

Reaxys 化學資料庫 教育訓練

www.reaxys.com

梁成芝 Olivia Liang
o.liang@elsevier.com

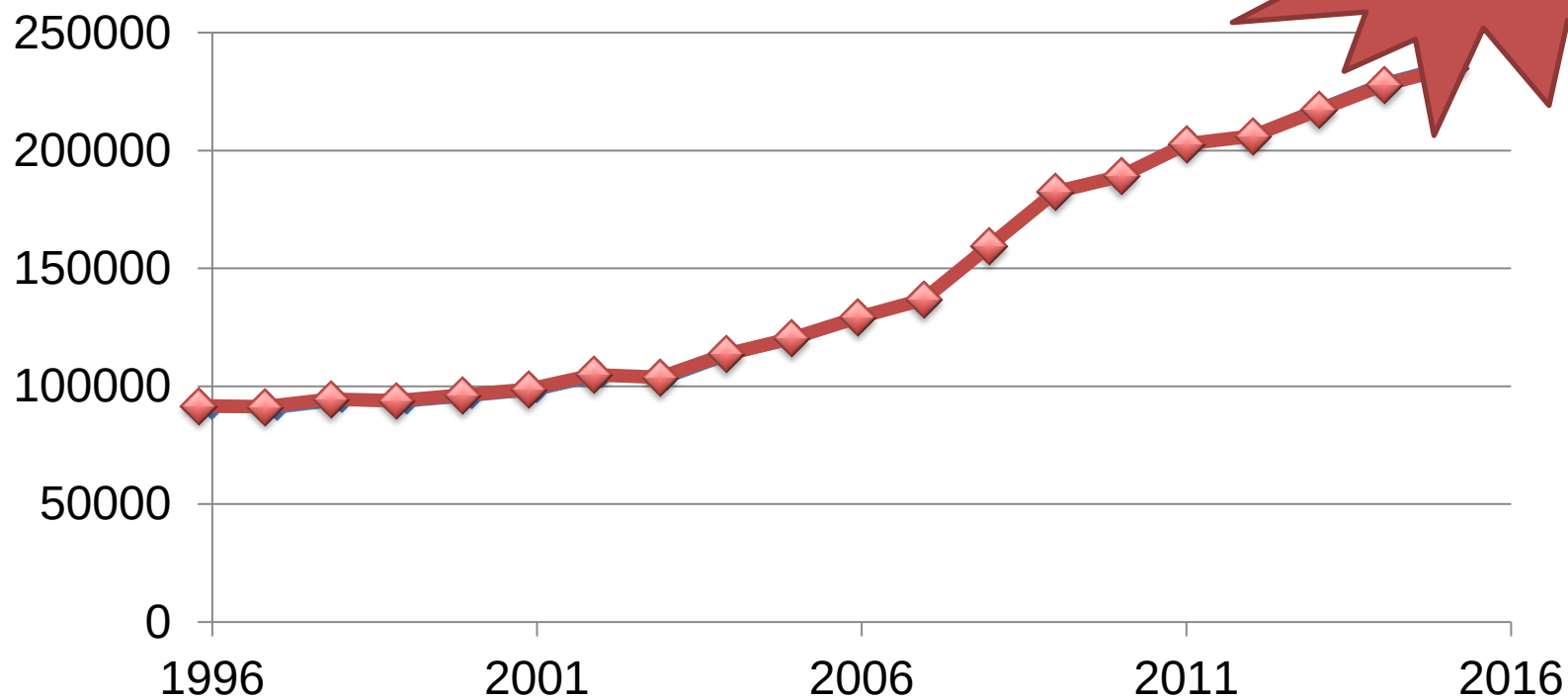
201608
Olivia Liang

Outline

- Reaxys introduction
- Case study & Demo
 - Keyword search
 - Ask Reaxys
 - Citation Basic Index
 - Structure Search
 - Marvin JS
 - Properties Search
 - Optical rotatory power
- New Reaxys

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

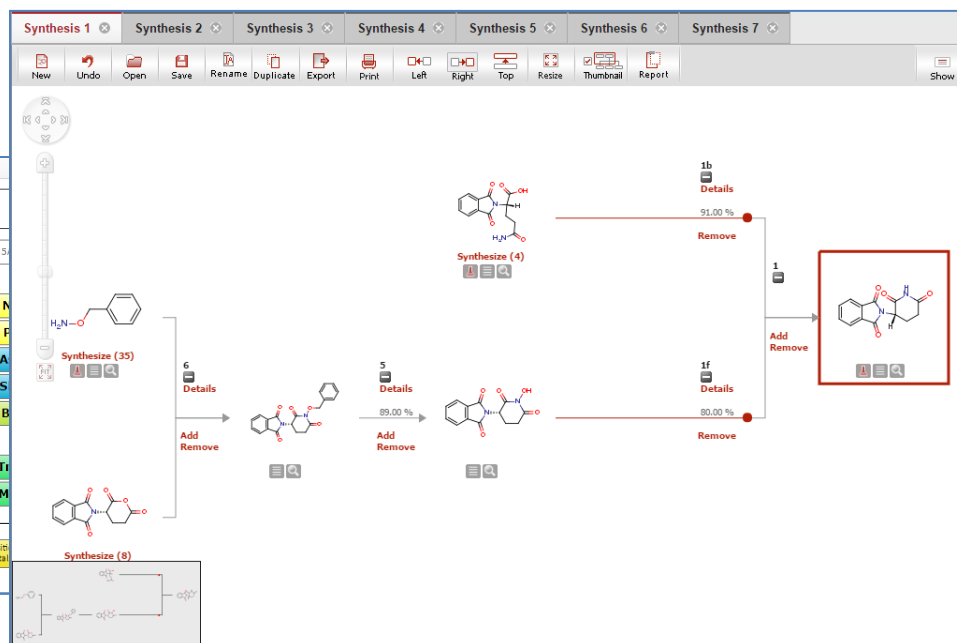
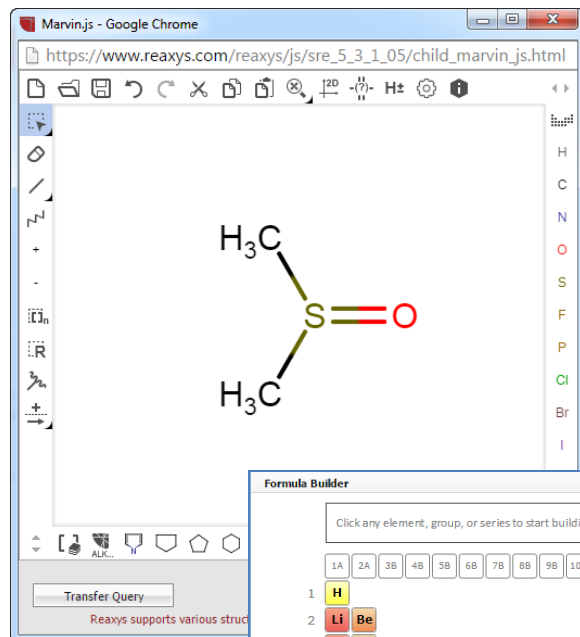
Show AND Buttons

<

<=

>

>=

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

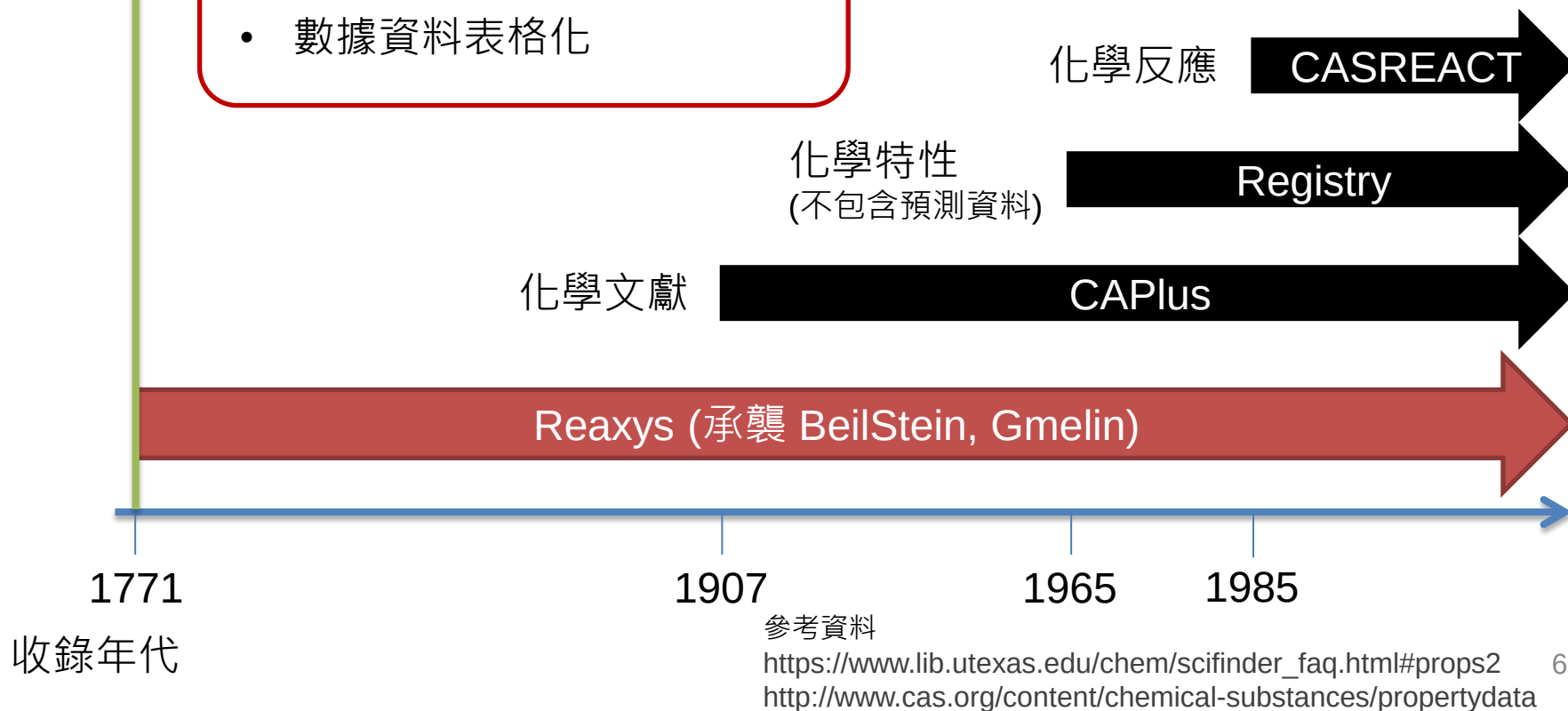
收錄 > 5億筆實驗數據
> 500種欄位
來自 > 130 個研究子領域

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



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

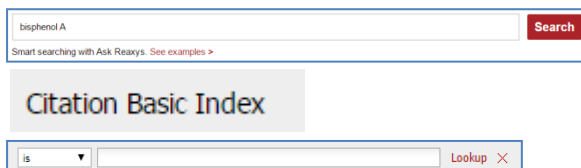
⚡ IR Spectroscopy (67 Hits out of 67 view all)				
Description (IR Spectroscopy)	Solvent (IR Spectroscopy)	Temperature (IR Spectroscopy)	Comment (IR Spectroscopy)	Reference
Bands	gaseous matrix			Maier, Guenther; Lautz, Christian
⚡ Physical Data				
⌵ Melting Point (10)				
⚡ Boiling Point (3)				
Boiling 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 500 種欄位可獨立或合併搜尋。

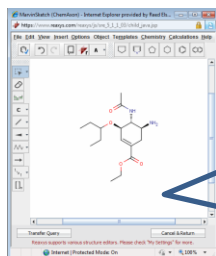
例如：搜尋包含34個碳，旋光度=18.2的所有化合物

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)

=

▼

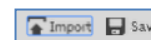
Lookup ×

分子式、合金、及其它 > 500 種欄位搜尋

布林邏輯



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)

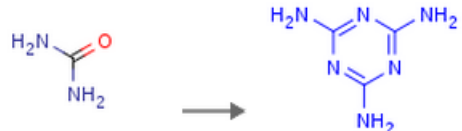
反應搜尋結果

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  

☐ 3	   Synthesize Find similar   Synthesize Find similar	Rx-ID: 748486 Find similar reactions Available through...  Accelrys' ACD  eMolecules  CambridgeSoft ACX
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)		

查看包裝價格

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.								
AgInS₂ Synthesize Hide Details Find similar	Chemical Name: silver indium disulfide 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	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) <table border="1"> <thead> <tr> <th>Melting Point</th> <th>Reference</th> </tr> </thead> <tbody> <tr> <td>871.84 °C</td> <td> 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 </td> </tr> <tr> <td>977 °C</td> <td> 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 </td> </tr> <tr> <td>872 °C</td> <td> 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 </td> </tr> </tbody> </table>						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
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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)

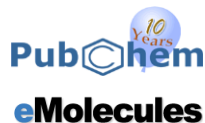
化合物*
(Substances)

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

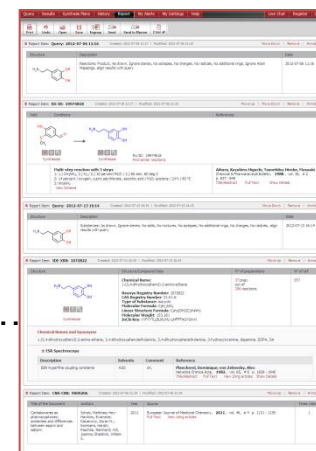
- 彙整各種搜尋結果
- 一鍵 e-mail 分享



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



Reaxys Demo & Case Study

Reaxys 中文線上學習平台

<http://taiwan.elsevier.com/elearning/reaxys>



<http://goo.gl/8WAMsk>

Reaxys 線上學習平台



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Reaxys 收錄期刊及專利資料，協助您搜尋整理好的化學反應、文獻、化合物及其特性與實驗數據，並輕鬆與他人分享
Reaxys 化學資料庫為國研院科資中心免費提供全國大專院校使用

熱門學習影片



Ask Reaxys
影片長度: 2:30
瀏覽次數: 46
最便捷的搜尋方式，輸入關鍵字由 Reaxys 自動辨識您想要的搜尋結果
[自我測驗](#)



Reaxys tree
影片長度: 1:35
瀏覽次數: 6
將 Reaxys 涵蓋的文獻分類並組成樹狀架構，您可搜尋特定概念並搜尋上下階層的文獻
[自我測驗](#)

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

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Performance Page

PRODUCT

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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.
AgInS₂  Synthesize Hide Details Find similar	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
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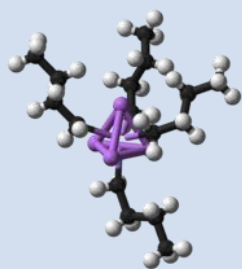
不同研究領域，適合不同的搜尋方式

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

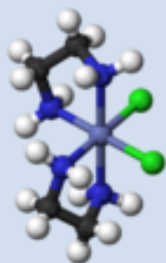
Found in KEYWORDS in REAXYS BIBLIOGRAPHIC
RECORDS



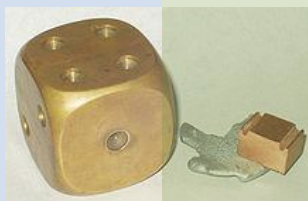
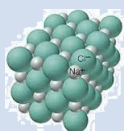
CLASSIC ORGANICS



ORGANOMETALLICS
COORDINATION
COMPOUNDS



CLASSIC INORGANICS

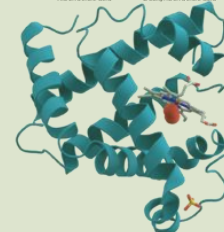
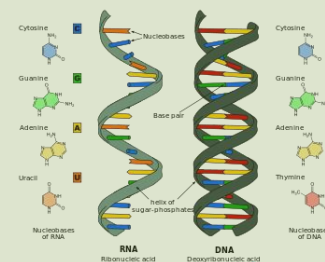
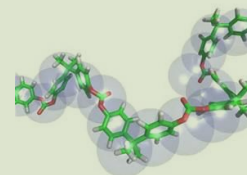


ALLOYS & METALS

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 X

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.

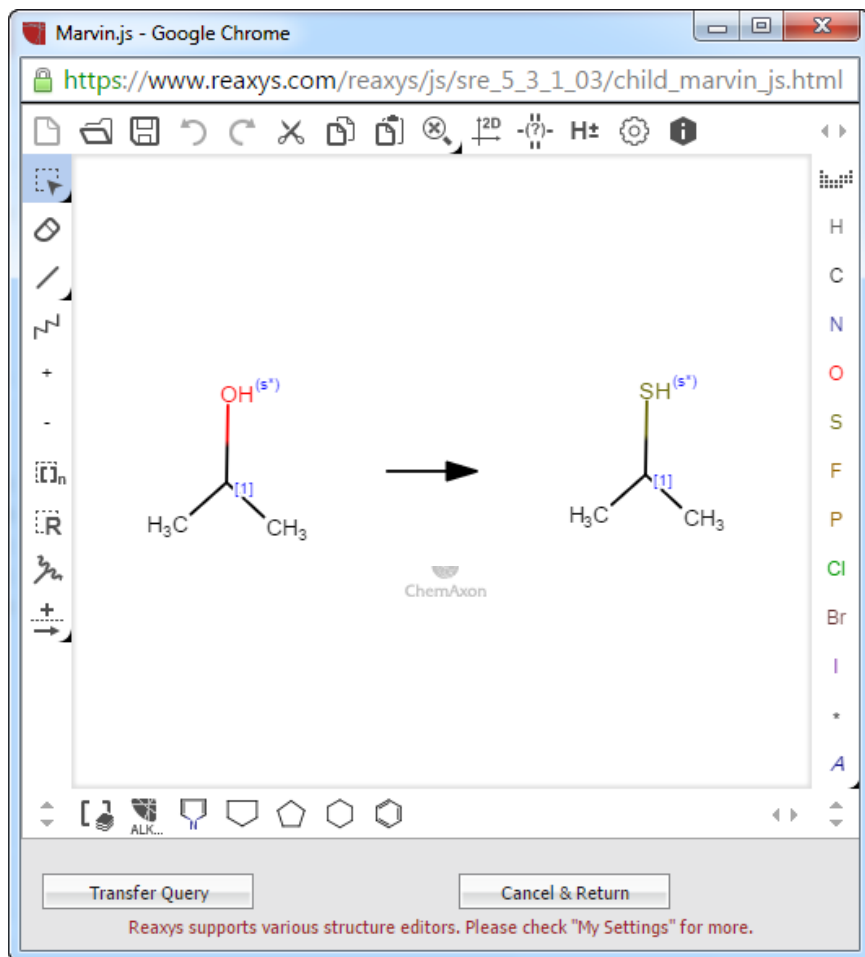
Keywords:
Author: economic optimization; ethylene plant; hydrocarbon pyrolysis; MPC; thermal cracker
Compendex Free Language: Economic optimization; Ethylene plants; hydrocarbon pyrolysis; MPC; Thermal cracker
Compendex Descriptor: Chemical plants; Cracking (chemical); Ethylene; Hydrocarbons; Model predictive 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

線上教學短片

<https://www.youtube.com/watch?v=46b3KXG0gxQ>

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)

物化特性搜尋 --

搜尋包含34個碳，旋光度=18.2的所有化合物

Molecular Formula

Molecular Formula Lookup × Formula Builder

Physical Data

Optical Rotatory Power (deg) = ▼

Show AND Buttons

Add to Query:

Structure Molecular Formula Alloy Add/Remove Fields...

搭配分子式搜尋
C34* 表示此分子含有47個碳，其餘未知

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

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)

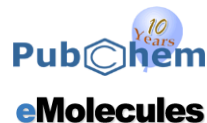
化合物*
(Substances)

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



Open Analysis View

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

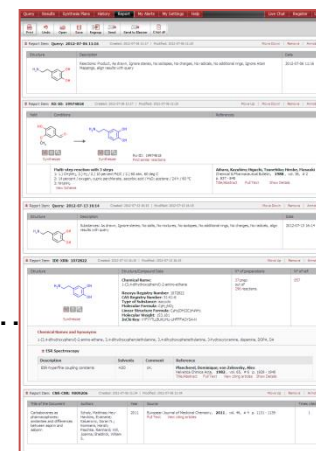


檔案格式：PDF、XML、Word、Excel、電子實驗記錄本、書目資料...

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



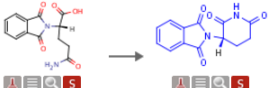
Report – 快速比較多種反應式並與同儕分享

可儲存 XML 檔案或直接以 e-mail 分享搜尋結果

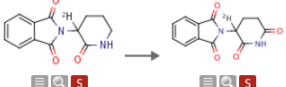
Query Results Synthesis Plans History **Report** My Alerts My Settings Help Register Login

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 three report items. The first item, 'Query: 2012-07-06 11:16', has a chemical structure of 1-(3,4-dihydroxyphenyl)-2-aminoethane and a description: 'Reactions: Product, As drawn, Ignore stereo, No isotopes, No charges, No radicals, No additional rings, Ignore Atom Mappings, align results with query'. The second item, 'Query: 2012-07-13 16:14', has a chemical structure of 1-(3,4-dihydroxyphenyl)-2-aminoethane and a description: 'Substances: As drawn, Ignore stereo, No salts, No mixtures, No isotopes, No additional rings, No charges, No radicals, align results with query'. The third item, 'IDE-XRN: 1072822', has a chemical structure of 1-(3,4-dihydroxyphenyl)-2-aminoethane and a description: 'Chemical Name: 1-(3,4-dihydroxyphenyl)-2-aminoethane, Reaxys Registry Number: 1072822, CAS Registry Number: 51-61-6, Type of Substance: isocyclic, Molecular Formula: C₈H₁₁NO₂, Linear Structure Formula: C₈H₁₁(OH)₂C₂H₄N₂, Molecular Weight: 153.181, InChI Key: Y1FYFTLLBULJHU-UHFFFAOYSA-N'. Below the chemical structure is a 'Synthesize' button. The 'Chemical Names and Synonyms' section lists: '1-(3,4-dihydroxyphenyl)-2-aminoethane, 3,4-dihydroxyphenylethylamine, 3,4-dihydroxyphenethylamine, 3-hydroxytyramine, dopamine, DOPA, DA'. The 'ESR Spectroscopy' section has a table with columns: 'Description', 'Solvents', 'Comment', and 'Reference'. The 'Description' is 'ESR-hyperfine coupling constants', 'Solvents' is 'H₂O', 'Comment' is '2H', and 'Reference' is 'Plancherel, Dominique; von Zelewsky, Alex. Helvetica Chimica Acta, 1982, vol. 65, # 6, p. 1929 - 1940. Title/Abstract Full Text View citing articles Show Details'. The bottom section, 'CHR-CHR: 9009206', has a table with columns: 'Title of the Document', 'Authors', 'Year', 'Source', and 'Times cited'. The 'Title of the Document' is 'Carboranes as pharmacophores: similarities and differences between aspirin and asbinn', 'Authors' is 'Scholz, Matthias; Hey-Hawkins, Evamarie; Kallerovic, Goran N.; Kommer, Haridh; Paschke, Reinhard; Will, Joanna; Sheldrick, William S.', 'Year' is '2011', 'Source' is 'European Journal of Medicinal Chemistry, 2011, vol. 46, # 4, p. 1131 - 1139. Full Text View citing articles', and 'Times cited' is '1'.

點 Report 查看
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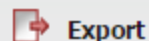
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及儲存資料給 Elsevier

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可儲存到 Report

Export 輸出搜尋文獻至 EndNote 或 Mendeley

Bioactivities (206)						Reactions (11671)						Substances (94)						Targets (3)						Citations (12434)					
Limit to						Exclude						Export						Print						Zoom in					
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

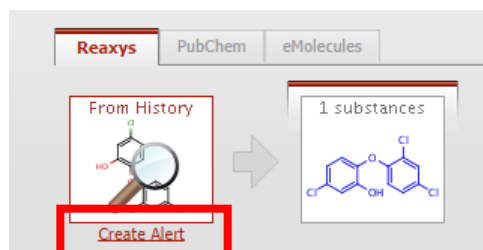
選擇檔案格式

選擇輸出範圍

輸出檔案

My Alerts – 持續關注特定主題

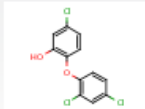
新知通報 (My Alerts)：訂閱常用搜尋條件，隨時閱讀最新資料。



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



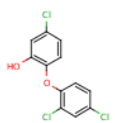
Recorded Webinar:
Solving tough chemistry problems Insights from an industry expert
Tuesday, Sept. 16, 9:00 AM EDT

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

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Reaxys PubChem eMolecules

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

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

New Reaxys 即將上市

Beta.reaxys.com (beta 測試版，可用現有 Reaxys 帳號密碼登入使用)

The screenshot shows the Reaxys Beta website search interface. At the top, the Reaxys logo is on the left, and navigation links for 'Quick search', 'Query builder', 'Results', 'Synthesis planner', and 'History' are in the center. On the right, there are links for 'Logout' and a help icon. Below the navigation bar, a large grey box contains the text 'Search substances, reactions, citations and bioactivity data'. Underneath this, there is a search input field with a magnifying glass icon and the placeholder text 'Substance Molecular Formula, e.g. Pt(PPh3)3'. Below the input field, the word 'AND' is centered. Under 'AND', there is a dashed box containing a chemical structure icon and the text 'Create Structure or Reaction Drawing'. To the right of the search input field, there is a blue speech bubble with the text '輸入關鍵字' (Enter keywords). Below the 'AND' section, there is another blue speech bubble with the text '輸入結構' (Enter structure). At the bottom right, there is a blue 'Search >' button. In the bottom right corner, there is a 'Feedback' link with a speech bubble icon.

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Search substances, reactions, citations and bioactivity data

輸入關鍵字

Q Substance Molecular Formula, e.g. Pt(PPh3)3

AND

輸入結構

Create Structure or Reaction Drawing

Search >

Feedback

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Reaxys Autoplan
影片長度: 4:18
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