

Reaxys 化學資料庫 教育訓練

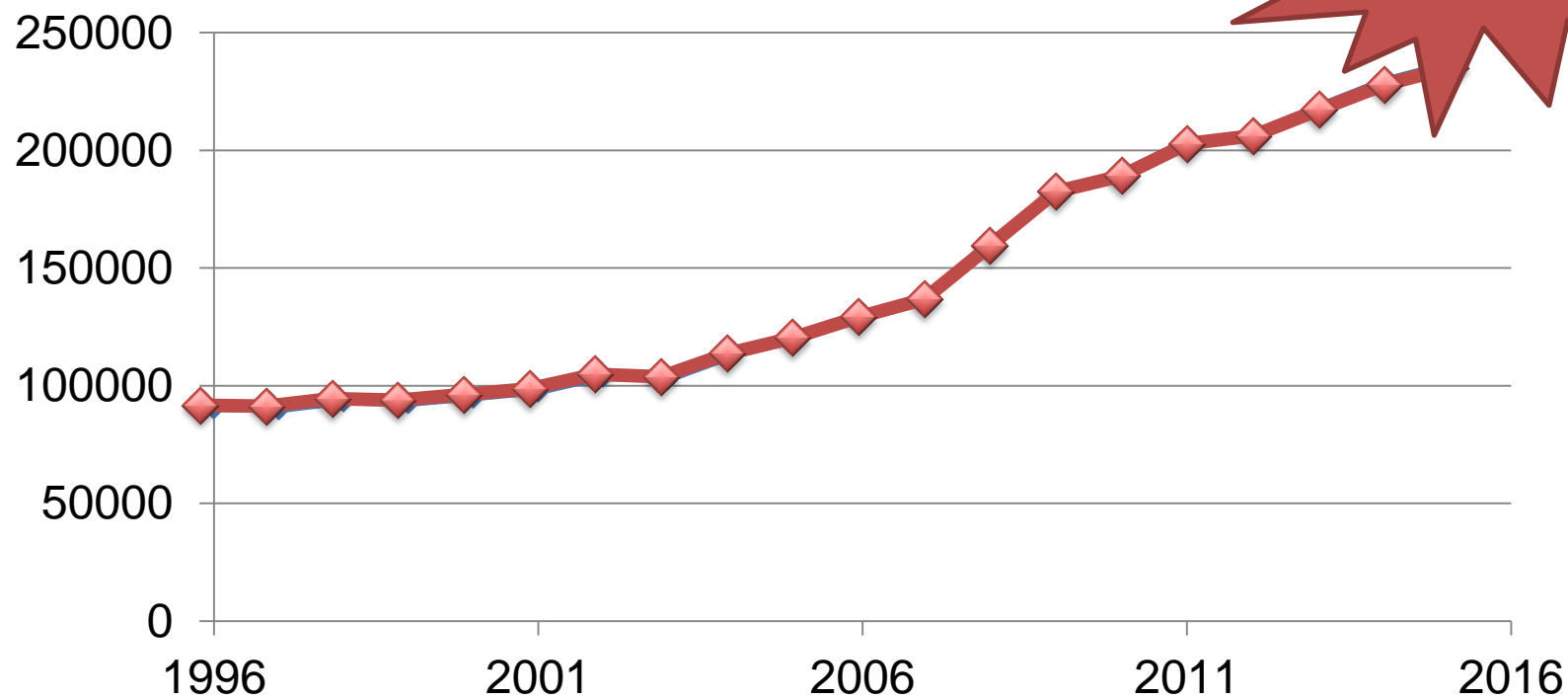
www.reaxys.com

梁成芝 Olivia Liang
o.liang@elsevier.com

201610
Olivia Liang

資訊爆炸的年代，是否有更好的選擇？

1996 - 2015 年化學領域發表文獻數量



更化學的搜尋方法

Ask Reaxys

AgInS2

SearchSmart searching with Ask Reaxys. [See examples >](#)**Physical Data**

Optical Rotatory Power (deg)

=

18.2

Show AND Buttons

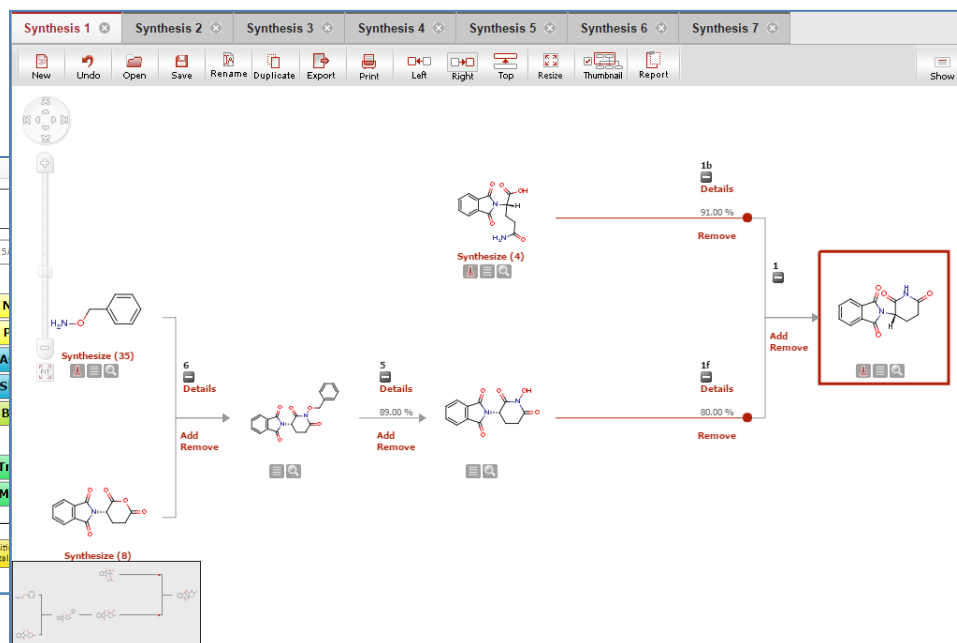
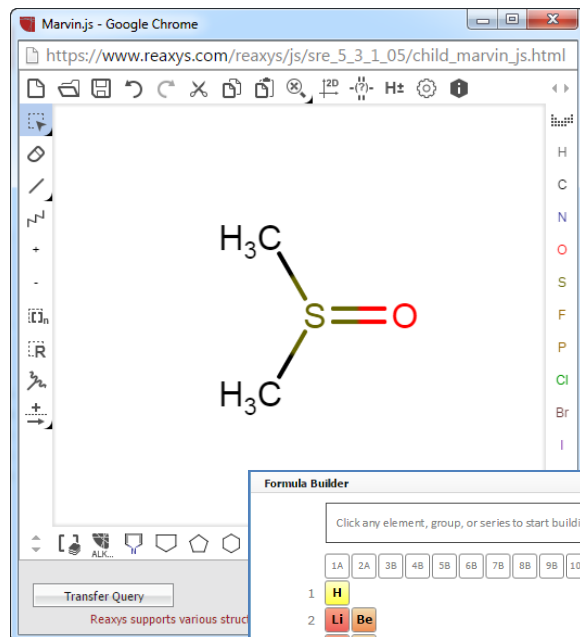
=

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<=

>

>=

Basic Indexes

Reaxys 可以用來搜尋哪些資料？

一般資料庫無法搜尋特定數值範圍的化學特性或實驗數據

搜尋結果

反應
(Reactions)

化合物
(Substances)

文獻
(Citations)

化學反應資料庫

收錄 > 4,100萬筆
單一或多步驟化學反應

化合物資料庫

收錄 > 2,650萬種
有機、無機、有機金屬
化合物

文獻資料庫

收錄 > 5,200萬筆資料
來自 >16,000種期刊及主要
專利局

特性資料庫

收錄 > 5億筆實驗數據
> 500種欄位
來自 > 130 個研究子領域

可直接瀏覽 281 本化學
期刊及專利全文中的合成
材料方法

可搜尋數值範圍。
例如：沸點 = 100°C 或沸
點 > 100 °C 的所有化合物

Reaxys 與 SciFinder 收錄內容比較

- Reaxys 收錄年代完整
- Reaxys 文獻多 **26%**
- Reaxys 特性資料多 **100倍**
- 數據資料表格化

Reaxys (承襲 BeilStein, Gmelin)

1771

1907

1965

1985

收錄年代

參考資料

https://www.lib.utexas.edu/chem/scifinder_faq.html#props2

<http://www.cas.org/content/chemical-substances/propertydata>

各種資料分門別類整理為表格，並抽出重要數據

表格中的文字皆可分類搜尋

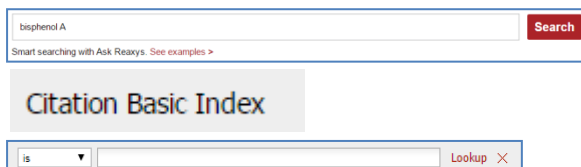
⚙ IR Spectroscopy (67 Hits out of 67 view all)				
Description (IR Spectroscopy)	Solvent (IR Spectroscopy)	Temperature (IR Spectroscopy)	Comment (IR Spectroscopy)	Reference
Bands	gaseous matrix			Maier, Guenther; Lautz, Christian
⚙ Physical Data				
⌵ Melting Point (10)				
⚙ Boiling Point (3)				
Boiling Point	Pressure (Boiling Point)	Reference		
1950 °C		Pourbaix, M. Bulletin des Societes Chimiques Belges, 1944 , vol. 53, p. 159 - 164 Full Text Show Details Gmelin Handbook: Zn: SVol., 235, page 802 - 803 Full Text Show Details		
1731 °C	600 Torr	Lemarchands, M.; Jacobs, M. Bulletin de la Societe Chimique de France, 1935 , vol. 2, p. 479 - 487 Full Text Show Details Gmelin Handbook: Zn: SVol., 235, page 802 - 803 Full Text Show Details		
2350 °C	760 Torr	Hagenbach; Langbein Arch. Sci. Phys. Nat., 1919 , vol. 1, p. 48 - 48 Full Text Show Details Gmelin Handbook: Zn: MVol., 43, page 126 - 128 Full Text Show Details		
				10284 Title/Abstract Full Text View citing articles Show Details

多元搜尋方式 -- 超過 400 種欄位可獨立或合併搜尋。

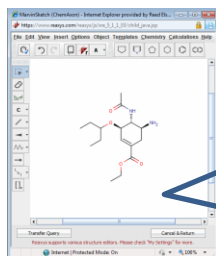
例如：搜尋包含34個碳，旋光度=18.2的所有化合物

關鍵字

Ask Reaxys



結構



- 支援 9 種繪圖軟體
- 強大衍生物搜尋功能
- Marvin JS 免安裝
JAVA

物質特性、實驗數據種類及其數值範圍

Physical Data

Optical Rotatory Power (deg)

=

▼

Show AND Buttons

Optical Rotatory Power (deg)

=

▼

Lookup ×

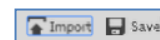
分子式、合金、及其它 > 500 種欄位搜尋

布林邏輯



Advanced

使用指令結合各種
搜尋條件 → 最完整



批次搜尋

History

結合多種搜尋條件



Merge 10 with 5



Overlap 10 with 5



Exclude 10 from 5



Exclude 5 from 10



反應
(Reactions)

化合物*
(Substances)

引用文獻
(Citations)

反應搜尋結果

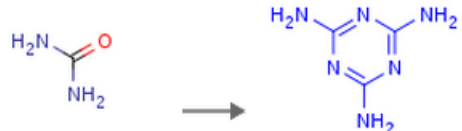







儲存勾選的反應資料

排序

☒ Limit to ☒ Exclude ☒ Export ☒ Print ☒ Zoom in ☒ Zoom out ☒ Hide

Sort by No of References  

查看包裝價格

<input type="checkbox"/> 3	<div>  <div>   </div> <div> Synthesize Find similar </div> </div> <div>   </div> <div> Synthesize Find similar </div> <div> Rx-ID: 748486 Find similar reactions </div>	<div> Available through...  Accelrys' ACD  eMolecules  CambridgeSoft ACX </div>
98%	Stage #1: T=140 - 160°C; P=6000.48 Torr; Stage #2: With ammonia ; γ-Al ₂ O ₃ P=750.06 - 1500.12 Torr;	erantsev; Tubolkin Chemistry, 2002 , vol. 75, # 11 p. 1883 - 1884 View citing articles Show Details
88.5%	in water Product distribution / selectivity; Show Experimental Procedure	EUROTECNICA MELAMINE, LUXEMBOURG, ZWEIGNIEDERLASSUNG IN ITTIGEN Patent: WO2007/119156 A2, 2007 ; Location in patent: Page/Page column 16-19 ; Title/Abstract Full Text Show Details
12.6%	With ammonia High Pressure; 70 to 300 at; at 350°C; 120 min;	Gmelin Handbook: C: MVol.D1, 45.11.4, page 449 - 450 Full Text Show Details Hunn, F. A. Diss. Zuerich T. H. 1959, S. 1/75 Full Text Show Details
⚡ Show Next 20 Details ⚡ Show All Remaining Details (31)		

搜尋結果 – substances

Bioactivities (0)

Reactions (35)

Substances (9)

Targets (0)

Citations (77)

go to Page Page 1 of 1

Limit to

Exclude

Export

Print

Zoom in

Zoom out

Hide

Sort by No of References

Display as

Exclude GOSTAR data

Structure	Structure/Compound Data	N° of preparations All Preps All Reactions	Available Data	Target	N° of ref.
<div> <div>AgInS₂</div> <div> <div>Synthesize</div> <div>Hide Details</div> <div>Find similar</div> </div> </div>	Chemical Name: silver indium disulfide Reaxys Registry Number: 15946194 Type of Substance: Solid solution Molecular Formula: AgInS ₂ Linear Structure Formula: AgInS ₂ Molecular Weight: 286.82 InChI Key: RDYBAOKQJVXEPR-UHFFFAOYSA-N	19 prep out of 22 reactions.	Druglikeness Identification Physical Data (88) Spectra (15) Use/Application (1) Quantum Chemical Data (4)	Show Targets	62

Chemical Names and Synonyms
 silver indium disulfide

Druglikeness

Identification

Physical Data

Melting Point (5)

Melting Point	Reference
871.84 °C	Bodnar'; Korzun; Yasyukevich Russian Journal of Inorganic Chemistry, 1998 , vol. 43, # 5 p. 771 - 774 Title/Abstract Full Text View citing articles Show Details Bodnar; Yasyukevich; Korzoun; Karoza Journal of Materials Science, 1998 , vol. 33, # 1 p. 183 - 188 Title/Abstract Full Text View citing articles Show Details
977 °C	Mal'sagov, A. U. Inorganic Materials (Transl. of Neorg. Mater.), 1989 , vol. 25, p. 17 - 20 Izvestiya Akademii Nauk SSSR, Neorganicheskie Materialy, 1989 , vol. 25, p. 22 - 29 Full Text Show Details
872 °C	Bodnar', I. V.; Orlova, N. S. Inorganic Materials (Transl. of Neorg. Mater.), 1989 , vol. 25, p. 330 - 335 Izvestiya Akademii Nauk SSSR, Neorganicheskie Materialy, 1989 , vol. 25, p. 382 - 387 Full Text Show Details Bodnar, I. V.; Korzun, B. V.; Chernyakova, A. P. Physica Status Solidi A: Applied Research, 1987 , vol. 101, p. 409 - 420 Full Text Show Details

Reaxys 搜尋結果分析及輸出

分析篩選搜尋結果，並輸出報告與同儕分享討論

搜尋結果

反應
(Reactions)

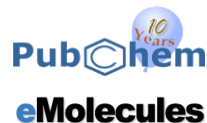
化合物*
(Substances)

引用文獻
(Citations)

合成路徑規畫

Synthesis Plans

資料庫連結



包裝價格資料

篩選功能：Analysis View 及 28 種 Filter



Filter by:

Substructure

多元資料儲存或輸出方式

Report

檔案格式：E-mail、HTML網頁、PDF

可儲存：搜尋條件、化合物、反應、文獻、合成路徑

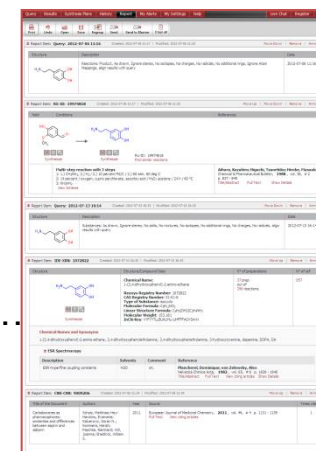
優點：適合儲存少量資料、操作簡便、格式簡明、保留超連結

- 彙整各種搜尋結果
- 一鍵 e-mail 分享

檔案格式：PDF、XML、Word、Excel、電子實驗記錄本、書目資料...

可儲存：化合物、反應、文獻、合成路徑

優點：可大量輸出搜尋結果、多種檔案格式可與進階分析軟體相容



New Reaxys 2016.10 更新




新版網頁 new.reaxys.com

- 內容擴充
 - 加入亞洲專利 (日本、韓國、中國、臺灣)
 - 摘錄 281 本期刊與專利的合成材料方法
 - 摘錄更多實驗數據內容，由 400 本擴充為 16000 本期刊
- 介面更新
 - 依據使用頻率重新調整介面

* 新版將與舊版並行至少半年


首頁 Quick Search

關鍵字搭配結構搜尋是使用頻率最高的搜尋方式

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


Search substances, reactions, citations and bioactivity data

輸入關鍵字搜尋



 Substance Property, e.g. solubility of vitamin D3

Search >

AND

 Create Structure or Reaction Drawing

繪製結構

 Version 1 Feedback 

進階搜尋 – Query Builder

整合超過 400 個欄位

The screenshot displays the Reaxys Query Builder interface. At the top, navigation tabs include 'Quick search', 'Query builder' (which is selected), 'Results', 'Synthesis planner', and 'History'. The user 'Olivia Liang' is logged in. Below the navigation bar, there are icons for 'Import', 'Save', 'Reset form', and 'Delete'. A 'Search Substances' button is also present. The main search area contains two criteria: 'Boiling Point' and 'Molecular Formula'. The 'Boiling Point' criterion is set to 'Boiling Point, °C' with a value of '100' and 'Pressure (Boiling Point), Torr'. The 'Molecular Formula' criterion is set to 'Molecular Formula' with a value of 'H2O'. A 'NOT' operator is visible between the two criteria. On the right side, a sidebar titled '1. 搜尋欄位' (Search Fields) lists various search fields under categories like 'Basic Indexes', 'Identification', 'Physical Properties', and 'Density'. The 'Physical Properties' category is expanded, showing fields like 'Melting Point', 'Boiling Point', 'Sublimation', 'Refractive Index', and 'Density'. A 'Feedback' button is at the bottom of the sidebar.

Reaxys[®] Quick search Query builder Results Synthesis planner History Olivia Liang

3. 搜尋 Search Substances

1. 搜尋欄位

Boiling Point

= Boiling Point, °C 100

= Pressure (Boiling Point), Torr

NOT

Molecular Formula

is Molecular Formula H2O

2. 輸入條件：
沸點 = 100 度
且分子式不是 H2O

Basic Indexes

Identification

Physical Properties

Melting Point

Boiling Point

Sublimation

Refractive Index

Density

Feedback

化學反應搜尋結果

83

Filters and Analysis

Yield

☐

>95 - 1002

☐

>80 - 851

☐

>75 - 801

☐

>30 - 352

☐

>15 - 201☐

Reagent/Catalyst

☐

hydrogenchloride9

☐

oxygen7☐☐☐☐☐

+

More

Quick searchQuery builderResultsSynthesis plannerHistory

Olivia Liang

83 Reactions

out of 72 Documents containing 96 Substances

0 selected: Limit ToExport

Reaxys Ranking

1



Find Similar Reactions

Yield	Conditions	Reference
99%	With hydrogenchloride; hydrogen palladium on activated charcoal In ethanol under 760 Torr for 24h Ambient temperature	Kohno; Sasao; Murahashi - Bulletin of the Chemical Society of Japan, 1990, vol. 63, # 4, p. 1252 - 1254

Full TextCited 11 timesShow details

ExportsFeedback

Autoplan 合成路徑規劃

Reaxys[®]

Synthesis Planner Edit

Autoplan 1 5

1 Plan 1

2 Plan 2

3 Plan 3

4 Plan 4

5 Plan 5

+ Create new

Plan 1

Import

Chemical reaction network diagram showing the synthesis of a target molecule from various starting materials. The network includes intermediates labeled 1, 2, 3, 4, and 5, with associated yields and reagents. For example, intermediate 2 is formed from 1f in 14% yield using oxygen, Cu(II) perchlorate, and ascorbic acid powder in water/acetone at 60°C for 24h. Intermediate 3 is formed from 4 in 67% yield using a specific reagent. The final product is formed from intermediate 1.

Conditions

Preparation - 2

Yield	Conditions	Reference
14%	With oxygen; Cu(II) perchlorate; ascorbic acid powder In water; acetone at 60°C for 24h	Aihara, Kazuhiro; Higuchi, Tsunehiko; Hirobe, Masaaki - Chemical & Pharmaceutical Bulletin, 1988, vol. 36, # 2, p. 837 - 840 Full Text Show details

Preparation - 3

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

Reaxys Demo & Case Study

Ask Reaxys

分子式 AgInS_2

Reaxys is changing! Join one of our webinars tomorrow to find out how. [Register here](#)

×



Anonymous user (198.176.84.34)

Query Results Synthesis Plans History Report My Alerts My Settings Help

Register Login ▾

Import Save

Ask Reaxys

AgInS2

Search

Smart searching with Ask Reaxys. [See examples >](#)

Reactions



Substances, Names, Formulas



Medicinal Chemistry



Literature



ReaxysTree



Start by specifying common ID fields such as CAS Registry number and more.

You can also search directly by these common property groups:



Physical



Spectra



Natural Product



Advanced

LIFE SCIENCE SOLUTIONS

Professional Services™
Pathway Studio®
Reaxys® Medicinal Chemistry
Reaxys®
PharmaPendium®
Emhace™

SUPPORT

Customer Support
Contact Us
Performance Page

PRODUCT

About Reaxys
Reaxys News and Events
Terms and Conditions
Privacy Policy

<https://www.reaxys.com/reaxys/secured/search.do#>

搜尋結果 – substances

Bioactivities (0) Reactions (35) **Substances (9)** Targets (0) Citations (77) go to Page Page 1 of 1

Limit to Exclude Export Print Zoom in Zoom out Hide Sort by No of References Display as Exclude GOSTAR data

Structure	Structure/Compound Data	N° of preparations All Preps All Reactions	Available Data	Target	N° of ref.								
<p>AgInS₂</p> <p>Synthesize Hide Details Find similar</p>	<p>Chemical Name: silver indium disulfide</p> <p>Reaxys Registry Number: 15946194 Type of Substance: Solid solution Molecular Formula: AgInS₂ Linear Structure Formula: AgInS₂ Molecular Weight: 286.82 InChI Key: RDYBAOKQJVXEPR-UHFFFAOYSA-N</p>	<p>19 prep out of 22 reactions.</p>	<p>Druglikeness Identification Physical Data (88) Spectra (15) Use/Application (1) Quantum Chemical Data (4)</p>	<p>Show Targets</p>	<p>62</p>								
<p>Chemical Names and Synonyms silver indium disulfide</p> <p>▼ Druglikeness</p> <p>▼ Identification</p> <p>▲ Physical Data</p> <p>▲ Melting Point (5)</p> <table border="1"> <thead> <tr> <th>Melting Point</th> <th>Reference</th> </tr> </thead> <tbody> <tr> <td>871.84 °C</td> <td> <p>Bodnar'; Korzun; Yasyukevich Russian Journal of Inorganic Chemistry, 1998, vol. 43, # 5 p. 771 - 774 Title/Abstract Full Text View citing articles Show Details</p> <p>Bodnar; Yasyukevich; Korzun; Karoza Journal of Materials Science, 1998, vol. 33, # 1 p. 183 - 188 Title/Abstract Full Text View citing articles Show Details</p> </td> </tr> <tr> <td>977 °C</td> <td> <p>Mal'sagov, A. U. Inorganic Materials (Transl. of Neorg. Mater.), 1989, vol. 25, p. 17 - 20 Izvestiya Akademii Nauk SSSR, Neorganicheskie Materialy, 1989, vol. 25, p. 22 - 29 Full Text Show Details</p> </td> </tr> <tr> <td>872 °C</td> <td> <p>Bodnar', I. V.; Orlova, N. S. Inorganic Materials (Transl. of Neorg. Mater.), 1989, vol. 25, p. 330 - 335 Izvestiya Akademii Nauk SSSR, Neorganicheskie Materialy, 1989, vol. 25, p. 382 - 387 Full Text Show Details</p> <p>Bodnar, I. V.; Korzun, B. V.; Chernyakova, A. P. Physica Status Solidi A: Applied Research, 1987, vol. 101, p. 409 - 420 Full Text Show Details</p> </td> </tr> </tbody> </table>						Melting Point	Reference	871.84 °C	<p>Bodnar'; Korzun; Yasyukevich Russian Journal of Inorganic Chemistry, 1998, vol. 43, # 5 p. 771 - 774 Title/Abstract Full Text View citing articles Show Details</p> <p>Bodnar; Yasyukevich; Korzun; Karoza Journal of Materials Science, 1998, vol. 33, # 1 p. 183 - 188 Title/Abstract Full Text View citing articles Show Details</p>	977 °C	<p>Mal'sagov, A. U. Inorganic Materials (Transl. of Neorg. Mater.), 1989, vol. 25, p. 17 - 20 Izvestiya Akademii Nauk SSSR, Neorganicheskie Materialy, 1989, vol. 25, p. 22 - 29 Full Text Show Details</p>	872 °C	<p>Bodnar', I. V.; Orlova, N. S. Inorganic Materials (Transl. of Neorg. Mater.), 1989, vol. 25, p. 330 - 335 Izvestiya Akademii Nauk SSSR, Neorganicheskie Materialy, 1989, vol. 25, p. 382 - 387 Full Text Show Details</p> <p>Bodnar, I. V.; Korzun, B. V.; Chernyakova, A. P. Physica Status Solidi A: Applied Research, 1987, vol. 101, p. 409 - 420 Full Text Show Details</p>
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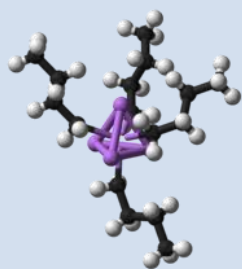
不同研究領域，適合不同的搜尋方式

Found in REAXYS SUBSTANCE RECORDS
... and ...

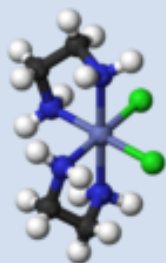
Found in KEYWORDS in REAXYS BIBLIOGRAPHIC
RECORDS



CLASSIC ORGANICS



ORGANOMETALLICS
COORDINATION
COMPOUNDS



CLASSIC INORGANICS

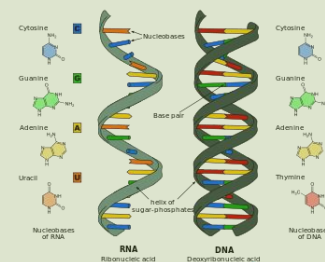
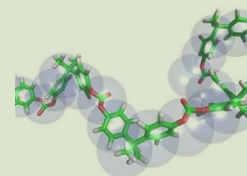


ALLOYS & METALS

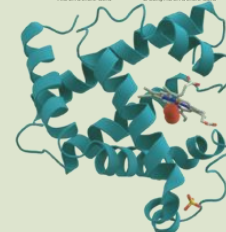
CERAMICS



POLYMERS



NUCLEIC ACIDS &
PROTEINS



搜尋化合物 Substances

搜尋文獻 Literature

關鍵字文獻搜尋 – 結合多個關鍵字

使用 Citation Basic Index 欄位或 Advanced Search

可使用多種指令
結合關鍵字

Citation Basic Index

布林邏輯 Boolean operators

- AND 涵蓋所有關鍵字
- OR 涵蓋任一關鍵字
- NOT 不涵蓋指定關鍵字

鄰近搜尋指令 Proximity Operators

- Next 兩個相鄰關鍵字依指定順序排列
- Near 兩個關鍵字無須依指定順序排列

其它搜尋指令

- 通用字元 * 可加在單字的左右側，用來搜尋不完整單字 (例如 cataly* 可找到 catalyst, catalysis 等)
- 括弧 () 優先運算括弧內指令
- 空格 = AND
- ; = OR
- - 連接詞彙 (例如 low-density)

輸入關鍵字並
預覽搜尋數量

Select index items and click 'Transfer'

Reaxys

Search for: thalidomide

thalidomide (21244)
thalidomide (celgene) (3)
thalidomide (contergan) (1)
thalidomide (durbin plc/gbr) (1)
thalidomide (glaxo smithkline) (1)
thalidomide (medimmune) (1)
thalidomide (penn/gbr) (1)
thalidomide (pharmion) (3)
thalidomide (schering) (1)
thalidomide (telik) (1)
thalidomide (thal) (1)
thalidomide - inhibition (12)
thalidomide - 19f nmr spectroscopy (2)
thalidomide - 1h-nmr spectroscopy (2)
thalidomide - 2d gel electrophoresis (2)
thalidomide - 4 aminobutyric acid uptake inhibitor (1)
thalidomide - 5-lipoxygenase-activating protein inhibitor (1)
thalidomide - abortifacient agent (1)
thalidomide - absolute configuration (3)
thalidomide - absorbent (1)

Page

小分子化合物文獻搜尋結果

乙烯裂解廠

Citation Basic Index

is

ethylene cracker plant

Lookup

Select index items and click 'Transfer'

Reaxys

Search for: ethylene crack

ethylene cracker (8)
ethylene cracker byproducts (1)
ethylene cracker complex (1)
ethylene cracker feed (3)
ethylene cracker feedstock (1)
ethylene cracker plant (1)
ethylene crackers (32)
ethylene cracking (36)

Economic optimization of a thermal cracker via model predictive control technology

Savu, Andreea R.; Muntean, Ionut; Lazea, Gheorghe; Agachi, Paul-Serban

2011

2011 19th Mediterranean Conference on Control and Automation, MED 2011, 2011, art. no. 5983153, p. 819 - 824
Full Text View citing articles

1

Title/Abstract

Economic optimization of a thermal cracker via model predictive control technology
An ethylene plant is one of the largest chemical plants and ethylene is industrially obtained through thermal cracking of hydrocarbons. The cracking furnace is the heart of such an installation and the frequent changes in feed mix, quality and prices; and the demand for its olefin products are influencing directly the production efficiency. Each reactant in the feed produces a certain distribution of products and in order to satisfy the demand constraints at the lowest cost; one needs to optimize the amounts of each reactant.

Keywords:
Author: economic optimization; ethylene plant; hydrocarbon pyrolysis; MPC; thermal cracker
Compendex Free Language: Economic optimization; Ethylene plants; hydrocarbon pyrolysis; MPC; Thermal cracker
Compendex Descriptor: Chemical plants; Cracking (chemical); Ethylene; Hydrocarbons; Model predictive control; Optimization; Petroleum chemistry
Compendex Mainhead: Predictive control systems
Reaxys Terms: cracking; thermal cracking

Page

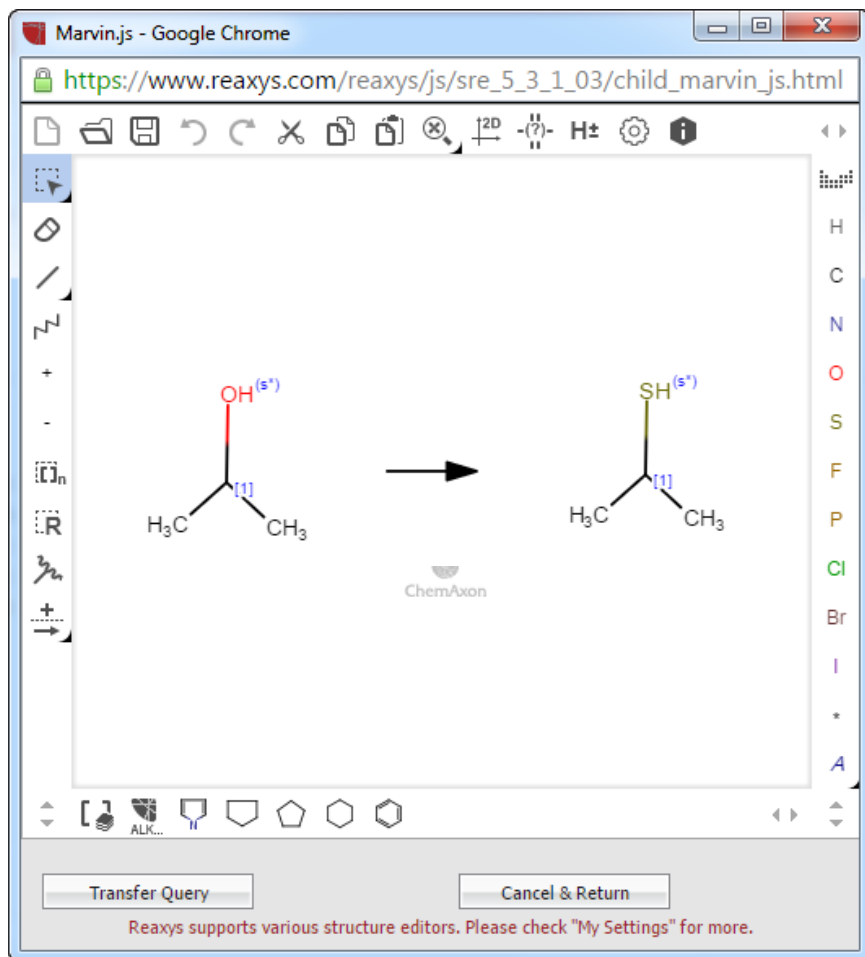
Transfer

Reset

Cancel

繪圖軟體 – Marvin JS

Reaxys 共支援 9 種繪圖軟體，包含常用的 Chemdraw, Accelrys, MarvinSketch 等



- 豐富的功能協助您搜尋各種衍生物與反應類型
 - 限定特定位置的鍵結、原子、或官能基種類，並具備多種彈性選項
 - R-group 功能
 - Substitution 限定特定原子是否接上官能基或接上鍵結的數量
 - Position variation bond 限定指定鍵結或官能基可能連接的多個位置
- 無須 Java 支援
- 可從 ChemDraw 複製貼上
- 繪製完畢的結構可存成去背圖檔，並可調整檔案大小

原廠線上教學短片


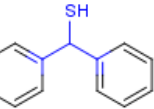
<https://docs.chemaxon.com/display/docs/Video+Tutorials+JS>

Reaction 搜尋結果

找到 1205 筆反應

Reactions (1205) Substances (1918) Citations (474) go to Page Page 1 of 134

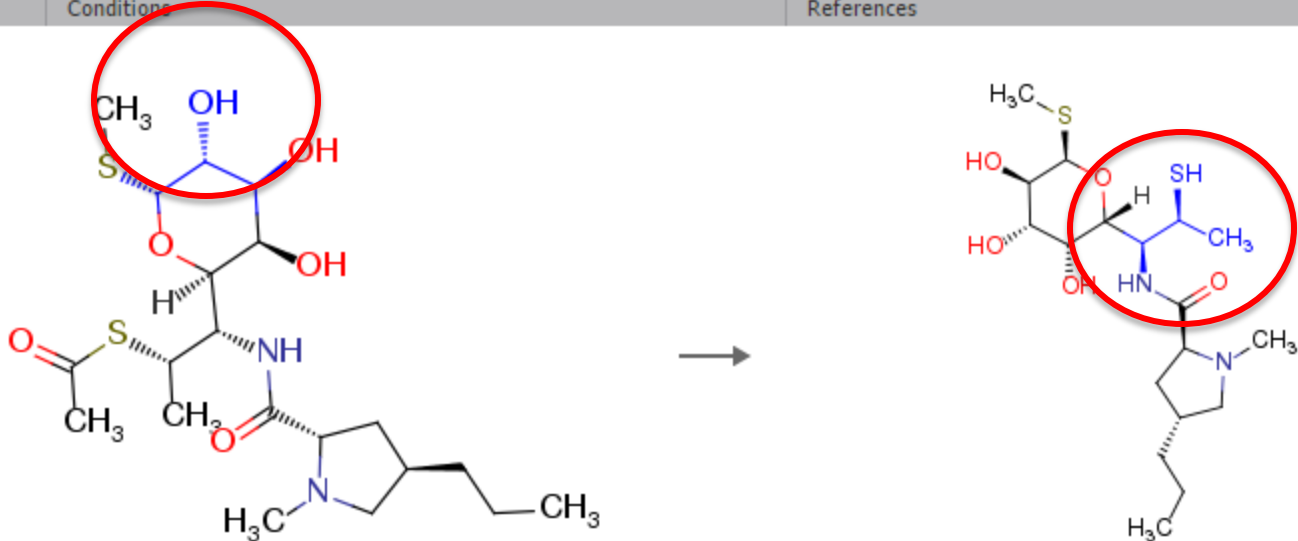




Limit to Exclude Export Print Zoom in Zoom out Hide Sort by Reaxys-Ranking

Yield	Conditions	References
<div><div><div><div>Synthesize</div><div>Find similar</div></div></div><div><div><div>Synthesize</div><div>Find similar</div></div></div><div>Rx-ID: 1786437 Find similar reactions</div></div> <td data-kind="ghost"></td> <td data-kind="ghost"></td>		
94%	With Lawessons reagent in toluene 0.5 h; Heating;	Nishio, Takehiko Journal of the Chemical Society, Perkin Transactions 1: Organic and Bio-Organic Chemistry (1972-1999), 1993 , # 10 p. 1113 - 1118 Title/Abstract Full Text View citing articles Show Details
94%	With Lawessons reagent in toluene 0.5 h; Heating;	Nishio, Takehiko Journal of the Chemical Society, Chemical Communications, 1989 , # 4 p. 205 - 206 Title/Abstract Full Text View citing articles Show Details
94%	With Lawessons reagent; water in toluene T=50°C;	Ohno, Michihiro; Miyamoto, Mitsuko; Hoshi, Kazuhiro; Takeda, Takahiro; Yamada, Naohiro; Ohtake, Atsushi Journal of Medicinal Chemistry, 2005 , vol. 48, # 16 p. 5279 - 5294 Title/Abstract Full Text View citing articles Show Details

Show All Remaining Details (4)

若不使用 atom mapping

找到 3158 個反應，但官能基的位置可能不同

Yield	Conditions	References
 <div data-bbox="357 949 473 1049"> Synthesize Find similar</div>	<p>With methanol; sodium methylate T=20°C; 0.333333 h; Show Experimental Procedure</p>	<p>Meiji Seika Kaisha, Ltd. Patent: EP1970377 A1, 2008 ; Location in patent: Page/Page column 48 ;</p> <div data-bbox="923 1192 1381 1220">Title/Abstract Full Text Show Details</div>
94%		<div data-bbox="1188 949 1304 1049"> Synthesize Find similar</div> <div data-bbox="1651 999 1864 1049">Rx-ID: 27887377 Find similar reactions</div>

合金搜尋

輸入元素成份搜尋合金、陶瓷複合材料

例如鈦合金 Ti-6Al-4V、貴金屬催化劑 Pd/C、

陶瓷材料Yttria(Y_2O_3)/Zirconia Ceramics (ZrO_2)

Alloy

合金成分

Component Formula

Ti

Fe or Fe2O3

Al

V

Percentage Type:

合金比例(範圍)

Percentage

Number or range: 20 or 20-40

Additional Components: ☐ 是否允許含有其他成分

合金成分比例單位

分子式搜尋

不完整分子式，例如只知道包含 34 個碳，輸入 C_{34}^*

多種分子數量組合，例如 Fe_xO_y , $x=2,3$ $y=2-4$

不同元素比例固定，例如 C_nH_{2n} , $n=2-4$

Formula Builder

Molecular Formula: Use this Formula

Periodic Table (Elements 1A to 8A, 1B to 2B, 3A to 8A):

Selected Element definition:

Fe

Charge(s): -

Count(s): -

Add

7 Nitrogen

N

Configuration [He] $2s^2 2p^3$

Isotopes ^{14}N ^{15}N

Density (kg/m³) 1.251

14.0067

0 more element(s) with arbitrary count

☐ Any more elements with any counts

Special groups:

Me Et Ph

Note: its also possible to enter

- ranges or enumerations defined via variables, e.g. Fe_xO_y $x=2,3$ $y=2-4$
- Arithmetic terms, e.g. C_nH_{2n+2} $n=3,4,5$

Classification: Metalloids, Nonmetals (Other Nonmetals, Halogens, Noble Gases), Metals (Alkali Metals, Alkaline Earth Metals, Lanthanoids, Actinoids, Transition Metals, Post Transition Metals)

分子式搭配其它欄位搜尋

分子式：氧化鋯 $\text{ZrO}[1-2]$

用途：牙科材料



Molecular Formula ✕

Molecular Formula Lookup ✕ Formula Builder

Use/Application

Use Pattern Lookup ✕

Show AND Buttons

Structure	Structure/Compound Data		N° of preparations All Preps All Reactions	Available Data	Target	N° of ref.
<div>O₂Zr</div> <div></div> <div>Synthesize Hide Details</div> <div>Find similar</div>	Chemical Name: zirconium oxide Reaxys Registry Number: CAS Registry Number: 7440-13-8 Type of Substance: Glass or compoundSolid solution Molecular Formula: O ₂ Zr Linear Structure Formula: Molecular Weight: 123.223 InChI Key: YYTCNKUFARLLT	Use Pattern			Reference	
		conventional particulate filler for fiber-reinforce composites used for dental applications			STICK TECH OY Patent: WO2008/917 A1, 2008 ; Title/Abstract Full Text Show Details	
		conventional particulate filler for fiber-reinforce composites used for dental appliances			STICK TECH OY Patent: WO2008/917 A1, 2008 ; Title/Abstract Full Text Show Details	
		conventional particulate filler for fiber-reinforce composites used for dental cavity fillings			STICK TECH OY Patent: WO2008/917 A1, 2008 ; Title/Abstract Full Text Show Details	
		conventional particulate filler for fiber-reinforce composites used for dental core composites			STICK TECH OY Patent: WO2008/917 A1, 2008 ; Title/Abstract Full Text Show Details	
		conventional particulate filler for fiber-reinforce composites used for dental provisional crown and bridge composites			STICK TECH OY Patent: WO2008/917 A1, 2008 ; Title/Abstract Full Text Show Details	
Chemical Names and Synonyms zirconium oxide, zirconia, ZrO ₂ , zirconium oxide mesoporous						
<div><div><div>⬆ Hit Data</div><div>⬇ Use (53 Hits out of 515 view all)</div></div></div>						

物化特性搜尋範例

搜尋包含34個碳，旋光度=18.2，且萃取自天然物的所有化合物

The screenshot shows a search interface with three main sections: Molecular Formula, Physical Data, and Natural Product. Each section has a 'Show AND Buttons' link. The Molecular Formula section contains a text input with 'C34*' and buttons for 'Lookup' and 'Formula Builder'. The Physical Data section contains a dropdown menu set to '=', a text input with '18.2', and a 'Show AND Buttons' link. The Natural Product section contains a checkbox labeled 'exists' and a 'Show AND Buttons' link. Callouts provide additional context: '搭配分子式搜尋 C34* 表示此分子含有34個碳，其餘未知' points to the Molecular Formula input; '選擇旋光度 optical rotatory power (deg) 選擇 = 輸入 18.2' points to the Physical Data dropdown and input; '天然物來源' points to the Natural Product checkbox; and '新增其它欄位' points to the 'Add/Remove Fields...' button in the bottom bar.

Molecular Formula

Molecular Formula Lookup

Physical Data

Optical Rotatory Power (deg) =

Show AND Buttons

Natural Product

Isolation from Natural Pro... ☒ exists

Show AND Buttons

Add to Query: Structure Molecular Formula Alloy

搭配分子式搜尋
C34* 表示此分子含有34個碳，其餘未知

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

天然物來源

新增其它欄位

Reaxys 搜尋結果分析及輸出

分析篩選搜尋結果，並輸出報告與同儕分享討論

搜尋結果

反應
(Reactions)

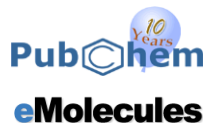
化合物*
(Substances)

引用文獻
(Citations)

合成路徑規畫

Synthesis Plans

資料庫連結



包裝價格資料

篩選功能：Analysis View 及 28 種 Filter



Filter by:

Substructure

多元資料儲存或輸出方式

Report

檔案格式：E-mail、HTML網頁、PDF

可儲存：搜尋條件、化合物、反應、文獻、合成路徑

優點：適合儲存少量資料、操作簡便、格式簡明、保留超連結

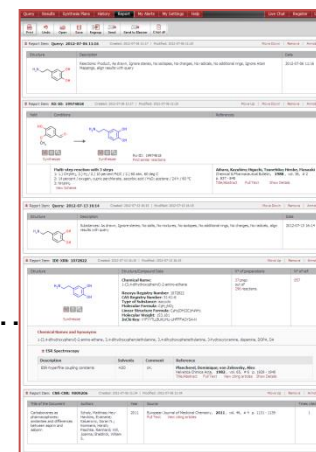
Export

檔案格式：PDF、XML、Word、Excel、電子實驗記錄本、書目資料...

可儲存：化合物、反應、文獻、合成路徑

優點：可大量輸出搜尋結果、多種檔案格式可與進階分析軟體相容

- 彙整各種搜尋結果
- 一鍵 e-mail 分享



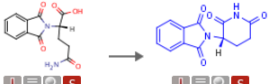
Report – 快速比較多種反應式並與同儕分享

可儲存 XML 檔案或直接以 e-mail 分享搜尋結果

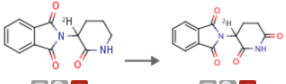
Query Results Synthesis Plans History **Report** My Alerts My Settings Help Register Login

Print Undo Open Save Regroup Send Send to Elsevier Clear all

Report Item: **RX-ID: 27910026** Created: 2015-12-18 18:38 | Modified: 2015-12-18 18:42 [Move Down](#) [Remove](#) [Annotation](#)

Yield	Conditions	References
 Synthesize Find similar Rx-ID: 27910026 Find similar reactions	91% With 1,1'-carbonyldiimidazole; 4-(N,N-dimethylamino)pyridine in acetonitrile 5 - 6 h; Heating / reflux; Show Experimental Procedure	MATRIX LABORATORIES LTD Patent: WO2008/35378 A2, 2008 ; Location in patent: Page/Page column 6; Title/Abstract Full Text Show Details

Report Item: **RX-ID: 29176469** Created: 2015-12-18 18:39 | Modified: 2015-12-18 18:42 [Move Up](#) [Move Down](#) [Remove](#) [Annotation](#)

Yield	Conditions	References
 Synthesize Find similar Rx-ID: 29176469 Find similar reactions	95% With ruthenium(IV) oxide; sodium periodate in dichloromethane; water; ethyl acetate T=40°C;	Yamamoto, Takeshi; Tokunaga, Etsuko; Nakamura, Shuichi; Shibata, Norio; Toru, Takeshi Chemical and Pharmaceutical Bulletin, 2010 , vol. 58, # 1 p. 110 - 112 Title/Abstract Full Text View citing articles Show Details

Report Item: **Synthesis Plan: Synthesis 8** Created: 2015-12-18 18:41 | Modified: 2015-12-18 18:42 [Move Up](#) [Remove](#) [Annotation](#)

Hide Synthesis Plan

Report – 儲存並分享規劃好的合成路徑

可使用 autoplan 自動規劃、瀏覽反應條件、產量、包裝價格、並挑選符合需求的路徑輸出成報告

Report Item: **Synthesis Plan: Synthesis 8** Created: 2015-12-18 18:41 | Modified: 2015-12-18 18:42 Move Up | Remove | Annotation

Hide Synthesis Plan

Hide Synthesis Details

Step	Yield	Conditions	References
1 Reaxys	34 mg	With ammonium cerium(IV) nitrate in acetonitrile T=20°C; 5 h;	Chang, Meng-Yang; Chang, Chung-Ho; Chen, Shui-Tein; Chang, Nein-Chen Journal of the Chinese Chemical Society, 2002 , vol. 49, # 3 p. 383 - 385 Title/Abstract Full Text View citing articles Show Details
	34 mg	With ammonium cerium(IV) nitrate in water; acetonitrile 5 h;	Chang, Meng-Yang; Chen, Shui-Tein; Chang, Nein-Chen Synthetic Communications, 2003 , vol. 33, # 8 p. 1375 - 1382 Title/Abstract Full Text View citing articles Show Details
2 Reaxys		With disodium hydrogenphosphate; sodium amalgam in methanol T=20°C; 1 h;	Chang, Meng-Yang; Chang, Chung-Ho; Chen, Shui-Tein; Chang, Nein-Chen Journal of the Chinese Chemical Society, 2002 , vol. 49, # 3 p. 383 - 385 Title/Abstract Full Text View citing articles Show Details
		With sodium amalgam; sodium salt of phosphorous acid in methanol T=20°C; 1 h;	Chang, Meng-Yang; Chen, Shui-Tein; Chang, Nein-Chen Synthetic Communications, 2003 , vol. 33, # 8 p. 1375 - 1382 Title/Abstract Full Text View citing articles Show Details

Report – 透過 e-mail 快速分享搜尋結果

The screenshot displays the Elsevier Report interface. At the top, a navigation bar includes 'Query', 'Results', 'Synthesis Plans', 'History', 'Report' (highlighted with a yellow box), 'My Alerts', 'My Settings', and 'Help'. Below this is a toolbar with icons for 'Print', 'Undo', 'Open', 'Save', 'Regroup', 'Send', 'Send to Elsevier', and 'Clear all'. The main content area shows a report for 'Query: 2012-07-06 11:16'. It includes a 'Structure' tab with a chemical structure of 1-(3,4-dihydroxyphenyl)-2-aminoethane, a 'Description' tab with search criteria, and a 'Date' column. Below this, there are sections for 'Yield', 'Conditions', and 'References'. A yellow arrow points from the 'Report' button in the navigation bar to a yellow box on the right. A blue callout box points to the 'Open' and 'Save' buttons. Another blue callout box points to the 'Send' button. A third blue callout box points to the 'Send to Elsevier' button. A fourth blue callout box points to the 'Send to Elsevier' button. A fifth blue callout box points to the 'Send to Elsevier' button. A yellow box on the right contains the text '點 Report 查看 儲存資料'. A yellow box on the right contains the text '搜尋指令、化合物 數據、反應、合成 路徑、文獻資料皆 可儲存到 Report'.

點 Report 查看 儲存資料

儲存或讀取 XML 檔

直接 E-mail 儲存資料

E-mail 搜尋問題 及儲存資料給 Elsevier

搜尋指令、化合物 數據、反應、合成 路徑、文獻資料皆 可儲存到 Report

Query

Results

Synthesis Plans

History

Report

My Alerts

My Settings

Help

Live Chat

Register

Login

Print

Undo

Open

Save

Regroup

Send

Send to Elsevier

Clear all

Report Item: Query: 2012-07-06 11:16

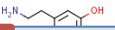
Created: 2012-07-06 11:17

Modified: 2012-07-06 11:20

Move Down

Remove

Annotation

Structure	Description	Date
	Reactions: Product, As drawn, Ignore stereo, No isotopes, No charges, No radicals, No additional rings, Ignore Atom Mappings, align results with query	2012-07-06 11:16

Regroup

Send

Send to Elsevier

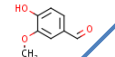
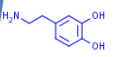
Clear all

Move Up

Move Down

Remove

Annotation

Yield	Conditions	References
		

直接 E-mail 儲存資料

E-mail 搜尋問題 及儲存資料給 Elsevier

Report Item: Query: 2012-07-13 16:14

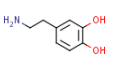
Created: 2012-07-13 16:15

Modified: 2012-07-13 16:15

Move Down

Remove

Annotation

Structure	Description	Date
	Substances: As drawn, Ignore stereo, No salts, No mixtures, No isotopes, No additional rings, No charges, No radicals, align results with query	2012-07-13 16:14

Report Item: IDE-XXR: 1072822

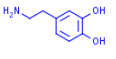
Created: 2012-07-13 16:15

Modified: 2012-07-13 16:15

Move Up

Remove

Annotation

Structure	Structure/Compound Data	N° of preparations	N° of ref.
	Chemical Name: 1-(3,4-dihydroxyphenyl)-2-aminoethane Reaxys Registry Number: 1072822 CAS Registry Number: 51-61-6 Type of Substance: isocyclic Molecular Formula: C ₈ H ₁₁ NO ₂ Linear Structure Formula: C ₈ H ₁₁ (OH) ₂ C ₂ H ₄ NH ₂ Molecular Weight: 153.181 InChI Key: Y1FYTTLBULJHU-UHFFFAOYSA-N	37 prep out of 296 reactions.	857

Chemical Names and Synonyms

1-(3,4-dihydroxyphenyl)-2-aminoethane, 3,4-dihydroxyphenylethylamine, 3,4-dihydroxyphenethylamine, 3-hydroxytyramine, dopamine, DOPA, DA

ESR Spectroscopy

Description	Solvents	Comment	Reference
ESR-hyperfine coupling constants	H ₂ O	2H.	Plancherel, Dominique; von Zelewsky, Alex Helvetica Chimica Acta, 1982 , vol. 65, # 6, p. 1929 - 1940 Title/Abstract Full Text View citing articles Show Details

Report Item: CHR-CHR: 9009206

Created: 2012-07-06 11:34

Modified: 2012-07-06 11:34

Move Up

Remove

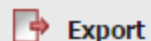
Annotation

Title of the Document	Authors	Year	Source	Times cited
Carbamoranes as pharmacophores: similarities and differences between aspirin and asborn	Scholz, Matthias; Hey-Hawkins, Evamarie; Kallerovic, Goran N.; Kommer, Haridh; Paschke, Reinhard; Will, Joanna; Sheldrick, William S.	2011	European Journal of Medicinal Chemistry, 2011 , vol. 46, # 4, p. 1131 - 1139 Full Text View citing articles	1

Export 輸出搜尋文獻至 EndNote 或 Mendeley

Bioactivities (206)						Reactions (11671)						Substances (94)						Targets (3)						Citations (12434)						go to Page <input type="text"/> Page 1 of 1382					
Limit to						Exclude						Export						Print						Zoom in						Zoom out					
Hide						Sort by						Relevance						Exclude GOSTAR data																	
Title of the Document						Authors						Year						Source						Times cited											
1						Cleansing articles for skin and/or hair which also deposit skin care actives						The Procter and Gamble Company						2002						Patent: US6338855 B1, 2002 ; Patent Family: WO1998/18445 A1; WO1998/18446 A1; WO1998/52537 A1; WO1999/12519 A1; EP935455 A1; ... Full Text											

Reaxys: Export Citation Results

**Export**

Substances Grid



Substances Report Table



Substances Reactions Table

Choose format

PDF/Print



XML*



Microsoft Word



Microsoft Excel*

Literature Management Systems
(e.g. ReferenceManager, EndNote etc.)

Electronic Lab Notebook



RD File

* these export formats allow to export bioactivity data

Export range

All hits



Range:

e.g. 1, 2-5, 10

Export contains

Include abstracts

Cancel

Export Data

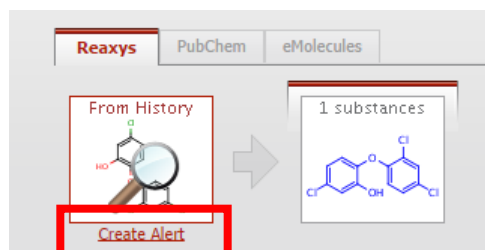
選擇檔案格式

選擇輸出範圍

輸出檔案

My Alerts – 持續關注特定主題

新知通報 (My Alerts) : 訂閱常用搜尋條件，隨時閱讀最新資料。



Query Results Synthesis Plans History Report **My Alerts** My Settings Help


Create Alert

Hint: please enter the name of the Alert and select the schedule (Frequency) in the form below. After each run of the Alert query you will receive an e-mail notification with a link to Reaxys allowing you to access the Alert results. [Privacy Policy](#)

Query  Ask Reaxys Substances: As drawn, Align results with query, (BP exists)

Name of Alert 輸入名稱

E-mail Address send copy to
e.g. a.smith@test.com; b.smith@test.com



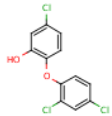
Recorded Webinar:
Solving tough chemistry problems Insights from an industry expert
Tuesday, Sept. 16, 9:00 AM EDT

Olivia Liang (o.liang@elsevier.com) is logged in

Query Results Synthesis Plans History Report **My Alerts** My Settings Help Logout

Reaxys PubChem eMolecules

To create a new Alert perform a new search and click the 'Create Alert' link on the results page

Name	Query	Description	Date created	Last run	Frequency
triclosanbp Modify alert	 Edit query	Ask Reaxys Substances: As drawn, Align results with query, (BP exists)	2014-09-22	Not yet run	After each update

中文線上學習平台

短片、應用範例、進階講座、線上測驗

- 網址：Taiwan.elsevier.com/reaxyshelp

Reaxys 線上學習平台



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