Reaxys 化學資料庫 教育訓練

www.reaxys.com

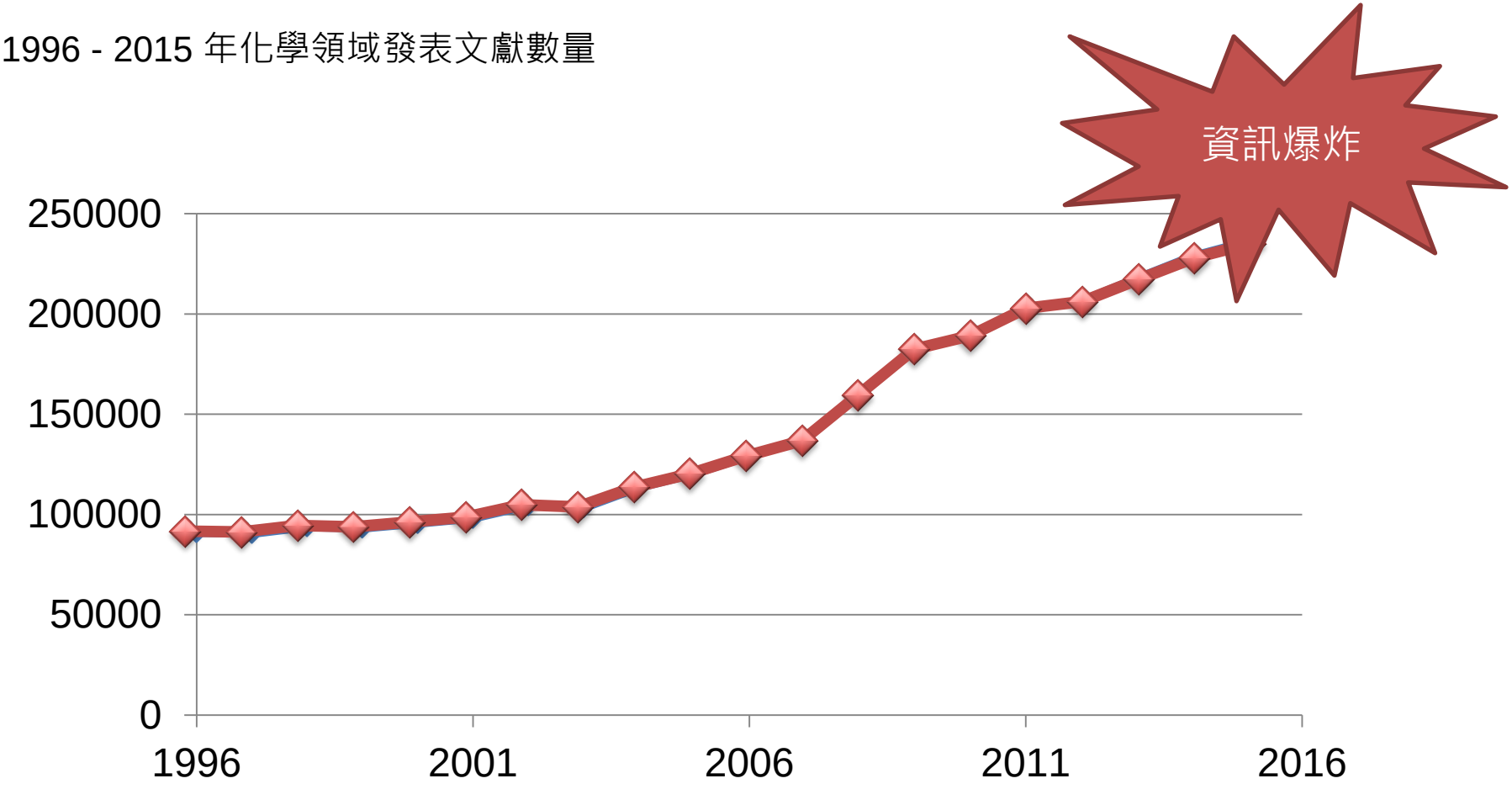
梁成芝 Olivia Liang
o.liang@elsevier.com

Outline

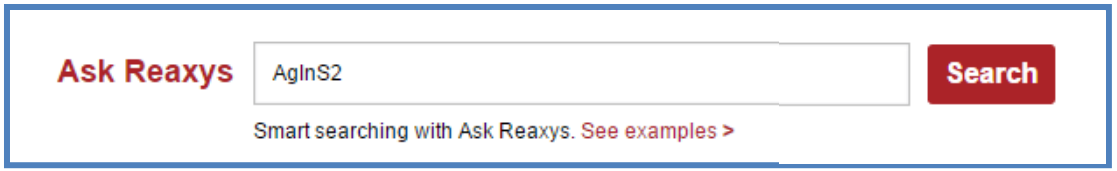
- Reaxys introduction
- Case study & Demo
  - Keyword search
    - Ask Reaxys
    - Citation Basic Index
  - Structure Search
    - Marvin JS
  - Properties Search
    - Optical rotatory power
- New Reaxys

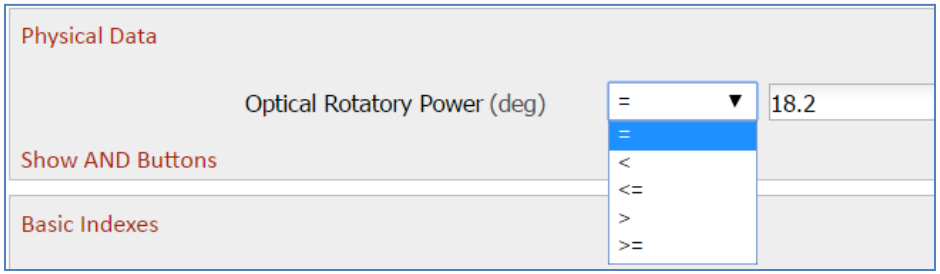
資訊爆炸的年代，是否有更好的選擇?

1996 - 2015 年化學領域發表文獻數量



更化學的搜尋方法


Ask Reaxys
AgInS2
Search
Smart searching with Ask Reaxys. See examples >


Physical Data
Optical Rotatory Power (deg)
=
18.2
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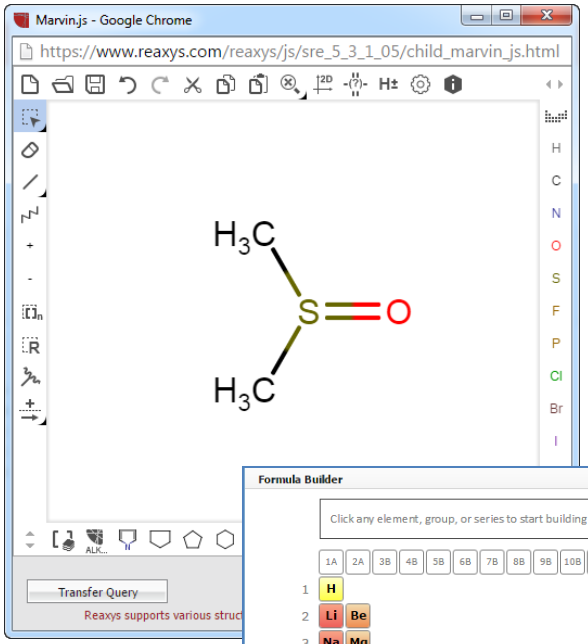
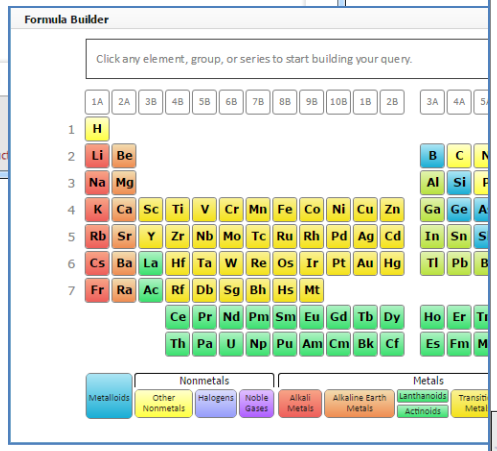
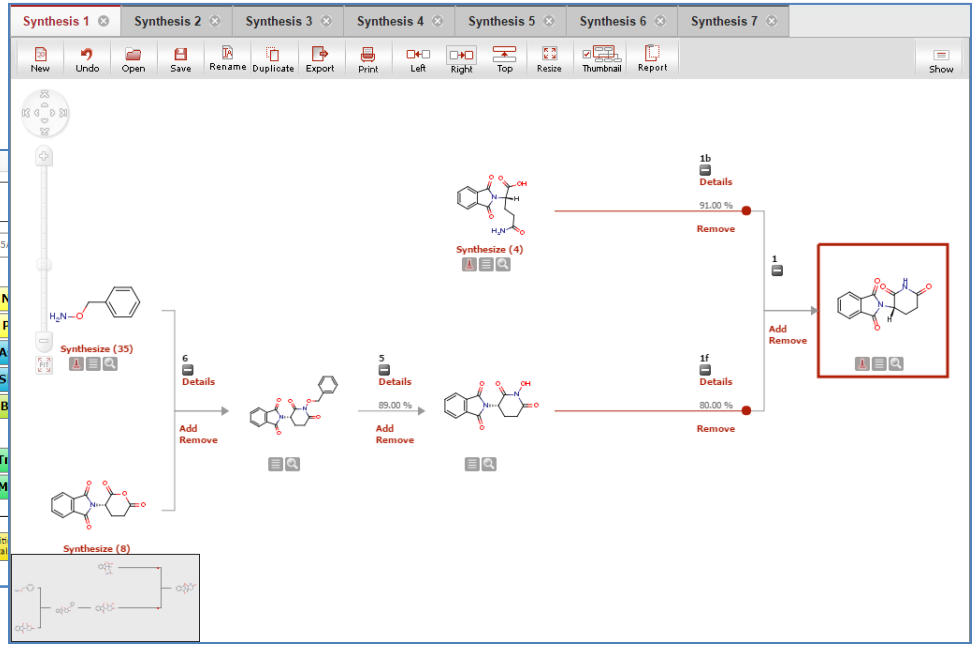
Show AND Buttons
Basic Indexes


Marvin.js - Google Chrome
https://www.reaxys.com/reaxys/js/sre_5_3_1_05/child_marvin_js.html
Transfer Query
Reaxys supports various struc


Formula Builder
Click any element, group, or series to start building your query.
Nonmetals
Metals


Synthesis 1
Synthesis 2
Synthesis 3
Synthesis 4
Synthesis 5
Synthesis 6
Synthesis 7
New
Undo
Open
Save
Rename
Duplicate
Export
Print
Left
Right
Top
Resize
Thumbnail
Report
Show
Synthesize (35)
Synthesize (8)
Synthesize (4)
Details
Add
Remove
91.00 %
89.00 %
80.00 %

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

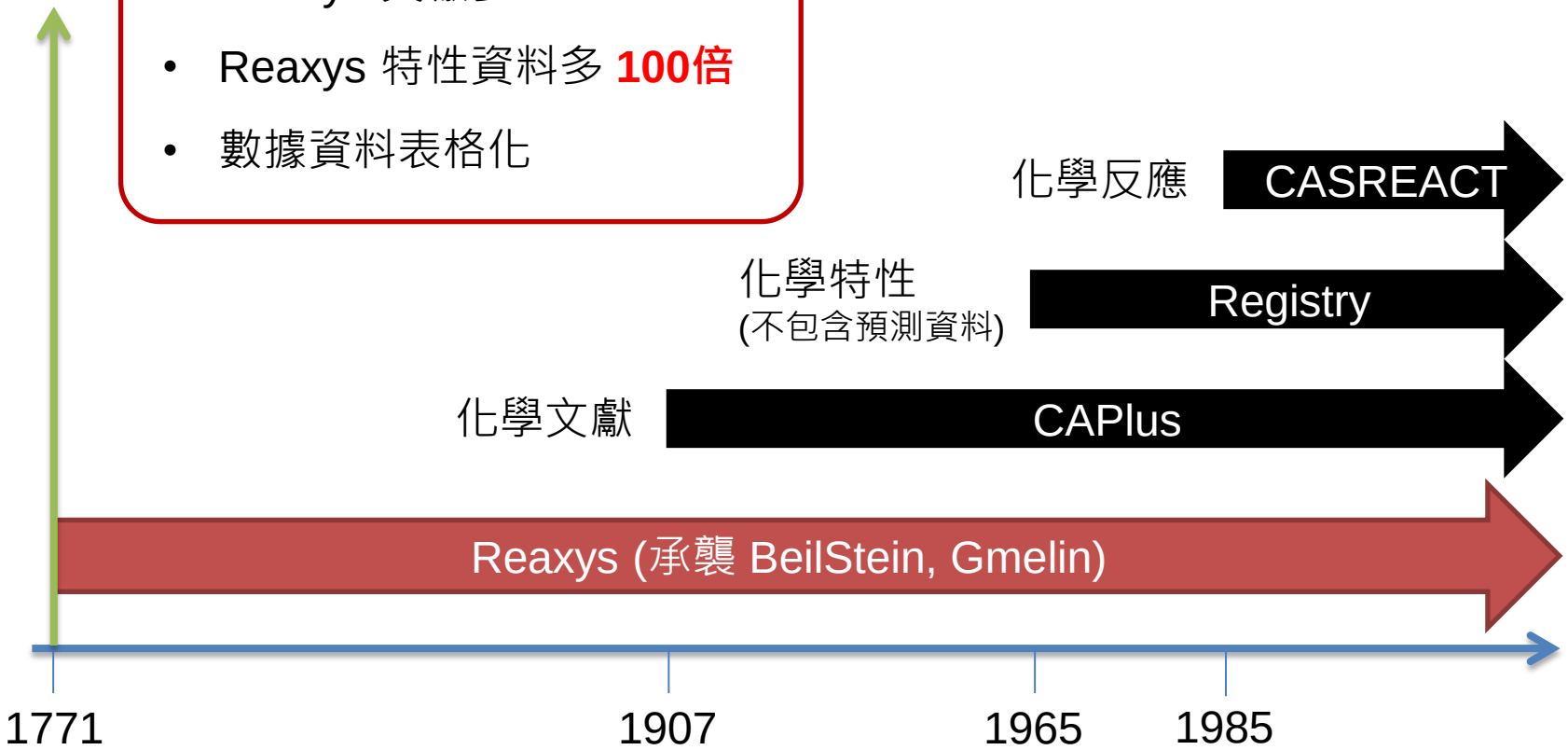
收錄 > 5億筆實驗數據
> 500種欄位
來自 > 130 個研究子領域

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



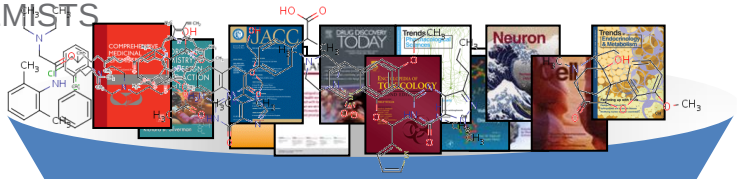
收錄年代

參考資料
https://www.lib.utexas.edu/chem/scifinder_faq.html#props2
http://www.cas.org/content/chemical-substances/propertydata

Reaxys 化學及藥物化學資料庫

我們的目標是為您節省更多時間

CATALOGUED AND TAXONMISED BY CHEMISTS FOR CHEMISTS



涵蓋 16,000 期刊及三大專利局

從 1776 年開始收錄

分類整理各種數據

高度相關的答案
RELEVANT ANSWERS

各種數據分門別類整理成表格

Structure	Structure/Compound Data	N° of preparations All Preps | All Reactions	Available Data	Target	N° of ref.
H_2C — CH_3 Synthesize | Hide Details Find similar	**Chemical Name:** propene **Reaxys Registry Number:** 1696878 **CAS Registry Number:** 187737-37-7 **Type of Substance:** acyclic **Molecular Formula:** C_3H_6 **Linear Structure Formula:** $C_2H_5CH_3$ **Molecular Weight:** 42.0806 **InChI Key:** QQONPFPTGQHPMA-UHFFFAOYSA-N	2824 prep out of 7655 reactions.	Hit Data (67) Druglikeness Bioactivity Identification Physical Data (1078) Spectra (183) Ecological Data (60) Use/Application (29) Natural Product (4)	Show Targets	9151

Chemical Names and Synonyms

propene, 1-propene, propylene

Hit Data

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** Angewandte Chemie - International Edition, **1999** , vol. 38, # 13-14 p. 2038 - 2041 Title/Abstract Full Text View citing articles Show Details
Spectrum	gas	26.9 °C	3500 - 500 cm**(-1)	**Street; Gellman** Journal of Physical Chemistry B, **1997** , vol. 101, # 8 p. 1389 - 1395 Title/Abstract Full Text View citing articles Show Details
Spectrum	solid matrix	-262.2 °C	3300 - 800 cm**(-1)	**Rowland, Brad; Hess, Wayne P.** Journal of Physical Chemistry A, **1997** , vol. 101, # 43 p. 8049 - 8056 Title/Abstract Full Text View citing articles Show Details
Bands	solid matrix	-262.2 °C	3086 - 916 cm**(-1)	**Rowland, Brad; Hess, Wayne P.** Journal of Physical Chemistry A, **1997** , vol. 101, # 43 p. 8049 - 8056 Title/Abstract Full Text View citing articles Show Details
Spectrum	solid matrix	-261.2 °C	3200 - 400 cm**(-1)	**Radziszewski, Juliusz G.; Downing, John W.; Gudipati, Murthy S.; Balaji; Thulstrup, Erik W.; Michl, Josef** Journal of the American Chemical Society, **1996** , vol. 118, # 42 p. 10275 - 10284 Title/Abstract Full Text View citing articles Show Details
Bands	solid matrix	-261.2 °C	3075 - 578 cm**(-1)	**Radziszewski, Juliusz G.; Downing, John W.; Gudipati, Murthy S.; Balaji; Thulstrup, Erik W.; Michl, Josef** Journal of the American Chemical Society, **1996** , vol. 118, # 42 p. 10275 - 10284 Title/Abstract Full Text View citing articles Show Details

Show next 20 Show next 47

Druglikeness

Bioactivity

Identification

Physical Data

Spectra

Ecological Data

Use/Application

Natural Product

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
				10284 Title/Abstract Full Text View citing articles Show Details

Physical Data

Melting Point (10)

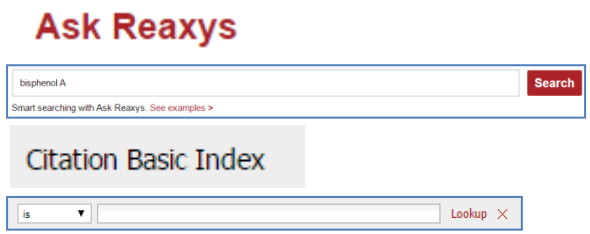
Boiling Point (3)

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

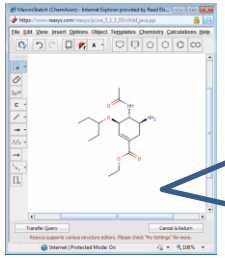
多元搜尋方式 -- 超過 500 種欄位可獨立或合併搜尋。

例如：搜尋包含34個碳，旋光度=18.2的所有化合物

關鍵字

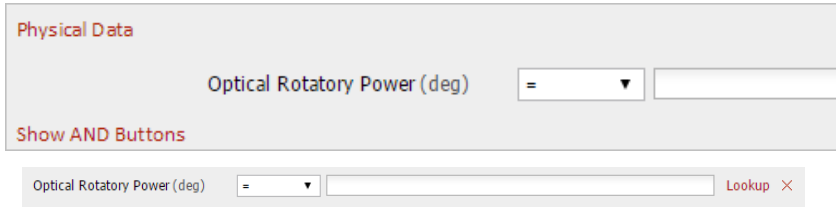


結構



- 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



分子式、合金、及其它 > 500 種欄位搜尋

布林邏輯

反應 (Reactions)

化合物* (Substances)

引用文獻 (Citations)

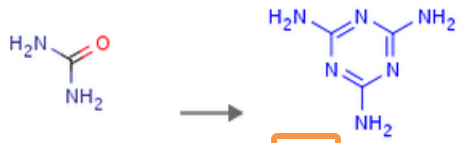
反應搜尋結果

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

查看包裝價格

Available through...
Accelrys' ACD
eMolecules
CambridgeSoft ACX

98%	Stage #1: T=140 - 160°C; P=6000.48 Torr; Stage #2: **With** ammonia; γ-Al_2O_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.
1 $AgInS_2$ 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

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

搜尋結果 -- Citations

Bioactivities (0) | Reactions (35) | Substances (9) | Targets (0) | Citations (77)

go to Page Page 1 of 9

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	Thermodynamic Stability of n-AgInSe2 in Photoelectrochemical Cells	Bicelli, Luisa Peraldo	1988	Journal of Physical Chemistry, **1988** , vol. 92, # 24 p. 6991 - 6997 Full Text View citing articles	
	Title/Abstract Show All Substances (5) Hit Substances in this article (1 out of 5)				
2	Photoelectrochemical study on the ternary semiconductors $AgInS_2$ and $AgInSe_2$	Odenweller; Grabner	1988	Berichte der Bunsengesellschaft/Physical Chemistry Chemical Physics, **1988** , vol. 92, # 11 p. 1330 - 1334 Full Text View citing articles	7
	Title/Abstract Show All Reactions (2) Show All Substances (6) Hit Substances in this article (1 out of 6)				
3	Solvothermal reaction route to nanocrystalline semiconductors $AgMS_2$ (M = Ga, In)	Hu, Junqing; Lu, Qingyi; Tang, Kaibin; Qian, Yitai; Zhou, Guien; Liu, Xianming	1999	Chemical Communications, **1999** , # 12 p. 1093 - 1094 Full Text View citing articles	40
	Title/Abstract Show All Reactions (2) Show All Substances (6) Hit Substances in this article (1 out of 6)				
4	A simple route to synthesize $MInS_2$ (M = Cu, Ag) nanorods from single-molecule precursors	Cui, Yong; Ren, Jin; Chen, Gang; Qian, Yitai; Xie, Yi	2001	Chemistry Letters, **2001** , # 3 p. 236 - 237 Full Text View citing articles	28

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

PubChem 10 Years

eMolecules

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

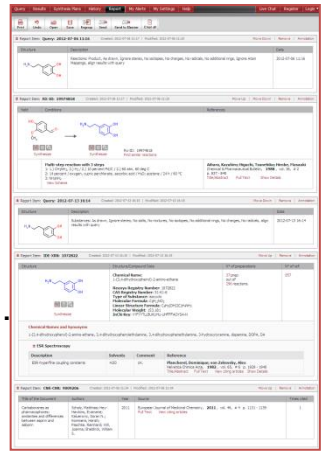
- 彙整各種搜尋結果
- 一鍵 e-mail 分享

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



ELSEVIER

Reaxys Demo & Case Study

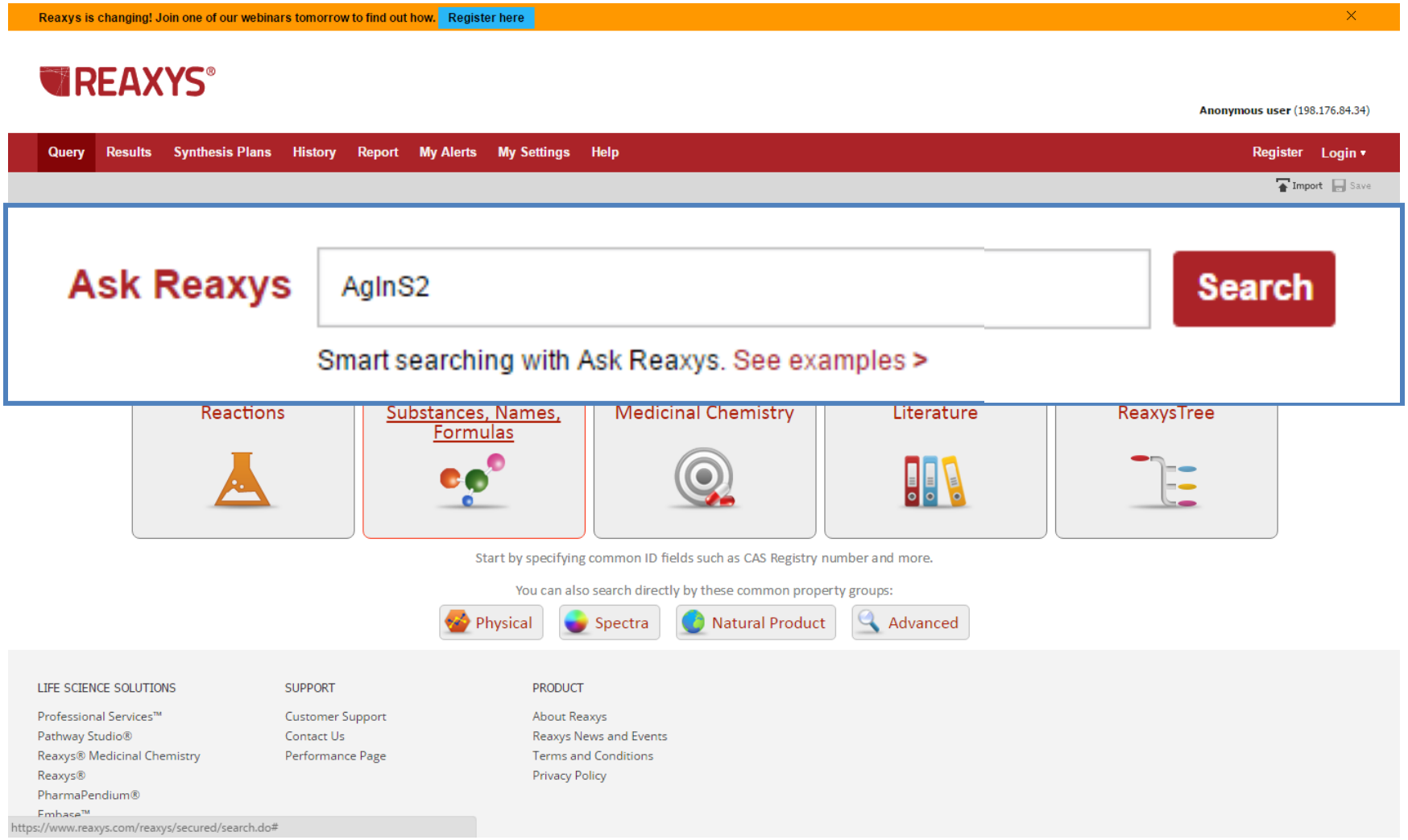
Reaxys 中文線上學習平台

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

http://goo.gl/8WAMsk

Ask Reaxys

分子式 $AgInS_2$



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.
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Chemical Names and Synonyms

silver indium disulfide

Druglikeness

Identification

Physical Data

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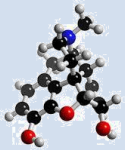
977 °C	**Mal'sagov, A. U.** Inorganic Materials (Transl. of Neorg. Mater.), **1989** , vol. 25, p. 17 - 20 Izvestiya Akademii Nauk SSSR, Neorganicheskie Materialy, **1989** , vol. 25, p. 22 - 29 Full Text Show Details
872 °C	**Bodnar', I. V.; Orlova, N. S.** Inorganic Materials (Transl. of Neorg. Mater.), **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

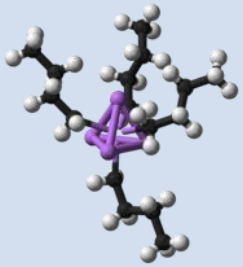
不同研究領域，適合不同的搜尋方式

Found in REAXYS SUBSTANCE RECORDS … and …

Found in KEYWORDS in REAXYS BIBLIOGRAPHIC RECORDS

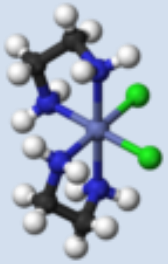


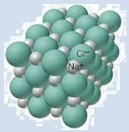
CLASSIC ORGANICS



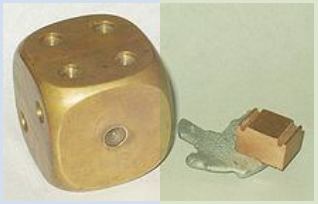
ORGANOMETALLICS

COORDINATION COMPOUNDS





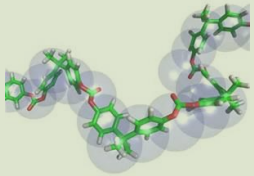
CLASSIC INORGANICS

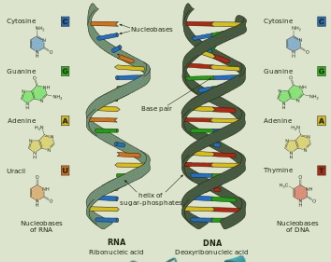


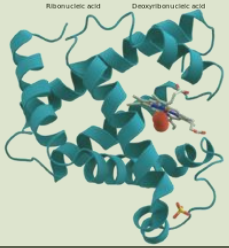
ALLOYS & METALS

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 | is ▼ | Lookup ✕

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

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.

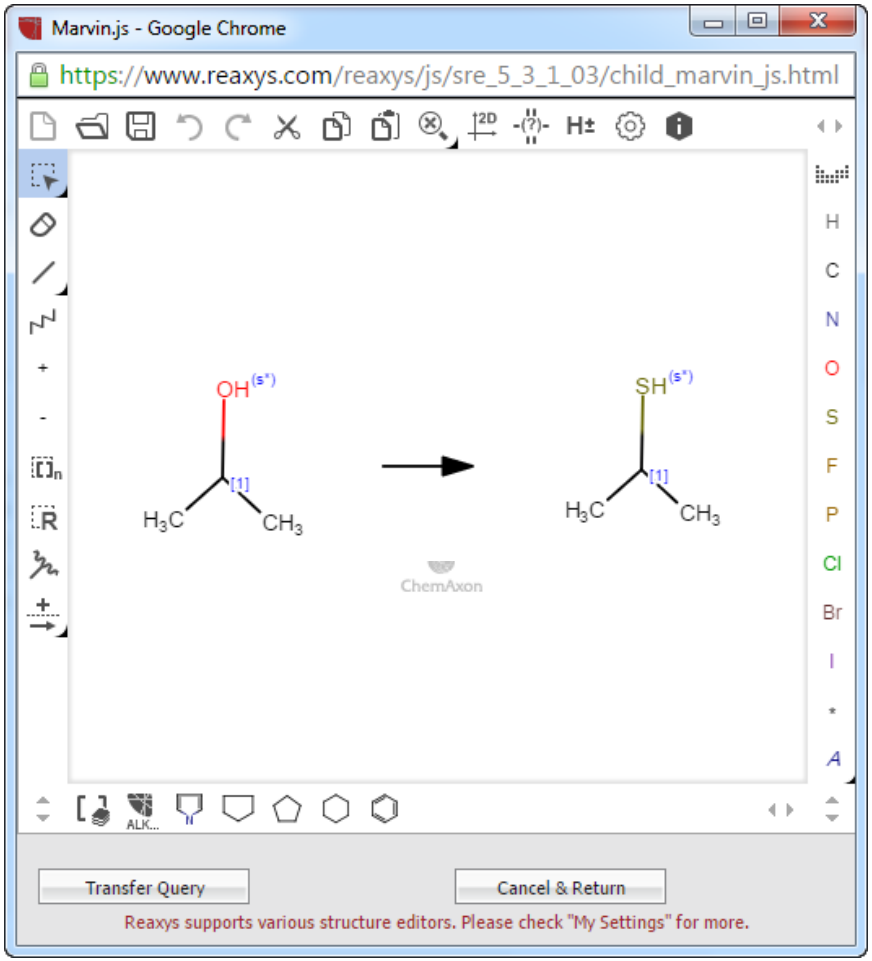
Keywords:
Author: economic optimization; ethylene plant; hydrocarbon pyrolysis; MPC; thermal cracker
Compendex Free Language: Economic optimization; Ethylene plants; hydrocarbon pyrolysis; MPC; Thermal cracker
Compendex Descriptor: Chemical plants; Cracking (chemical); Ethylene; Hydrocarbons; Model predictive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

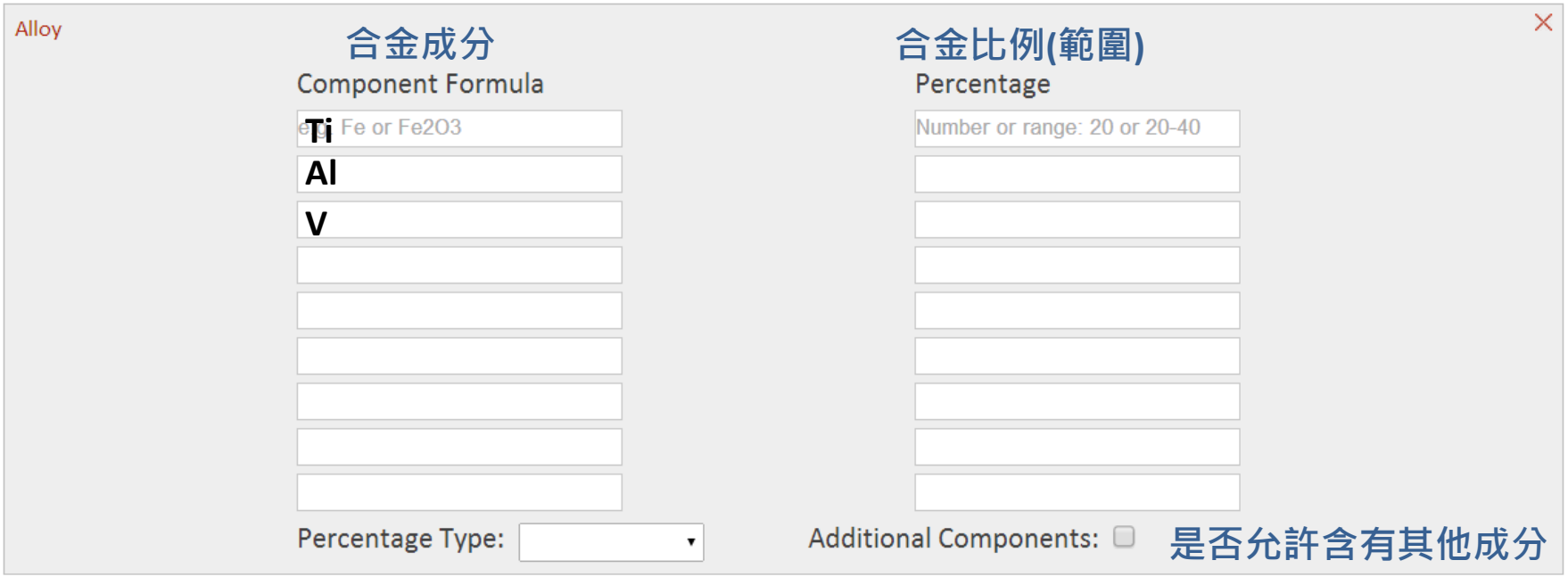


- 豐富的功能協助您搜尋各種衍生物與反應類型
  - 限定特定位置的鍵結、原子、或官能基種類，並具備多種彈性選項
  - R-group 功能
  - Substitution 限定特定原子是否接上官能基或接上鍵結的數量
  - Position variation bond 限定指定鍵結或官能基可能連接的多個位置
- 無須 Java 支援
- 可從 ChemDraw 複製貼上
- 繪製完畢的結構可存成去背圖檔，並可調整檔案大小

線上教學短片
https://www.youtube.com/watch?v=46b3KXG0gxQ

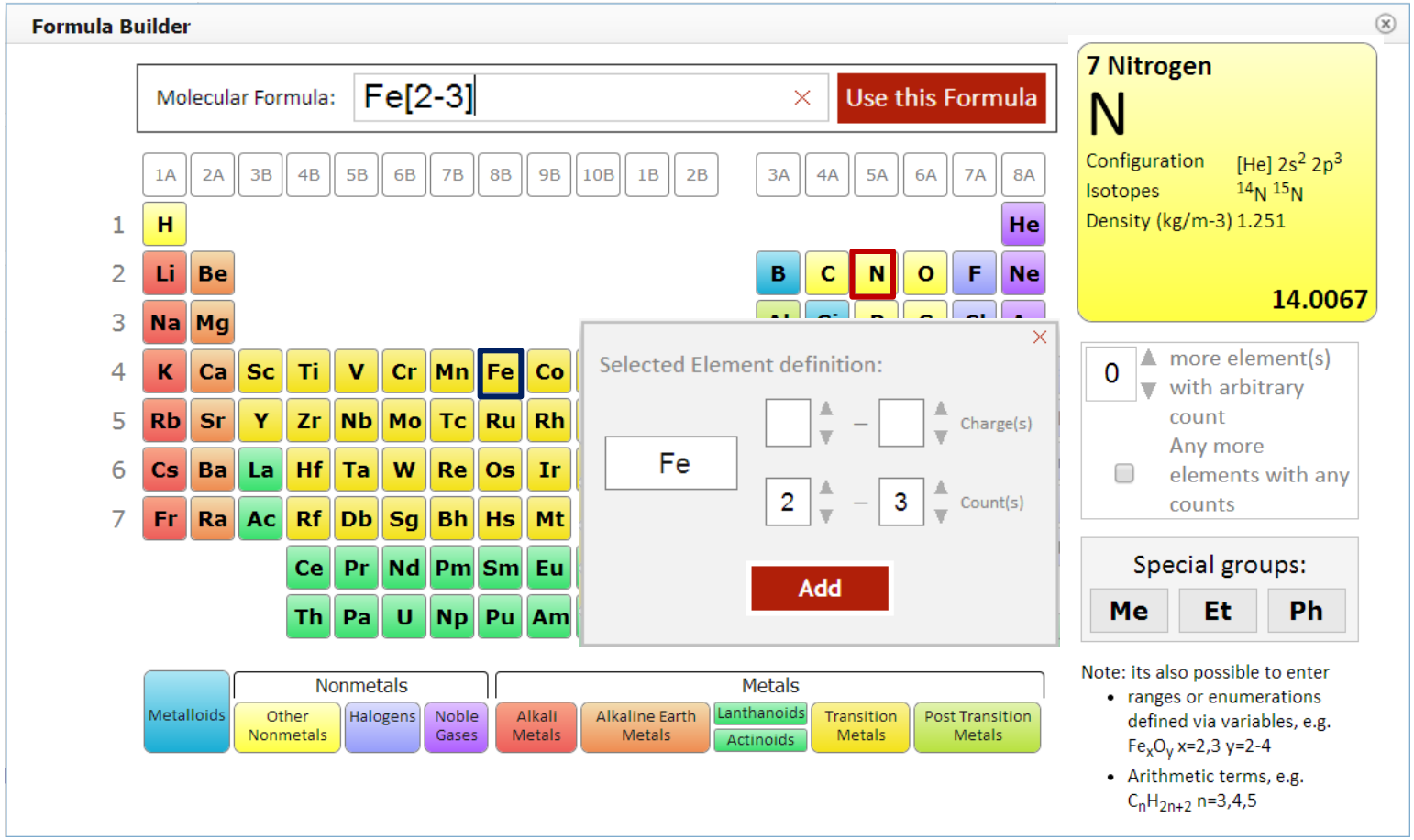
合金搜尋

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(y2o3)/Zirconia Ceramics (ZrO2)



分子式搜尋

不完整分子式，例如只知道包含 34 個碳，輸入 C34*
多種分子數量組合，例如 FexOy, X=2,3 Y=2-4
不同元素比例固定，例如 CnH2n, n=2-4



物化特性搜尋 --

搜尋包含34個碳，旋光度=18.2的所有化合物

搭配分子式搜尋
C34* 表示此分子含有47個碳，其餘未知

Molecular Formula

Molecular Formula C34* Lookup Formula Builder

Physical Data

Optical Rotatory Power (deg) = 18.2

Show AND Buttons

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

Add to Query: Structure Molecular Formula Alloy Add/Remove Fields...

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

PubChem (10 Years)

eMolecules

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

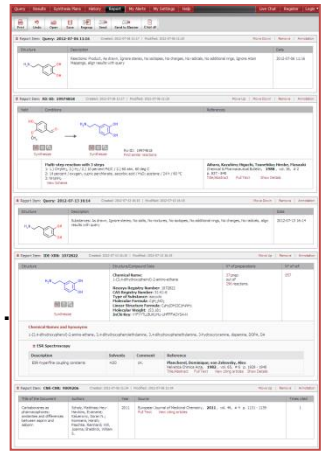
- 彙整各種搜尋結果
- 一鍵 e-mail 分享

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

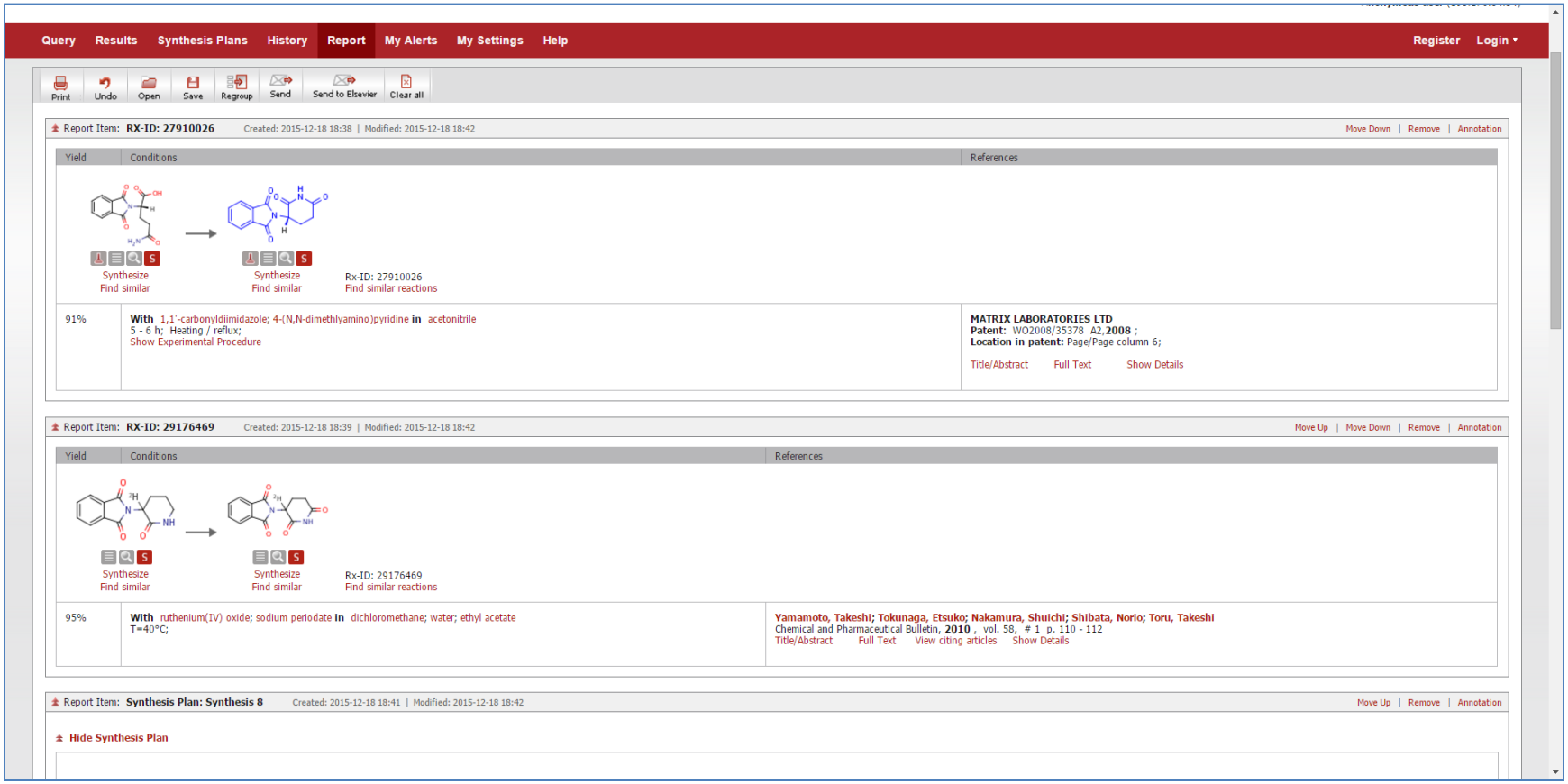
Export

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



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

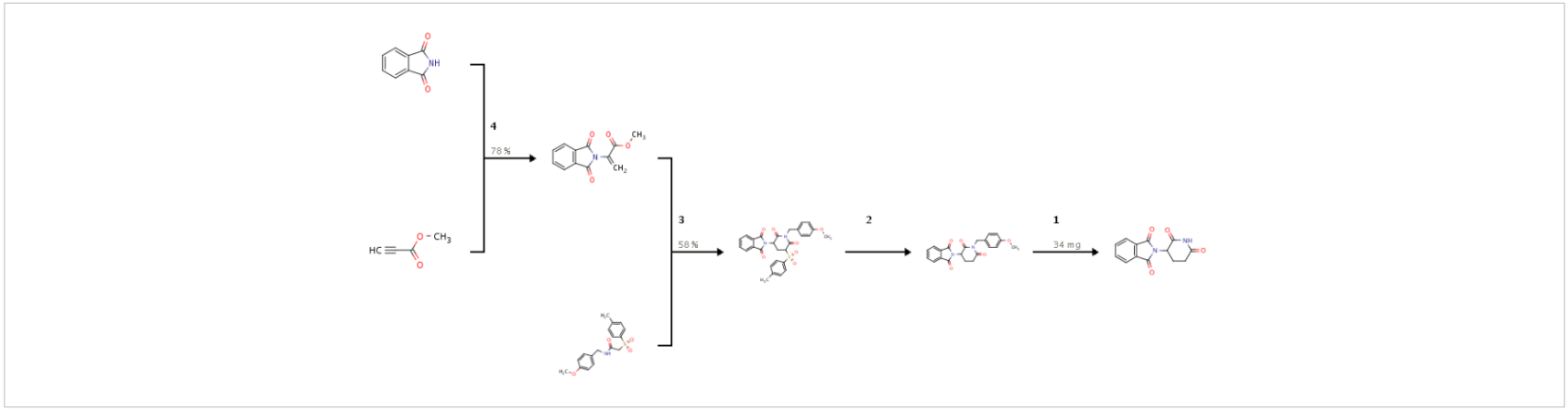


Report – 儲存並分享規劃好的合成路徑

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

點 Report 查看儲存資料

儲存或讀取 XML 檔

直接 E-mail 儲存資料

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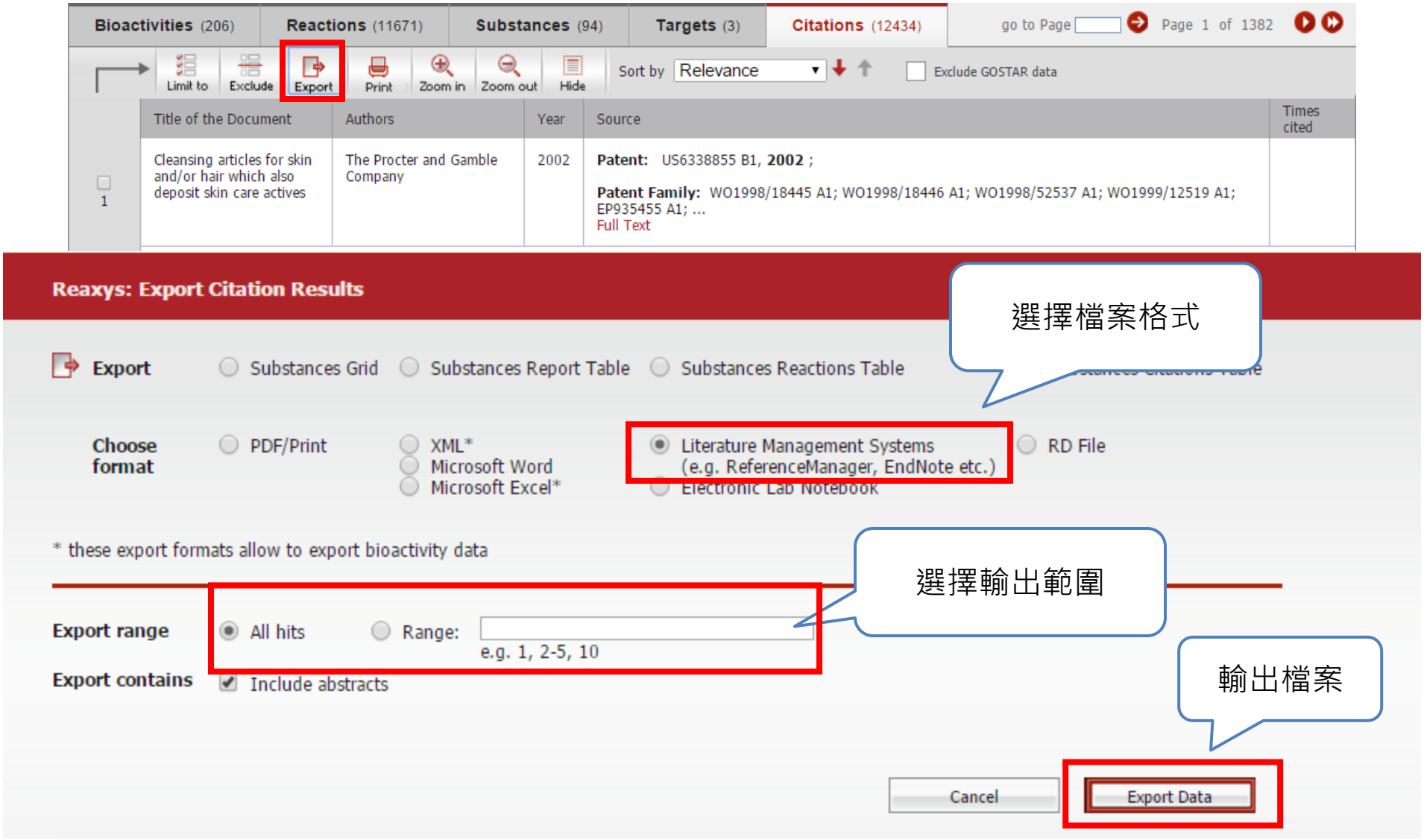
搜尋指令、化合物數據、反應、合成路徑、文獻資料皆可儲存到 Report

Export 輸出搜尋文獻至 EndNote 或 Mendeley



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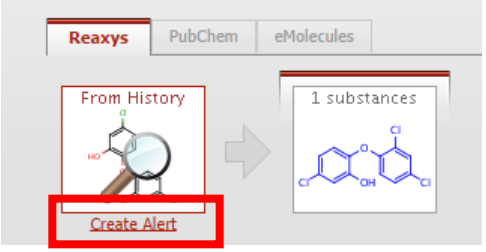
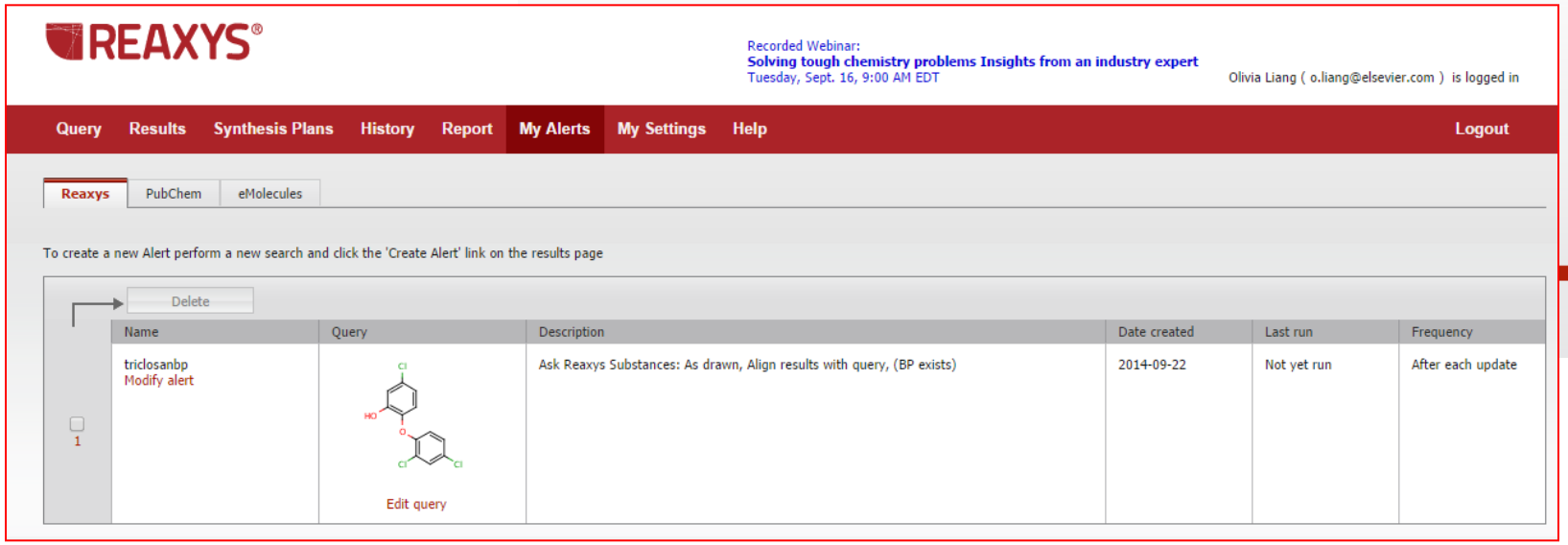
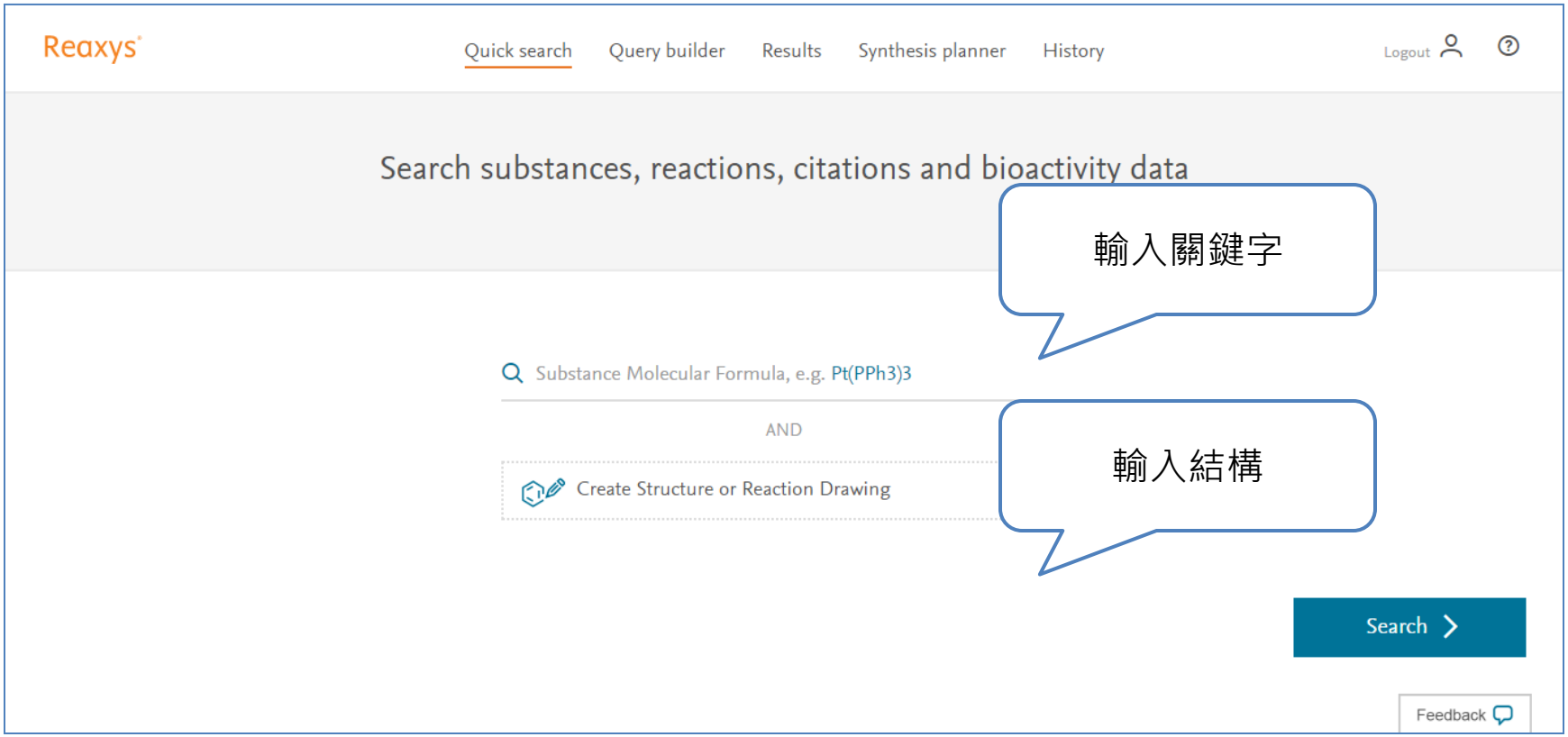




New Reaxys 即將上市

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



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