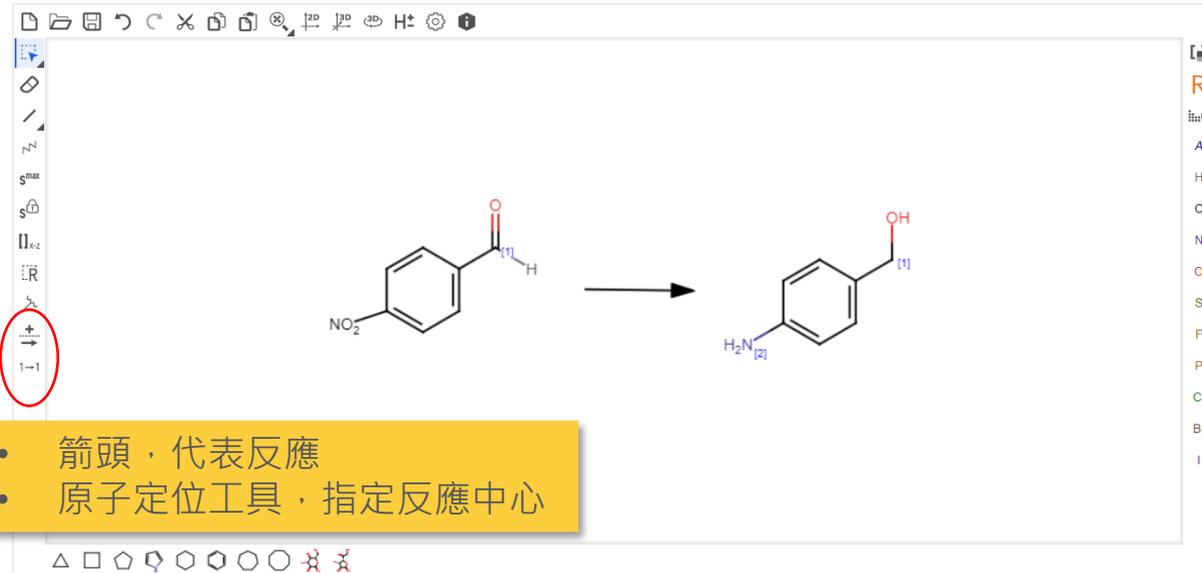
Quick search Query builder Results Retrosynthesis History

Register >

Sign in 

Structure editor selected: MarvinJS ChemDrawJS

Insert structure from name >



Search this structure as:

As drawn

As substructure

Similar

Tautomers

Stereo

Additional ring closures

Related Markush

Salts

Mixtures

Isotopes

Charges

Radicals

+ More options

- 箭頭，代表反應
- 原子定位工具，指定反應中心

反應式搜尋的基本工具

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

11,49 K Filters Limit to > Exclude >

By Structure Yield Reagent/Catalyst Solvent Catalyst Classes Solvent Classes Product Availability Reactant Availability Reaction Classes Document Type Publication Year

0 selected Limit To Exclude Export Show Conditions

Sort by No of References

隱藏實驗條件

11,489 Reactions out of 6,833 Documents, containing 12,995 Substances, 2,202 Targets

1

986 Conditions Find Similar > Reaction ID: 601797

篩選研究主題有興趣的催化劑/溶劑/反應類型

511 Conditions Find Similar > Reaction ID: 608056

3

篩選有實驗材料方法的反應式

利用Query Builder 指定反應條件

The screenshot displays the Reaxys Query Builder interface. At the top, the Reaxys logo is on the left, and navigation links for 'Quick search', 'Query builder', 'Results', 'Retrosynthesis', 'History', and 'Alerts' are in the center. A user profile 'Ryan Huang' is on the right. Below the navigation, there are buttons for 'Reactions', 'Targets', 'Substances', and 'Documents'. A toolbar includes 'Import', 'Save', 'Reset form', and 'Delete all'. The main workspace shows a chemical reaction: benzaldehyde (O=Cc1ccccc1) reacting to form benzyl alcohol (OCC1=CC=CC=C1). Below the reaction, the text 'As drawn' is visible. A search criteria panel is open, showing 'Group 1' with two conditions: 'Yield (numerical) >= 96' and 'Time (Reaction Details) <= 0.25'. A right-hand sidebar lists search fields such as 'Topics and Keywords', 'Identification', 'Physical Properties', 'Spectra', 'MedChem', 'Other', 'Reactions', 'Bibliography', 'PubChem', and 'Commercial Substances'.

- 時間單位為Hr
- 同一個資料格裡面必須用 Proximity (相鄰)串在一起

[\(152\) Reaxys 反應式搜尋 - 如何定義反應條件 - YouTube](#)

使用Query Builder 結合關鍵字搜尋Experimental Procedure

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

Search in: Reactions > Targets > Substances > Documents >

Import Save Reset form Delete all

Patent Assignee Structure Molecular Formula CAS RN TI, AB & KW

Group 3 Ungroup

Structure



On all atoms

AND Reaction Data & Condi... is NMR

Search fields

- Fields
- Forms
- History
- Reaxys
- Topics and Keywords
- Identification
- Physical Properties
- Spectra
- MedChem
- Other
- Reactions
- Bibliography
- PubChem
- Commercial Substances

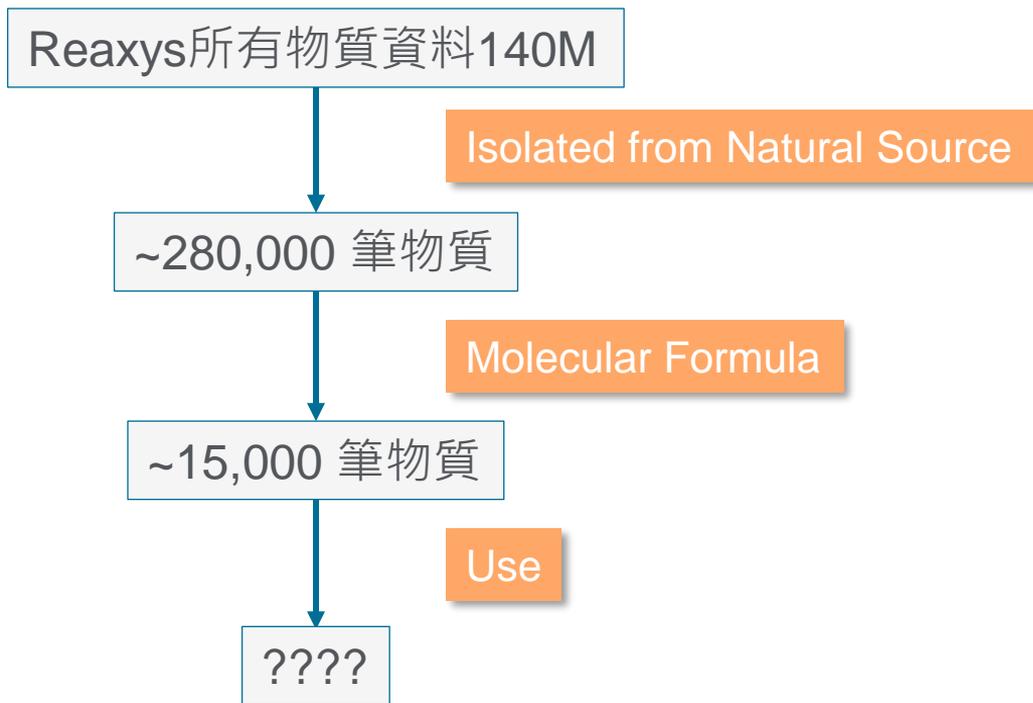
搜尋Experimental Procedure裡面的文字

Query Builder 問題範例

- 搜尋天然物質，在結構上至少有30個C原子，且曾經被報導有抗菌的效果？
- 靈芝(*Ganoderma lucidum*) 的萃取物發現有興趣的活性，經過分子量測定約426.7，尋找符合條件物質的NMR圖譜？
- (示範)如何尋找被報導抑制冠狀病毒 (RdRp聚合酶)的化合物，已經做過*in vitro* 細胞試驗，且IC₅₀濃度需低於1μM

Query Builder

- 搜尋天然物質，在結構上至少有30個C原子，且曾經被報導有抗菌的效果？



Query Builder

- 搜尋天然物質，在結構上至少有30個C原子，且曾經被報導有抗菌的效果？

The screenshot shows the Reaxys Query Builder interface. At the top, there are navigation tabs: Quick search, Query builder (selected), Results, Synthesis planner, History, and Alerts. The user's name, Ryan Huang, is visible in the top right. Below the navigation, there are search filters: Reactions, Targets, Substances, and Documents. A search bar contains the text 'isolated'. Below the search bar, there are icons for Import, Save, Reset form, and Delete all. To the right, there are icons for Structure, Molecular Formula, CAS RN, and TI, AB & KW. The main search area shows a search field with the text 'Isolated from Natural...' and a 'Find any' button. A red circle with the number '3' highlights the 'Find any' button. To the right, there is a list of search fields, with 'Isolated from Natural Source' highlighted by a red circle and the number '2'. A red dashed box highlights the search fields area, with a red circle and the number '1' indicating the search fields list.

1. 在右上方搜尋欄位“Isolated from Natural Source”
2. 左鍵點擊，將天然物搜尋加到左邊
3. 點選Find any → 不限定物種來源

Query Builder

- 搜尋天然物質，在結構上至少有30個C原子，且曾經被報導有抗菌的效果？

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

Search in: Reactions Targets Substances Documents

Import Save Reset form Delete all

Structure **Molecular Formula** CAS RN TI, AB & KW

Isolated from Natural... Find any Show fields (Isolated from Natural Source)

AND Molecular Formula is C30*

AND Use Find any Show fields (Laboratory Use and Handling, Use Pattern)

Search fields use

Reaxys

1. 點選Molecular Formula
2. 輸入C30 *(星號代表可以有更多的元素)

Query Builder

- 搜尋天然物質，在結構上至少有30個C原子，且曾經被報導有抗菌的效果？

Reaxys® Quick search **Query builder** Results Synthesis planner History Alerts Ryan Huang

Search in: Reactions Targets Substances Documents

Import Save Reset form Delete all Structure Molecular Formula CAS RN TI, AB & KW

Isolated from Natural... Find any Show fields (Isolated from Natural Source)

AND Molecular Formula is C30*

AND Use Find any Show fields (Laboratory Use and Handling, Use Pattern)

Search fields use

Use

1. 在右上方搜尋欄位 “Use“
2. 左鍵點擊，將用途搜尋器加到左邊

Query Builder

- 搜尋天然物質，在結構上至少有30個C原子，且曾經被報導有抗菌的效果？

Reaxys® Quick search Query builder Results Synthesis planner History Alerts Ryan Huang

Search in: Reactions > Targets > **Substances >** Documents >

Import Save Reset form Delete all Structure Molecular Formula CAS RN TI, AB & KW

Isolated from Natural... Find any Show fields (Isolated from Natural Source)

AND Molecular Formula is C30*

AND Use Find any Hide fields

Laboratory Use and Handling

is antimicrobial

antimicrobial
antimicrobialagent
antimicrobialantipruritic
antimicrobialcomponent
antimicrobially

Search fields use

Reaxys ^

Use

輸入“antimicrobial*”
(*星號，可以容許後面有更多同義詞
增加搜尋範圍)



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Reaxys Retrosynthesis Page

合成路徑面板



登入Reaxys – 註冊免費帳號

Reaxys®

[Quick search](#) [Query builder](#) ^{New} [Results](#) [Synthesis planner](#) [History](#) [Alerts](#)

Ryan Huang  

Search for 184475-35-2

Import 

Search Reaxys

184475-35-2

如果要深入的使用Reaxys，可以免費申請Reaxys帳號：

- 更久的掛網時間
- 能夠匯出資料
- 儲存、管理搜尋結果
- 設定被動接收更新內容
- 可以有自己的 **Retrosynthesis** 面板

Create account

Your IP: 198.176.125.21 

First Name

Last Name

Email address

Password

Confirm password

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(Do not use on a shared computer!)

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[Content Overview](#) | Latest update: 11. September 2019 >

118M [Substances](#) 49M [Reactions](#) 59M [Documents](#) 37M [Bioactivities](#) 1.5M [Targets](#)

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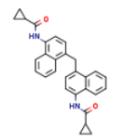
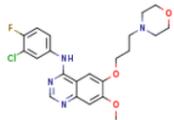
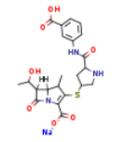
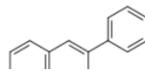
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逆合成面板 (規劃合成路徑、合成材料與反應條件)

Reaxys

Quick search Query builder Results **Retrosynthesis** History Alerts

Ryan Huang  

No.	Date/Time	Project name		No. of routes
5623	01 Oct 2021 03:06	Project #5623	 Delete  Edit 	Predicted  In progress Published 0 View 
5622	01 Oct 2021 02:58	Project #5622	 Delete  Edit 	Predicted 13 Published 5 View 
5146	28 Sep 2021 08:01	Project #5146	 Delete  Edit 	Predicted 0 Published 4 View 
4556	17 Sep 2021 03:25	Project #4556	 Delete  Edit 	Predicted 18 Published 5

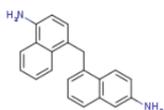
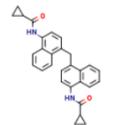
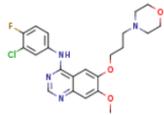
畫出專屬於你的結構

View the results

逆合成面板 (規劃合成路徑、合成材料與反應條件)

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

Draw new structure

No.	Date/Time	Project name		No. of routes
5625	01 Oct 2021 03:12	Project #5625	 Delete	Published Click here for options
5623	01 Oct 2021 03:06	Project #5623	 Delete	6 Published 0 View
5622	01 Oct 2021 02:58	Project #5622	 Delete	Predicted 13 Published 5 View
5146	28 Sep 2021 08:01	Project #5146	 Delete	Predicted 0 Published 4

如果查詢不到100%相似的結構，可用相似結構查詢

逆合成面板 (規劃合成路徑、合成材料與反應條件)

Reaxys®

Quick search Query builder Results **Retrosynthesis** History Alerts

Ryan Huang

Export Legend

Hide Reaxys Examples **Tree view** Table view

Output complete synthesis plan

Predicted route #1

Step 1 Step 2 Step 3 Step 4 Step 5

1

Reaction ID: 11291703

Conditions	Yield	Reference
With pyridine; dmap In 1,2-dichloro-ethane at 100°C; for 3h;		Jenkins, Tracy J.; Guan, Bing; Dai, Mingshi; Li, Gang; Lightburn, Thomas E.; Huang, Shan; Freeze, B. Scott; (...) Ocain, Timothy D.; Harriman, Geraldine C. [Journal of Medicinal Chemistry, 2007, vol. 50, # 3, p. 566 - 584] Full Text ↗ Cited 29 times ↗ Details > Abstract >

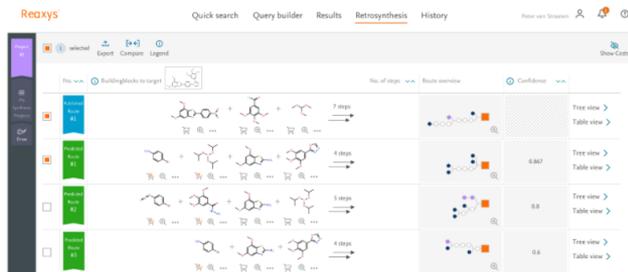
1 out of 1

The screenshot displays the Reaxys retrosynthesis software interface. At the top, there are navigation tabs for 'Quick search', 'Query builder', 'Results', 'Retrosynthesis', 'History', and 'Alerts'. The user's name 'Ryan Huang' is visible in the top right. The main workspace shows a retrosynthetic analysis of a complex molecule, with the predicted route broken down into five steps. A yellow callout box highlights the 'Export' button and contains the text '輸出完整的合成計畫' (Output complete synthesis plan). The right-hand panel provides detailed information for the first step of the route, including the reaction scheme, reagents (pyridine, dmap), solvent (1,2-dichloro-ethane), temperature (100°C), and time (3h). A reference is provided: Jenkins, Tracy J.; Guan, Bing; Dai, Mingshi; Li, Gang; Lightburn, Thomas E.; Huang, Shan; Freeze, B. Scott; (...) Ocain, Timothy D.; Harriman, Geraldine C. [Journal of Medicinal Chemistry, 2007, vol. 50, # 3, p. 566 - 584].

公開演講資訊 10/5 (二) 10:00-11:00 利用retrosynthesis AI引擎來預測合成路徑

Reaxys 新面貌 - 逆合成預測模組上線 當化學遇上 AI 系列活動第三場

[Reaxys 新面貌 - 逆合成預測模組上線](#)
[當化學遇上 AI 系列活動第三場](#)
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給想要擁有逆合成預測模組的您：全新 Reaxys Predictive Retrosynthesis 模組，以神經網路 (Neural Network) 技術作為核心引擎，畫出您想的目標分子，10 分鐘內預測全合成路徑，內建 AI 評分機制，追蹤材料價格、供應商、文獻證據強度，協助您做出更有效率的判斷。

公開演講資訊 10/7 (四) 22:00-23:00 化學反應條件預測



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Reaction condition prediction using Reaxys: from raw data to best-in-class model

📅 Oct 07 2021, 10:00pm 🌐 | Duration: 45 mins

▶ Upcoming webinar part of Big Data in Chemistry webinar series



Reaction condition prediction using Reaxys: from raw data to best-in-class model

Speaker:
Timur Madzhidov,
Assistant Professor at Department of Organic and
Medicinal Chemistry, Kazan Federal University

When:
Thursday October 7
4 PM / CEST, 10AM / EDT



[Reaction condition prediction using Reaxys: from raw data to best-in-class model \(brighttalk.com\)](#)

俄羅斯喀山國立大學 (Kazan Federal University) 有機與藥物化學系系主任 Timur Madzhidov 副教授



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Reaxys Commercial Substances

供應商物質資料庫



新增分類"Commercial Substances"於預視頁面

- Quick Search輸入CAS#，或畫結構搜尋您要購買的物質

Reaxys® [Quick search](#) Query builder Results Synthesis planner History Alerts Ryan Huang

Results for "186519-92-6" New Edit

	1	Substances CAS# : 186519-92-6 Edit in Query Builder Create Alert	Preview Results View Results
	0	Documents Titles, Abstracts, Keywords : "186519-92-6" Edit in Query Builder Create Alert	
	2	Commercial Substances CAS# : 186519-92-6 Edit in Query Builder Create Alert	Preview Results View Results



物質頁面購物車新增分類”Commercial Substances”

- 或點擊右上方切換資料庫為Commercial Substances

Reaxys® Quick search Query builder **Results** Synthesis planner History Alerts Ryan Huang

1 Substances out of 5 Documents, containing 11 Reactions, 0 Targets

0 selected Limit To Exclude Export Preparations Sort by No of References

Grid Heatmap

Reaxys - 1

Reaxys - 1

- Reaxys - 1
- Commercial Substances - 2
- eMolecules - 2
- LabNetwork - 0
- PubChem - 1
- SigmaAldrich - 1

4-chloro-7H-pyrrolo[2,3-d]pyrimidine-5-carboxylic acid
C₇H₄ClN₃O₂ 197.581 14006617 186519-92-6

Identification
Druglikeness
Physical Data - 1
Spectra - 2

Substance Availability

- Commercial Substances
- Accelrys' ACD
- CambridgeSoft ACX
- Sigma Aldrich
- eMolecules

ELSEVIER 509 6241 eMolecules

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Reaxys Commercial Substances 為每一筆物質提供詳細的供應商列表(A)包括純度、價格、包裝及到貨時間。您可利用篩選工具(B)加速挑選過程，並點擊供應商商品頁面連結(C)造訪供應商網頁。

Reaxys[®] Quick search Query builder Results Synthesis planner History Alerts Ryan Huang

0 selected Limit To Exclude Export Sort by Commercial Substance ID ↑ Grid

Please take a moment to check individual supplier websites for the most up-to-date information on pricing and availability

Supplier (A)	Product	Purity	Package size & price		Availability
Enamine - USA USA	186519-92-6 EN300-152527 ↗		mg		Tier Time: Tier 2 Last updated: 2020-06-01
eMolecules Enamine - USA USA	4-chloro-7H-pyrrolo[2,3-d]pyrimidine-5-carboxylic acid 186519-92-6 EN300-152527 ↗	95%	500 mg	159 USD	Shipment time: 2-10 days Tier Time: Tier 2 Last updated: 2020-06-01
eMolecules Manchester Organics Ltd USA	4-Chloro-7H-pyrrolo[2,3-d]pyrimidine-5-carboxylic acid 186519-92-6 F45799 ↗		1 g	994 USD	Shipment time: 12 weeks Tier Time: Tier 4 Last updated: 2020-06-01
eMolecules Oakwood Chemicals USA	4-Chloro-7H-pyrrolo[2,3-d]pyrimidine-5-carboxylic acid 186519-92-6 076916 ↗	95%	250 mg	134 USD	Shipment time: 1-5 days Tier Time: Tier 1 Last updated: 2020-06-01
eMolecules Oakwood Chemicals USA	4-Chloro-7H-pyrrolo[2,3-d]pyrimidine-5-carboxylic acid 186519-92-6 076916 ↗	95%	1 g	241 USD	Shipment time: 1-5 days Tier Time: Tier 1 Last updated: 2020-06-01
eMolecules Pharmablock USA	4-chloro-7H-pyrrolo[2,3-d]pyrimidine-5-carboxylic acid 186519-92-6 PB02420 ↗		10 g	670 USD	Shipment time: 4 weeks Tier Time: Tier 3 Last updated: 2020-06-01
eMolecules Pharmablock USA	4-chloro-7H-pyrrolo[2,3-d]pyrimidine-5-carboxylic acid 186519-92-6 PB02420 ↗		50 g	2241 USD	Shipment time: 4 weeks Tier Time: Tier 3 Last updated: 2020-06-01

Show Less ^

Feedback

(B)

(C)



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Search Result Management & Data Export

資料儲存管理/匯出



設定郵件提醒 - 新文獻

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

6,561 Documents with 3,870 Substances, 2,154 Reactions, 0 Targets

6,561 Documents
Today 11:28
Quick Search: ""perovskite solar cell""

Alert

當有最新的研究發表，通知您的私人信箱

Is machine learning...
Parikh, Nishi; Karamita, Meera; Raay, Vena; Mani, Ravathi; Monammas; Prochowicz, Daniel; Akin, Seekin; Kalam, Abul; Satapathi, Soumitra; Yadav, Pankaj [Journal of Energy Chemistry, 2022, vol. 66, p. 74 - 90]

Index Terms hit: {...Metal halide perovskites, Perovskite solar cell...}

High-performance perovskite solar cells based on dopant-free hole-transporting material fabricated by a thermal-assisted blade-coating method with efficiency exceeding 21%
Lee, Kun-Mu; Chiu, Wei-Hao; Tsai, Yu-Hsiang; Wang, Chao-Shian; Tao, Yu-Tai; Lin, Yan-Duo [Chemical Engineering Journal, 2022, vol. 427]

Index Terms hit: {...Dopant-free hole-transporting material, Fully printed perovskite solar cell, Thermal-assisted blade-coating...}

Exploring low-temperature processed multifunctional HEPES-Au NSSs-modified SnO₂ for efficient planar perovskite solar cells

Feedback



01.10.2021

設定郵件提醒 - 相似結構

1
22
Preview

Filters

Limit to > Exclude >

22 Substances

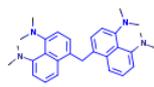
Today 11:47
Quick Search: 

Parameters >
Substance Classes >
Molecular Weight > 2
Number of Fragments >
Availability >
Availability in other databases >
Available Data >
Document Type >

22 Substances out of 21 Documents, containing 51 Reactions, 0 Targets

Alert 

Alerts

Chemical structure: 

Query: Quick Search: 

Alert name: alert1

Send alerts to: r.huang@elsevier.com 

Frequency: Every week  on: Friday 

Send alert: Upon first appearance in the database  

Do not send alerts with zero results 

ADVANCED ALERT CONTENT: 

From databases: Reaxys

Include in email: Title and bibliographic information
 Abstract
 Full abstract
 Partial abstract
 Hit details (keywords, substances, reactions or targets)

Email alerts will produce an email with a maximum of 99 records. 

Cancel > Create >

Reaxys - 22 

Sort by No of References  Grid  Heatmap 

Preparations - 18 >
Reactions - 19 >
Documents - 9 >

Preparations - 4 >
Reactions - 4 >
Documents - 4 >

Quick search Query builder Results Retrosynthesis History Alerts Ryan Huang

Export substances Reaxys

Choose a format: PDF/Print

Range: All results - 22

Export:

- All available data
- Identification data only
- Hit data only
- Choose specific data + Add datapoints

Include structures

Include a description in the document

Disclaimer: please refer to our [Terms and Conditions](#) before downloading data.

Export >

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- 須登入帳號
- 每次上限5000筆
- 每24小時上限25次

限制資料類型來減少資料下載量



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