

Reaxys 化學資料庫 教育訓練

www.reaxys.com

Elsevier 生命科學解決方案經理

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2015.9.24

學術文獻發表量急遽增加



一般資料庫的搜尋結果無法滿足化學領域的特殊需求

The image shows a Google search for 'tamiflu'. The search results include a link to a Taiwanese website (www.ktgh.com.tw) and a Wikipedia entry for Oseltamivir. Below these, there is a search result from PubMed. The PubMed result is titled 'Oseltamivir-resistant influenza A(H1N1) viruses found in ...' and lists several authors and a PMID. A large red 'X' is overlaid on the PubMed search result, indicating that general search results like these do not meet the specialized needs of the chemical field.

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...
囊, 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 /osəl'tæmivɪr/, me...
medication used to prevent and treat...

Tamiflu Uses, Dosage & Side Effects
www.drugs.com > Conditions > In...
Tamiflu is is an antiviral medication u...
Learn about side effects, interactions...

Tamiflu & Relenza: how effective are they?
www.cochrane.org > Features > 翻...
2014年4月10日 - The BMJ and Cochr...
makers to review guidance on use of...

PubMed.gov
National Library of Medicine
Institutes of Health

Search
Advanced
Help

Summary ▾ 20 per page
Recently Added ▾

Results: 1 to 20 of 3144

1. **Oseltamivir-resistant influenza A(H1N1) viruses found in ...**
permissive mutations, which compensate for fitness impairment caused by...
Souza TM, Fintelman-Rodrigues N, Resende...
Fernandes SB, Cury AL, Rediger IN, Siqueira...
Mem Inst Oswaldo Cruz. 2015;27(02):110(1):101-105. Epub...
PMID: 25742269 [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...**

Filters: Manage Filters

New feature
Try the new Display Settings option - Sort by Relevance

Results by year

Download CSV

Related searches
tamiflu effectiveness
tamiflu prophylaxis
tamiflu influenza
tamiflu renal
tamiflu cochrane

PMC Images search for tamiflu

Smarter Chemistry



MarvinSketch (ChemAvon) - 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

Formula Builder

Click

1 H 2

2 Li B

3 Na M

Synthesize (27)

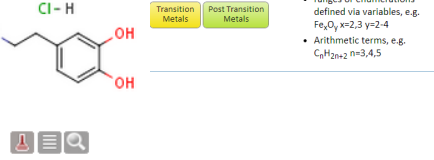
2 Details

Add Remove

Synthesize (158)

Mass Spectrometry (17)

Description	Peak	Location	Comment	Reference
spectrum		Paragraph 0124		SHANGHAI INSTITUTE OF ORGANIC CHEMISTRY, CHINESE ACADEMY OF SCIENCES; LIANHE CHEMICAL TECHNOLOGY CO., L Qianghui Patent: US2014/221662 A1, 2014 ;
electrospray ionisation (ESI) spectrum				Hu, Zhe-Yi; Boucher, Bradley A.; Laizure, S. Case Journal of Mass Spectrometry, 2013 , vol. 48, # 8 Title/Abstract Full Text View citing articles
Spectrum		supporting information		Kongkamnerd, Jarinrat; Cappelletti, Luca; Prandi Cattoli, Giovanni; Terregino, Calogero; Capua, Ilia Biorganic and Medicinal Chemistry, 2012 , vol. 20, Title/Abstract Full Text View citing articles
APCI (atmospheric pressure chemical ionization) spectrum		supporting information		Chuanopparat, Nutthawat; Kongkathip, Ngampor Tetrahedron Letters, 2012 , vol. 53, # 46 p. 6209 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, Ngampor Tetrahedron Letters, 2012 , vol. 53, # 46 p. 6209 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 Foundati Patent: EP2201911 A1, 2011 ;
ESI (Electrospray ionisation)				Ishikawa, Hayato; Bondzic, Bojan P.; Hayashi, Yu defined by variables, e.g. Fe ₂ O ₃ , x=2.3, y=2-4 • Arithmetic terms, e.g. C ₁₀ H ₁₂ +n=3,4,5



Query Results Synthesis Plans History Report My Alerts My Settings Help

Live Chat Register Login

Print Undo Open Save Refgroup Send To Elsevier Clear All

Report Item: Query: 2012-07-06 11:16 Created: 2012-07-06 11:17 Modified: 2012-07-06 11:20 Move Down Remove Annotation

Structure Description Date

Reactions: Product, As drawn, Ignore stereo, No isotopes, No charges, No radicals, No additional rings, Ignore Atom

Neoprops, align results with query

2012-07-06 11:16

Report Item: RX-ID: 19974818 Created: 2012-07-06 11:17 Modified: 2012-07-06 11:20 Move Up Move Down Remove Annotation

Yield Conditions References

Synthesize Synthesize Rx-ID: 19974818 Find similar reactions

Multi-step reaction with 3 steps

1: 13) Chrom. 2) 10% 3) 50 percent Pd/C / 2) 50 atm, 60 deg C

2: 14 percent / oxygen, cupric perchlorate, ascorbic acid / H₂O acetone / 24 h / 60 °C

3: 10 min

View Scheme

Aihara, Kazuhiko; Higuchi, Tsunenobu; Hirobe, Haseaki
Chemical & Pharmaceutical Bulletin, **1988**, vol. 36, # 2
p. 837-840
Title/Abstract Full Text Show Details

Report Item: Query: 2012-07-13 16:14 Created: 2012-07-13 16:15 Modified: 2012-07-13 16:15 Move Down Remove Annotation

Structure Description Date

Substances: As drawn, Ignore stereo, No salts, No mixtures, No isotopes, No additional rings, No charges, No radicals, align results with query

2012-07-13 16:14

Report Item: IDE-XR#: 1072822 Created: 2012-07-13 16:15 Modified: 2012-07-13 16:15 Move Up Remove Annotation

Structure Compound Data N° of Preparations N° of ref.

1-(3,4-dihydroxyphenyl)-2-amino-ethane 37 prep out of 236 reactions. 837

Chemical Name: 1-(3,4-dihydroxyphenyl)-2-amino-ethane

Reaxys Registry Number: 1072822

CAS Registry Number: 51-61-6

Type of Substance: basic

Molecular Formula: C₈H₁₁NO₂

Linear Structure Formula: C₈H₉O₂NC₂H₄NH₂

Molecular Weight: 153.181

Index Key: YFFYYTULQJUNHJFHFADYSA-N

Chemical Names and Synonyms

1-(3,4-dihydroxyphenyl)-2-amino-ethane, 3,4-dihydroxyphenylethylamine, 3,4-dihydroxyphenylethylamine, 3-hydroxytyramine, dopamine, DOPA, DA

ESR Spectroscopy

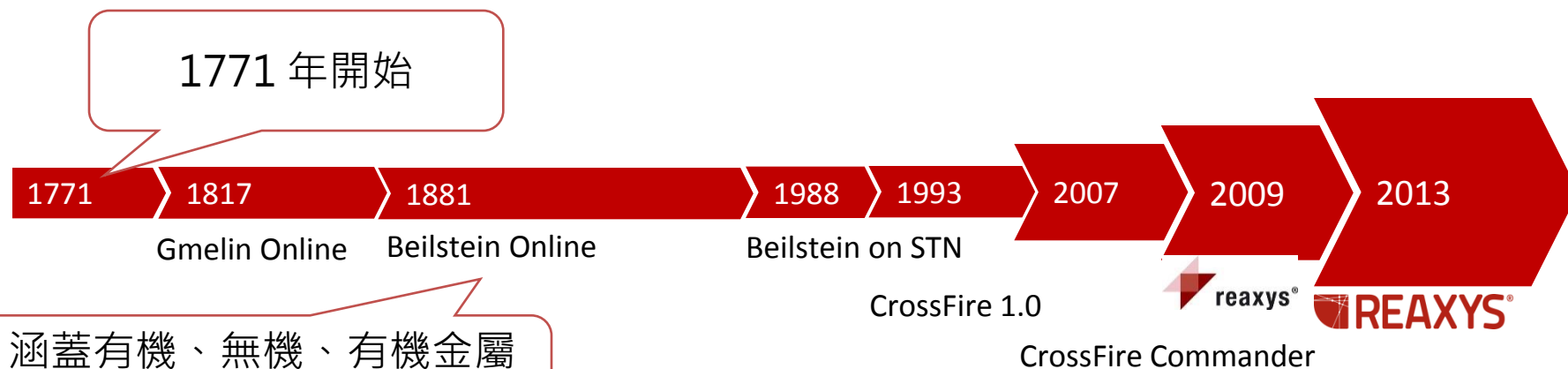
Description	Solvents	Comment	Reference
ESR-hyperfine coupling constants	H2O	DH	Plancherel, Dominique; von Zelevsky, Alex Helvetica Chim Acta, 1982 , vol. 65, # 6 p. 1929-1940 Title/Abstract Full Text View citing articles Show Details

Report Item: CBR-CNR: 9009206 Created: 2012-07-06 11:34 Modified: 2012-07-06 11:34 Move Up Remove Annotation

Title of the Document	Authors	Year	Source	Times cited
Carbamoranes as pharmacophores; similarities and differences between epiorn and asborn	Scholz, Matthias; Heyderlind, Svenja; Kollerovic, Goran N.; Komosa, Marija; Paschle, Reinhard; Vill, Simona; Sheddik, William S.	2011	European Journal of Medicinal Chemistry, 2011 , vol. 46, # 4 p. 1131-1139 Full Text View citing article	1

Reaxys 的過去與現在

承襲 Gmelin, Beilstein, 與 CrossFire 資料庫



涵蓋有機、無機、有機金屬
領域 400種核心期刊

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 2015

文獻資料

A Bibliographic Database

>46 million records
(from ~16,000 journal titles
plus records from key patent
organisations)

A Substance Database

~ 90 million substances
(total)
~ 57 million substances
(unique)

Reaxys
2015

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

> 36 million single- and
multi-step reactions

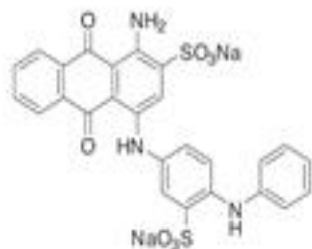
A Property Database

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

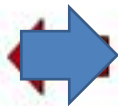
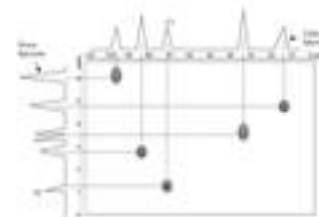
> 500 個欄位
可獨立或合併搜尋

REAXYS資料擷取方式

從文獻中分別擷取出化學結構、物理化學特性、藥理資訊以及化學合成反應式等資訊，再整理 SUBSTANCES、REACTIONS 及 CITATIONS 三類，共超過 500個欄位



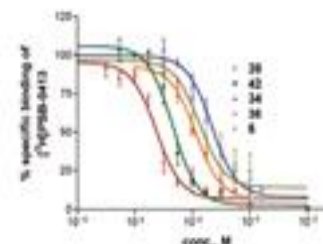
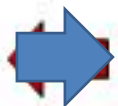
Chemical Structures

Physicochemical Properties



Chemical Synthesis



Pharmacology



> 500 個欄位
可獨立或合併搜尋

Smarter Chemistry



多元化搜尋管道

結構

分子式 合金 Reaxys Tree

> 500 個欄位

Reaction Basic Index is Sharpless Lookup X

A screenshot of the Reaxys search interface. It shows a search bar with 'Sharpless' entered, a dropdown menu with 'is', and a 'Lookup X' button. Above the search bar are several icons representing different search methods: 'Structure' (a chemical structure), 'Molecular Formula' (a periodic table), 'Alloys' (a table of properties), and 'Reaxys Tree' (a hierarchical tree structure).

Ask Reaxys Sharpless 自動辨識關鍵字屬性 Go

Examples

A search bar with the text 'Sharpless' and '自動辨識關鍵字屬性' (Automatic identification of keyword attributes). To the right is a red 'Go' button. Below the search bar is a small icon and the word 'Examples'.

化合物
(Substance)



反應
(Reaction)



文獻
(Literature)

搜尋結果


Ask Reaxys 搜尋範例


EASY OF USE

Ask Reaxys

A set of examples have been implemented providing users with an overview about Ask Reaxys capabilities, helping them to get the most out of this feature.

Ask Reaxys

 [Examples](#)



Query Examples X

What is Ask Reaxys?

You can query the Reaxys database without learning how to construct complex queries. Please try out these examples below.

Substances

Substance name "Atenolol" Substance name will be translated into a structure and searched	CAS-NO "102625-70-7" CAS-NO will be looked up and searched on success	Molecular Formula "Pt(PPh3)3" Molecular Formula will be searched as formula
<input type="button" value="Try it"/>	<input type="button" value="Try it"/>	<input type="button" value="Try it"/>

Substance Properties

MELTING POINT "melting point of xylitol" "Xylitol" will be translated into a structure and combined with a search for	SOLUBILITY "solubility of vitamin D3" "Vitamin D3" will be translated into a structure and combined with a	FERROELECTRICITY "ferroelectric materials" Substances with ferroelectric data will be searched
---------------------------------------------------------------------------------------------------------------------------------	----------------------------------------------------------------------------------------------------------------------	----------------------------------------------------------------------------------------------------------

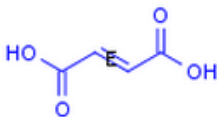



Ask Reaxys 搜尋應用範例

順丁烯二酸 + HPLC 檢測方法 (Maleic Acid + HPLC)

Ask Reaxys

maleic acid HPLC

Go

Structure	Structure/Compound Data	N° of preparations All Preps All Reactions	Available Data	Target	N° of ref.
    Synthesize Hide Details Find similar	Chemical Name: (2E)-but-2-enedioic acid Reaxys Registry Number: 605763 CAS Registry Number: 110-17-8 Type of Substance: acyclic Molecular Formula: C ₄ H ₄ O ₄ Linear Structure Formula: COOHCHCHCOOH Molecular Weight: 116.073 InChI Key: VZCYOOQTPOCHFL-OWOJBTEDSA-N Highest Clinical Phase: Marketed	452 prep out of 4930 reactions.	Hit Data (2) Druglikeness Bioactivity Identification Physical Data (505) Spectra (150) Ecological Data (22) Use/Application (628) Natural Product (57)	Show Targets	3563

Chemical Names and Synonyms

(2E)-but-2-enedioic acid, but-2-en-1,4-dioic acid, Fumaric acid, (E)-2-butenedioic acid, trans-butenedioic acid, fumaric acid, fumarate

Hit Data

Chromatographic Data (2 Hits out of 2 view all)

Chromatographic data	Location	Reference
HPLC (High performance liquid chromatography)		Silva, Luis R.; Azevedo, Jessica; Pereira, Maria J.; Carro, Lorena; Velazquez, Encarna; Peix, Alvaro; Valentao, Patricia; Andrade, Paula B. Journal of Agricultural and Food Chemistry, 2014 , vol. 62, # 3 p. 557 - 564 Title/Abstract Full Text View citing articles Show Details Espinoza, C.; Contreras, N.; Berros, C.; Salazar, R. Journal of the Chilean Chemical Society, 2014 , vol. 59, # 2 p. 2507 - 2511 Title/Abstract Full Text View citing articles Show Details
HPLC (High performance liquid chromatography)	supporting information	Upendar Reddy; Lo, Rabindranath; Roy, Sovan; Banerjee, Tanmay; Ganguly, Bishwajit; Das, Amitava Chemical Communications, 2013 , vol. 49, # 84 p. 9818 - 9820 Title/Abstract Full Text View citing articles Show Details

Ask Reaxys

切換自動辨識結果

The interface shows three tabs: Reaxys (selected), PubChem, and eMolecules. Below the tabs is a 'Query' input area with a magnifying glass icon and a chemical structure of maleic acid. A 'Create Alert' button is visible. To the right, a box displays '70 substances' and the same chemical structure, with a 'Show Query' button highlighted in orange.

可預覽搜尋結果，協助判斷採用何種辨識方式

Ask Reaxys - Analysis

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

Suggested Query	Results	Select Action
<p>maleic acid HPLC</p> <p>Result: substances Show query</p>	70 substances in Reaxys	<p>Search</p> <p>Edit query in Advanced</p>
<p>maleic acid HPLC</p> <p>Result: citations Show query</p>	182 citations in Reaxys	<p>Search</p> <p>Edit query in Advanced</p>

Legend: Bibliography Compound Concept Date Keyword Bioactivity Ignored

Cancel

Ask Reaxys 搜尋應用範例

棉酚檢測方式 (Gossypol Detection)

Ask Reaxys

Gossypol detection

Go

Title of the Document	Authors	Year	Source	Times cited
Detection of ultra trace amount gossypol with chemiluminescence using capillary electrophoresis as injection techniques	Liu, Er Bao; Zhang, Min; Xue, Bing Chun; Zhao, Peng Xiang; Liu, Yin	2005	Chinese Chemical Letters, 2005 , vol. 16, # 12 p. 1649 - 1651 Full Text View citing articles	2
<div style="border: 1px solid blue; border-radius: 15px; padding: 5px; display: inline-block;"> 檢測方式：毛細管電泳 (Capillary electrophoresis) </div>				
A validated HPLC assay for the determination of R-(-)-gossypol in human plasma and its application in clinical pharmacokinetic studies	Lin, Hongxia; Gounder, Murugesan K.; Bertino, Joseph R.; Kong, Ah-Ng Tony; DiPaola, Robert S.; Stein, Mark N.	2012	Journal of Pharmaceutical and Biomedical Analysis, 2012 , vol. 66, p. 371 - 375 Full Text View citing articles	2
<div style="border: 1px solid blue; border-radius: 15px; padding: 5px; display: inline-block;"> 檢測方式：HPLC </div>				
Capillary electrophoresis to quantitate gossypol enantiomers in cotton flower petals and seed	Vshivkov, Sergey; Pshenichnov, Egor; Golubenko, Zamira; Akhunov, Alik; Namazov, Shadman; Stipanovic, Robert D.	2012	Journal of Chromatography B: Analytical Technologies in the Biomedical and Life Sciences, 2012 , vol. 908, p. 94 - 97 Full Text View citing articles	4
<div style="border: 1px solid blue; border-radius: 15px; padding: 5px; display: inline-block;"> 檢測方式：Flow Injection </div>				
Determination of gossypol in trace level by flow injection analysis with chemiluminescence detection	Xue, Bing Chun; Liu, Er Bao	2006	Chinese Chemical Letters, 2006 , vol. 17, # 1 p. 57 - 60 Full Text View citing articles	2
Accumulation of gossypol enantiomers in ovine tissues	Kim; Calhoun; Stipanovic	1996	Comparative Biochemistry and Physiology - B Biochemistry and Molecular Biology, 1996 , vol. 113, # 2 p. 417 - 420 Full Text View citing articles	35

Reaxys 搜尋架構



一、Reaxys 搜尋架構

選擇合適的搜尋管道

多元化搜尋管道

Ask Reaxys

Examples

結構

分子式 合金 Reaxys Tree

> 500 個欄位

Reaction Basic Index

布林邏輯



Advanced

使用指令結合各種
搜尋條件 → 最完整

Import Save

批次搜尋

History

結合多種搜尋條件

搜尋結果

化合物
(Substance)

反應
(Reaction)

文獻
(Literature)

結構搜尋 – Marvin JS

REAXYS[®]

Query Results Synthesis Plans History Report My Alerts My Settings Help

Start Over

Ask Reaxys e.g. Ask Re

Smart search

無須 Java 支援



Reactions



Substances



MedChemistry



Literature



ReaxysTree



Physical



Spectra

Structure

MarvinJS
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

PASTE

STRUCTURE EDITOR

Create Structure Template from Name

Identification

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

Submit

Cancel

Marvin.js - Google Chrome

https://www.reaxys.com/reaxys/js/sre_5_3_1_03/child_marvin_js.html

ChemAxon

Transfer Query Cancel & Return

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

Search Substances

Click to start Search

Clear Query

Marvin JS – Basic search function

Marvin.js - Google Chrome
https://www.reaxys.com/reaxys/js/sre_5_3_1_03/child_marvin_js.html

COOH

搜尋官能基

Transfer Query Cancel & Return

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

Drawing 畫筆



Abbreviated groups

COO

Expand

COOEt

COOH

COOiAm

COOK

COONa

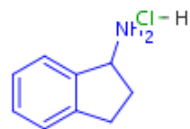
COOPh

COOsBu

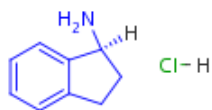
Ok

Marvin JS – substructure search

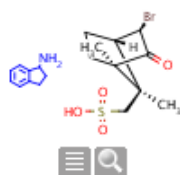
Marvin JS – substructure search



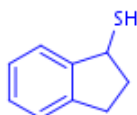
Synthesize | Show Details



Synthesize | Show Details



Synthesize | Show Details



Synthesize | Show Details

4 Oc1c2ccccc12 5 Nc1c2ccccc12

Periodic System

Periodic Table | Advanced

Name: Chromium (Cr)
 Atomic number: 24
 Mass: 51.9961
 Electronegativity: 1.6
 Ox. state(s): 0,1,2,3,4,5,6

1	2											13	14	15	16	17	18	
1	H	He											B	C	N	O	F	Ne
2	Li	Be											Al	Si	P	S	Cl	Ar
3	Na	Mg	3	4	5	6	7	8	9	10	11	12	Al	Si	P	S	Cl	Ar
4	K	Ca	Sc	Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn	Ga	Ge	As	Se	Br	Kr
5	Rb	Sr	Y	Zr	Nb	Mo	Tc	Ru	Rh	Pd	Ag	Cd	In	Sn	Sb	Te	I	Xe
6	Cs	Ba	La	Hf	Ta	W	Re	Os	Ir	Pt	Au	Hg	Tl	Pb	Bi	Po	At	Rn
7	Fr	Ra	Ac	Rf	Db	Sg	Bh	Hs	Mt									

Atom list: Ce, Pr, Nd, Pm, Sm, Eu, Gd, Tb, Dy, Ho, Er, Tm, Yb, Lu
 NOT list: Th, Pa, U, Np, Pu, Am, Cm, Bk, Cf, Es, Fm, Md, No, Lr
 Clear list

Color schema: CPK Standard state Blocks Metals/Nonmetals
 Color legend:

Close

搜尋指令

結構搜尋

廣瀨教授：

我曾對醇類及胺類的醯化

(acylation) 反應感興趣，一般來

說胺化作用 (amination) 比酯化

作用 (esterification) 更容易發生，

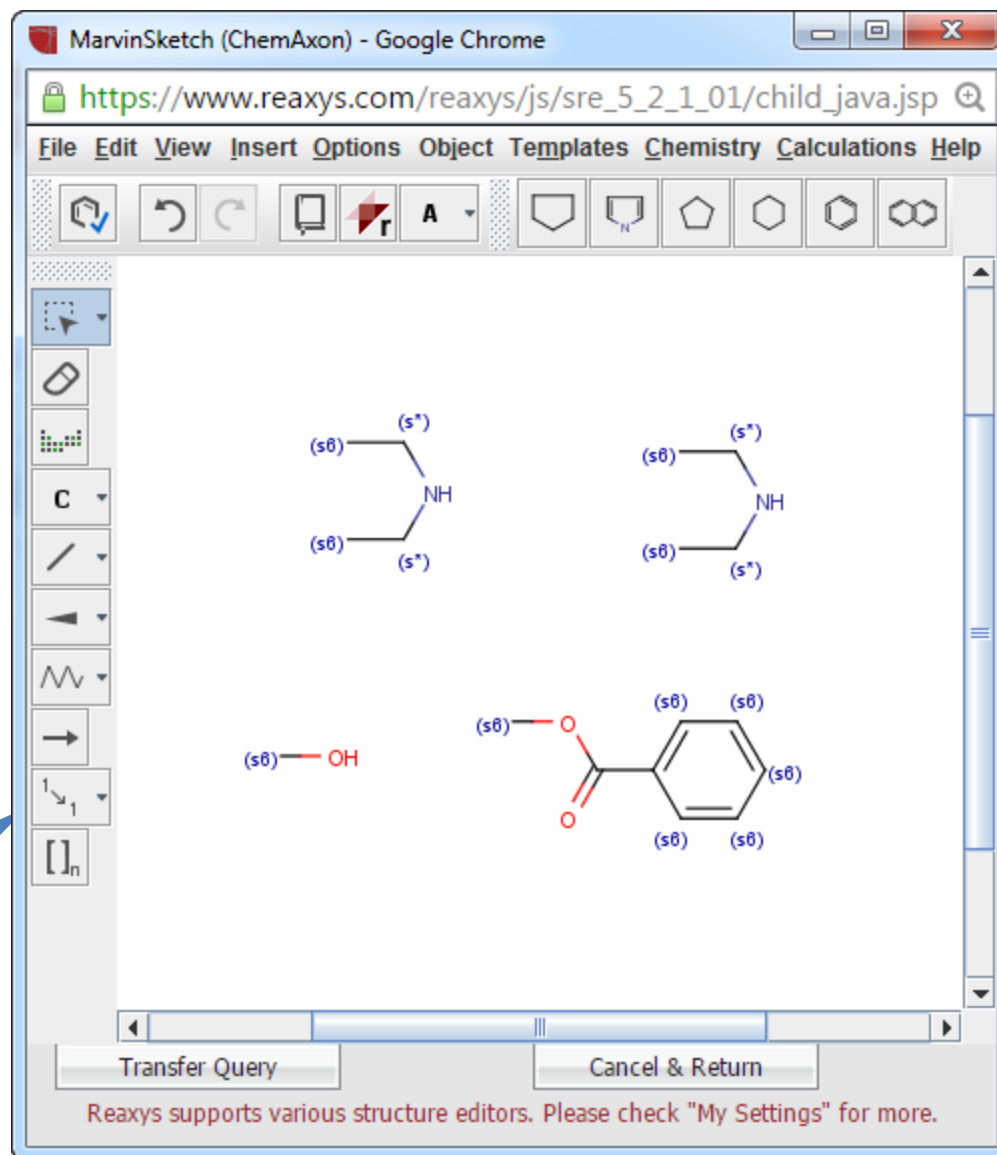
因此通常胺基比羥基更容易反應，

但我想找出羥基有反應而不改變

胺基的反應

特殊搜尋技巧：

- Substitution count
- Atom mapping



搜尋結果

129 reactions out of 43 bioactivities and 198 substances and 12 targets and 39 citations

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

go to Page Page 1 of 15

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

Yield	Conditions	References
1	<p>A B</p> <p>Synthesize Find similar</p>	<p>Rx-ID: 25608814 Find similar reactions</p> <p>With sodium tetrahydroborate in methanol T=-75 - 25°C; Show Experimental Procedure</p> <p>Chellquist, Eric; Doubleday, Mary; Gilbert, Charles; Zhang, Xuehai; McLane, Michael; Ambruster, Kyle; Levitt, Roy C. Patent: US2007/10504 A1, 2007 ; Location in patent: Page/Page column 10-11 ;</p> <p>Title/Abstract Full Text Show Details</p>
2	<p>Synthesize Synthesize Synthesize</p>	<p>A B</p> <p>Synthesize Synthesize</p>

檢視現有合成路徑

點選 VIEW SCHEME 檢視合成路徑圖

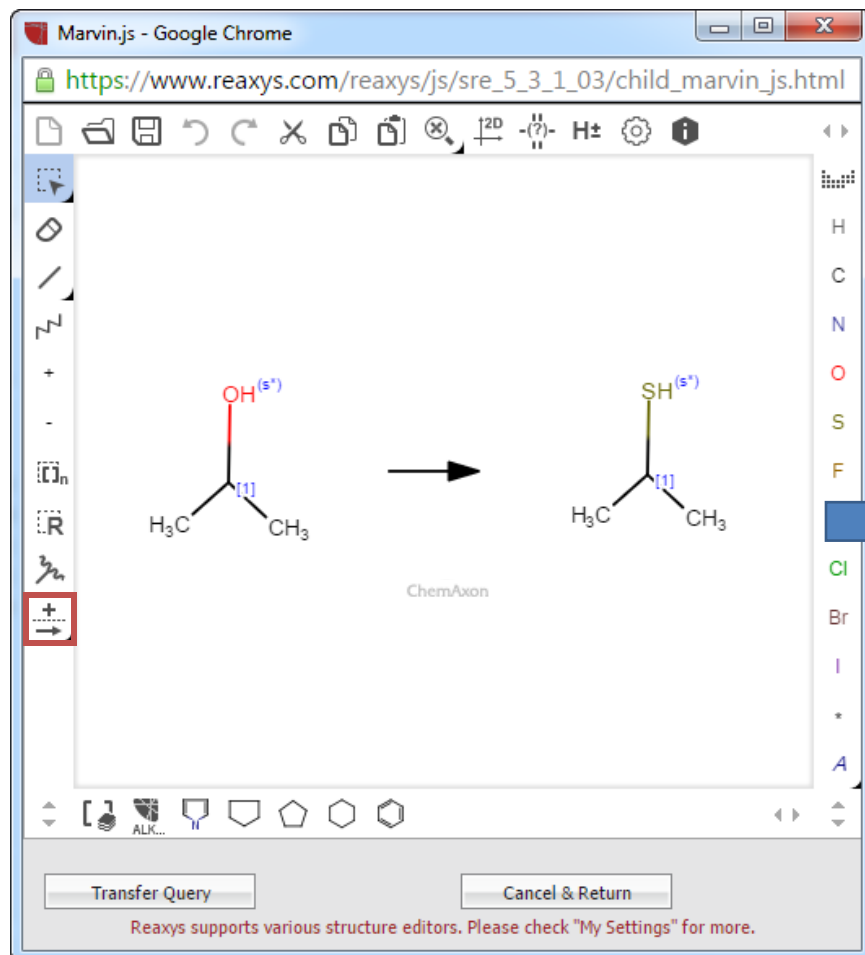
The screenshot displays the Reaxys software interface for viewing a synthesis scheme. The window title is "Synthesis 1". The top toolbar includes icons for New, Undo, Open, Save, Rename, Duplicate, Export, Print, Left, Right, Top, Resize, Thumbnail, Report, and Show. On the left, there are navigation and zoom controls.

The main area shows a synthesis scheme with the following components:

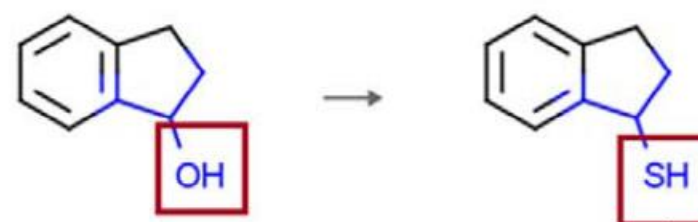
- Top Left:** A chemical structure of a dimethylchlorosilane derivative: CC(C)(Cl)Si.
- Step 4:** Labeled "Synthesize (99)", showing a reaction with a 95% yield. The reagent is a complex multi-ring system. Below it are "Add" and "Remove" buttons.
- Step 3:** Labeled "Synthesize (265)", showing a reaction with a 78% yield. The reagent is a complex multi-ring system. Below it are "Add" and "Remove" buttons.
- Step 2:** Labeled "Synthesize (21)", showing a reaction with a 78% yield. The reagent is a complex multi-ring system. Below it are "Add" and "Remove" buttons.
- Step 1:** Labeled "Synthesize (11)", showing a reaction with a 78% yield. The reagent is a complex multi-ring system. Below it are "Add" and "Remove" buttons.
- Bottom Left:** A chemical structure of a complex multi-ring system, labeled "Synthesize (265)".
- Bottom Center:** A chemical structure of a complex multi-ring system, labeled "Synthesize (11)".
- Bottom Right:** A chemical structure of a complex multi-ring system, labeled "Synthesize (21)".

The final product of the synthesis is a complex multi-ring system, highlighted with a red box. The interface also includes a "Fit" button and a "Thumbnail" view in the bottom left corner.

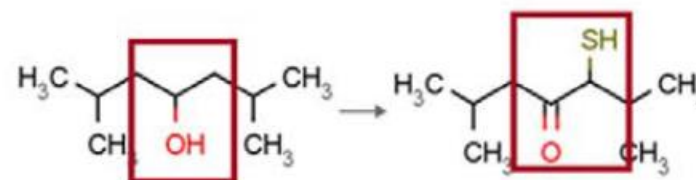
Marvin JS – atom mapping



結果差異



Mapped reaction result



Unmapped reaction result

Marvin JS – Substitution

Right click to add atom properties

Duplicate
+ R-group attachment
- R-group attachment
Atom properties
Absolute stereo (chiral)

Transfer Query Cancel & Return

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

Atom properties

Change to Element

Basic Advanced

Total H (H)	<input type="text"/>	<input type="checkbox"/>
Implicit H (h)	<input type="text"/>	<input type="checkbox"/>
Bond orders (v)	<input type="text"/>	<input type="checkbox"/>
Connections (X)	<input type="text"/>	<input type="checkbox"/>
Ring count (R)	<not set>	<input type="checkbox"/>
Smallest ring size (r)	<input type="text"/>	<input type="checkbox"/>
Ring bond (rb)	<not set>	<input type="checkbox"/>
Substitutions (s)	as drawn	<input type="checkbox"/>
Unsaturated (u)	<not set>	<input type="checkbox"/>
Aromaticity (a/A)	<not set>	<input type="checkbox"/>

Ok

Marvin JS – Substitution

Atom properties ×

Change to

Basic **Advanced**

Total H (H)

Implicit H (h)

Bond orders (v)

Connections (X)

Ring count (R)

Smallest ring size (r)

Ring bond (rb)

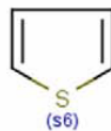
Substitutions (s)

Unsaturated (u)

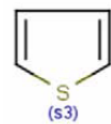
Aromaticity (a/A)

結構搜尋指令

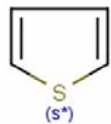
.s6



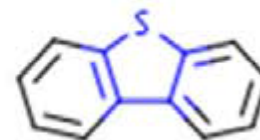
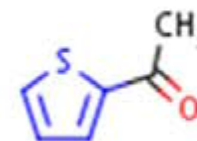
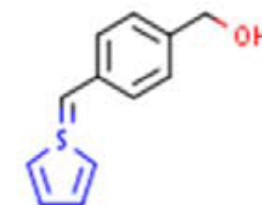
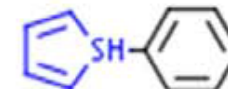
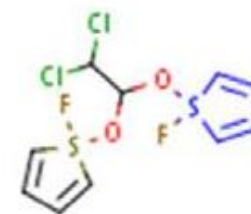
.s3



.s*



結果差異




結構搜尋其他設定選項

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

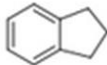
- As drawn
- Substructure **衍生物**
 - on heteroatoms
 - on all atoms
- Similarity **相似結構**

- 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...

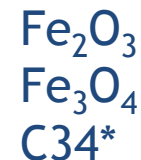
Click on one of the hyperlinks below for getting similar compounds according to the selected scope:

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

Cancel

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	Transition Metals	Post Transition Metals
						Actinoids		

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
Pb/C
yttria/zirconia ceramics

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

Alloy

合金成分

Component Formula

Fe ₂ O ₃ Fe2O3
Al ₂ O ₃
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

Reactions
Substances
Literature
ReaxysTree
Physical
Spectra
Natural Product
Advanced

Bibliographic Data

Document Type	is	
Authors	is	
Common Patent Number	starts with	
Patent Country Code	ends with	
Journal Title	contains	
Publication Year	is	
DOI	=	
Title	is	
Abstract	is	
Keywords	is	
Citation Basic Index	is	

Show AND Buttons

Select index items and click 'Transfer'

Reaxys

Search for:

- 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)
- short survey (437392)

Transfer

Reset

Cancel

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

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

Available to add

Already selected

Searches in multiple databases

文獻搜尋預設欄位

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

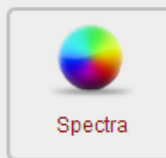
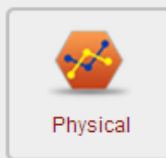
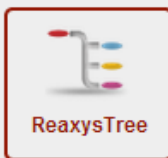
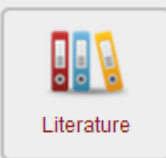
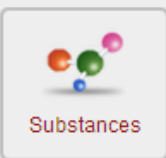
Remove all

Add Defaults

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.

Reset Select All Highlighted Deselect All

- ReaxysTree**
- chemical transformations**
(chemical reaction classification, chemical reaction classifications, chemical transformation, ...)
- chemical reaction class**
(chemical reaction type, Reaction Class, Reaction classification, reaction classifications, re...)
- condensation reaction**
(condensation reactions)
- polycondensation**
(polycondensations)

Clear Query

Search Literature

按下 Search

合併搜尋條件 -- History

結合多個搜尋條件 – 萊克多巴胺 + 毒性 (Ractopamine + Toxicity)

Select how you want to combine the hitsets

19 citations out of 0 reactions and 0 bioactivities and 0 substances and 0 targets

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

Limit to Exclude Export Print Zoom in Zoom out Hide Sort by Relevance

	Title of the Document	Authors	Year	Source	Times cited
<input type="checkbox"/> 1	Major food safety episodes in Taiwan: Implications for the necessity of international collaboration on safety assessment and management	Li, Jih-Heng; Yu, Wen-Jing; Lai, Yuan-Hui; Ko, Ying-Chin	2012	Kaohsiung Journal of Medical Sciences, 2012 , vol. 28, # 7 SUPPL. p. S10-S16 Full Text View citing articles	1
▼ Title/Abstract					
<input type="checkbox"/> 2	Multi-spectroscopic methods combined with molecular modeling dissect the interaction mechanisms of ractopamine and calf thymus DNA	Chai, Jun; Wang, Juyuan; Xu, Qifei; Hao, Fang; Liu, Rutao	2012	Molecular BioSystems, 2012 , vol. 8, # 7 p. 1902 - 1907 Full Text View citing articles	10
▼ Title/Abstract					
<input type="checkbox"/> 3	Segmental arterial mediolysis - An iatrogenic vascular disorder induced by ractopamine	Slavin, Richard E.; Yaeger, Micheal J.	2012	Cardiovascular Pathology, 2012 , vol. 21, # 4 p. 334 - 338 Full Text View citing articles	6
▼ Title/Abstract					

二、Reaxys 搜尋結果與分析

精準篩選搜尋結果

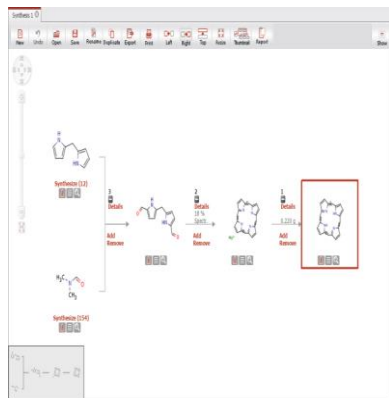
搜尋結果

化合物
(Substance)

反應
(Reaction)

文獻
(Literature)

合成路徑規畫



連結外部
資料庫

小分子資料

PubChem ^{10 Years}

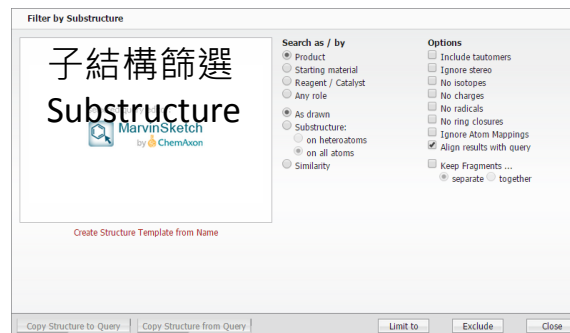
供應商資料

eMolecules

Scopus

篩選功能：Analysis View 及 28 種 Filter

Open Analysis View



子結構篩選
Substructure
MarvinSketch
by ChemAxon

Search as / by

- Product
- Starting material
- Reagent / Catalyst
- Any role
- As drawn
- Substructure:
 - on heteroatoms
 - on all atoms
- Similarity

Options

- Include tautomers
- Ignore stereo
- No isotopes
- No charges
- No radicals
- No ring closures
- Ignore Atom Mappings
- Align results with query
- Keep Fragments ...
 - separate
 - together

Create Structure Template from Name

Copy Structure to Query | Copy Structure from Query | Limit to | Exclude | Close

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

Document Type

Authors

Patent Assignee

Journal Title

Publication Year

Substructure

Yield

Record Type

Reagent/Catalyst

Solvent

Reaction Type

No. of Steps

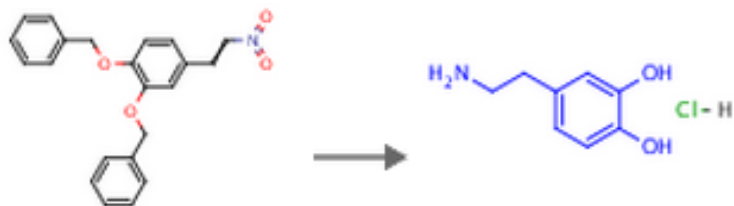
Product Availability

Reactant Availability

Availability in other DBs

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

Reaction step: CC(C)(C)OC(=O)NCC1=CC=C(O)C=C1 + Cl → NCC1=CC=C(O)C=C1 (100.00% yield)

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

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

Synthesis 1 x Synthesis 2 x Synthesis 3 x Synthesis 4 x Synthesis 5 x

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

Synthesize (27)

Synthesize (158)

2 Details

Add Remove

1 Details

99 %

Add Remove

Available through...

- Accelrys' ACD
- eMolecules
- CambridgeSoft ACX
- PharmaPendium

Safety Data...

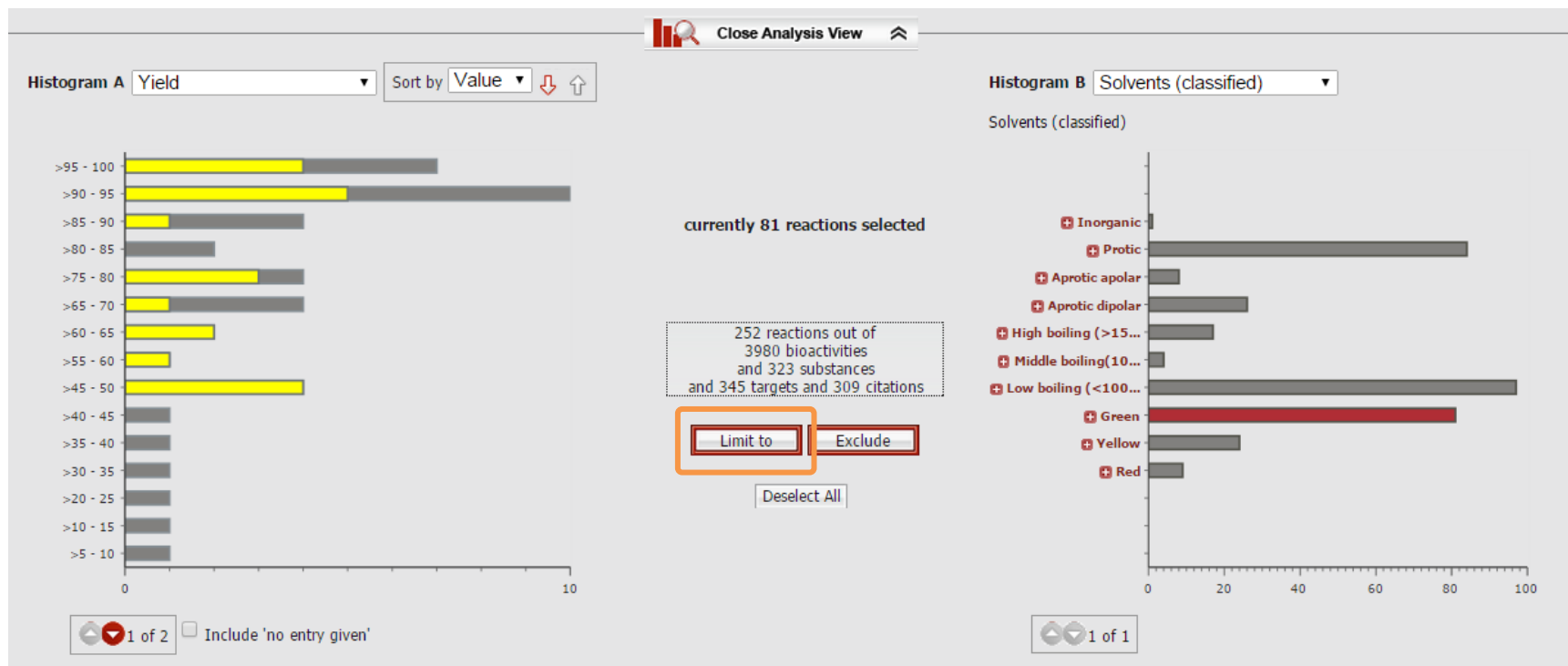
Reaxys-RN: 3656720
 MF: C8H12NO2*Cl
 MW: 189.642
 CAS-RN: 62-31-7

Show Details

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

Analysis View 視覺化分析系統

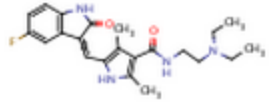
範例：使用環保溶劑，合成反應的產率分布



結果畫面相似結構搜尋

DISCOVERABILITY

Structure



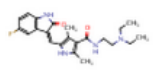
Synthesize | Show Details

Find similar



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
	7	80	137	231	351

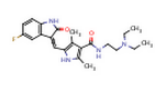
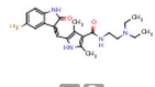
Cancel



80 substances out of 313 reactions and 5701 bioactivities and 949 targets and 420 citations

Heatmap Reactions Substances (Grid) **Substances (Report)** Targets Citations go to Page Page 1 of 9

Limit to Exclude Export Print Zoom in Zoom out Hide Sort by Similarity

Structure	% Similarity	Structure/Compound Data	N° of preparations All Preps All Reactions	Available Data	Target	N° of ref.
 Synthesize Show Details Find similar	100.0%	Chemical Name: N-[2-(diethylamino)ethyl]-5-[(5-fluoro-1,2-dihydro-2-oxo-3H-indol-3-ylidene)methyl]-2,4-dimethyl-1H-pyrrole-3-carboxamide Reaxys Registry Number: 9364276 CAS Registry Number: 557795-19-4 Type of Substance: heterocyclic Molecular Formula: C ₂₂ H ₂₇ FN ₄ O ₂ Linear Structure Formula: C ₂₂ H ₂₇ FN ₄ O ₂ Molecular Weight: 398.48 InChI Key: WINHZLLDWRZWR-ATVHPVEESA-N	32 prep out of 91 reactions.	Druglikeness Bioactivity Identification Physical Data (19) Spectra (28) Use/Application (330)	Show Targets	334
 Synthesize Show Details Find similar	100.0%	Chemical Name: [18F]SU11248 Reaxys Registry Number: 10127360 Type of Substance: heterocyclic Molecular Formula: C ₂₂ H ₂₇ FN ₄ O ₂ Linear Structure Formula: C ₂₂ H ₂₇ (¹⁸ F)N ₄ O ₂ Molecular Weight: 397.482 InChI Key: WINHZLLDWRZWR-RLPLYDDSA-N	1 prep out of 1 reactions.	Druglikeness Identification	Show Targets	1

結構相似性排序

Similarity sorting

- 結果畫面可直接點“Find similar”做相似結構搜尋
- 相似搜尋結果可依照相似性排序

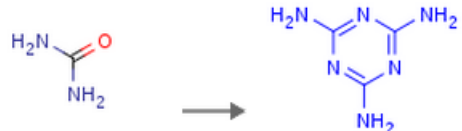
反應搜尋結果

儲存勾選的反應資料

排序

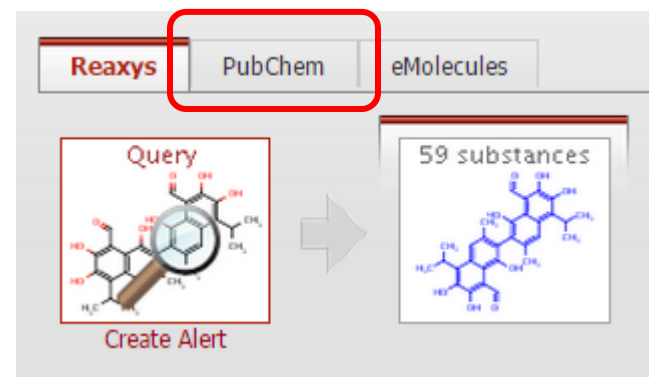
Limit to Exclude Export Print Zoom in Zoom out Hide

Sort by **No of References** ↓ ↑

<p>3</p>	 <p>Synthesize Find similar</p>	<p>Rx-ID: 748486 Find similar reactions</p> <p>查看包裝價格</p>
<p>98%</p>	<p>Stage #1: T=140 - 160°C; P=6000.48 Torr; Stage #2: With ammonia; γ-Al₂O₃ P=750.06 - 1500.12 Torr;</p>	<p>Available through...</p> <ul style="list-style-type: none"> Accelrys' ACD eMolecules CambridgeSoft ACX <p>erantsev; Tubolkin Chemistry, 2002, vol. 75, # 11 p. 1883 - 1884 View citing articles Show Details</p>
<p>88.5%</p>	<p>in water Product distribution / selectivity; Show Experimental Procedure</p>	<p>EUROTECNICA MELAMINE, LUXEMBOURG, ZWEIGNIEDERLASSUNG IN ITTIGEN Patent: WO2007/119156 A2, 2007 ; Location in patent: Page/Page column 16-19 ;</p> <p>Title/Abstract Full Text Show Details</p>
<p>12.6%</p>	<p>With ammonia High Pressure; 70 to 300 at; at 350°C; 120 min;</p>	<p>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</p>
<p>⌵ Show Next 20 Details ⌵ Show All Remaining Details (31)</p>		

PubChem 搜尋結果

切換至 PubChem 資料庫



PubChem | OPEN CHEMISTRY DATABASE

Search Compounds



Compound Summary for CID 3503

Download

Print

Share

Help

Gossypol

[Read about the new page format and features](#) [Go to the legacy page](#)



Vendors



Drug Information



Pharmacology



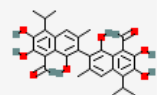
Literature



Patents



Bioactivities



PubChem CID:	3503
Chemical Names:	gossypol; 303-45-7; Pogosin; (-)-Gossypol; (+)-Gossypol; Tash 1; More...
Molecular Formula:	C ₃₀ H ₃₀ O ₈
Molecular Weight:	518.5544 g/mol
InChI Key:	QBKSWRVVCFDOT-UHFFFAOYSA-N
Modify Date:	2015-04-11
Create Date:	2005-03-25

[Cite this Record](#)

A dimeric sesquiterpene found in cottonseed (GOSSYPOLIUM). The (-) isomer is active as a male contraceptive (CONTRACEPTIVE AGENTS, MALE) whereas toxic symptoms are associated with the (+) isomer. *from MeSH [4]*

文獻搜尋結果 – 連結至 Scopus (世界大學排名採用系統)

COLLABORATION

Citations Author names, which can also be found in Scopus are now hyperlinks, so that information about affiliation and publications can be immediately looked up in Scopus.

The image shows a Reaxys interface with a search result for a document. The document title is "Asymmetric synthesis of andavadoic acid via base-catalyzed 5-exo-tet cyclization of a β -hydroperoxy epoxide". The authors listed are Barnych, Bogdan; Fenet, Bernard; Vatele, Jean-Michel. The year is 2013, and the source is Tetrahedron, 2013, vol. 69, # 1 p. 334 - 340. A blue arrow points from the author name "Vatele, Jean-Michel" in the citation to the Scopus author profile for "Vatèle, Jean Michel".

The Scopus profile for "Vatèle, Jean Michel" shows the following information:

- Universite Claude Bernard Lyon 1, Equipe SURCOOF Bât Raulin, Villeurbanne, France
- Author ID: 7004270318
- Documents: 73
- Citations: 1233 total citations by 857 documents
- h-index: 21
- Co-authors: 46
- Subject area: Biochemistry, Genetics and Molecular Biology, Chemistry

The Scopus profile also includes a graph showing the number of documents and citations over time (2005 to 2015). The graph shows a general upward trend in both documents and citations, with a peak in 2015.

The Scopus profile also includes a list of documents, with the following entries:

Document Title	Author	Year	Journal	Cited by
Regioselective oxidative cleavage of benzylidene acetals of glycopyranosides with periodic acid catalyzed by tetrabutylammonium bromide	Vatèle, J.-M.	2014	Synlett 25 (1), ST-2013-D0847-L, pp. 115-119	0
Erratum: Regioselective oxidative cleavage of benzylidene acetals of glycopyranosides with periodic acid catalyzed by tetrabutylammonium bromide (Synlett (2014) 1 (115))	Vatèle, J.-M.	2014	Synlett	0
One-pot oxidative conversion of alcohols into nitriles by using a TEMPO/Ph(OAc) ₂ /NH ₄ OAc system	Vatèle, J.-M.	2014	Synlett	0

三、Reaxys 搜尋結果分析及輸出

輸出報告與同儕分享討論

搜尋結果

化合物
(Substance)

反應
(Reaction)

文獻
(Literature)

合成路徑規畫

Synthesis Plans

資料庫連結

Pubchem
10 Years
eMolecules

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

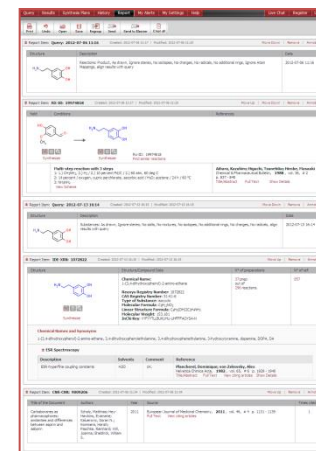
優點：適合儲存少量資料、操作簡便、格式簡明、保留超連結

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



多樣化結果輸出功能 -- 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

Report Item: **Query: 2012-07-06 11:16** Created: 2012-07-06 11:17 | Modified: 2012-07-06 11:20

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

Report Item: **RX-ID: 19974818** Created: 2012-07-06 11:17 | Modified: 2012-07-06 11:20

Yield	Conditions	References
	Rx-ID: 19974818 Find similar reactions	Aihara, Kazuhiro; Higuchi, Tsunehiko; Hirobe, Masaaki Chemical & Pharmaceutical Bulletin, 1988 , vol. 36, # 2 p. 837-840 Title/Abstract Full Text Show Details

Multi-step reaction with 3 steps
1: 1) CH₂Br₂, 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: Nal/Hg
View Scheme

Report Item: **Query: 2012-07-13 16:14** Created: 2012-07-13 16:15 | Modified: 2012-07-13 16:15

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

Report Item: **IDE-XRN: 1072822** Created: 2012-07-13 16:15 | Modified: 2012-07-13 16:15

Structure	Structure/Compound Data	N° of preparations	N° of ref.
	Chemical Name: 1-(3,4-dihydroxyphenyl)-2-amino-ethane Reaxys Registry Number: 1072822 CAS Registry Number: 51-61-6 Type of Substance: azydic Molecular Formula: C ₈ H ₁₂ NO ₂ Linear Structure Formula: C ₈ H ₂ (OH) ₂ C ₂ H ₄ N ₂ Molecular Weight: 153.181 InChi Key: Y1FYFTLLBULJHU-UHFFFAOYSA-N	37 prep out of 296 reactions.	857

Chemical Names and Synonyms
1-(3,4-dihydroxyphenyl)-2-amino-ethane, 3,4-dihydroxyphenylethylamine, 3,4-dihydroxyphenethylamine, 3-hydroxytyramine, dopamine, DOPA, DA

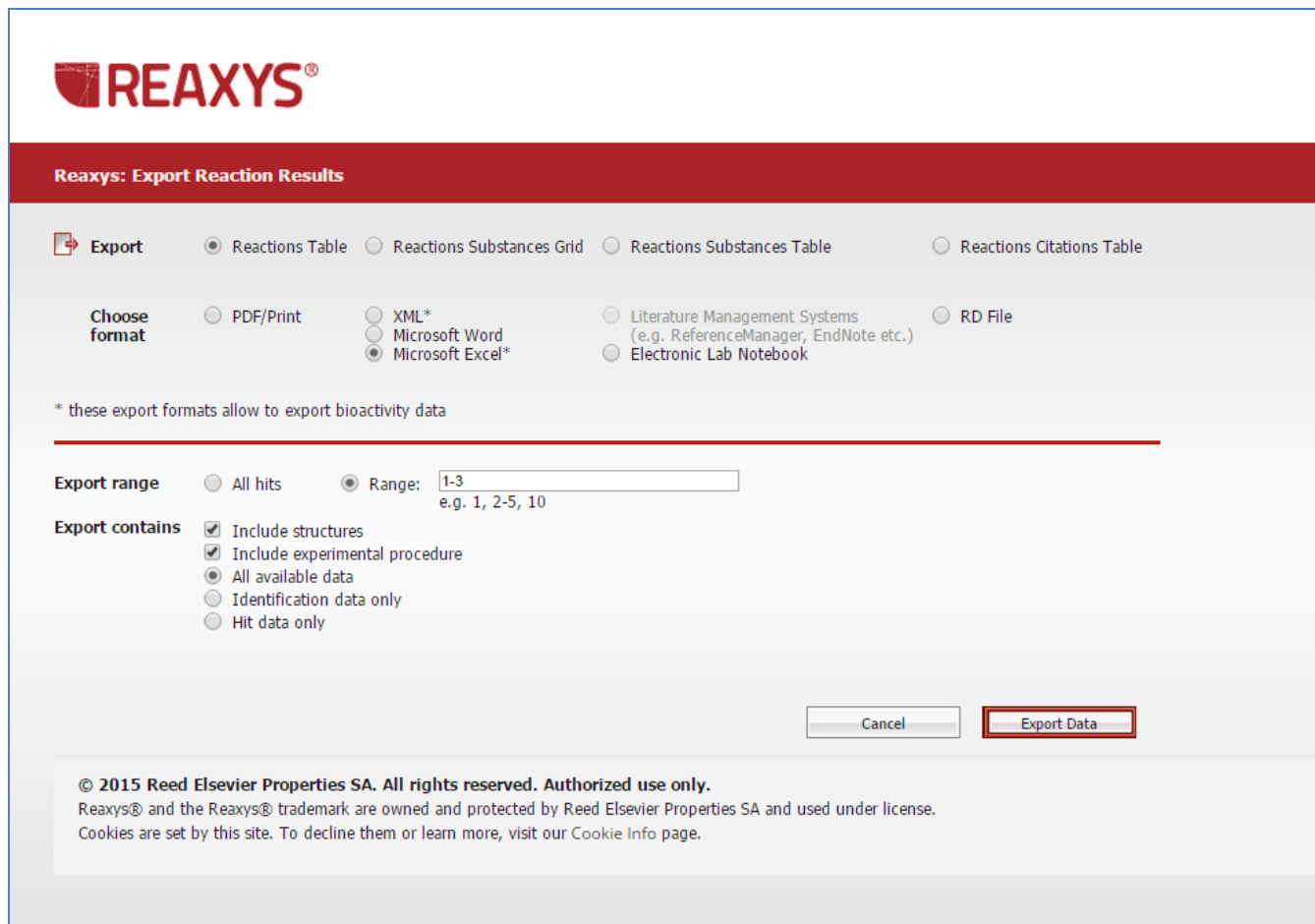
ESR Spectroscopy

Description	Solvents	Comment	Reference
ESR-hyperfine coupling constants	H2O	1H.	Plancherel, Dominique; von Zelewsky, Alex Helvetica Chimica Acta, 1982 , vol. 65, # 6, p. 1929-1940 Title/Abstract Full Text View citing articles Show Details

Report Item: **CHR-CHR: 9009206** Created: 2012-07-06 11:34 | Modified: 2012-07-06 11:34

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

輸出搜尋結果



REAXYS®

Reaxys: Export Reaction Results

Export Reactions Table Reactions Substances Grid Reactions Substances Table Reactions Citations Table

Choose format PDF/Print XML* Literature Management Systems (e.g. ReferenceManager, EndNote etc.) RD File
 Microsoft Word Microsoft Excel* Electronic Lab Notebook

* these export formats allow to export bioactivity data

Export range All hits Range:
e.g. 1, 2-5, 10

Export contains Include structures Include experimental procedure
 All available data Identification data only Hit data only



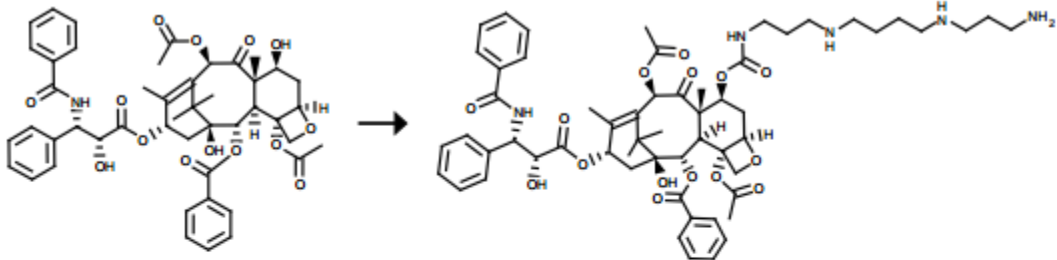
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https://www.reaxys.com/reaxys/printing/reaxys_anonymous_20150513_102021_206.pdf

分享搜尋結果

PDF EXPORT RESULT

Query

	Query	Results	Date
1. Query		80 reactions in Reaxys	2015-05-13 10h:09m:06s (EST)
2. Query	 <p>Search as: Product, As drawn, No salt</p> <p>filtered by Number of Reaction</p>		Rx-ID: 12697962 View in Reaxys 1/1
		Yield Conditions & References	
		Reaction Steps: 4 1: imidazole; DMAP 2: DMAP 3: 78 percent / HF*pyridine 4: CH ₂ Cl ₂ ; propan-2-ol With 1H-imidazole, 4-(N,N-dimethylamino)pyridine, pyridine hydrogenfluoride in dichloromethane, isopropyl alcohol Battaglia, Arturo; Guerrini, Andrea; Baldelli, Eleonora; Fontana, Gabriele; Varchi, Greta; Samori, Cristian; Bombardelli, Ezio; Tetrahedron Letters; vol. 47; nb. 16; (2006); p. 2667 - 2670 View in Reaxys	

個人化功能

註冊及登錄

個人化功能

1. Report: 輸出報告
2. History: 搜尋紀錄
3. My Alerts: 新知通報
4. My Settings: 個人化設定

輸入英文資料

密碼建議包含大小寫、
數字及特殊符號(*_.)

點擊送出資料

The screenshot displays the Elsevier registration and login page. At the top, a navigation bar includes links for Query, Results, Synthesis Plans, History, Report, My Alerts, My Settings, and Help. The main content area is divided into two sections: 'Register' and 'Login'.

Register Section:

- Title:** A dropdown menu with 'Mr' selected.
- First Name:** A text input field.
- Last Name:** A text input field.
- Email:** A text input field.
- Job title:** A text input field.
- Institution:** A text input field.
- Location:** A text input field.
- Password:** A text input field.
- Confirm password:** A text input field.

Registration Options:

- I have read and understand the **Registered User Agreement** and agree to be bound by all of its terms.*
- I wish to sign-up to receive product update bulletins and the bi-monthly Reaxys newsletter.
- I wish to receive special offers and promotions from Elsevier Information Systems GmbH and its affiliates about related products and services.

Login Section:

- User name:** A text input field containing 'o.liang@elsevi'.
- Password:** A text input field with masked characters.
- Remember me on this computer
- [Forgotten password](#)
- [Institution Login](#)


Buttons:

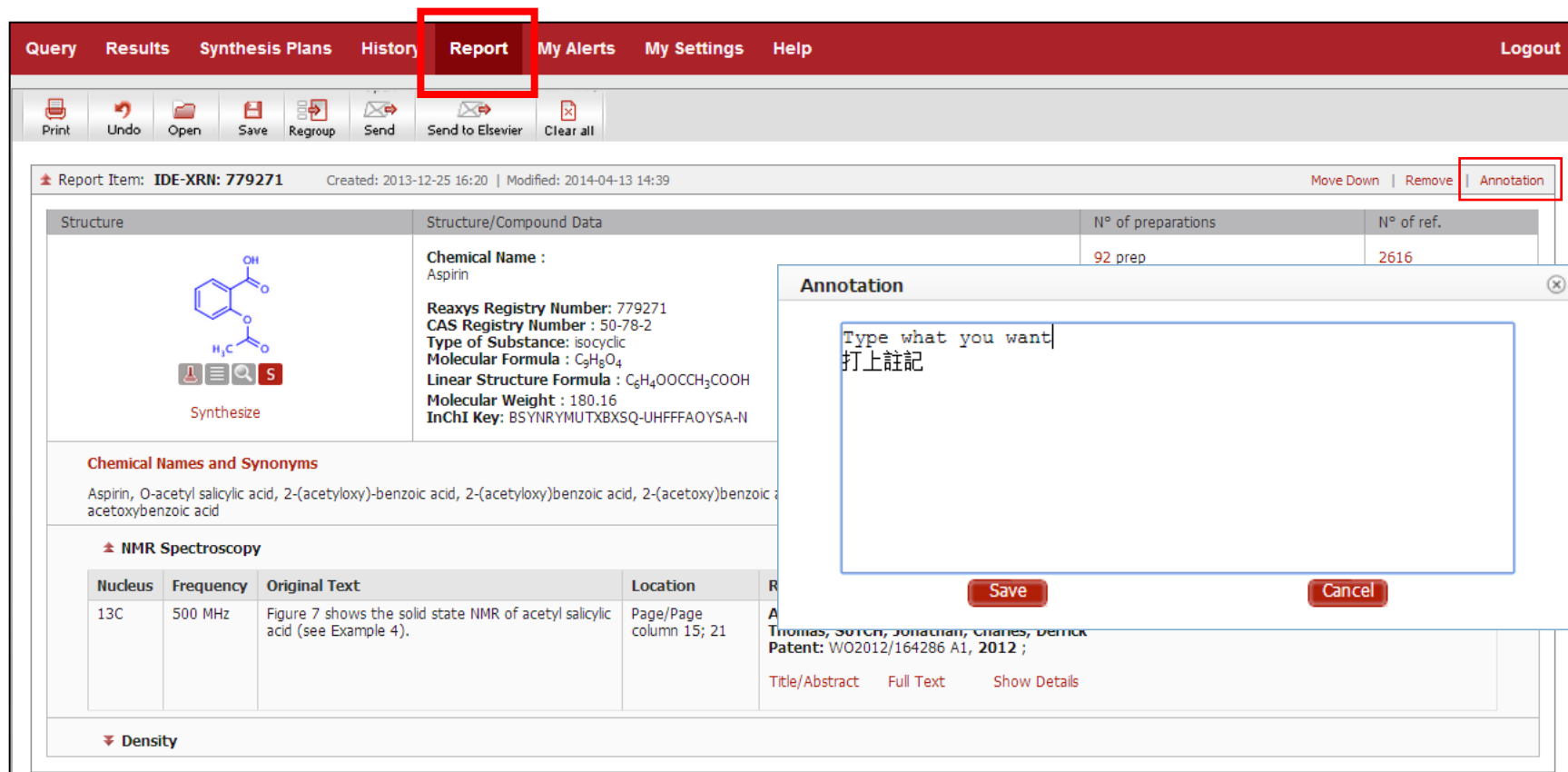
- Register:** A button at the bottom of the registration form.
- Go:** A button next to the login password field.

Annotations:

- A callout box points to the 'Title' dropdown with the text '輸入英文資料'.
- A callout box points to the 'Password' field with the text '密碼建議包含大小寫、數字及特殊符號(*_.)'.
- A callout box points to the 'Register' button with the text '點擊送出資料'.

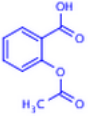
1. Report

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。



The screenshot displays the Reaxys software interface. The top navigation bar includes 'Query', 'Results', 'Synthesis Plans', 'History', 'Report', 'My Alerts', 'My Settings', 'Help', and 'Logout'. The 'Report' menu item is highlighted with a red box. Below the navigation bar is a toolbar with icons for Print, Undo, Open, Save, Regroup, Send, Send to Elsevier, and Clear all. The main content area shows a report for 'IDE-XRN: 779271' (Aspirin). The report includes a chemical structure, chemical name, registry numbers, molecular formula, and a table of NMR spectroscopy data. An 'Annotation' dialog box is open, allowing users to add notes to the report. The dialog box contains a text input field with the placeholder text 'Type what you want' and the Chinese characters '打上註記'. The dialog box also has 'Save' and 'Cancel' buttons.

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

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

Density

多樣化結果輸出功能 -- 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 'Report' section of the Reaxys interface, which is organized into several report items. Each item is color-coded and linked to a specific output category:

- Report Item: Query: 2012-07-06 11:16** (Blue box): Shows search results for a query, including a chemical structure and a description of reaction mappings.
- Report Item: RX-ID: 19974818** (Purple box): Displays a reaction scheme with reagents and conditions, along with a reference to a scientific paper.
- Report Item: Query: 2012-07-13 16:14** (Red box): Shows search results for a specific compound, including its structure and a description.
- Report Item: IDE-XRN: 1072822** (Red box): Provides detailed compound data such as chemical name, CAS number, molecular formula, and ESR spectroscopy information.
- Report Item: CHR-CHR: 9009206** (Green box): Lists search results for chemical literature, including document titles, authors, years, and sources.

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

合併搜尋

結合多個搜尋條件

Select how you want to combine the hitsets



Merge 104 with 99



Overlap 104 with 99



Exclude 104 from 99



Exclude 99 from 104

Cancel

Combine hitsets

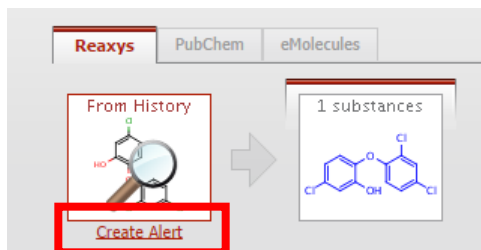
Select at least two hitsets for combining



	Query	Temporary result description			Date
<input type="checkbox"/>	105	19 citations Overlap 2 items from History	View	Store	2015-04-19 16:58
<input checked="" type="checkbox"/>	104 Edit Create Alert Literature: (Citation Basic Index = 'toxic*')	974822 citations Literature: (Citation Basic Index = 'toxic*')	View	Store	2015-04-19 16:57
<input type="checkbox"/>	103	591110 reactions	View	Store	
<input type="checkbox"/>	102	1098618 bioactivities	View	Store	
<input type="checkbox"/>	101	472699 substances	View	Store	
<input type="checkbox"/>	100	6322 targets	View	Store	
<input checked="" type="checkbox"/>	99 Edit Create Alert Literature: (Citation Basic Index = "Ractopamine*")	604 citations Literature: (Citation Basic Index = "Ractopamine*")	View	Store	2015-04-19 16:57
<input type="checkbox"/>	98	40 reactions	View	Store	
<input type="checkbox"/>	97	738 bioactivities	View	Store	
<input type="checkbox"/>	96	202 substances	View	Store	
<input type="checkbox"/>	95	12 targets	View	Store	

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。



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

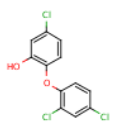
E-mail Address send copy to

REAXYS[®] Recorded Webinar: **Solving tough chemistry problems Insights from an industry expert** Tuesday, Sept. 16, 9:00 AM EDT Olivia Liang (o.liang@elsevier.com) is logged in

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

Reaxys PubChem eMolecules

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

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

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

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。

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 Dotmatic'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

線上資源

WEBINAR & HELP

Ease of Use: 首頁上方，不定期提供產品最新消息，如資料庫更新、線上講座訊息等。

Professor Forest Robertson of Western Connecticut State University explains how he uses Reaxys to further educational goals. [Read the article.](#)



Query Results Synthesis Plans History Report My Alerts My Settings Help

REAXYS[®] AND REAXYS[®] Medicinal Chemistry

Search for help...

Contact Us

Ease of Use: 使用 HELP 時，系統自動辨認使用者權限，並提供對應的說明

All Questions

New Features (5)

General Information

Admin Tools (2)

Guides, Videos and Workflows

Webinars

Queries Q&A

Results Q&A

Settings Q&A (9)

Structure Editors Q&A (4)

Alerts Q&A (2)

Searching for Literature in Reaxys

You can view a video tutorial on 'Searching for Literature in Reaxys' below. Spanish, Portuguese or French subtitles are also available. Please click on the 'CC' option, to access the language...

Reactions Search Options

On the Reactions query page, you can input a full reaction or just one substance. Data can be searched alone or with a substance/reaction. Click the Role radio button located...

Finding Reactions in Reaxys

You can view a video tutorial on 'Finding Reactions in Reaxys' below.

Ask Reaxys

Reaxys contains a huge amount of synthesis details, has a rich data set of substance properties, and includes vast literature coverage and index terms. Ask Reaxys is designed to help you get...

How do I set up a reaction query?

Click the 'Reactions' icon. On the 'Reactions query page', you can input a full reaction or just one substance. Data can be searched alone or with a substance/reaction. Click the 'Role radio' button...

中文線上資源

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Query 搜尋頁面介紹

Substances - Result Page 化合物搜尋

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由化學家專為化學家所設計

進入Reaxys化學資料庫

Reaxys中文支援

Reaxys研究迷俱樂部

加入粉絲團

Scopus

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REAXYS

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WIX PAGES

776

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

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- Elsevier 台灣電子報 - 2013年一月號
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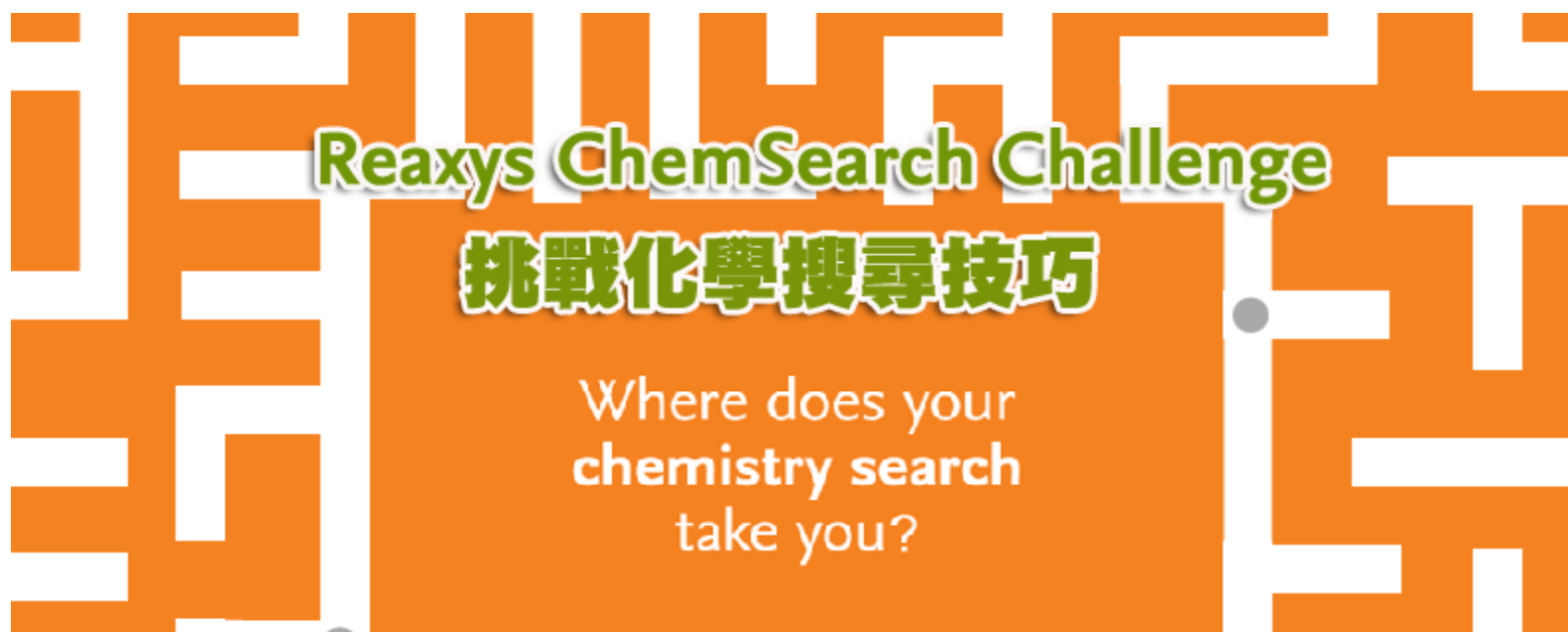
近期活動 – ChemSearch Challenge

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挑戰化學搜尋技巧

Where does your
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take you?

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Thank you!



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