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CAS / SciFinder Web

Basic Training

2009.10

A division of the American Chemical Society
www.cas.org

內容綱要

- SciFinder Web新介面介紹
- 文獻檢索(Explore Reference)
- 物質檢索(Explore Substance)
- 反應檢索(Explore Reaction)

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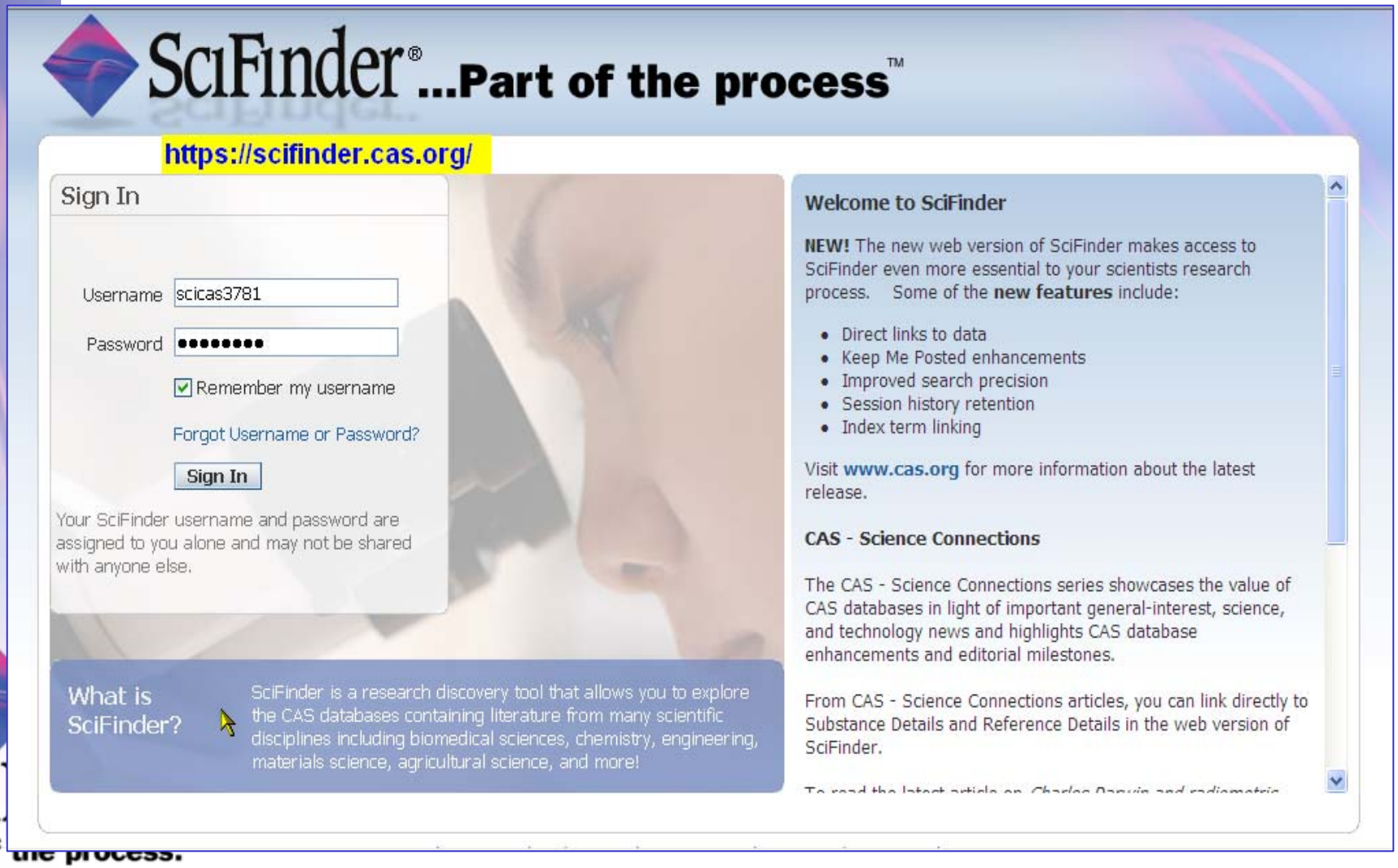
SciFinder Web網址 https://scifinder.cas.org

-https 連線透過 “port 443”; IP: 134.243.5.42

-Windows / Mac : IE, FireFox, Safari, Chrome

-Java Runtime Environment (JRE 6.x) ; Java Plug-In



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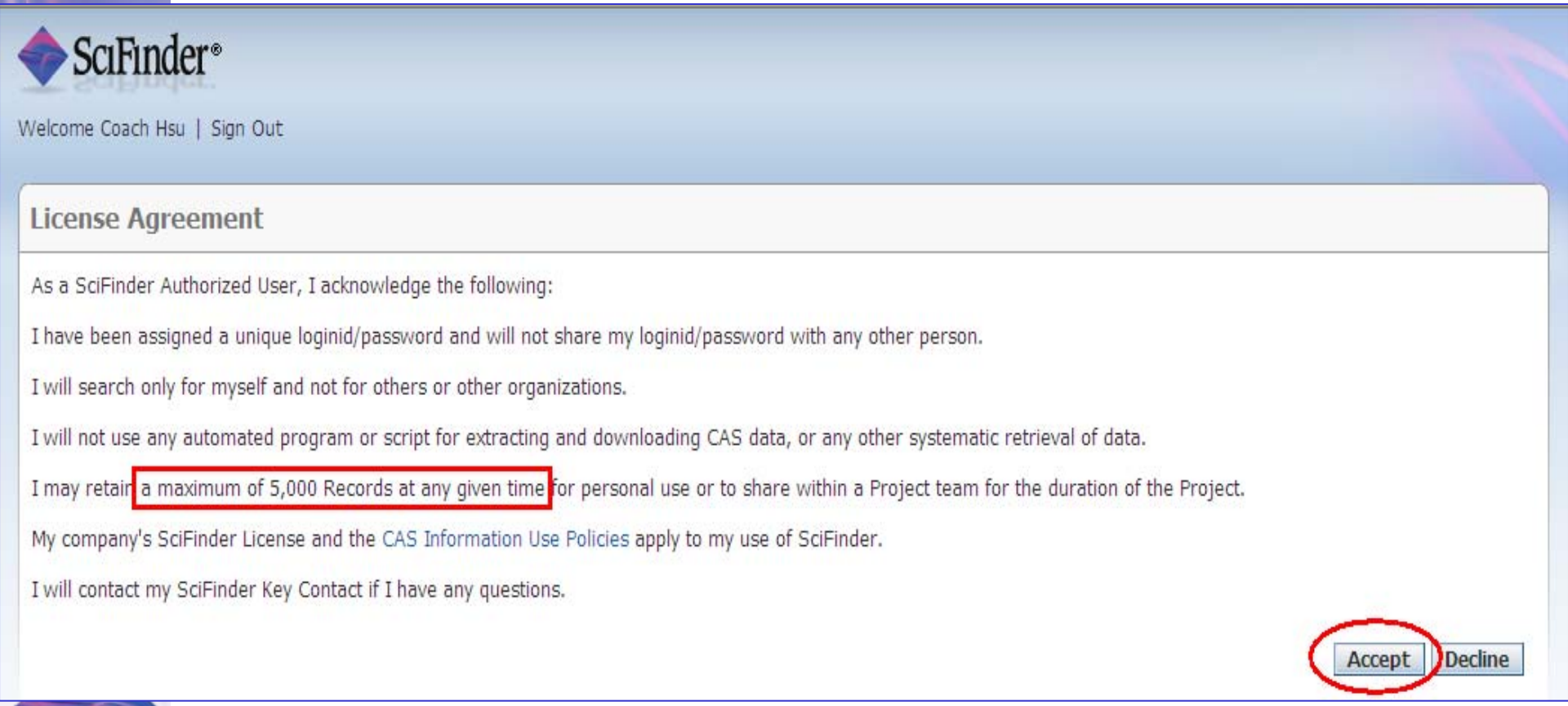
請尊重智財權及著作權，
勿違法使用及大量下載~



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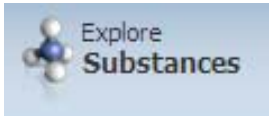
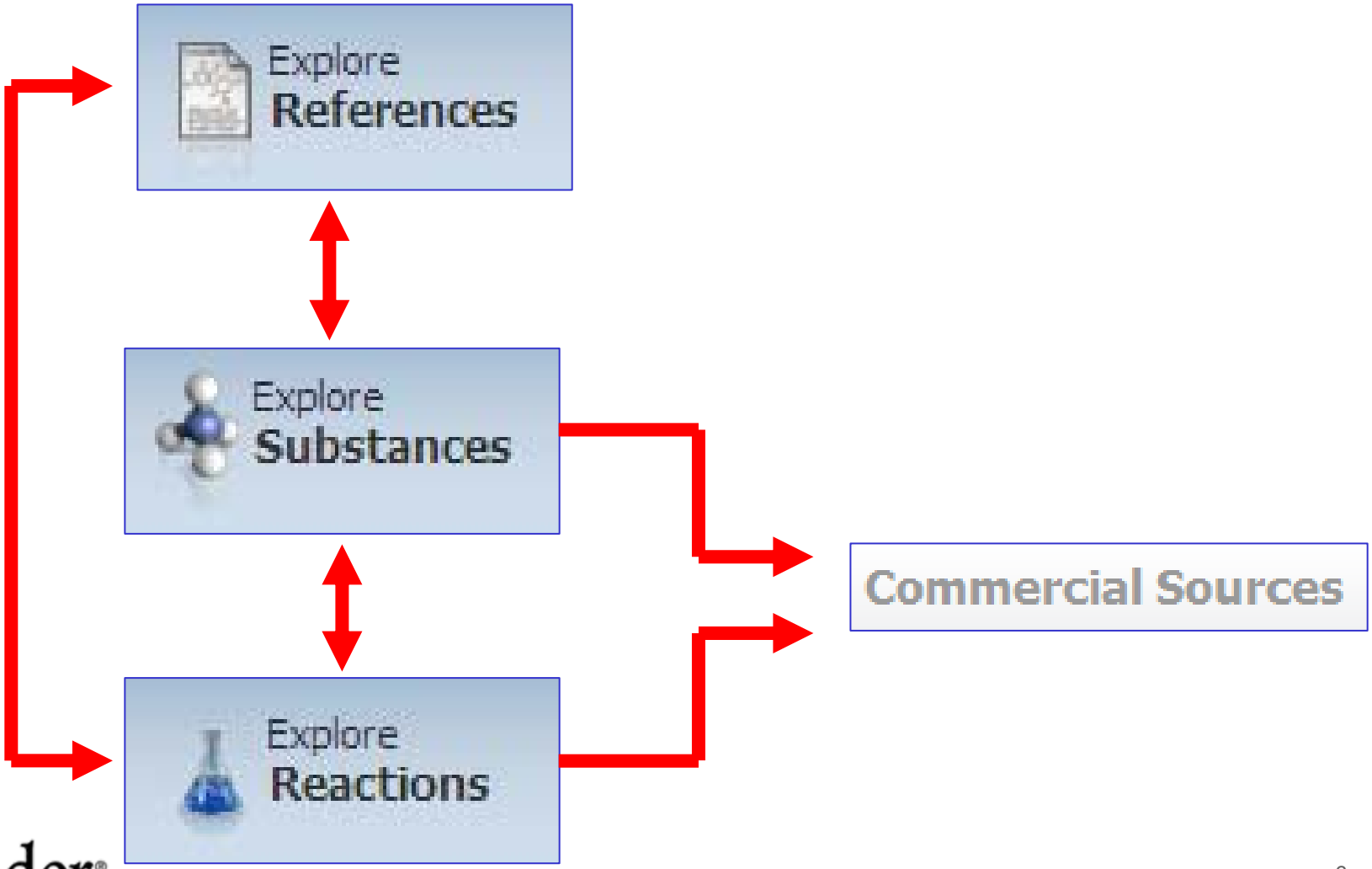
輕鬆選擇從何種角度出發進行檢索

Type of information	Content and coverage	Starting points for locating chemical synthesis information
	•>31 million references from 59 patent authorities worldwide and >10,000 major scientific journals • >18 million references from MEDLINE® •1907 to present, plus selected pre-1907 articles and patents	•Research topic
	•>50 million organic and inorganic substances •>61 million sequences •>1.9 billion predicted and experimental properties, spectra, and data tags, plus •>23.8 million proton NMR spectra 1957 to present, plus selected substances back to the early 1900s •Commercial source information from >900 suppliers for >26 million substances •Regulatory information for more than 245,000 substances	•Chemical name or CAS Registry Number® •Molecular formula •Chemical structure drawing
	•>29 million preparations, including •>18 million single- and multi-step reactions •1840 to present	•Reaction structure drawing •Functional group transformation

自由地想像，在不同類型資料中恣意轉換與串連，獲得最精準與最廣泛的訊息 !!



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透過SciFinder可以在6個資料庫進行整合查詢，其中包含CAS 最重要的5個化學資料庫!!

CAplus℠	CAS REGISTRY℠	CASREACT®	CHEMCATS®	CHEMLIST®
• >31M bibliographic records • >10K journals covered • Patents from 59 patent offices • Updated daily (~3K daily) • Links to almost 400 publishers and 5 patent offices • Literature back to early 1800s • Cited articles from 1997 onward	• >50M small molecules • >61M sequences • Updated daily (>12K daily) • Substances reported comprehensively in literature back to 1957 • Includes nomenclature, spectra, and properties (experimental and predicted)	• >18M single and multi-step reactions • Extracted from patents and journal articles • Updated weekly (~30K weekly) • Reactions back to 1840 • Reaction conditions starting in 2003	• >24M commercially available compounds • >900 suppliers • >1000 chemical catalogs • Updated when new or revised catalogs are available • Contact/ordering information including quantity and pricing (when available)	• >248K inventoried / regulated substances • >100 inventories & regulated lists from 1979 to present • Updated weekly (~50 additions) • Contains regulatory requirements for substances

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以及NLM製作的MEDLINE®資料庫，可檢索生物醫學相關領域的文獻!

MEDLINE®

- >18M bibliographic records
- 4,800 biomedical journals
- Updated 5 times per week
- 1950 -1966 from OLDMEDLINE database

更多資訊，請上網..

http://www.cas.org/expertise/cascontent/caplus/patcoverage/worldcov.html
http://www.cas.org/expertise/cascontent/caplus/corejournals.html
http://www.cas.org/expertise/cascontent/ataglance/index.html
http://www.cas.org/cgi-bin/cas/regreport.pl

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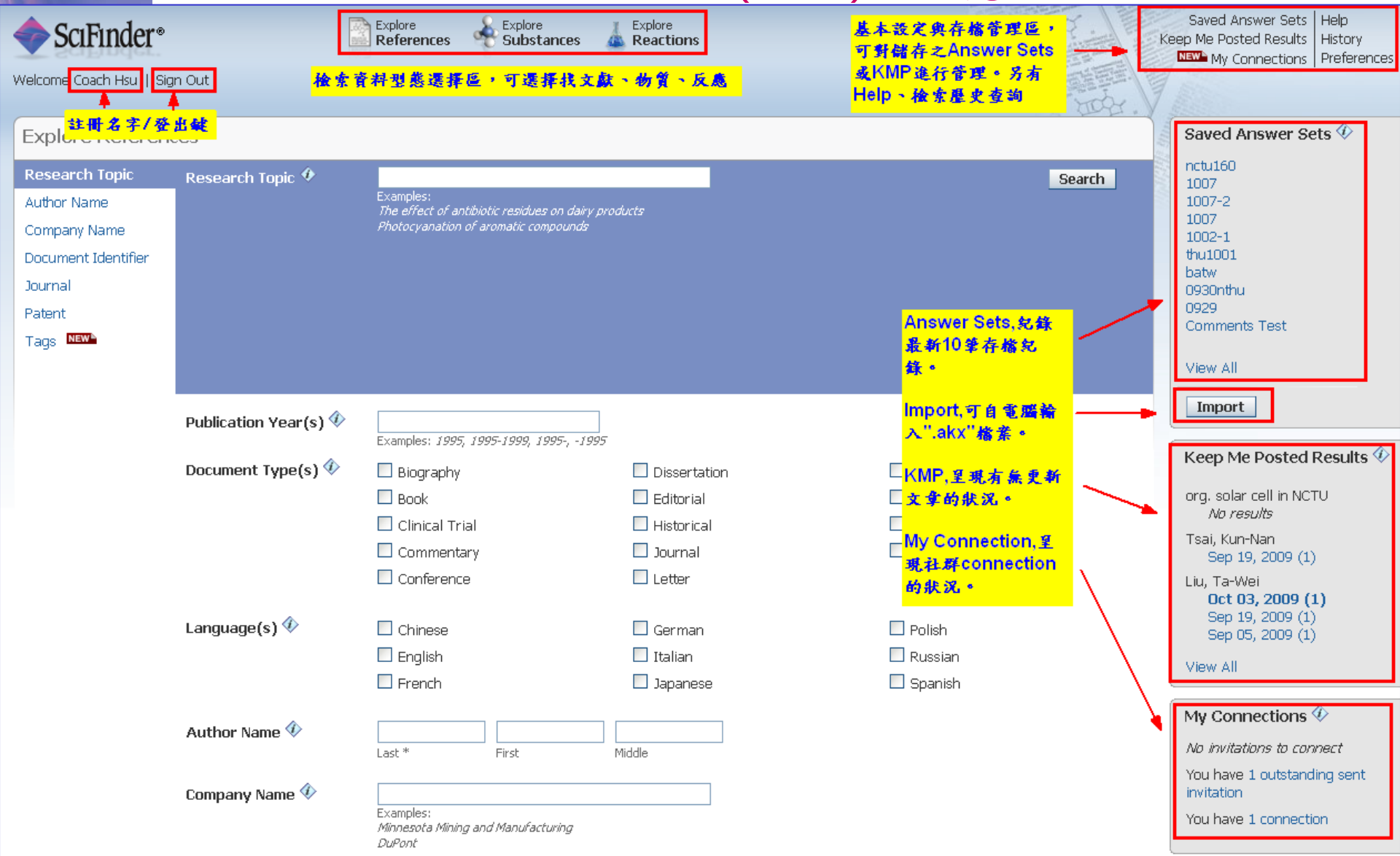
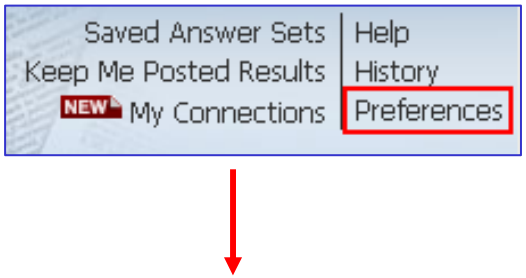
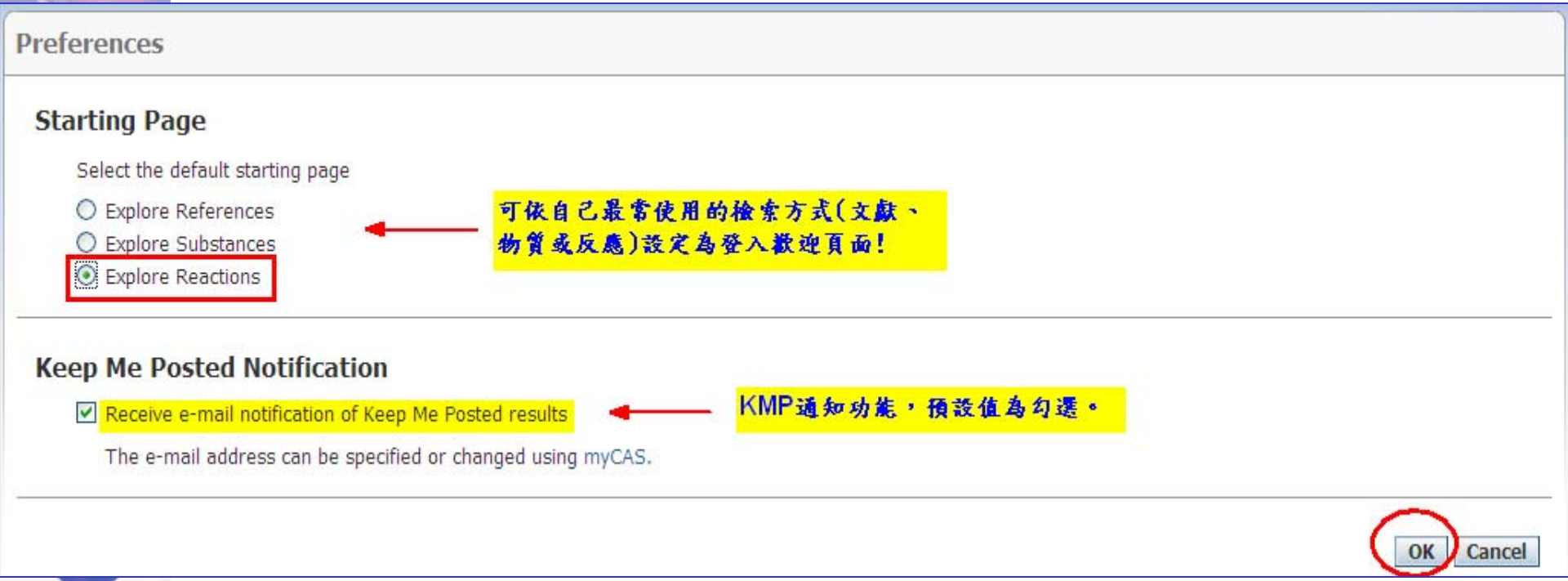
SciFinder Web新介面介紹:

全新介面，加強個人化功能(KMP)與直覺式檢索頁面.....

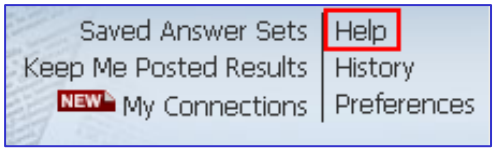


Preferences: 可設定常用的檢索方式為歡迎頁面，以及KMP的通知功能~





Help: 可幫助您更容易了解SF Web的使用方式，任何時間點選 亦可連結至說明頁面~



Contents | Index | Search

- SciFinder Overview
- INTRODUCTION
- EXPLORE TASKS
- USING ANSWER SETS
- COLLABORATION
- KEEP ME POSTED
- LINK RESOURCES
- HISTORY
- OBTAINING DOCUMENTS
- PREFERENCES
- MISCELLANEOUS

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SciFinder Overview

What's New

The latest browser-based SciFinder® provides many new capabilities.

Reactions

- Solvent limiter for a reaction search
- Search for similar reactions
- Reaction search results sorted by product yield, number of steps, or publication date

Substances

- Refine a substance result answer set by property values
- Export substance property values to data table
- ACD predicted carbon-13 Nuclear Magnetic Resonance (NMR) spectra data

Collaboration

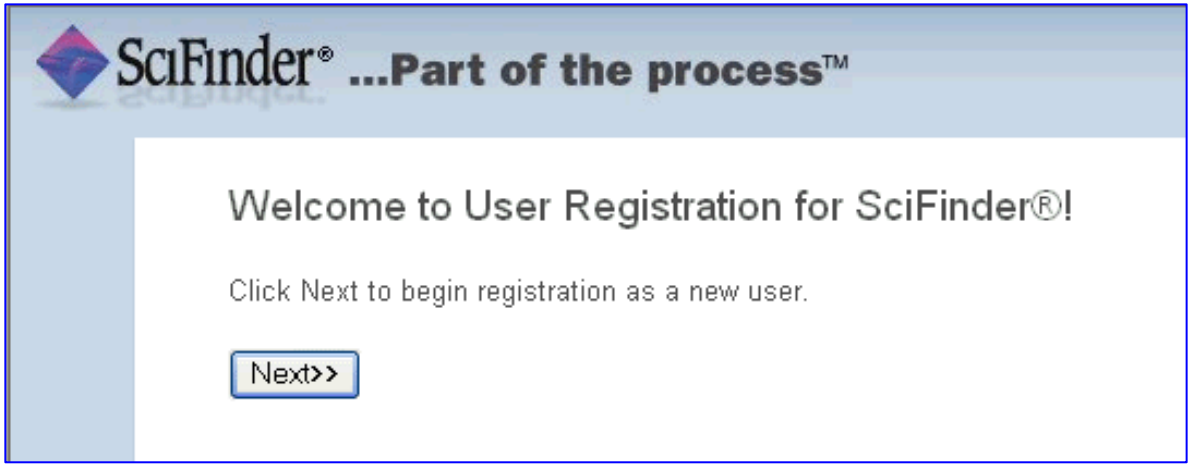
- Collaborate with colleagues at your research site using My Connections
- Tags for grouping references and sharing them with colleagues at your research site
- Commenting for references and for sharing with colleagues at your research site

Usability Enhancements

- Specify a search type for reaction and substance explore pages
- Search short cut from substance and reaction search results
- One step transfer of queries between structure and reaction explores
- Linked CAplus roles to explore references from substances
- CAS Structure Drawing window resize
- Page view preferences
- Reference results viewing options
- Substance results columns per page options
- Reaction results viewing options
- Links from ACS articles to SciFinder substances and reactions search
- Combine Keep Me Posted results
- Task Billing

立即申請 !!

- 請向學校圖書館洽詢SciFinder Web 註冊URL，點選後進入註冊畫面..



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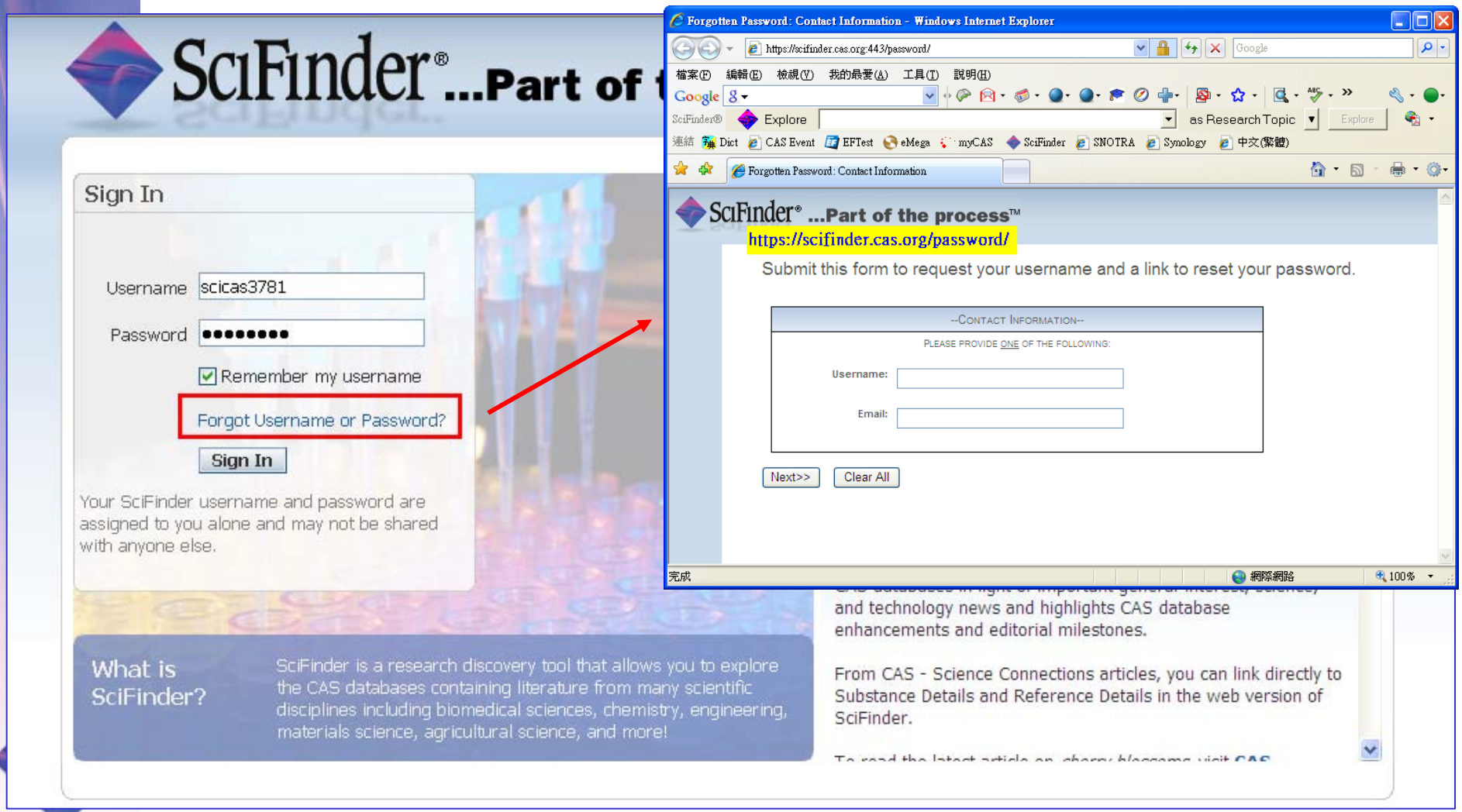
忘記密碼時...



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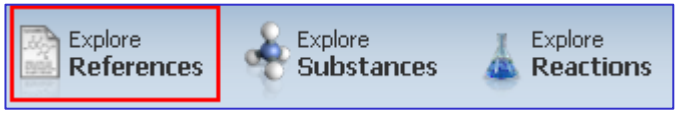
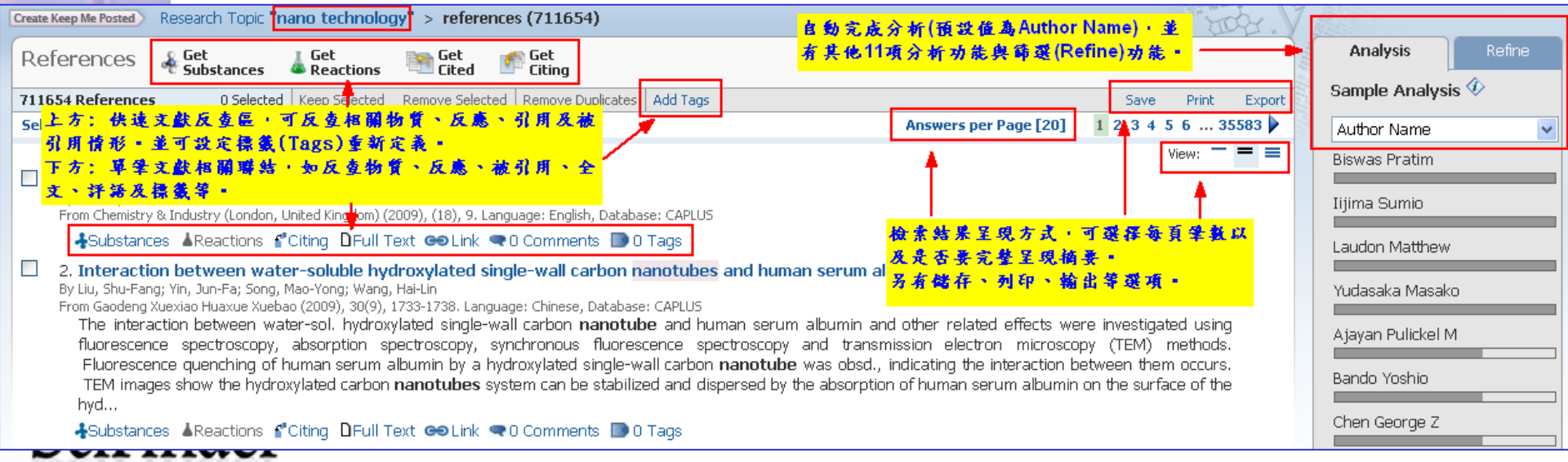
文獻檢索:

有多種方式查詢文獻，如主題、作者名、公司名...等!!下方並有限制條件區可供設定。



文獻檢索結果在上方有快速反查區，以及單筆文獻的相關聯結，並可調整結果呈現方式。右方則是自動分析作者名稱與篩選功能。



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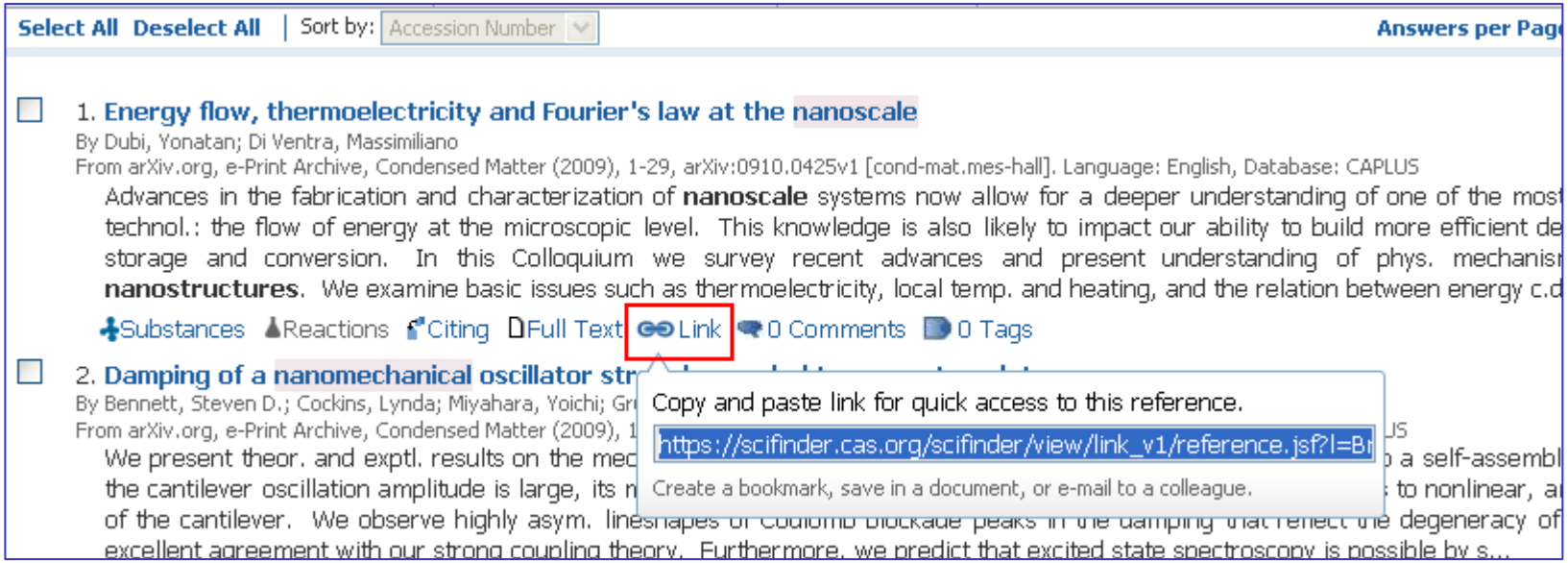
感興趣(或最終篩選得到)的文章，可透過"Link"功能快速複製一串URL(物質/反應檢索亦同)，此URL可分享給他人。只要登入SF Web並貼上此URL即可快速獲得此篇文獻，減少重複查詢的工作。



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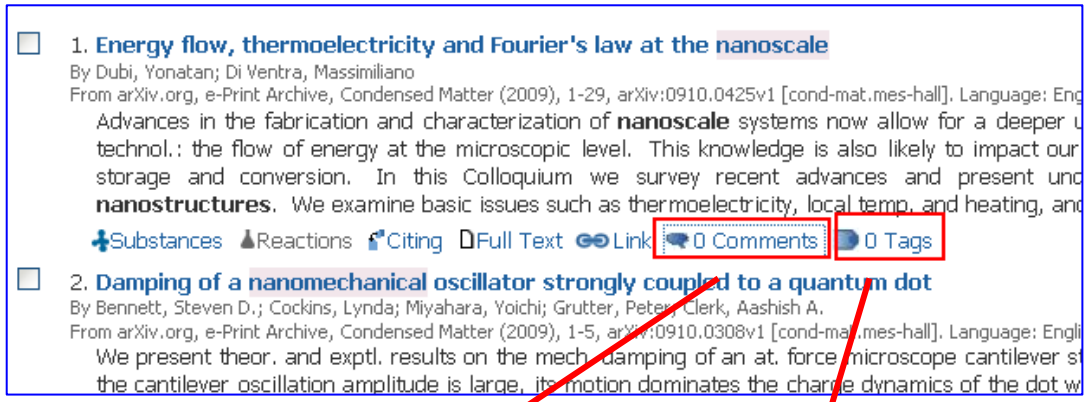
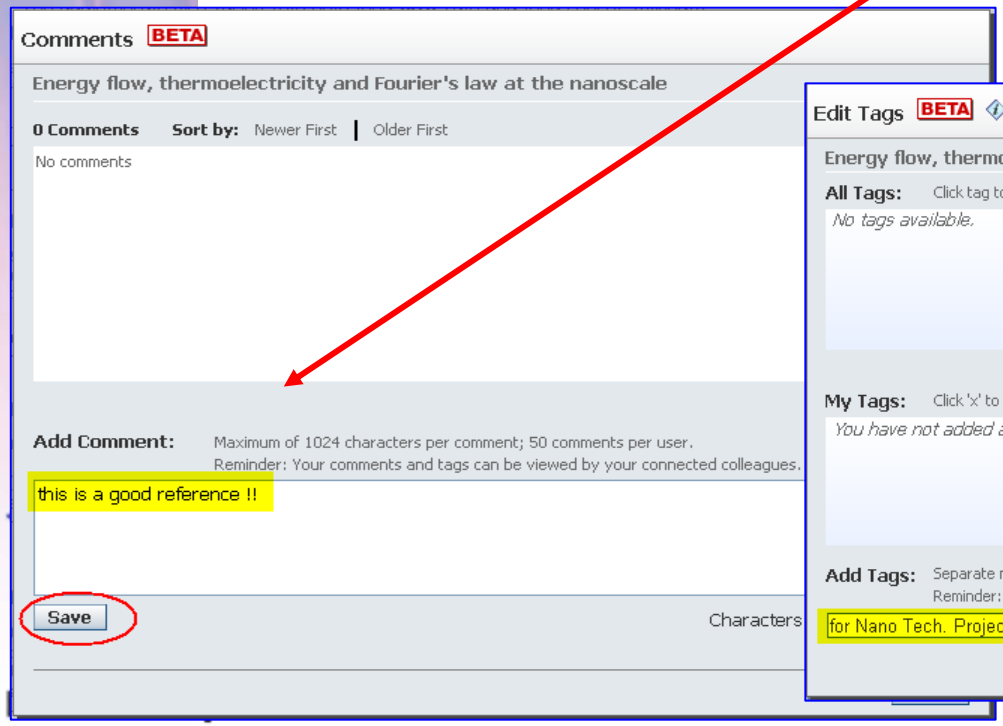
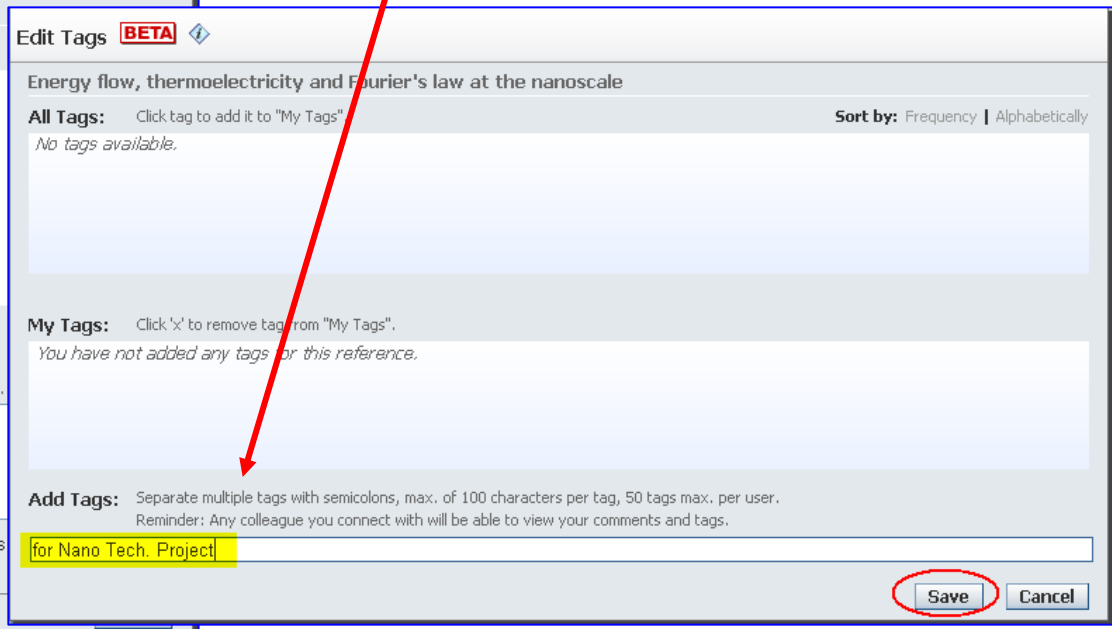
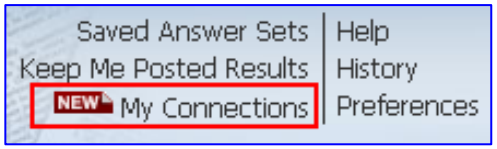
感興趣(或最終篩選得到)的文章，可增加Comments以及Tags，可分享給"My Connection"設定的朋友。

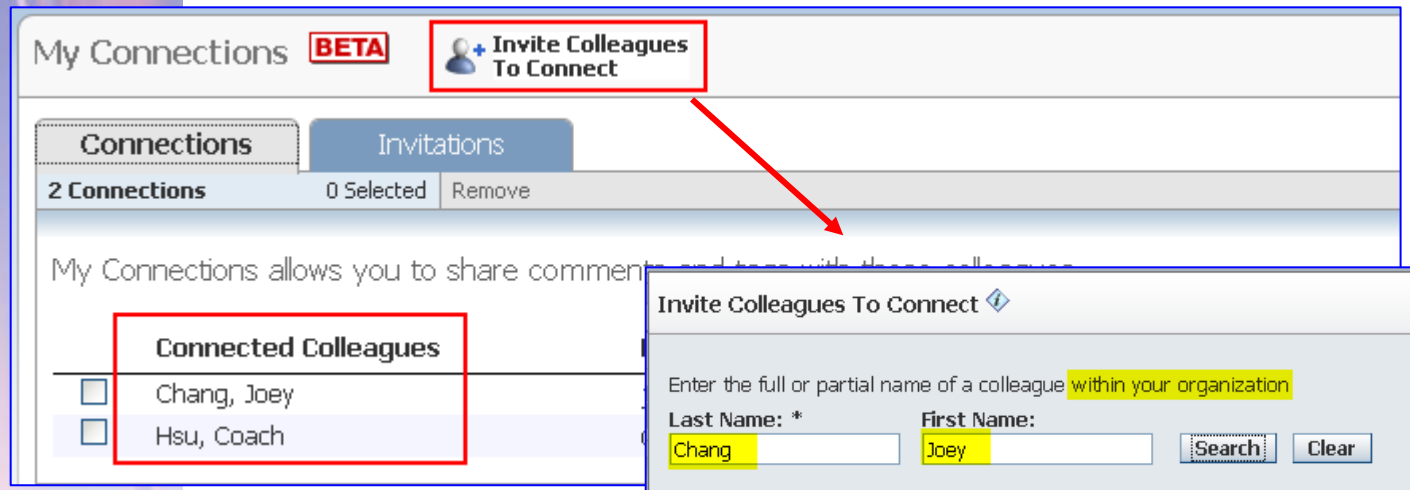


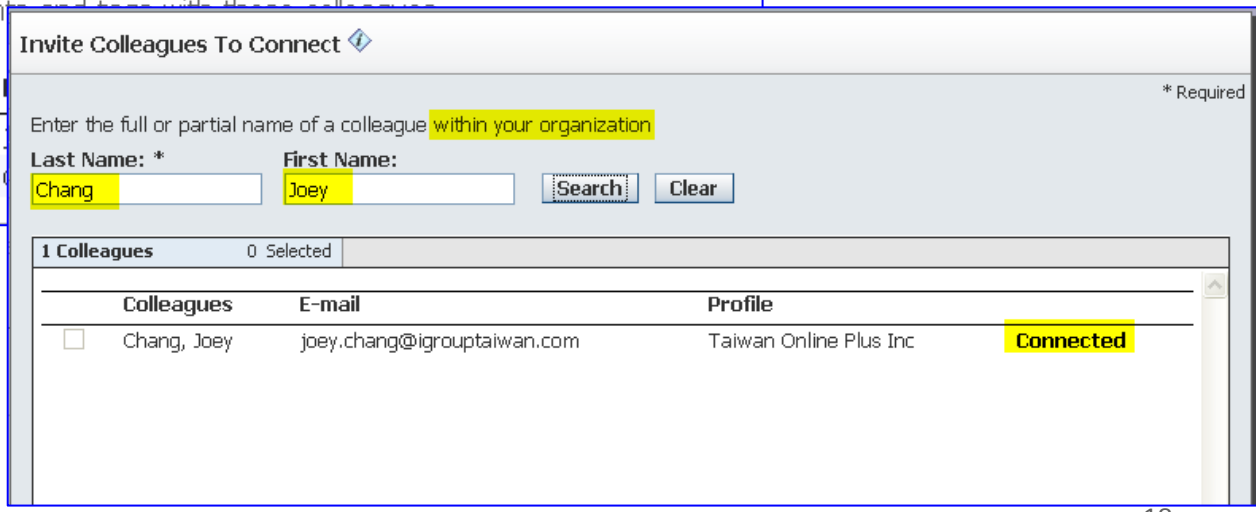




My Connections:於同一訂購單位(學校)中，可設定多組社群連結，設為連結的人員可互相查看"Comments"以及"Tags"資料。







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Tags:於文獻檢索區中可點選Tags查看自己與連結人員所設定的資料，以加速文獻分享與團隊合作研究。

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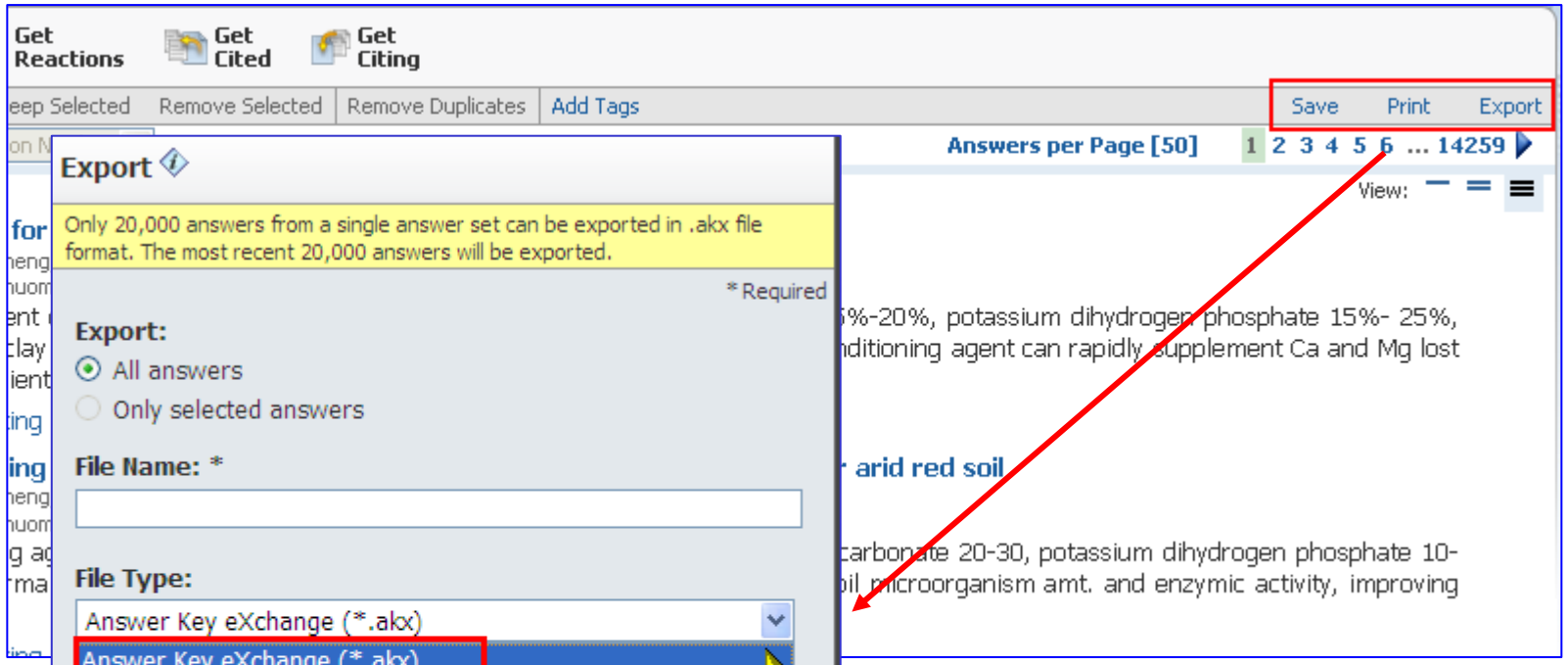
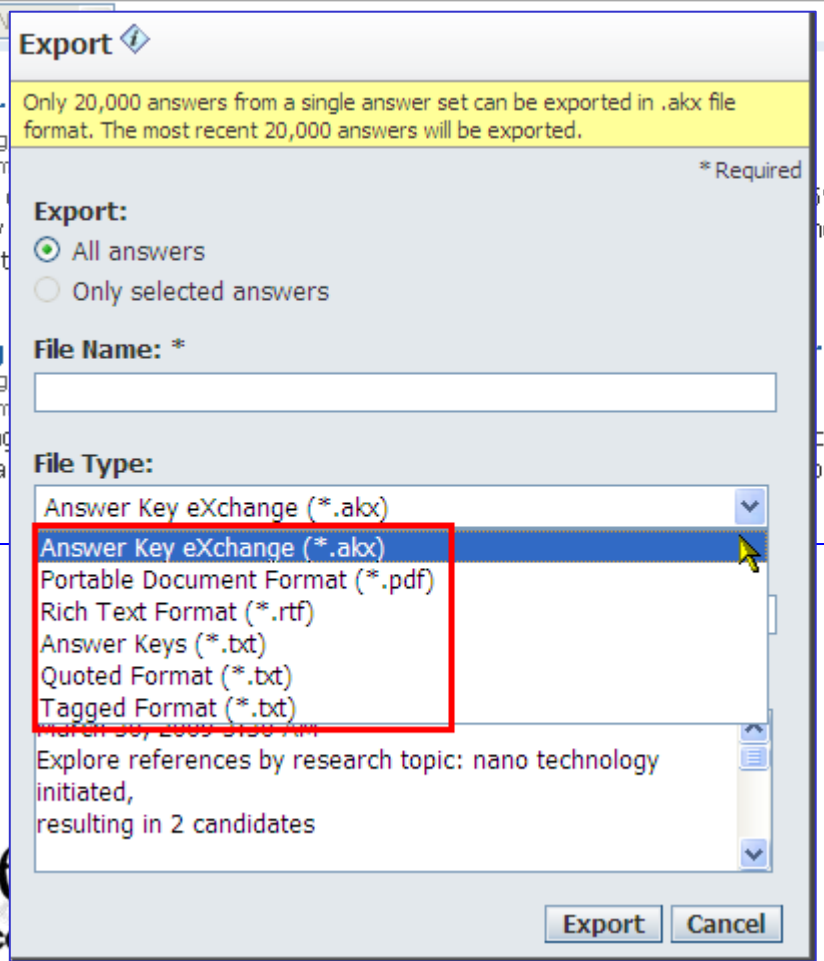
文獻結果可進行”Save”(Answer Set)、“Print”、“Export”等動作。Export可輸出成多種格式，如akx, pdf, rtf, txt等。”Save”與”Export”皆有最大存檔/輸出筆數限制。





文獻結果可以不同形式排序，如登錄號、作者名、發表年份、標題等

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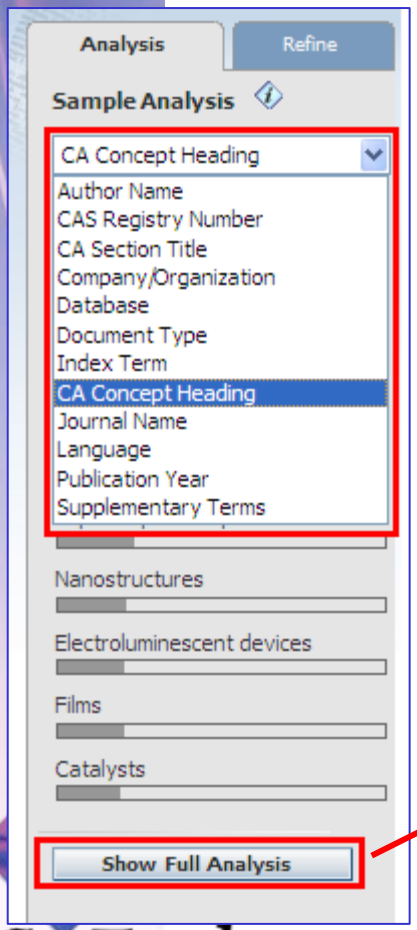
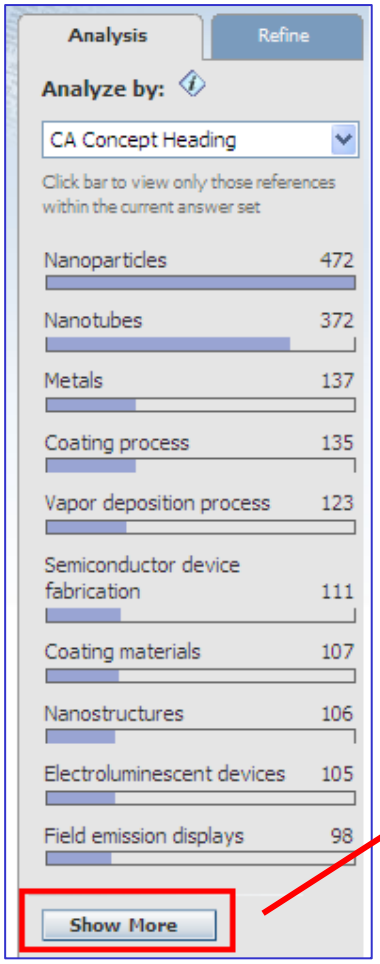
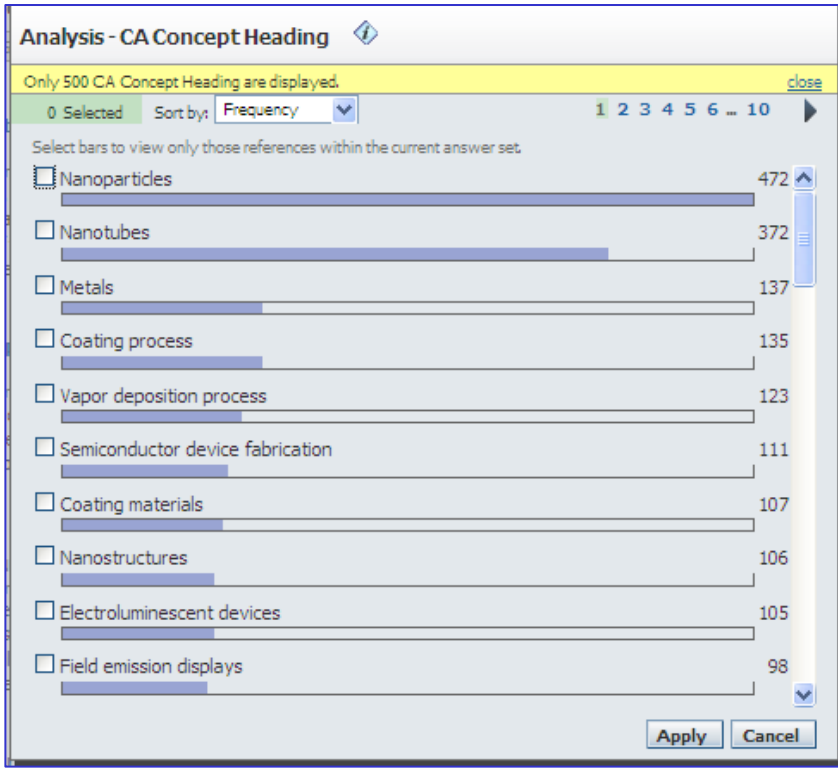
分析欄位增加"CA Concept Heading"，可更清楚了解文獻檢索結果中包含的"重要觀念"。點選"Full Analysis"可秀出每個分析選項的筆數，也可點選"more"做完整的分析查看。







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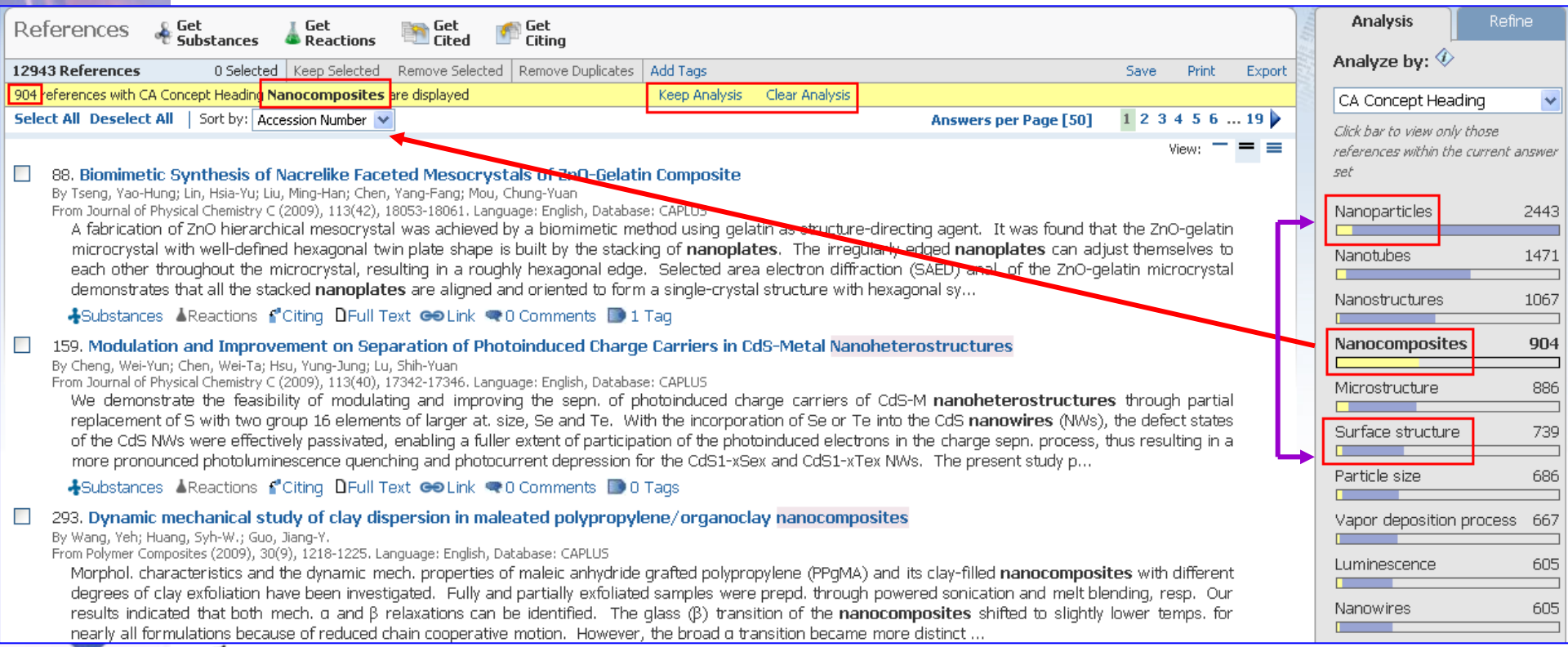
點選感興趣的分析項目(ex. Nanocomposites)，結果會先以黃色區塊表示，並在其他分析項目中以黃色表示重複文章所佔比例。若此分析結果為所需，則點選"keep analysis"!!



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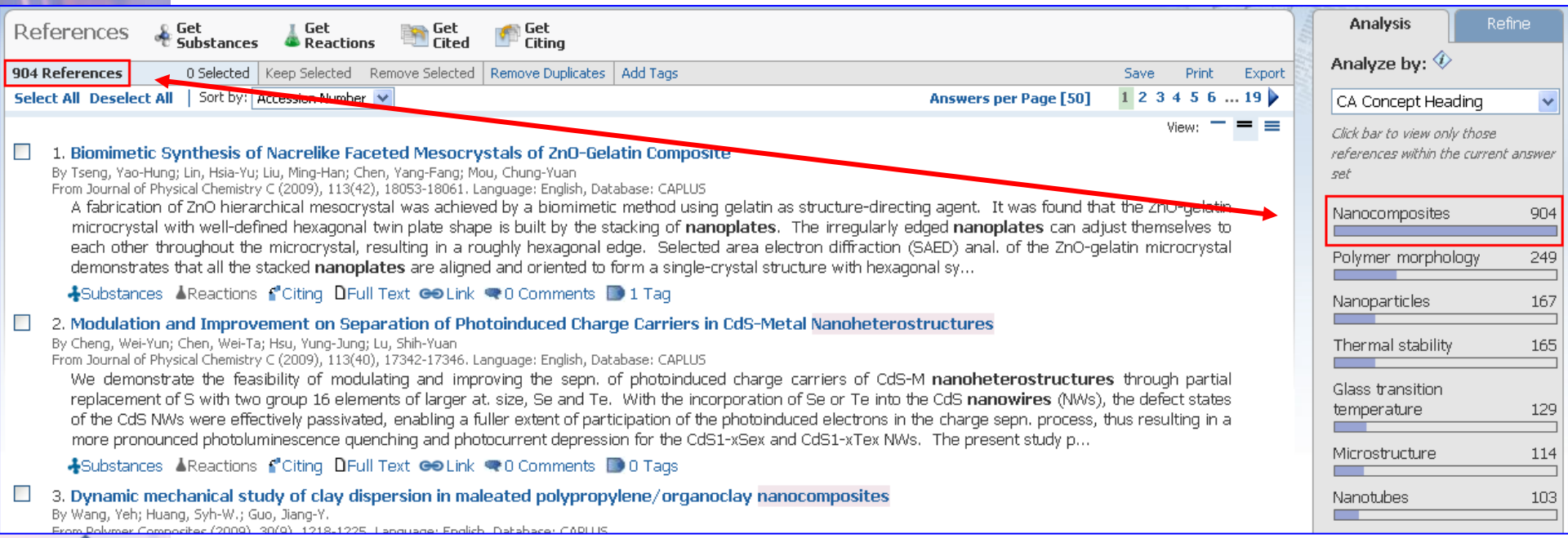
Keep analysis結果!!



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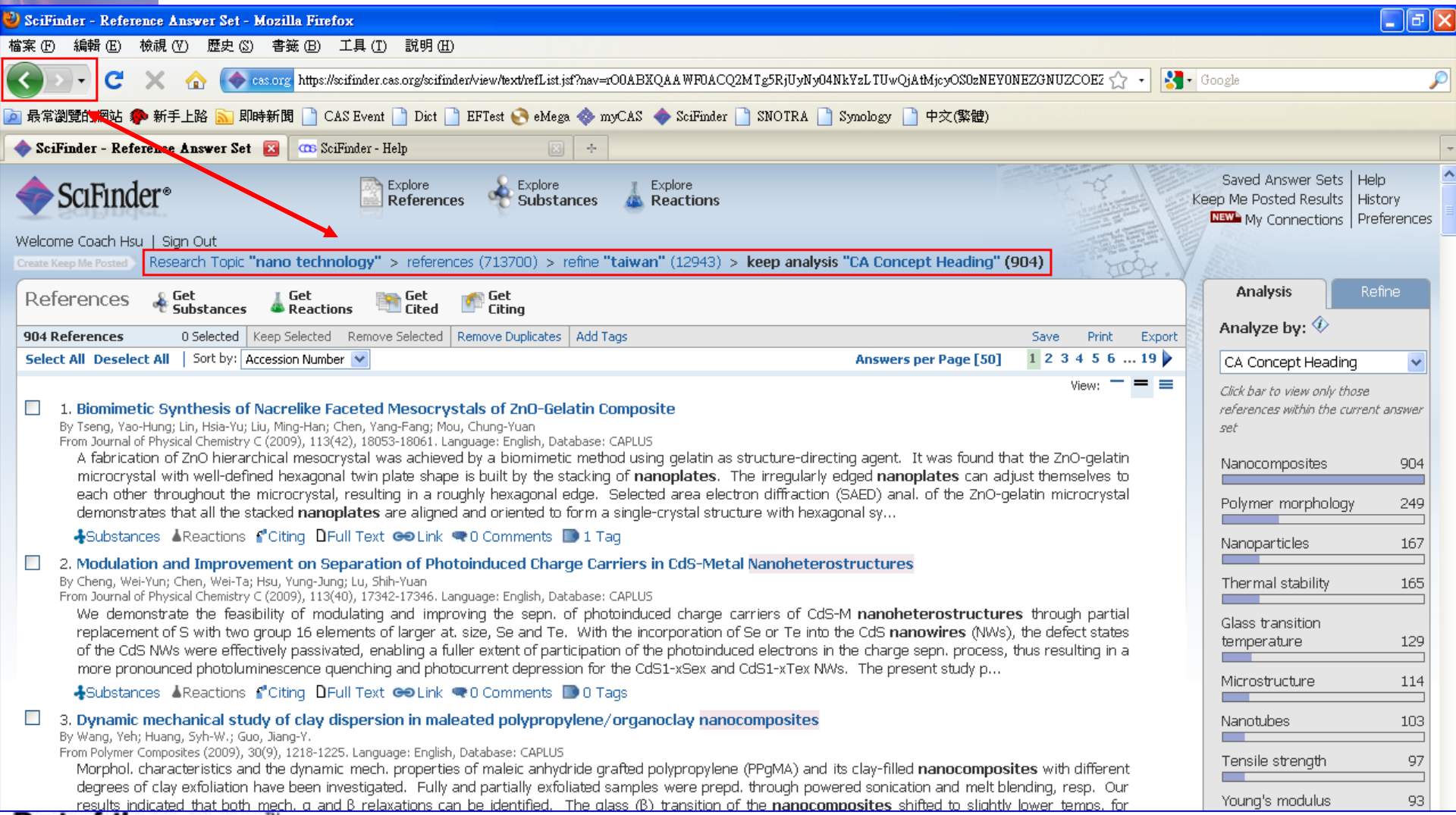
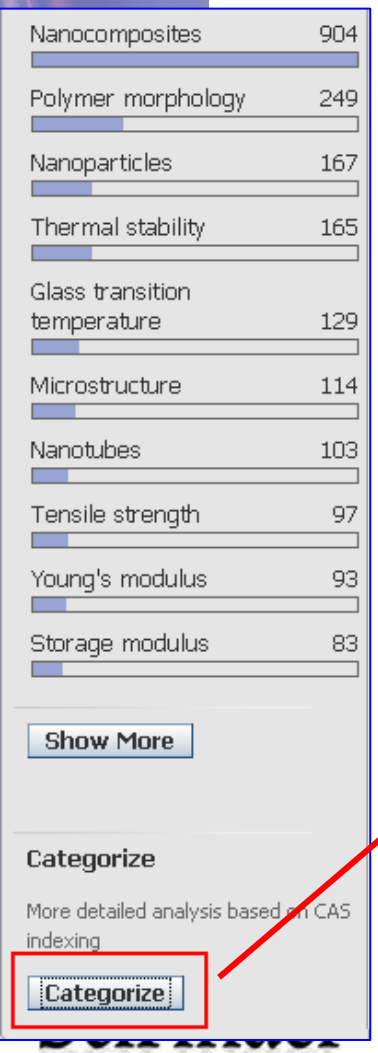
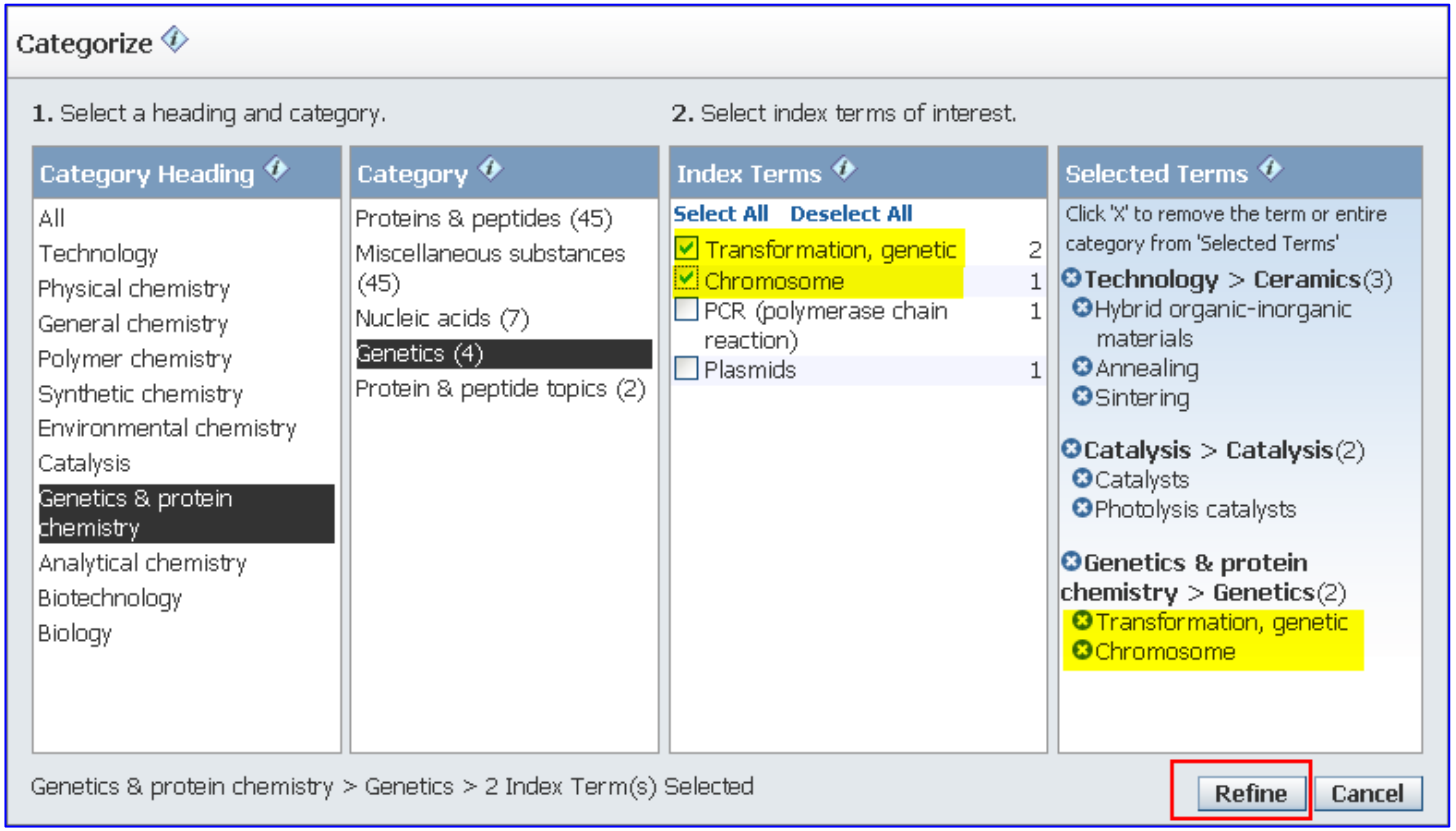
檢索策略/步驟會以"字串路徑"的方式於上方保留下來，不再需要點選"上一步"，直接點選檢索策略中的路徑任何一步驟，即可回到該檢索結果!!

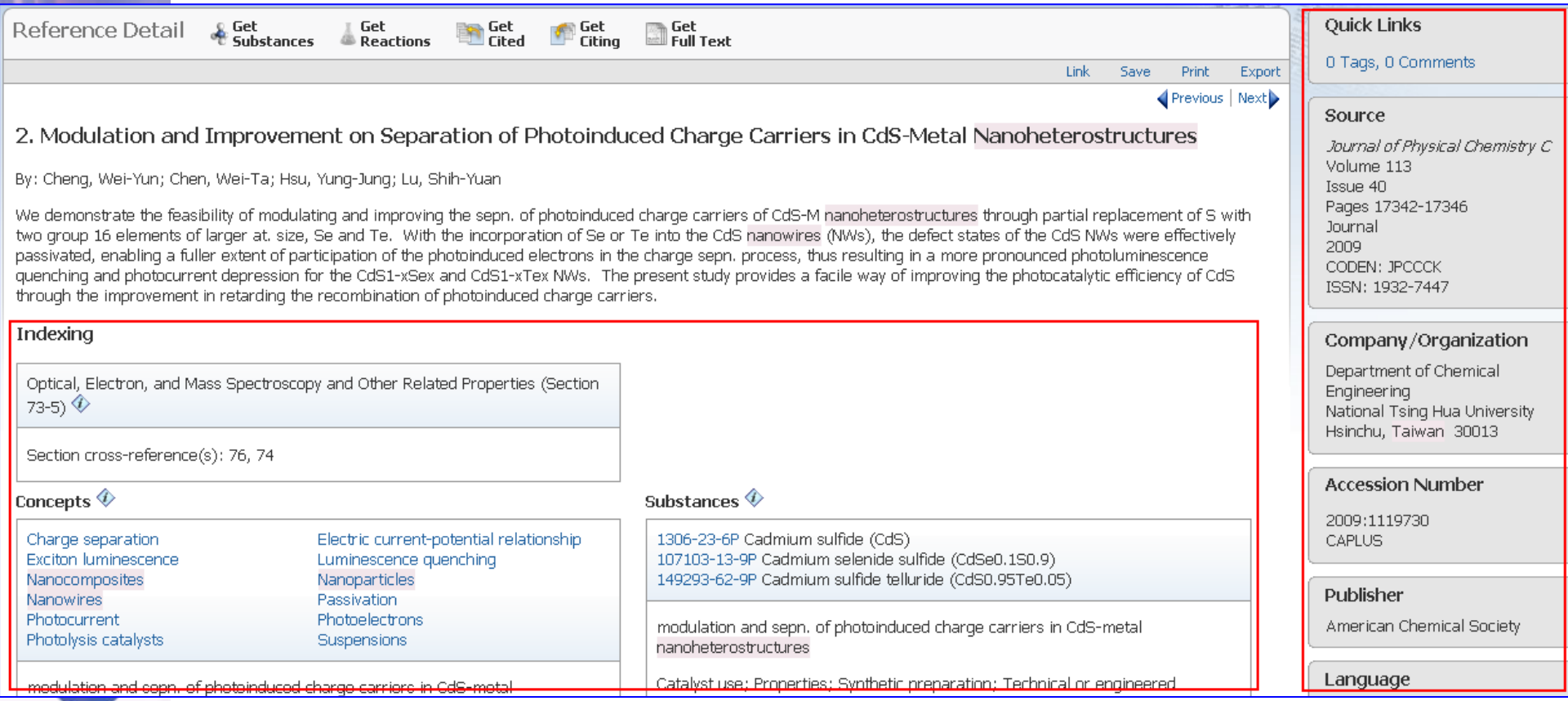


分類(Categorize)，位於分析欄位下方，點選後會出現大型對話框，選擇每一階層感興趣的欄位，點選”Refine”即可進行分類!!





點選文章進入後，右側是文章相關資訊，下方為經CA科學家整理後的精華區塊，如Indexing、Concepts、Substances..等!!



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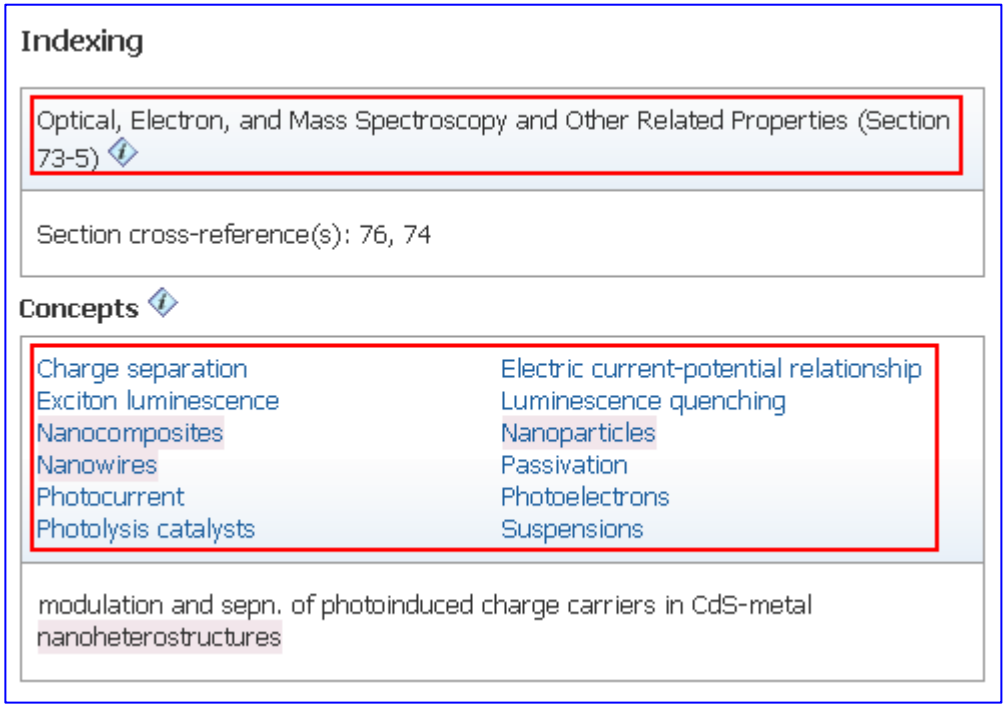
Concepts區塊提供超連結點選，方便研究人員快速轉換至相關主題!!



Indexing

Optical, Electron, and Mass Spectroscopy and Other Related Properties (Section 73-5)

Section cross-reference(s): 76, 74

Concepts

Charge separation	Electric current-potential relationship
Exciton luminescence	Luminescence quenching
Nanocomposites	Nanoparticles
Nanowires	Passivation
Photocurrent	Photoelectrons
Photolysis catalysts	Suspensions

modulation and sepn. of photoinduced charge carriers in CdS-metal nanoheterostructures

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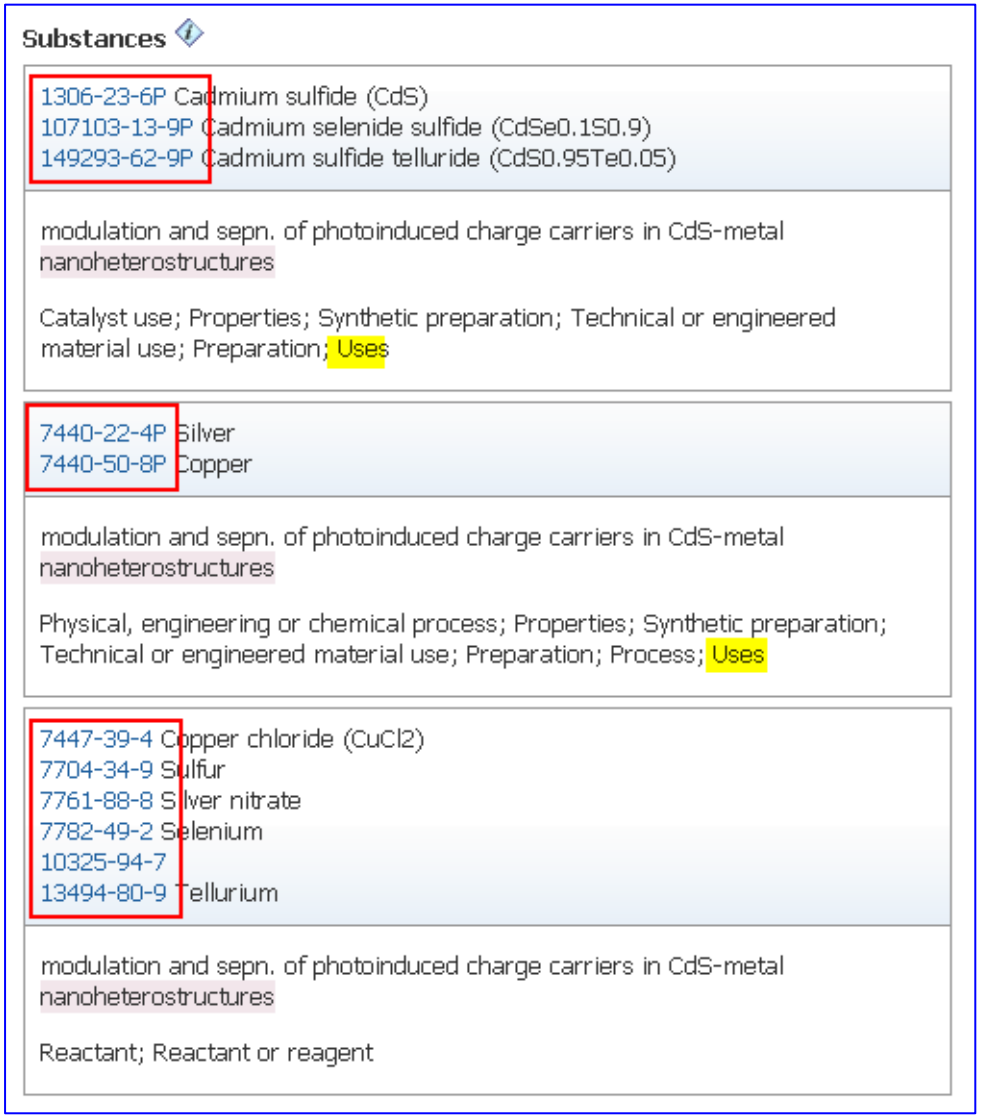
Substances區塊提供本文章中相關物質超連結點選，方便研究人員快速查看相關物質資訊，下方並有此物質在本文章中扮演的角色說明!!



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物質檢索：

可選擇直接繪製結構(點小圖出現畫板)，或可利用分子式、物質定義來進行查詢! 下方有限制條件區可供設定。

Explore Substances

Chemical Structure
Molecular Formula
Substance Identifier

Chemical Structure

Click image to draw or import structure

Search

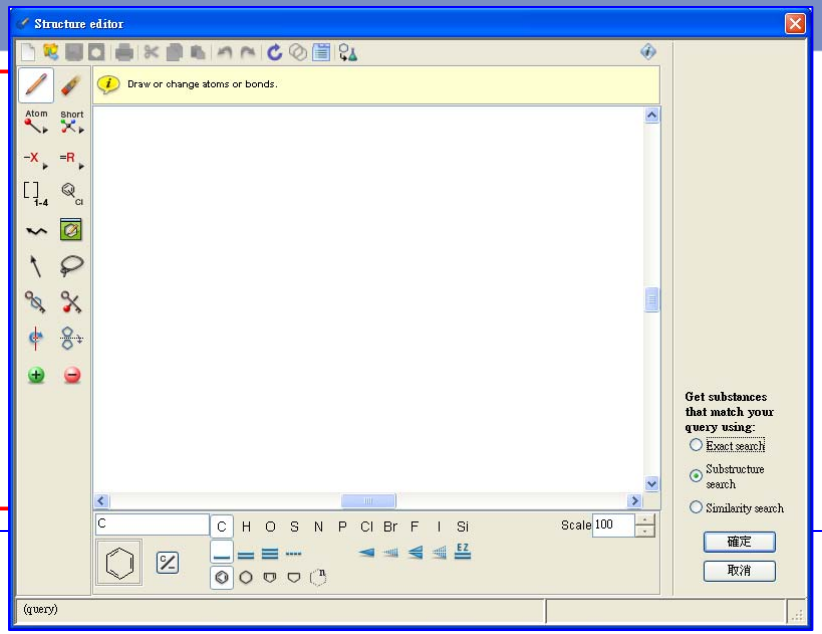
第一次執行畫板系統會自動偵測JAVA版本是否為最新，並會提示安裝下載，請安裝完後重新啟動SciFinder。

可從畫板直接繪製結構，或可利用分子式、物質定義來查詢。
下方有限制條件區。

Characteristic(s)
- Single component
- Commercially available
- Included in reference(s)

Class(es)
- Alloys
- Coordination compounds
- Incompletely defined

Studies
- Analytical
- Biological



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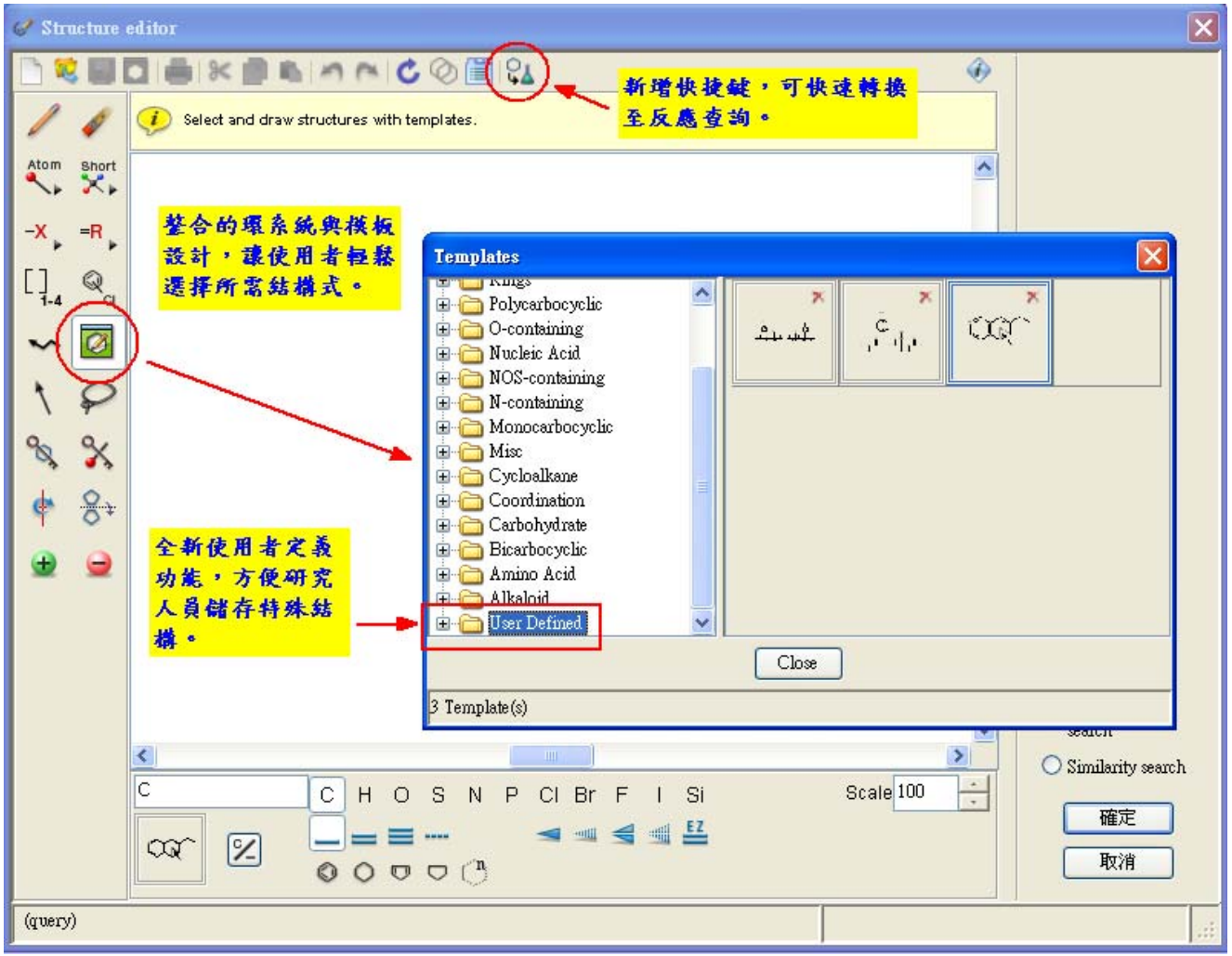
承接軟體版強大的工具列設計理念，方便使用者更輕鬆的選擇功能。如整合的環系統與模板設計、使用者定義功能....



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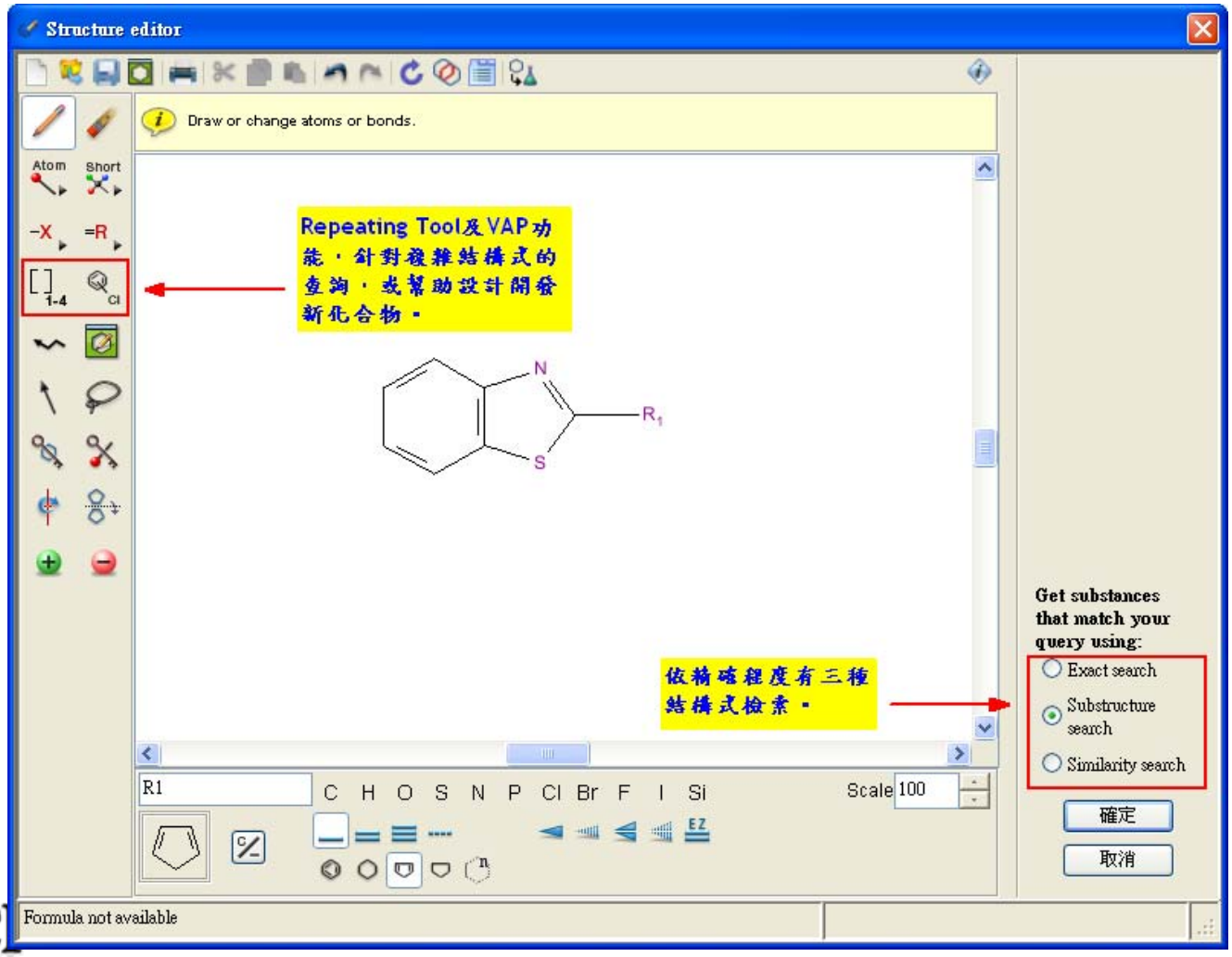
Repeating tool及VAP可針對複雜結構進行模糊參數設定，檢索時亦有SSM模組(Substructure, Similarity)可供模糊比對搜尋。



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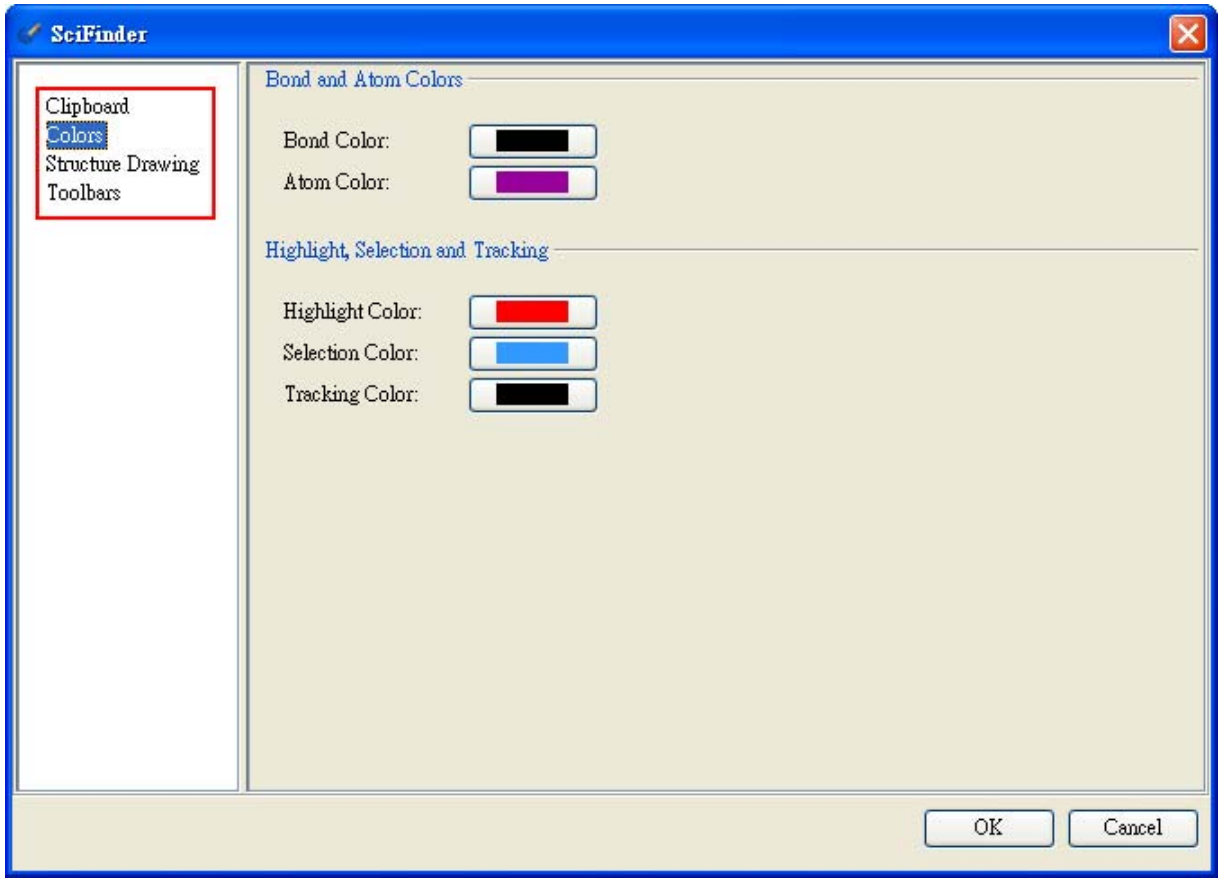
Preference可針對畫板顏色、工具列項目等進行調整。



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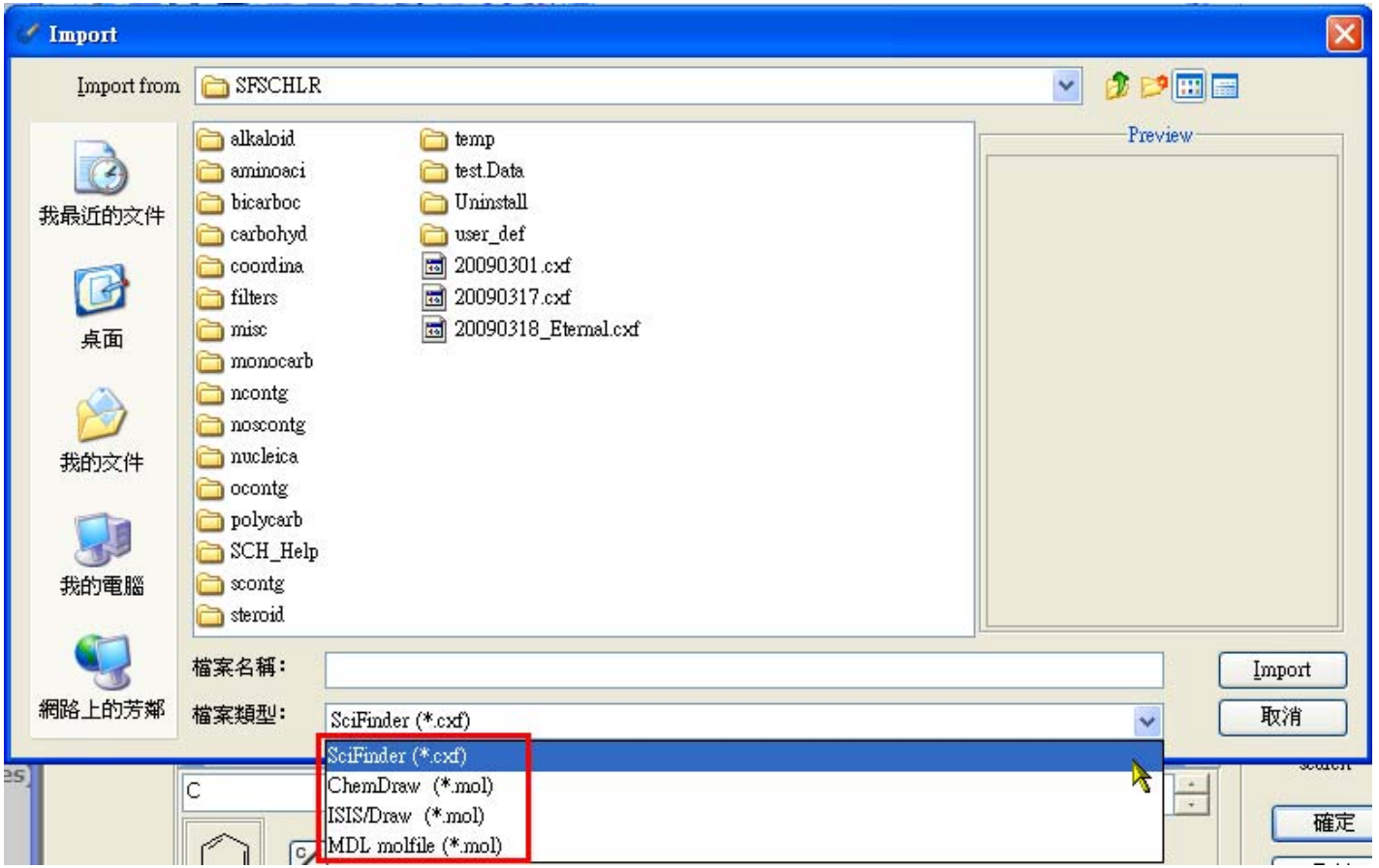
支援多種Import/Export格式，方便研究人員快速轉換，如ChemDraw, ISIS/Draw, MDL等。



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Substance Detail：更清楚易懂的排列方式，讓研究人員快速掌握物質的相關性質與連結相關資訊。

Substance Detail | Get References | Get Reactions | Get Commercial Sources | Get Regulatory Information

Link | Save | Print | Export

Previous | Next

快速反查區，可找此物質相關"文獻"、"反應"、"供應商"及"管制資訊"。

Link功能，複製特定URL以供後續快速進入或分享檢索結果。

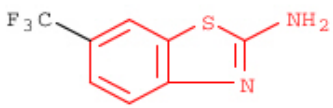
8151.

CAS Registry Number: 777-12-8

$C_8 H_5 F_3 N_2 S$

2-Benzothiazolamine, 6-(trifluoromethyl)-

Benzothiazole, 2-amino-6-(trifluoromethyl)- (6CI,7CI,8CI); 2-Amino-6-(trifluoromethyl)benzothiazole; 2-Amino-6-trifluoromethyl-1,3-benzothiazole; 6-(Trifluoromethyl)-1,3-benzothiazol-2-ylamine; 6-Trifluoromethylbenzothiazol-2-ylamine



~44 References

Document Types: Journal, Patent

CAplus Role	Patents	Nonpatents
Biological study	✓	✓
Preparation	✓	✓
Properties		✓
Reactant or reagent	✓	✓
Uses	✓	✓

討論此物質的文獻型態，可依類型快速串連至不同文獻。

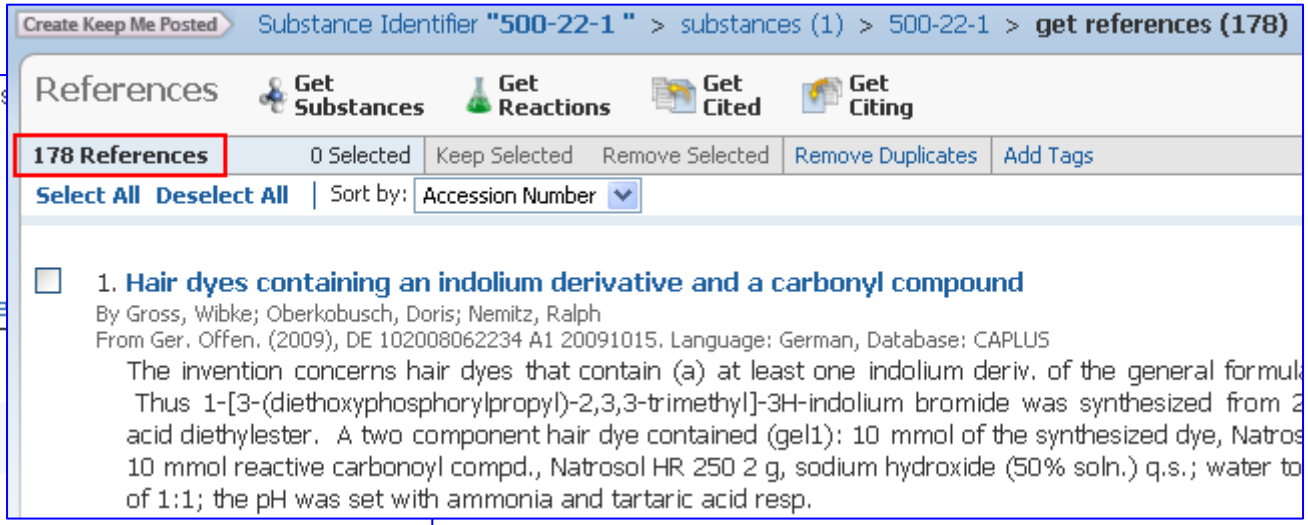
物質"預測性"數據

Predicted Properties: Biological | Chemical | Density | Lipinski and Related | Spectra | Structure-related | Thermal

Biological Properties	Value	Conditions	Notes
Bioconcentration Factor	1.0	pH 1 Temp: 25 °C	(4)
Bioconcentration Factor	1.78	pH 2 Temp: 25 °C	(4)
Bioconcentration Factor	12.4	pH 3 Temp: 25 °C	(4)

Top

Substance Detail：可點選感興趣的類別，即可快速串連至相關文獻。專利中屬於預測性的物質(Prophetic)亦會被特別標示。



Substance Detail：經由系統推導演算所預測的物質特性包含NMR光譜，並已完整分類。可點選預測性光譜圖(見下頁)。

Predicted Properties: Biological Chemical Density Lipinski and Related Spectra Structure-related Thermal

Biological Properties	Value	Conditions	Notes	Top
Bioconcentration Factor	1.0	pH 1 Temp: 25 °C	(50)	
Bioconcentration Factor	1.0	pH 2 Temp: 25 °C	(50)	
Bioconcentration Factor	1.0	pH 3 Temp: 25 °C	(50)	
Bioconcentration Factor	1.25	pH 4 Temp: 25 °C	(50)	
Bioconcentration Factor	1.55	pH 5 Temp: 25 °C	(50)	
Bioconcentration Factor	1.59	pH 6 Temp: 25 °C	(50)	
Bioconcentration Factor	1.59	pH 7 Temp: 25 °C	(50)	
Bioconcentration Factor	1.59	pH 8 Temp: 25 °C	(50)	
Bioconcentration Factor	1.59	pH 9 Temp: 25 °C	(50)	
Bioconcentration Factor	1.59	pH 10 Temp: 25 °C	(50)	

Chemical Properties	Value	Conditions	Notes	Top
Koc	1.0	pH 1 Temp: 25 °C	(50)	
Koc	1.88	pH 2 Temp: 25 °C	(50)	
Koc	13.2	pH 3 Temp: 25 °C	(50)	

Lipinski and Related Properties	Value	Conditions	Notes	Top
Freely Rotatable Bonds	1		(50)	
H Acceptors	2		(50)	
H Donors	0		(50)	
H Donor/Acceptor Sum	2		(50)	
logP	0.568±0.258	Temp: 25 °C	(50)	
Molecular Weight	107.11		(50)	

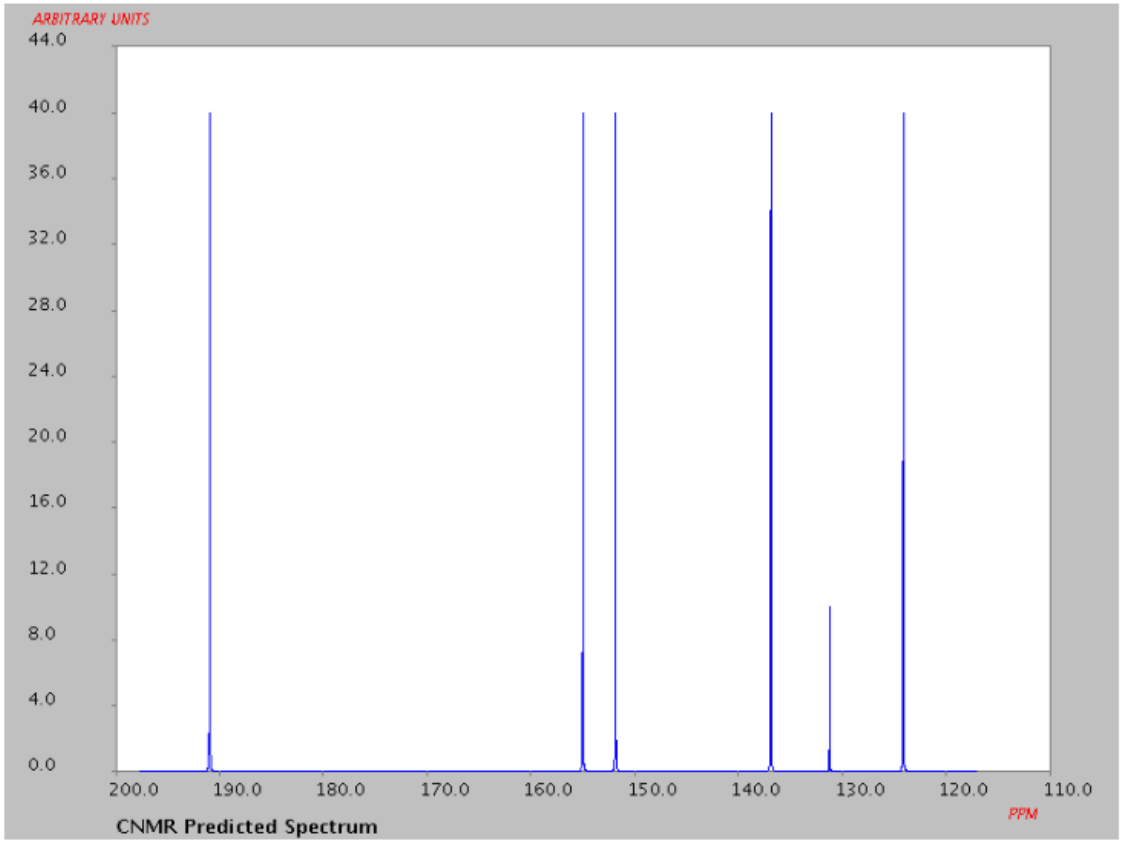
Spectra Properties	Value	Conditions	Notes	Top
Carbon-13 NMR Spectrum NEW	See spectrum		(51)	
Proton NMR Spectrum	See spectrum		(51)	

Part of the process.

Substance Detail：Carbon-13 NMR光譜，由ACD/Labs以軟體推導演算得出。

Carbon-13 NMR Spectrum

Print



Spectrum ID
500221-CNMR

Nucleus
13C

Standard
Tetramethylsilane (75-76-3)

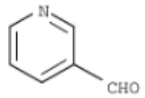
Temperature
25 °C

Source
Predicted NMR data calculated using Advanced Chemistry Development, Inc. (ACD/Labs) Software V9.07 (© 1994-2009 ACD/Labs)

CAS Registry Number: 500-22-1

C_6H_5NO

3-Pyridinecarboxaldehyde



Part of the process.

Substance Detail：經由實驗所得到的物質特性包含各式光譜圖，並已完整分類。可點選各類型的光譜圖參考(見下頁)。

Experimental Properties: Biological Chemical Optical and Scattering Spectra Thermal

Biological Properties	Value	Conditions	Notes	Top
LC50	See full text		(41) CAS	
LC50	See full text		(42) CAS	
Median Lethal Dose(LD50)	900 mg/kg	Organism: mouse Route: intravenous	(12) CAS	

Chemical Properties	Value	Conditions	Notes	Top
Acid/Base Dissociation Constant (Ka/Kb)	See full text		(1) CAS	
Solubility	See full text		(41) CAS	

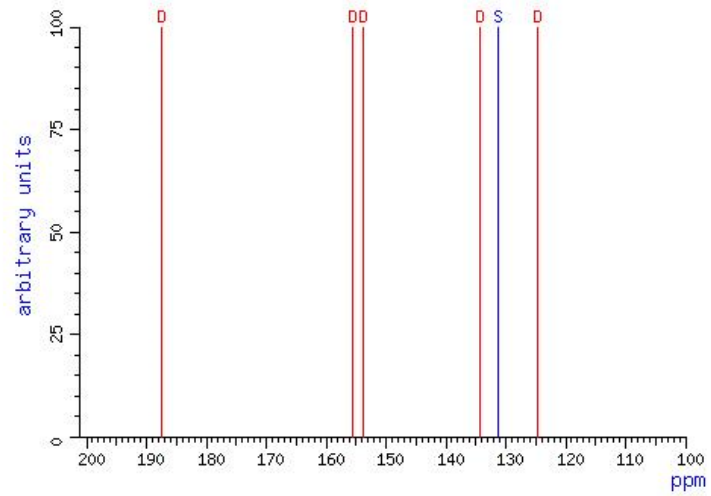
Optical and Scattering Properties	Value	Conditions	Notes	Top
Refractive Index	1.5507	Wavlen: 589.3 nm; Temp: 20 °C	(49) CAS	
Refractive Index	1.5475	Wavlen: 589.3 nm; Temp: 20 °C	(3) CAS	

Spectra Properties	Value	Conditions	Notes	Top
Carbon-13 NMR Spectrum	See spectrum		(25) WSS	
Carbon-13 NMR Spectrum	See spectrum		(26) WSS	
Carbon-13 NMR Spectrum	See spectrum		(27) WSS	
Carbon-13 NMR Spectrum	See spectrum		(27) WSS	
Carbon-13 NMR Spectrum	See spectrum		(27) WSS	
Carbon-13 NMR Spectrum	See spectrum		(28) WSS	
Carbon-13 NMR Spectrum	See spectrum		(28) WSS	
Carbon-13 NMR Spectrum	See spectrum		(29) AIST	
Carbon-13 NMR Spectrum	See full text		(30) CAS	
Carbon-13 NMR Spectrum	See full text		(31) CAS	
Carbon-13 NMR Spectrum	See full text		(32) CAS	
Carbon-13 NMR Spectrum	See full text		(33) CAS	
Carbon-13 NMR Spectrum	See full text		(34) CAS	

Substance Detail：右側顯示來源資料。

Carbon-13 NMR Spectrum

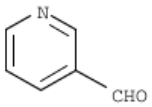
Print



CAS Registry Number: 500-22-1

C_6H_5NO

3-Pyridinecarboxaldehyde



Spectrum ID

CNCC-78983-177P

Nucleus

13C

Source

Spectral data were obtained from Wiley Subscription Services, Inc. (US)

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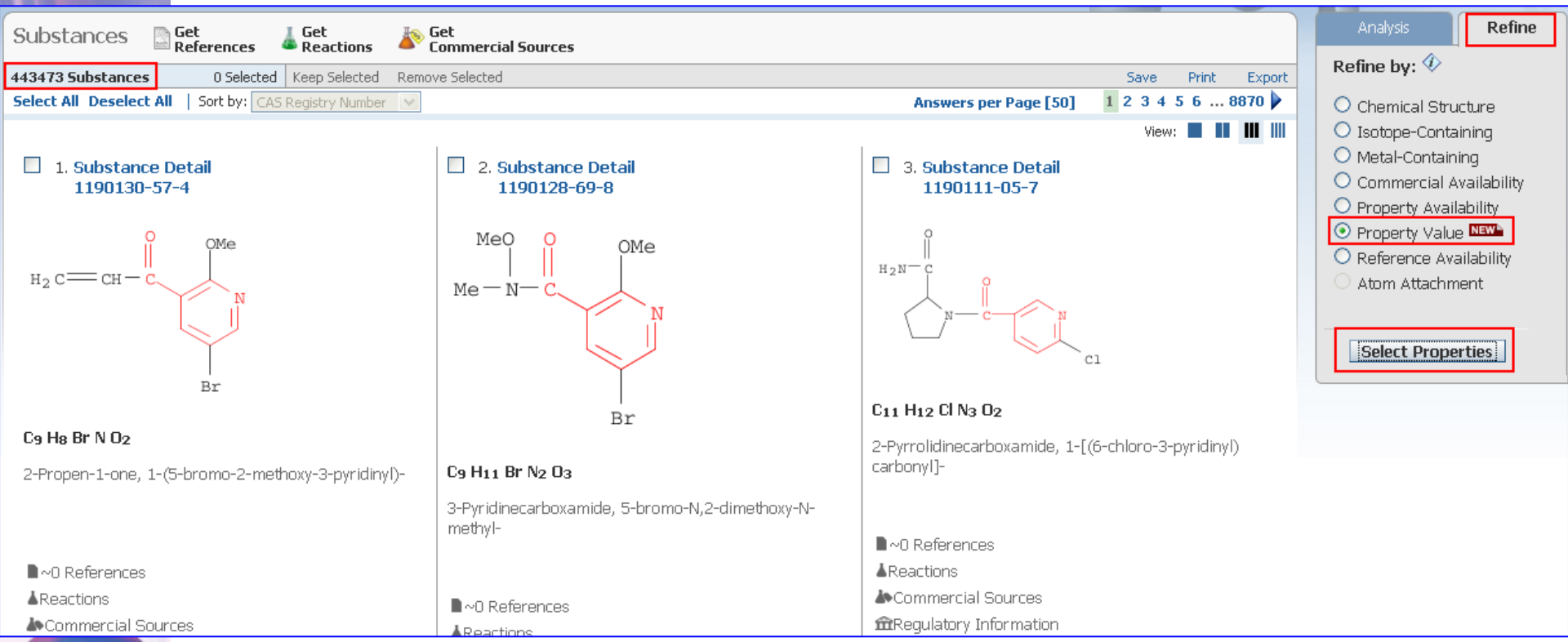
New features：若物質檢索有多筆資料，可透過Refine功能”Property Value”進行篩選。(見下頁)



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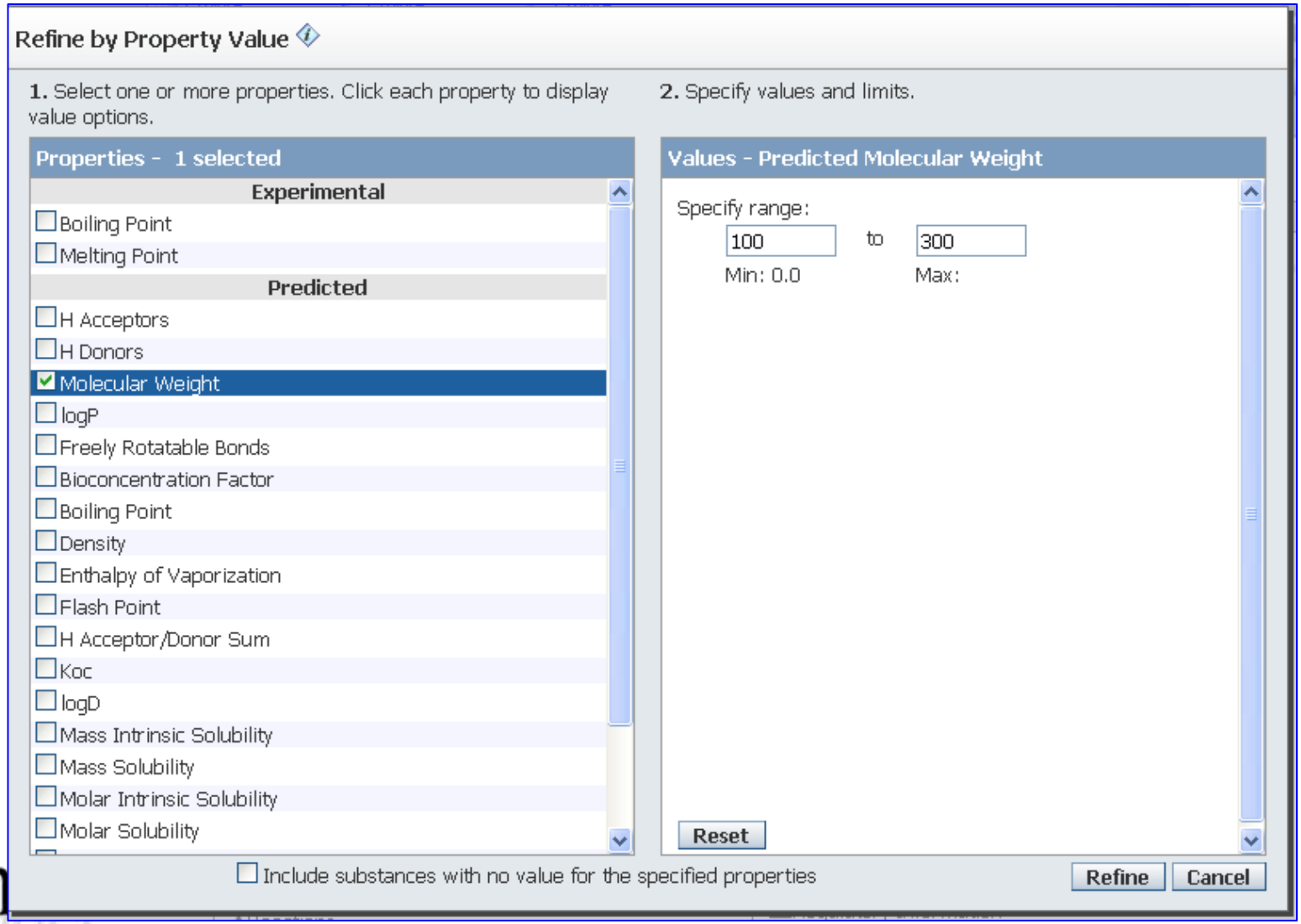
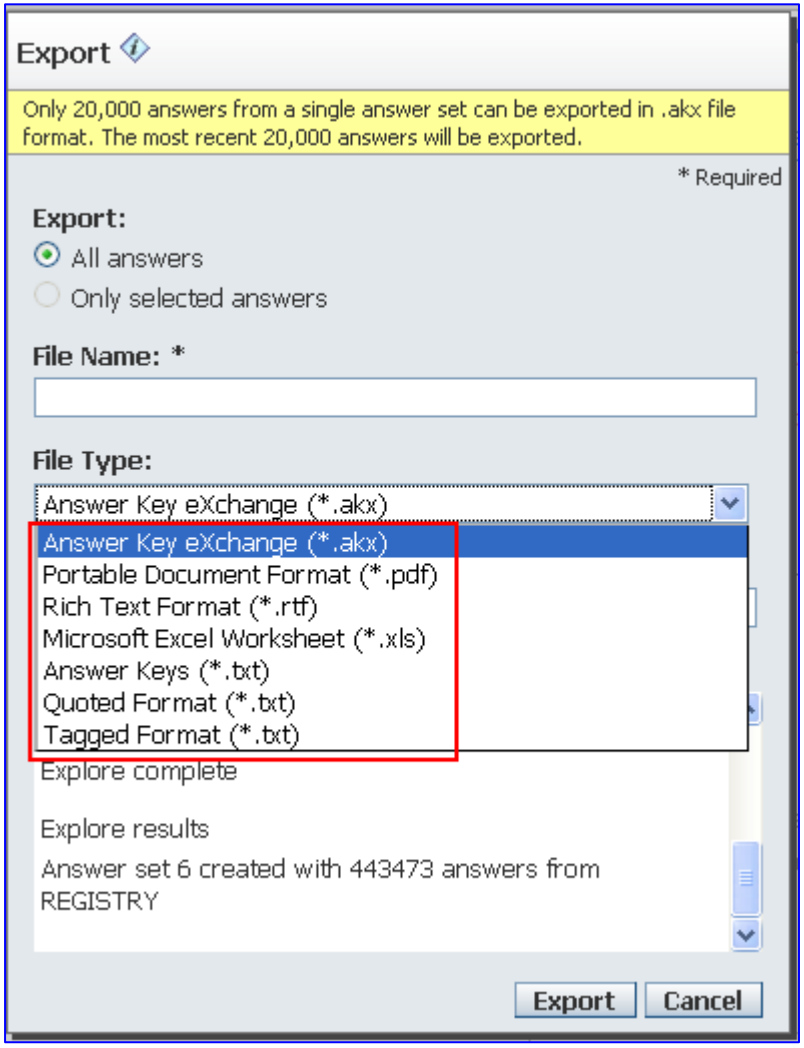
Refine：透過指定分子量的大小來限縮檢索結果。



Export檔案支援多種格式，如 akx, pdf, rtf, xls, txt。



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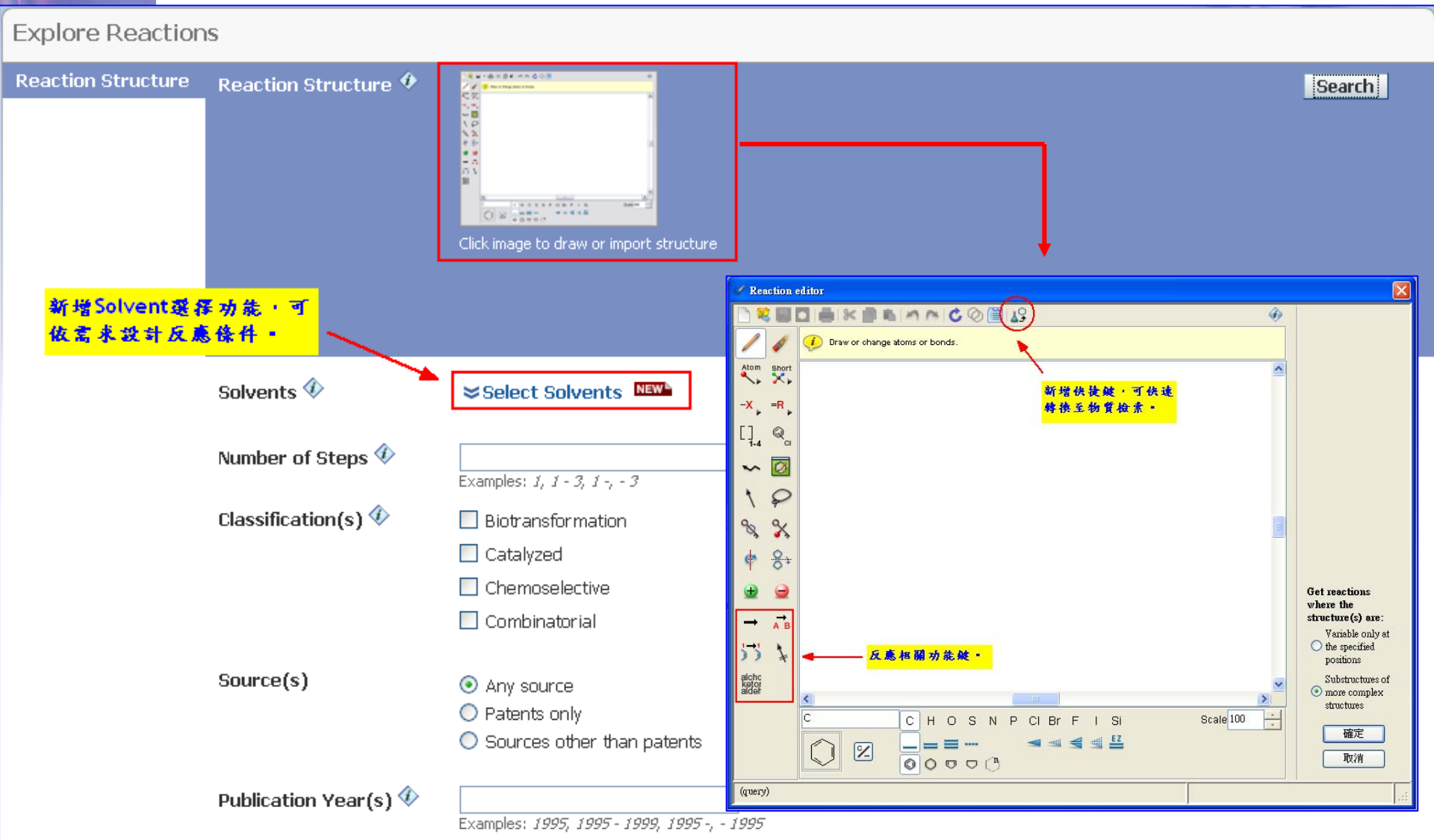
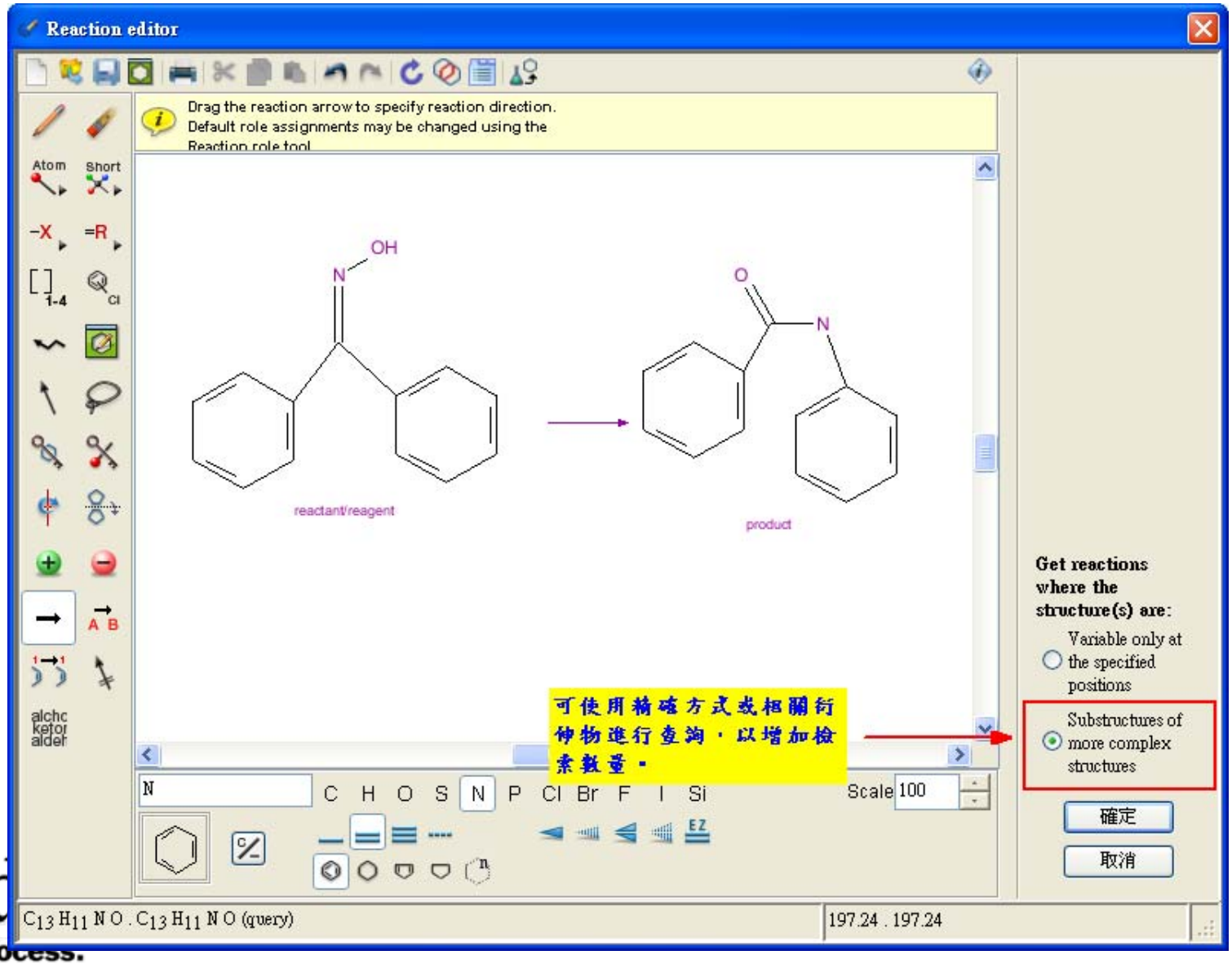
反應檢索:

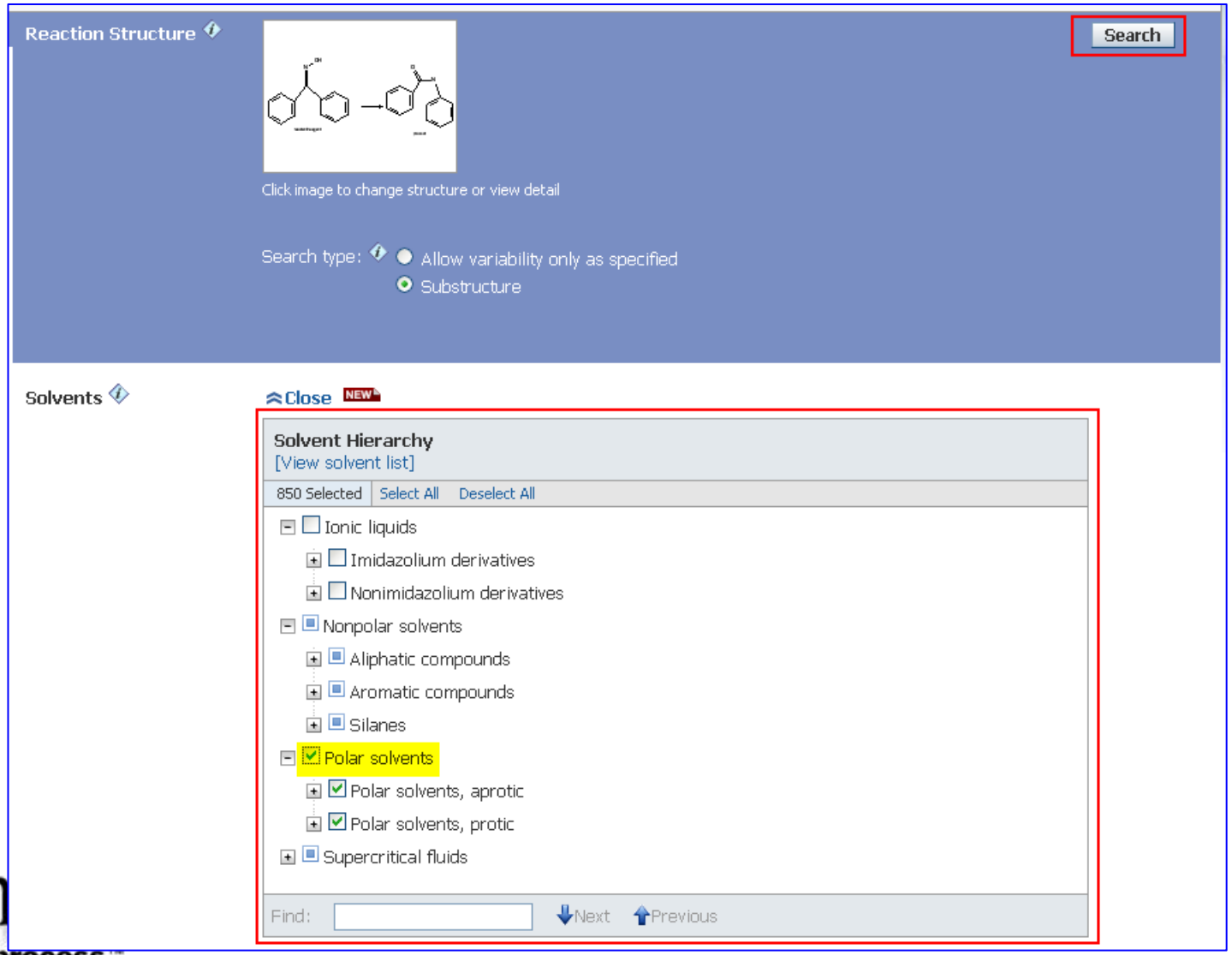
新增Solvent選擇功能，可依需求設計反應條件。點選小圖後出現畫板，較物質檢索多出5個專屬按鍵，下方有限制條件區可供設定。



承接軟體版強大的工具列設計理念，方便使用者更輕鬆的選擇功能。



進行檢索之前，可選擇特定Solvents以限縮檢索結果。



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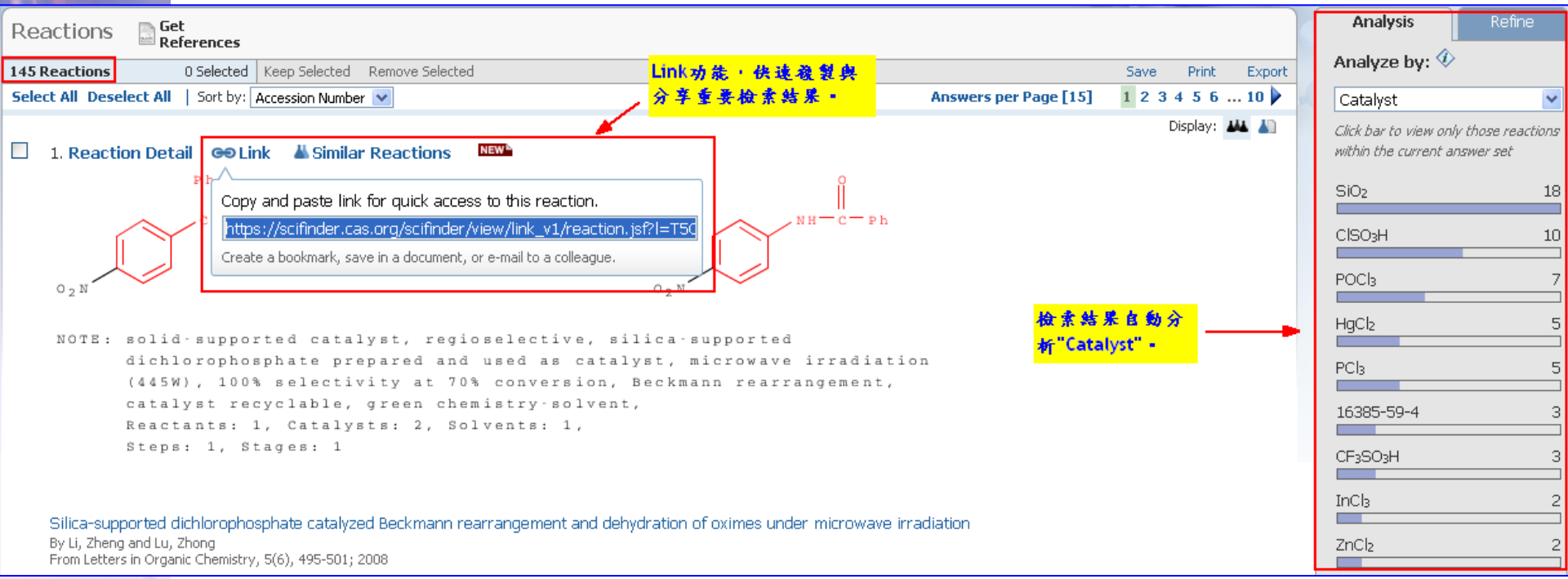
簡潔的檢索結果瀏覽頁面，自動完成分析統計；Link功能快速複製與分享重要檢索結果。



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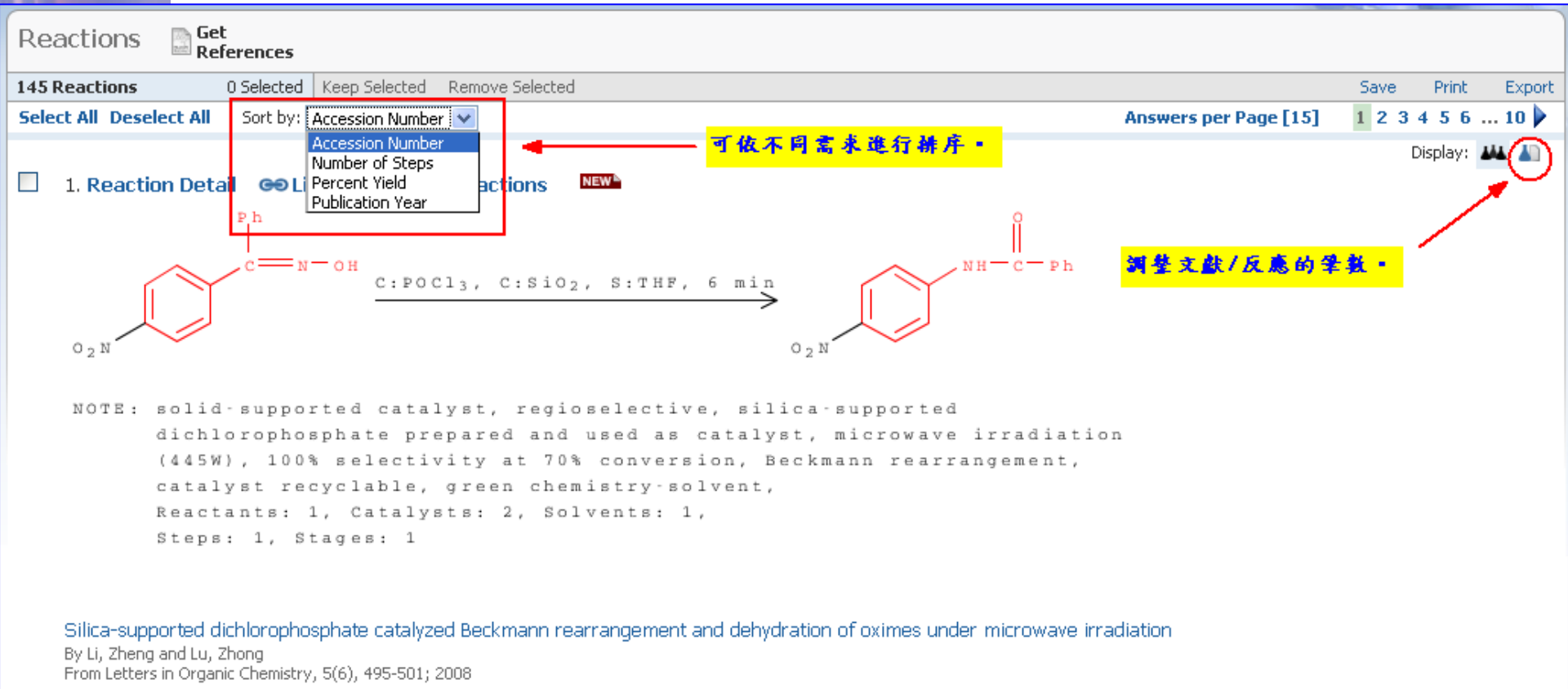
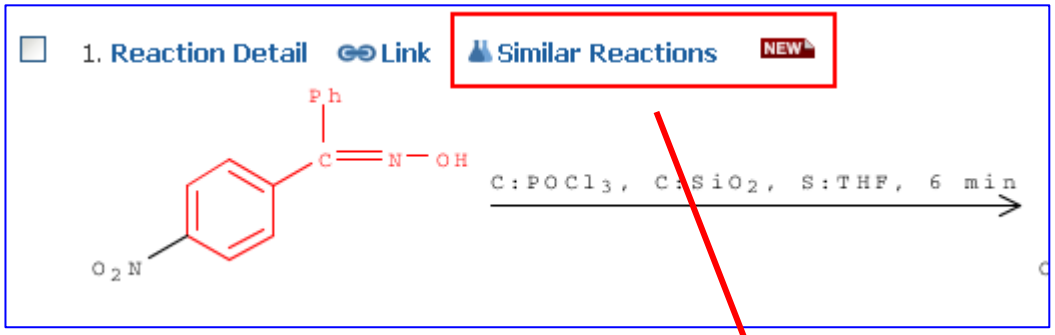
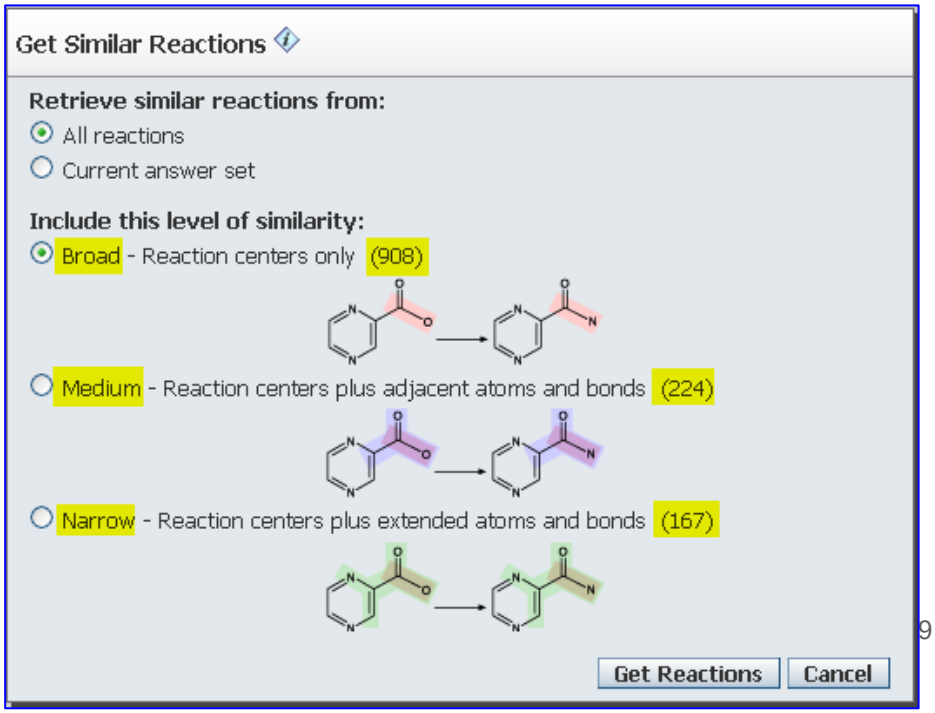
可依照不同需求進行排序，以及調整文獻/反應的筆數(one reaction per reference)。



新功能: Similar Reaction，可依照相似程度不同(筆數多寡)，勾選適合的相似反應。





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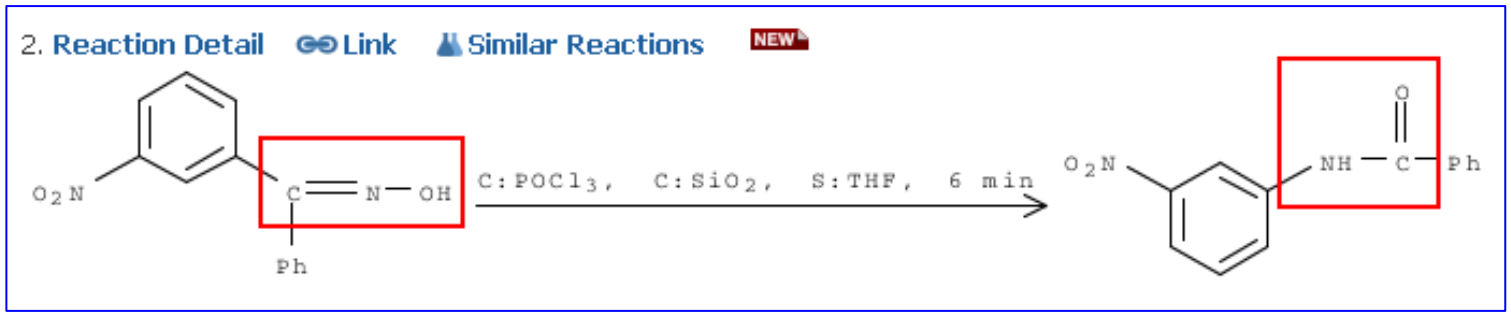
執行similar reaction結果。



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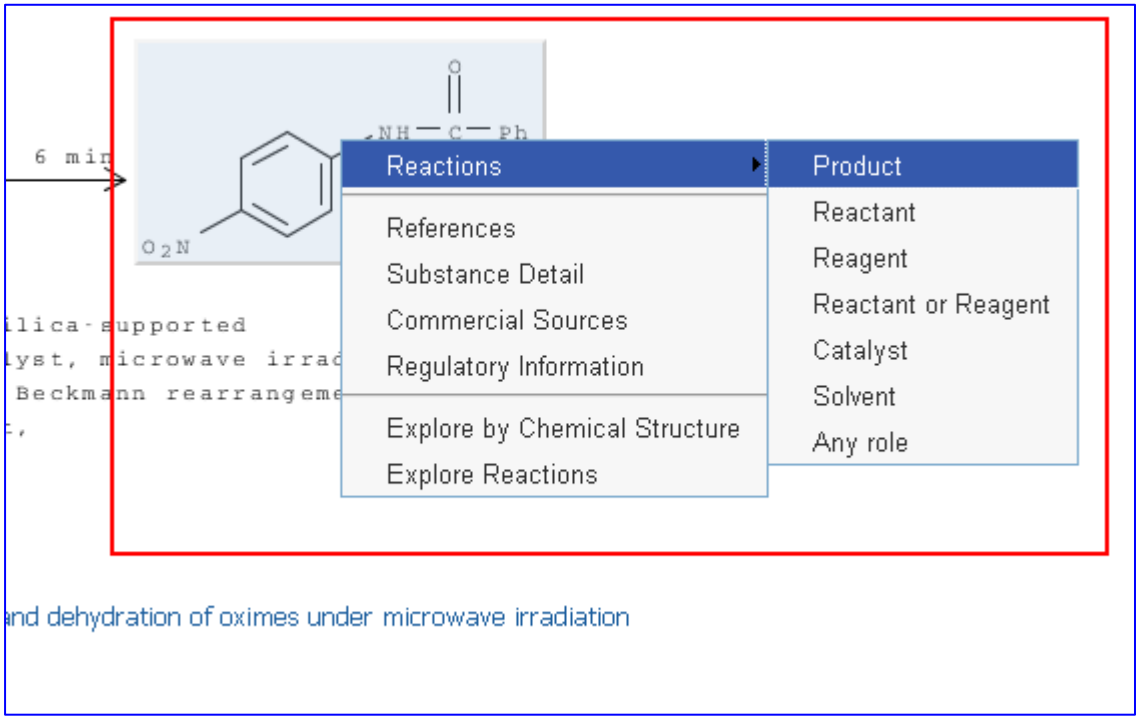
直接點選感興趣物質，可再進行相關查詢。



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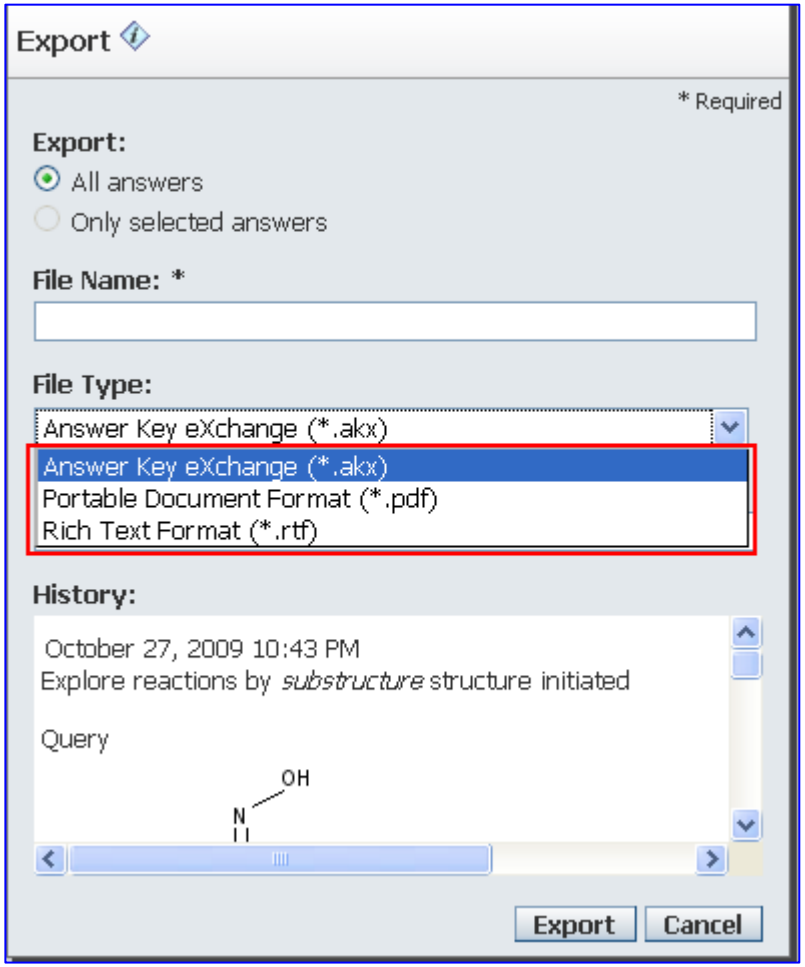
Export檔案支援多種格式，如 akx, pdf, rtf。



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其他常用功能:

Answer Sets: 可對2個以上的答案群集進行combine功能。

History: 可下載最新10筆檢索歷程，方便研究人員熟悉檢索策略。

KMP results: 檢索結果更新通知功能設定。

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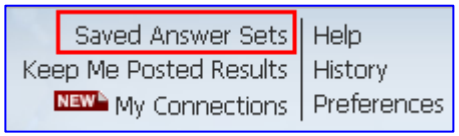

可個別以"文獻"、"物質"、"反應"進行2個以上答案群集的combine功能。

Saved Answer Sets | Combine Answer Sets

References (55) | Substances (10) | Reactions (3)

55 Answer Sets | 3 Selected | Delete Selected

Reference Answer Set Details			Date Saved
IPAMA_CY with Ak repeat_patent (18) Combine with tyrosinase and dopamine Combine Reference Answer Sets "IPA IPAMA_CY with Ak repeat_patent"	Edit	Link	Oct 20, 2009
IPAMA_CY with Ak repeat_patent (4) By dopamine Opened saved answer set "IPAMA_CY remove 0 references (485) > refine "d			0, 2009
IPAMA_CY with Ak repeat_patent (14) By tyrosinase Opened saved answer set "IPAMA_CY remove 0 references (485) > refine "ty			0, 2009
IPAMA_CY based_patent (53) Combine with tyrosinase and dopamine Combine Reference Answer Sets "IPA IPAMA_CY based_patent" (53) > remove 0 references (53)			0, 2009
IPAMA_CY based_patent (19) By dopamine Chemical Structure substructure > substances (11890) > get references (4882) > refine "Patents only" (2488) > remove 106 references (2382) > refine "dopamine" (19)	Edit	Link	Oct 20, 2009

Combine Answer Sets

Select an option for combining the selected saved answer sets:

- Combine — Include all references from all selected answers
- Intersect — Include only references that appear in all selected sets

Combine Answer Sets | Cancel

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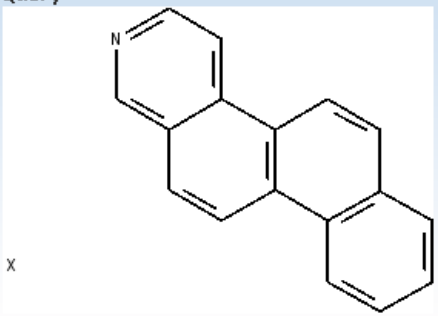
可下載最新10筆歷程並以Word程式開啟，方便研究人員了解檢索策略。

History

Print Export

Session began October 27, 2009 at 8:20 PM

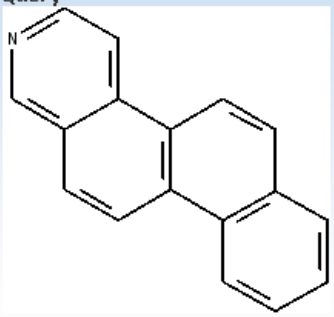
Explore substances by *substructure* structure initiated October 27, 2009 8:26 PM
Query



Explore complete
Explore results
Answer set 1 created with 2 answers from REGISTRY

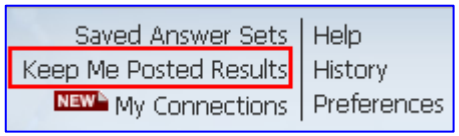
Detailed display from Answer set 1 of 472986-99-5

Explore substances by *substructure* structure initiated October 27, 2009 8:28 PM
Query

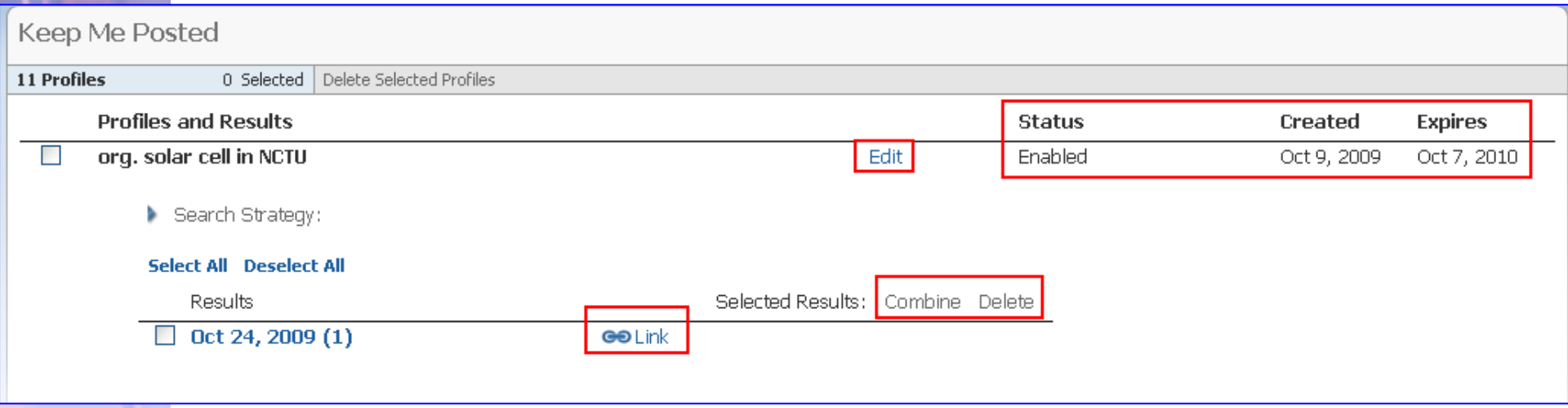


Previous Sessions

SFSessionHistory-2009-10-27_101211.rtf
SFSessionHistory-2009-10-23_040541.rtf
SFSessionHistory-2009-10-23_040401.rtf
SFSessionHistory-2009-10-22_011910.rtf
SFSessionHistory-2009-10-20_235046.rtf
SFSessionHistory-2009-10-20_233906.rtf
SFSessionHistory-2009-10-20_201623.rtf
SFSessionHistory-2009-10-20_200924.rtf
SFSessionHistory-2009-10-20_105129.rtf
SFSessionHistory-2009-10-20_052239.rtf



可隨時對KMP更新通知進行調整，如Edit/Link/Combine/Delete。



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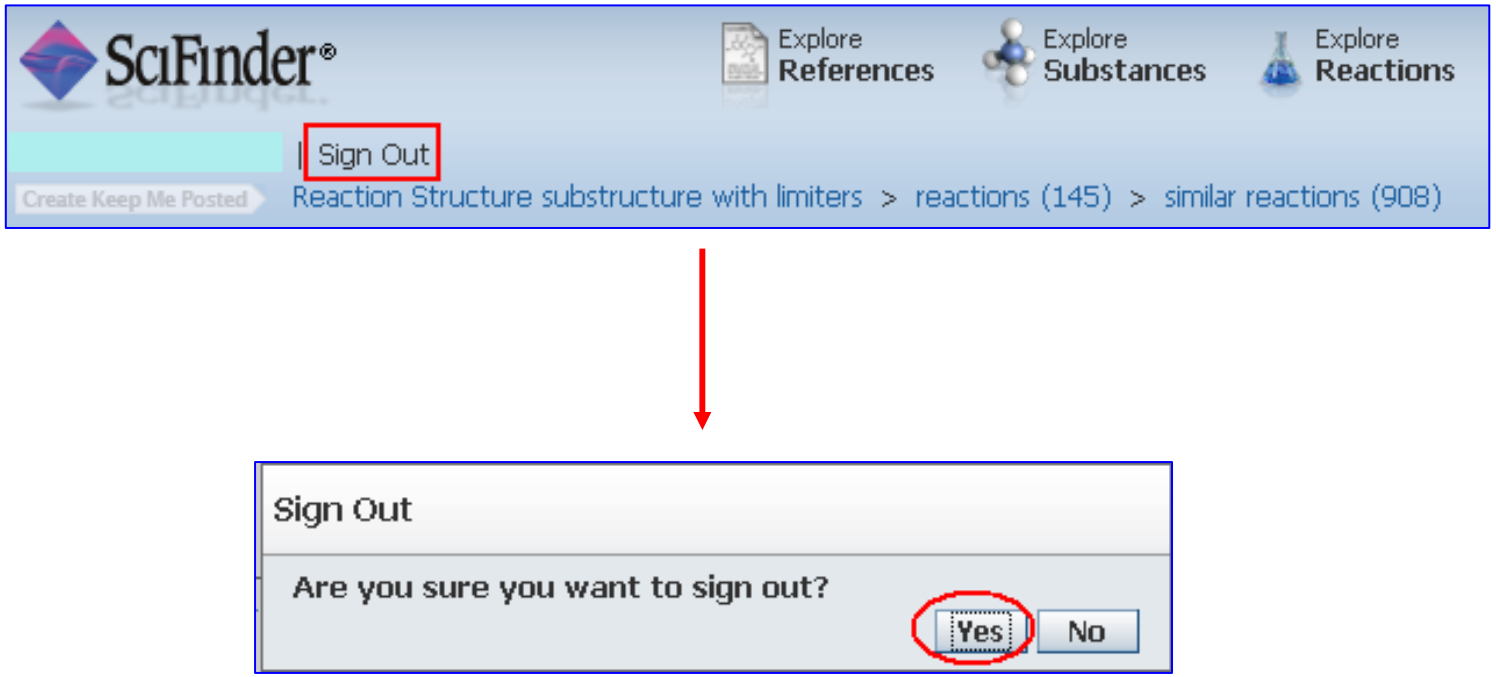
使用完畢記得點選"Sign Out"登出，
以免影響其他人使用權益。



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當發現Web版連線速度變慢時...

- 與網管人員確認Web版伺服器不要設定防火牆

  port: 443 IP:134.243.5.42
- 更新 瀏覽器或JAVA(結構/反應畫板需要)版本
- 關閉 不必要的程式或網頁
- 改用其他瀏覽器, 如: FireFox, Safari, Chrome

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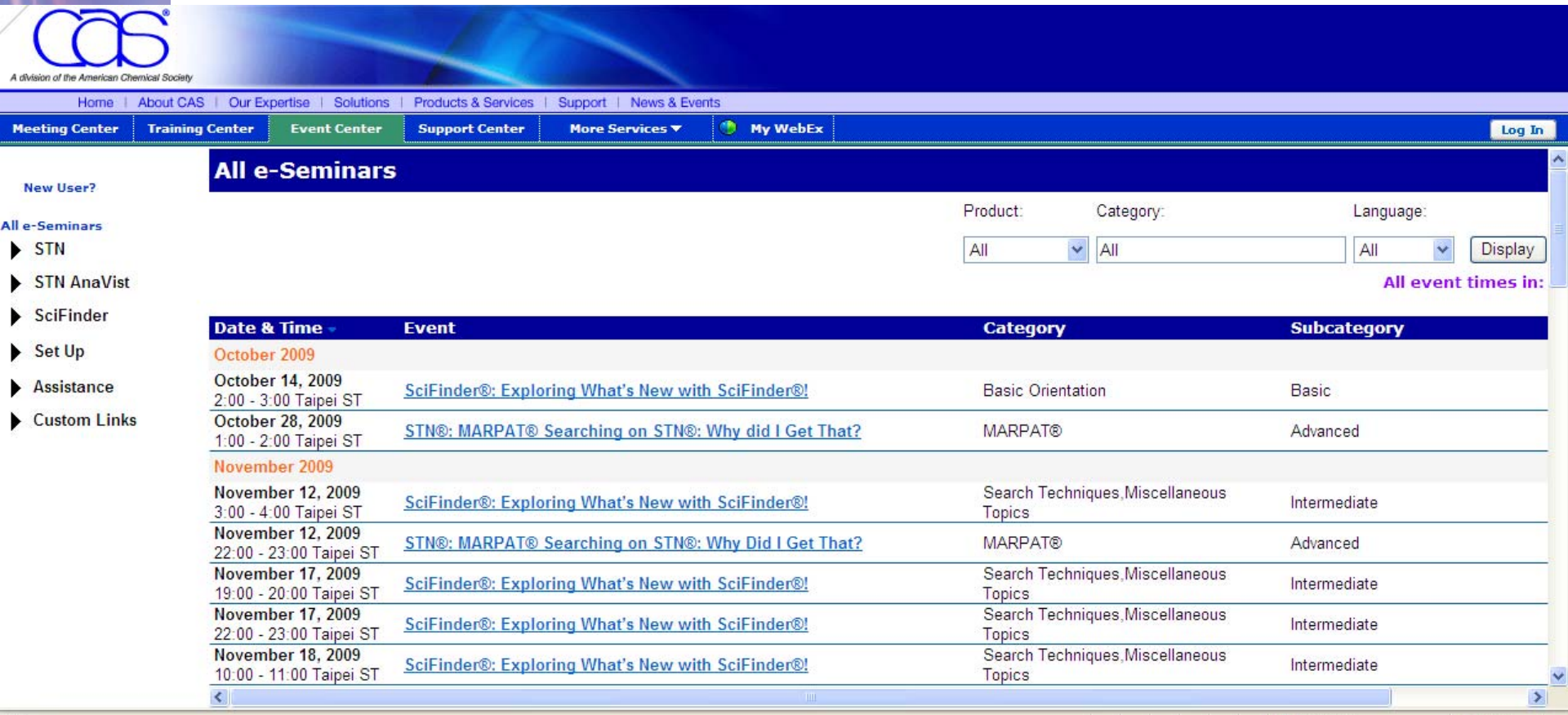
透過線上學習更多關於Web版的檢索技巧

→ https://casevents.webex.com



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&

Link the Science World~

CAS 台灣代表

CAS: www.cas.org 、 TW: www.igrouptaiwan.com

若您需要進一步資訊，請與我們連絡～

Tel：(02) 2707 8588

鄭淮辰：ext. 226 E-mail：brad.cheng@igrouptaiwan.com

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