網址

www.reaxys.com

REAXYS 教育訓練

梁成芝

ELSEVIER 生命科學解決方案經理

o.liang@elsevier.com

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HOW YOU THINK HOW YOU WORK

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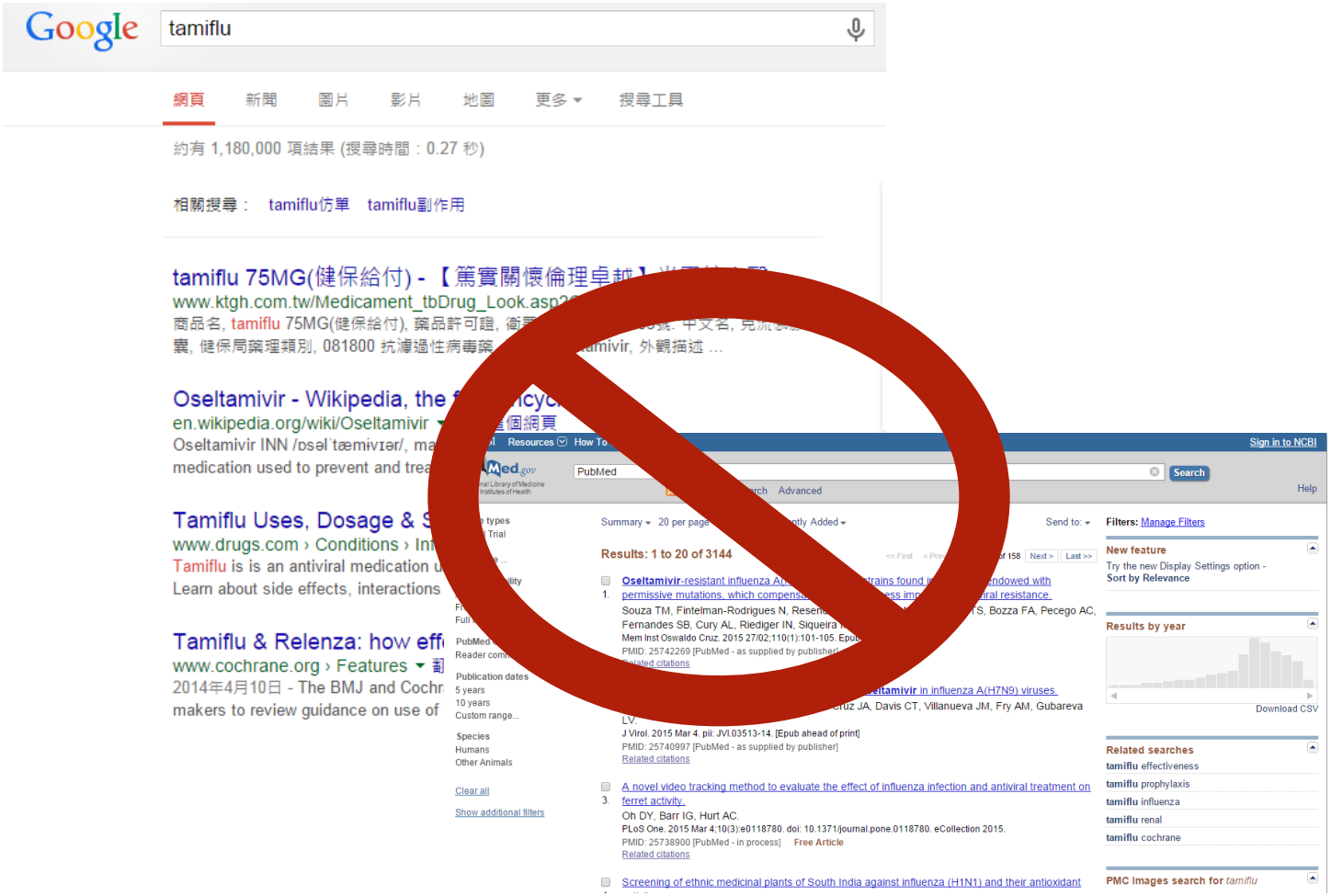
HOW YOU THINK HOW YOU WORK



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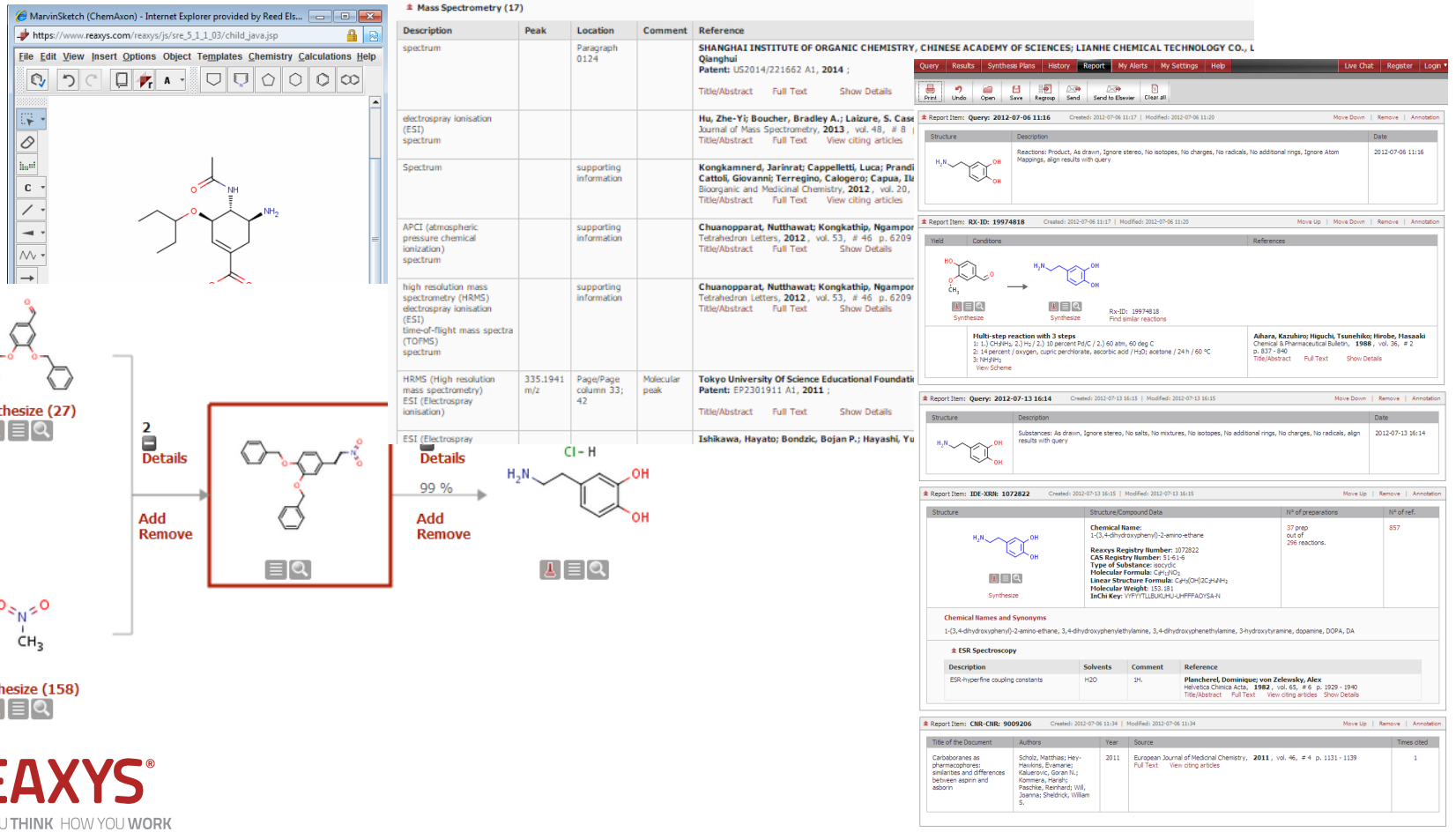
Smarter Chemistry



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Reaxys 獨有資料
小分子藥物最大資料庫

搜集大量文獻

摘錄重要資訊

搜尋介面

節省文獻閱讀時間

更多搜尋管到
精準找到所需資料

快速回答問題

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ELSEVIER

30%
FASTER

23%
LESS COSTLY

REAXYS化學資料庫收錄內容

1771 年開始

1771 → 1817 → 1881 → 1988 → 1993 → 2007 → 2009 → 2013

Gmelin Online　Beilstein Online　Beilstein on STN　CrossFire 1.0　CrossFire Commander

reaxys®　REAXYS®

包含有機、無機、
有機金屬三大領域

資料來自
超過 16000 種期刊
經實驗驗證的數據

三大專利資料庫：
USTPO, EPO, WIPO

Reaxys 資料庫含有：

5,500 萬 個有機、無機及有機金屬化合物

3,600 萬 個化學反應

5 億 項已出版的實驗結果

獨特資料來源：

16,000 篇化學相關定期刊物

130 個學科主題—比其他任何研究解決方案都來得多

超過 240 年的化學研究發展時間（1771 年至今）

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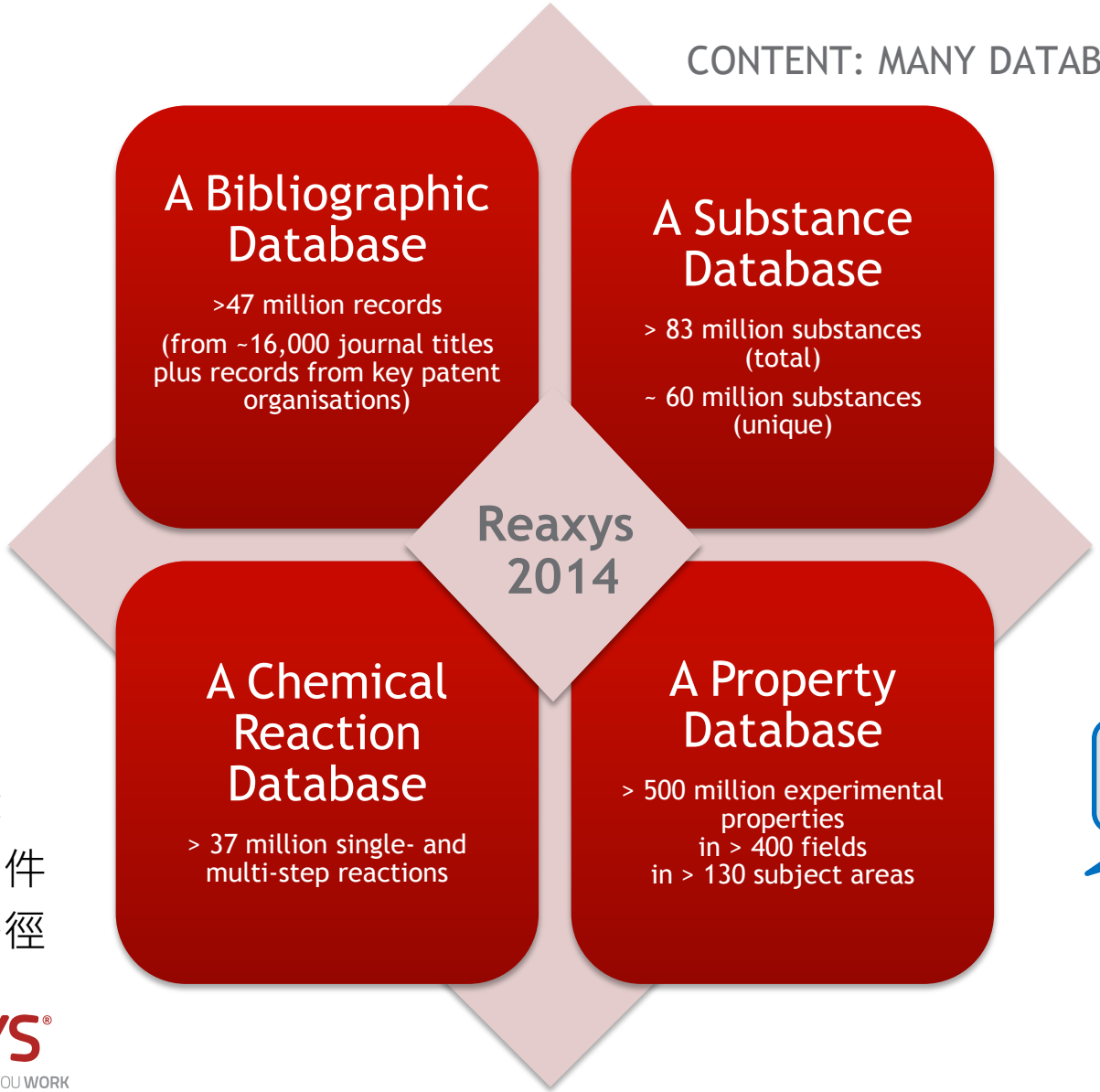
REAXYS 資料庫可以找到哪些資訊?

CONTENT: MANY DATABASES ALL IN ONE

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

> 400 個欄位可獨立或合併搜尋

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REAXYS 搜尋流程

建立搜尋指令

- **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

結果呈現方式

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

篩選分析

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

個人化功能

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

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SEARCH IN REAXYS

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REAXYS 首頁

REAXYS化學資料庫使用介面簡單且**不受使用人數限制**！

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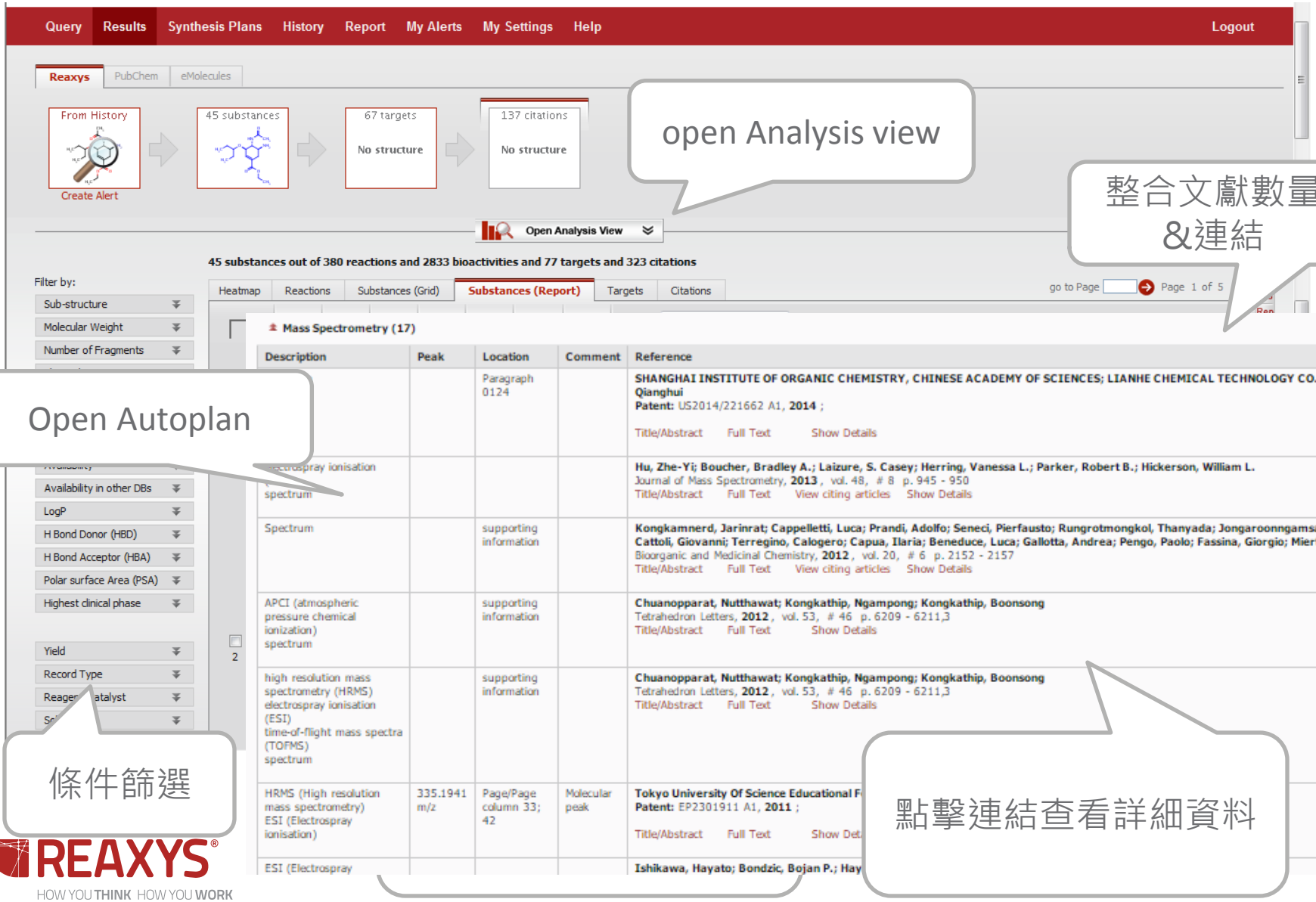
REAXYS 化合物搜尋結果畫面



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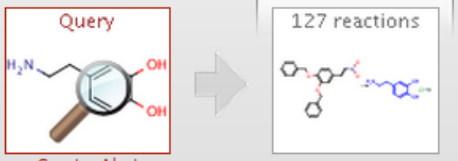
反應搜尋結果畫面

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



Open Analysis View

Filters

Filter by:

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

127 reactions out of 154 substances and 90 citations

Reactions | Substances (Grid) | Substances (Table) | Citations

go to Page | Page 1 of 15

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

	Yield	Conditions	References
1	99% 產率	**With** hydrogenchloride; hydrogen; palladium on activated charcoal **in** ethanol P=760 Torr; 24 h; Ambient temperature; 反應條件	文獻來源出處 **Kohno; Murahashi; Sasao** Bulletin of the Chemical Society of Japan, **1990**, vol. 63, # 4 p. 1252 - 1254 Title/Abstract Full Text View citing articles Show Details
2			

Synthesize | Synthesize | Rx-ID: 2154254 | Find similar reactions

Synthesize | Synthesize | Rx-ID: 336756 | Find similar reactions

文獻搜尋結果畫面

REAXYS®

Anonymous user (145.36.147.151)

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

Reaxys | PubChem | eMolecules

Query — Create Alert

173 substances — Show Query

Open Analysis View

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

Filter by:

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

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

go to Page | Page 1 of 243

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

	Title of the Document	Authors	Year	Source	Times cited
1		Culvenor,C.C.J.; Ham,N.S.	1974	Australian Journal of Chemistry, **1974**, vol. 27, p. 2191 - 2198 Full Text	
	Show All Substances (26) **Hit Substances in this article (1 out of 26)**				
2	2-Amino-1,2,3,4,-tetrahydronaphthalene derivatives with cardiovascular activity, [illegible] their preparation and pharmaceutical compositions containing them	CHIESI FARMACEUTICI S.p.A.	1991	**Patent:** EP405344 A2, **1991**; **Patent Family:** EP405344 A2; EP405344 B1; Full Text	
	Title/Abstract **Front page Information** **Show All Reactions (7)** **Show All Targets** **Show All Substances (26)** **Hit Substances in this article (1 out of 26)**				
3	Substituted aryl and aralkyl amides in the treatment of parkinsonism	Schering Corporation	1976	**Patent:** US3944675 A1, **1976**; **Patent Family:** US3944675 A1; US4053509 A1; Full Text	
	Title/Abstract **Front page Information** **Show All Reactions (23)** **Show All Substances (50)** **Hit Substances in this article (1 out of 50)**				

標題 | 作者 | 年份 | 文獻來源出處 | 引用次數

列出文獻中所有化合物結構、反應式、專利資訊及相關連結

Ask Reaxys 實際範例

Ask Reaxys | Enter a keyword, concept or author | Go

Examples

Substances

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

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

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

Substance Properties

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

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

FERROELECTRICITY
"ferroelectric materials" Substances with ferroelectric data will be searched
Try it

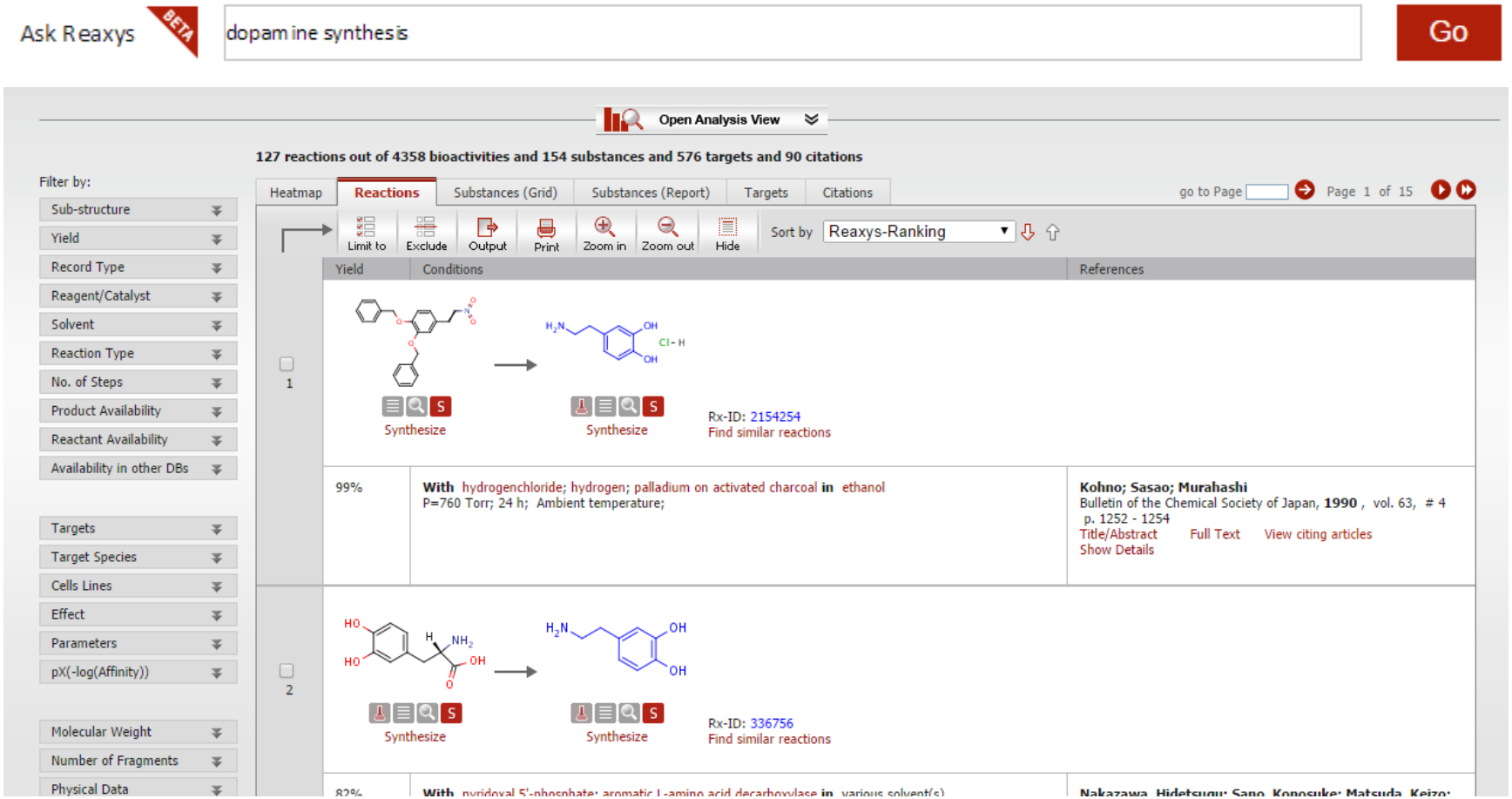
Reactions

SYNTHESIS
"preparation of porphyrine" Reactions with porphrine (structured) as product will be searched
Try it

REACTION TYPE
"phosphorylation" Reactions with reaction type phosphorylation will be searched
Try it

NAMED REACTION
"Suzuki coupling" Reactions with reaction type Suzuki coupling will be searched
Try it

實例說明 1
DOPAMINE 合成方法



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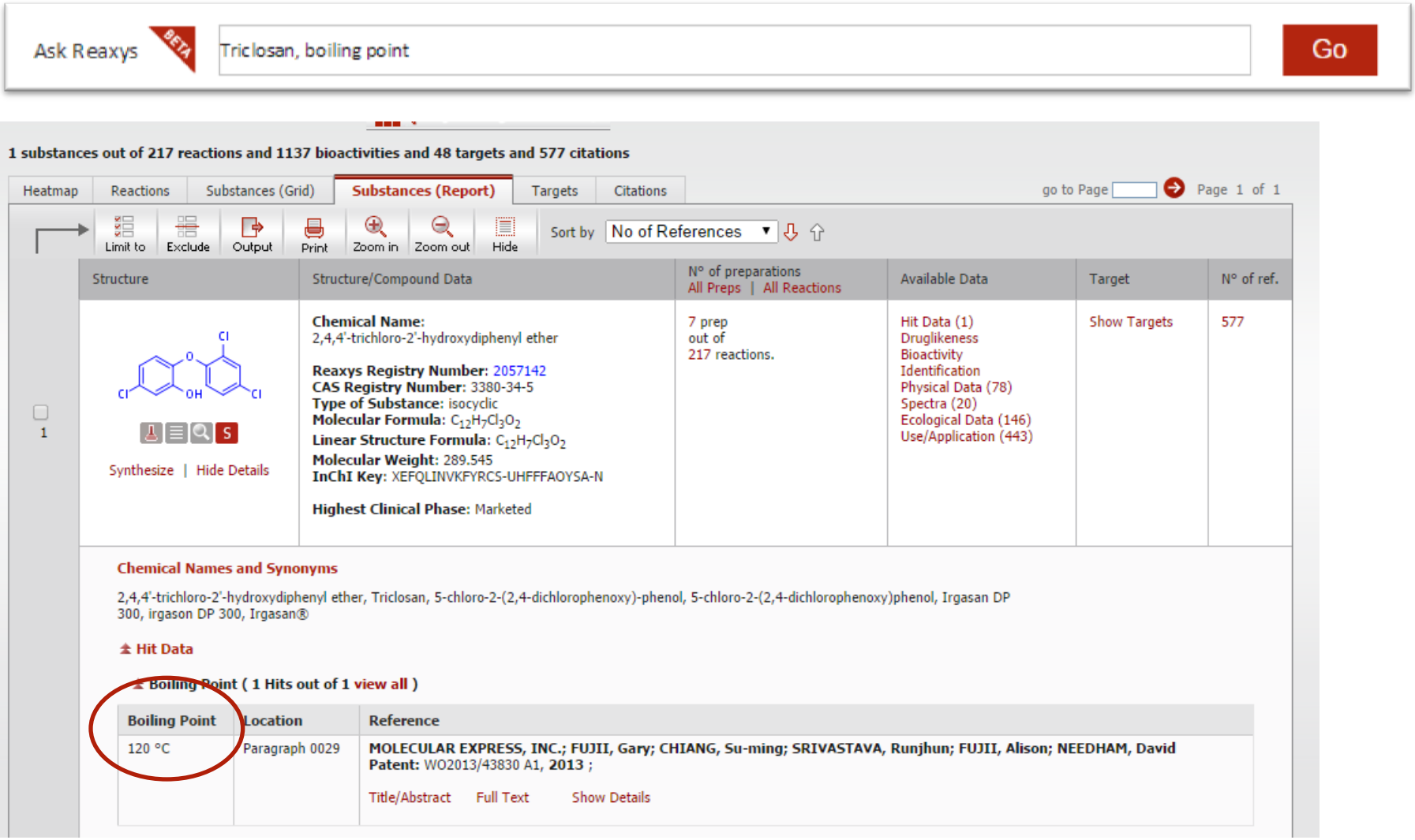
實例說明2
TRICLOSAN, BOILING POINT



Ask Reaxys

智慧辨認輸入的關鍵字

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

Import | Save

Ask Reaxys - Analysis

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

Suggested Query	Results	Select Action
superconductors 2013 **Result: citations** Show query	2085 citations in Reaxys	Search Edit query in Advanced
superconductors 2013 **Result: citations** Show query	123 citations in Reaxys	Search Edit query in Advanced

Legend: Bibliography | Compound | Concept | Date | Keyword | Bioactivity | ~~Ignored~~

Cancel

You can also search directly by these common property groups:

Physical | Spectra | Natural Product | Advanced

影片介紹

Ask Reaxys

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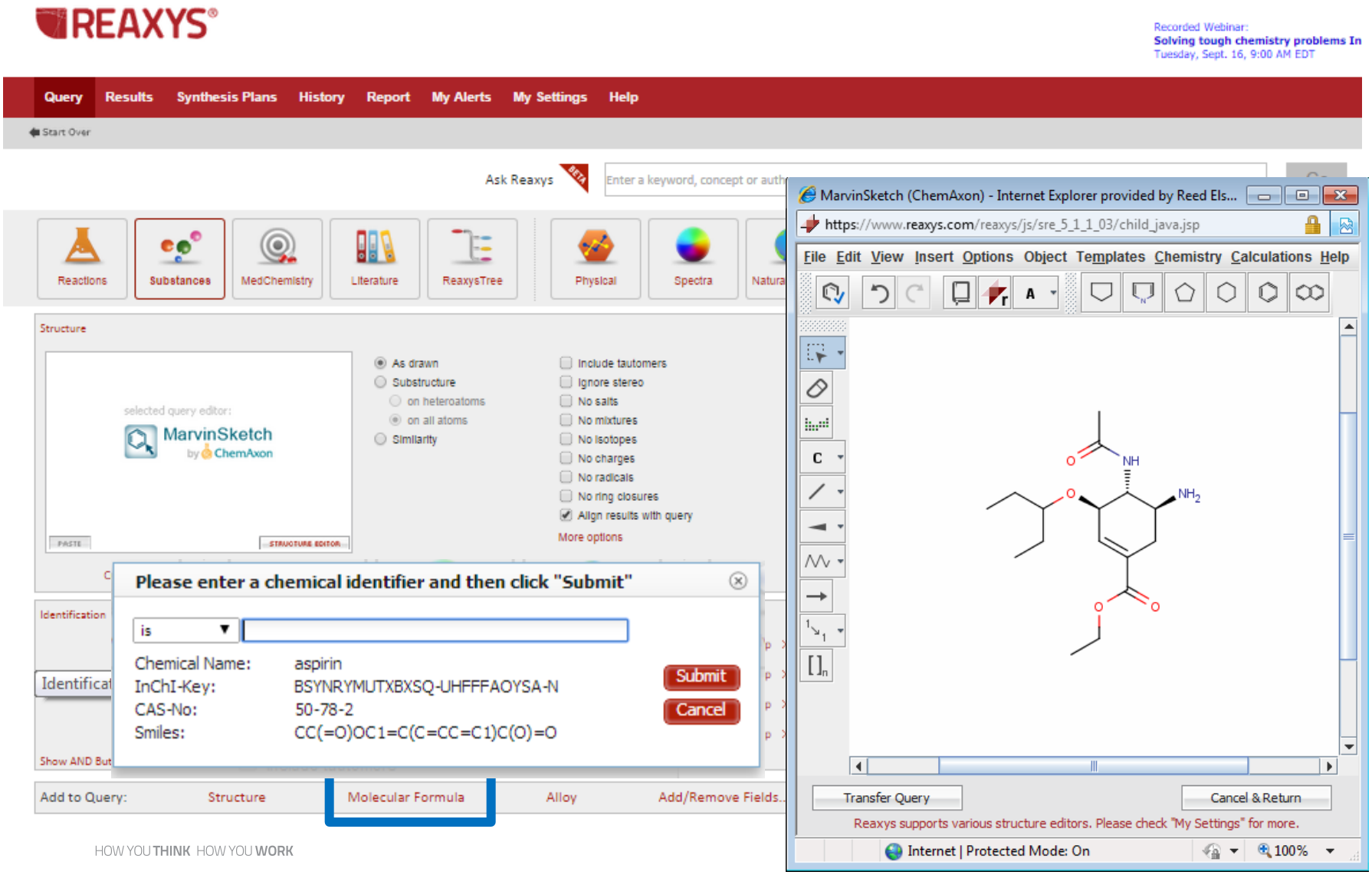
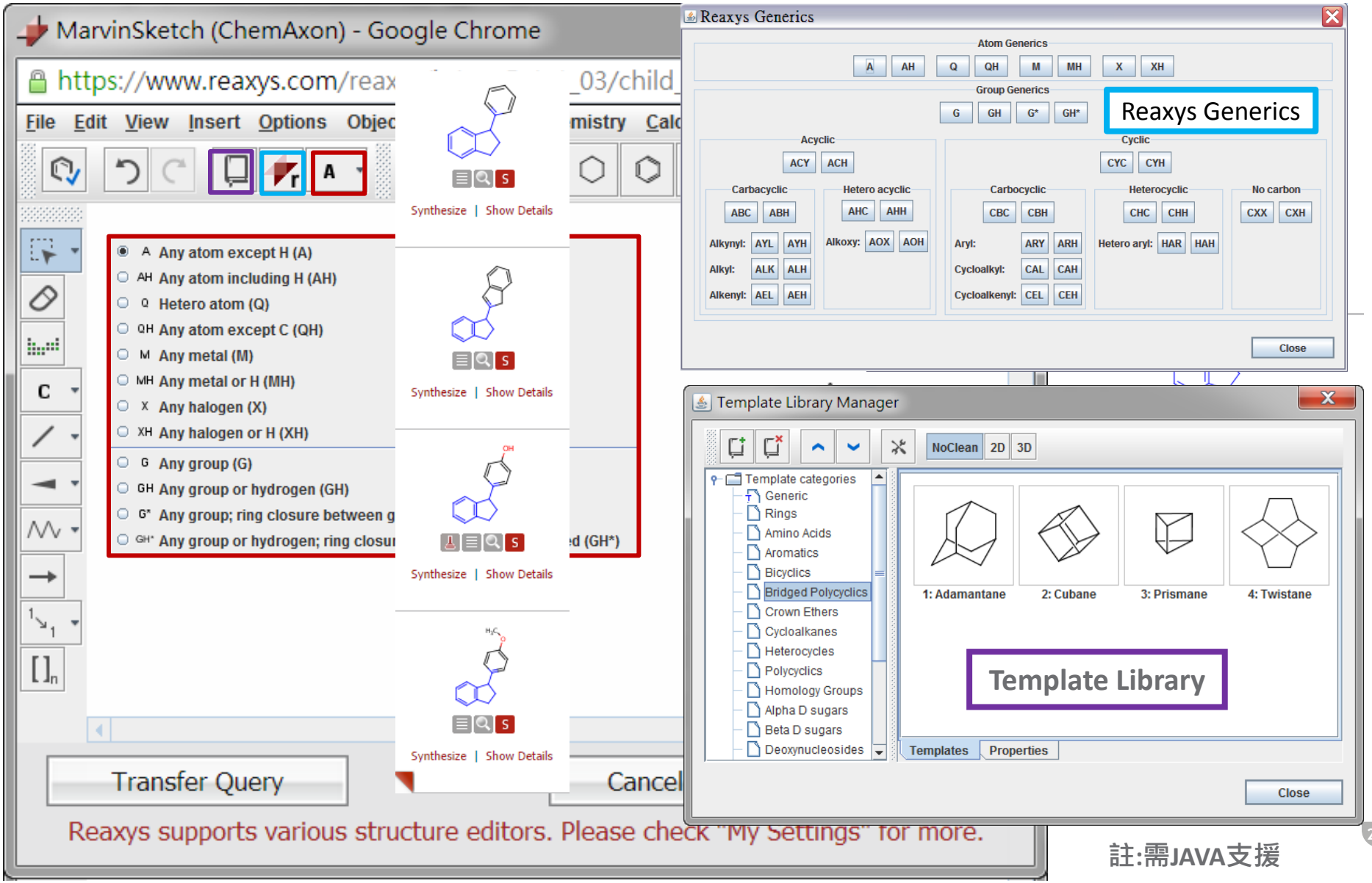
REAXYS 搜尋介面


REAXYS
Recorded Webinar:
Solving tough chemistry problems In
Tuesday, Sept. 16, 9:00 AM EDT
Query
Results
Synthesis Plans
History
Report
My Alerts
My Settings
Help
Start Over
Ask Reaxys
Enter a keyword, concept or auth
Reactions
Substances
MedChemistry
Literature
ReaxysTree
Physical
Spectra
Structure
selected query editor:
MarvinSketch
by ChemAxon
As drawn
Substructure
on heteroatoms
on all atoms
Similarity
Include tautomers
Ignore stereo
No salts
No mixtures
No isotopes
No charges
No radicals
No ring closures
Align results with query
More options
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
Identification
Identificat
Show AND But
Add to Query:
Structure
Molecular Formula
Alloy
Add/Remove Fields...
MarvinSketch (ChemAxon) - Internet Explorer provided by Reed Els...
https://www.reaxys.com/reaxys/js/sre_5_1_1_03/child_java.jsp
File Edit View Insert Options Object Templates Chemistry Calculations Help
Transfer Query
Cancel & Return
Reaxys supports various structure editors. Please check "My Settings" for more.
Internet | Protected Mode: On
100%

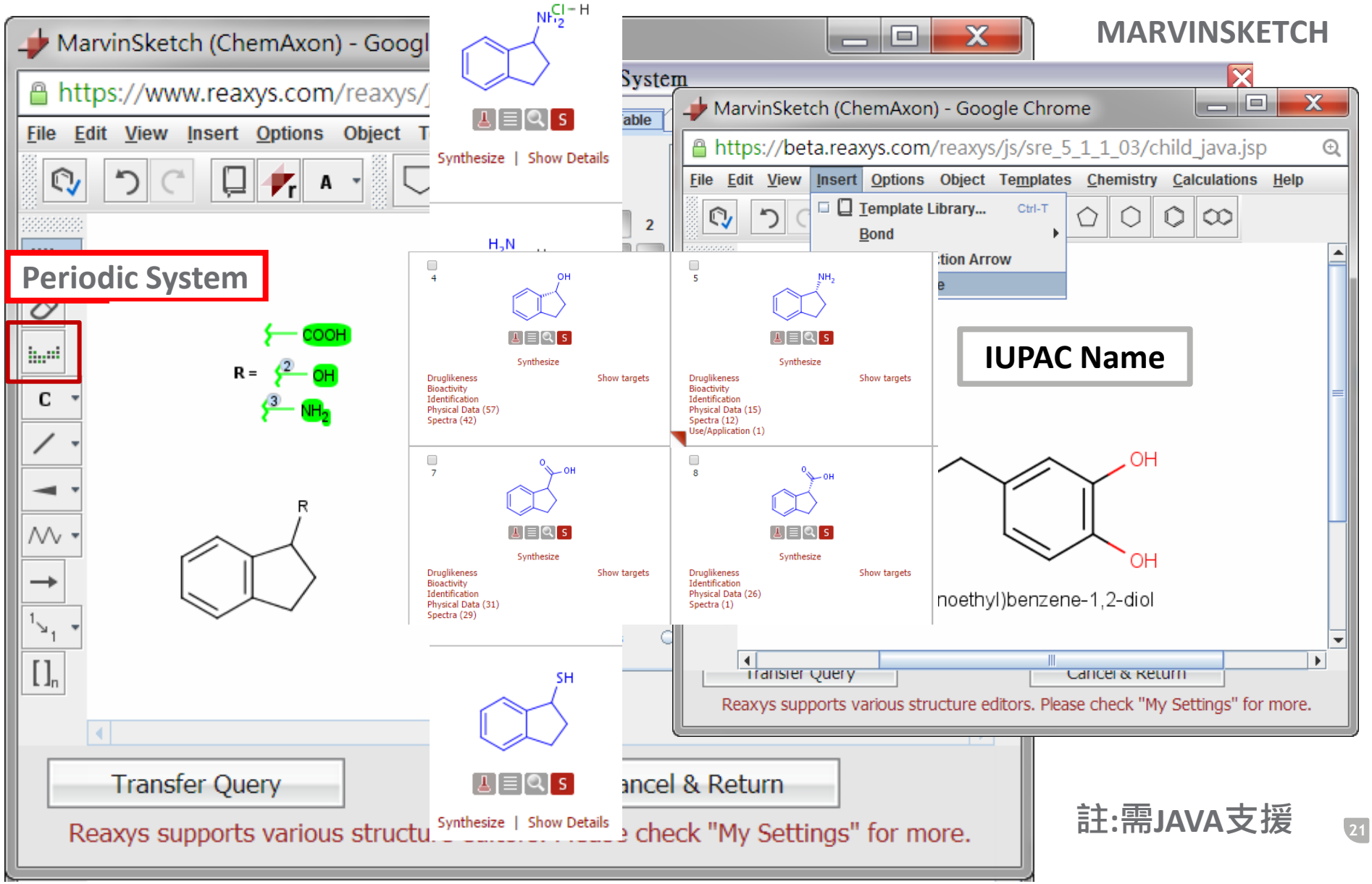
繪圖軟體 - MARVINSKETCH



註:需JAVA支援

繪圖軟體 - MARVINSKETCH

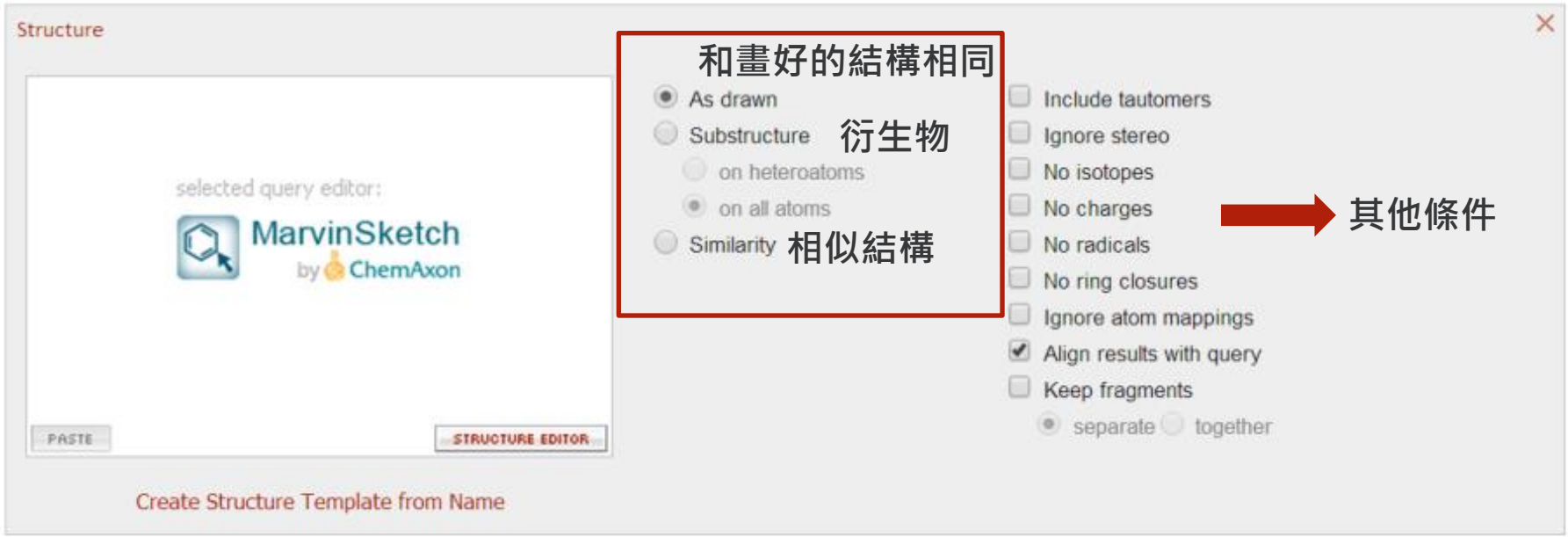
MARVINSKETCH

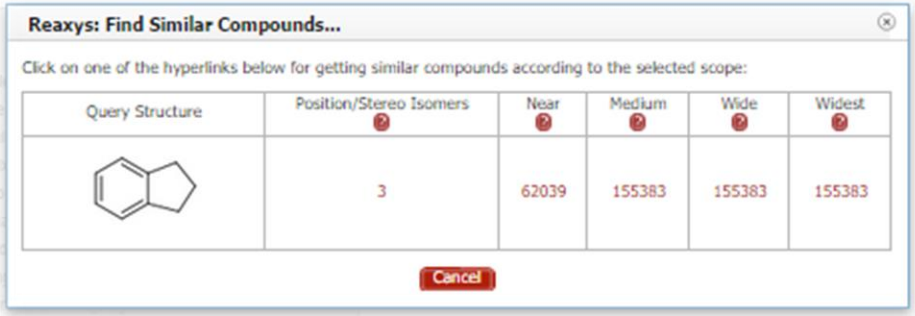


註:需JAVA支援

衍生物搜尋

REAXYS 可以針對您的需求，搜尋各式各樣的衍生物





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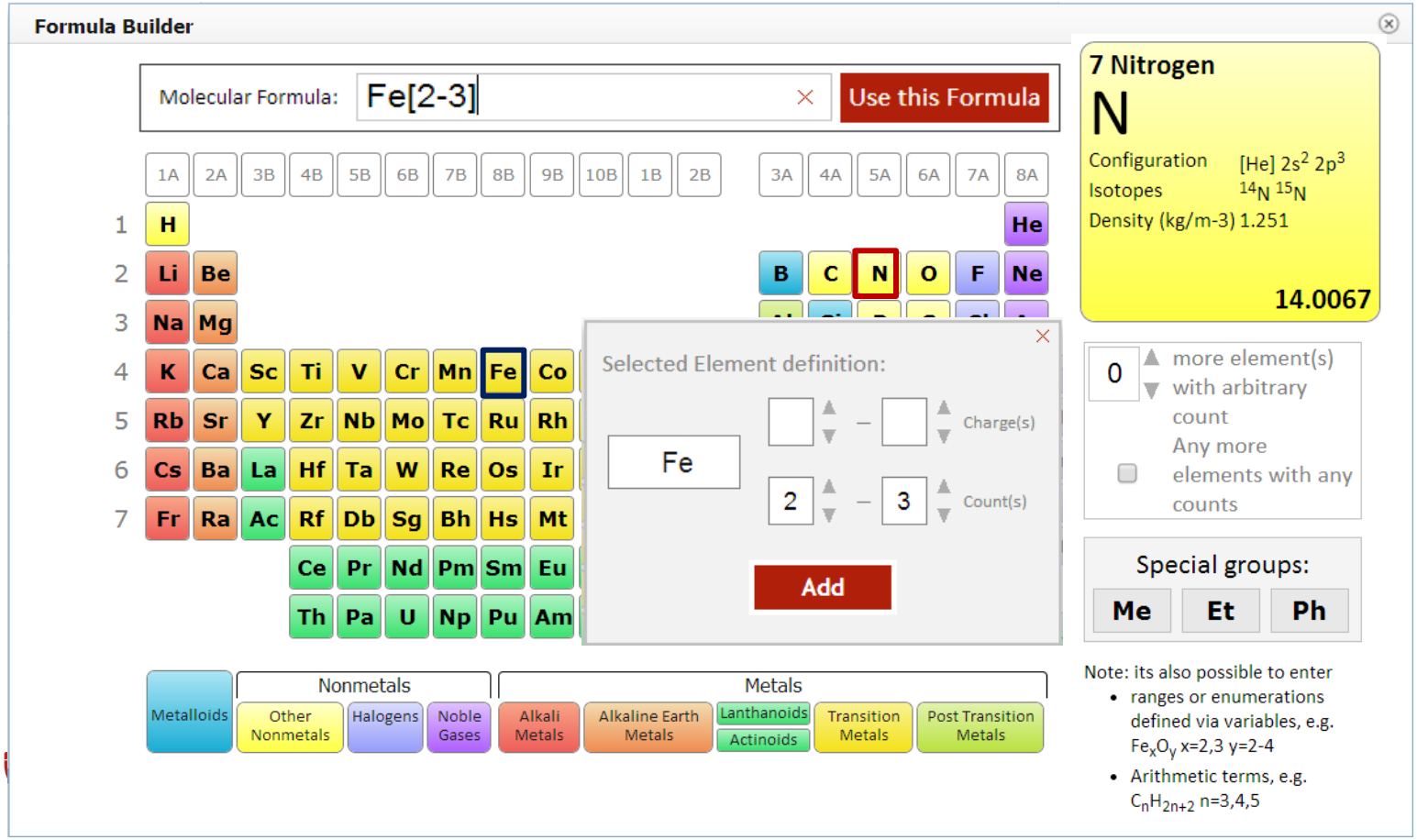
Fe2O3
Fe3O4
AlGaO

建立搜尋指令-分子式
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

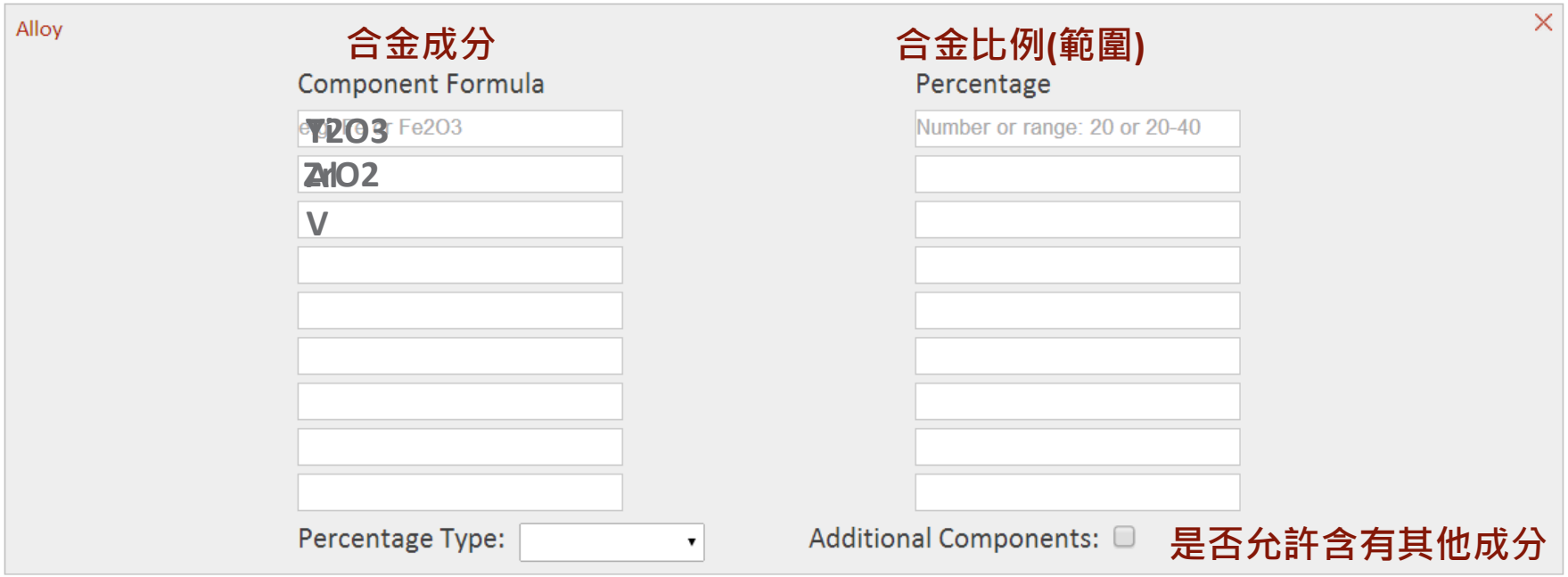
Query Builder

建立搜尋指令-合金

Alloy

Ti-6Al-4V

yttria/zirconia ceramics



或者您也可以使用Advanced Search

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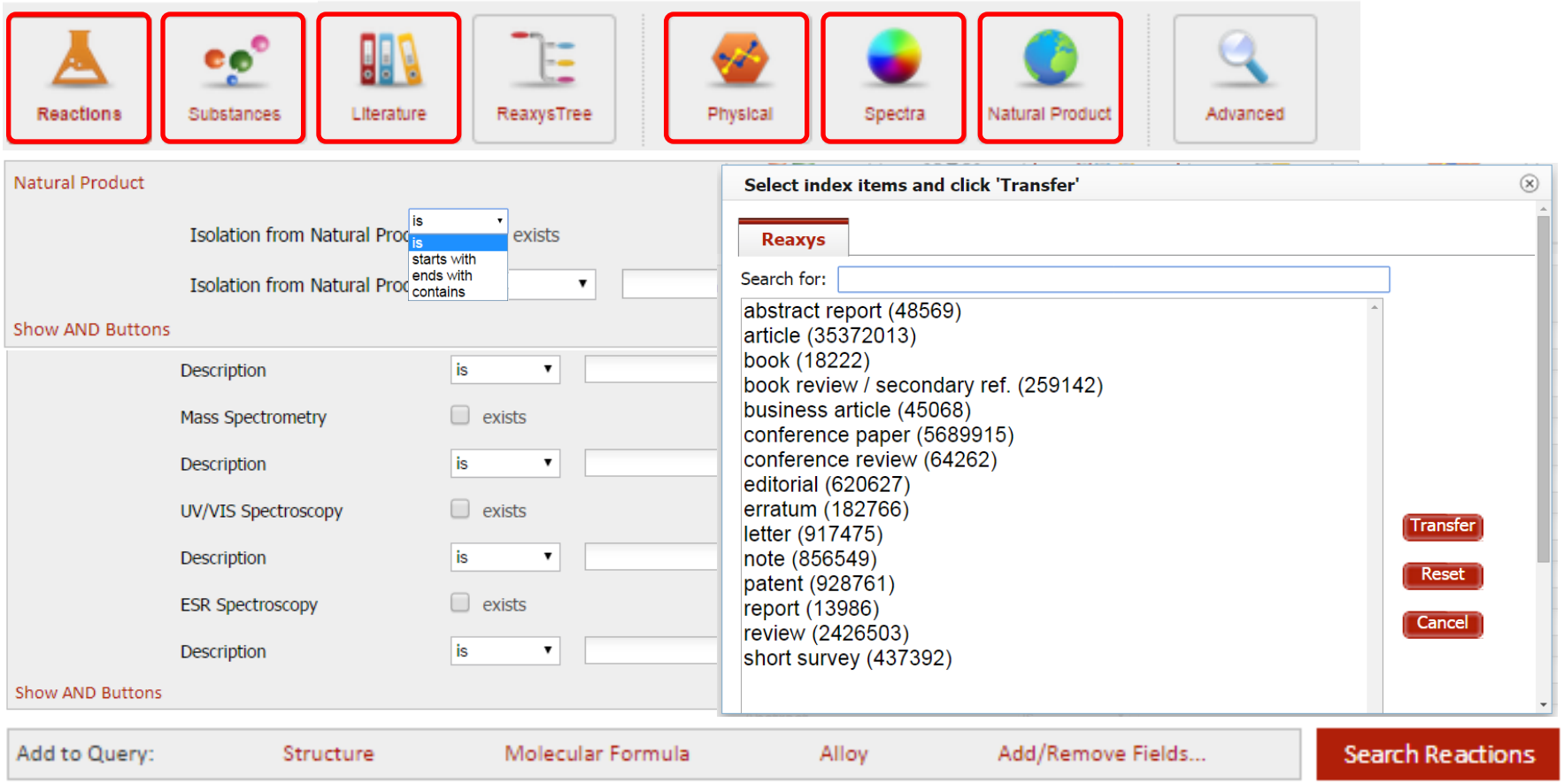
欄位搜尋

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



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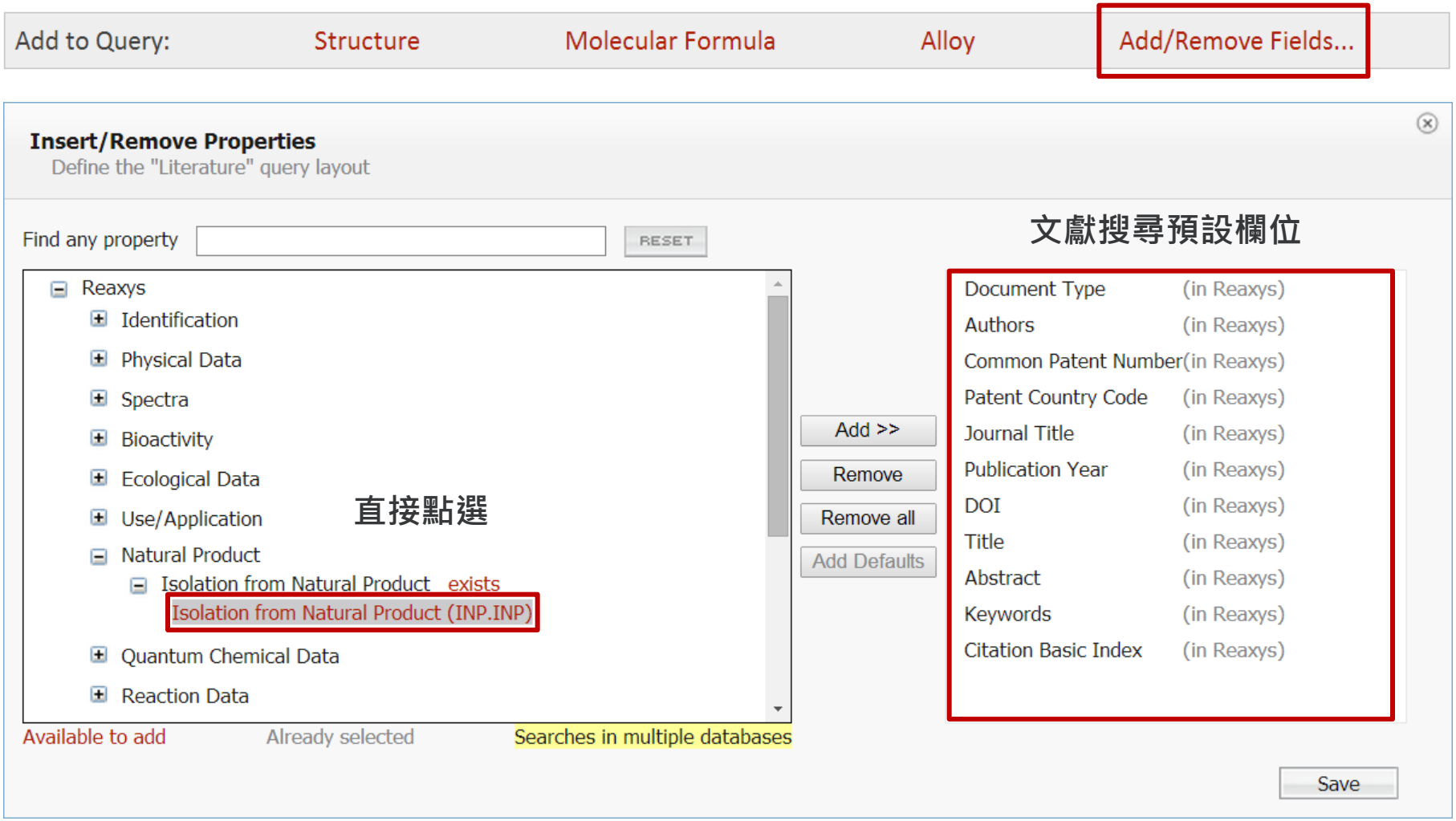
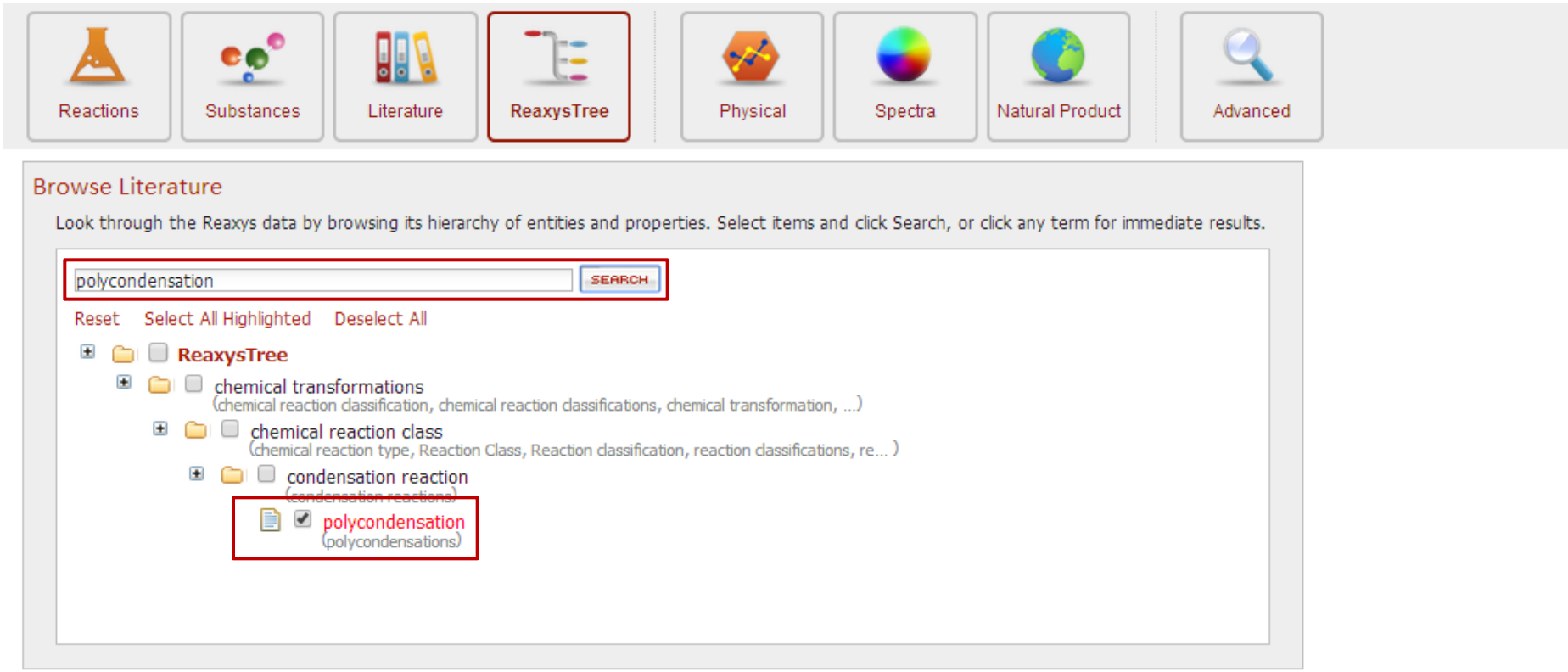
新增欄位
Fields


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

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REAXYS 搜尋流程

建立搜尋指令

- **Ask Reaxys: 關鍵字智慧搜尋**
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- Analysis View: 視覺化分析系統
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- AutoPlan: 規畫合成路徑

個人化功能

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

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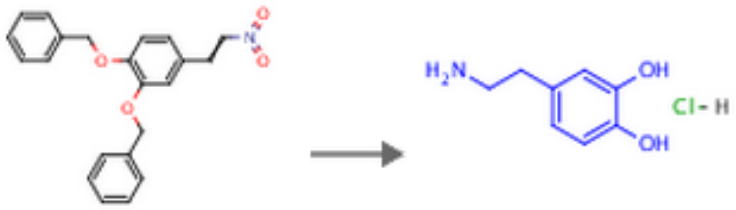
建立合成計畫
Synthesis Plans



Synthesize

Synthesize

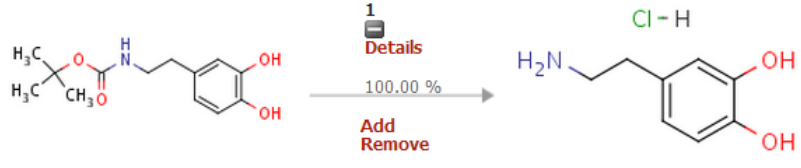
Rx-ID: 2154254
Find similar reactions

Manually
by Autoplan
by Autoplan (with options)

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

Synthesis 1 | Synthesis 2 | Synthesis 3 | Synthesis 4

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



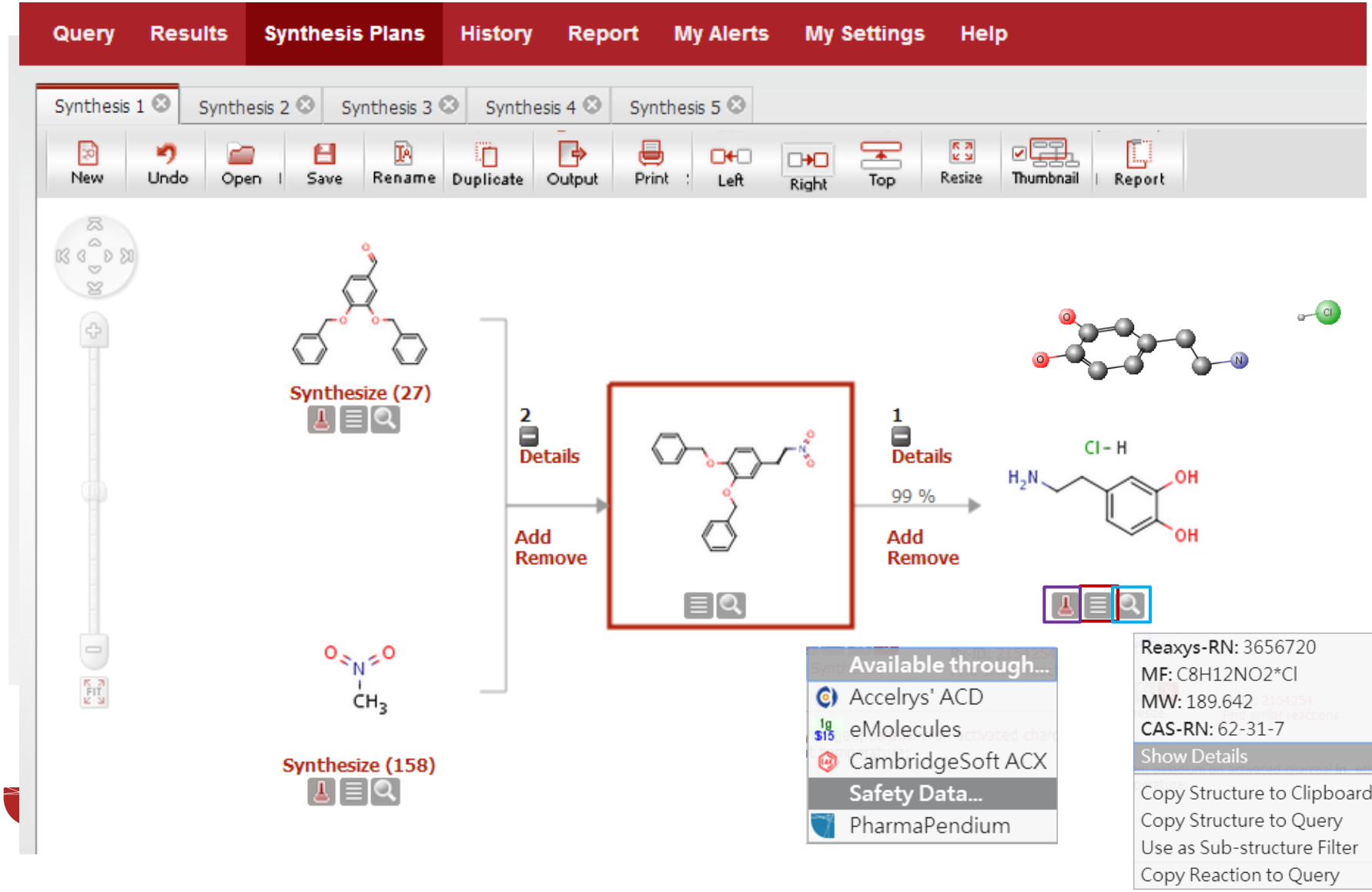
Synthesize (7)

Manually
by Query
by Autoplan
by Autoplan (with options)

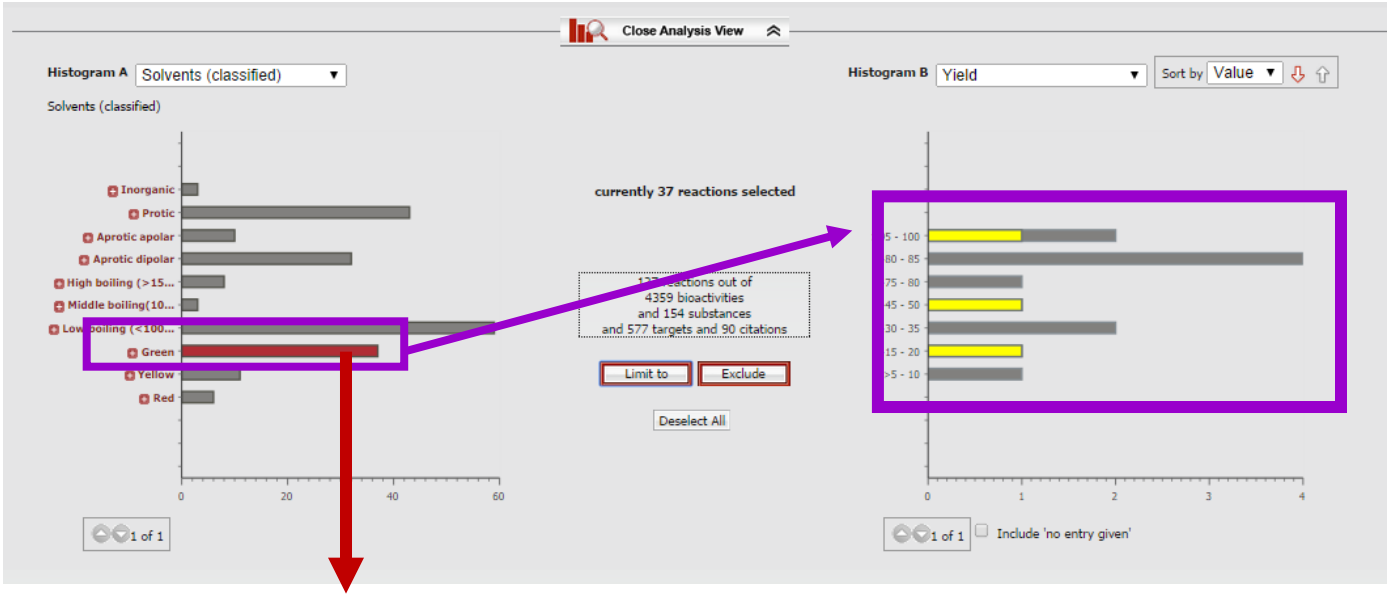
Hide selected details | Hide all details | Show all details

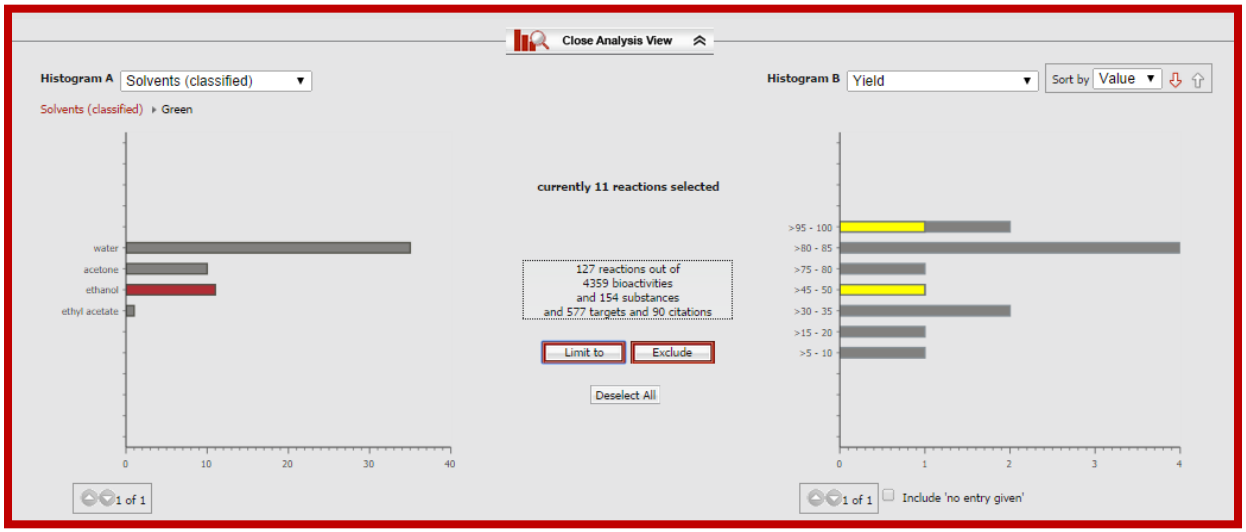
Step	Yield	Conditions	References
1 Reaxys	100%	With methanol; chloro-trimethyl-silane 3 h; Reflux;	Barontini, Maurizio; Bernini, Roberta; Crisante, Fernanda; Fabrizi, Giancarlo Synthesis, 2009 , # 22 art. no. P09409SS, p. 3838 - 3842 Title/Abstract Full Text View citing articles Show Details

建立合成計畫
manually



視覺化分析工具 -- Analysis View





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多樣化結果輸出功能 - ENHANCED REPORT

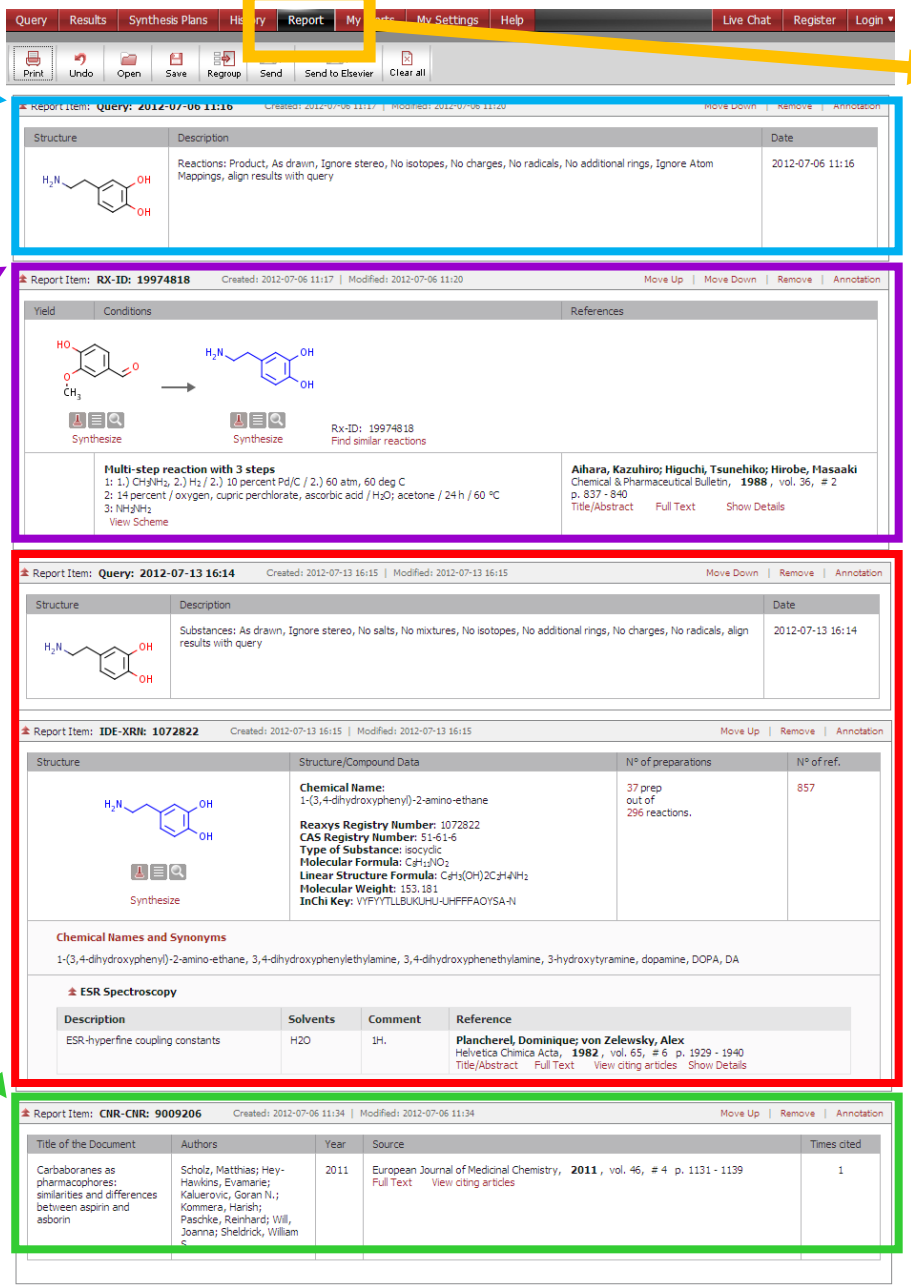
搜尋紀錄輸出

反應搜尋結果輸出

化合物搜尋結果輸出

文獻搜尋結果輸出

輸出結果



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- My Settings: 個人化設定

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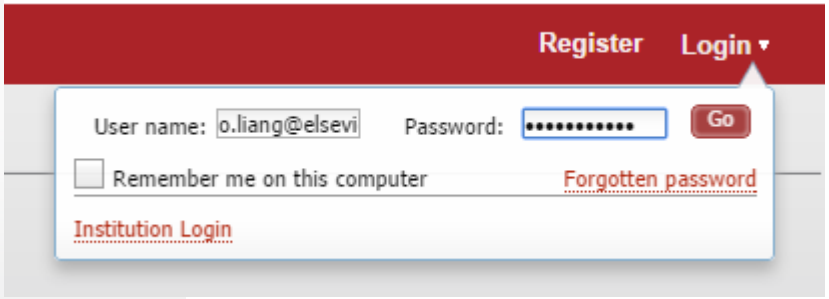
個人化功能
註冊及登錄



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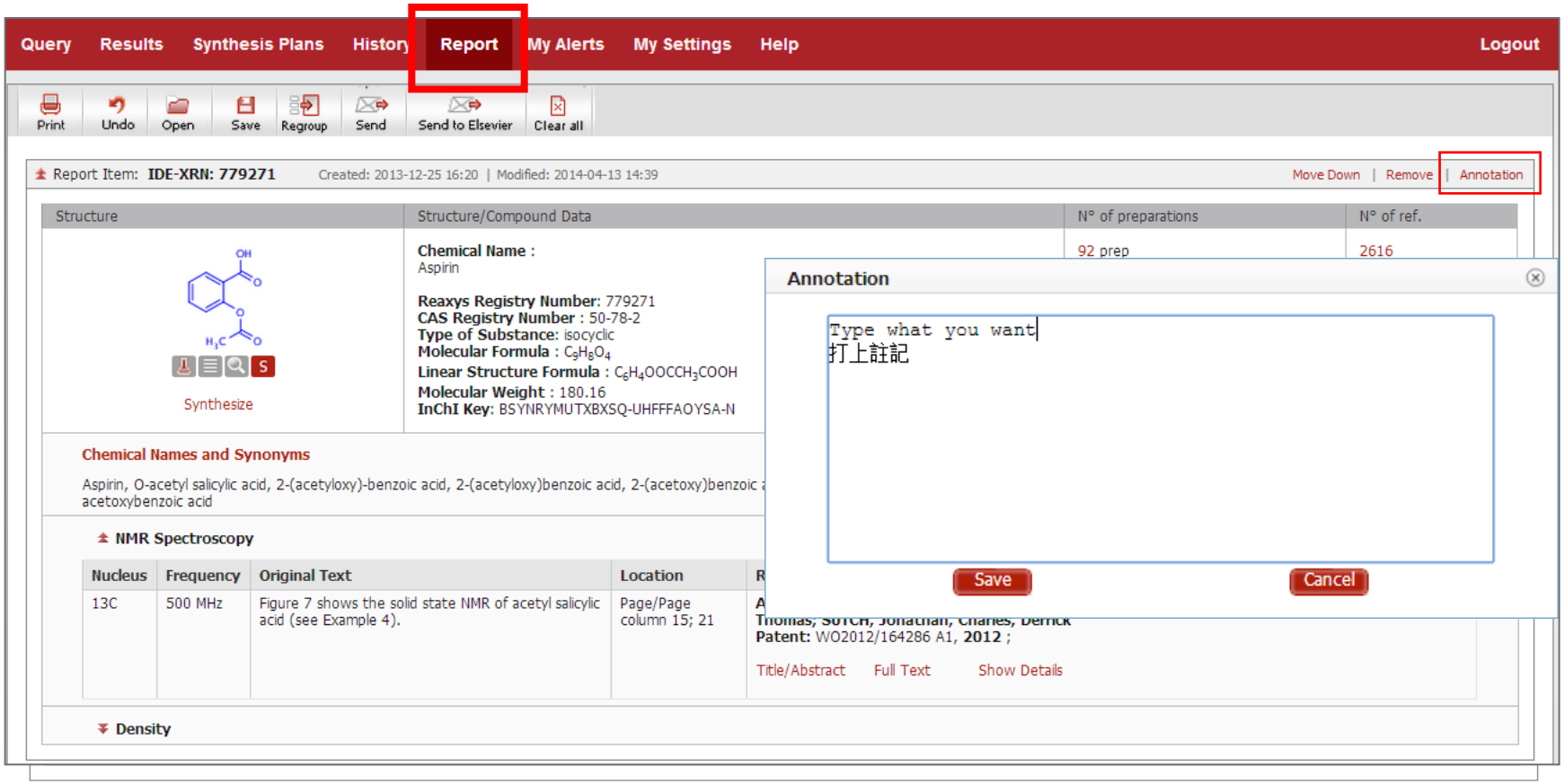
主題 1 : Report

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



多樣化結果輸出功能 - ENHANCED REPORT

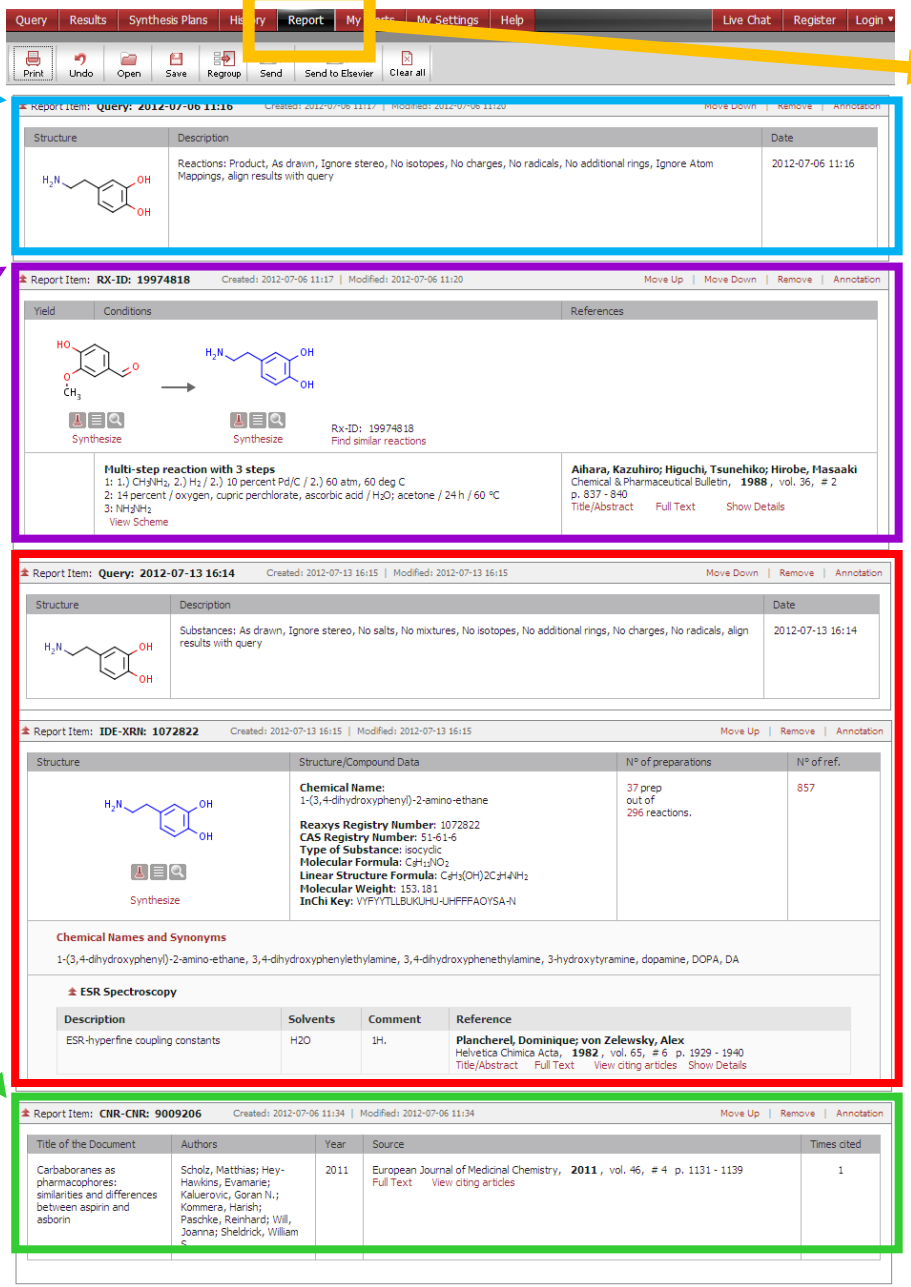
搜尋紀錄輸出

反應搜尋結果輸出

化合物搜尋結果輸出

文獻搜尋結果輸出

輸出結果



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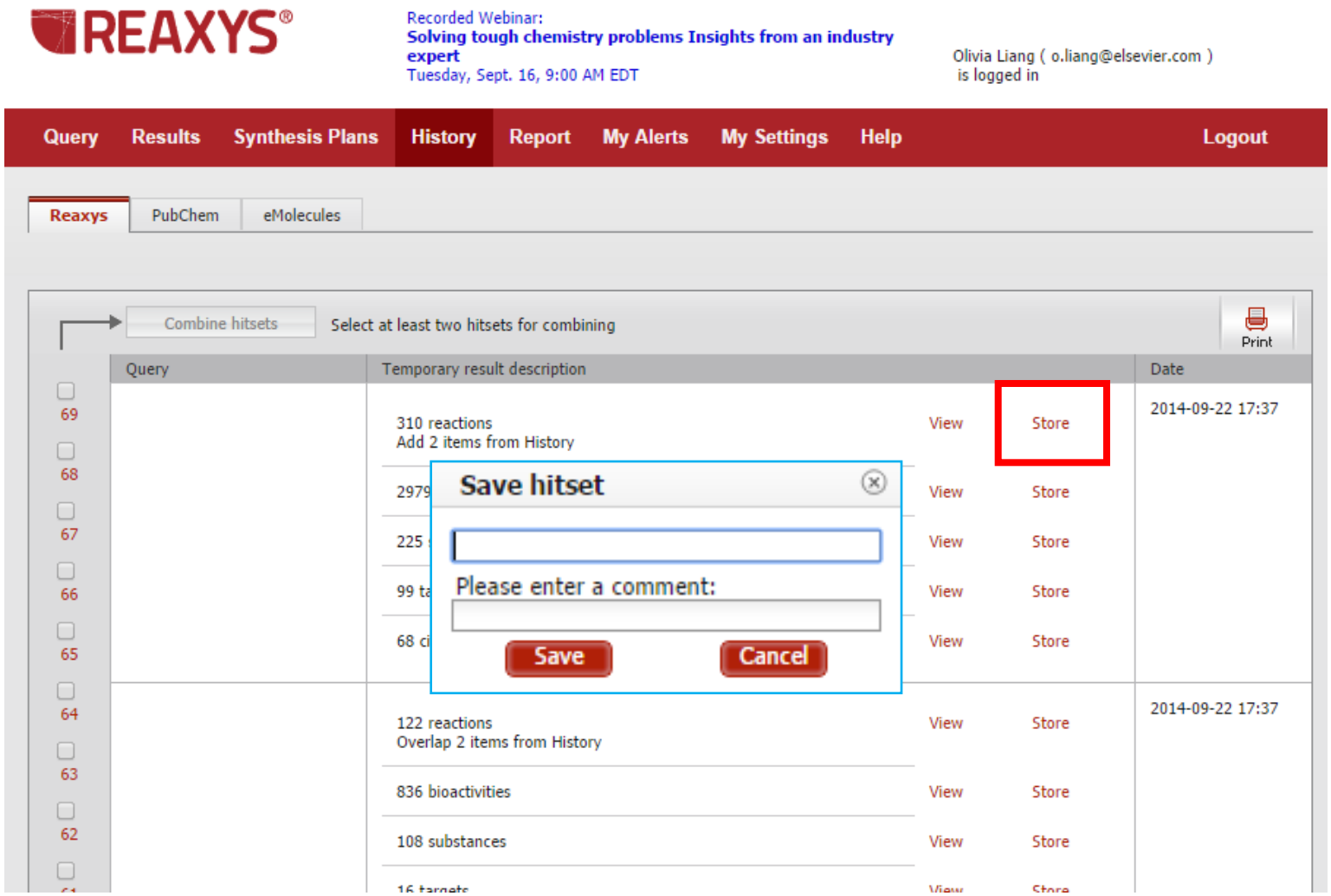
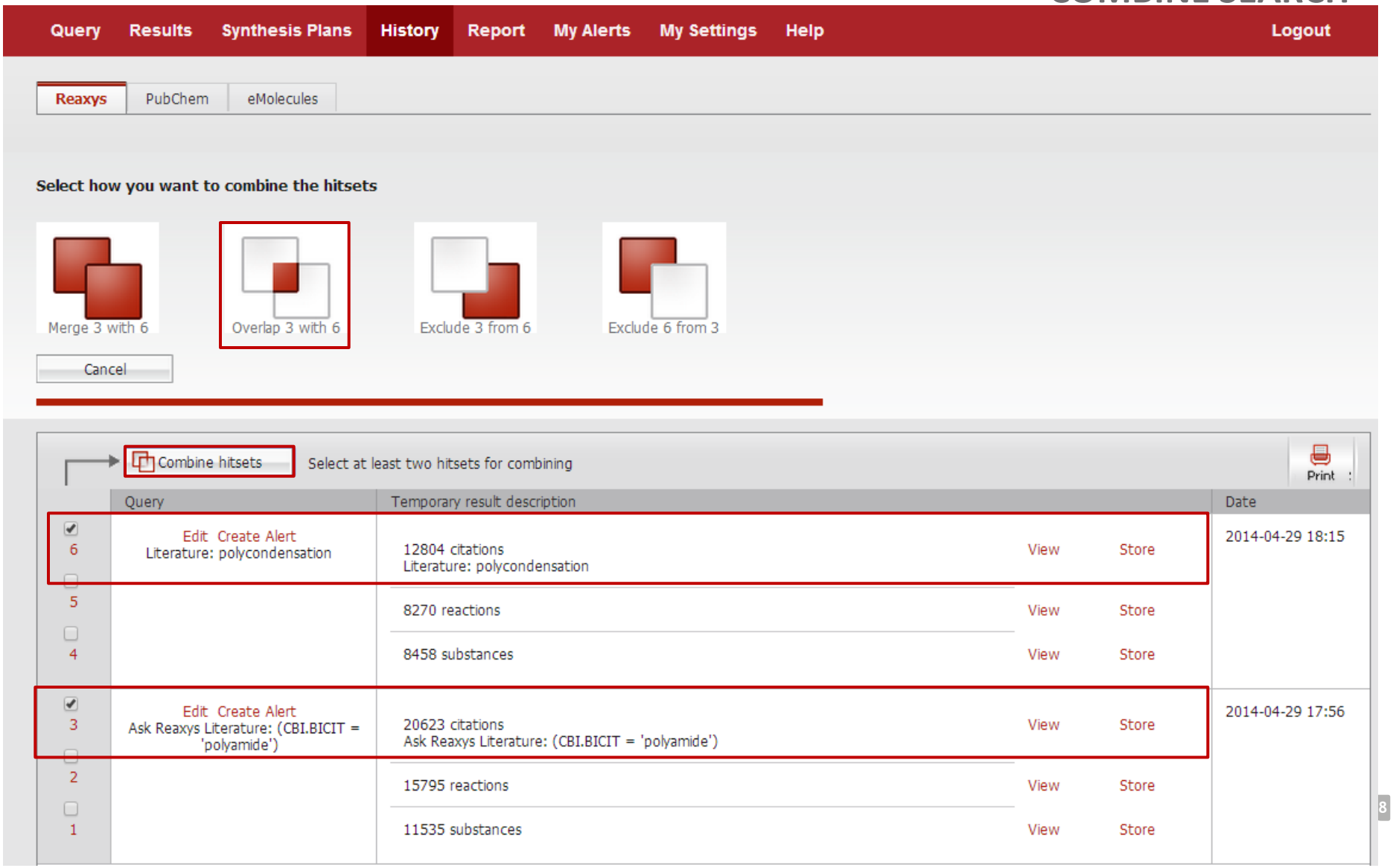
主題 2 : History

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



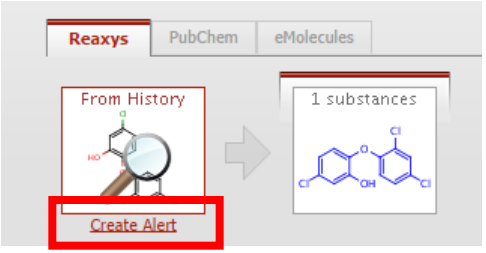
SEARCH HISTORY

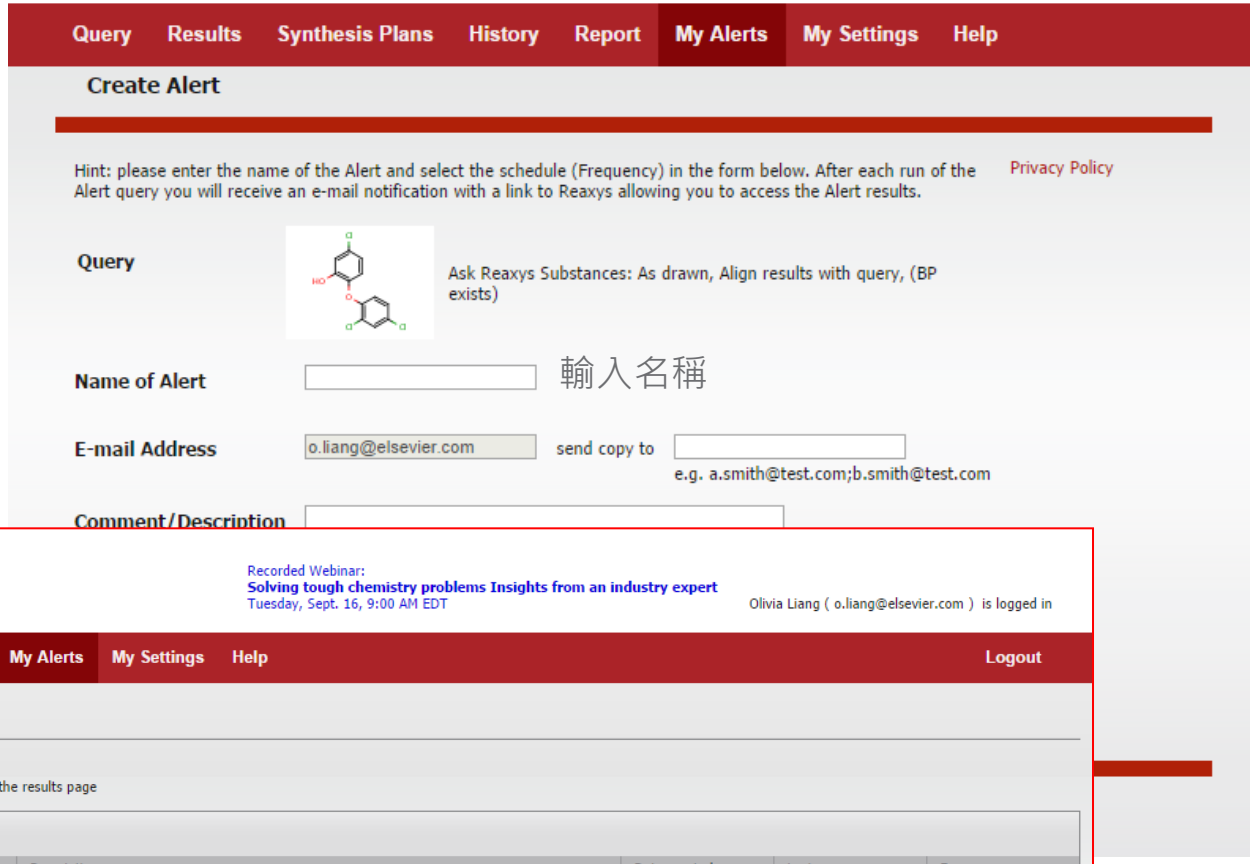
COMBINE SEARCH

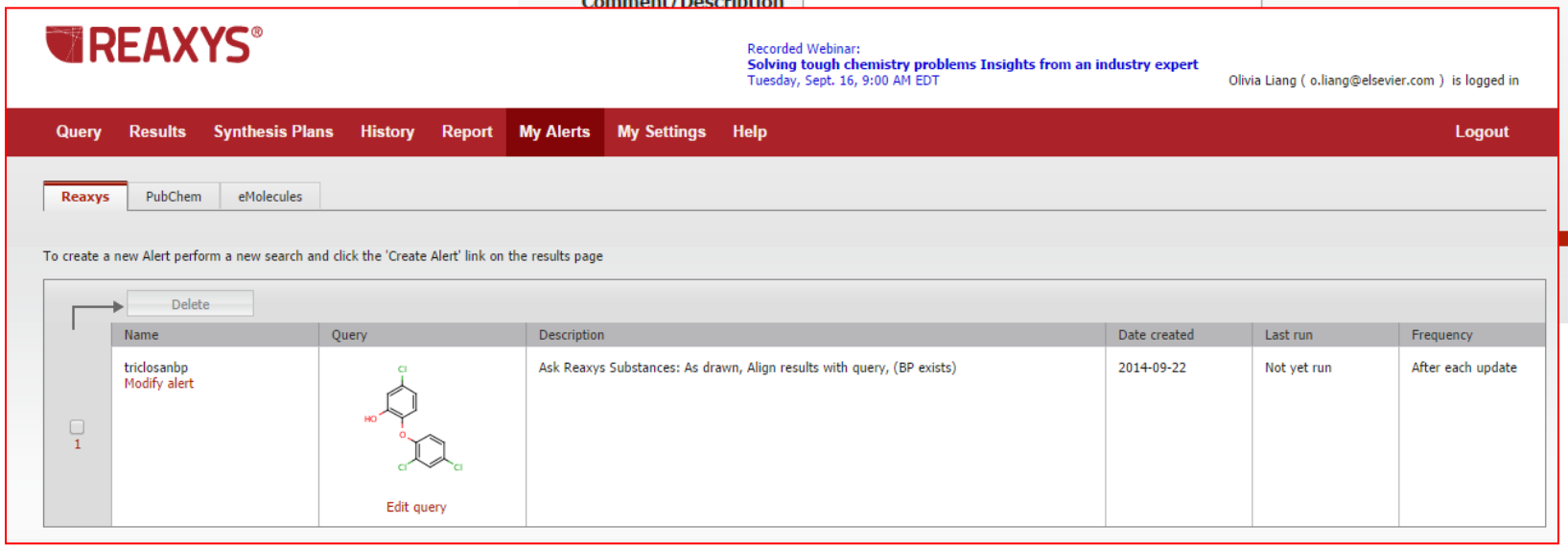


主題 3 : My Alerts

新知通報 (MY ALERTS)：訂閱常用搜尋條件，隨時閱讀最新資料。

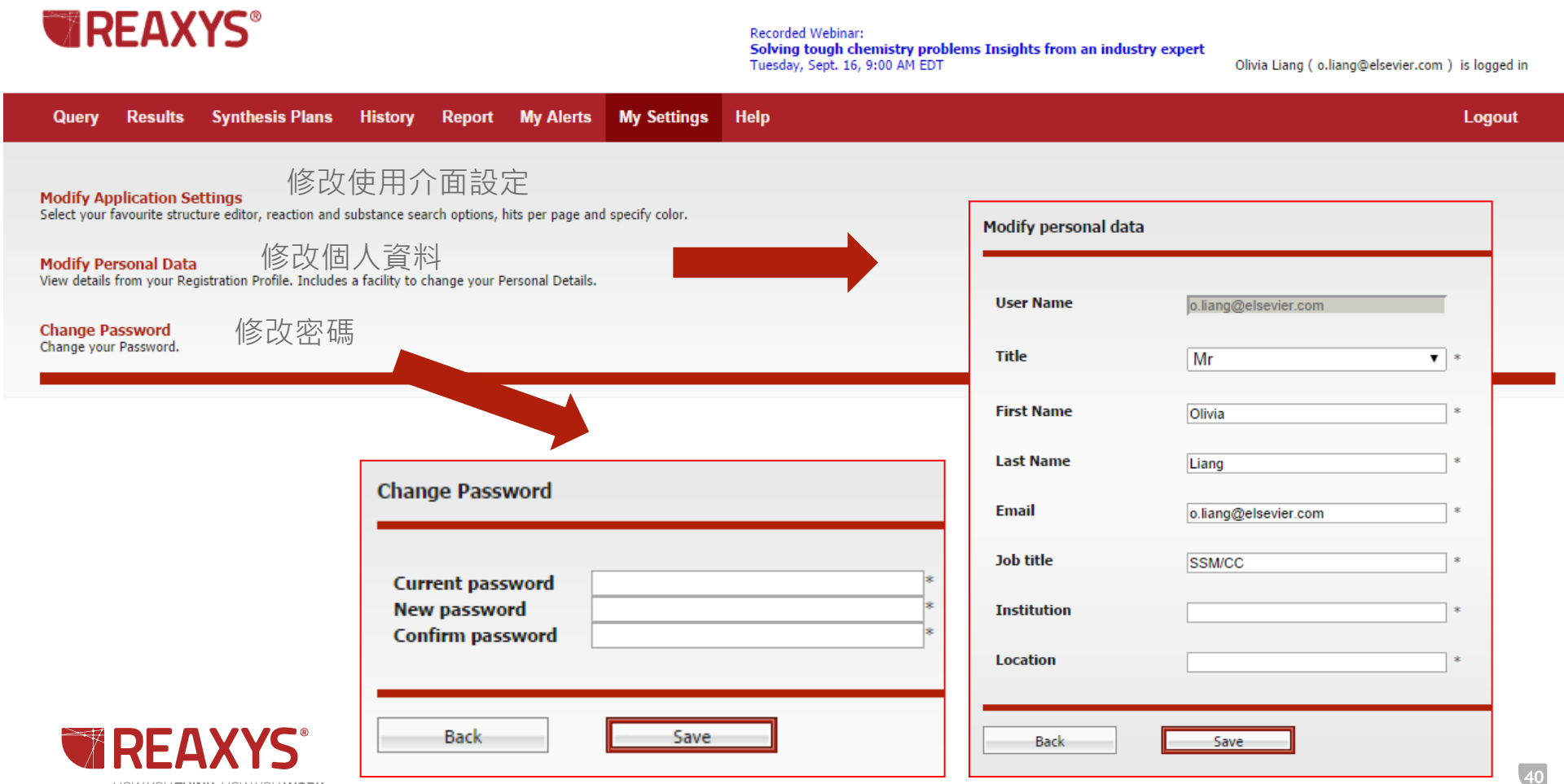






主題 4 : My Setting

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



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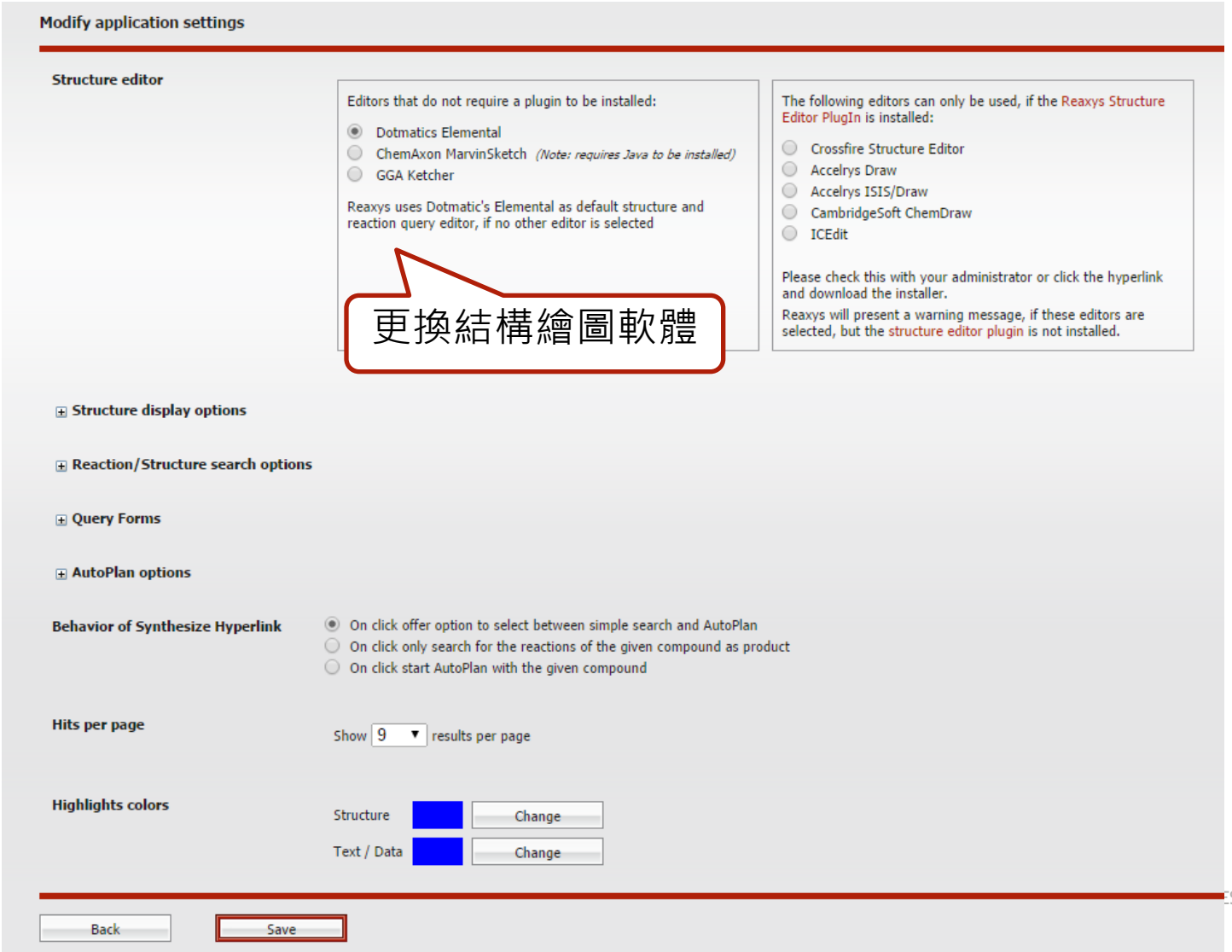
修改使用介面設定


Modify application settings
Structure editor
Editors that do not require a plugin to be installed:
Dotmatics Elemental
ChemAxon MarvinSketch (Note: requires Java to be installed)
GGA Ketcher
Reaxys uses Dotmatic's Elemental as default structure and reaction query editor, if no other editor is selected
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.
更換結構繪圖軟體
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 9 results per page
Highlights colors
Structure
Change
Text / Data
Change
Back
Save

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如有相關問題請連絡

梁 成 芝

LIFE SCIENCE CUSTOMER CONSULTANT

O.LIANG@ELSEVIER.COM

電話:(02)2522-5937

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