Reaxys 化學資料庫
教育訓練

www.reaxys.com

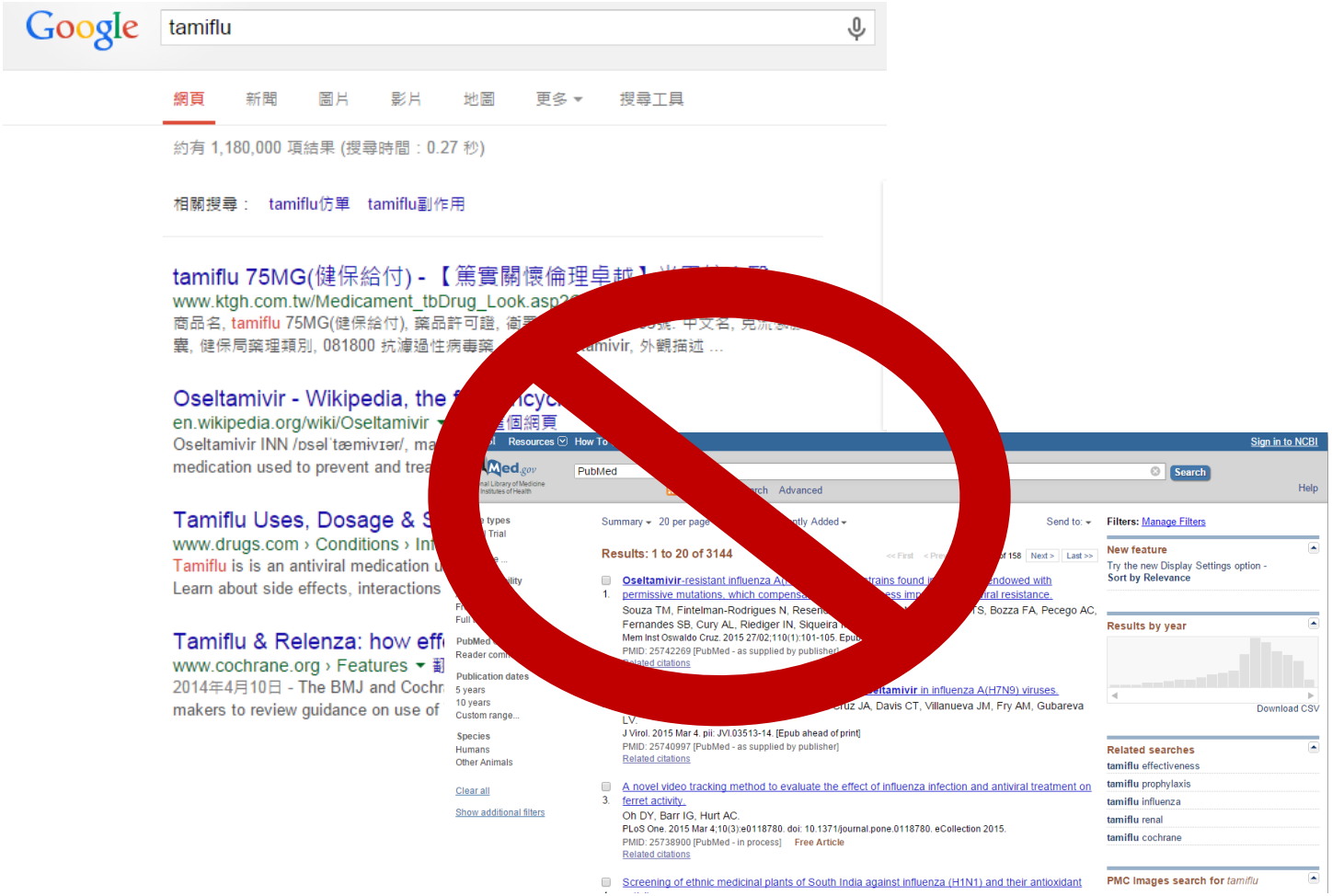
Elsevier 生命科學解決方案經理

Olivia Liang 梁成芝

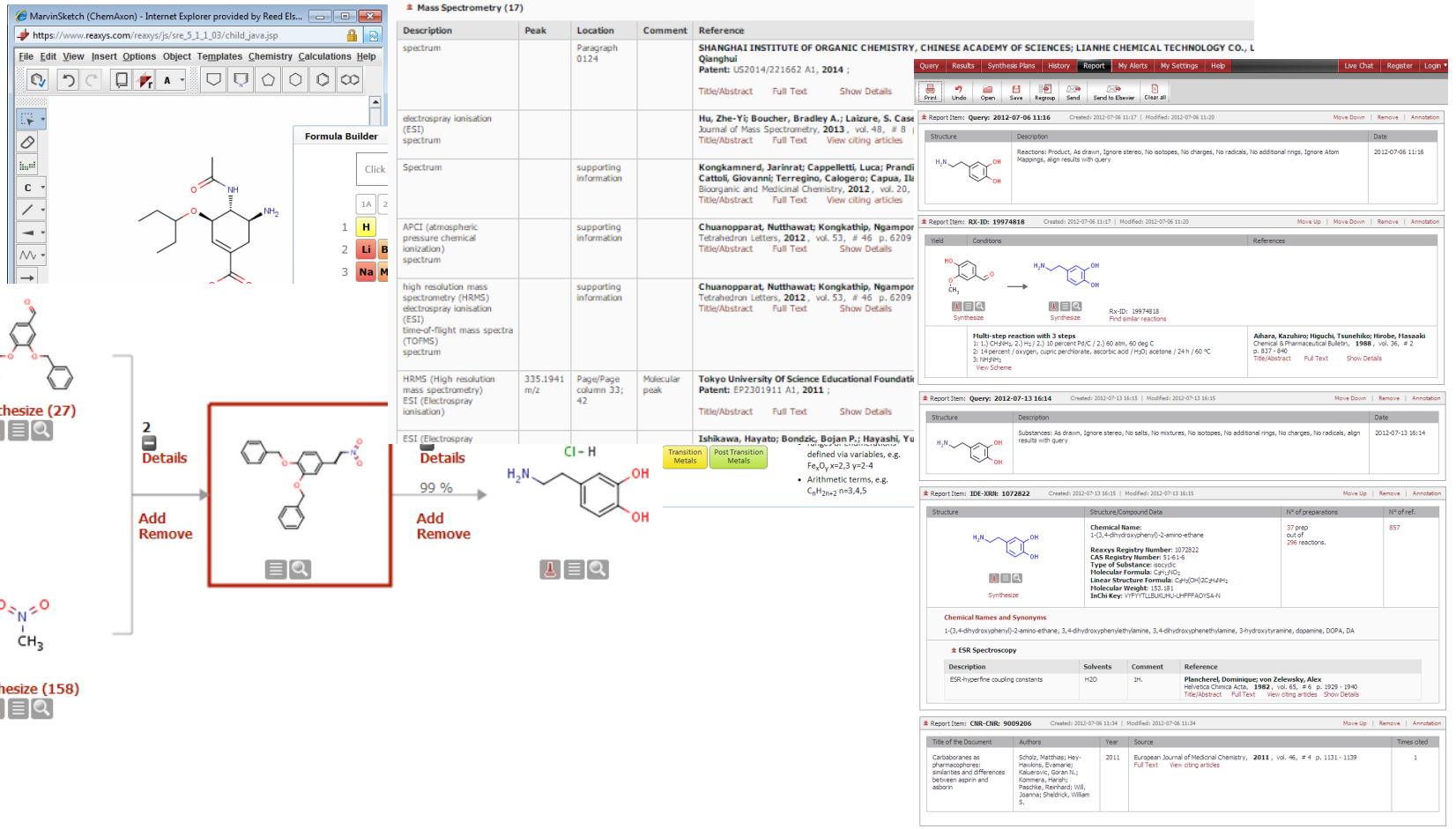
2015.9.24

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

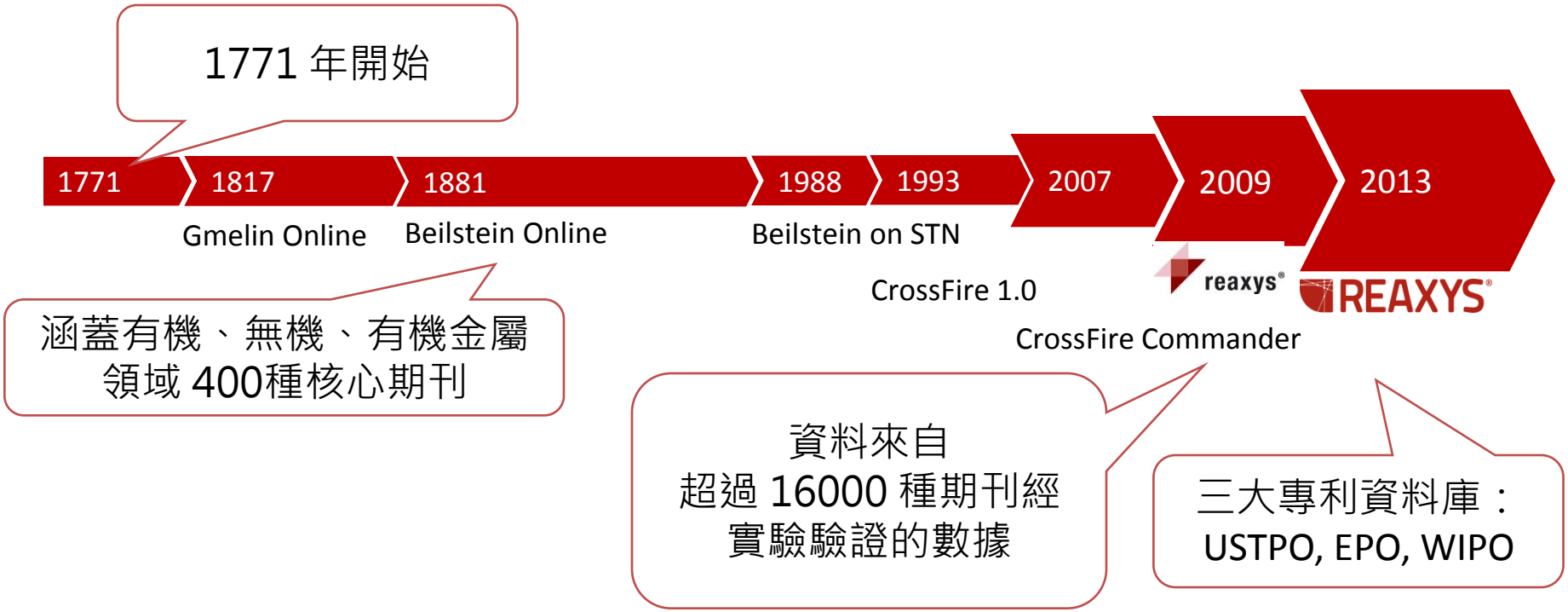


Smarter Chemistry



Reaxys 的過去與現在

承襲 Gmelin, Beilstein, 與 CrossFire 資料庫



Reaxys 2015

文獻資料

化合物

- 物化特性
- 實驗數據

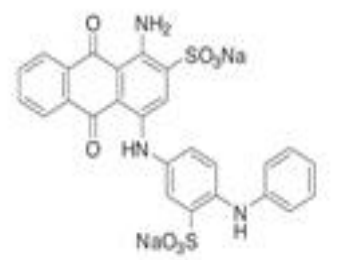
化學反應

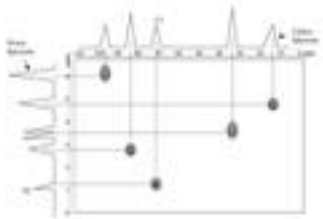
- 反應式
- 反應條件
- 合成路徑

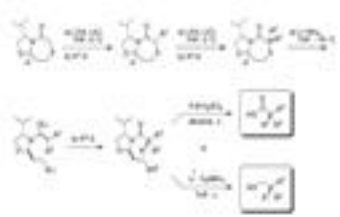
> 500 個欄位
可獨立或合併搜尋

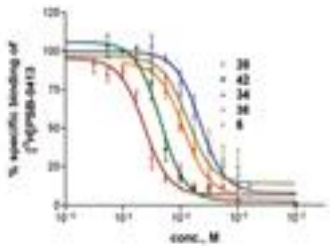
REAXYS資料擷取方式

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





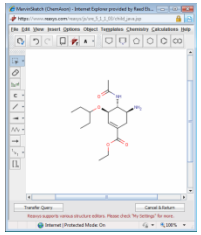




> 500 個欄位
可獨立或合併搜尋

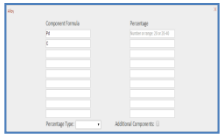
多元化搜尋管道

結構



分子式

合金



Reaxys Tree

> 500 個欄位

Reaction Basic Index | is | Sharpl* | Lookup

Ask Reaxys | Sharpless | 自動辨識關鍵字屬性 | Go

Examples

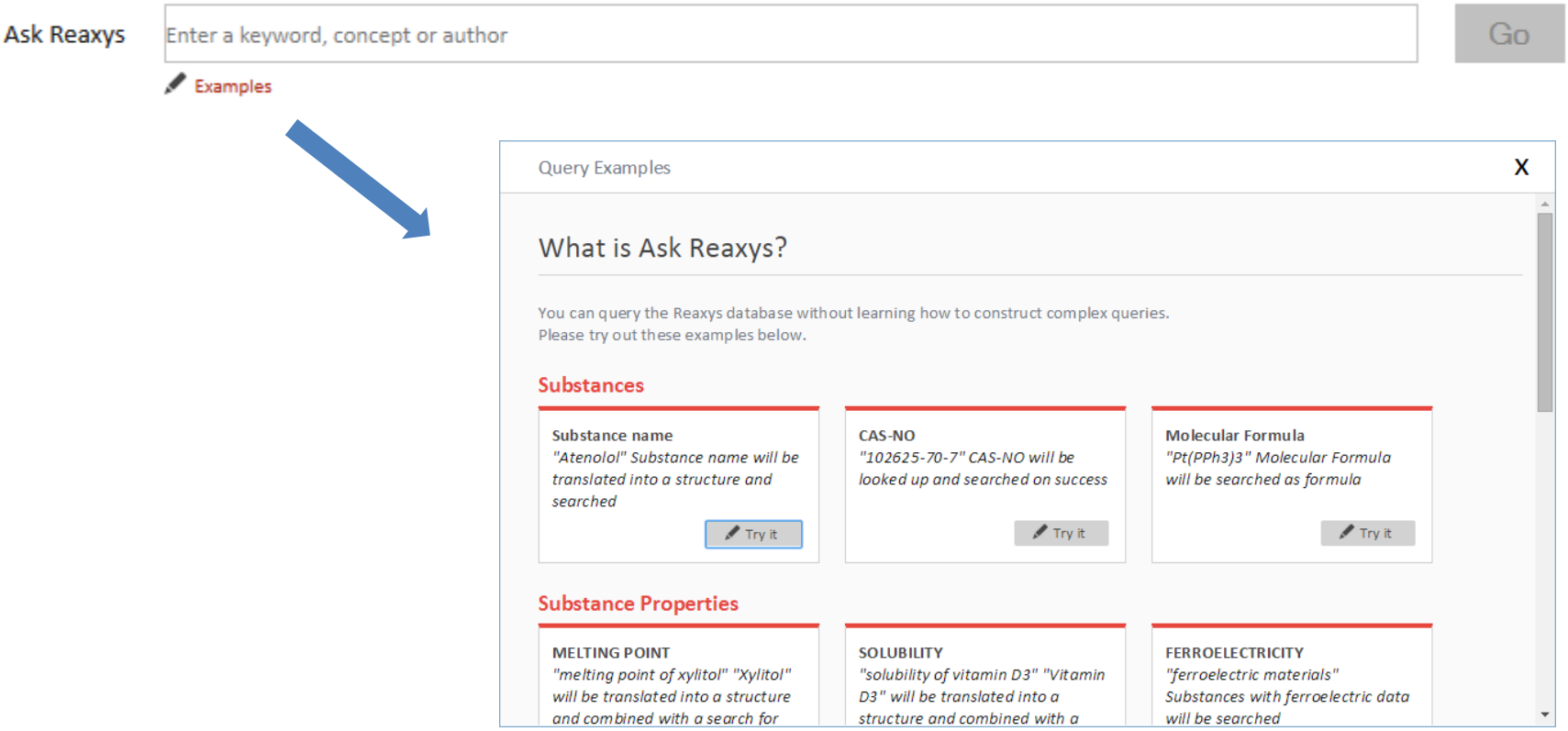
搜尋結果

- 化合物 (Substance)
- 反應 (Reaction)
- 文獻 (Literature)

Ask Reaxys 搜尋範例

EASY OF USE

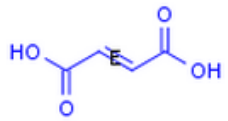
Ask Reaxys
A set of examples have been implemented providing users with an overview about Ask Reaxys capabilities, helping them to get the most out of this feature.



Ask Reaxys 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:** $C_4H_4O_4$ **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

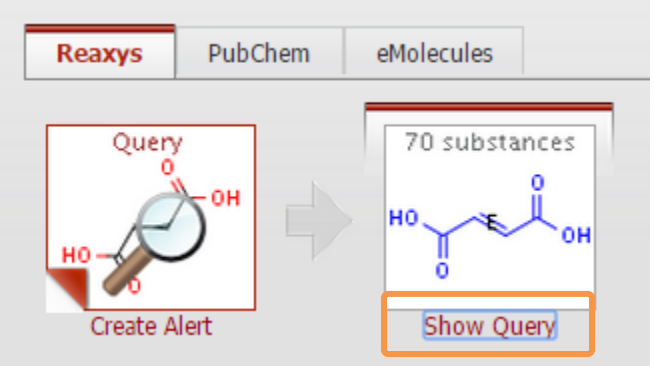
Hit Data

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



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
maleic acid HPLC **Result: substances** Show query	70 substances in Reaxys	Search Edit query in Advanced
maleic acid HPLC **Result: citations** Show query	182 citations in Reaxys	Search Edit query in Advanced

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
Title/Abstract				
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
Title/Abstract				
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
Title/Abstract				
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
Title/Abstract				
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
Title/Abstract				

檢測方式：毛細管電泳
(Capillary electrophoresis)

檢測方式：HPLC

檢測方式：Flow Injection

Reaxys 搜尋架構

建立搜尋指令

搜尋結果

篩選分析

資料儲存與輸出

- **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

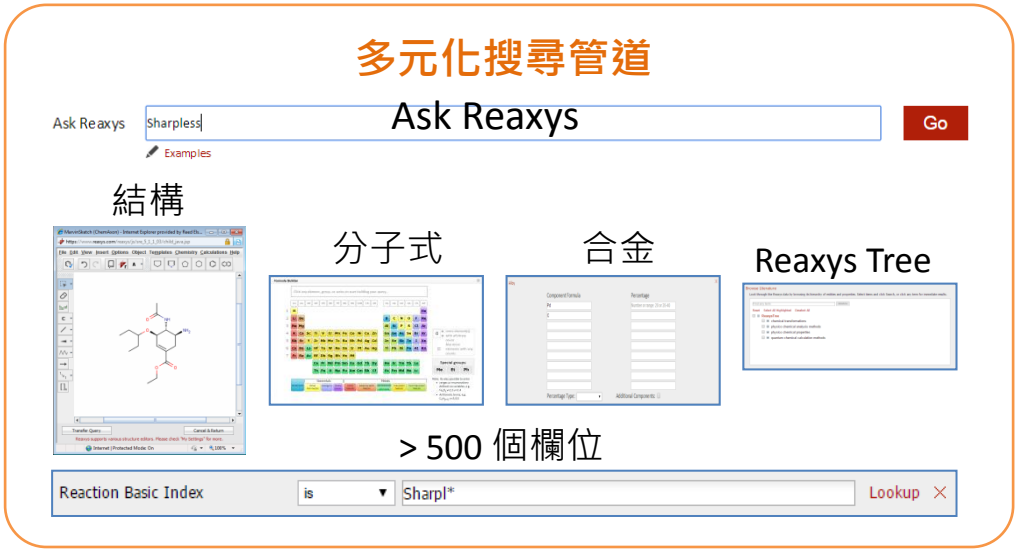
- Reaction: 反應
- Substance: 化合物
- Literature: 文獻

- AutoPlan: 自動規劃合成路徑
- 連結外部資料庫
- Analysis View 及 filter: 資料篩選

- Report 報告格式
- Export 輸出資料

一、Reaxys 搜尋架構

選擇合適的搜尋管道

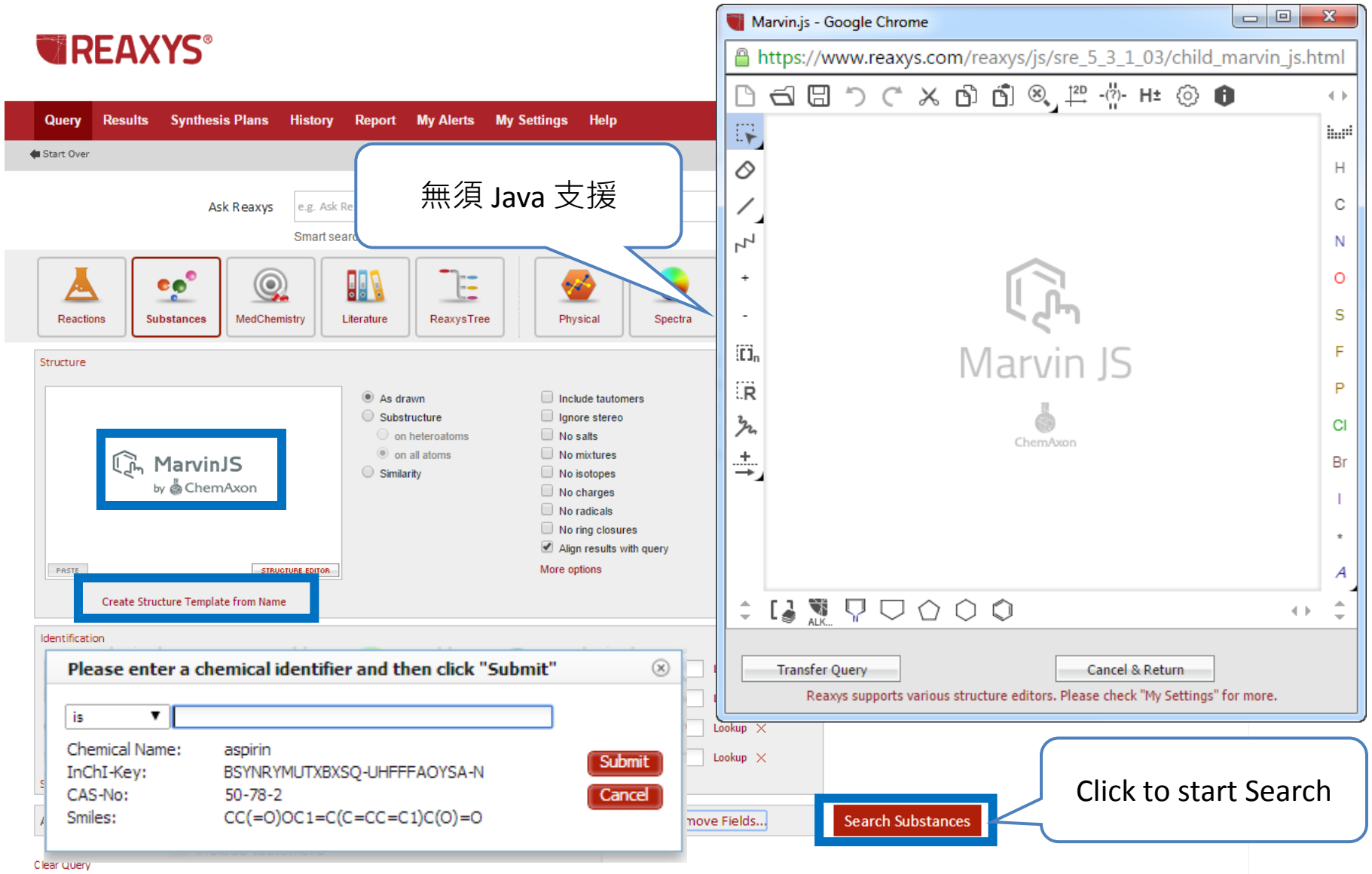


布林邏輯

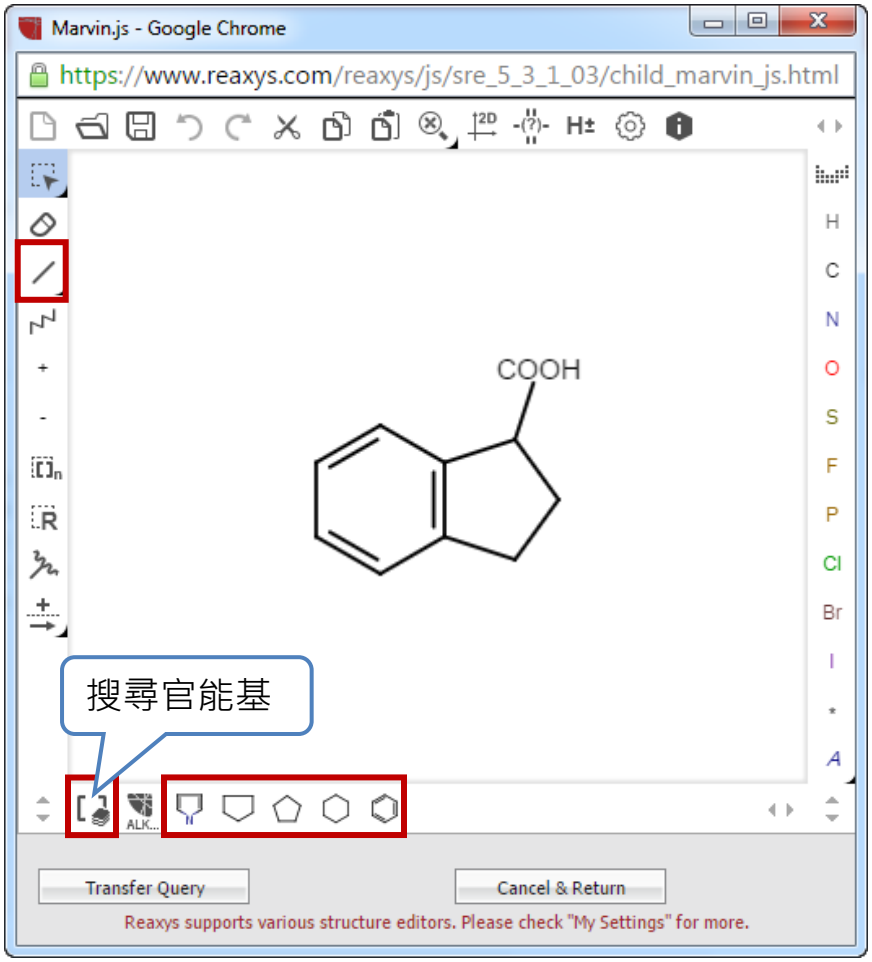
搜尋結果

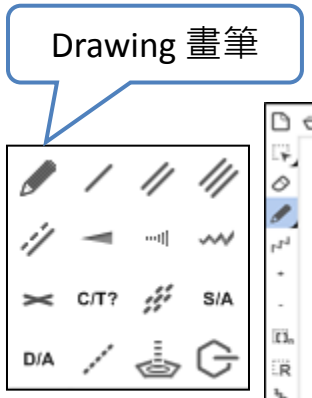
- 化合物 (Substance)
- 反應 (Reaction)
- 文獻 (Literature)

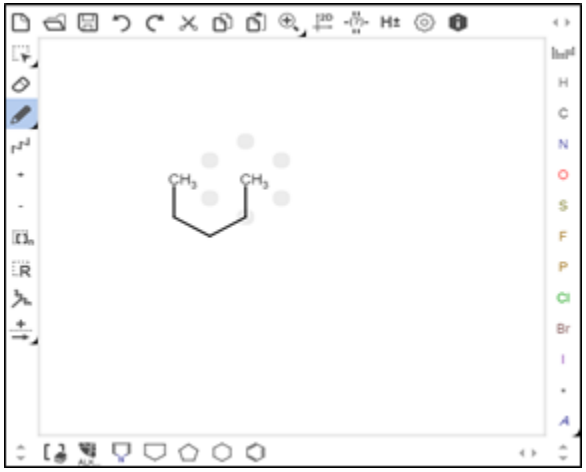
結構搜尋 – Marvin JS

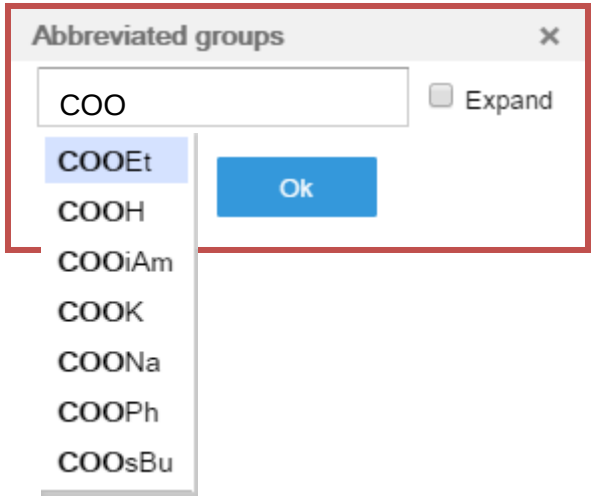


Marvin JS – Basic search function

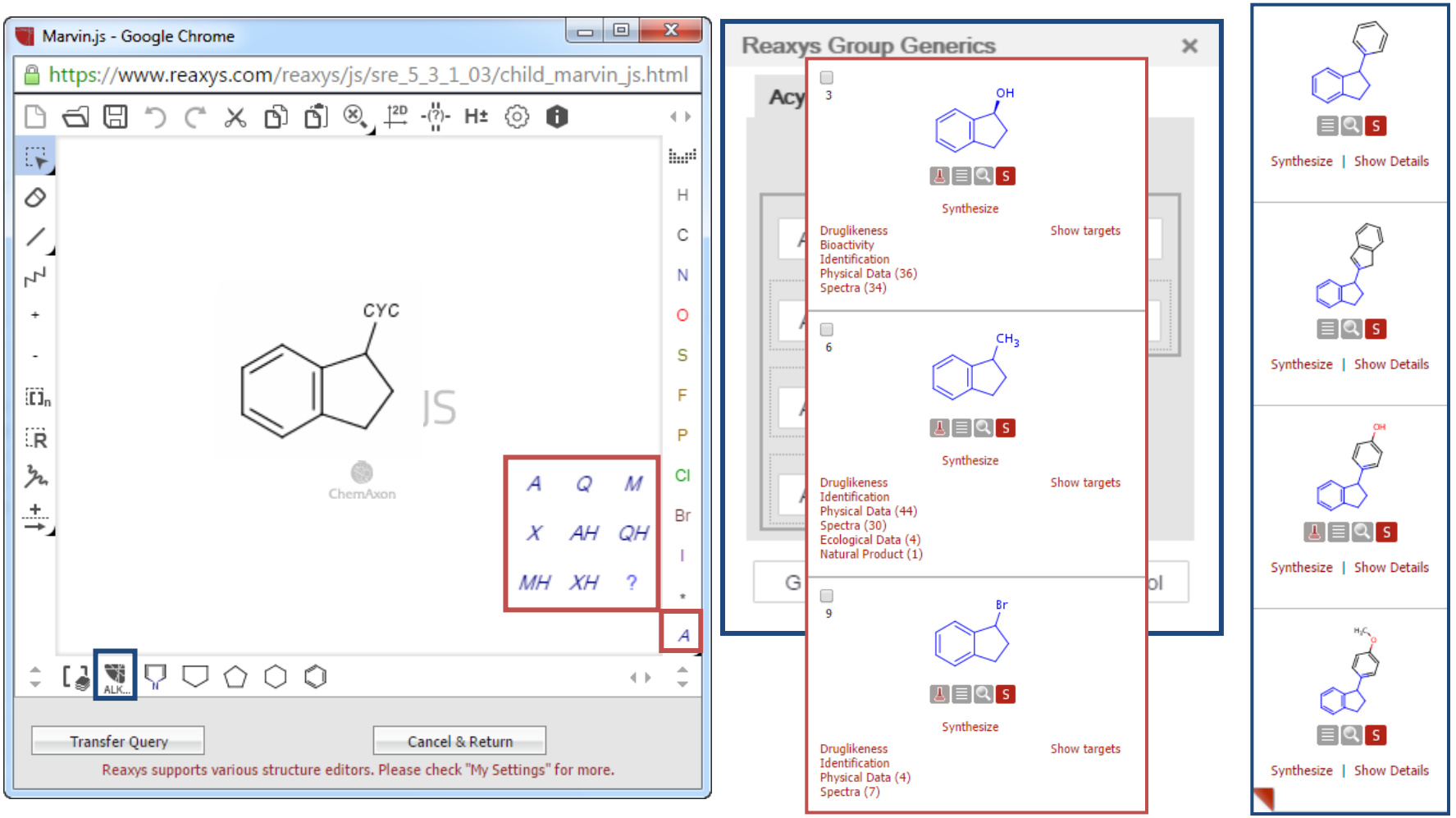




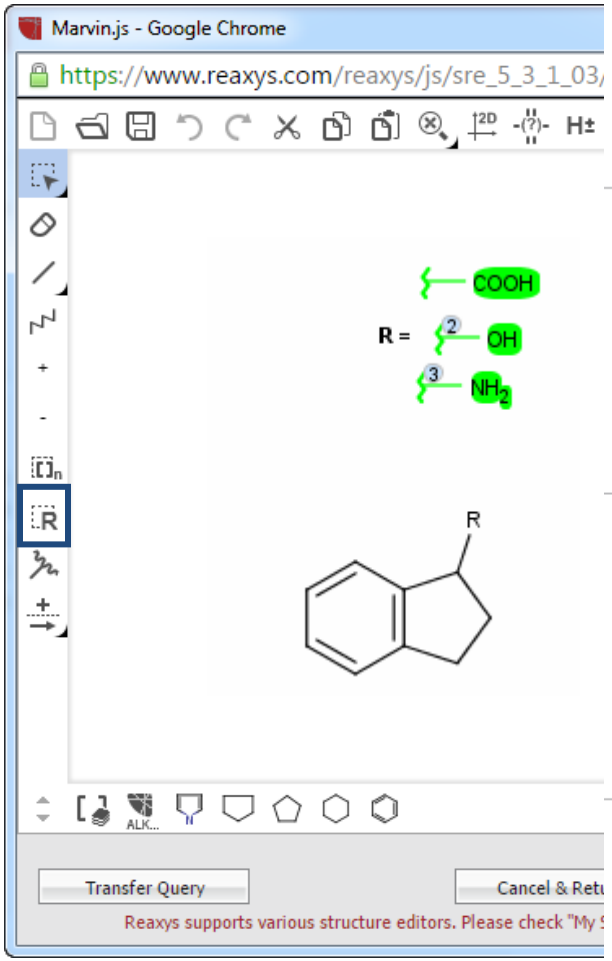


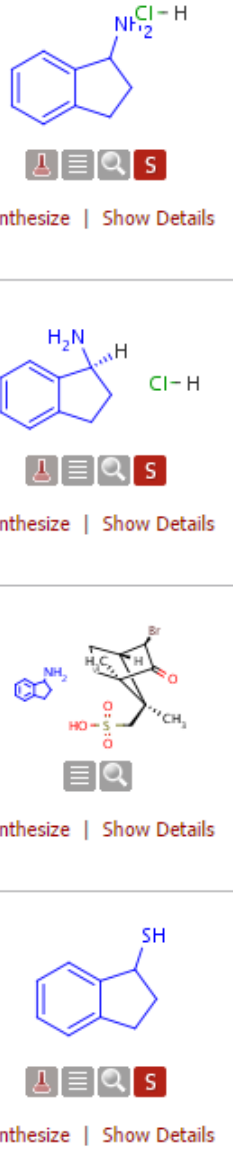


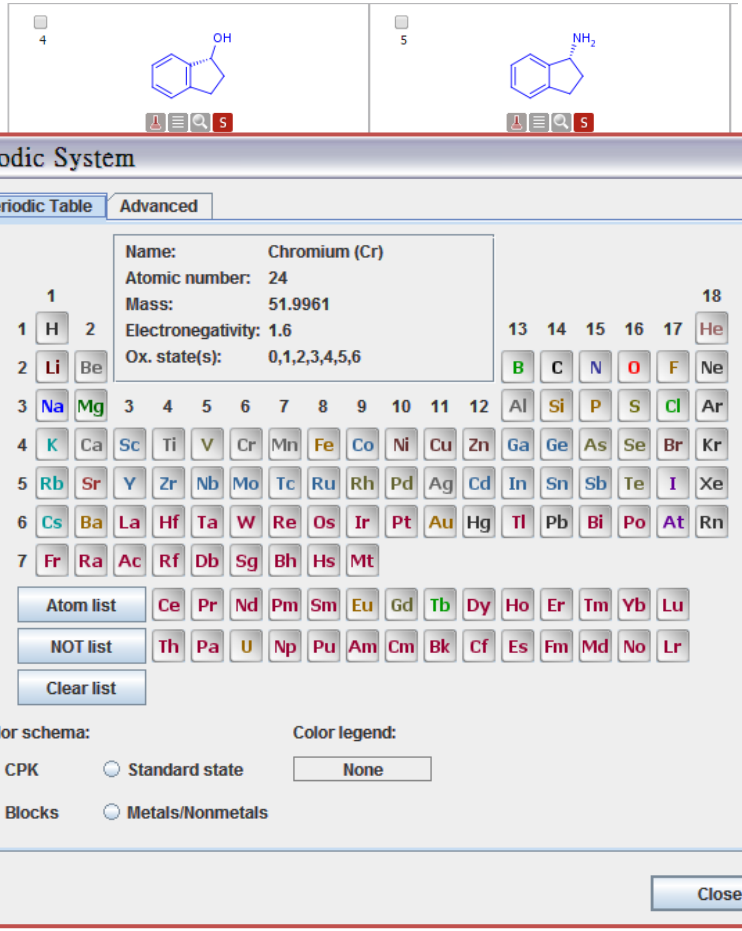
Marvin JS – substructure search



Marvin JS – substructure search







搜尋指令

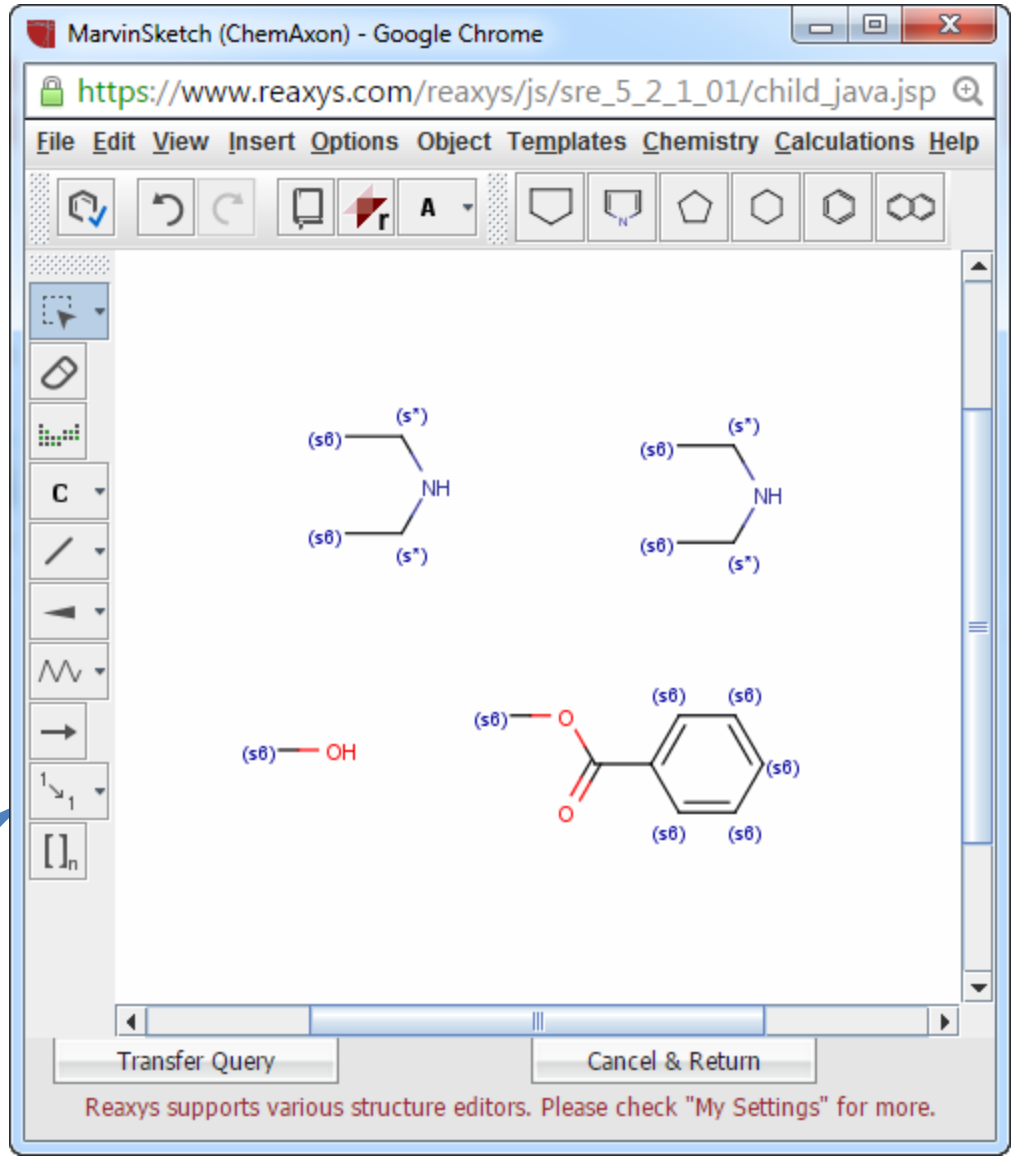
結構搜尋

廣瀨教授：

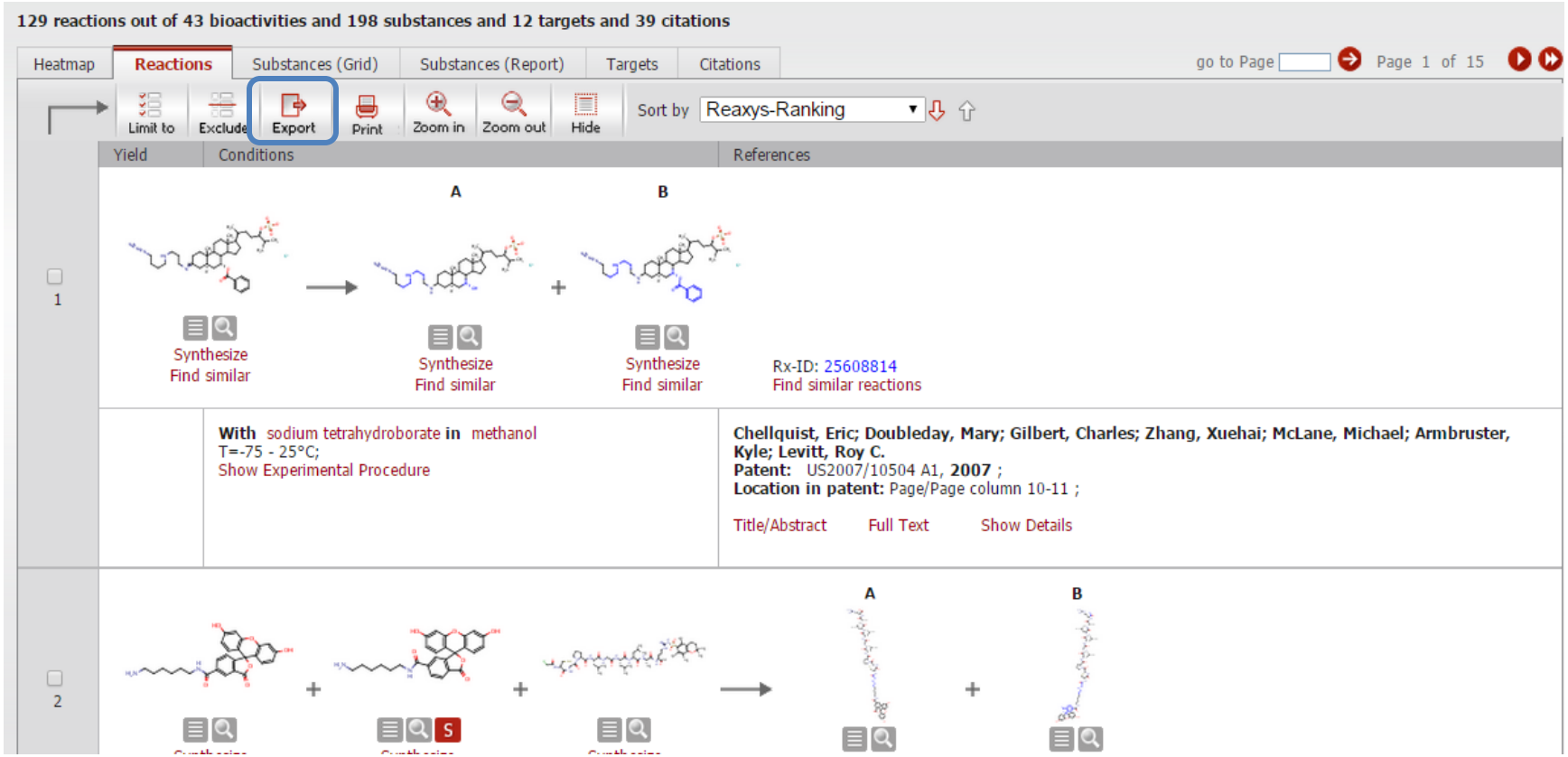
我曾對醇類及胺類的醯化 (acylation) 反應感興趣，一般來說胺化作用 (amination) 比酯化作用 (esterification) 更容易發生，因此通常胺基比羥基更容易反應，但我想找出羥基有反應而不改變胺基的反應

特殊搜尋技巧：

- Substitution count
- Atom mapping

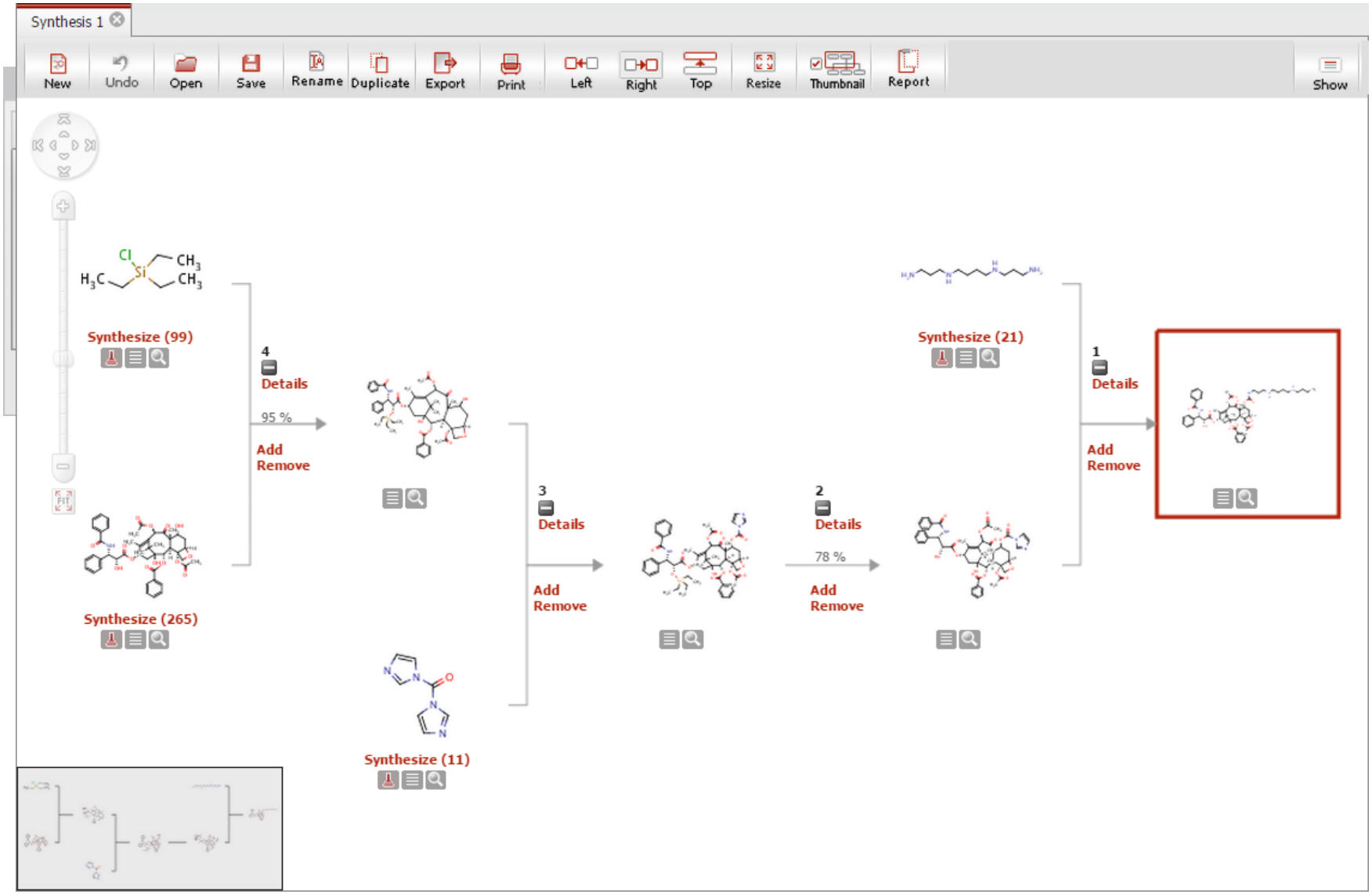


搜尋結果

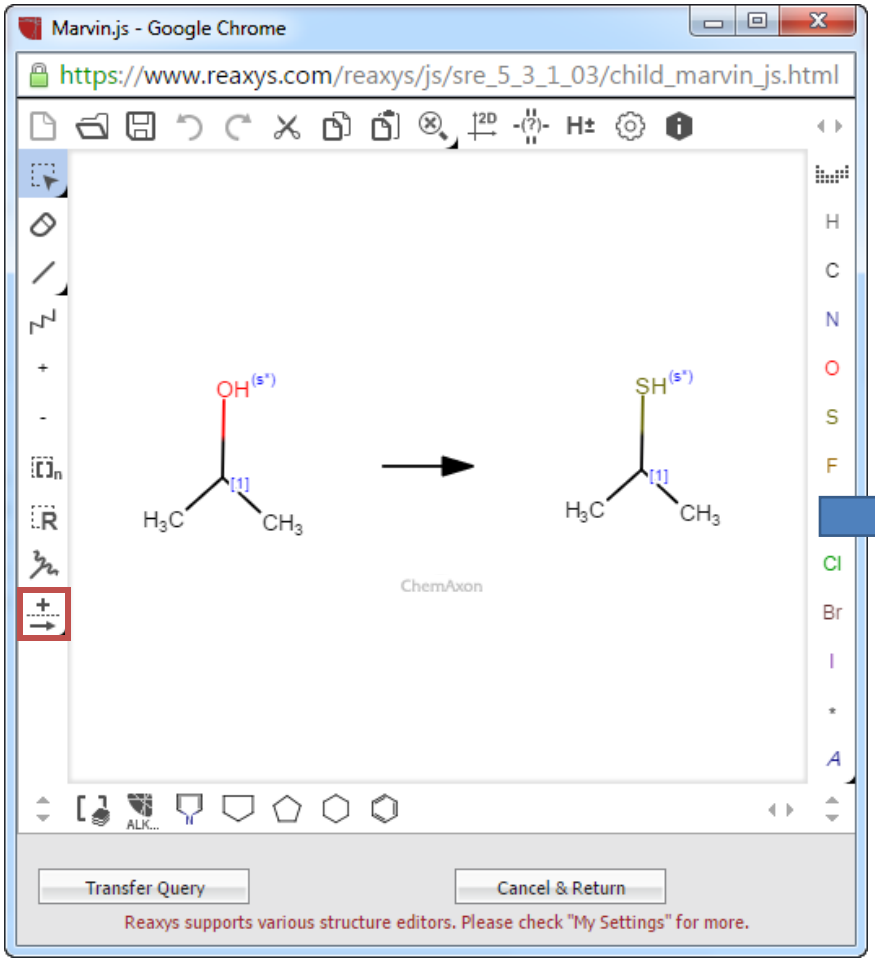

129 reactions out of 43 bioactivities and 198 substances and 12 targets and 39 citations
Heatmap
Reactions
Substances (Grid)
Substances (Report)
Targets
Citations
go to Page
Page 1 of 15
Limit to
Exclude
Export
Print
Zoom in
Zoom out
Hide
Sort by
Reaxys-Ranking
Yield
Conditions
References
A
B
1
Synthesize
Find similar
Synthesize
Find similar
Synthesize
Find similar
Rx-ID: 25608814
Find similar reactions
With sodium tetrahydroborate in methanol
T=-75 - 25°C;
Show Experimental Procedure
Chellquist, Eric; Doubleday, Mary; Gilbert, Charles; Zhang, Xuehai; McLane, Michael; Armbruster, Kyle; Levitt, Roy C.
Patent: US2007/10504 A1, 2007 ;
Location in patent: Page/Page column 10-11 ;
Title/Abstract
Full Text
Show Details
2
A
B

檢視現有合成路徑

點選 VIEW SCHEME 檢視合成路徑圖

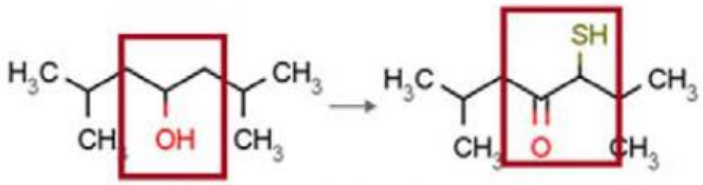


Marvin JS – atom mapping



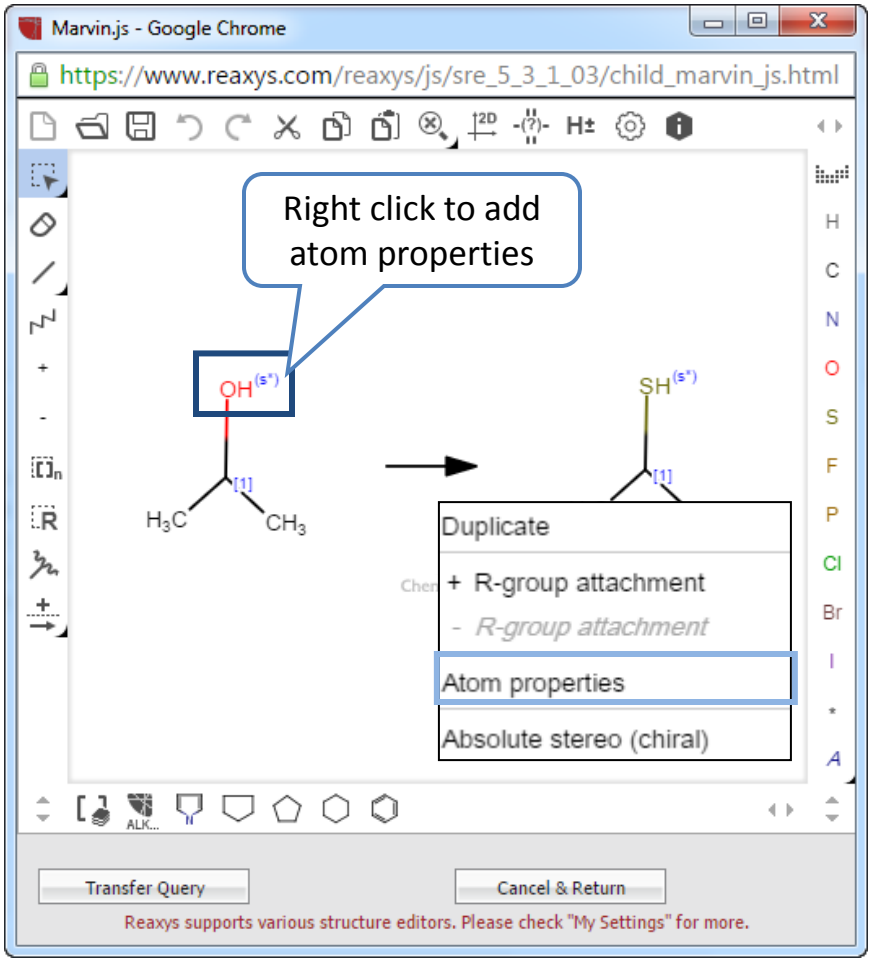
結果差異

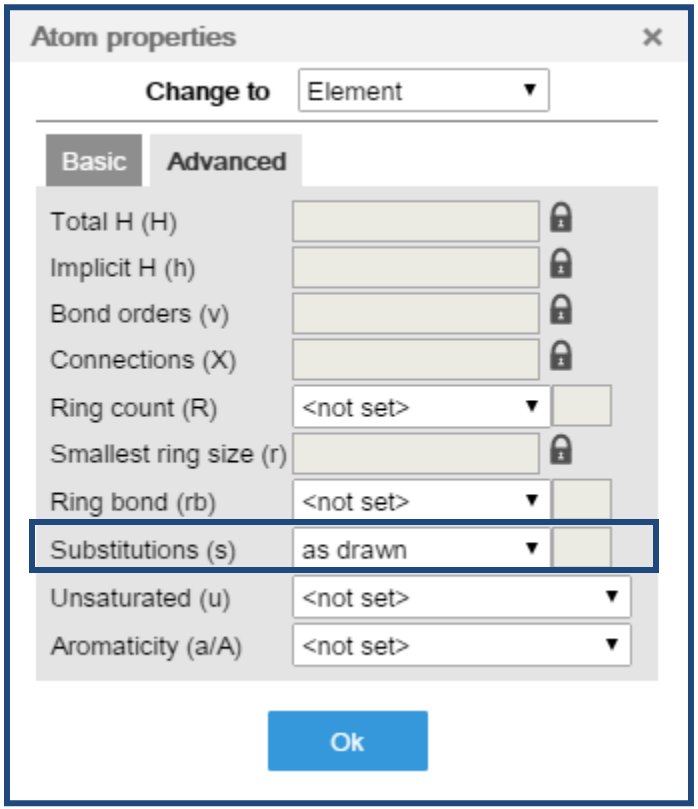
Mapped reaction result



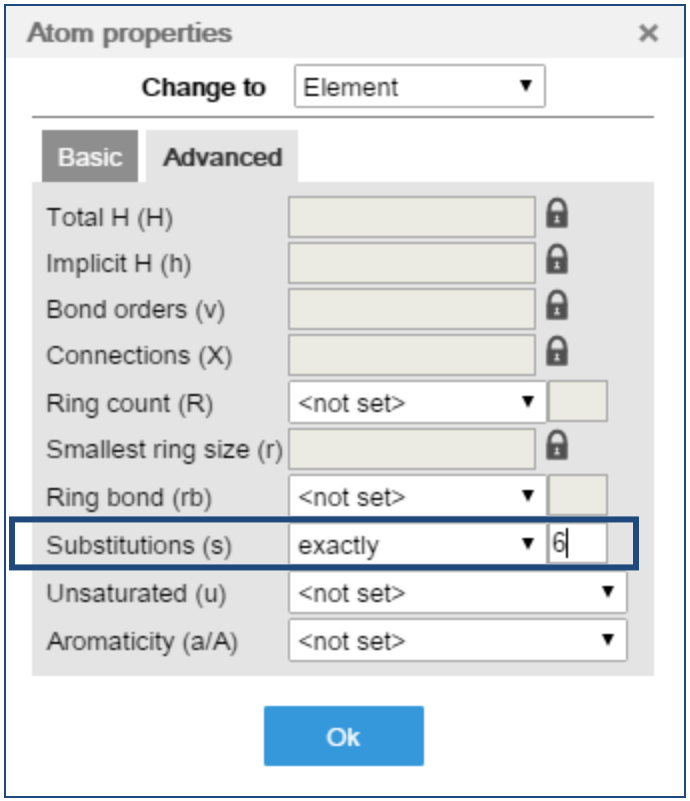
Unmapped reaction result

Marvin JS – Substitution





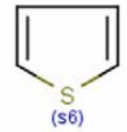
Marvin JS – Substitution

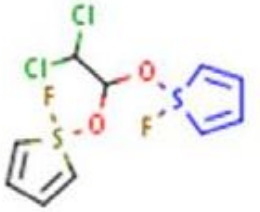


結構搜尋指令

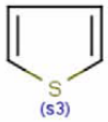
結果差異

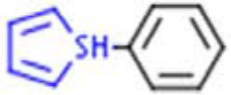
.s6

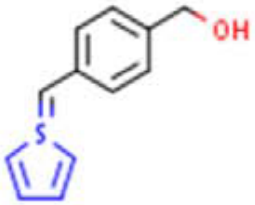




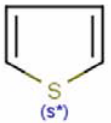
.s3

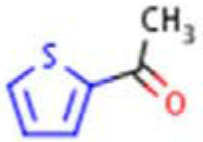


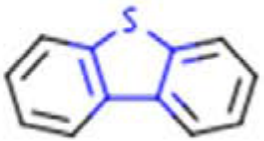




.s*

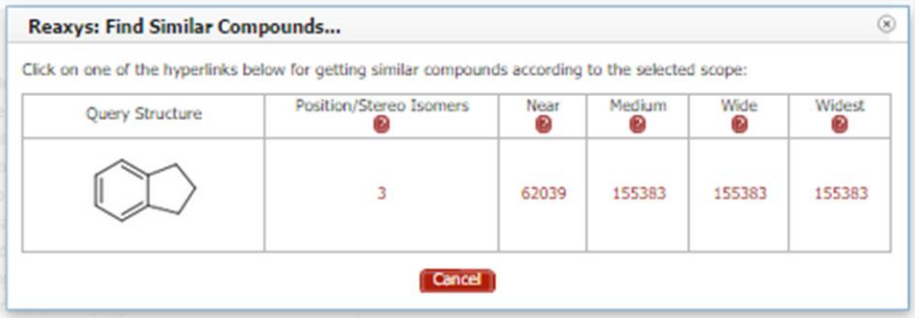






結構搜尋其他設定選項

REAXYS 可以針對您的需求，搜尋各式各樣的衍生物

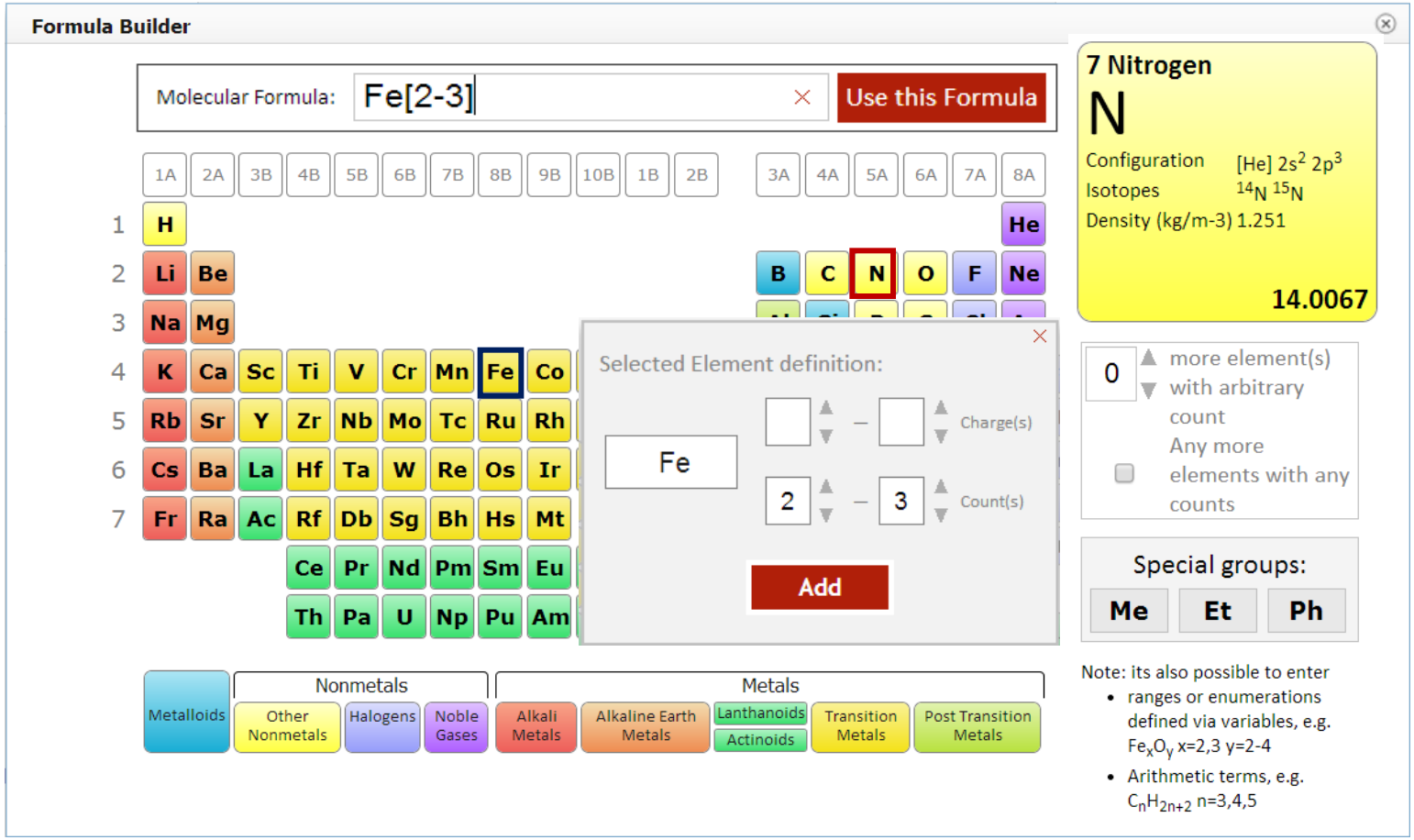


建立搜尋指令-分子式

Fe_2O_3
Fe_3O_4
C34*

Molecular Formula

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



將滑鼠移到元素上方即可預覽該元素詳細資訊

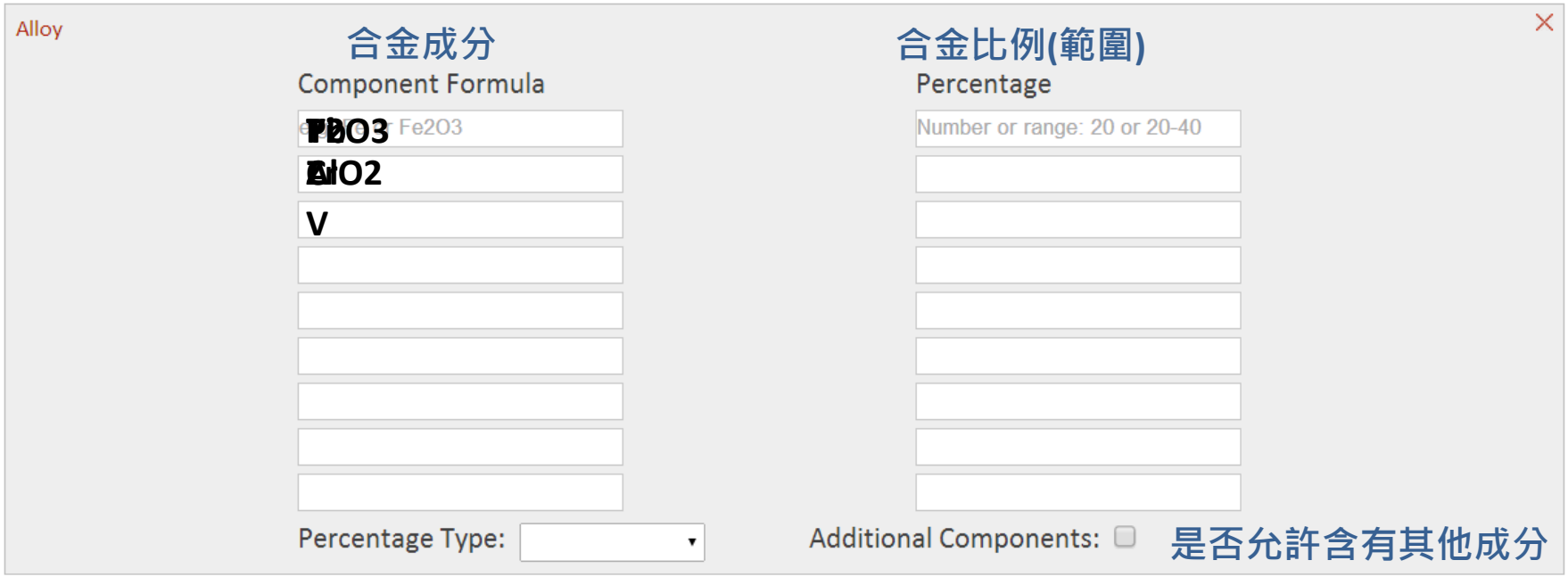
影片介紹

Query Builder

建立搜尋指令-合金

Alloy

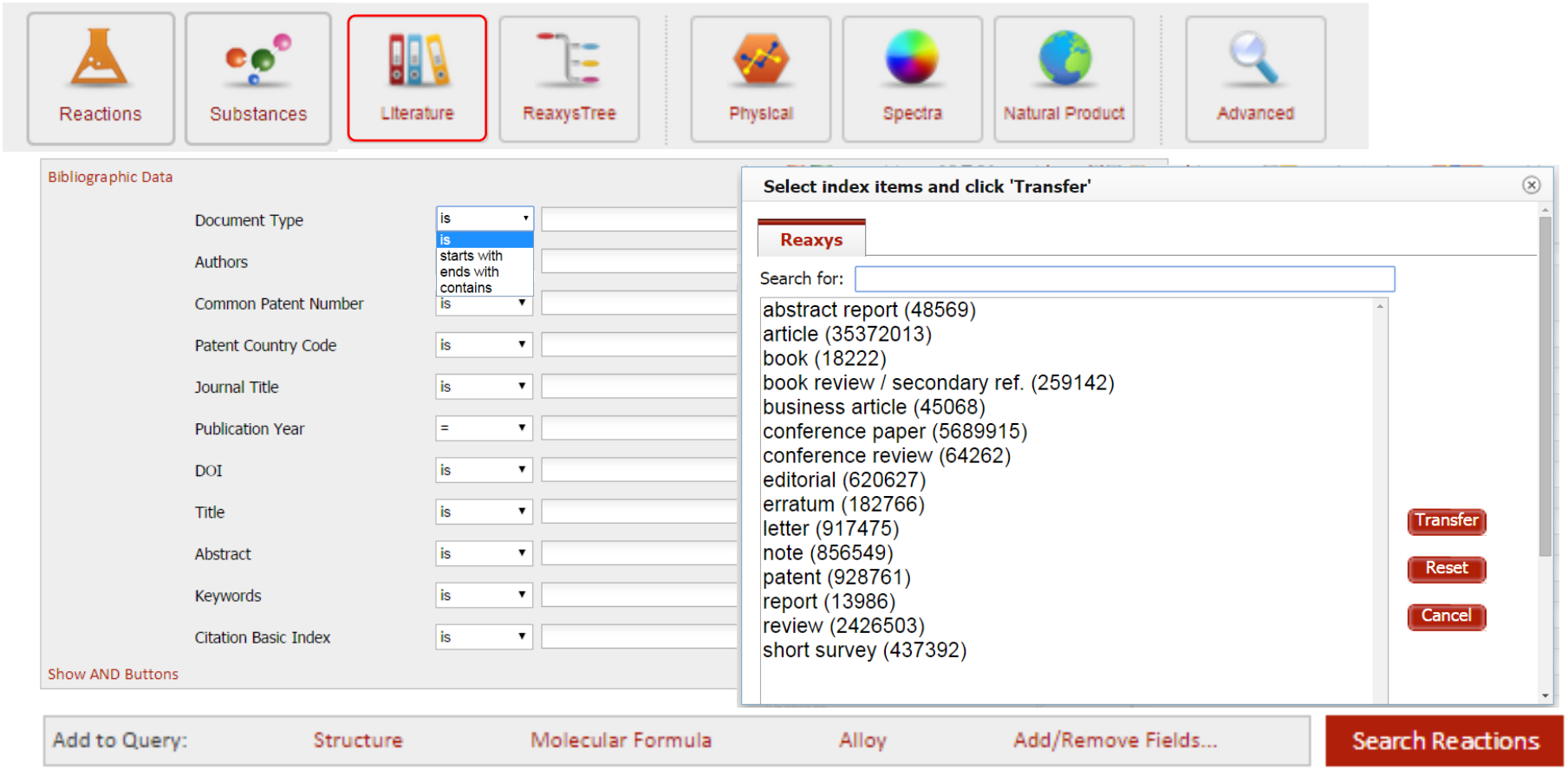
Ti-6Al-4V
Pb/C
yttria/zirconia ceramics



合金成分比例單位

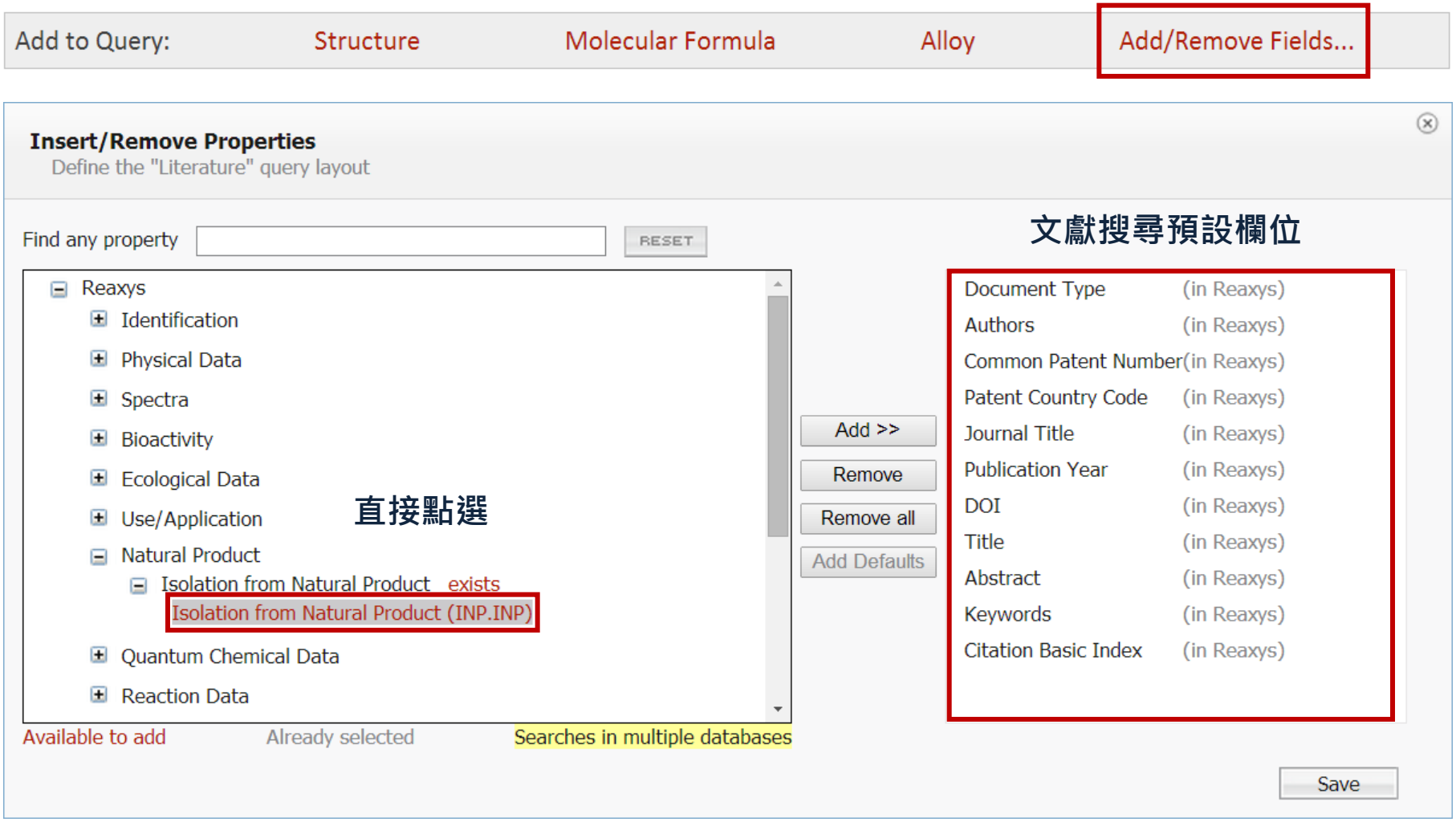
或者您也可以使用Advanced Search

欄位搜尋


Reactions
Substances
Literature
ReaxysTree
Physical
Spectra
Natural Product
Advanced
Bibliographic Data
Document Type
is
is
starts with
ends with
contains
Authors
Common Patent Number
Patent Country Code
Journal Title
Publication Year
DOI
Title
Abstract
Keywords
Citation Basic Index
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

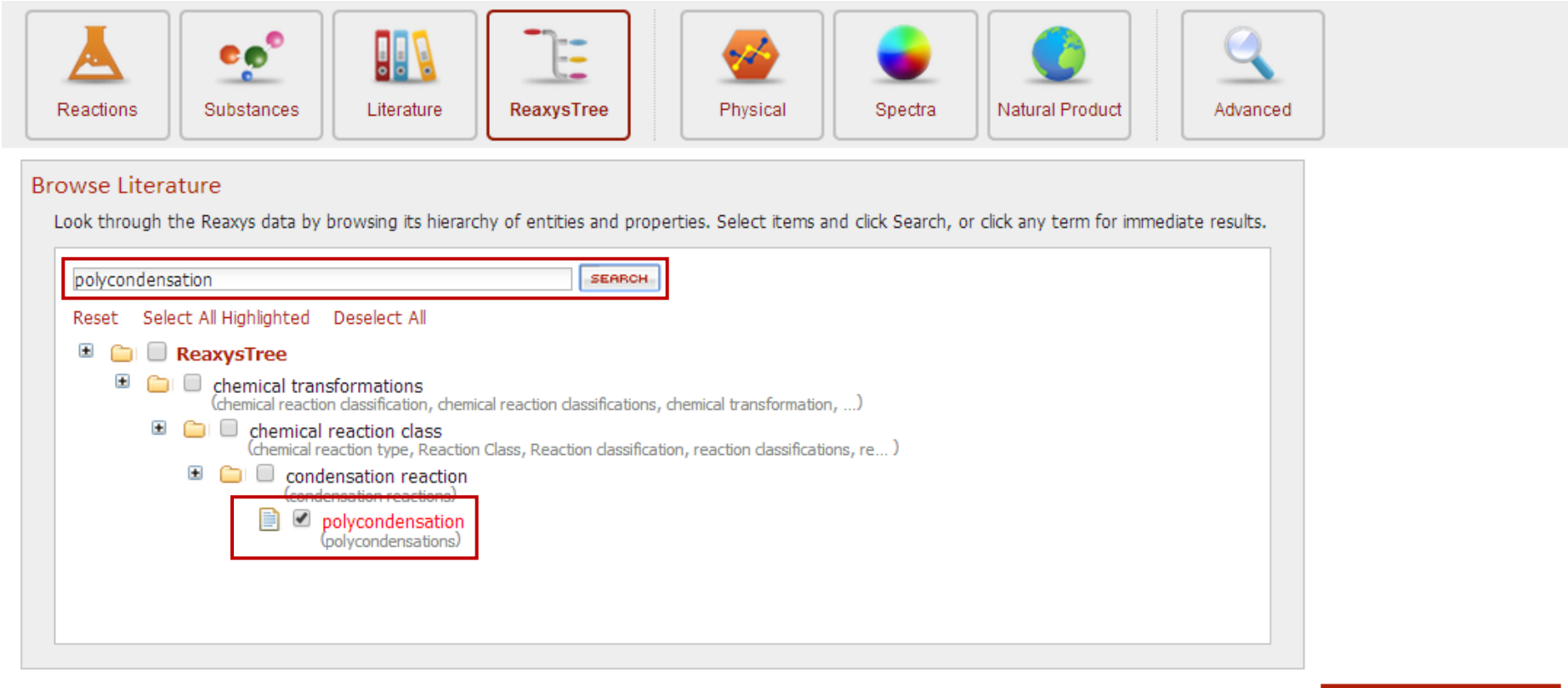
新增欄位

Fields


Add to Query:
Structure
Molecular Formula
Alloy
Add/Remove Fields...
Insert/Remove Properties
Define the "Literature" query layout
Find any property
RESET
文獻搜尋預設欄位
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
Add >>
Remove
Remove all
Add Defaults
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)
Available to add
Already selected
Searches in multiple databases
Save

REAXYS TREE

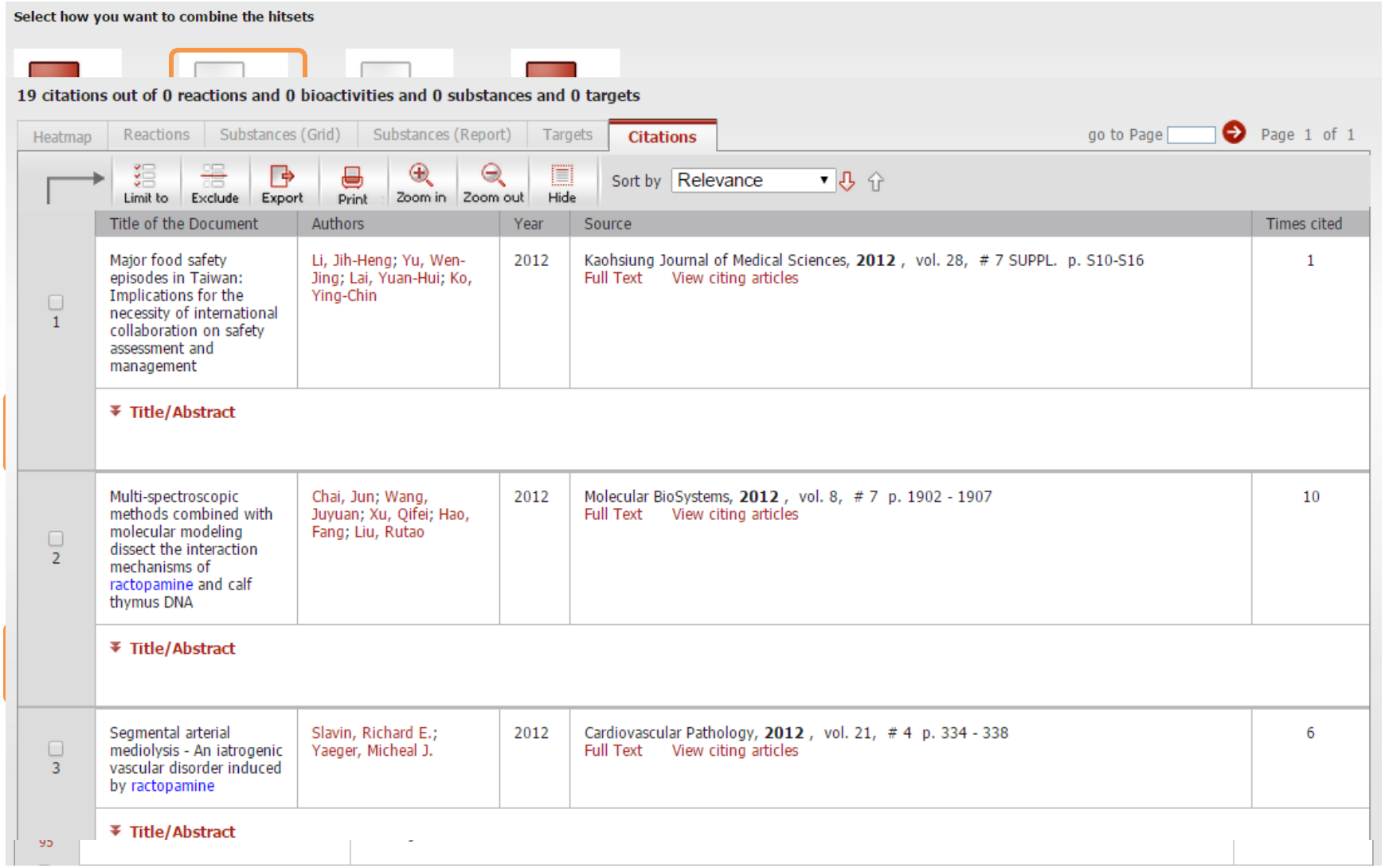
POLYCONDENSATION



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
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				
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				
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

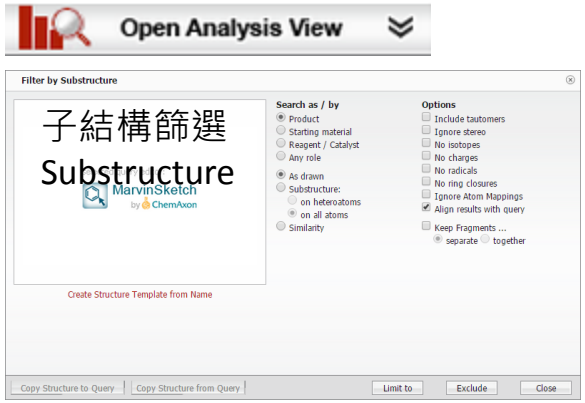
PubChem (10 Years)

供應商資料

eMolecules

Scopus

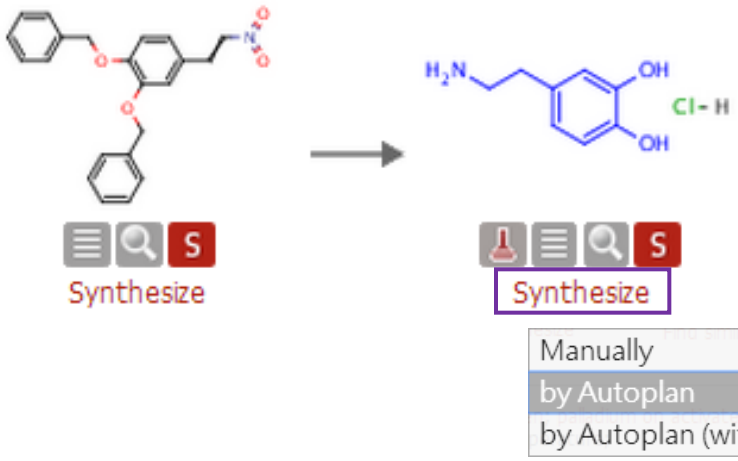
篩選功能：Analysis View 及 28 種 Filter

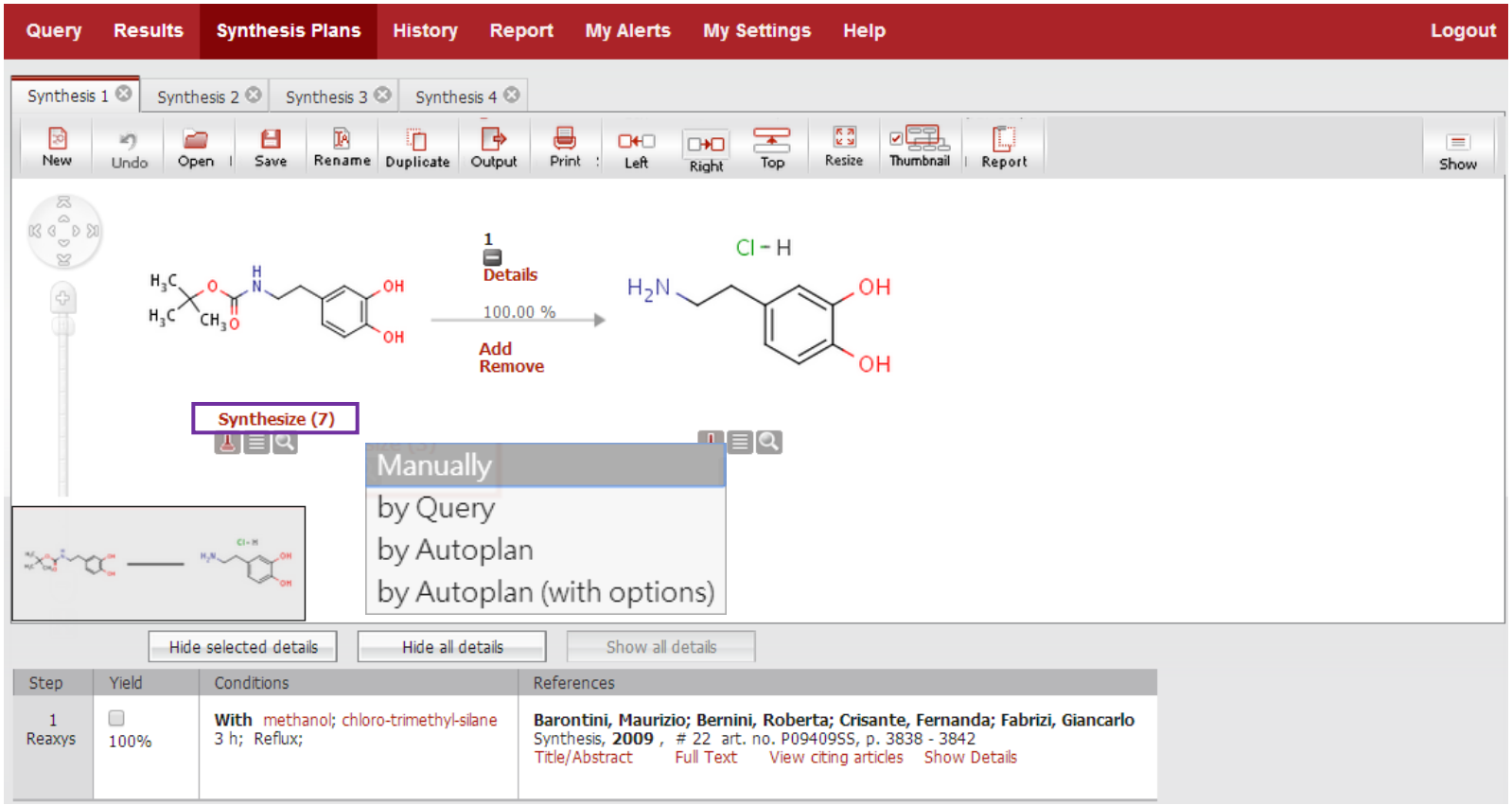


- Molecular Weight
- Number of Fragments
- Physical Data
- Spectroscopic Data
- Ecological Data
- Natural Product
- Availability
- Availability in other DBs
- LogP
- H Bond Donor (HBD)
- H Bond Acceptor (HBA)
- Polar surface Area (PSA)
- Highest clinical phase

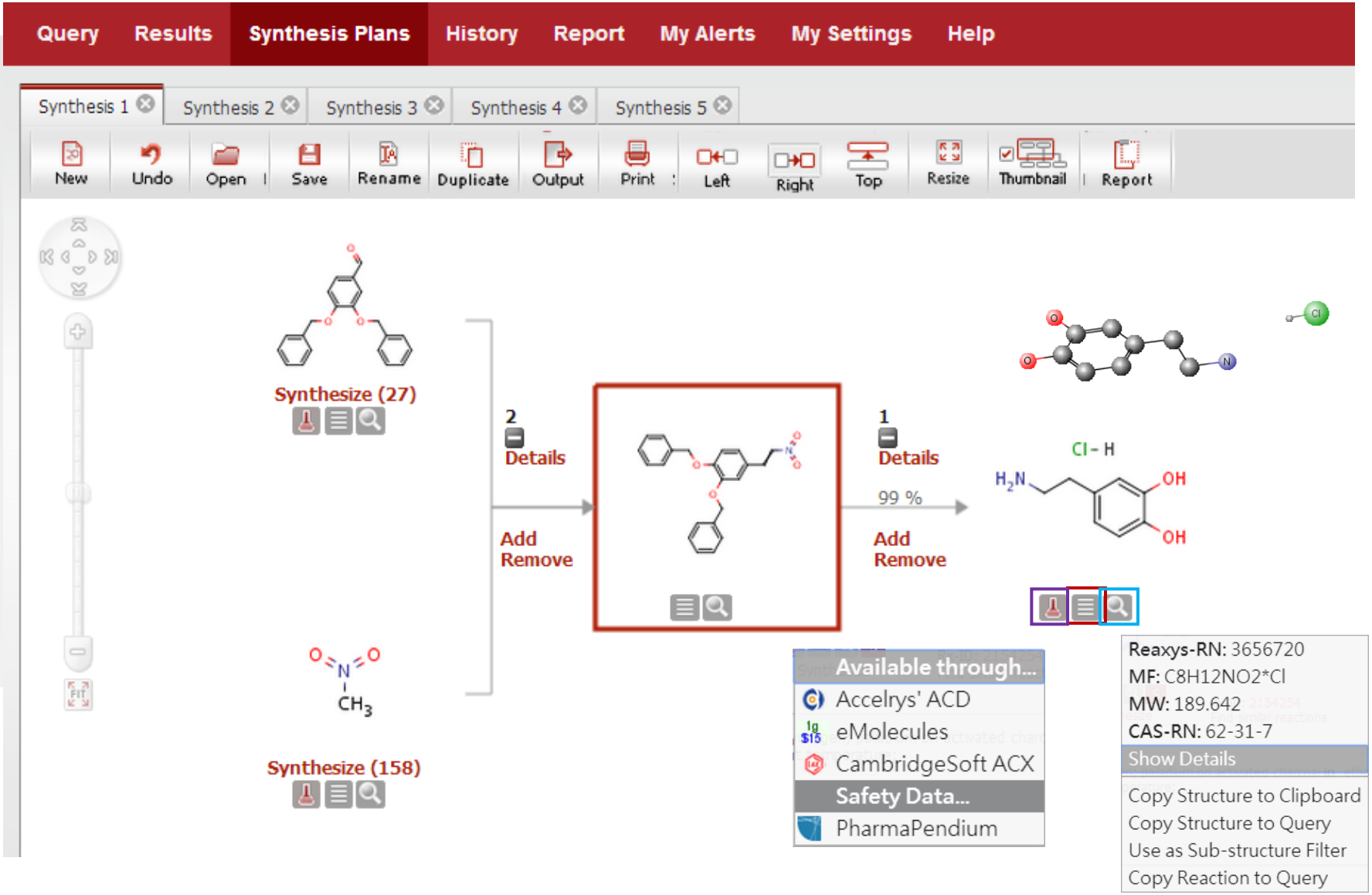
- Document Type
- Authors
- Patent Assignee
- Journal Title
- Publication Year
- Substructure
- Yield
- Record Type
- Reagent/Catalyst
- Solvent
- Reaction Type
- No. of Steps
- Product Availability
- Reactant Availability
- Availability in other DBs

建立合成計畫
Synthesis Plans



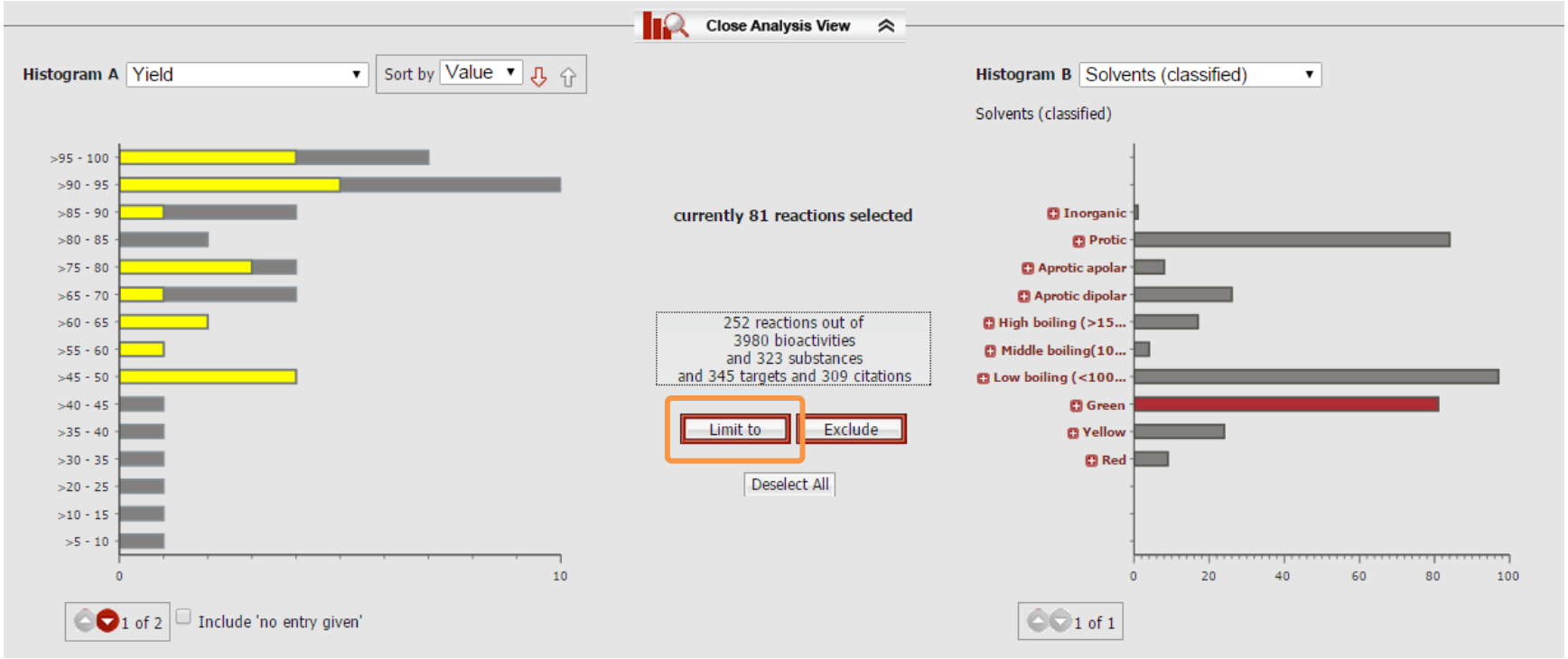


建立合成計畫


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)
2
Details
Add
Remove
1
Details
99 %
Add
Remove
Cl - H
OH
OH
Synthesize (158)
Available through...
Accelrys' ACD
eMolecules
CambridgeSoft ACX
Safety Data...
PharmaPendium
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

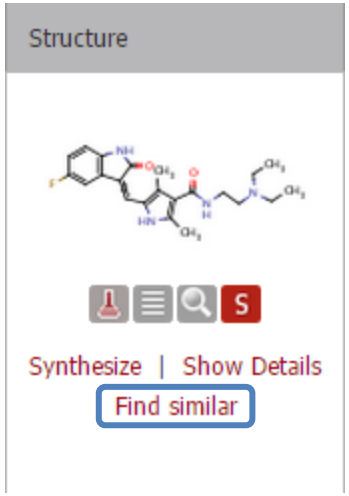
Analysis View 視覺化分析系統

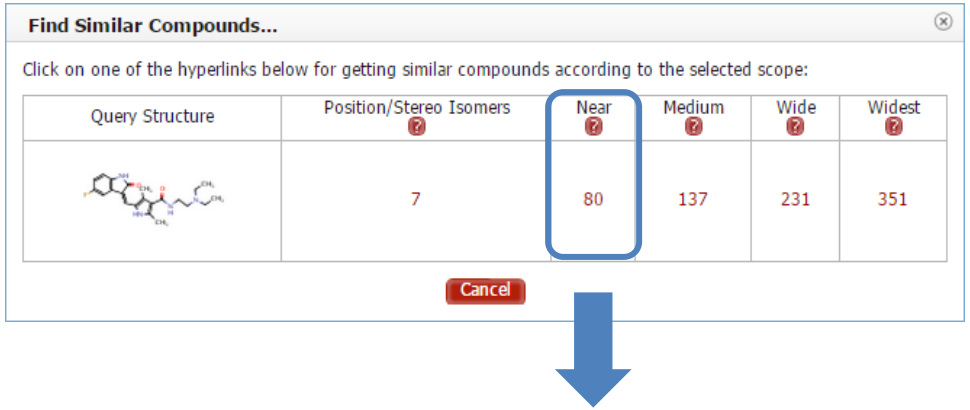
範例：使用環保溶劑，合成反應的產率分布

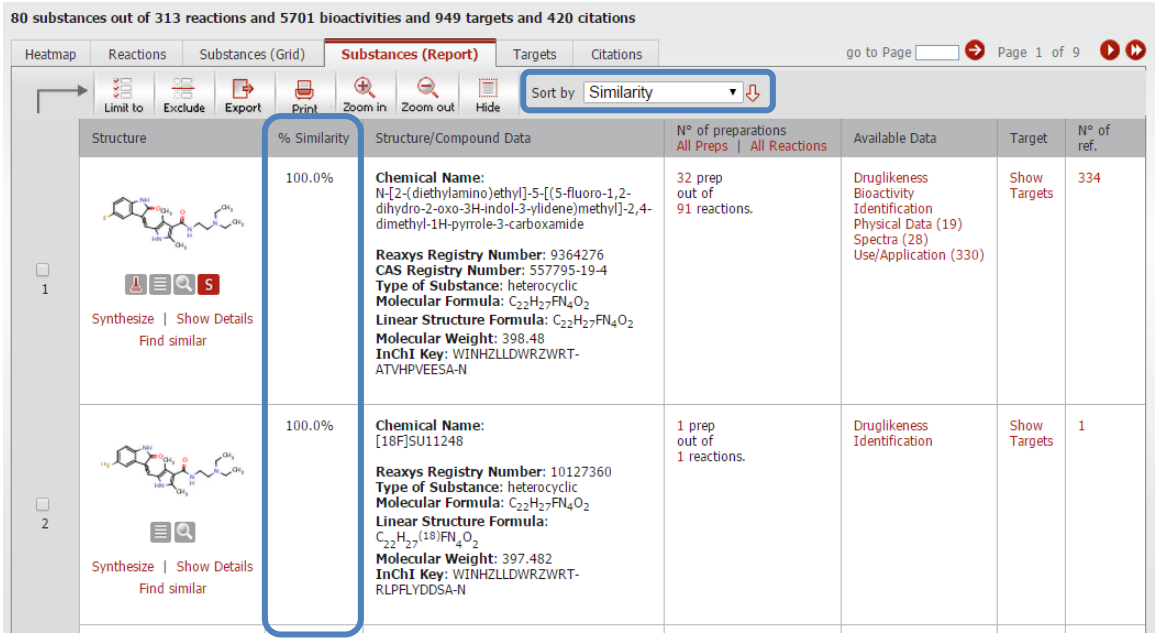


結果畫面相似結構搜尋

DISCOVERABILITY







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

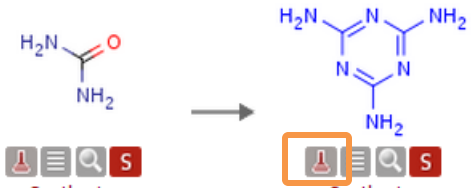
反應搜尋結果

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

3



Synthesize
Find similar

Synthesize
Find similar

Rx-ID: 748486
Find similar reactions

查看包裝價格

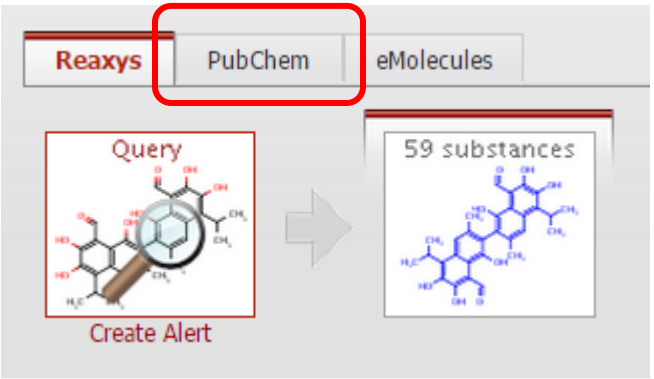
Available through...
Accelrys' ACD
eMolecules
CambridgeSoft ACX

98%	Stage #1: T=140 - 160°C; P=6000.48 Torr; Stage #2: **With** ammonia; γ-Al_2O_3 P=750.06 - 1500.12 Torr;	**erantsev; Tubolkin** Chemistry, **2002** , vol. 75, # 11 p. 1883 - 1884 View citing articles Show Details
88.5%	**in** water Product distribution / selectivity; Show Experimental Procedure	**EUROTECNICA MELAMINE, LUXEMBOURG, ZWEIGNIEDERLASSUNG IN ITTIGEN** **Patent:** WO2007/119156 A2, **2007** ; **Location in patent:** Page/Page column 16-19 ; Title/Abstract Full Text Show Details
12.6%	**With** ammonia High Pressure; 70 to 300 at; at 350°C; 120 min;	**Gmelin Handbook:** C: MVol.D1, 45.11.4, page 449 - 450 Full Text Show Details **Hunn, F. A.** Diss. Zuerich T. H. 1959, S. 1/75 Full Text Show Details

Show Next 20 Details **Show All Remaining Details (31)**

PubChem 搜尋結果

切換至 PubChem 資料庫



PubChem OPEN CHEMISTRY DATABASE

Search Compounds

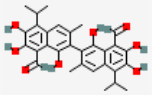
Compound Summary for CID 3503 | Download | Print | Share | Help

Gossypol

Read about the new page format and features | Go to the legacy page

Vendors | Drug Information | Pharmacology | Literature | Patents | Bioactivities

Cite this Record



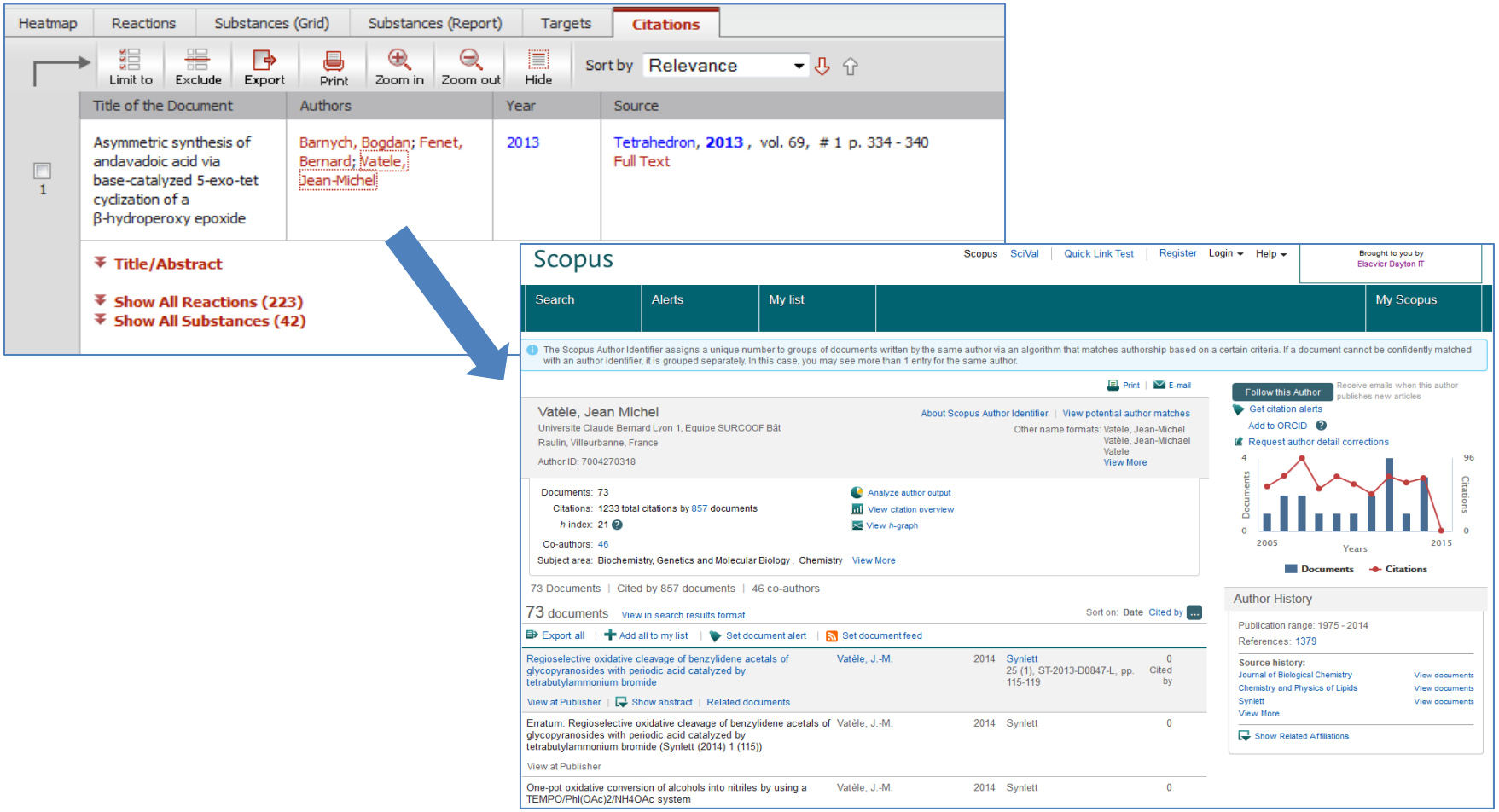
PubChem CID:	3503
Chemical Names:	gossypol; 303-45-7; Pogosin; (-)-Gossypol; (+)-Gossypol; Tash 1; More...
Molecular Formula:	$C_{30}H_{30}O_8$
Molecular Weight:	518.5544 g/mol
InChI Key:	QBKSWRVVCFFDOT-UHFFFAOYSA-N
Modify Date:	2015-04-11
Create Date:	2005-03-25

A dimeric sesquiterpene found in cottonseed (GOSSYPIUM). 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.



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

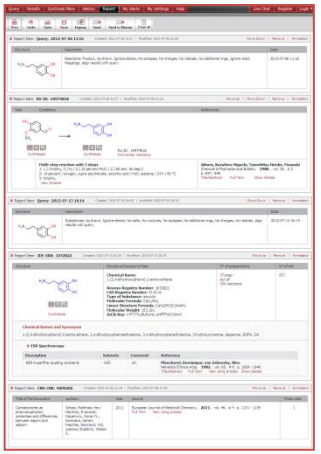
多元資料儲存或輸出方式

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



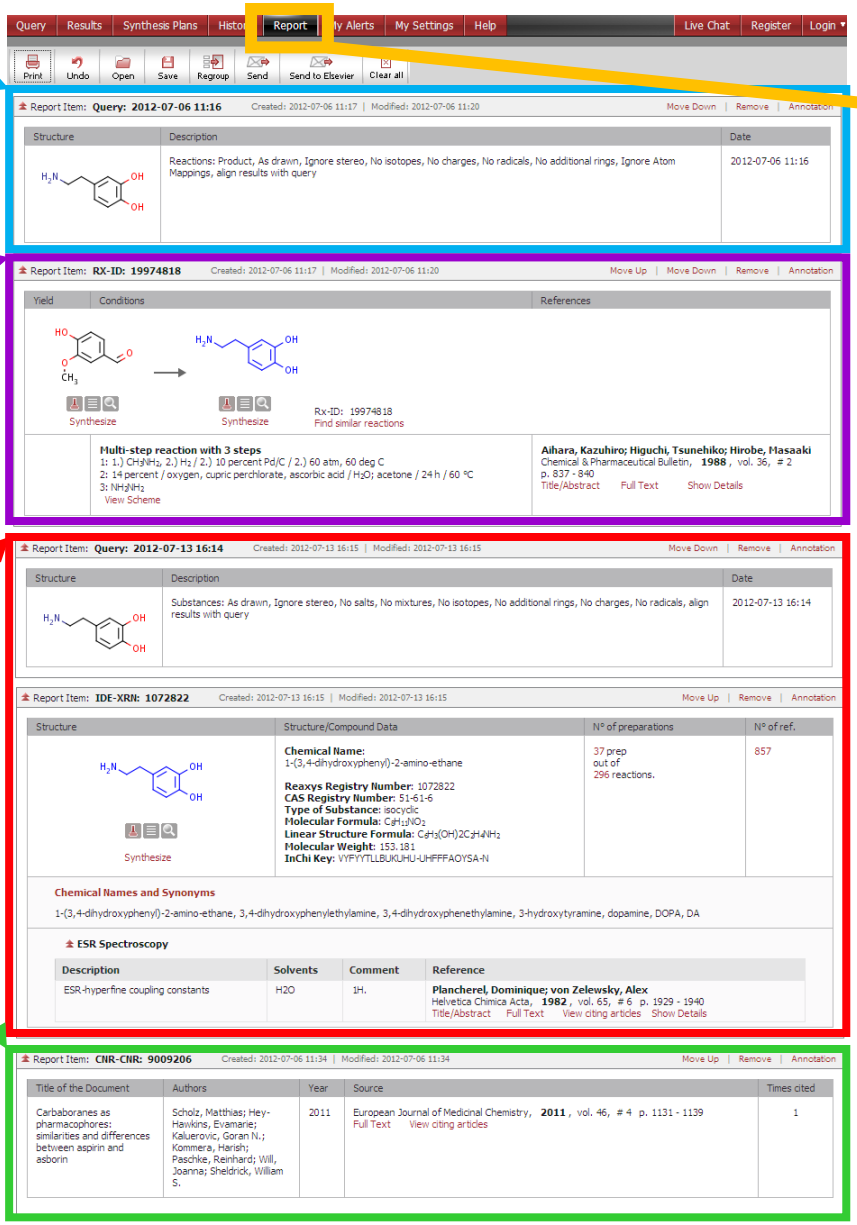
多樣化結果輸出功能 -- REPORT

搜尋紀錄輸出

反應搜尋結果輸出

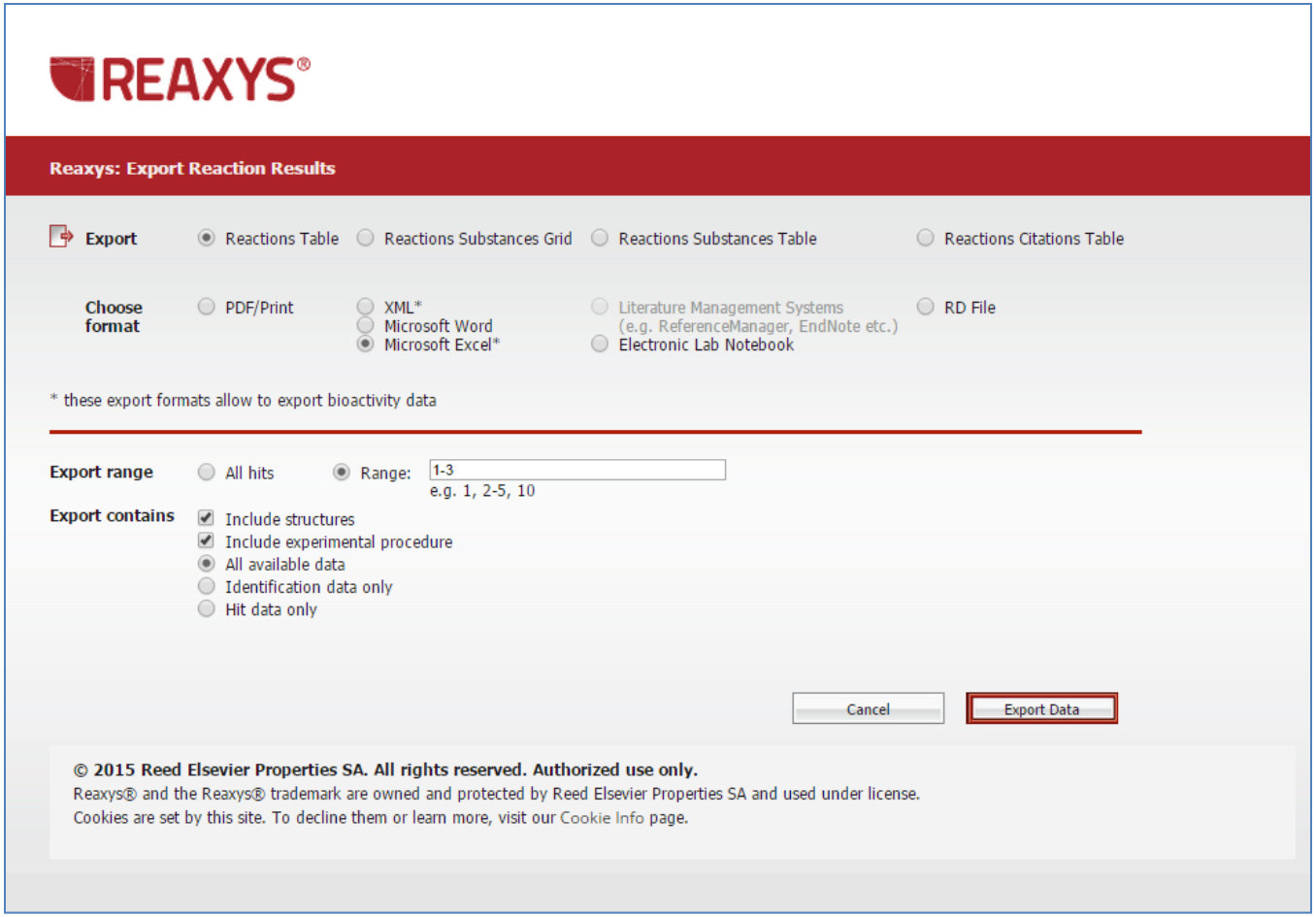
化合物搜尋結果輸出

文獻搜尋結果輸出



輸出結果

輸出搜尋結果

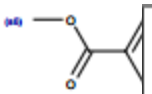


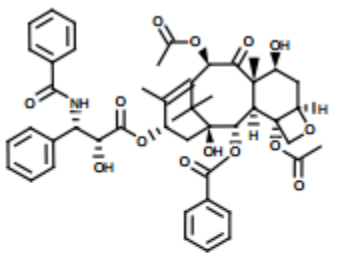
https://www.reaxys.com/reaxys/printing/reaxys_anonymous_20150513_102021_206.pdf

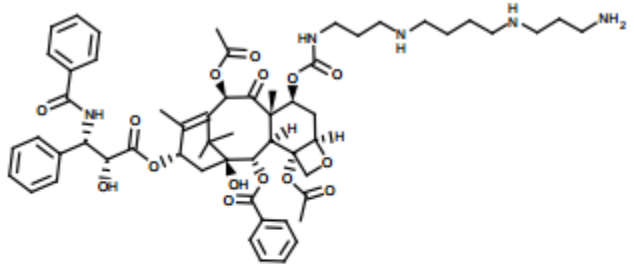
分享搜尋結果

PDF EXPORT RESULT

Query

	Query	Results	Date
1. Query	   Search as: Product, As drawn, No sal	80 reactions in Reaxys	2015-05-13 10h:09m:06s (EST)
2. Query	filtered by Number of Reactio		





Rx-ID: 12697962 View in Reaxys 1/1

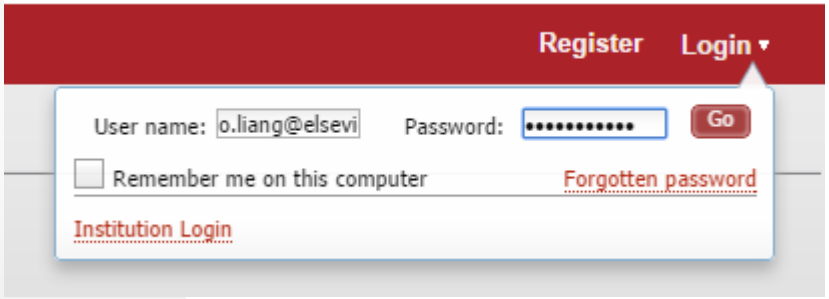
Yield	Conditions & References
	Reaction Steps: 4 1: imidazole; DMAP 2: DMAP 3: 78 percent / HF*pyridine 4: CH_2Cl_2; propan-2-ol **With** 1H-imidazole, 4-(N,N-dimethlyamino)pyridine, pyridine hydrogenfluoride **in** dichloromethane, isopropyl alcohol **Battaglia, Arturo; Guerrini, Andrea; Baldelli, Eleonora; 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

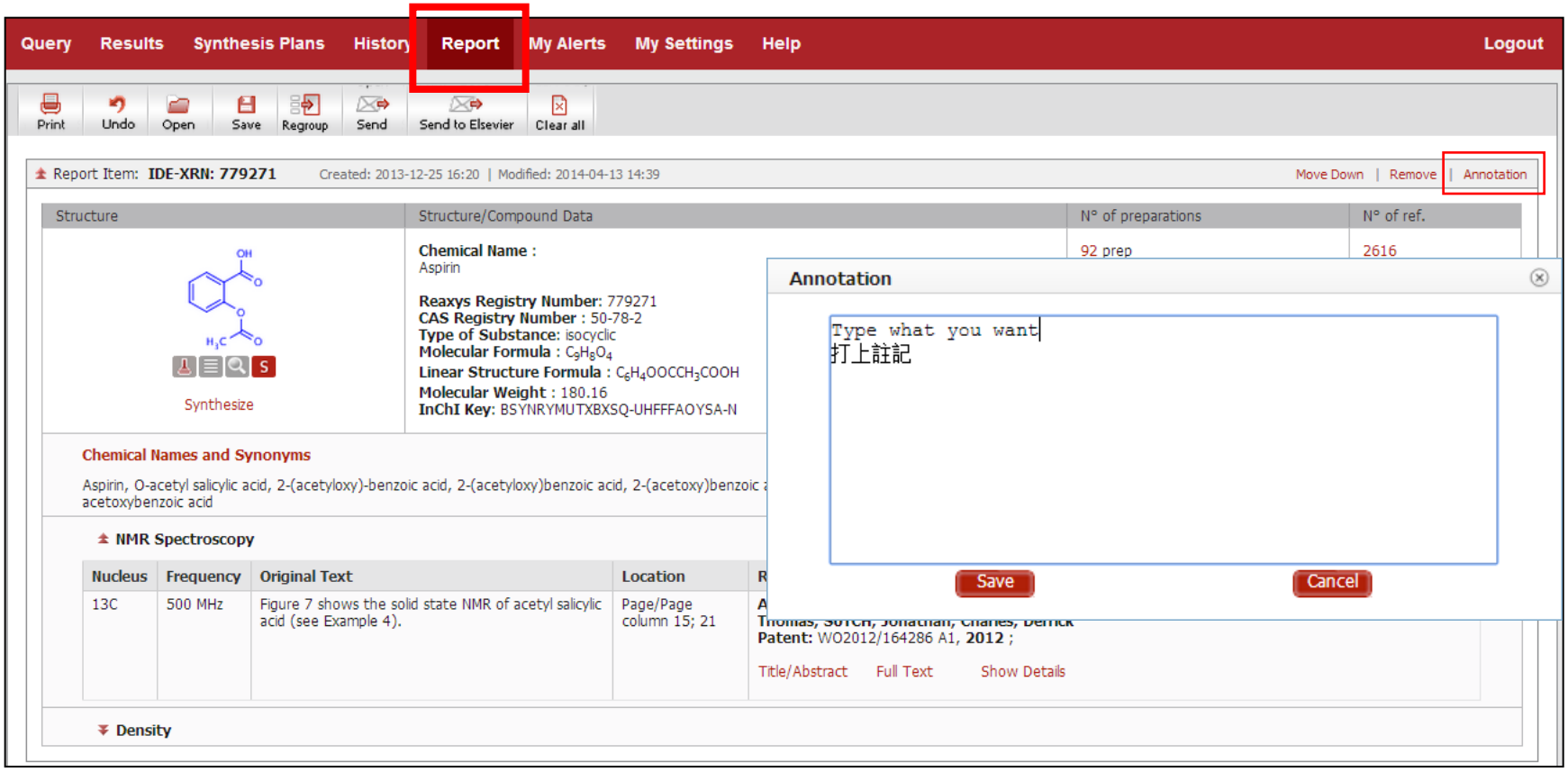
1. Report: 輸出報告
2. History: 搜尋紀錄
3. My Alerts: 新知通報
4. My Settings: 個人化設定



密碼建議包含大小寫、數字及特殊符號(*_.)

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。



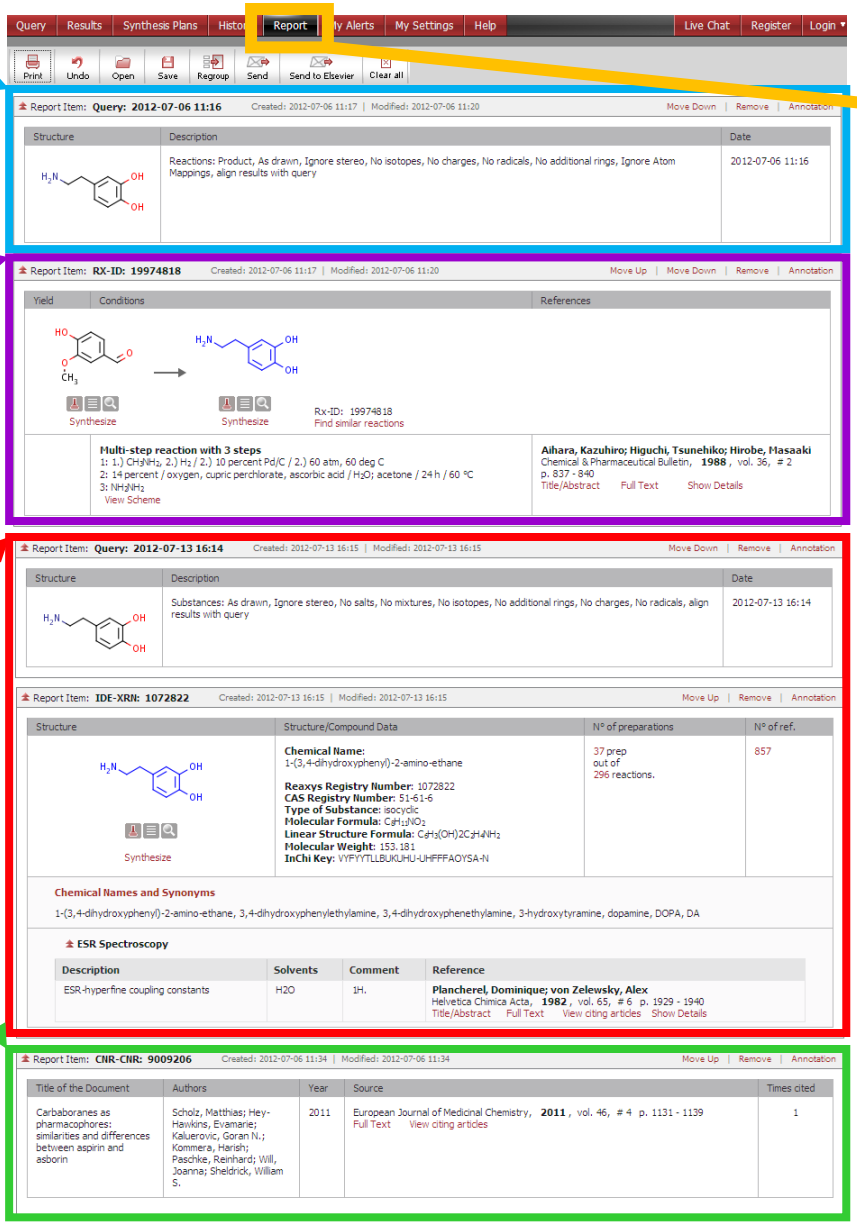
多樣化結果輸出功能 -- REPORT

搜尋紀錄輸出

反應搜尋結果輸出

化合物搜尋結果輸出

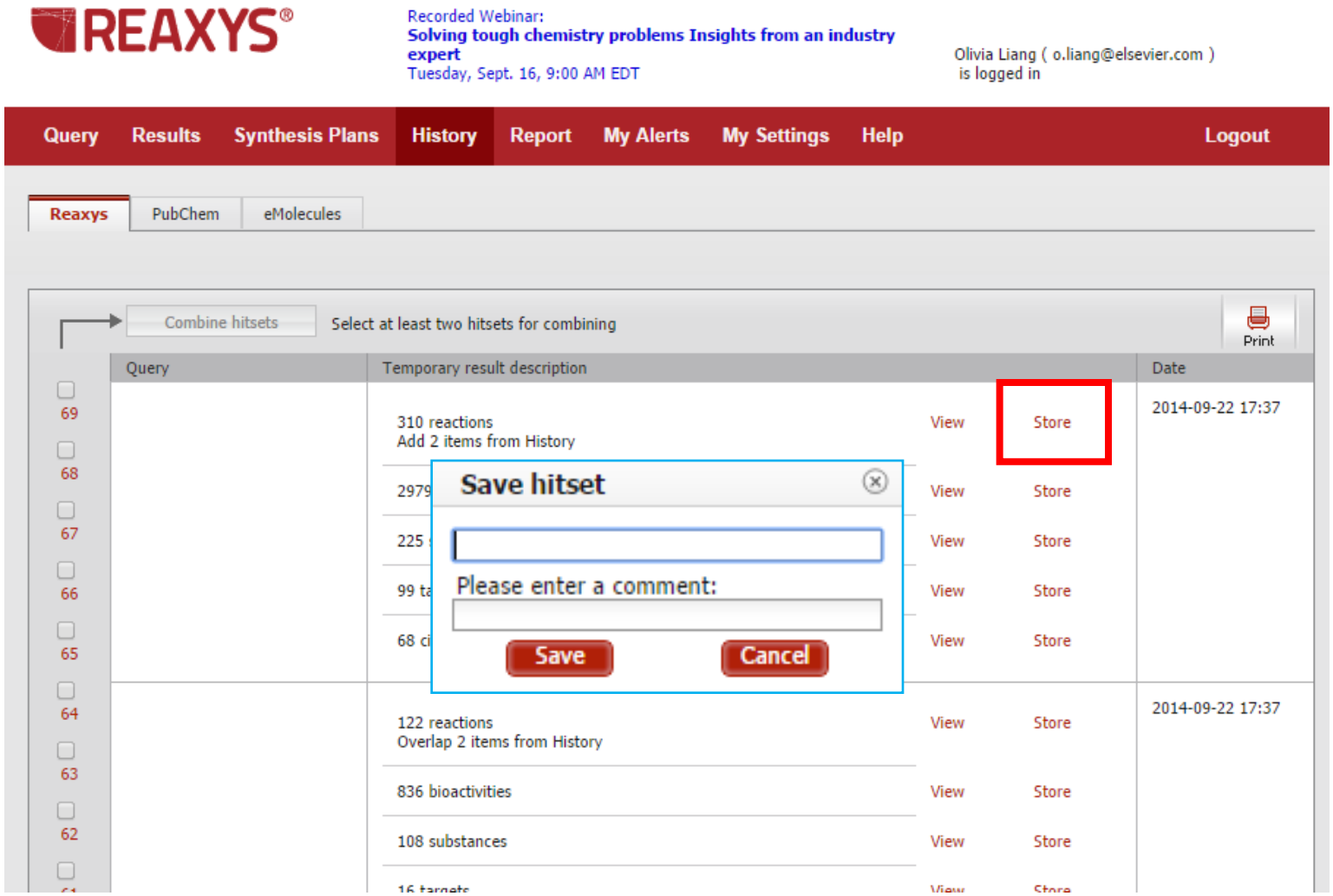
文獻搜尋結果輸出



輸出結果

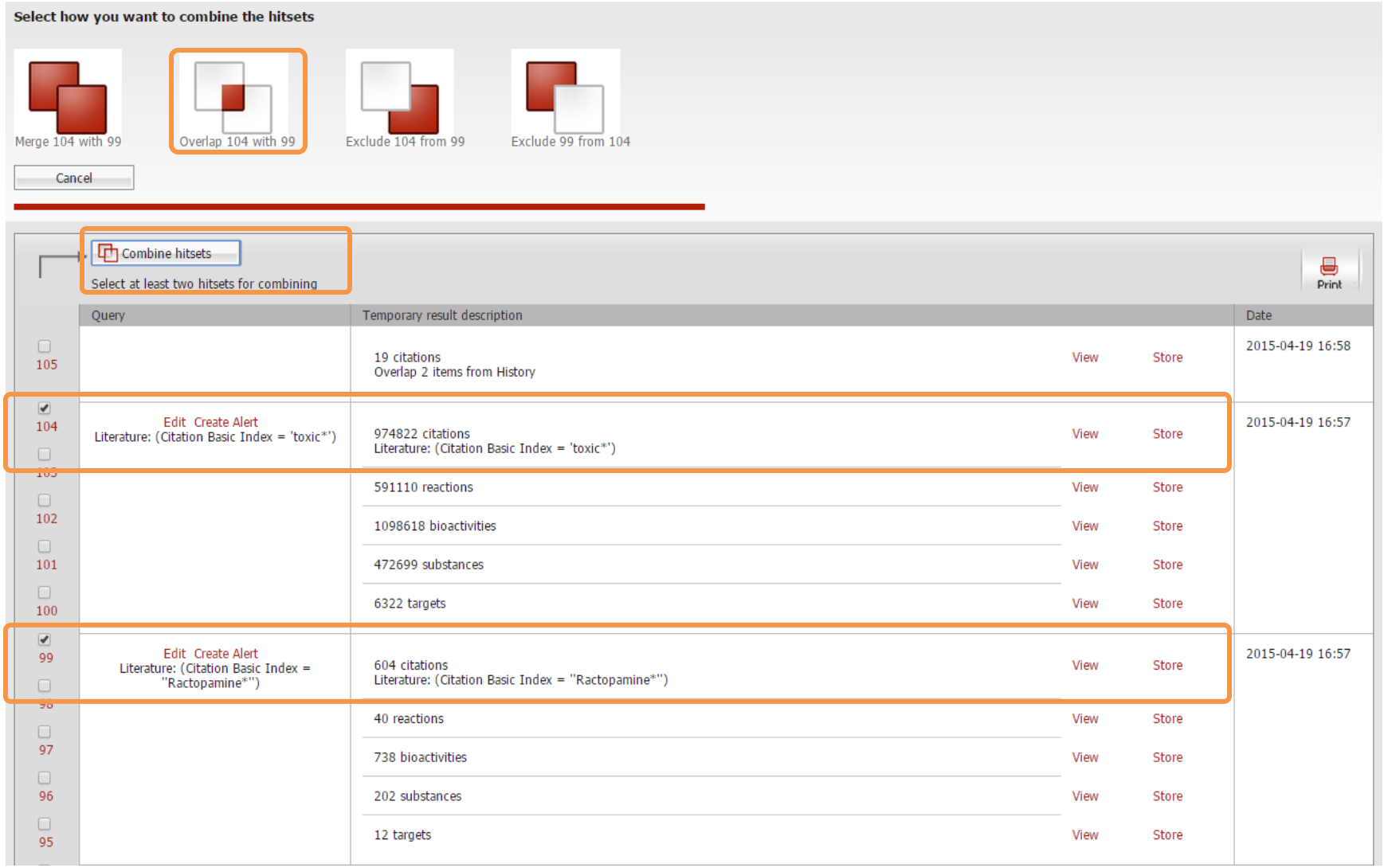
2. History

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。



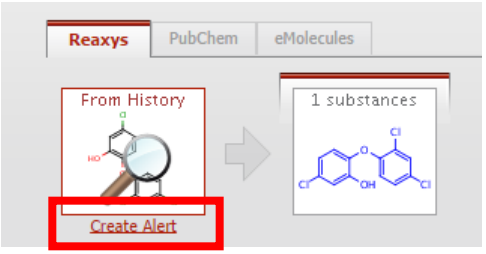
合併搜尋

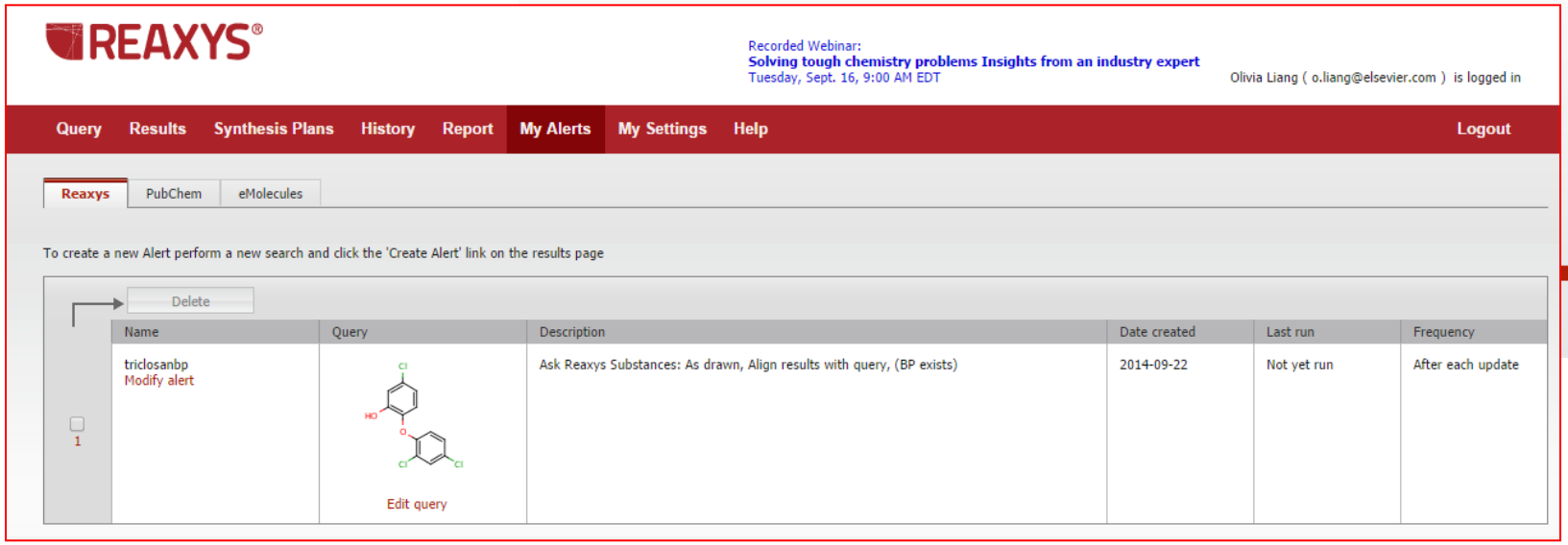
結合多個搜尋條件



3. My Alerts

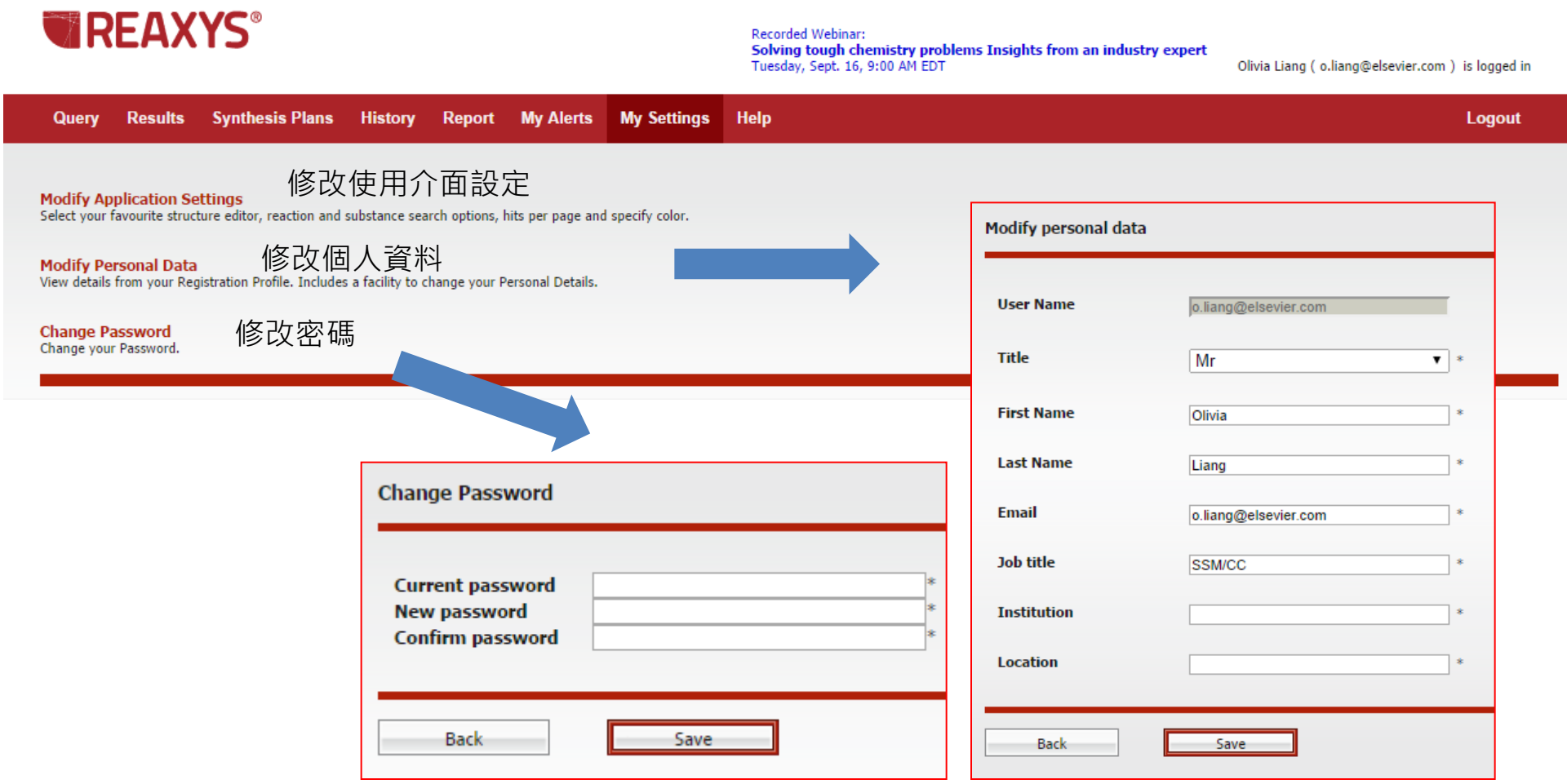
新知通報 (MY ALERTS)：訂閱常用搜尋條件，隨時閱讀最新資料。





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。



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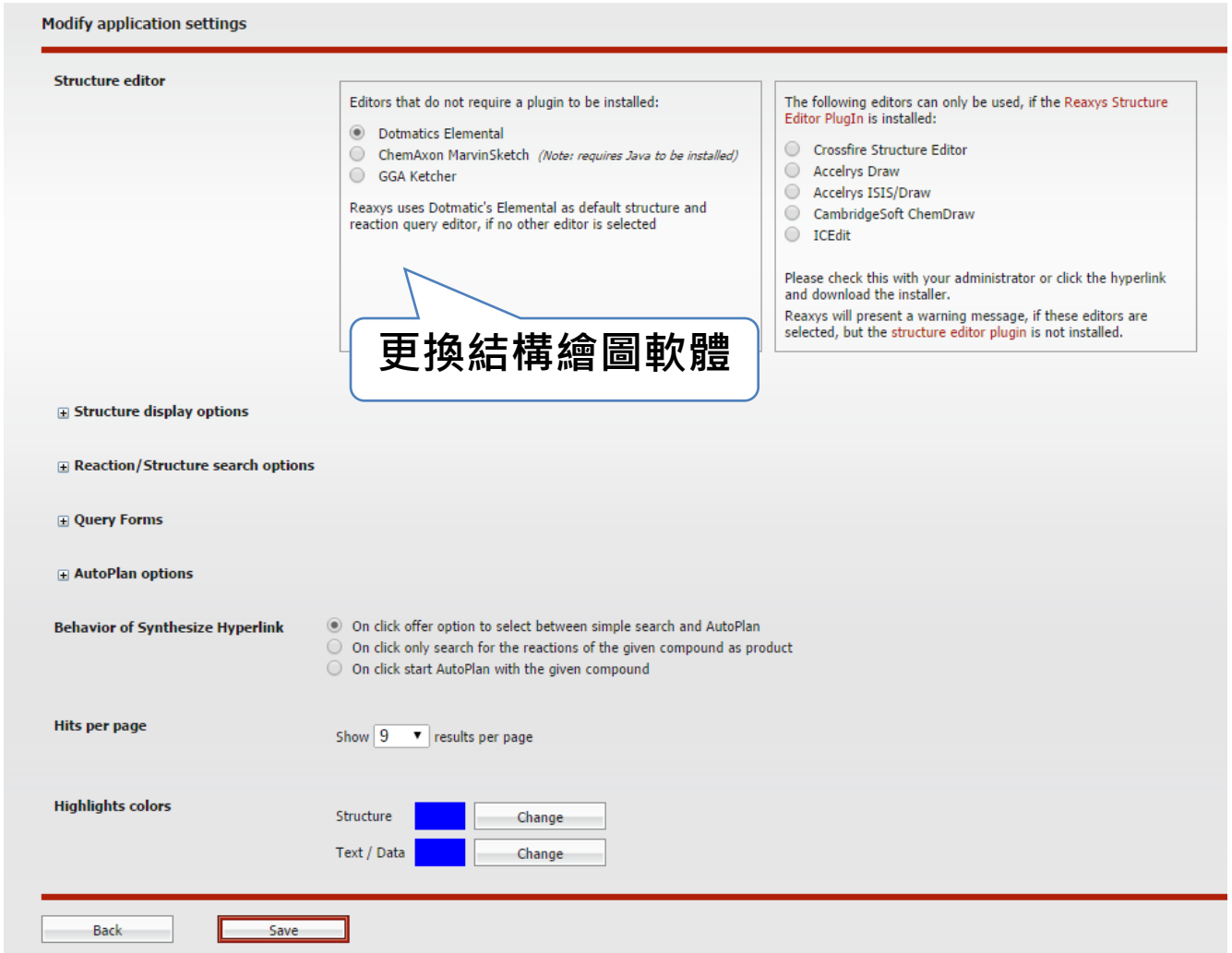

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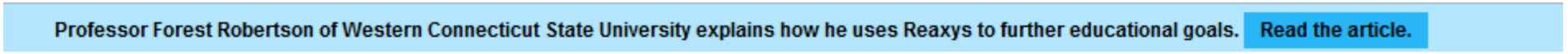
WEBINAR & HELP

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。



REAXYS®

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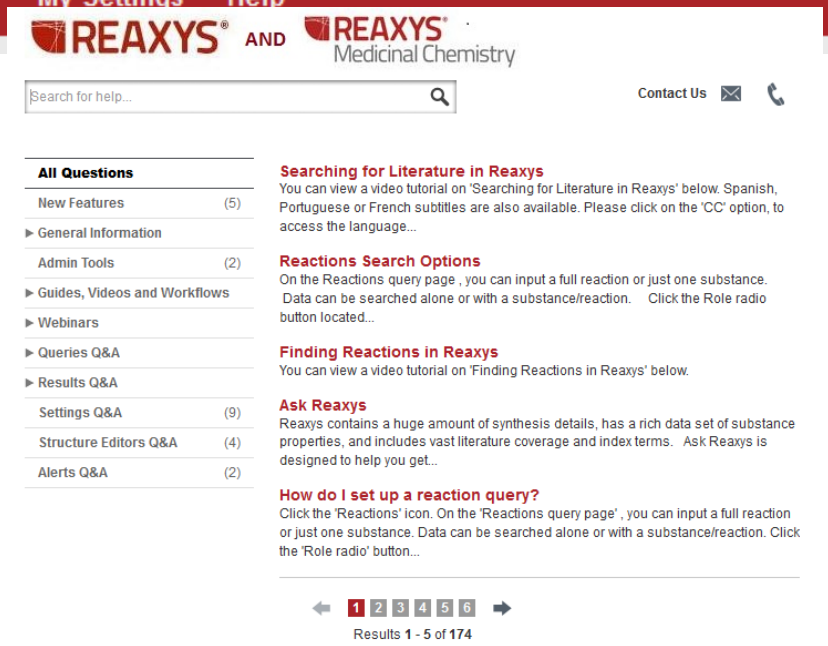
Ease of Use: 使用 HELP 時，系統自動辨認使用者權限，並提供對應的說明



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如果你的朋友問你，該如何馬上去除狗身上的臭味，你多快可以找到另他驚豔的方法並展現自己的化學搜尋實力呢?

Thank you!

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