

網址

www.reaxys.com

REAXYS 教育訓練

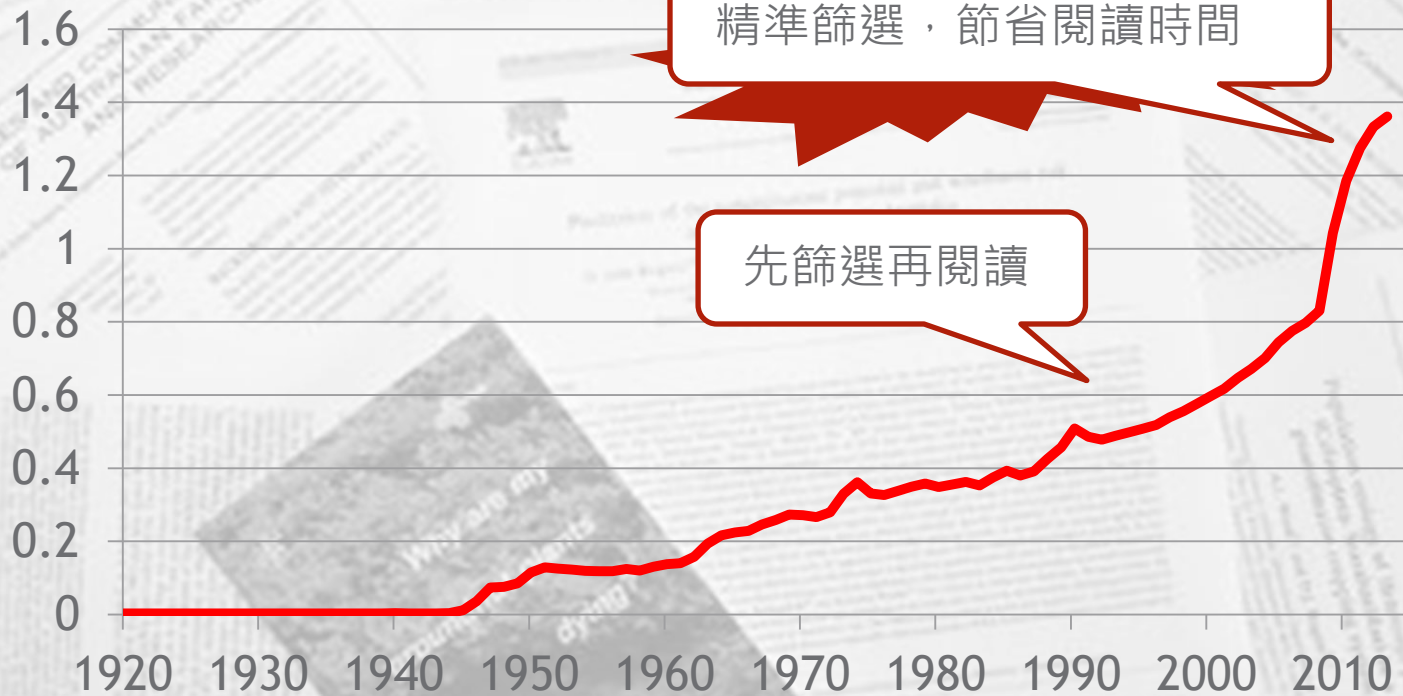
梁成芝

ELSEVIER 生命科學解決方案經理

o.liang@elsevier.com



Millions



精準篩選，節省閱讀時間

先篩選再閱讀

Google

網頁 新聞 圖片 影片 地圖 更多 搜尋工具

約有 1,180,000 項結果 (搜尋時間: 0.27 秒)

相關搜尋: tamiflu仿單 tamiflu副作用

tamiflu 75MG(健保給付) - 【篤實關懷倫理卓越】
www.ktgh.com.tw/Medicament_tbDrug_Look.asp?
 商品名, tamiflu 75MG(健保給付), 藥品許可證, 衛署... 中文名, 克流感... 藥, 健保局藥理類別, 081800 抗濾過性病毒藥, amivir, 外觀描述...

Oseltamivir - Wikipedia, the free encyclopedia
en.wikipedia.org/wiki/Oseltamivir
 Oseltamivir INN /ɒsəlˈtæmɪvɪər/, medication used to prevent and treat

Tamiflu Uses, Dosage & Side Effects
www.drugs.com > Conditions > Infections
 Tamiflu is an antiviral medication used to prevent and treat influenza. Learn about side effects, interactions, and more.

Tamiflu & Relenza: how effective are they?
www.cochrane.org > Features > Reviews
 2014年4月10日 - The BMJ and Cochrane Reviewers have made a new Cochrane Review to review guidance on use of

PubMed
 Search
 Results: 1 to 20 of 3144
 1. **Oseltamivir-resistant influenza A(H3N2) viruses found in Hong Kong associated with permissive mutations, which compensate for fitness impairment and confer resistance.**
 Souza TM, Fintelman-Rodrigues N, Resende M, et al. *J Virol*. 2015 Mar 4; pii: JVI.03513-14. [Epub ahead of print]
 PMID: 25740997 [PubMed - as supplied by publisher] [Related citations](#)

2. **A novel video tracking method to evaluate the effect of influenza infection and antiviral treatment on ferret activity.**
 Oh DY, Barr IG, Hurt AC. *PLoS One*. 2015 Mar 4;10(3):e0118780. doi: 10.1371/journal.pone.0118780. eCollection 2015.
 PMID: 25738900 [PubMed - in process] Free Article [Related citations](#)

3. **Screening of ethnic medicinal plants of South India against influenza (H1N1) and their antioxidant activity.**
 ...

Filters: Manage Filters
 New feature: Try the new Display Settings option - Sort by Relevance
 Results by year: [Bar chart showing results over time]
 Related searches: tamiflu effectiveness, tamiflu prophylaxis, tamiflu influenza, tamiflu renal, tamiflu cochrane
 PMC Images search for tamiflu



Smarter Chemistry



30%
FASTER

23%
LESS COSTLY



ELSEVIER

Reaxys 獨有資料
小分子藥物最大資料庫

搜集大量文獻

節省文獻閱讀時間

摘錄重要資訊

更多搜尋管到
精準找到所需資料

搜尋介面

快速回答問題

 **REAXYS**[®]

HOW YOU THINK HOW YOU WORK

 **REAXYS**[®]

HOW YOU THINK HOW YOU WORK

REAXYS化學資料庫收錄內容

1771 年開始



包含有機、無機、
有機金屬三大領域

資料來自
超過 16000 種期刊
經實驗驗證的數據

三大專利資料庫：
USTPO, EPO, WIPO

Reaxys 資料庫含有：

5,500 萬

個有機、
無機及有機金屬化合物

3,600 萬

個化學反應

5 億

項已出版的
實驗結果

獨特資料來源：

16,000

篇化學相關定期刊物

130

個學科主題—比其他任何研
究解決方案都來得多

超過 **240**

年的化學研究發展時間
(1771 年至今)

REAXYS 資料庫可以找到哪些資訊?

CONTENT: MANY DATABASES ALL IN ONE

文獻資料

A Bibliographic Database

>47 million records
(from ~16,000 journal titles
plus records from key patent
organisations)

A Substance Database

> 83 million substances
(total)
~ 60 million substances
(unique)

Reaxys
2014

化合物

- 物化特性
- 實驗數據

化學反應

- 反應式
- 反應條件
- 合成路徑

A Chemical Reaction Database

> 37 million single- and
multi-step reactions

A Property Database

> 500 million experimental
properties
in > 400 fields
in > 130 subject areas

> 400 個欄位可獨立或合併搜尋

REAXYS 搜尋流程

建立搜尋指令



結果呈現方式



篩選分析



• Ask Reaxys: 關鍵字智慧搜尋

- Structure: 結構
- Formula: 分子式
- Alloy: 合金
- Fields: 欄位
- Reaxys Tree: 群組搜尋

- Reaction: 反應
- Substance: 化合物
- Literature: 文獻

- Analysis View: 視覺化分析系統
- Filter: 篩選搜尋結果
- AutoPlan: 規畫合成路徑

個人化功能

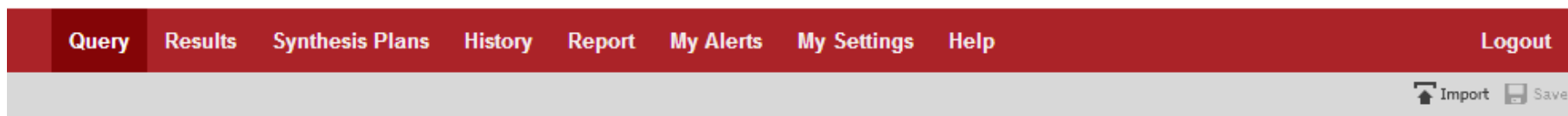
- Report: 輸出報告
- History: 搜尋紀錄
- My Alerts: 新知通報
- My Settings: 個人化設定

SEARCH IN REAXYS

discover

REAXYS 首頁

REAXYS化學資料庫使用介面簡單且不受使用人數限制！



Ask Reaxys

NEW 智慧型搜尋欄位 (使用關鍵字)

Find substances, reactions, bioactivity data, citations, patents, and more from Reaxys, PubChem, and eMolecules

<p>Reactions</p> <p>反應搜尋</p>	<p>Substances, Names, Formulas</p> <p>化合物搜尋</p>	<p>Literature</p> <p>文獻搜尋</p>	<p>ReaxysTree BETA</p> <p>NEW Reaxys 索引詞彙 (可做群組搜尋)</p>
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You can also search directly by these common property groups:

<p>Physical</p>	<p>Spectra</p>	<p>Natural Product</p>	<p>Advanced</p>
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附加搜尋條件設定

進階搜尋

REAXYS 化合物搜尋結果畫面

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

Reaxys PubChem eMolecules

From History 45 substances 67 targets 137 citations

Create Alert No structure No structure

open Analysis view

整合文獻數量 &連結

45 substances out of 380 reactions and 2833 bioactivities and 77 targets and 323 citations

Filter by: Sub-structure Molecular Weight Number of Fragments

Heatmap Reactions Substances (Grid) **Substances (Report)** Targets Citations go to Page Page 1 of 5

Open Autoplan

Condition Selection

條件篩選

Mass Spectrometry (17)

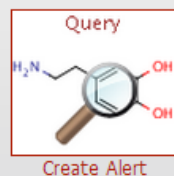
Description	Peak	Location	Comment	Reference
		Paragraph 0124		SHANGHAI INSTITUTE OF ORGANIC CHEMISTRY, CHINESE ACADEMY OF SCIENCES; LIANHE CHEMICAL TECHNOLOGY CO., L Qianghui Patent: US2014/221662 A1, 2014 ; Title/Abstract Full Text Show Details
Electrospray ionisation spectrum				Hu, Zhe-Yi; Boucher, Bradley A.; Laizure, S. Casey; Herring, Vanessa L.; Parker, Robert B.; Hickerson, William L. Journal of Mass Spectrometry, 2013, vol. 48, # 8 p. 945 - 950 Title/Abstract Full Text View citing articles Show Details
Spectrum		supporting information		Kongkamnerd, Jarinrat; Cappelletti, Luca; Prandi, Adolfo; Seneci, Pierfausto; Rungrotmongkol, Thanyada; Jongaroonngamsan, Cattoli, Giovanni; Terregino, Calogero; Capua, Iliaria; Beneduce, Luca; Gallotta, Andrea; Pengo, Paolo; Fassina, Giorgio; Miertus Bioorganic and Medicinal Chemistry, 2012, vol. 20, # 6 p. 2152 - 2157 Title/Abstract Full Text View citing articles Show Details
APCI (atmospheric pressure chemical ionization) spectrum		supporting information		Chuanopparat, Nutthawat; Kongkathip, Ngampong; Kongkathip, Boonsong Tetrahedron Letters, 2012, vol. 53, # 46 p. 6209 - 6211,3 Title/Abstract Full Text Show Details
high resolution mass spectrometry (HRMS) electrospray ionisation (ESI) time-of-flight mass spectra (TOFMS) spectrum		supporting information		Chuanopparat, Nutthawat; Kongkathip, Ngampong; Kongkathip, Boonsong Tetrahedron Letters, 2012, vol. 53, # 46 p. 6209 - 6211,3 Title/Abstract Full Text Show Details
HRMS (High resolution mass spectrometry) ESI (Electrospray ionisation)	335.1941 m/z	Page/Page column 33; 42	Molecular peak	Tokyo University Of Science Educational F Patent: EP2301911 A1, 2011 ; Title/Abstract Full Text Show Det
ESI (Electrospray				Ishikawa, Hayato; Bondzic, Bojan P.; Hay

點擊連結查看詳細資料

REAXYS® HOW YOU THINK HOW YOU WORK

反應搜尋結果畫面

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



127 reactions

Open Analysis View

127 reactions out of 154 substances and 90 citations

- ### Filters
- Filter by:
- Sub-structure
 - Yield
 - Record Type
 - Reagent/Catalyst
 - Solvent
 - Reaction Type
 - No. of Steps
 - Product Availability
 - Reactant Availability
 - Availability in other DBs
 - Molecular Weight
 - Number of Fragments
 - Physical Data
 - Spectroscopic Data
 - Bioactivity
 - Ecological Data
 - Natural Product
 - Availability
 - Availability in other DBs

Reactions Substances (Grid) Substances (Table) Citations go to Page 1 of 15

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

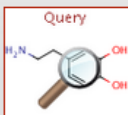
Yield	Conditions	References
99%	With hydrogenchloride; hydrogen; palladium on activated charcoal in ethanol P=760 Torr; 24 h; Ambient temperature;	Kohno; Murahashi; Sasao Bulletin of the Chemical Society of Japan, 1990, vol. 63, # 4 p. 1252 - 1254 Title/Abstract Full Text View citing articles Show Details

產率 99%

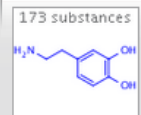
反應條件 With hydrogenchloride; hydrogen; palladium on activated charcoal in ethanol P=760 Torr; 24 h; Ambient temperature;

文獻來源出處
Kohno; Murahashi; Sasao
Bulletin of the Chemical Society of Japan, 1990, vol. 63, # 4 p. 1252 - 1254
Title/Abstract
Full Text View citing articles Show Details

Reaxys PubChem eMolecules



Create Alert



Show Query

Open Analysis View

173 substances out of 1150 reactions and 4219 bioactivities and 542 targets and 2183 citations

Filter by:

- Substructure
- Molecular Weight
- Number of Fragments
- Physical Data
- Spectroscopic Data
- Ecological Data
- Natural Product
- Availability
- Availability in other DBs
- LogP
- H Bond Donor (HBD)
- H Bond Acceptor (HBA)
- Polar surface Area (PSA)
- Highest clinical phase
- Yield
- Record Type
- Reagent/Catalyst
- Solvent
- Reaction Type
- No. of Steps
- Product Availability
- Reactant Availability
- Availability in other DBs

Heatmap	Reactions	Substances (Grid)	Substances (Report)	Targets	Citations
go to Page <input type="text"/> Page 1 of 243					
<div style="display: flex; justify-content: space-between;"> <div> <p>Limit to Exclude Export Print Zoom in Zoom out Hide</p> </div> <div>Sort by Relevance</div> </div>					
	Title of the Document	Authors	Year	Source	Times cited
<input type="checkbox"/> 1		Culvenor,C.C.J.; Ham,N.S.	1974	Australian Journal of Chemistry, 1974 , vol. 27, p. 2191 - 2198 Full Text	
<p> Show All Substances (26) Hit Substances in this article (1 out of 26) </p>					
<input type="checkbox"/> 2	2-Amino-1,2,3,4-tetrahydronaphthalene derivatives with cardiovascular activity. 標題	CHIESI FARMACEUTICI S.p.A.	1991	Patent: EP405344 A2, 1991 ; Patent Family: EP405344 A2; EP405344 B1; Full Text	引用次數
<p> Title/Abstract Front page Information Show All Reactions (7) Show All Targets Show All Substances (26) Hit Substances in this article (1 out of 26) </p>					
<input type="checkbox"/> 3	Substituted aryl and aralkyl amides in the treatment of parkinsonism	Schering Corporation	1976	Patent: U53944675 A1, 1976 ; Patent Family: U53944675 A1; U54053509 A1; Full Text	
<p> Title/Abstract Front page Information Show All Reactions (23) Show All Substances (50) Hit Substances in this article (1 out of 50) </p>					


列出文獻中所有化合物結構、反應式、專利資訊及相關連結

Ask Reaxys 實際範例

Ask Reaxys

Enter a keyword, concept or author

Go

 Examples

Substances

Substance name

"Atenolol" Substance name will be translated into a structure and searched

 Try it

CAS-NO

"102625-70-7" CAS-NO will be looked up and searched on success

 Try it

Molecular Formula

"Pt(PPh₃)₃" Molecular Formula will be searched as formula

 Try it

Substance Properties

MELTING POINT

"melting point of xylitol" "Xylitol" will be translated into a structure and combined with a search for any melting point data

 Try it

SOLUBILITY

"solubility of vitamin D3" "Vitamin D3" will be translated into a structure and combined with a search for any solubility data

 Try it

FERROELECTRICITY

"ferroelectric materials" Substances with ferroelectric data will be searched

 Try it

Reactions

SYNTHESIS

"preparation of porphyrine" Reactions with porphyrine (structured) as product will be searched

 Try it

REACTION TYPE

"phosphorylation" Reactions with reaction type phosphorylation will be searched

 Try it

NAMED REACTION

"Suzuki coupling" Reactions with reaction type Suzuki coupling will be searched

 Try it

實例說明 1

DOPAMINE 合成方法

Ask Reaxys



dopamine synthesis

Go

Open Analysis View

127 reactions out of 4358 bioactivities and 154 substances and 576 targets and 90 citations

Filter by:

- Sub-structure
- Yield
- Record Type
- Reagent/Catalyst
- Solvent
- Reaction Type
- No. of Steps
- Product Availability
- Reactant Availability
- Availability in other DBs
- Targets
- Target Species
- Cells Lines
- Effect
- Parameters
- pX(-log(Affinity))
- Molecular Weight
- Number of Fragments
- Physical Data

Heatmap Reactions Substances (Grid) Substances (Report) Targets Citations

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

Yield	Conditions	References
<input type="checkbox"/> 1	 Synthesize	Rx-ID: 2154254 Find similar reactions
99%	With hydrogenchloride; hydrogen; palladium on activated charcoal in ethanol P=760 Torr; 24 h; Ambient temperature;	Kohno; Sasao; Murahashi Bulletin of the Chemical Society of Japan, 1990 , vol. 63, # 4 p. 1252 - 1254 Title/Abstract Full Text View citing articles Show Details
<input type="checkbox"/> 2	 Synthesize	Rx-ID: 336756 Find similar reactions
82%	With pyridoxal 5'-phosphate; aromatic L-amino acid decarboxylase in various solvent(s)	Nakazawa Hidetsugu; Sano Kenzoku; Matsuda Keizo

實例說明2

TRICLOSAN, BOILING POINT

Ask Reaxys



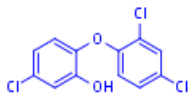
Triclosan, boiling point

Go

1 substances out of 217 reactions and 1137 bioactivities and 48 targets and 577 citations

Heatmap Reactions Substances (Grid) **Substances (Report)** Targets Citations go to Page Page 1 of 1

Limit to Exclude Output Print Zoom in Zoom out Hide Sort by No of References

Structure	Structure/Compound Data	N° of preparations All Preps All Reactions	Available Data	Target	N° of ref.
 Synthesize Hide Details	Chemical Name: 2,4,4'-trichloro-2'-hydroxydiphenyl ether Reaxys Registry Number: 2057142 CAS Registry Number: 3380-34-5 Type of Substance: isocyclic Molecular Formula: C ₁₂ H ₇ Cl ₃ O ₂ Linear Structure Formula: C ₁₂ H ₇ Cl ₃ O ₂ Molecular Weight: 289.545 InChI Key: XEFQLINVKFYRCS-UHFFFAOYSA-N Highest Clinical Phase: Marketed	7 prep out of 217 reactions.	Hit Data (1) Druglikeness Bioactivity Identification Physical Data (78) Spectra (20) Ecological Data (146) Use/Application (443)	Show Targets	577

Chemical Names and Synonyms

2,4,4'-trichloro-2'-hydroxydiphenyl ether, Triclosan, 5-chloro-2-(2,4-dichlorophenoxy)-phenol, 5-chloro-2-(2,4-dichlorophenoxy)phenol, Irgasan DP 300, irgason DP 300, Irgasan®

Hit Data

Boiling Point (1 Hits out of 1 view all)

Boiling Point	Location	Reference
120 °C	Paragraph 0029	MOLECULAR EXPRESS, INC.; FUJII, Gary; CHIANG, Su-ming; SRIVASTAVA, Runjhun; FUJII, Alison; NEEDHAM, David Patent: WO2013/43830 A1, 2013 ; Title/Abstract Full Text Show Details

Ask Reaxys

智慧辨認輸入的關鍵字

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

Import Save

Ask Reaxys - Analysis

Reaxys found several possibilities to answer your query. Please select from the list:

Suggested Query	Results	Select Action
<p>superconductors 2013</p> <p>Result: citations Show query</p>	2085 citations in Reaxys	<p>Search</p> <p>Edit query in Advanced</p>
<p>superconductors 2013</p> <p>Result: citations Show query</p>	123 citations in Reaxys	<p>Search</p> <p>Edit query in Advanced</p>

Legend: Bibliography Compound Concept Date Keyword Bioactivity Ignored

Cancel

You can also search directly by these common property groups:

Physical Spectra Natural Product Advanced

REAXYS 搜尋介面

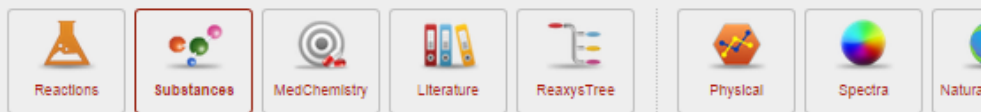


Recorded Webinar:
Solving tough chemistry problems In
Tuesday, Sept. 16, 9:00 AM EDT

Query Results Synthesis Plans History Report My Alerts My Settings Help

Start Over

Ask Reaxys BETA Enter a keyword, concept or author



Structure

selected query editor:
 MarvinSketch
by ChemAxon

As drawn
 Substructure
 on heteroatoms
 on all atoms
 Similarity

Include tautomers
 Ignore stereo
 No salts
 No mixtures
 No isotopes
 No charges
 No radicals
 No ring closures
 Align results with query

More options

Identification

Identificat

Show AND But

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

Please enter a chemical identifier and then click "Submit"

is

Chemical Name: aspirin
InChI-Key: BSYNRYMUTXBXSQ-UHFFFAOYSA-N
CAS-No: 50-78-2
Smiles: CC(=O)OC1=C(C=CC=C1)C(O)=O

MarvinSketch (ChemAxon) - Internet Explorer provided by Reed Els...

https://www.reaxys.com/reaxys/js/sre_5_1_1_03/child_java.jsp

File Edit View Insert Options Object Templates Chemistry Calculations Help

Transfer Query

Reaxys supports various structure editors. Please check "My Settings" for more.

Internet | Protected Mode: On 100%

繪圖軟體 - MARVINSKETCH

MarvinSketch (ChemAxon) - Google Chrome

https://www.reaxys.com/reax

File Edit View Insert Options Object

Synthesize | Show Details

- A Any atom except H (A)
- AH Any atom including H (AH)
- Q Hetero atom (Q)
- QH Any atom except C (QH)
- M Any metal (M)
- MH Any metal or H (MH)
- X Any halogen (X)
- XH Any halogen or H (XH)
- G Any group (G)
- GH Any group or hydrogen (GH)
- G* Any group; ring closure between g
- GH* Any group or hydrogen; ring closure

Transfer Query

Reaxys Generics

Atom Generics: A, AH, Q, QH, M, MH, X, XH

Group Generics: G, GH, G*, GH*

Reaxys Generics

Acyclic: ACY, ACH

Cyclic: CYC, CYH

Carbocyclic: ABC, ABH, CBC, CBH

Hetero acyclic: AHC, AHH

Heterocyclic: CHC, CHH

No carbon: CXX, CXH

Alkynyl: AVL, AYH

Alkoxy: AOX, AOH

Aryl: ARY, ARH

Cycloalkyl: CAL, CAH

Cycloalkenyl: CEL, CEH

Hetero aryl: HAR, HAH

Close

Template Library Manager

NoClean 2D 3D

Template categories:

- Generic
- Rings
- Amino Acids
- Aromatics
- Bicyclics
- Bridged Polycyclics
- Crown Ethers
- Cycloalkanes
- Heterocycles
- Polycyclics
- Homology Groups
- Alpha D sugars
- Beta D sugars
- Deoxynucleosides

1: Adamantane 2: Cubane 3: Prismane 4: Twistane

Template Library

Templates Properties

Close

Reaxys supports various structure editors. Please check "My Settings" for more.

註:需JAVA支援

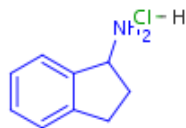
繪圖軟體 - MARVINSKETCH

MARVINSKETCH

MarvinSketch (ChemAxon) - Google Chrome

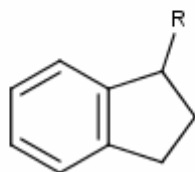
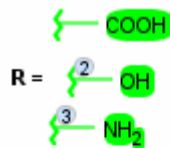
<https://www.reaxys.com/reaxys/>

File Edit View Insert Options Object T



Synthesize | Show Details

Periodic System



4

Synthesize

Druglikeness
Bioactivity
Identification
Physical Data (57)
Spectra (42)

Show targets

7

Synthesize

Druglikeness
Bioactivity
Identification
Physical Data (31)
Spectra (29)

Show targets

Synthesize | Show Details

MarvinSketch (ChemAxon) - Google Chrome

https://beta.reaxys.com/reaxys/js/sre_5_1_1_03/child_java.jsp

File Edit View Insert Options Object Templates Chemistry Calculations Help

Template Library... Ctrl-T

Bond

Insertion Arrow

IUPAC Name

noethyl)benzene-1,2-diol

Transfer Query Cancel & Return

Reaxys supports various structure editors. Please check "My Settings" for more.

Transfer Query

Cancel & Return

Reaxys supports various structu... check "My Settings" for more.


註:需JAVA支援

衍生物搜尋

REAXYS 可以針對您的需求，搜尋各式各樣的衍生物

Structure

selected query editor:



PASTE STRUCTURE EDITOR

Create Structure Template from Name

和畫好的結構相同

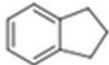
- As drawn
- Substructure **衍生物**
 - on heteroatoms
 - on all atoms
- Similarity **相似結構**

- Include tautomers
- Ignore stereo
- No isotopes
- No charges
- No radicals
- No ring closures
- Ignore atom mappings
- Align results with query
- Keep fragments
 - separate together

→ 其他條件

Reaxys: Find Similar Compounds...

Click on one of the hyperlinks below for getting similar compounds according to the selected scope:

Query Structure	Position/Stereo Isomers	Near	Medium	Wide	Widest
	3	62039	155383	155383	155383

Cancel

Fe2O3
Fe3O4
AlGaO

建立搜尋指令-分子式

Molecular Formula

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

Formula Builder

Molecular Formula: Use this Formula

	1A	2A	3B	4B	5B	6B	7B	8B	9B	10B	1B	2B	3A	4A	5A	6A	7A	8A	
1	H																	He	
2	Li	Be											B	C	N	O	F	Ne	
3	Na	Mg																	
4	K	Ca	Sc	Ti	V	Cr	Mn	Fe	Co										
5	Rb	Sr	Y	Zr	Nb	Mo	Tc	Ru	Rh										
6	Cs	Ba	La	Hf	Ta	W	Re	Os	Ir										
7	Fr	Ra	Ac	Rf	Db	Sg	Bh	Hs	Mt										
			Ce	Pr	Nd	Pm	Sm	Eu											
			Th	Pa	U	Np	Pu	Am											

Selected Element definition:

- Charge(s)

- Count(s)

Add

7 Nitrogen

N

Configuration [He] 2s² 2p³
Isotopes ¹⁴N ¹⁵N
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

Metalloids	Nonmetals			Metals					
	Other Nonmetals	Halogens	Noble Gases	Alkali Metals	Alkaline Earth Metals	Lanthanoids	Actinoids	Transition Metals	Post Transition Metals

將滑鼠移到元素上方即可預覽該元素詳細資訊

影片介紹



Query Builder

建立搜尋指令-合金 Alloy

Ti-6Al-4V
yttria/zirconia ceramics

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

Alloy

合金成分

Component Formula

Y2O3 example: Fe2O3

ZrO2

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

或者您也可以使用Advanced Search

欄位搜尋

欄位搜尋：輸入想要搜尋的欄位，如：Chromatographic data 或 Natural Product

The screenshot displays the Reaxys search interface. At the top, there are eight category icons: Reactions, Substances, Literature, ReaxysTree, Physical, Spectra, Natural Product, and Advanced. The 'Natural Product' icon is highlighted with a red box. Below the icons, the 'Natural Product' section is active, showing search criteria for 'Isolation from Natural Product' with a dropdown menu set to 'is'. Below this, there are several search criteria for 'Description' with dropdown menus set to 'is'. A 'Show AND Buttons' link is visible. On the right, a 'Select index items and click 'Transfer'' window is open, showing a search for 'Reaxys' and a list of results including 'abstract report (48569)', 'article (35372013)', 'book (18222)', 'book review / secondary ref. (259142)', 'business article (45068)', 'conference paper (5689915)', 'conference review (64262)', 'editorial (620627)', 'erratum (182766)', 'letter (917475)', 'note (856549)', 'patent (928761)', 'report (13986)', 'review (2426503)', and 'short survey (437392)'. The 'Transfer' button is highlighted in red. At the bottom, there is a 'Search Reactions' button and a bar with 'Add to Query:' and 'Add/Remove Fields...' options.

新增欄位 Fields

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

Insert/Remove Properties ✕

Define the "Literature" query layout

Find any property RESET

- Reaxys
 - Identification
 - Physical Data
 - Spectra
 - Bioactivity
 - Ecological Data
 - Use/Application
 - Natural Product
 - Isolation from Natural Product exists
 - Isolation from Natural Product (INP.INP)
 - Quantum Chemical Data
 - Reaction Data

直接點選

Document Type (in Reaxys)

Authors (in Reaxys)

Common Patent Number(in Reaxys)

Patent Country Code (in Reaxys)

Journal Title (in Reaxys)

Publication Year (in Reaxys)

DOI (in Reaxys)

Title (in Reaxys)

Abstract (in Reaxys)

Keywords (in Reaxys)

Citation Basic Index (in Reaxys)

Add >>

Remove

Remove all

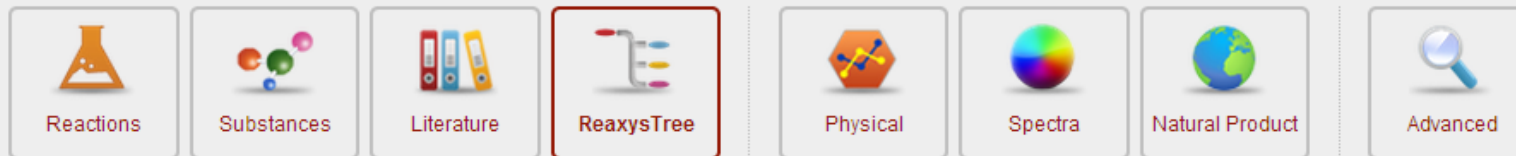
Add Defaults

Available to add Already selected Searches in multiple databases

Save

REAXYS TREE

POLYCONDENSATION



Browse Literature

Look through the Reaxys data by browsing its hierarchy of entities and properties. Select items and click Search, or click any term for immediate results.

A screenshot of the Reaxys search interface. At the top, a search bar contains the text "polycondensation" and a "SEARCH" button. Below the search bar are three links: "Reset", "Select All Highlighted", and "Deselect All". The main area displays a tree view of search results. The root node is "ReaxysTree" (folder icon). It has a sub-node "chemical transformations" (folder icon) with the description "(chemical reaction classification, chemical reaction classifications, chemical transformation, ...)". Under "chemical transformations" is "chemical reaction class" (folder icon) with the description "(chemical reaction type, Reaction Class, Reaction classification, reaction classifications, re...)". Under "chemical reaction class" is "condensation reaction" (folder icon) with the description "(condensation reactions)". Under "condensation reaction" is "polycondensation" (document icon) with the description "(polycondensations)". The "polycondensation" item is selected, indicated by a checked checkbox and a red border around its label and description.

Clear Query

Search Literature

按下 Search

REAXYS 搜尋流程

建立搜尋指令



結果呈現方式



篩選分析



• Ask Reaxys: 關鍵字智慧搜尋

- Structure: 結構
- Formula: 分子式
- Alloy: 合金
- Fields: 欄位
- Reaxys Tree: 群組搜尋

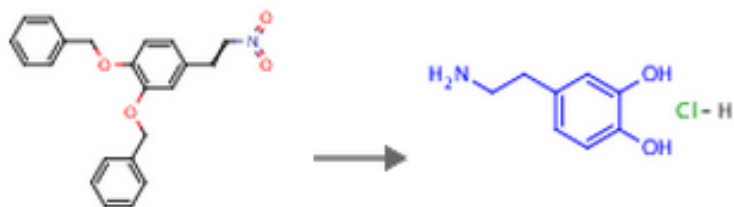
- Reaction: 反應
- Substance: 化合物
- Literature: 文獻

- Analysis View: 視覺化分析系統
- Filter: 篩選搜尋結果
- AutoPlan: 規畫合成路徑

個人化功能

- Report: 輸出報告
- History: 搜尋紀錄
- My Alerts: 新知通報
- My Settings: 個人化設定

建立合成計畫 Synthesis Plans



Synthesize

Synthesize

Rx-ID: 2154254
Find similar reactions

- Manually
- by Autoplan
- by Autoplan (with options)

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

Synthesis 1 x Synthesis 2 x Synthesis 3 x Synthesis 4 x

New Undo Open Save Rename Duplicate Output Print Left Right Top Resize Thumbnail Report Show

Synthesize (7)

- Manually
- by Query
- by Autoplan
- by Autoplan (with options)

Hide selected details Hide all details Show all details

Step	Yield	Conditions	References
1 Reaxys	100%	With methanol; chloro-trimethyl-silane 3 h; Reflux;	Barontini, Maurizio; Bernini, Roberta; Crisante, Fernanda; Fabrizi, Giancarlo Synthesis, 2009, # 22 art. no. P0940955, p. 3838 - 3842 Title/Abstract Full Text View citing articles Show Details

建立合成計畫 manually

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

Synthesis 1 ✕ Synthesis 2 ✕ Synthesis 3 ✕ Synthesis 4 ✕ Synthesis 5 ✕

New Undo Open Save Rename Duplicate Output Print Left Right Top Resize Thumbnail Report

Synthesize (27)

Synthesize (158)

2 Details

Add Remove

1 Details

Add Remove

99 %

Available through...

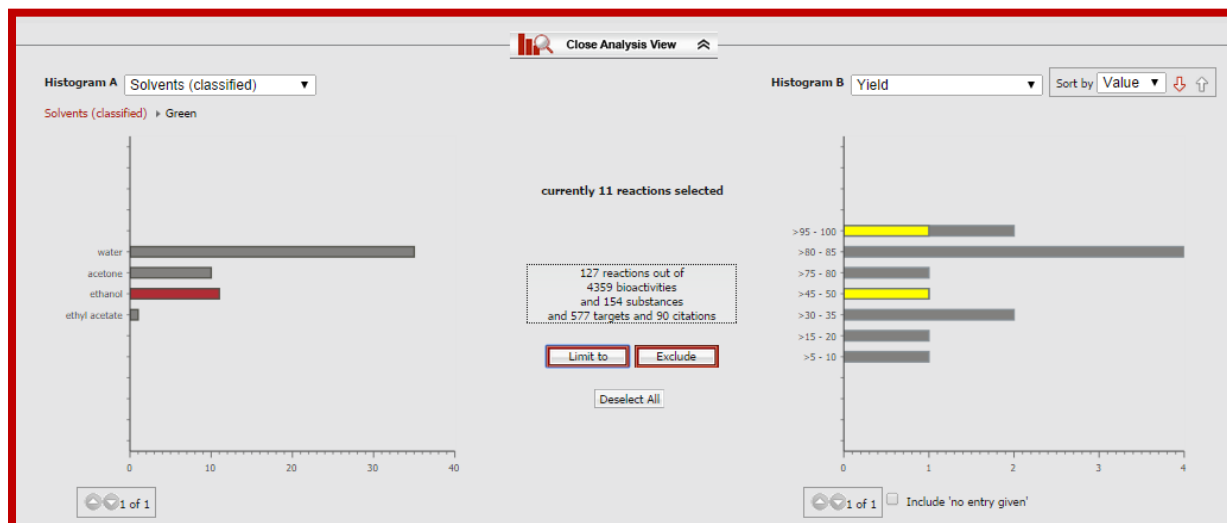
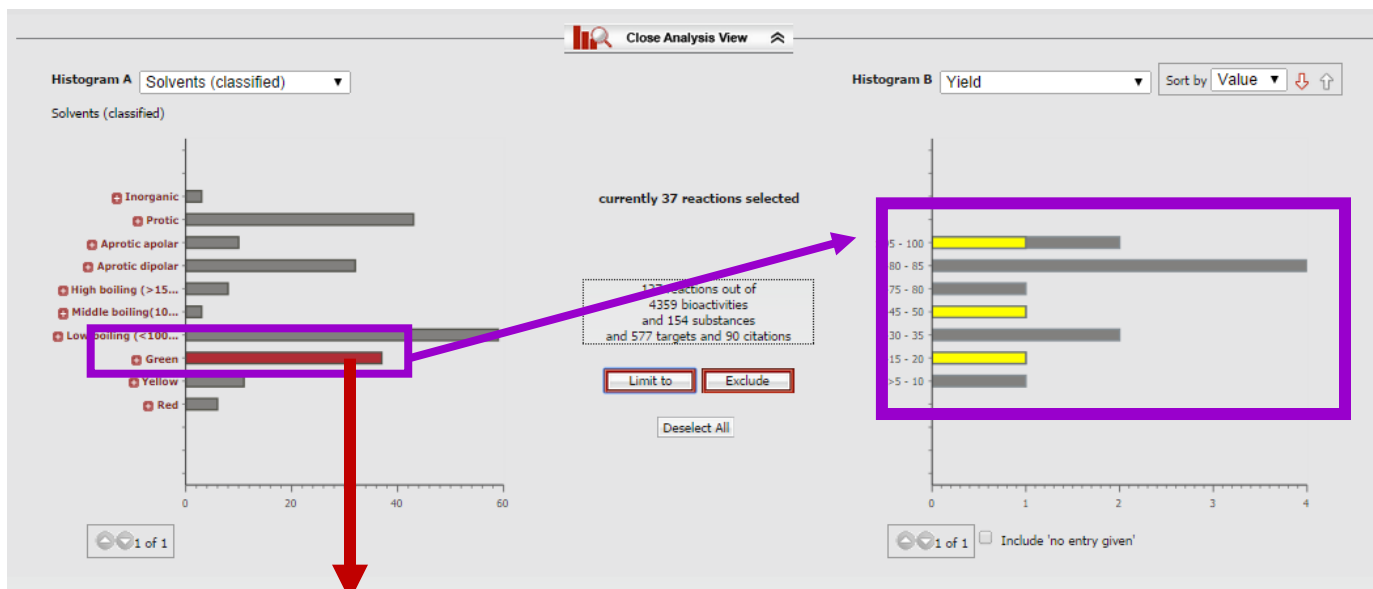
- Accelrys' ACD
- eMolecules
- CambridgeSoft ACX
- PharmaPendium

Safety Data...

Reaxys-RN: 3656720
MF: C8H12NO2*Cl
MW: 189.642
CAS-RN: 62-31-7
[Show Details](#)

Copy Structure to Clipboard
 Copy Structure to Query
 Use as Sub-structure Filter
 Copy Reaction to Query

視覺化分析工具 -- Analysis View



多樣化結果輸出功能 - ENHANCED REPORT

搜尋紀錄輸出

反應搜尋結果輸出

化合物搜尋結果輸出

文獻搜尋結果輸出

輸出結果

The screenshot displays the REAXYS interface with several report items, each highlighted by a colored box and an arrow pointing to a label:

- Report Item: Query: 2012-07-06 11:16** (Blue box): Shows a table with columns for Structure, Description, and Date. The structure is 3,4-dihydroxyphenylethylamine.
- Report Item: RX-ID: 19974818** (Purple box): Shows a reaction scheme for the synthesis of 3,4-dihydroxyphenylethylamine from 3,4-dihydroxybenzaldehyde. It includes reaction conditions and a reference to Aihara et al. (1988).
- Report Item: Query: 2012-07-13 16:14** (Red box): Shows a table with columns for Structure, Description, and Date. The structure is 3,4-dihydroxyphenylethylamine.
- Report Item: IDE-XRN: 1072822** (Red box): Shows a table with columns for Structure, Structure/Compound Data, N° of preparations, and N° of ref. It includes chemical name, CAS number, and molecular formula.
- Report Item: CNR-CNR: 9009206** (Green box): Shows a table with columns for Title of the Document, Authors, Year, Source, and Times cited. It lists a document about carbaboranes as pharmacophores.

REAXYS 搜尋流程

建立搜尋指令



結果呈現方式



篩選分析



• Ask Reaxys: 關鍵字智慧搜尋

- Structure: 結構
- Formula: 分子式
- Alloy: 合金
- Fields: 欄位
- Reaxys Tree: 群組搜尋

- Reaction: 反應
- Substance: 化合物
- Literature: 文獻

- Analysis View: 視覺化分析系統
- Filter: 篩選搜尋結果
- AutoPlan: 規畫合成路徑

個人化功能

- Report: 輸出報告
- History: 搜尋紀錄
- My Alerts: 新知通報
- My Settings: 個人化設定

個人化功能 註冊及登錄

Query Results Synthesis Plans History Report My Alerts My Settings Help

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Last Name *

Email *

Job title *

Institution *

Location *

Password *

Confirm password *

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Register

點擊送出資料

Register Login

User name: Password:


Remember me on this computer [Forgotten password](#)

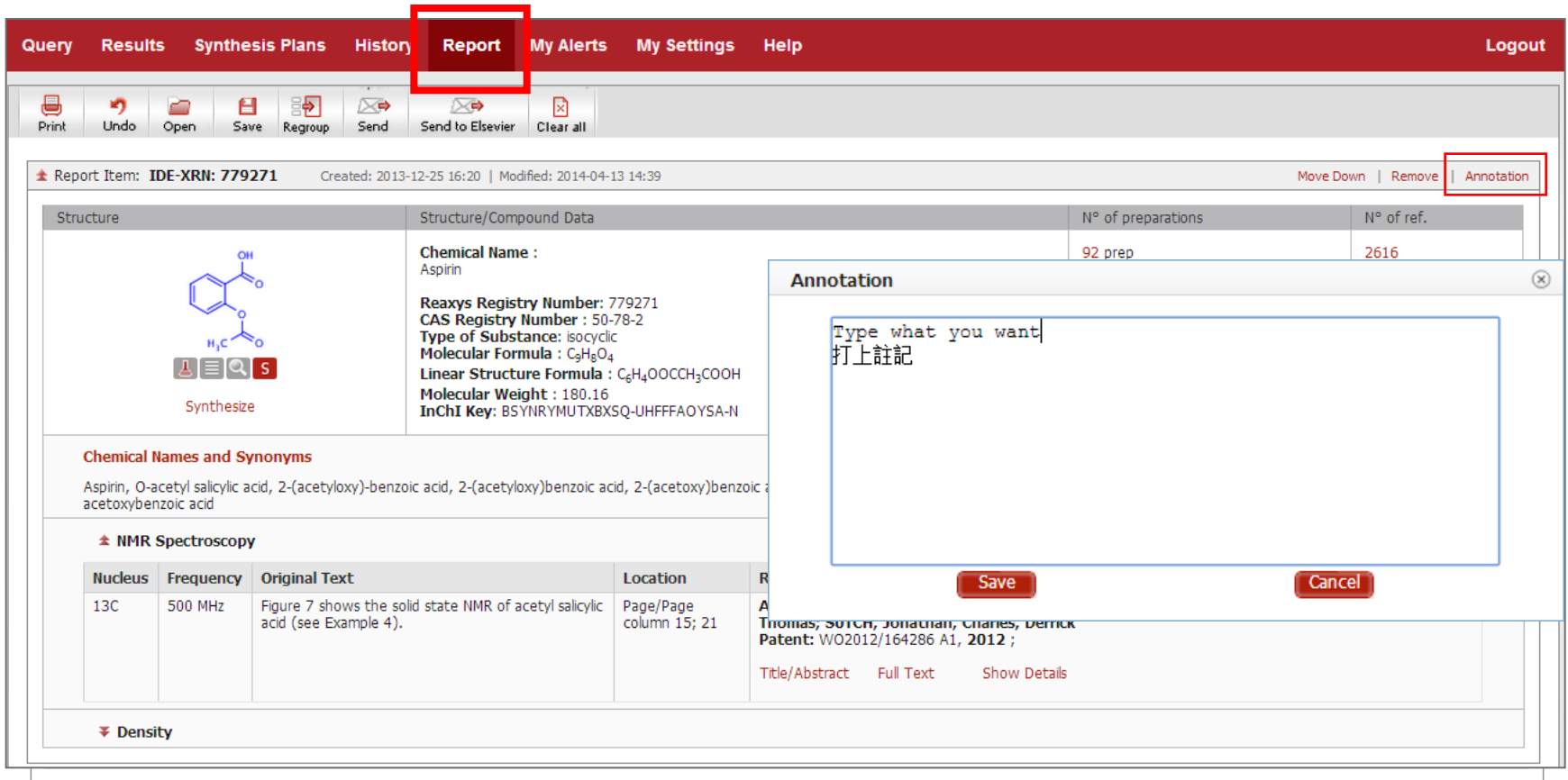
[Institution Login](#)

密碼建議包含大小寫、
數字及特殊符號(*_.)



主題 1 : Report

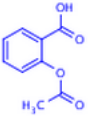
多樣化結果輸出功能 (REPORT) : 只要有  圖示處皆可輸出至REPORT , 如 : 搜尋條件、搜尋結果及合成計畫等。



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

Print Undo Open Save Regroup Send Send to Elsevier Clear all

Report Item: IDE-XRN: 779271 Created: 2013-12-25 16:20 Modified: 2014-04-13 14:39 Move Down Remove Annotation

Structure	Structure/Compound Data	N° of preparations	N° of ref.
 Synthesize	Chemical Name : Aspirin Reaxys Registry Number: 779271 CAS Registry Number : 50-78-2 Type of Substance: isocyclic Molecular Formula : C ₉ H ₈ O ₄ Linear Structure Formula : C ₆ H ₄ OOCCH ₃ COOH Molecular Weight : 180.16 InChI Key : BSYNRYMUTXBXSQ-UHFFFAOYSA-N	92 prep	2616

Chemical Names and Synonyms
Aspirin, O-acetyl salicylic acid, 2-(acetyloxy)-benzoic acid, 2-(acetyloxy)benzoic acid, 2-(acetoxy)benzoic acid, acetoxybenzoic acid

NMR Spectroscopy

Nucleus	Frequency	Original Text	Location
13C	500 MHz	Figure 7 shows the solid state NMR of acetyl salicylic acid (see Example 4).	Page/Page column 15; 21

Annotation

Type what you want
打上註記

Save Cancel

Thomas, Ulrich, Jonathan, Charles, Derrick
Patent: WO2012/164286 A1, 2012 ;
Title/Abstract Full Text Show Details

Density

多樣化結果輸出功能 - ENHANCED REPORT

搜尋紀錄輸出

反應搜尋結果輸出

化合物搜尋結果輸出

文獻搜尋結果輸出

輸出結果

The screenshot displays the REAXYS Enhanced Report interface with several report items. A yellow box highlights the 'Report' menu in the top navigation bar. Colored arrows point from external labels to specific report sections: a blue arrow points to the first report (search record), a purple arrow to the second report (reaction search), a red arrow to the third report (compound search), and a green arrow to the fourth report (literature search).

Report Item: Query: 2012-07-06 11:16
 Structure: NCC1=CC=C(O)C(O)=C1
 Description: Reactions: Product, As drawn, Ignore stereo, No isotopes, No charges, No radicals, No additional rings, Ignore Atom Mappings, align results with query
 Date: 2012-07-06 11:16

Report Item: RX-ID: 19974818
 Yield: CC1=C(O)C(=O)C=C1 → NCC1=CC=C(O)C(O)=C1
 Conditions: 1: 1) CH₃NH₂, 2) H₂ / 2.) 10 percent Pd/C / 2.) 60 atm, 60 deg C
 2: 14 percent / oxygen, cupric perchlorate, ascorbic acid / H₂O; acetone / 24 h / 60 °C
 3: NH₂NH₂
 References: Aihara, Kazuhiro; Higuchi, Tsunehiko; Hirobe, Masaaki
 Chemical & Pharmaceutical Bulletin, 1988, vol. 36, # 2
 p. 837 - 840
 Title/Abstract Full Text Show Details

Report Item: Query: 2012-07-13 16:14
 Structure: NCC1=CC=C(O)C(O)=C1
 Description: Substances: As drawn, Ignore stereo, No salts, No mixtures, No isotopes, No additional rings, No charges, No radicals, align results with query
 Date: 2012-07-13 16:14

Report Item: IDE-XRN: 1072822
 Structure: NCC1=CC=C(O)C(O)=C1
 Structure/Compound Data:
 Chemical Name: 1-(3,4-dihydroxyphenyl)-2-amino-ethane
 Reaxys Registry Number: 1072822
 CAS Registry Number: 51-61-6
 Type of Substance: isocyclic
 Molecular Formula: C₈H₁₂N₂O₂
 Linear Structure Formula: C#N(OH)2C#H4H2
 Molecular Weight: 153.151
 InChi Key: VYFYTLBLKJHU-UHFFFAOYSA-N
 N° of preparations: 37 prep out of 296 reactions.
 N° of ref.: 857
 Chemical Names and Synonyms: 1-(3,4-dihydroxyphenyl)-2-amino-ethane, 3,4-dihydroxyphenylethylamine, 3,4-dihydroxyphenethylamine, 3-hydroxytyramine, dopamine, DOPA, DA
 ESR Spectroscopy:
 Description: ESR-hyperfine coupling constants
 Solvents: H2O
 Comment: 1H.
 Reference: 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: CNR-CNR: 9009206
 Title of the Document: Carboranes as pharmacophores: similarities and differences between aspirin and asborin
 Authors: Scholz, Matthias; Hey-Havikons, Evamarie; Kaluerovic, Goran N.; Kammer, Harish; Paschke, Reinhard; Will, Joanna; Sheldrick, William C.
 Year: 2011
 Source: European Journal of Medicinal Chemistry, 2011, vol. 46, # 4 p. 1131 - 1139
 Times cited: 1

主題 2 : History

搜尋紀錄 (HISTORY) : 保存重要搜尋結果。如：搜尋條件、搜尋結果及合成計畫等。




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

Combine hitsets Select at least two hitsets for combining 

	Query	Temporary result description			Date
<input type="checkbox"/>	69	310 reactions Add 2 items from History	View	Store	2014-09-22 17:37
<input type="checkbox"/>	68	2979	View	Store	
<input type="checkbox"/>	67	225	View	Store	
<input type="checkbox"/>	66	99 ta	View	Store	
<input type="checkbox"/>	65	68 d	View	Store	
<input type="checkbox"/>	64	122 reactions Overlap 2 items from History	View	Store	2014-09-22 17:37
<input type="checkbox"/>	63	836 bioactivities	View	Store	
<input type="checkbox"/>	62	108 substances	View	Store	
<input type="checkbox"/>	61	16 targets	View	Store	

Save hitset 

Please enter a comment:

Save **Cancel**


SEARCH HISTORY

COMBINE SEARCH


[Query](#)
[Results](#)
[Synthesis Plans](#)
[History](#)
[Report](#)
[My Alerts](#)
[My Settings](#)
[Help](#)
[Logout](#)

Reaxys
PubChem
eMolecules


Select how you want to combine the hitsets




Merge 3 with 6



Overlap 3 with 6




Exclude 3 from 6



Exclude 6 from 3

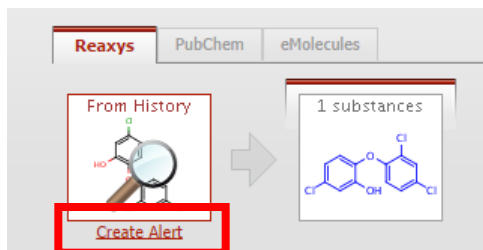
Combine hitsets Select at least two hitsets for combining

 Print

	Query	Temporary result description		Date
<input checked="" type="checkbox"/>	Edit Create Alert Literature: polycondensation	12804 citations Literature: polycondensation	View Store	2014-04-29 18:15
<input type="checkbox"/>	5	8270 reactions	View Store	
<input type="checkbox"/>	4	8458 substances	View Store	
<input checked="" type="checkbox"/>	Edit Create Alert Ask Reaxys Literature: (CBI.BICIT = 'polyamide')	20623 citations Ask Reaxys Literature: (CBI.BICIT = 'polyamide')	View Store	2014-04-29 17:56
<input type="checkbox"/>	2	15795 reactions	View Store	
<input type="checkbox"/>	1	11535 substances	View Store	

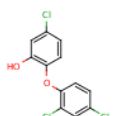
主題 3 : My Alerts

新知通報 (MY ALERTS) : 訂閱常用搜尋條件，隨時閱讀最新資料。



The 'Create Alert' form is displayed on a dark red background. It includes a navigation bar with 'Query', 'Results', 'Synthesis Plans', 'History', 'Report', 'My Alerts', 'My Settings', and 'Help'. The form contains a hint, a 'Query' field with a chemical structure and a description, a 'Name of Alert' field with the placeholder '輸入名稱', an 'E-mail Address' field with 'o.liang@elsevier.com' and a 'send copy to' field with 'e.g. a.smith@test.com;b.smith@test.com', and a 'Comment/Description' field.

The screenshot shows the 'My Alerts' page in the Reaxys interface. The top navigation bar includes 'Query', 'Results', 'Synthesis Plans', 'History', 'Report', 'My Alerts', 'My Settings', 'Help', and 'Logout'. The page header features the Reaxys logo and a recorded webinar notice. Below the navigation, there is a 'Delete' button and a table of alerts.

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

主題 4 : My Setting

個人化設定 (MY SETTINGS)：修改個人資料、修改密碼、或依照自己的喜好設定REAXYS 介面。如，更換繪圖軟體、挑選常用搜尋欄位等等。



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

修改使用介面設定

Modify Application Settings

Select your favourite structure editor, reaction and substance search options, hits per page and specify color.

修改個人資料

Modify Personal Data

View details from your Registration Profile. Includes a facility to change your Personal Details.

修改密碼

Change Password

Change your Password.

Change Password

Current password *
New password *
Confirm password *

Back

Save

Modify personal data

User Name
Title *
First Name *
Last Name *
Email *
Job title *
Institution *
Location *

Back

Save

修改使用介面設定

Modify application settings

Structure editor

Editors that do not require a plugin to be installed:

- Dotmatics Elemental
- ChemAxon MarvinSketch *(Note: requires Java to be installed)*
- GGA Ketcher

Reaxys uses Dotmatics's Elemental as default structure and reaction query editor, if no other editor is selected

更換結構繪圖軟體

The following editors can only be used, if the **Reaxys Structure Editor PlugIn** is installed:

- Crossfire Structure Editor
- Accelrys Draw
- Accelrys ISIS/Draw
- CambridgeSoft ChemDraw
- ICEdit

Please check this with your administrator or click the hyperlink and download the installer.

Reaxys will present a warning message, if these editors are selected, but the **structure editor plugin** is not installed.

Structure display options

Reaction/Structure search options

Query Forms

AutoPlan options

Behavior of Synthesize Hyperlink

- On click offer option to select between simple search and AutoPlan
- On click only search for the reactions of the given compound as product
- On click start AutoPlan with the given compound

Hits per page

Show results per page

Highlights colors

Structure

Text / Data

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REAXYS
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線上影音教學

- Query 搜尋頁面介紹
- Substances - Result Page 化合物搜尋

由化學家專為化學家所設計

進入Reaxys化學資料庫

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WIX PAGES

線上合成 - Synthe planning介紹(中文 Reaxys入門第四步, 合成工具介紹, 總

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 - Elsevier 台灣電子報 - 2013年二月號
 - Elsevier 台灣電子報 - 2013年一月號
 - Elsevier 台灣電子報 - 十二月號
 - Elsevier 台灣電子報 - 十一月號
 - Elsevier 台灣電子報 - 十月號
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