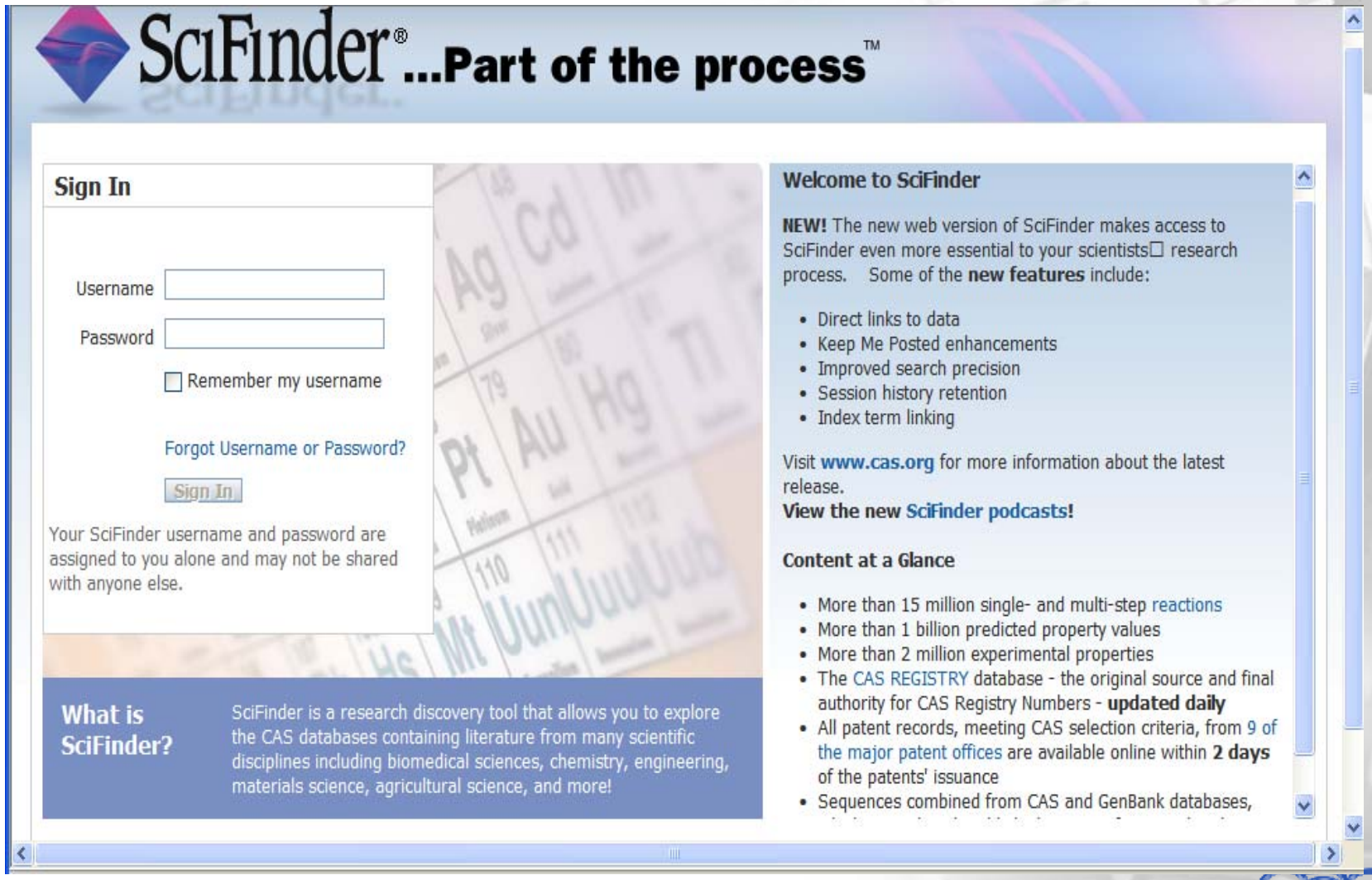
Web version of SciFinder®: new interface and features

Bhawat Ruangying, CAS representative

Updated at 22 Dec 2009

SciFinder web interface



Technical aspects of SciFinder Web

- SciFinder URL : http://scifinder.cas.org
  - Windows-based browsers Internet Explorer 6.x and 7.x as well as FireFox 2.x
  - Mac browser support for Firefox and Safari
  - Java applet (J2SE Runtime Environment 6.0, which installs Java 1.6 version) installed on users' computers for CASDraw to operate
- No software or sife.prf required
- Network requirement:
  - https (SSL) connection via port 443 to scifinder.cas.org
  - http connection on port 80 to chemport.cas.org
- Client based SciFinder will continue to be fully supported by CAS

Online user registration consists of two steps

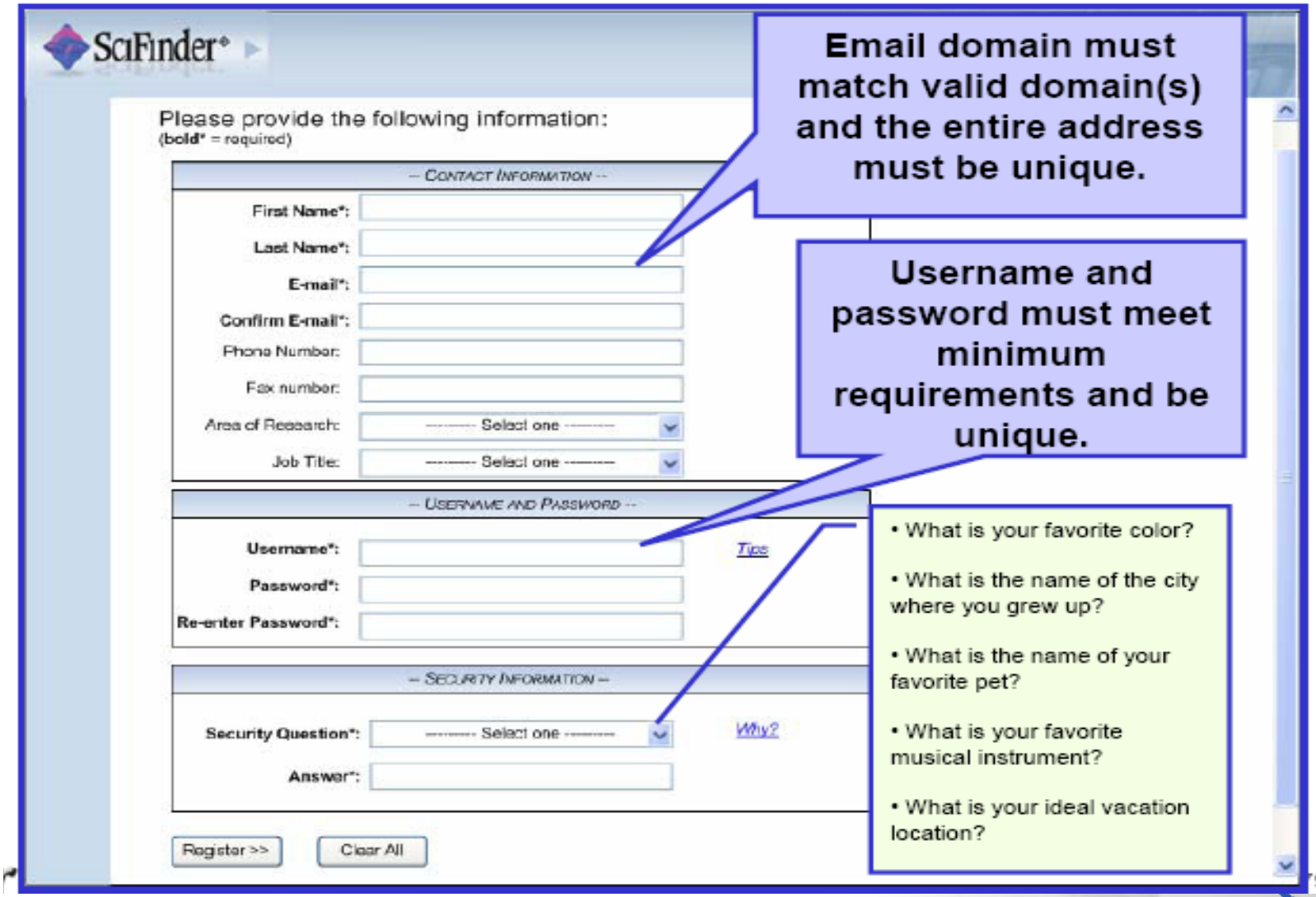
Key Contact Setup

- Log on to myCAS to use set-up registration capabilities
- Verifies email domain(s) are correct and sufficient
- Sends CAS corrections or updates as needed
- Generates unique registration URL for distribution to users

User Registration

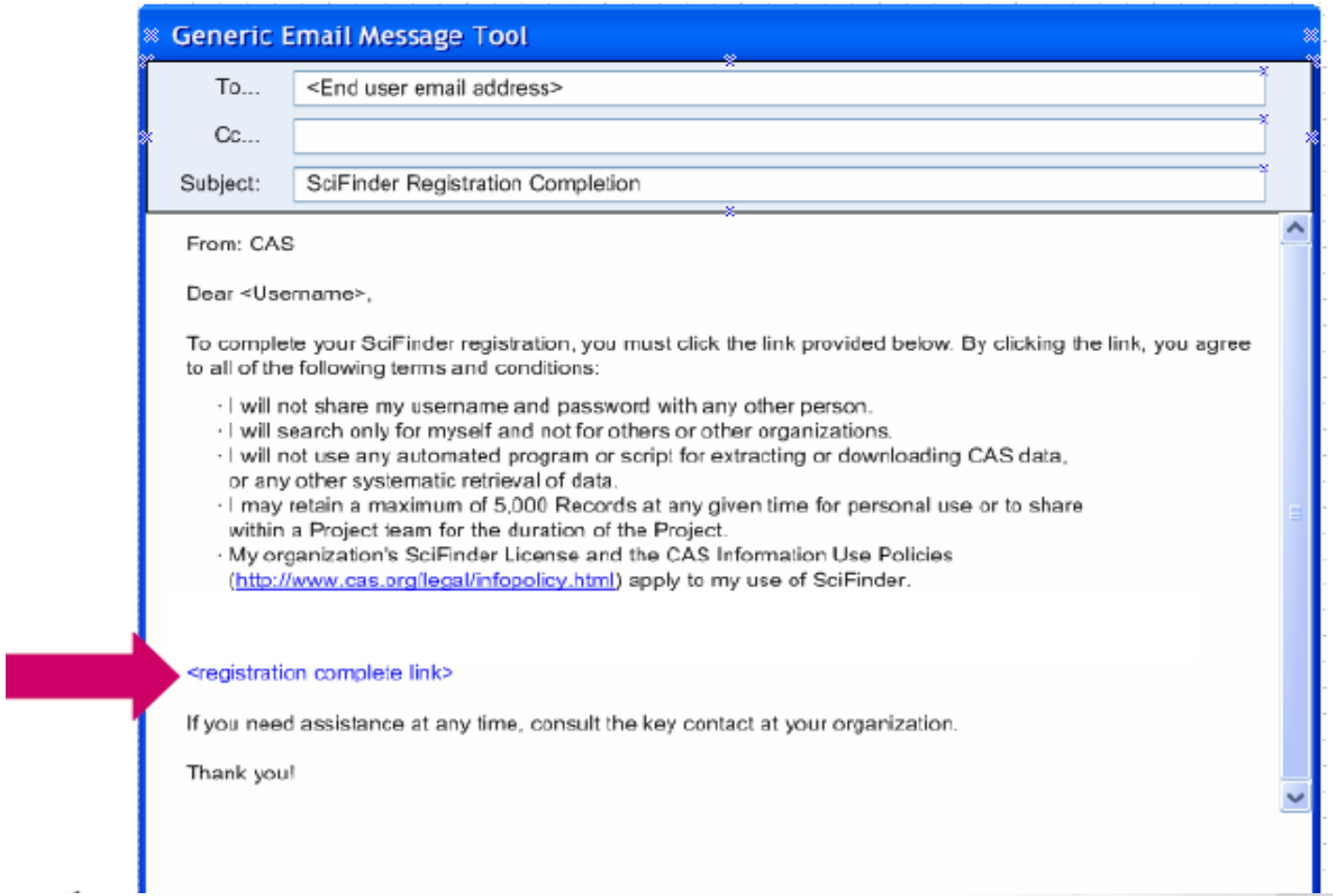
- Obtains the registration URL
- Creates a new username and password online
- Enters required email address and other information
- Confirms registration via email

User enters the information

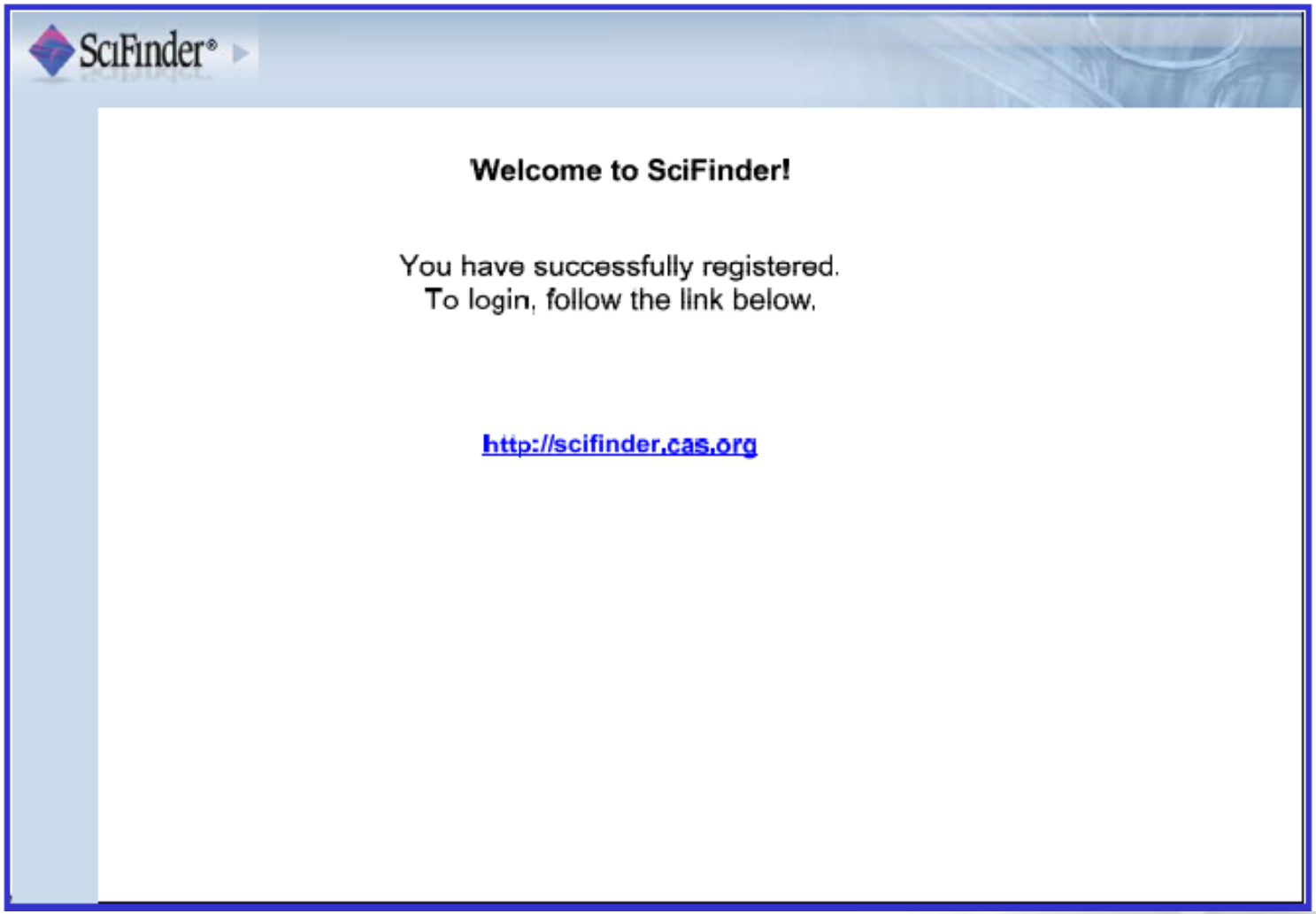


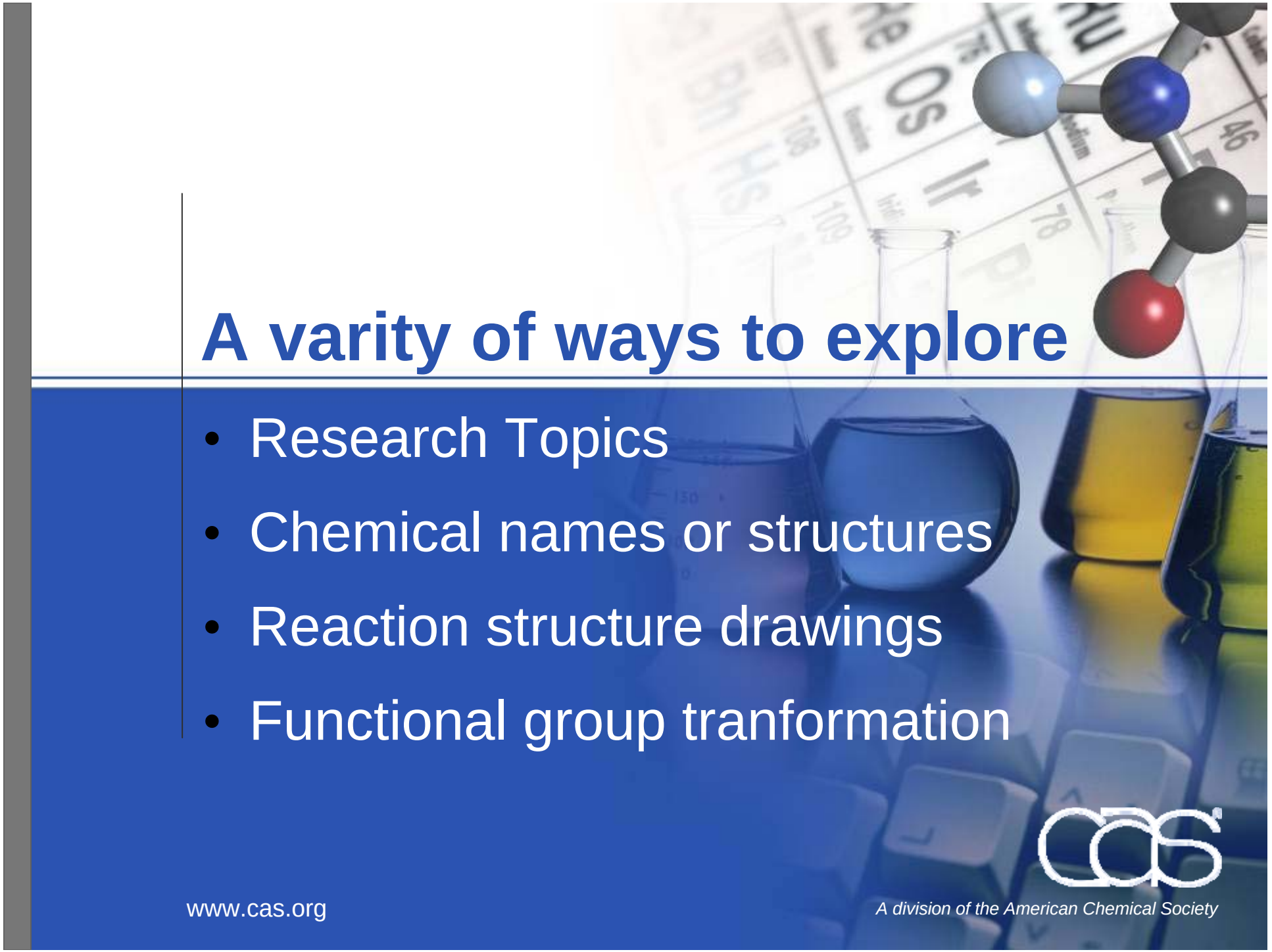
Email validation for new IDs

User receives email confirmation



User is now ready to access

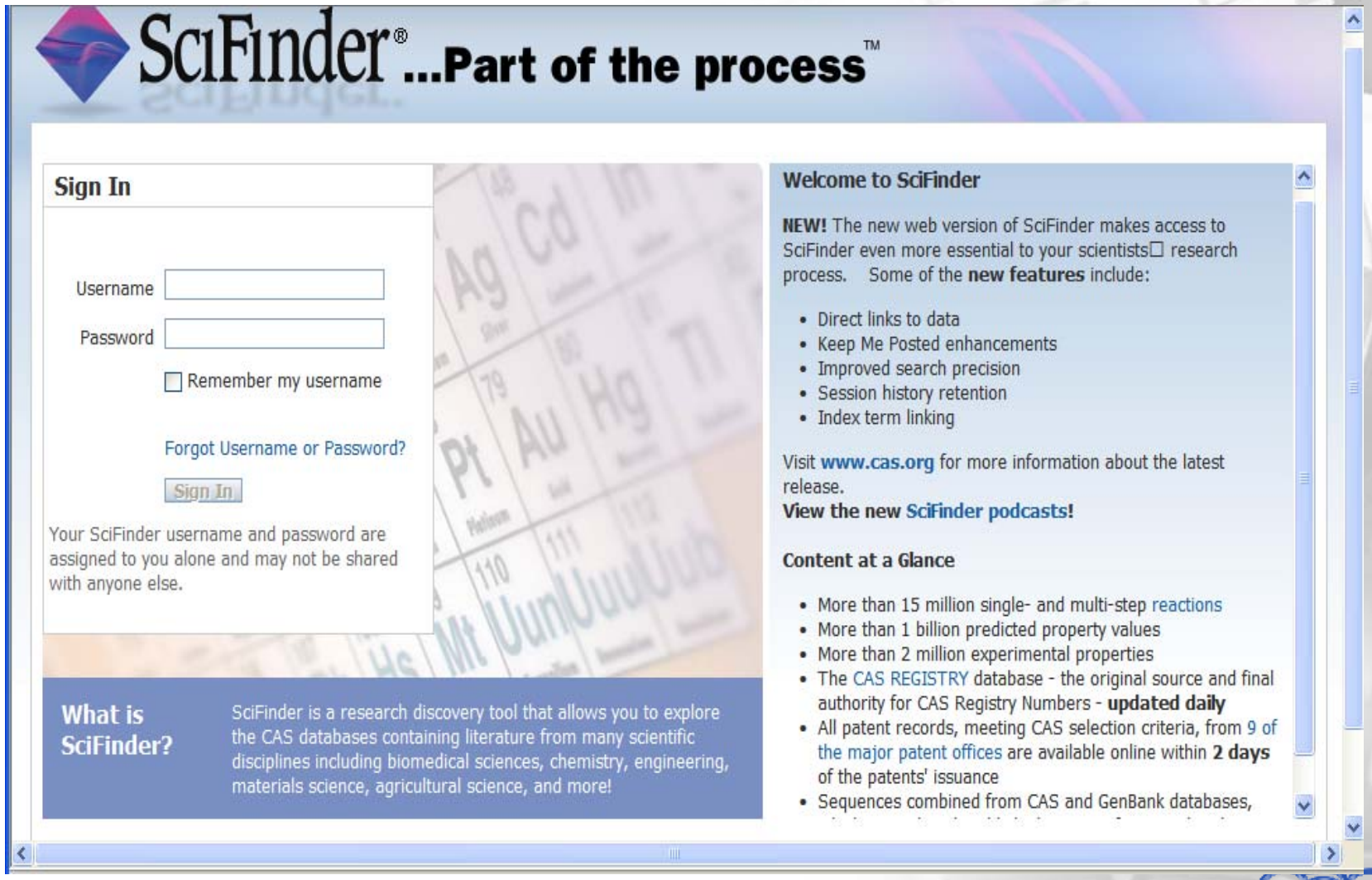




A varity of ways to explore

- Research Topics
- Chemical names or structures
- Reaction structure drawings
- Functional group tranformation

SciFinder web interface

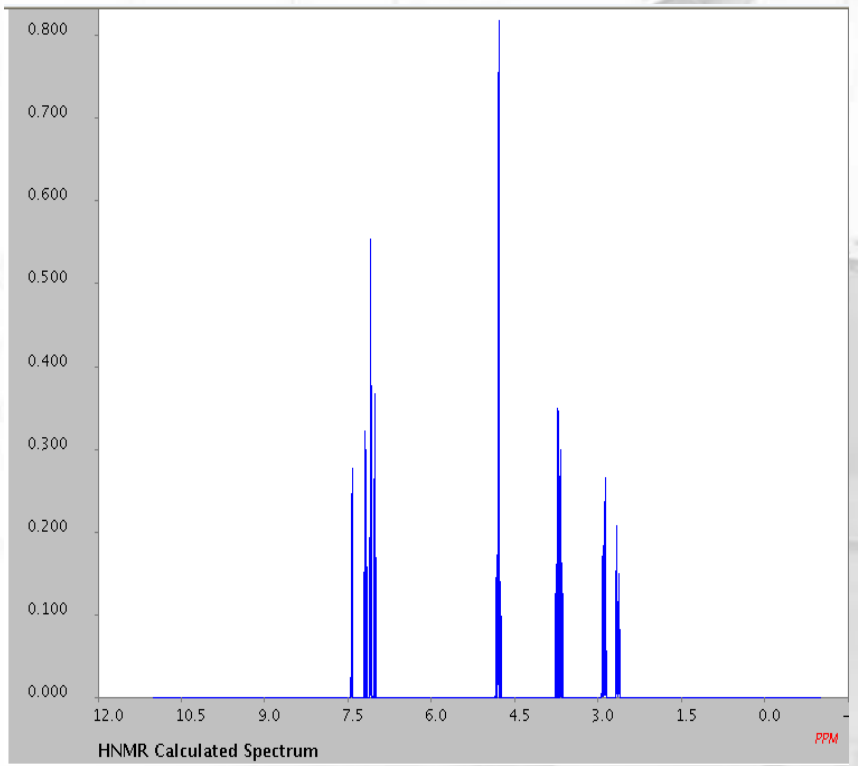


SciFinder allows for integrated searching of these essential resources for scientists

Type of information	Content and coverage	Starting points for locating chemical synthesis information
References	• >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
Substances	• >51 million organic and inorganic substances • >61 million sequences • >2.6 billion predicted and experimental properties, spectra, and data tags, plus >29.6 million proton NMR spectra and 29.7 million predicted ^{13}C-NMR spectra • 1957 to present, plus selected substances back to the early 1900s • Commercial source information from >1,000 suppliers for >38 million substances • Regulatory information for > 270,000 substances	• Chemical name or CAS Registry Number® • Molecular formula • Chemical structure drawing
Reactions	• >29 million preparations, including >21 million single- and multi-step reactions • 1840 to present	• Reaction structure drawing • Functional group transformation

New content added – more property data

- 1.9 billion predicated and experimental properties, spectra and data tags
- 23.8 million newly released predicted proton NMR spectra
- Thousands of new experimental NMR, IR, and Mass spectra as well as experimental physical properties now appear in Substance Details



Prophetic Substance

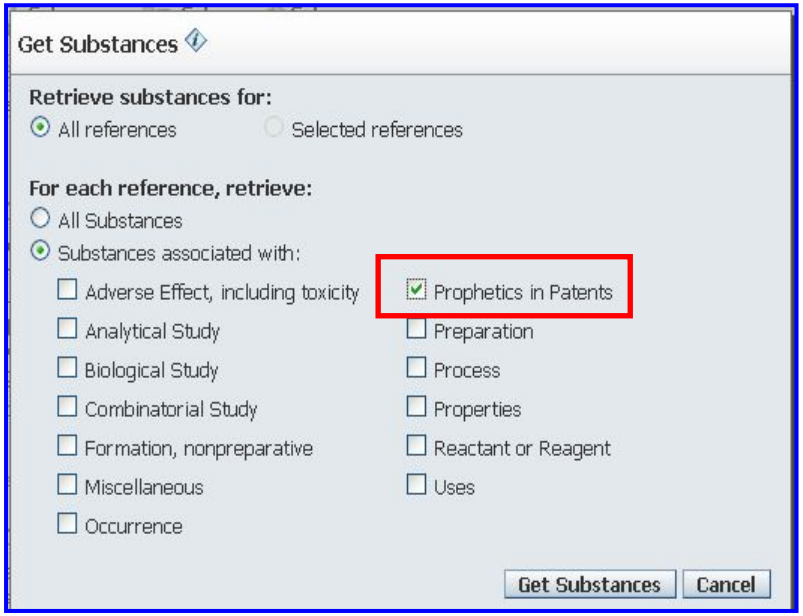
A new role for substances indexed as prophetics. It is a specific substance located in the examples of a patent that has no supporting data (e.g property data or yields)

7758-29-4 Sodium tripolyphosphate

antimicrobial compns. and methods to eradicate and remove fungi and bacteria from indoor and outdoor structures and materials

Other use, unclassified; Technical or engineered material use; Uses; Prophetic

Reference Detail



Role	Patents	Nonpatents	Nonspecific Derivatives from Patents	Nonspecific Derivatives from Nonpatents
Analytical study	✓	✓		
Biological study	✓	✓	✓	✓
Formation, nonpreparative	✓	✓		
Miscellaneous		✓		
Occurrence		✓		
Preparation	✓	✓	✓	
Process	✓	✓		
Properties	✓	✓		
Prophetic in patents	✓			
Reactant or reagent	✓	✓		
Uses	✓	✓		

Substance Detail

New content added – New reaction information

- More than 29 million preparations
- Thousands of evaluated reactions from several Wiley reference works:
  - Encyclopedia of Reagents for Organic Synthesis (EROS)
  - Organic Syntheses
  - Organic Reactions
- Giving access to important older reactions

Reference Search

www.cas.org

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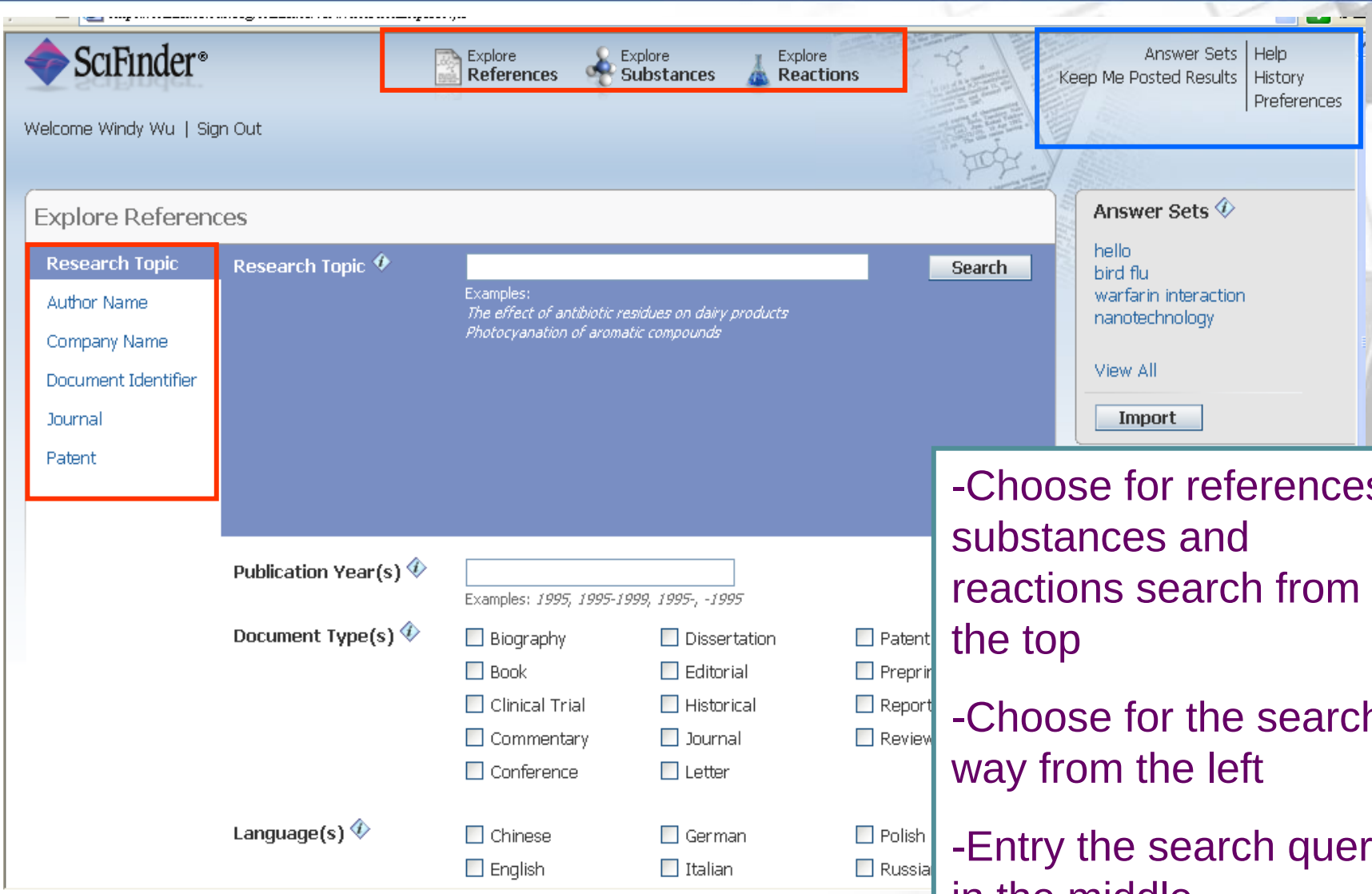
Clear search interface at one page

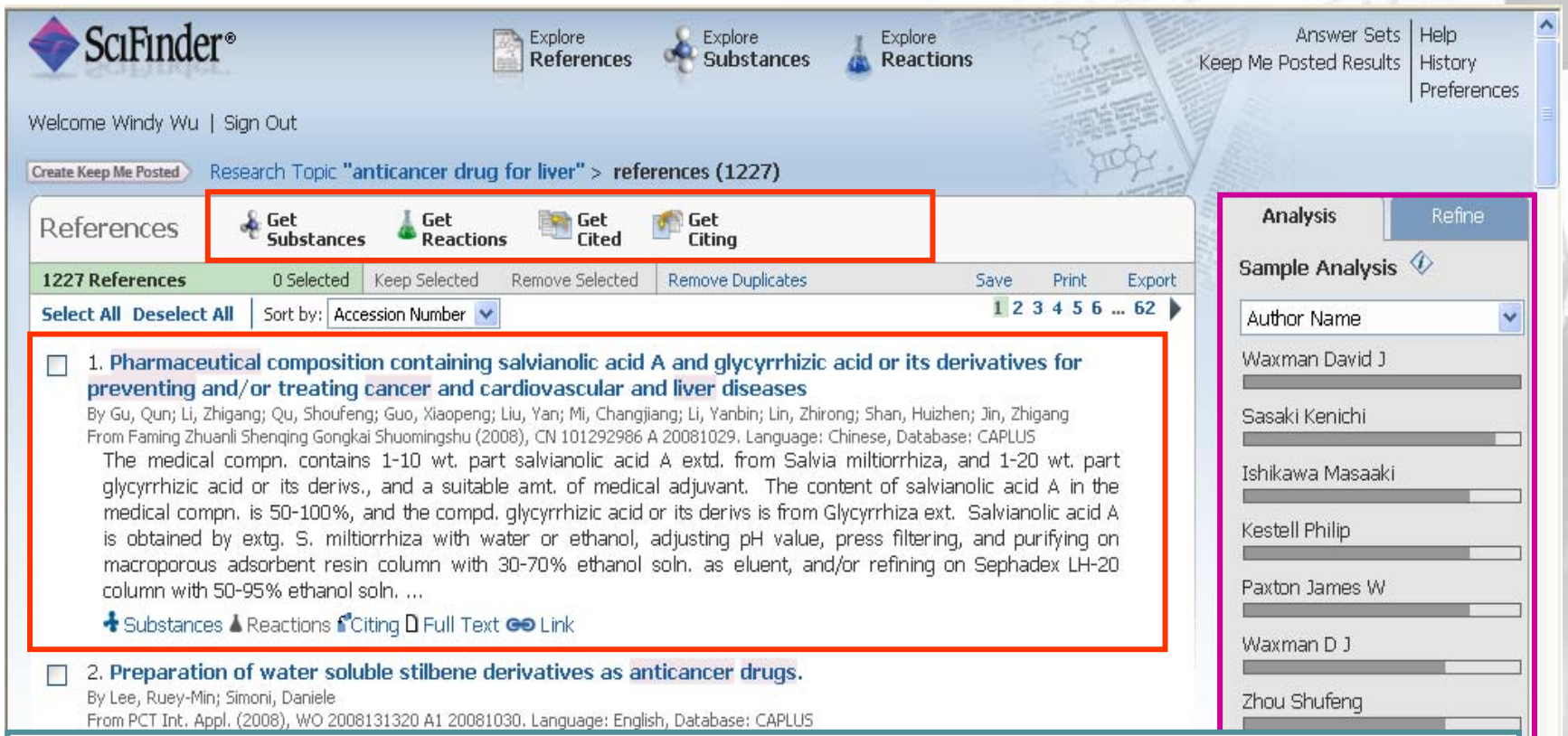


-Choose for references, substances and reactions search from the top

-Choose for the search way from the left

-Entry the search queries in the middle

Informative references answer page

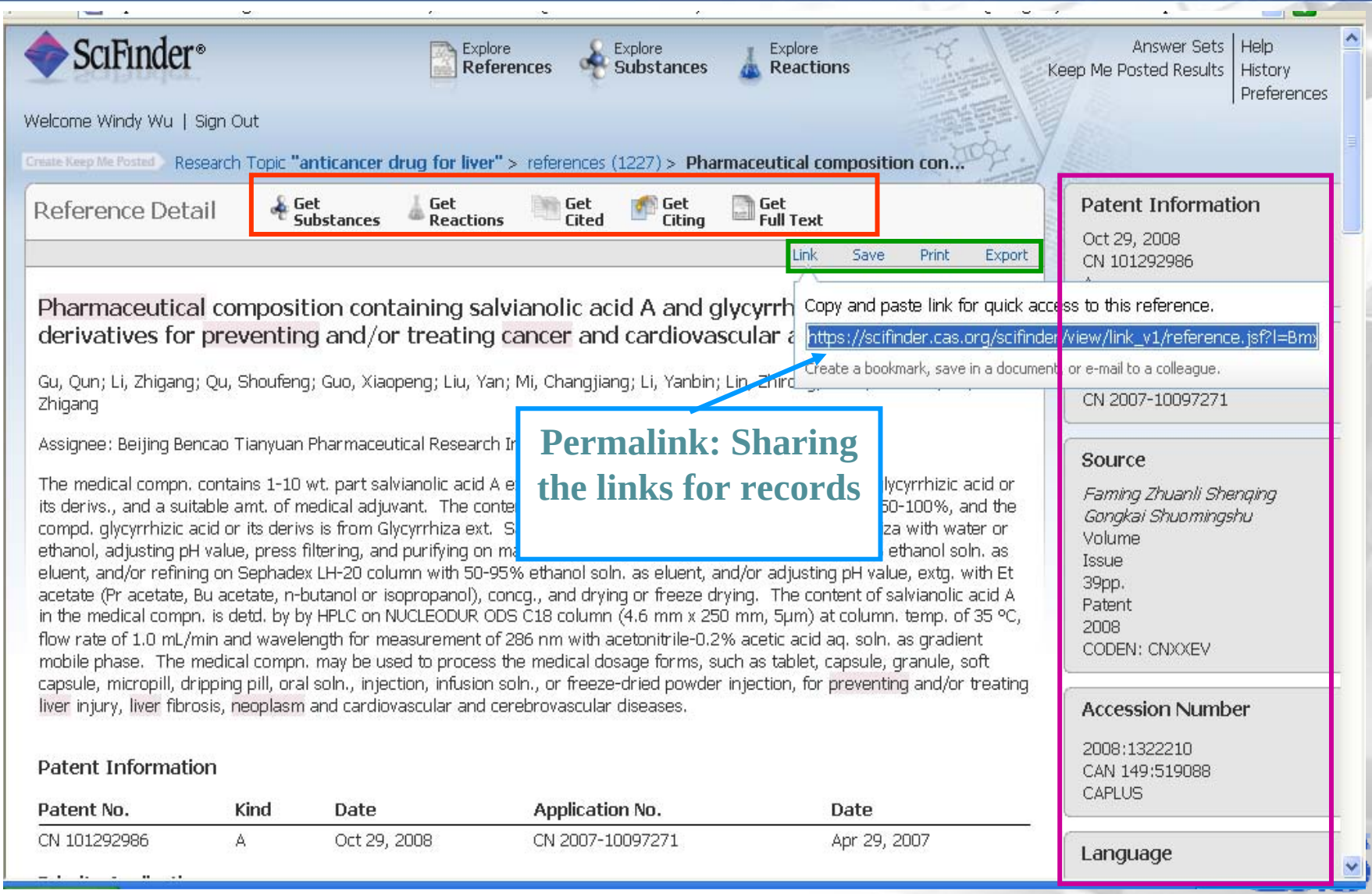


-Abstract information for quick reference, with the keyword highlighted

-Get related information for particular or all references

-Analyses are performed automatically for getting more ideas of answer set

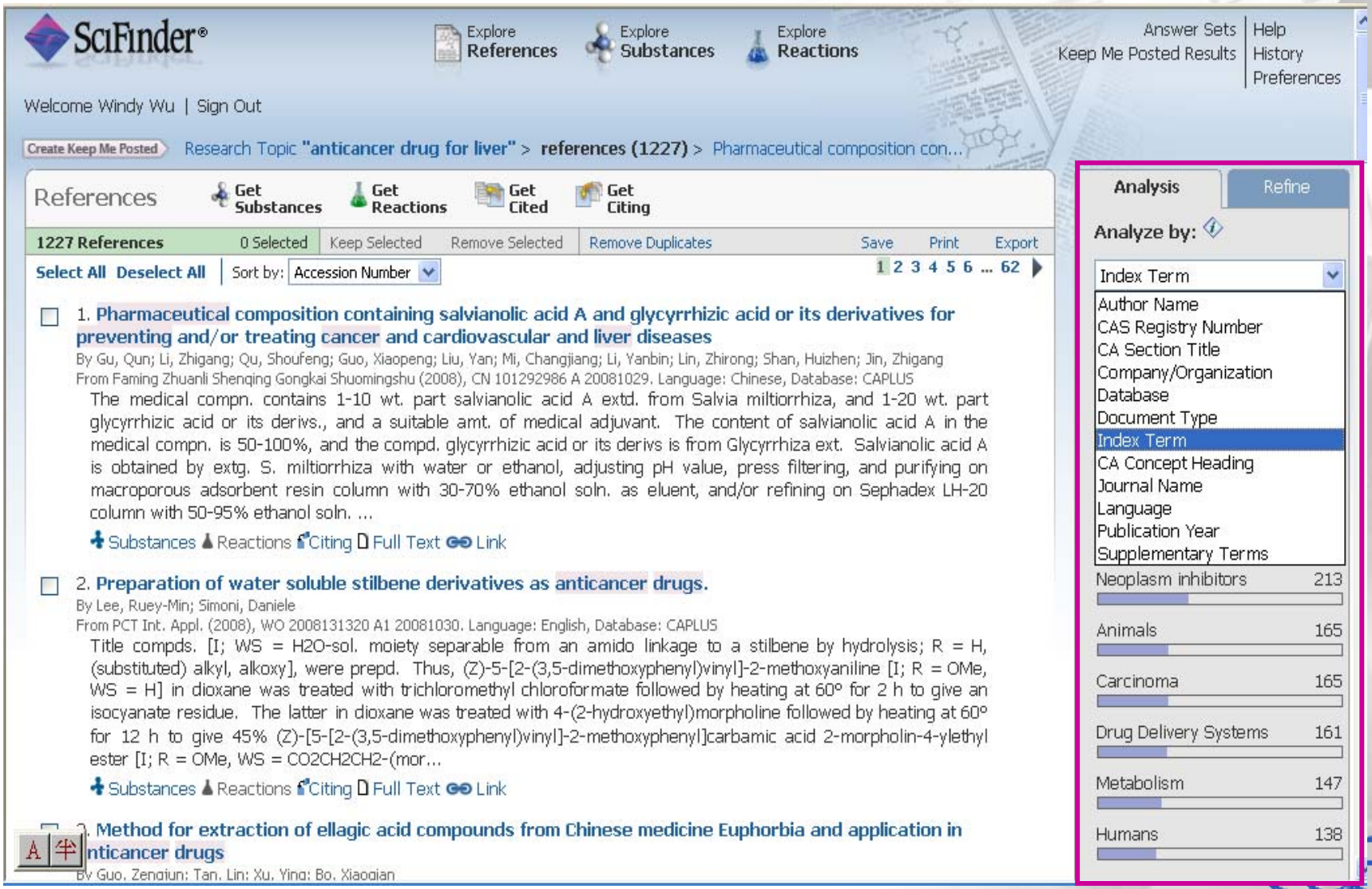
A CAplus record (1)



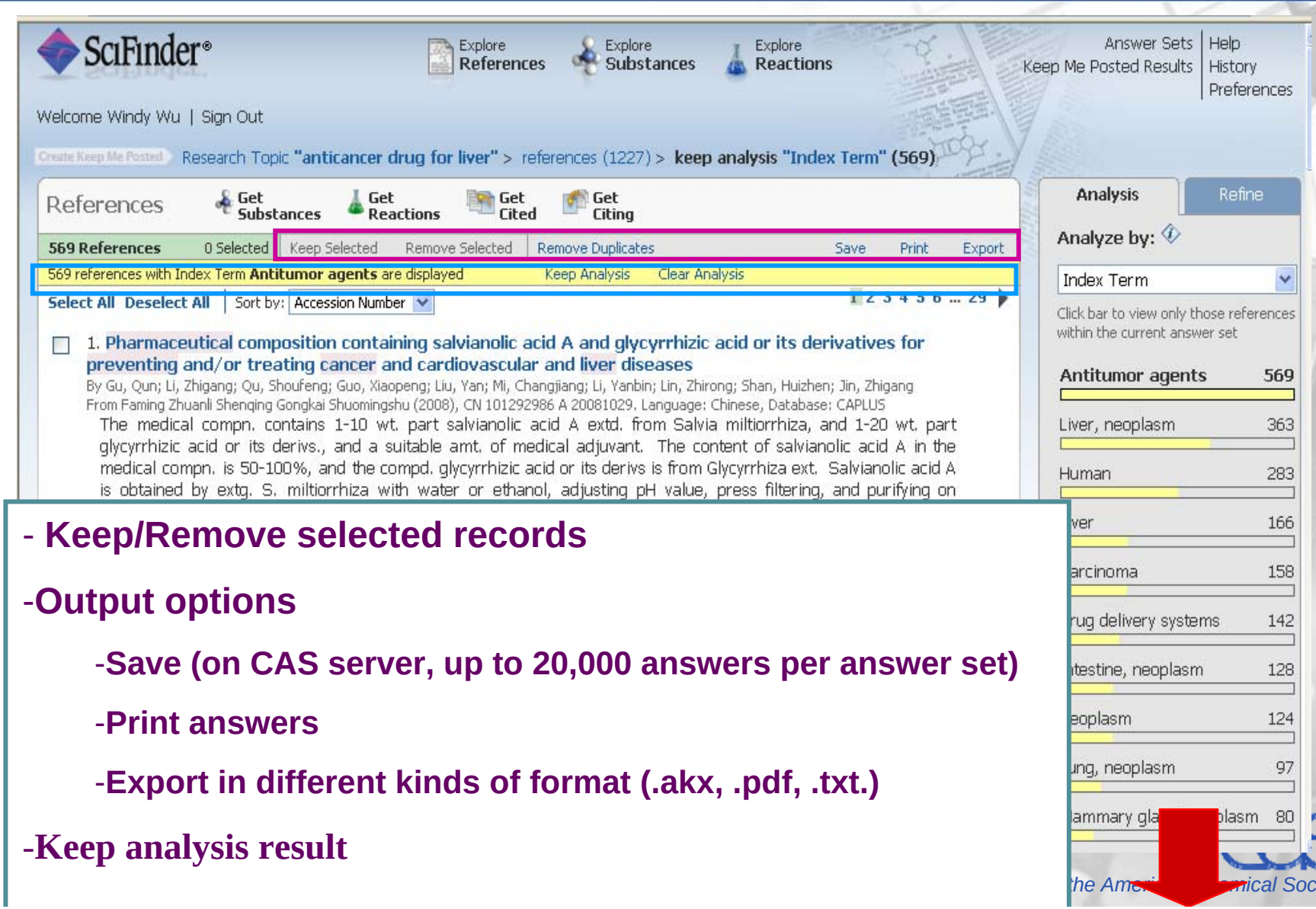
A CAplus record (2)

- CAS scientists index for novel concepts and substances
- Concepts heading with sub-heading for detailed information
- Index terms are linked for faster exploring
- CAS registry number is indexed for substance with specific role

Analyze the results by different ways



Keep selected records and analysis display



- Keep/Remove selected records

-Output options

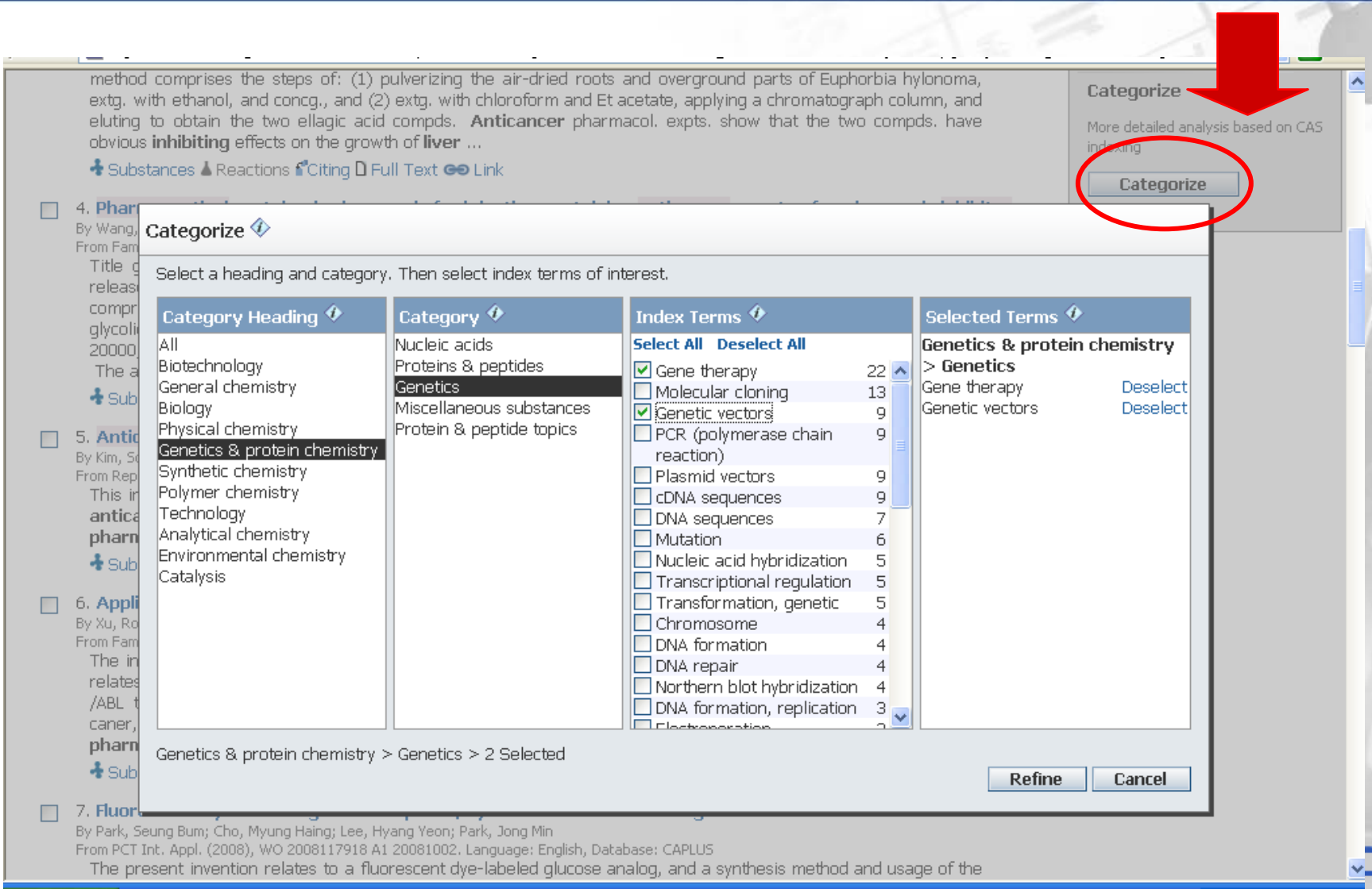
  -Save (on CAS server, up to 20,000 answers per answer set)

  -Print answers

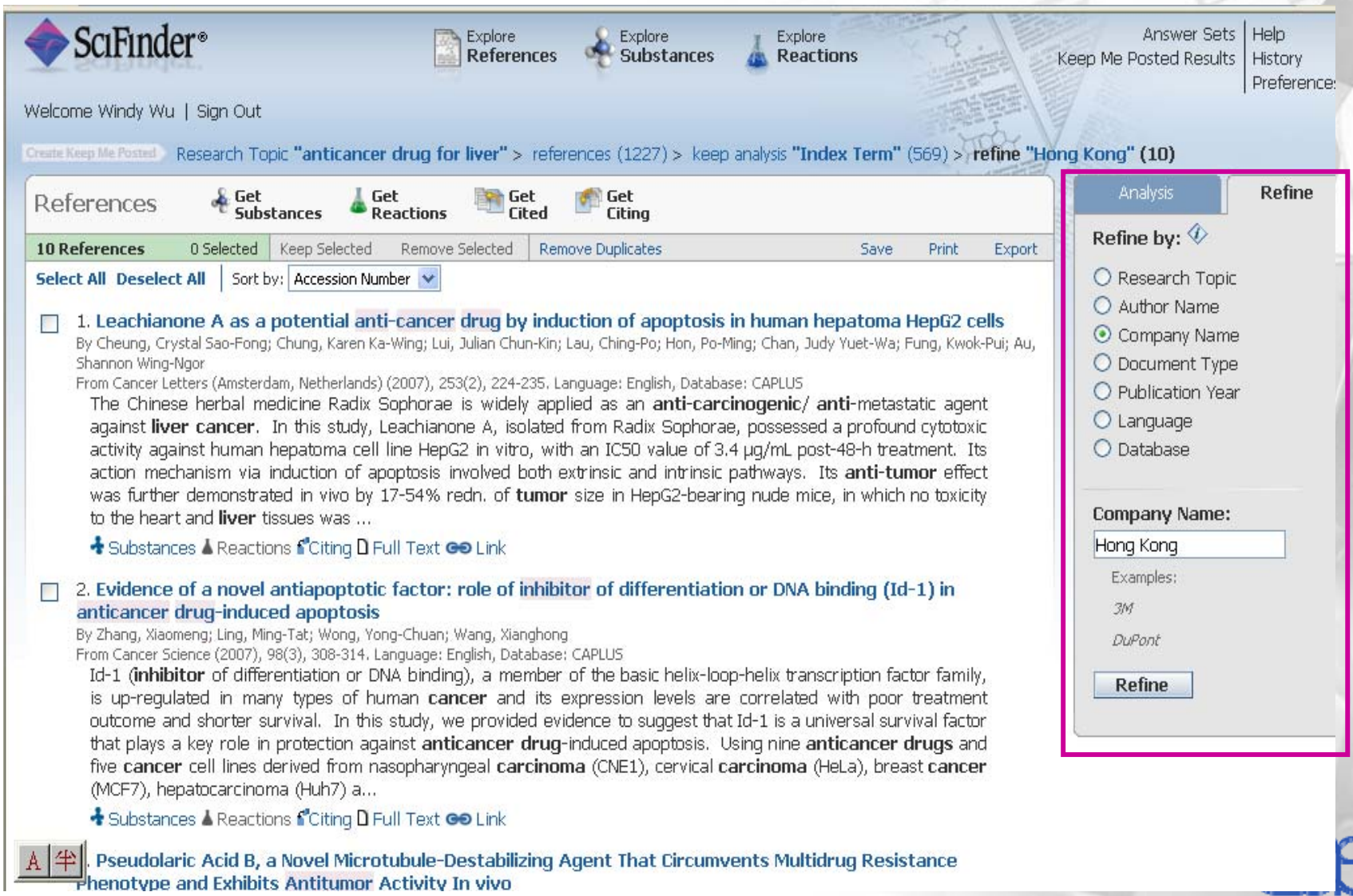
  -Export in different kinds of format (.akx, .pdf, .txt.)

-Keep analysis result

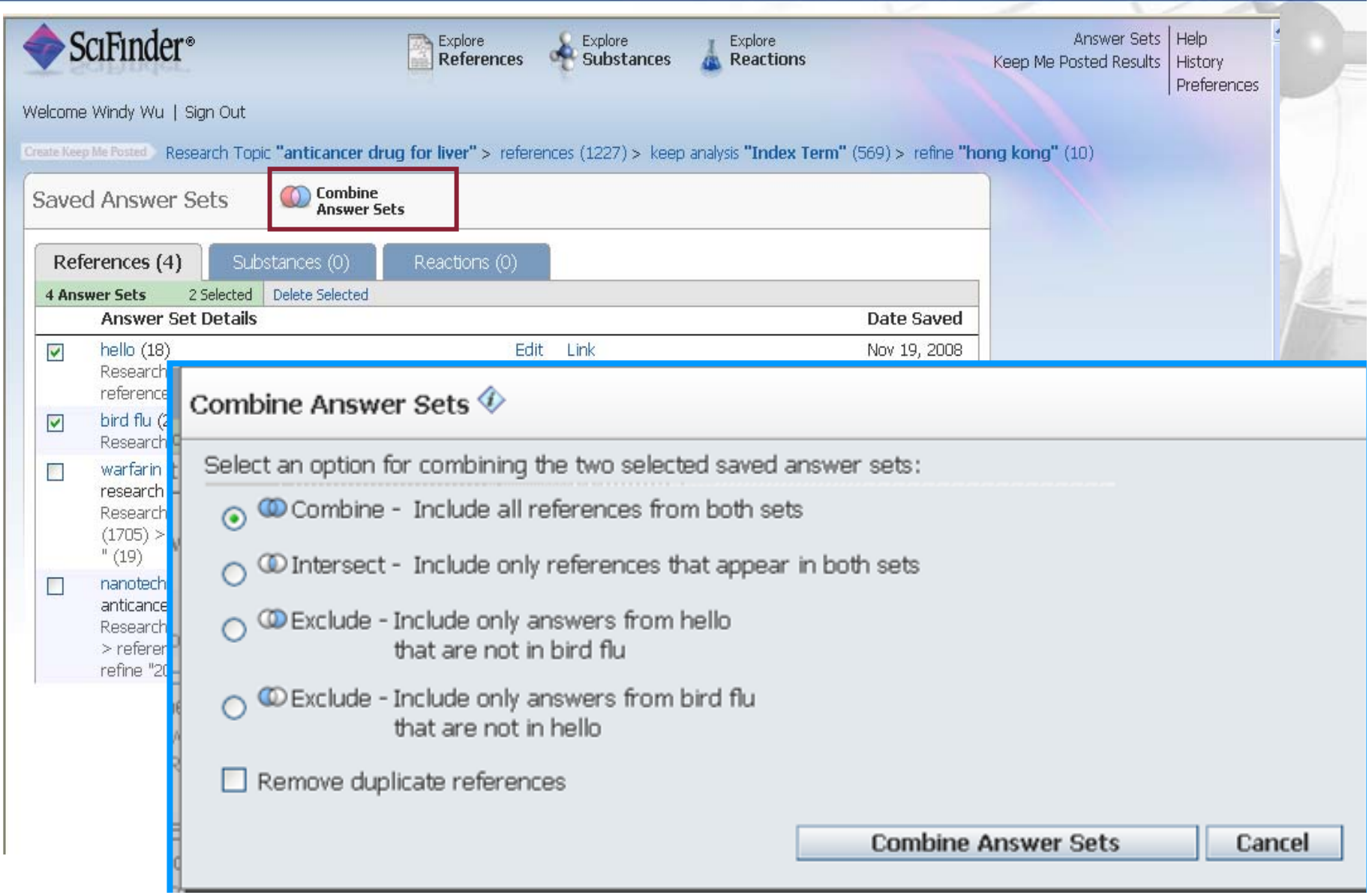
Categorize helps to refine to specific index terms



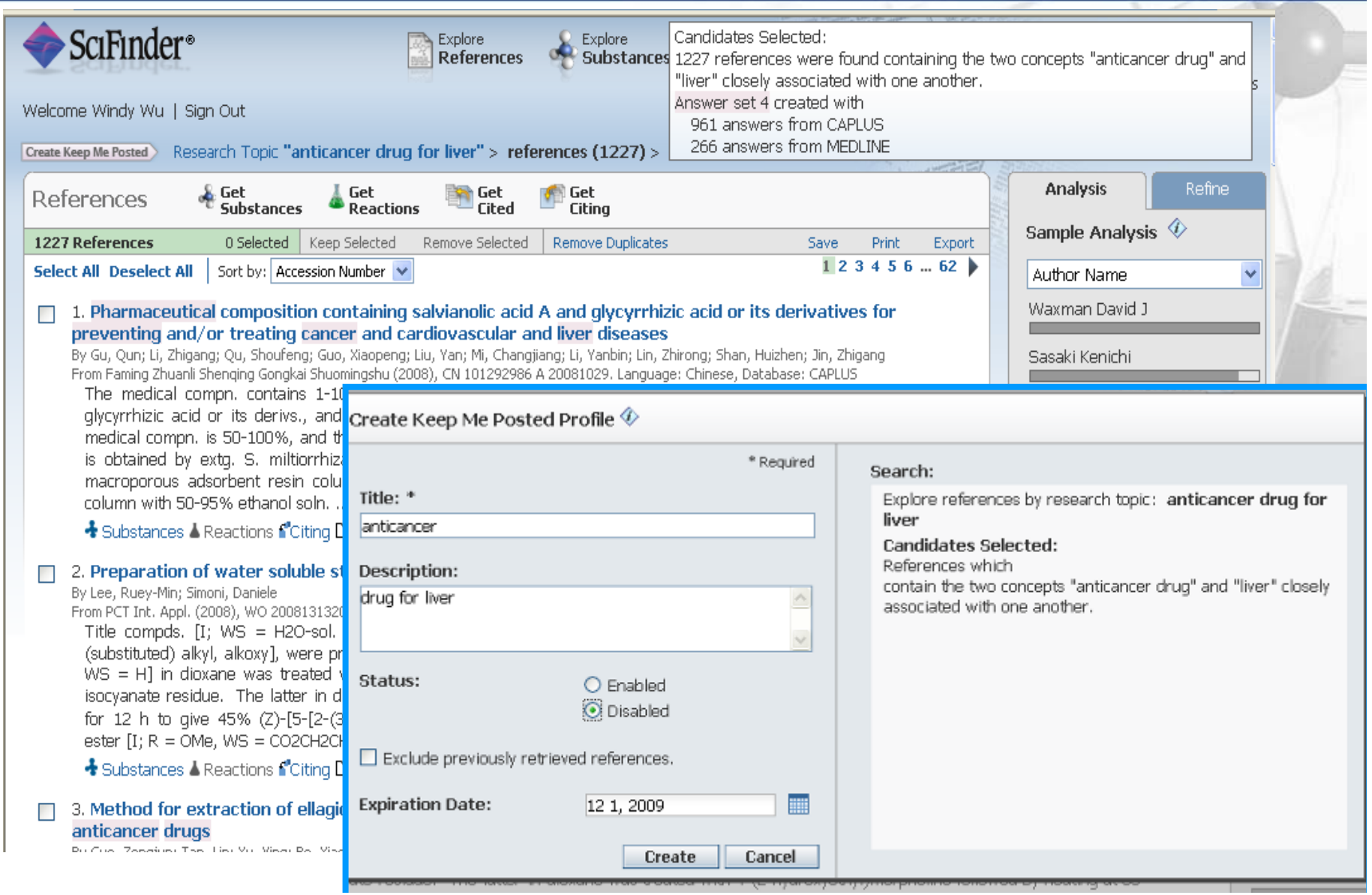
Refine the answer sets to particular interest



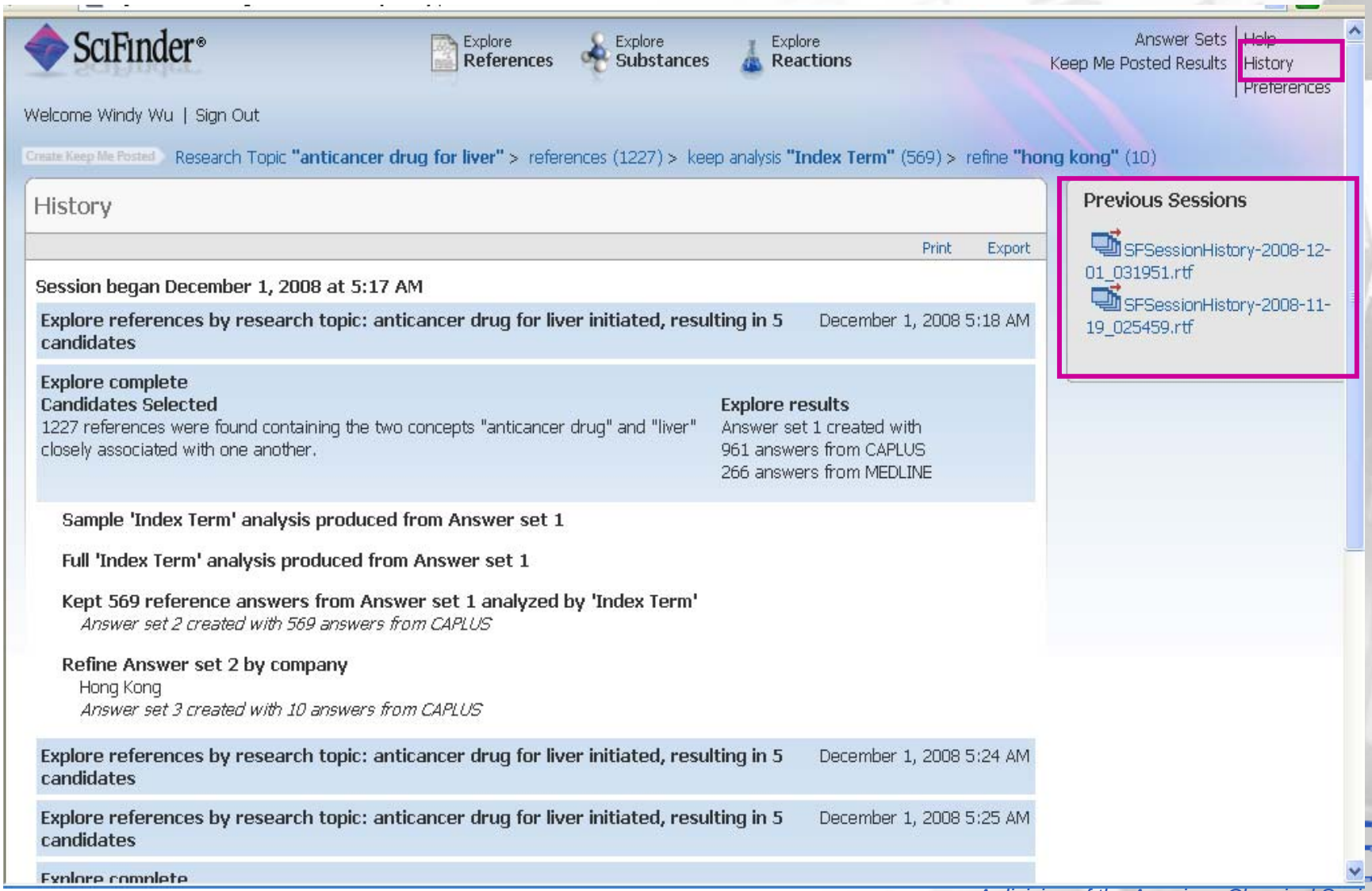
Combine answer sets for references, substances and reactions



Keep me posted for references



Download up to 10 previous history sessions



Structure search

www.cas.org

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Structure Drawing Tools

Icon	Tool	Icon	Tool
	Pencil (default selection)		Eraser
	Atom Menu		Shortcut Menu
	Chain		Template
	Selection		Lasso
	Rotation		Flip Structure
	Positive Charge		Negative Charge

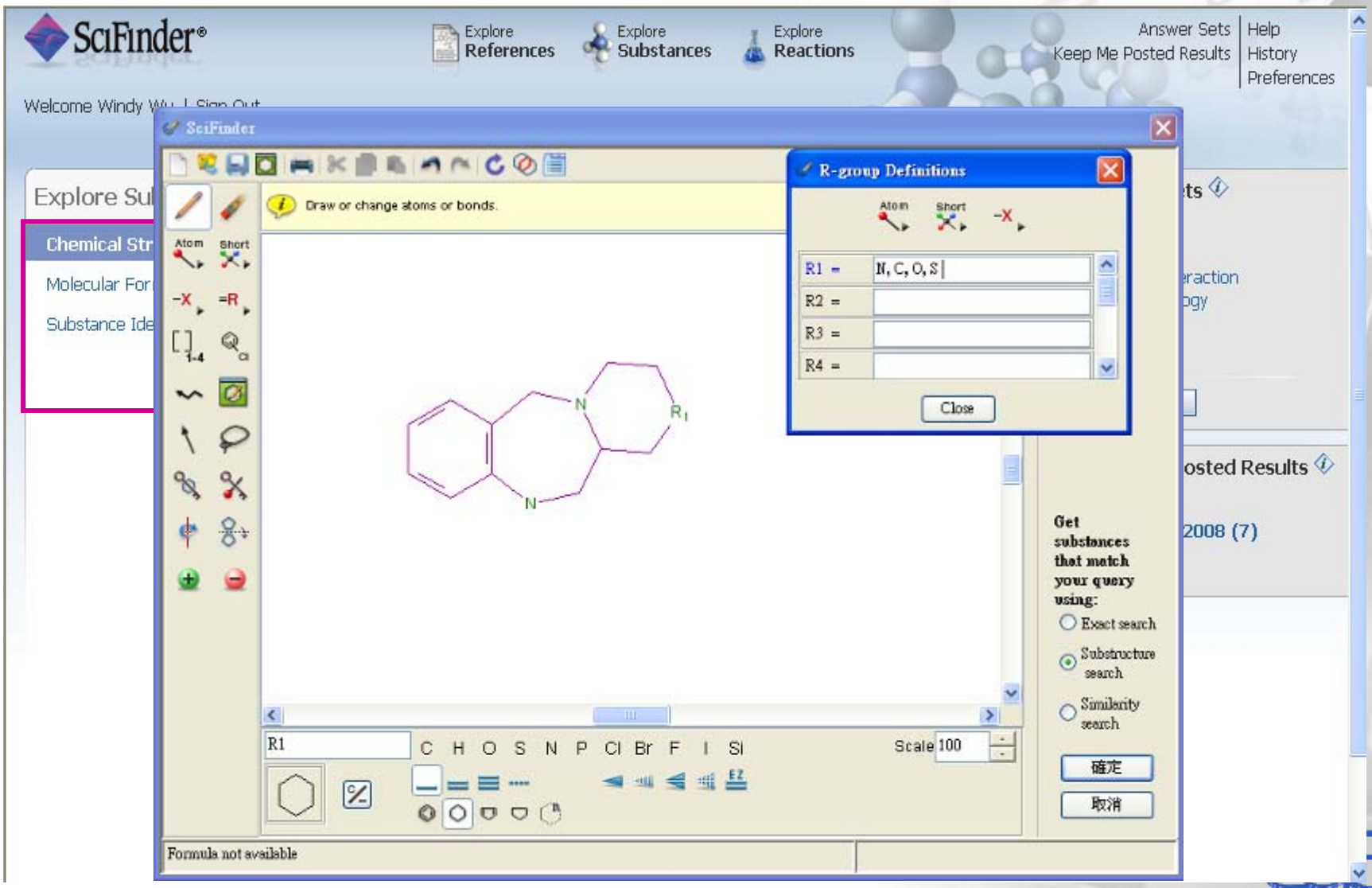
Structure searching with SSM – If you have the SciFinder Substructure Module (SSM), six additional drawing tools are available.

Icon	Tools	Icon	Tools
	Variables (X Menu)		R-group
	Repeating Group		Variable Attachment Position
	Lock Rings		Lock Atoms

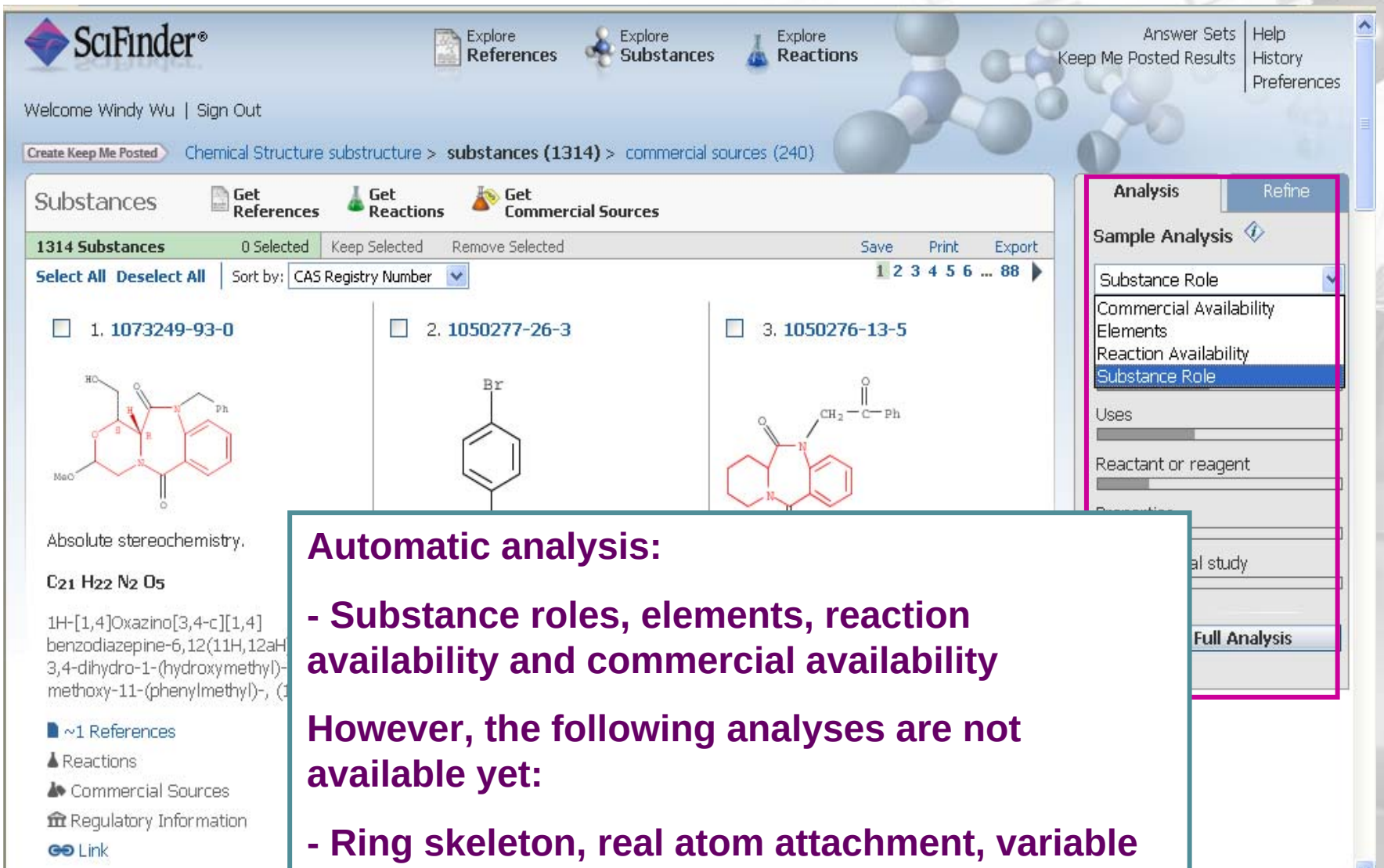
Reaction searching – If you are performing a Reaction search, five additional reaction-specific tools are available.

Icon	Tools	Icon	Tools
	Reaction Arrow		Reaction Role
	Atom Mapping		Reaction Site Marking
	Functional Group		

Structure search java plug-in



Structure search result



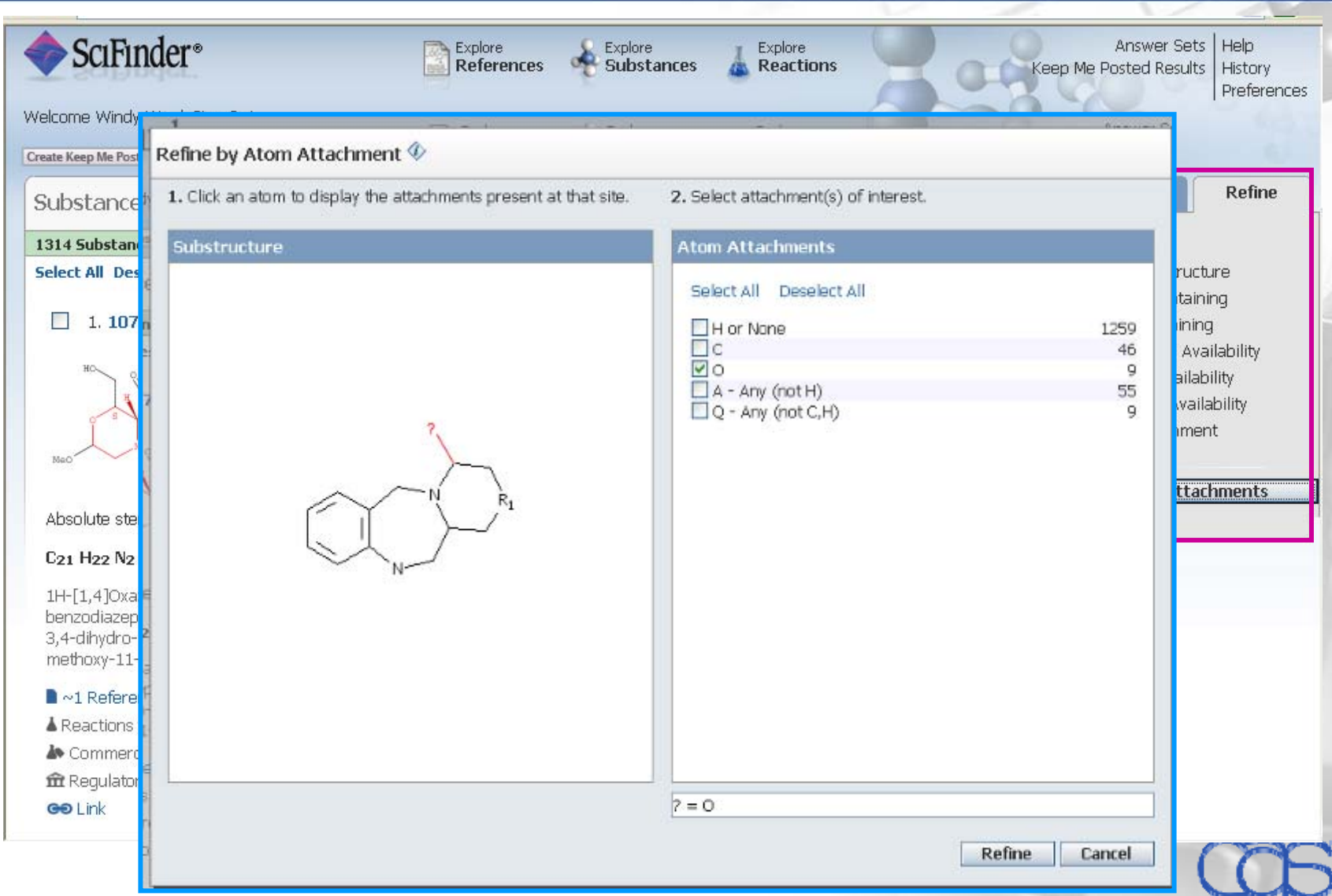
Automatic analysis:

- Substance roles, elements, reaction availability and commercial availability

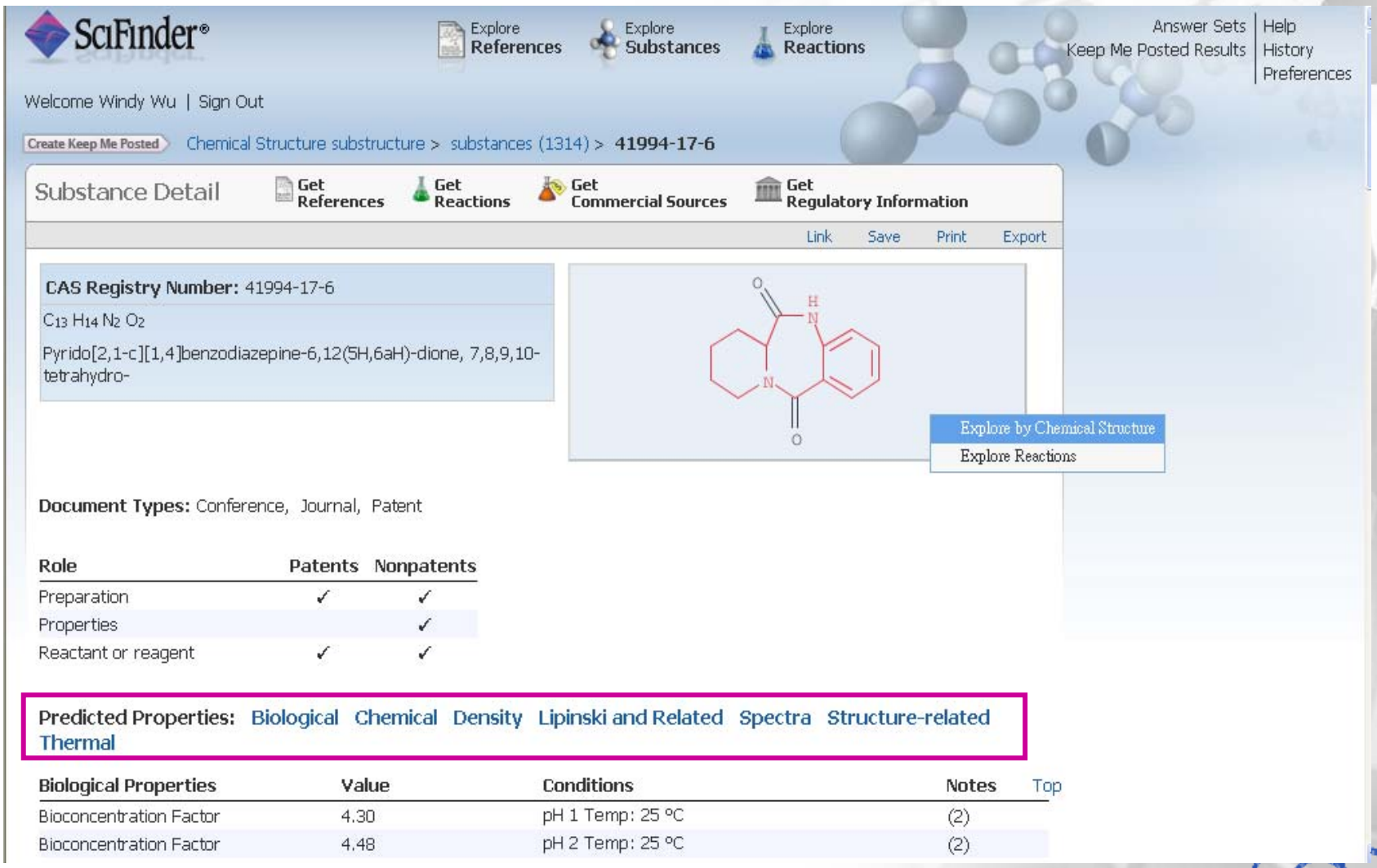
However, the following analyses are not available yet:

- Ring skeleton, real atom attachment, variable group and R-Group

Refine structure results by atom attachment



A substance record (1)



A substance record (2)

H Donors	1		(2)
H Donor/Acceptor Sum	5		(2)
logP	1.162±0.409	Temp: 25 °C	(2)
Molecular Weight	230.26		(2)

Spectra Properties	Value	Conditions	Notes	Top
Proton NMR Spectrum	See spectrum		(3)	

Structure-related Properties

Polar Surface Area

Thermal Properties

Boiling Point

Enthalpy of Vaporization

Flash Point

(2) Calculated using Advanced C
(3) Predicted NMR data calculat
ACD/Labs)

Experimental Properties:

Spectra Properties

Carbon-13 NMR Spectrum

IR Absorption Spectrum

Mass Spectrum

Proton NMR Spectrum

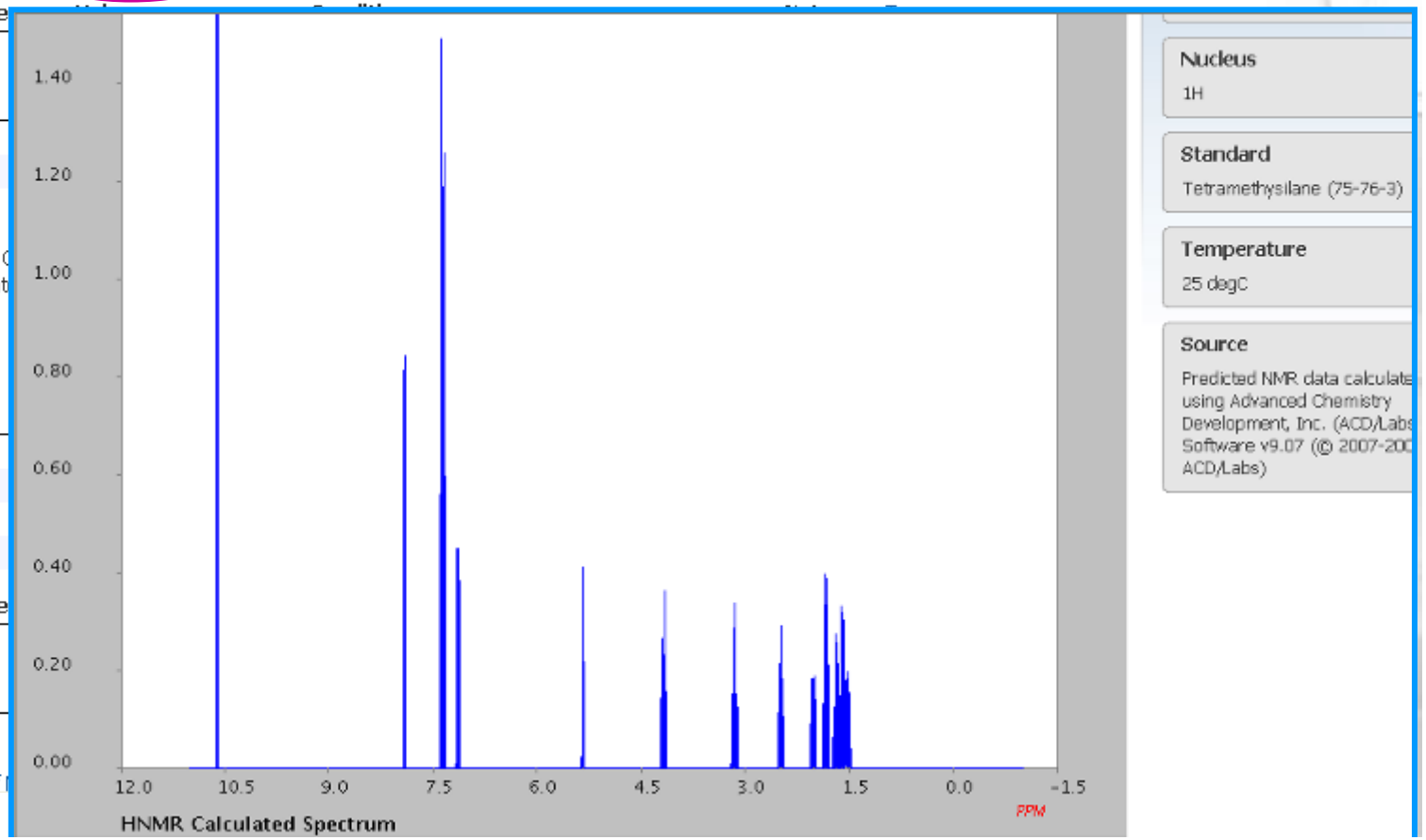
Structure-related Properties

Crystal Structure

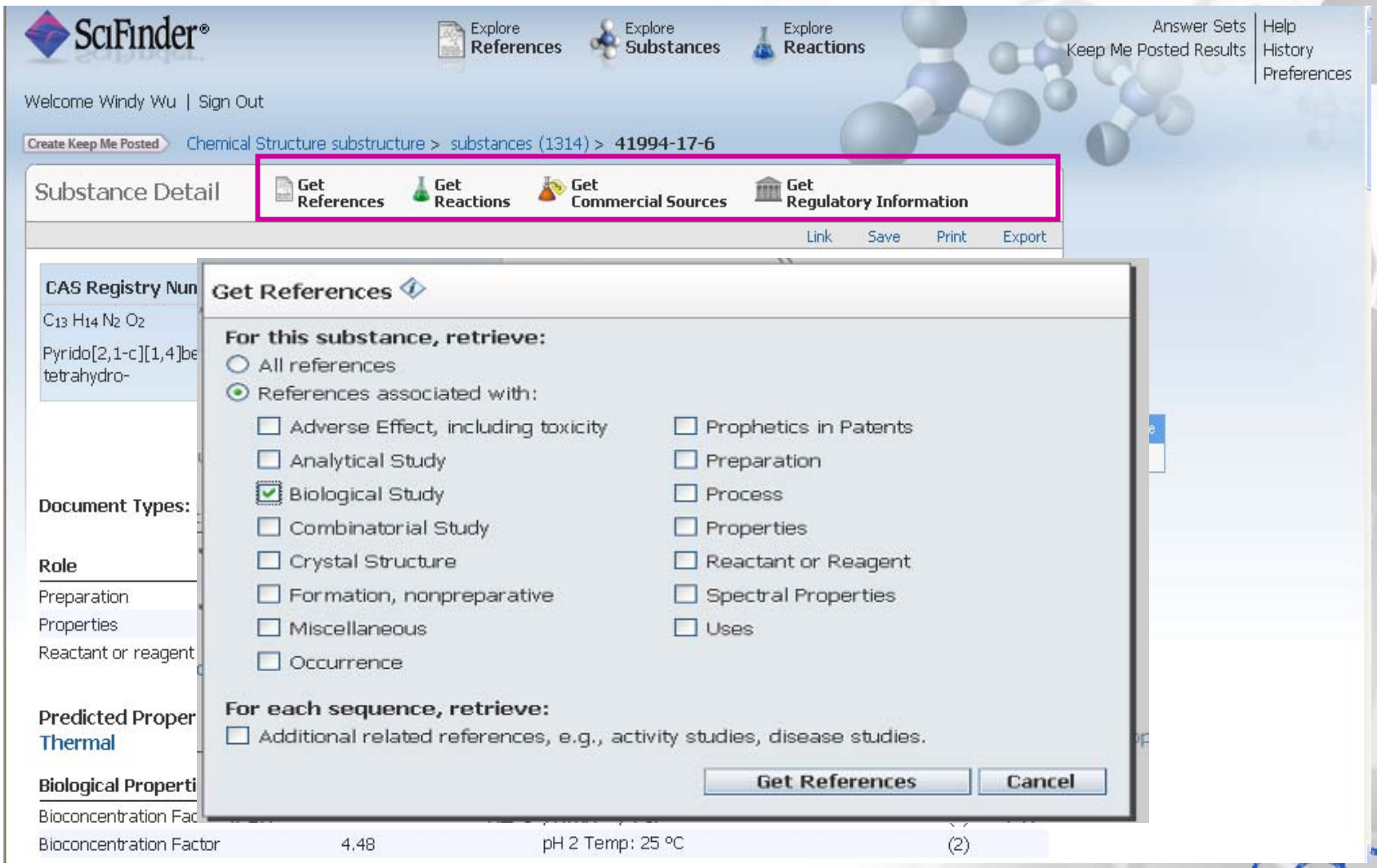
Thermal Properties

Melting Point

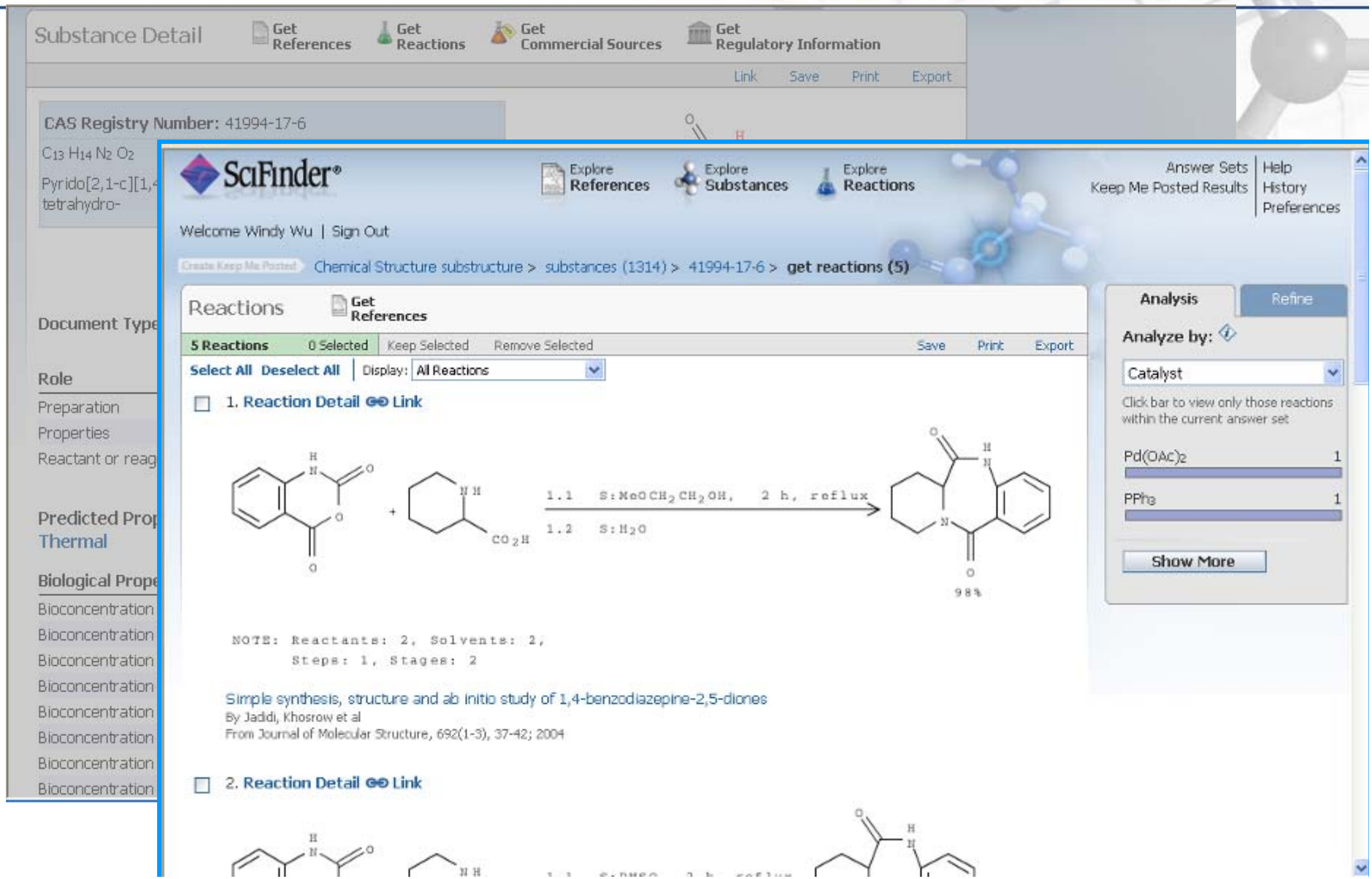
(1) Jadidi, Khosrow; Journal of



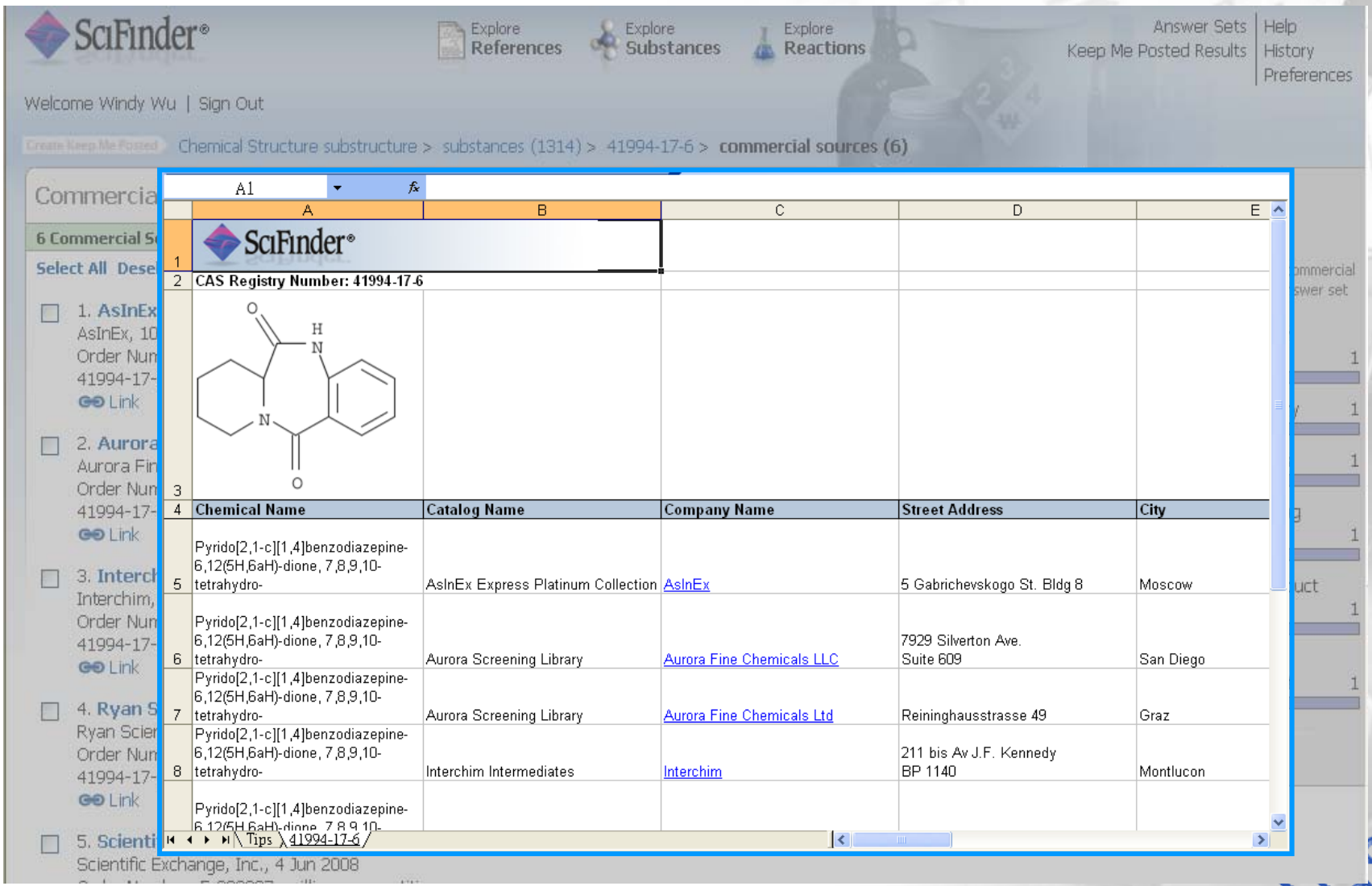
Get interest references for substance



Get reaction information with detailed condition



Export supplier information to excel table



Structure search (New Enhancements)

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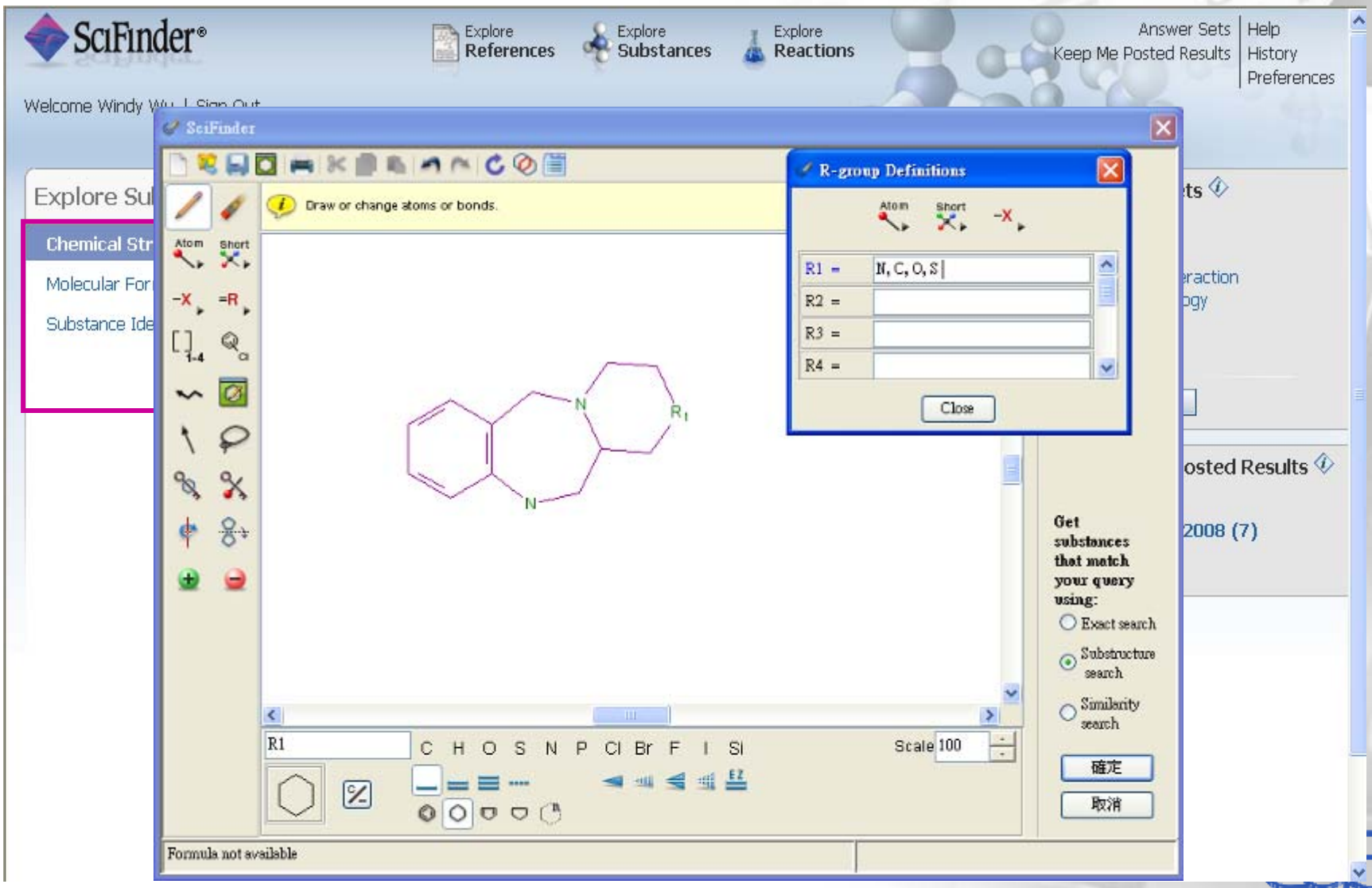
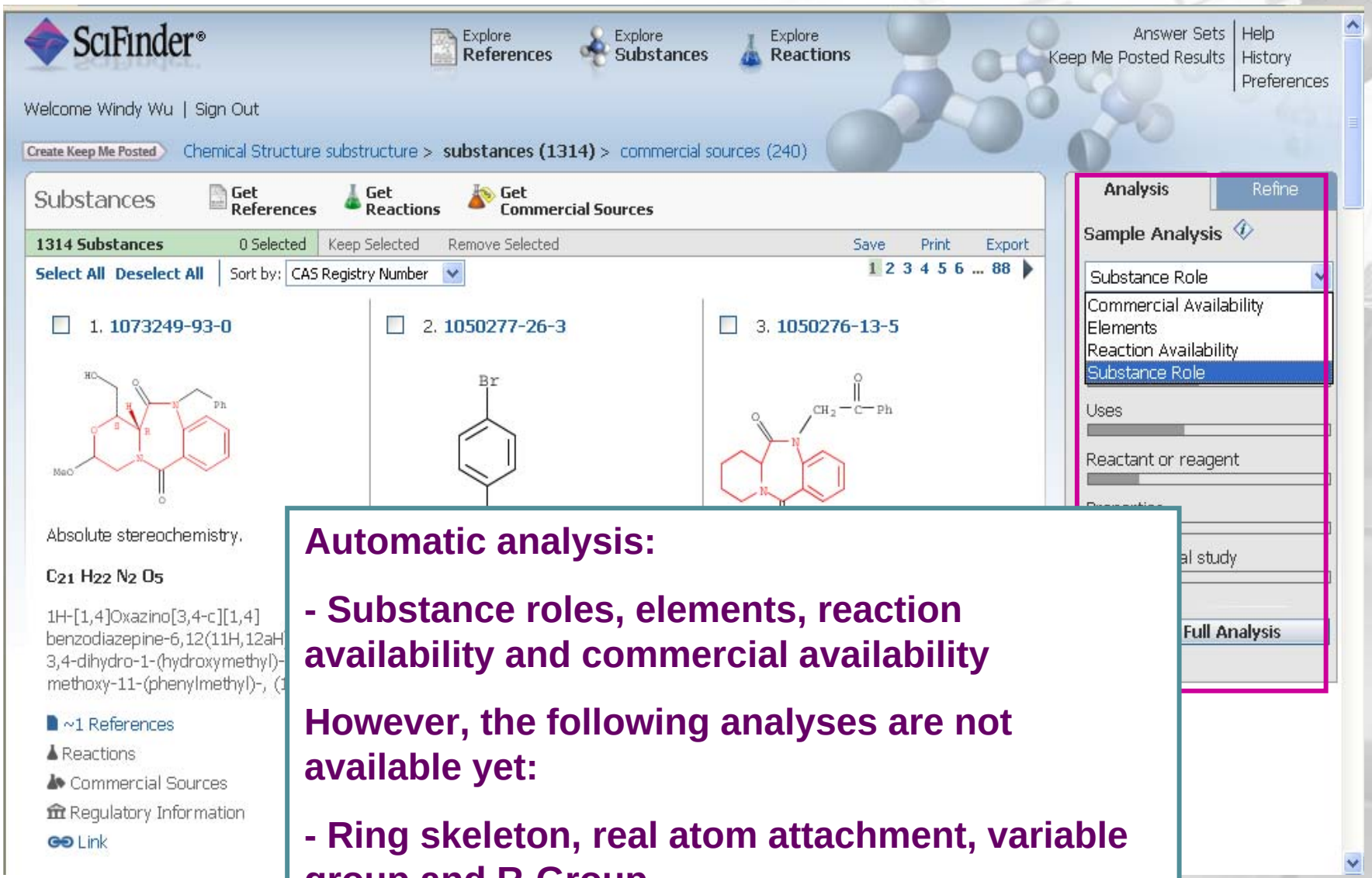
Structure search java plug-in



Structure search result



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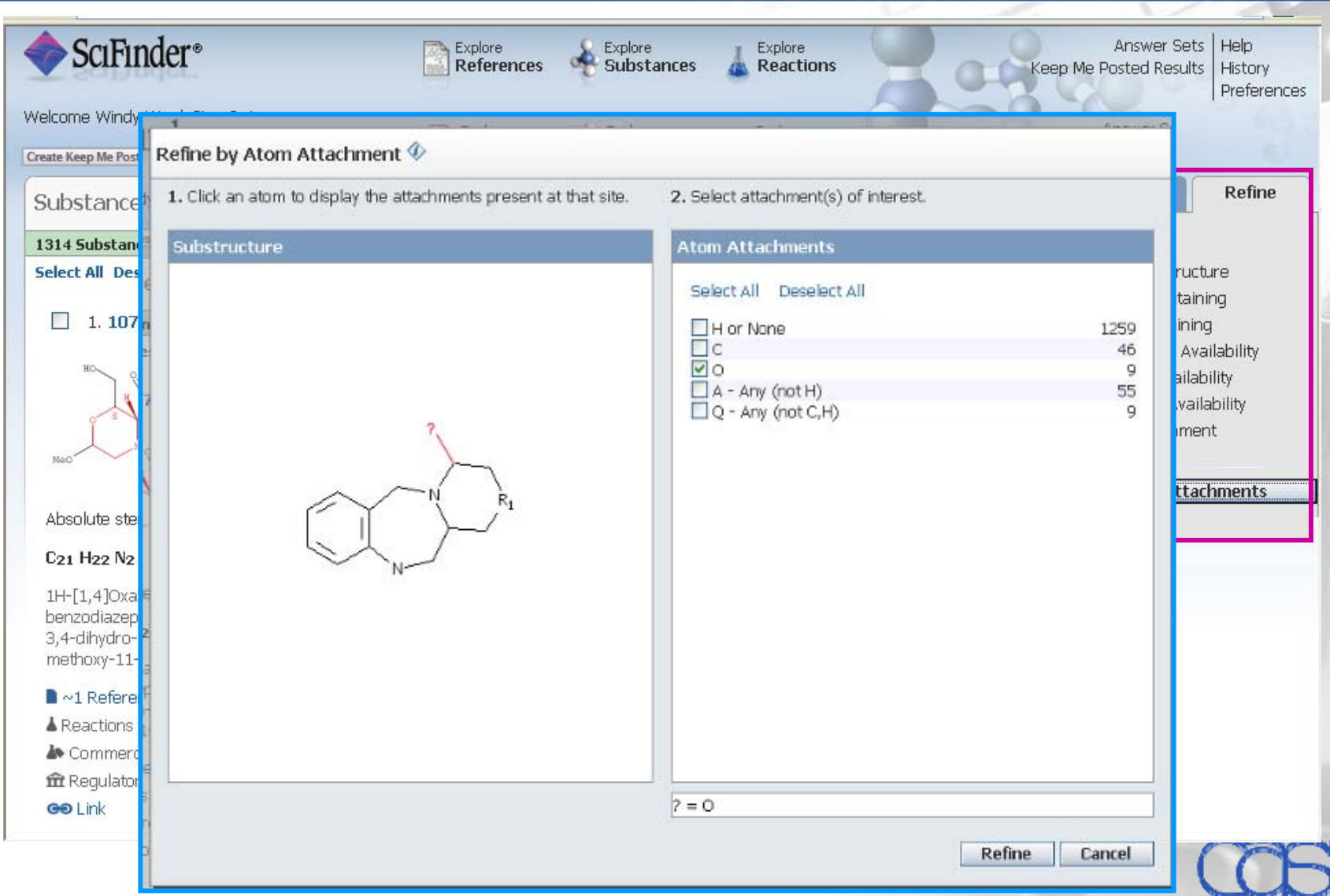

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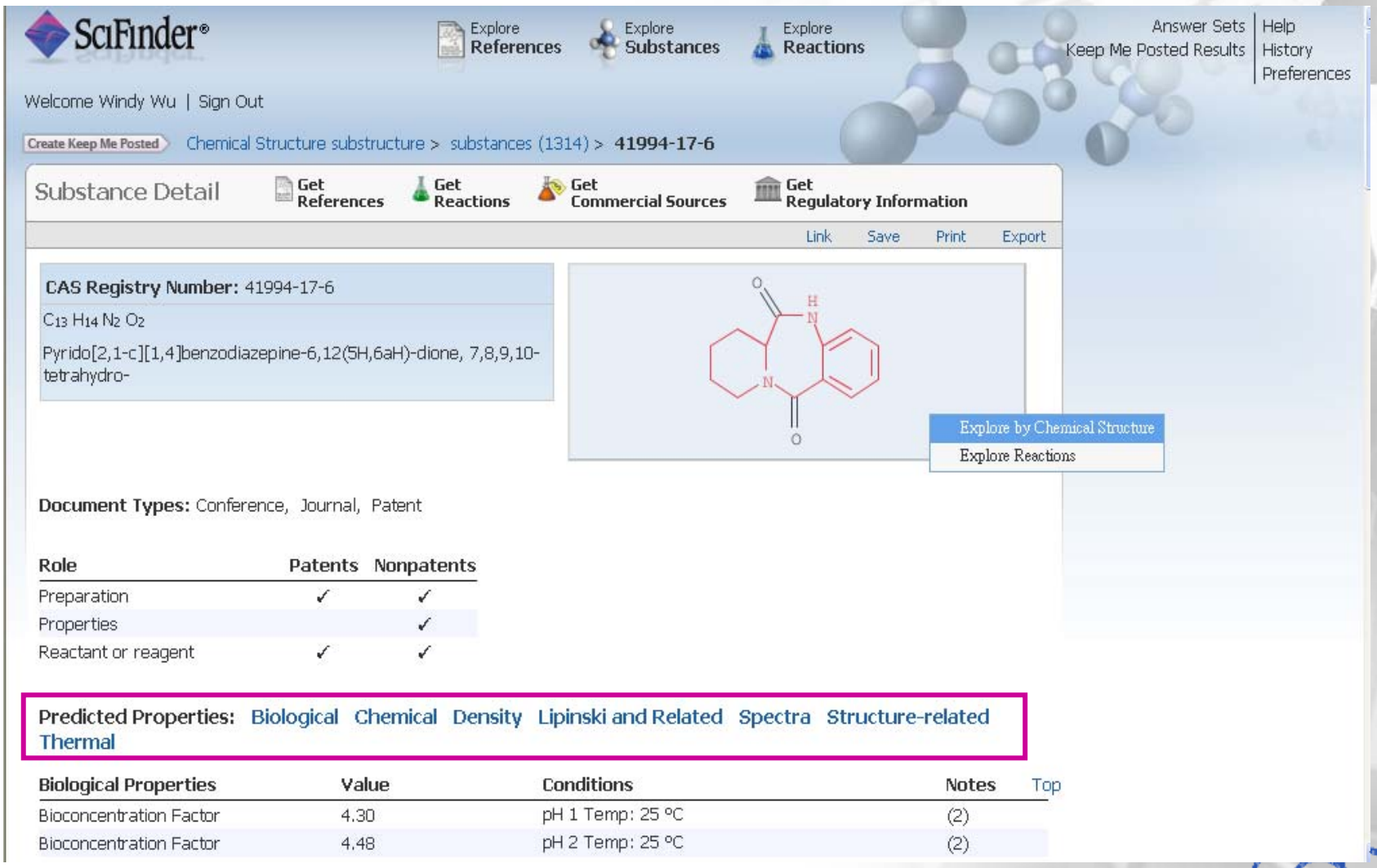

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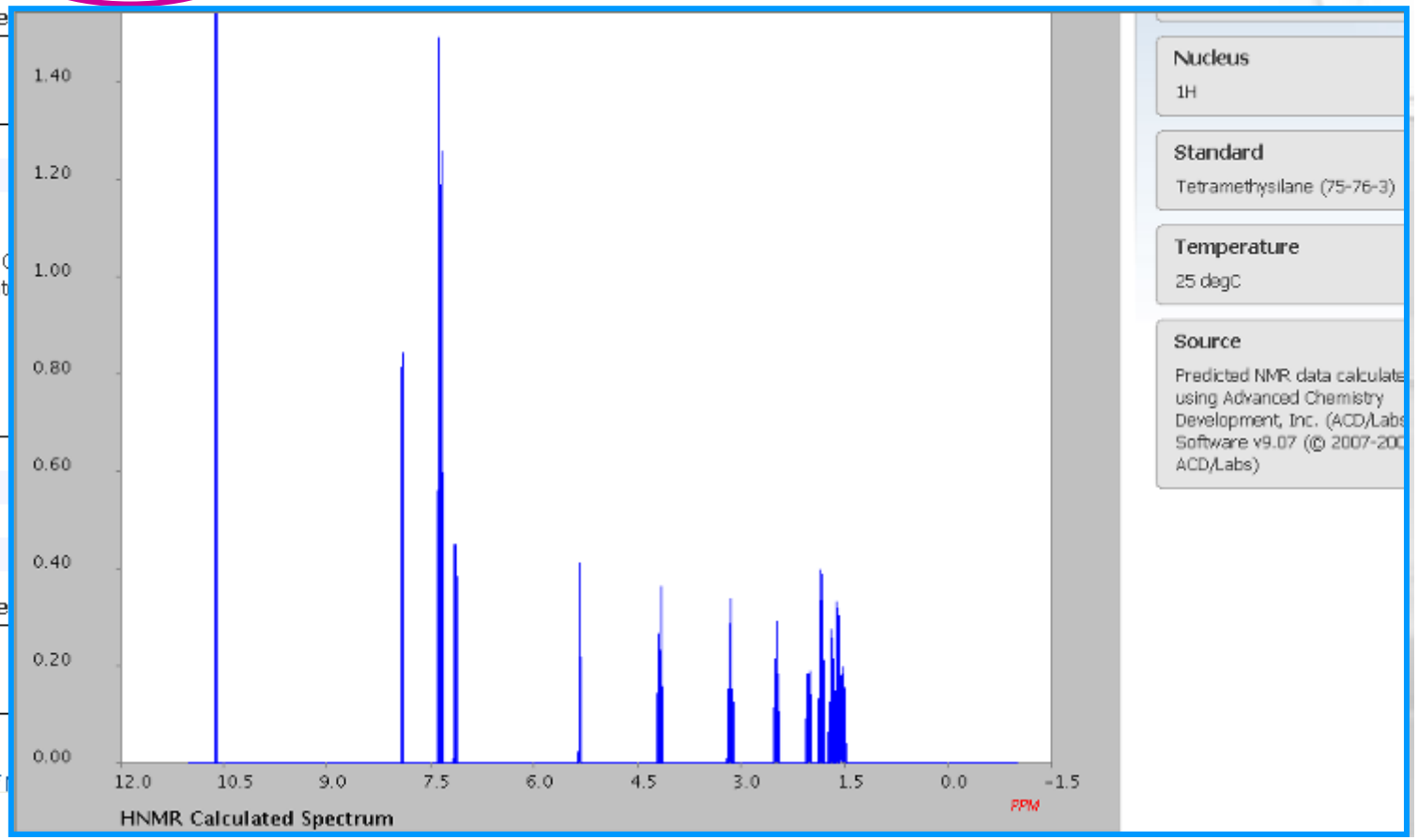
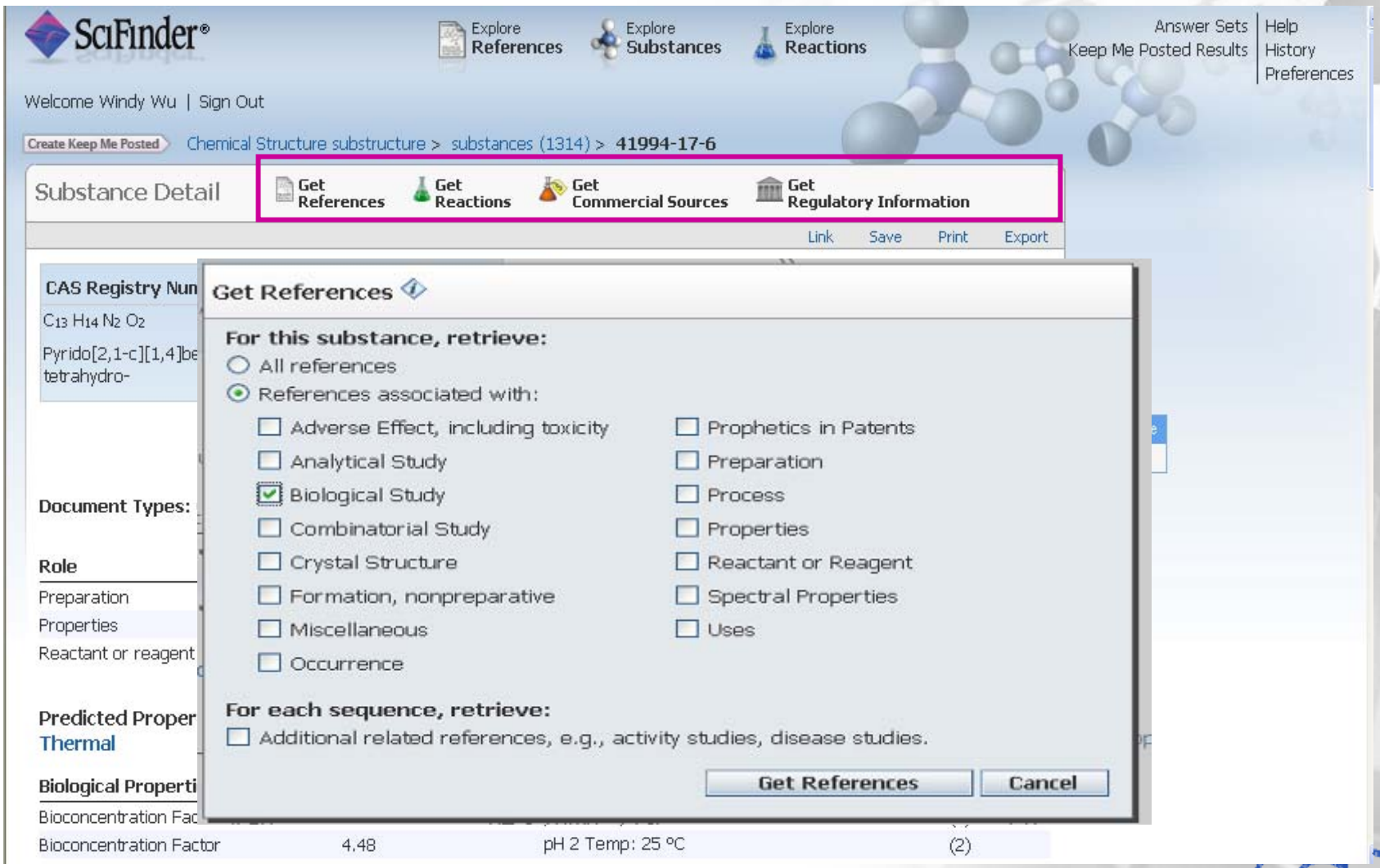
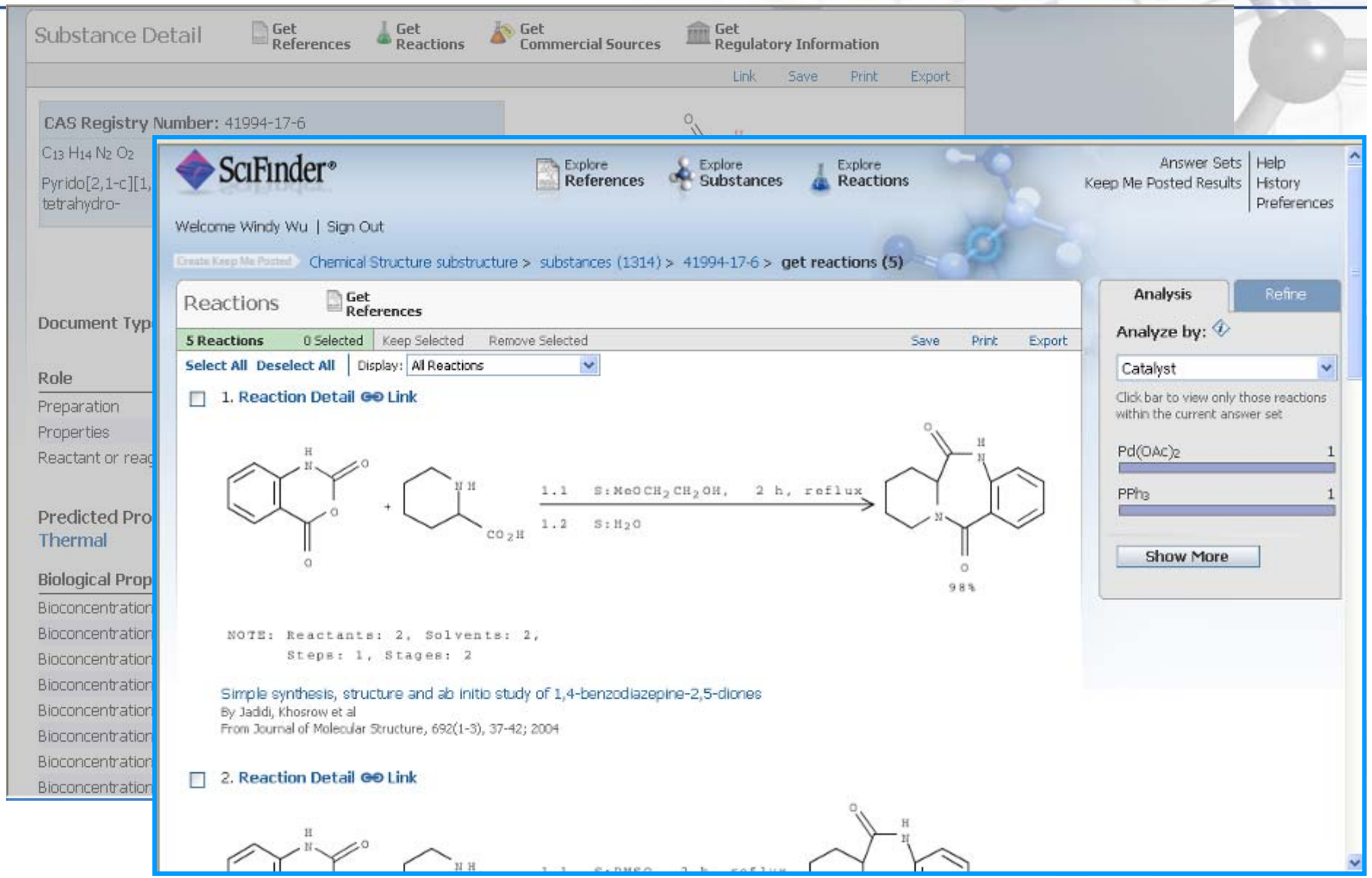


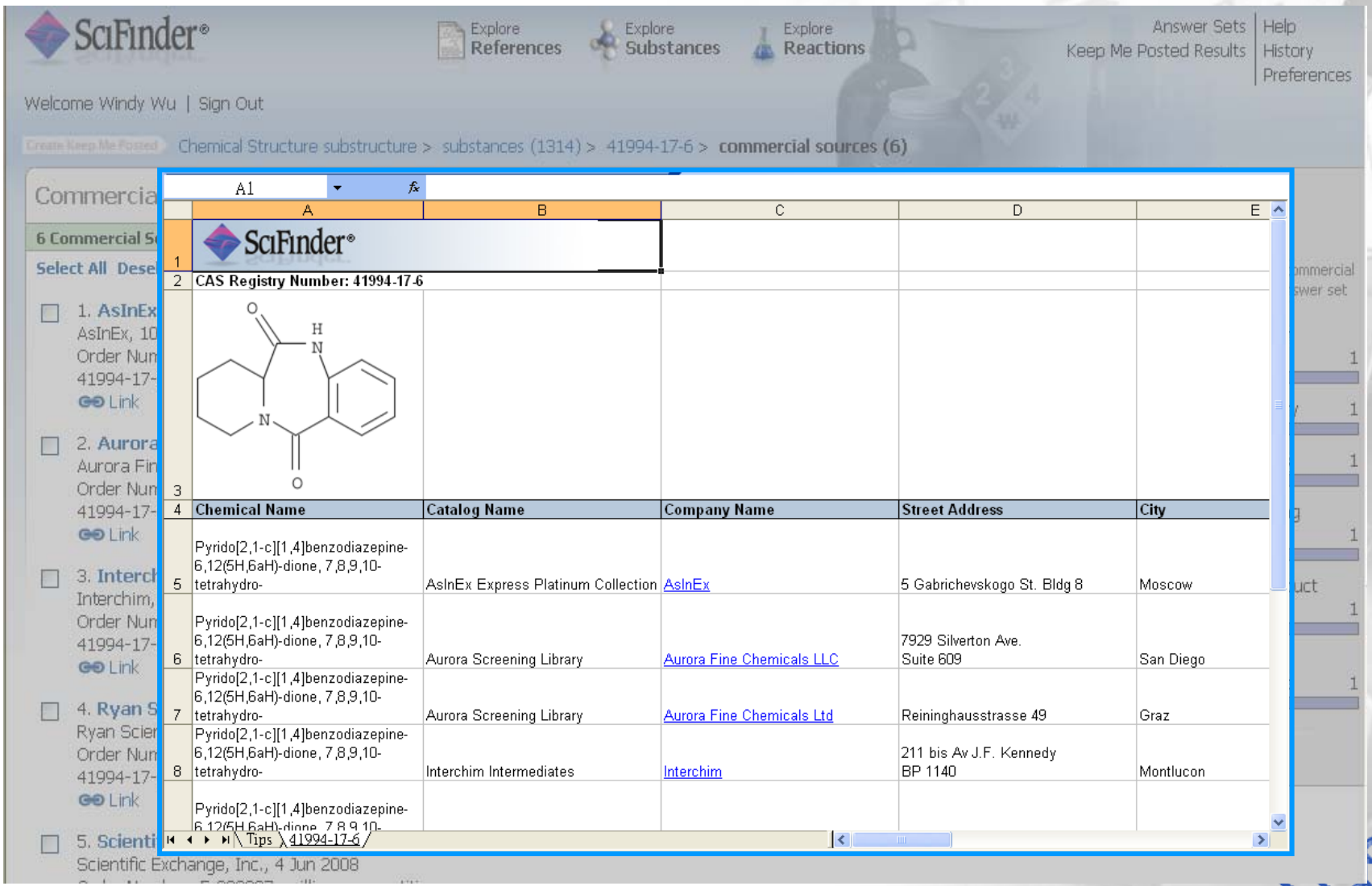
Get interest references for substance



Get reaction information with detailed condition



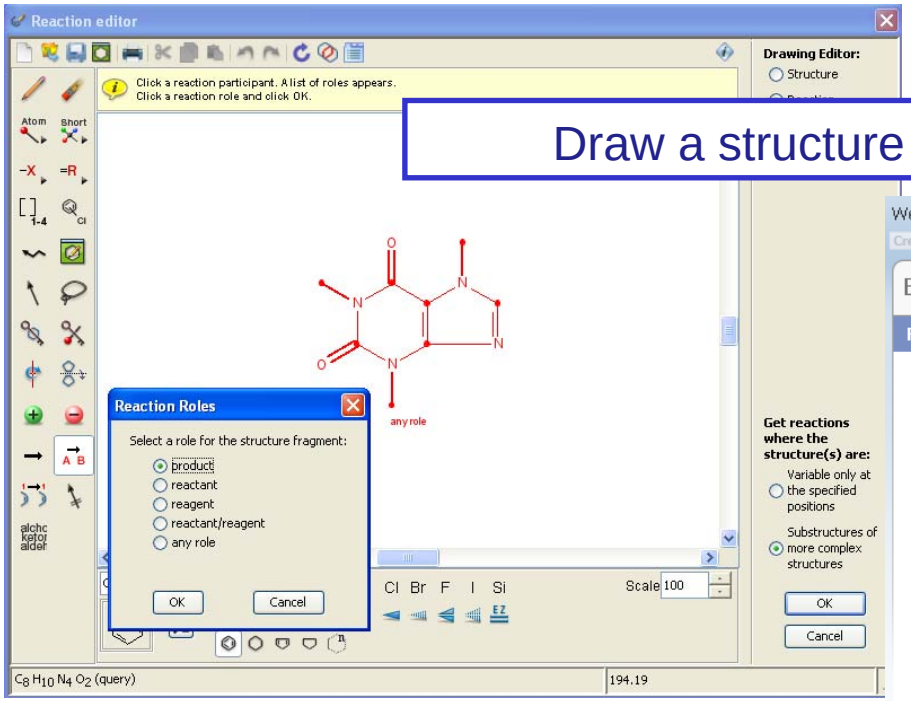
Export supplier information to excel table



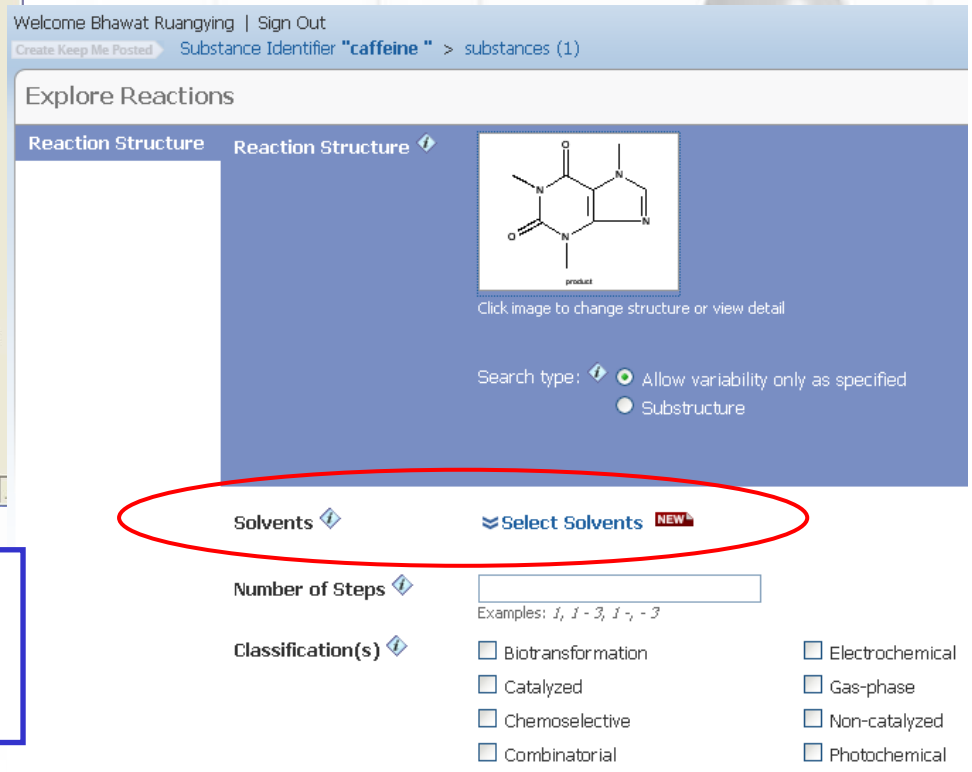
Summary of Scifinder Web

- Provide quick access and user friendly interface to search for scientific information
- New features that are tailor made for the needs of researchers
- Enhanced content for properties, spectra, registration, reaction information and etc
- Personalization features (keep me posted and save as)

Explore Reaction (Ex. Caffeine : Step 1)



Draw a structure or Search by common name

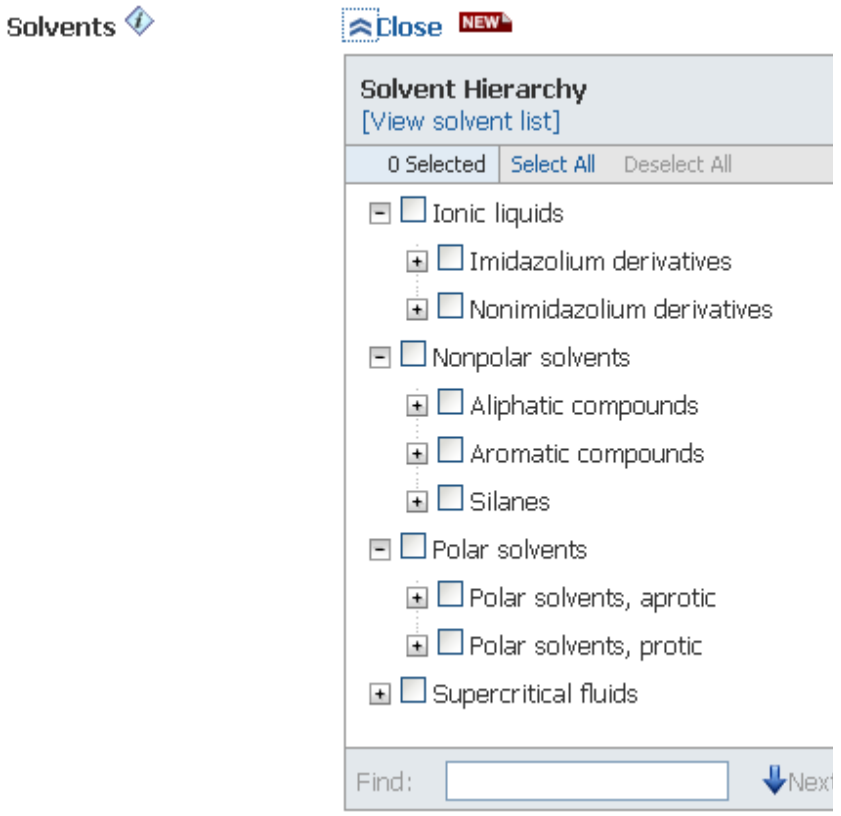


1. Draw a structure or Search by common name : Caffeine
2. Select Solvent list

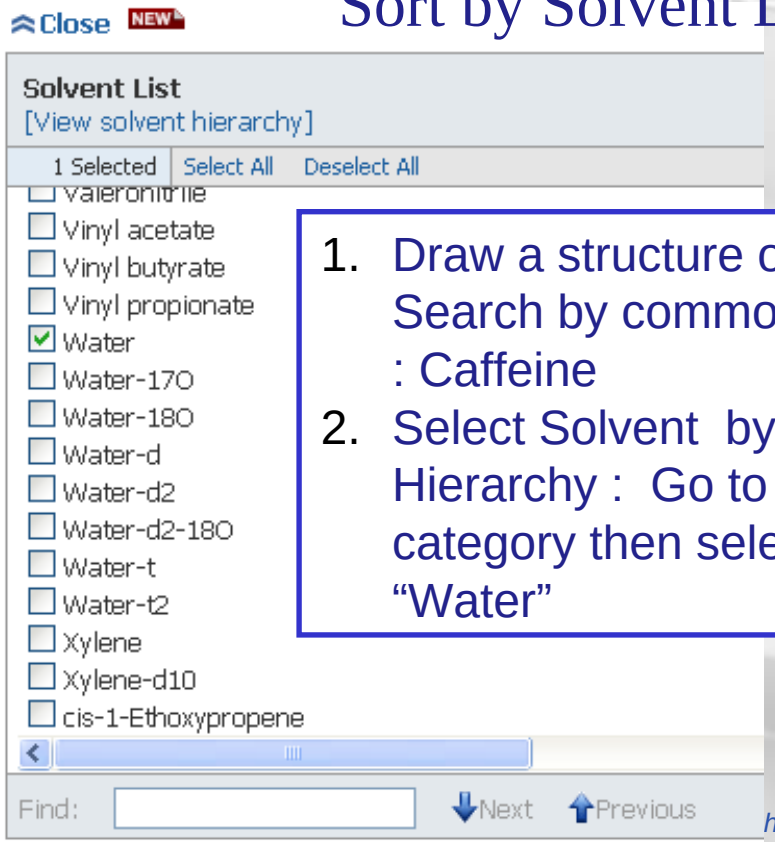
Select Solvent Limiter (Step 2)

Focus your reaction results by specifying one or more solvents.

Sort by Solvent Hierarchy



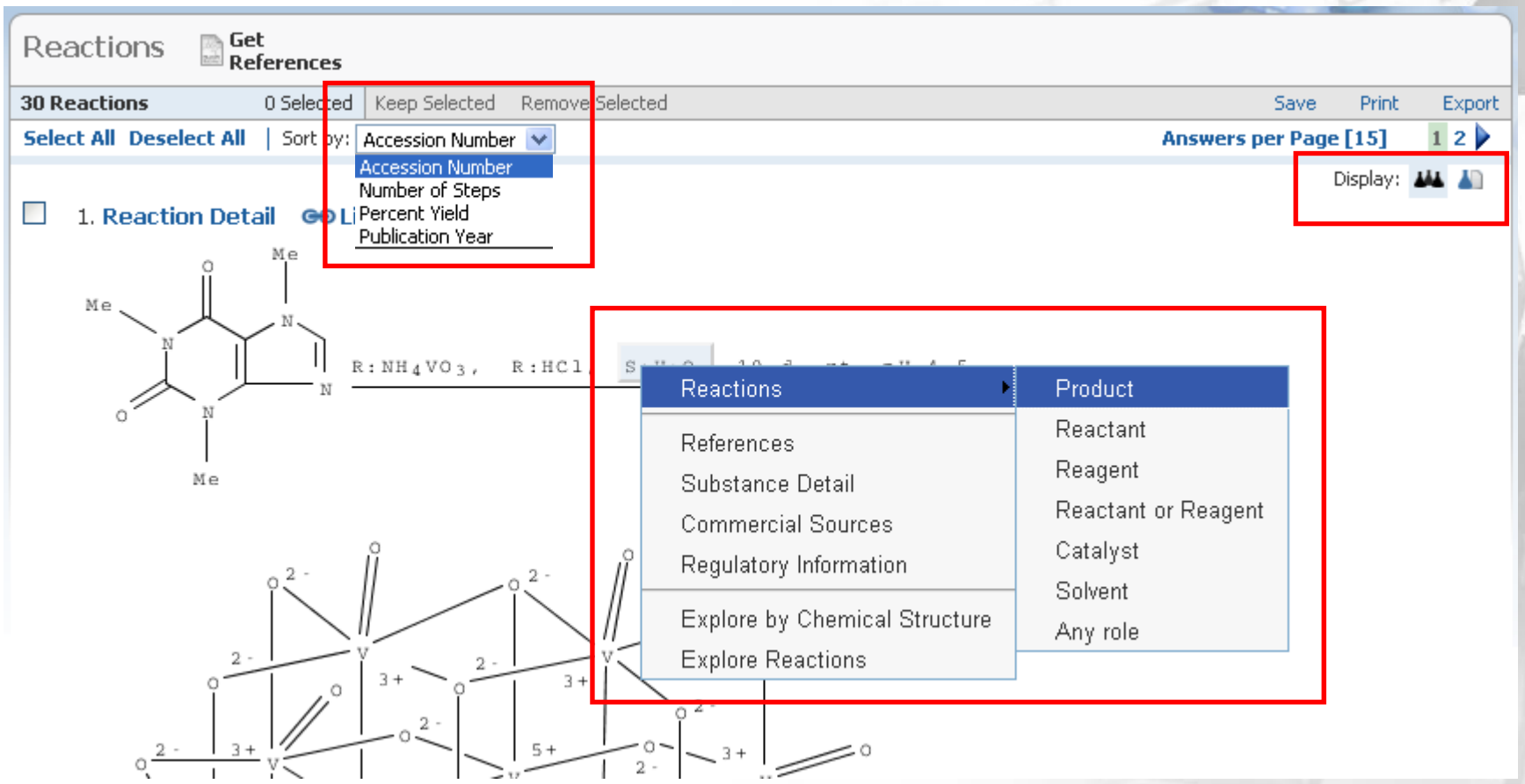
Sort by Solvent List



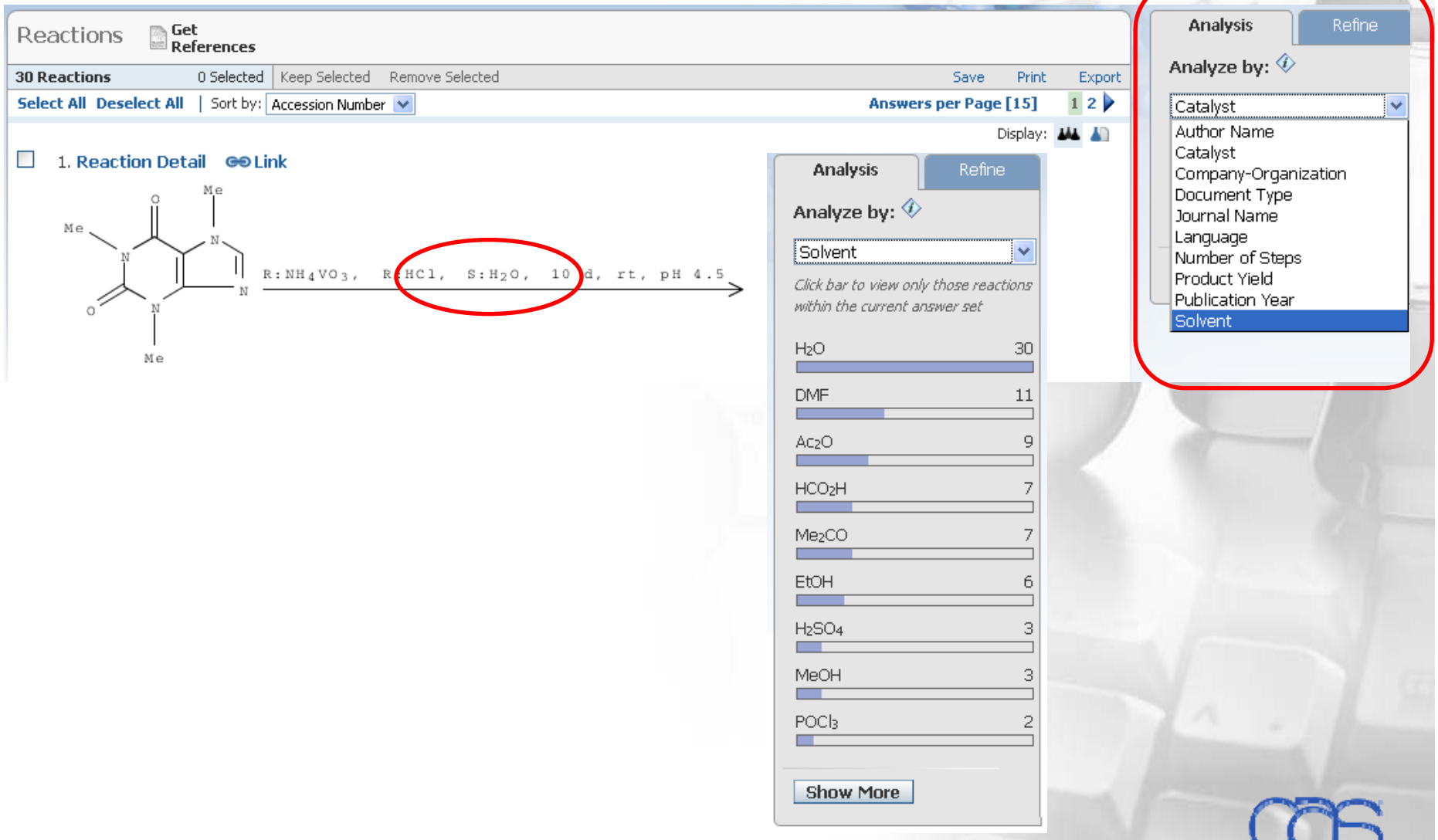
1. Draw a structure or Search by common name : Caffeine
2. Select Solvent by Solvent Hierarchy : Go to SCF category then select "Water"

hemical Society

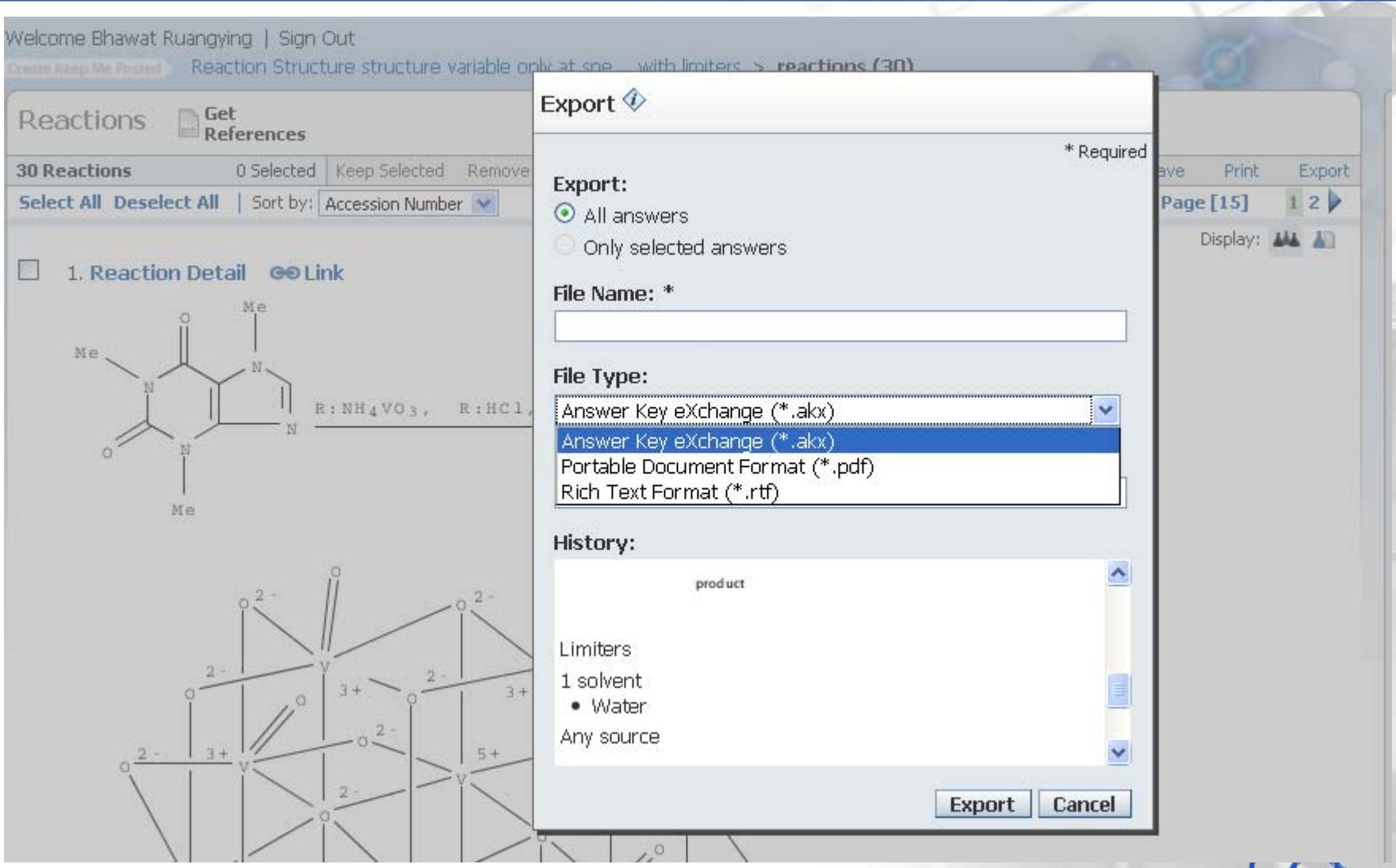
Reaction Answer Set Sort/ Solvent Exploring (Step 3)



Analyze by Solvent (Step 4)

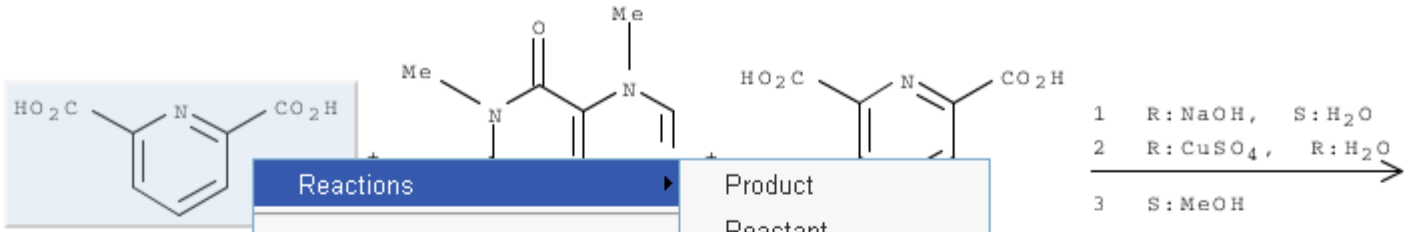


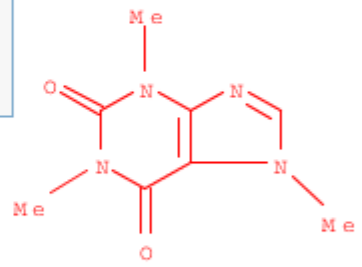
Export Feature (Step 5)



Quick Search from reaction result set (Step 6)

3. **Reaction Detail** Link





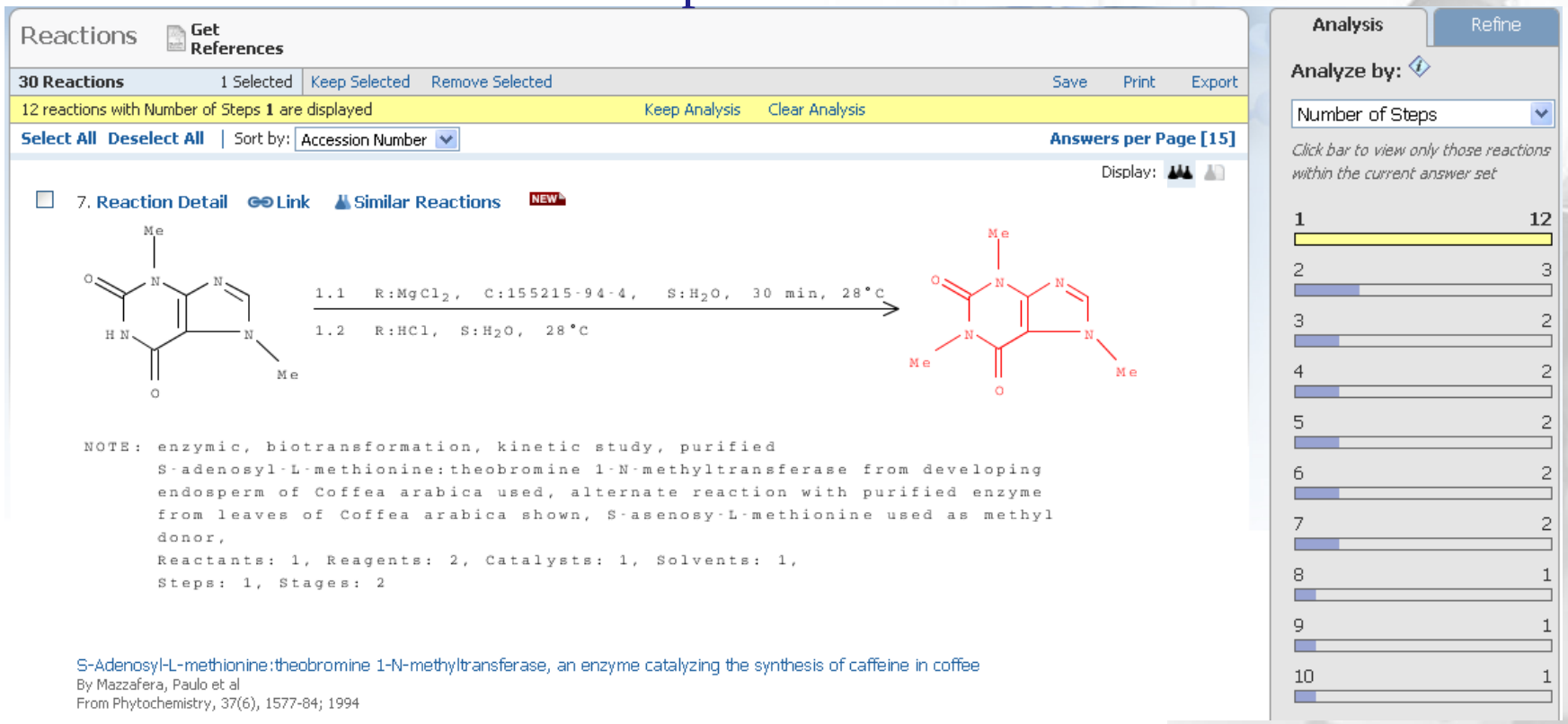
copper pyridinedicarboxylato complex

NOTE: Reactants: 2, Reagents: 4, Solvents: 2,
Steps: 3, Stages: 3

Copper(II) pyridine-2,6-dicarboxylates. Coordination and distortion isomers of [Cu(pydca)(H2O)2]
By Koman, M. et al
From Polish Journal of Chemistry, 75(7), 957-964; 2001

Get Similar Reactions (Step 7.1)

Find reactions that undergo similar transformations for all single step reactions

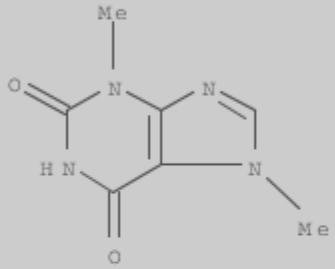


A division of the American Chemical Society

Get Similar Reactions (Step 7.2)

Thiocyanatochromium(III) complexes with urotropine
By Ganescu, I. et al
From Analele Stiintifice ale Universitatii "Al. I. C

7. Reaction Detail Link Sim



1.1
1.2

NOTE: enzymic, biotransf
S-adenosyl-L-methi
endosperm of Coffe
from leaves of Cof
donor,
Reactants: 1, Reag
Steps: 1, Stages:

S-Adenosyl-L-methionine:theobromine 1-N-methyltransferase, an enzyme catalyzing the synthesis of caffeine in coffee
By Mazzafera, Paulo et al
From Phytochemistry, 37(6), 1577-84; 1994

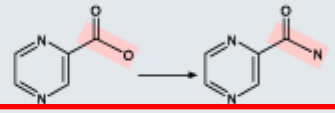
Get Similar Reactions

Retrieve similar reactions from:

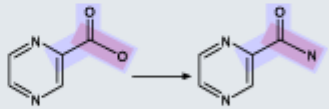
- (•) All reactions
- ( ) Current answer set

Include this level of similarity:

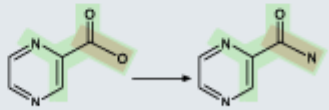
- (•) Broad - Reaction centers only (18793)



- ( ) Medium - Reaction centers plus adjacent atoms and bonds (1595)



- ( ) Narrow - Reaction centers plus extended atoms and bonds (76)



Get Reactions Cancel

Similarity Matches

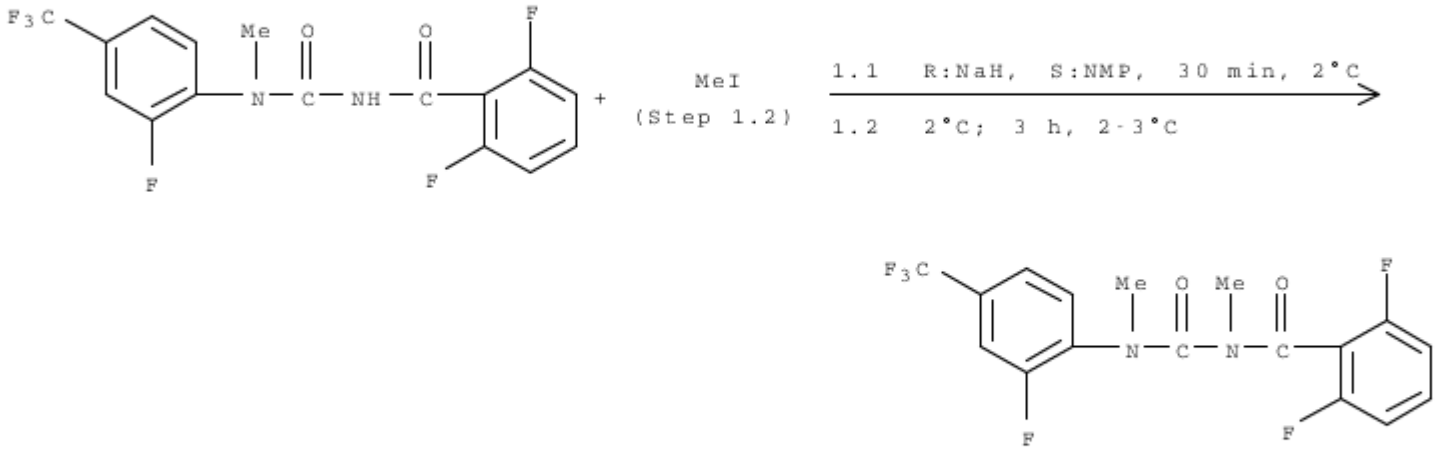
Reactions | Get References

1595 Reactions | 0 Selected | Keep Selected | Remove Selected | Save | Print | Export

Select All | Deselect All | Sort by: Similarity | Answers per Page [15] | 1 2 3 4 5 6 ... 107

Display:

1. Reaction Detail | Link | Similar Reactions NEW



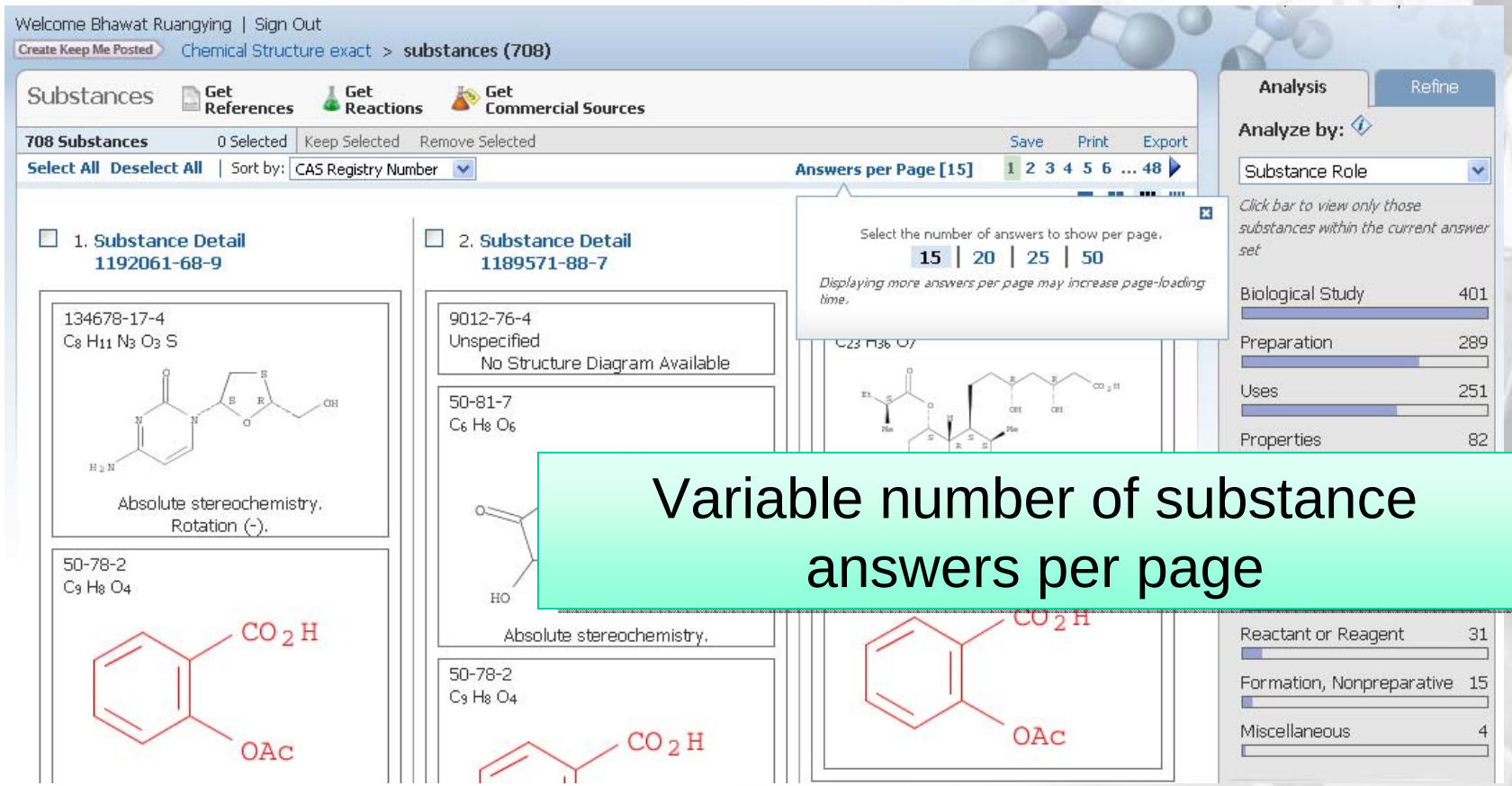
NOTE: Reactants: 2, Reagents: 1, Solvents: 1,
Steps: 1, Stages: 2

Novel use of (n'-methyl)benzoylurea compound for preventing a plant from damage by insect pest after germination

By Sakamoto, Norihisa and Konobe, Masato

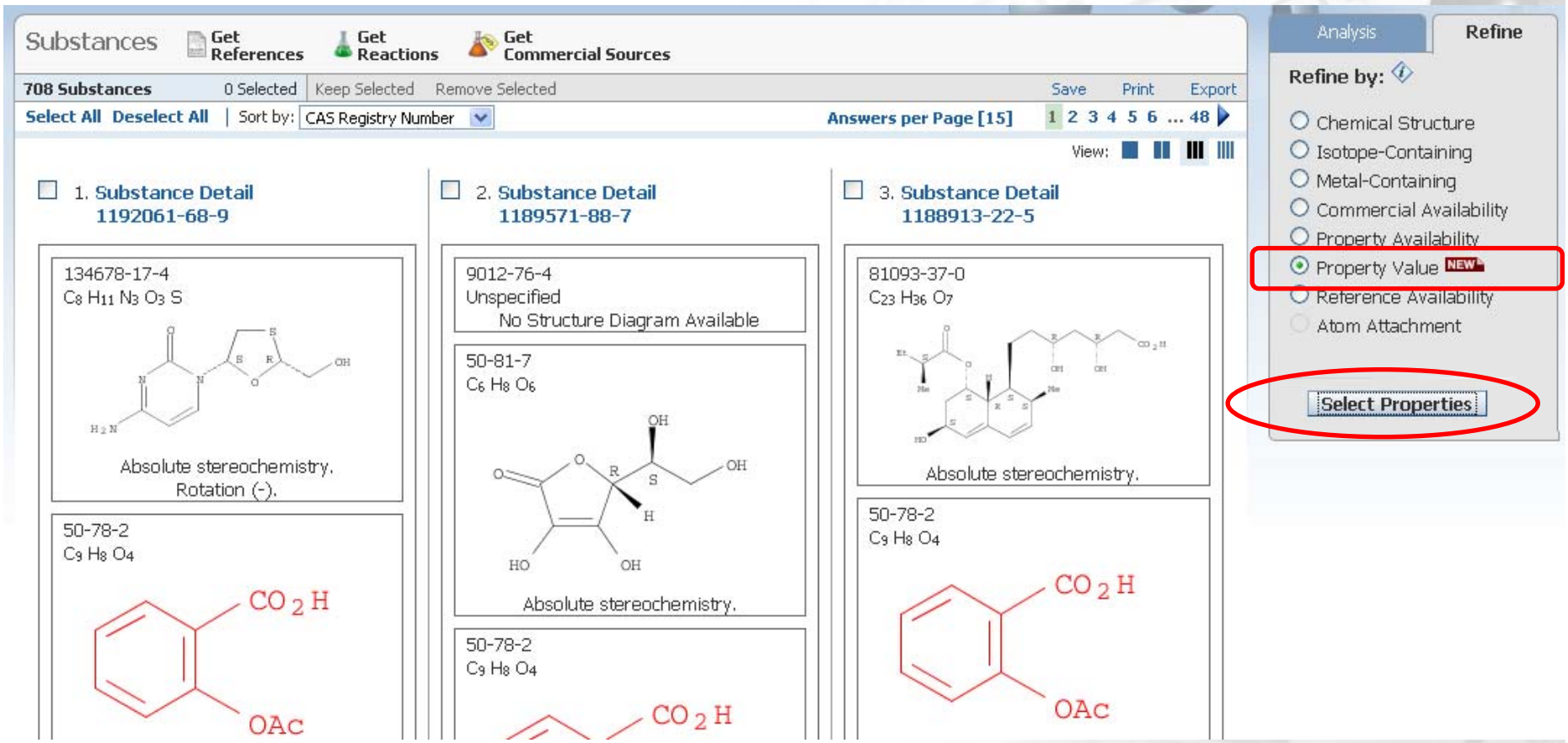
From U.S. Pat. Appl. Publ., 2008274884, 06 Nov 2008

Explore Substance (Ex. Aspirin, Step 1)

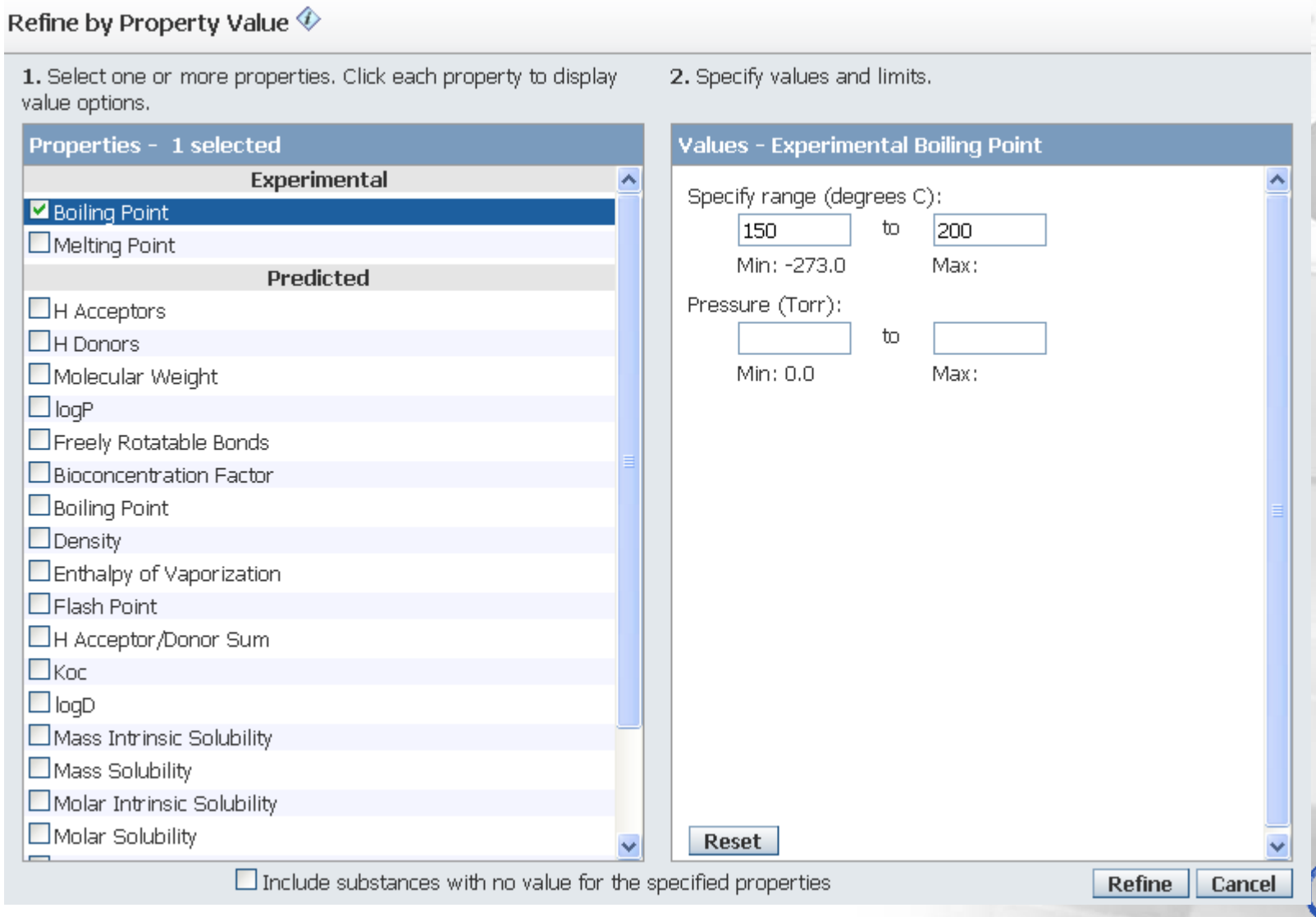


Variable number of substance answers per page

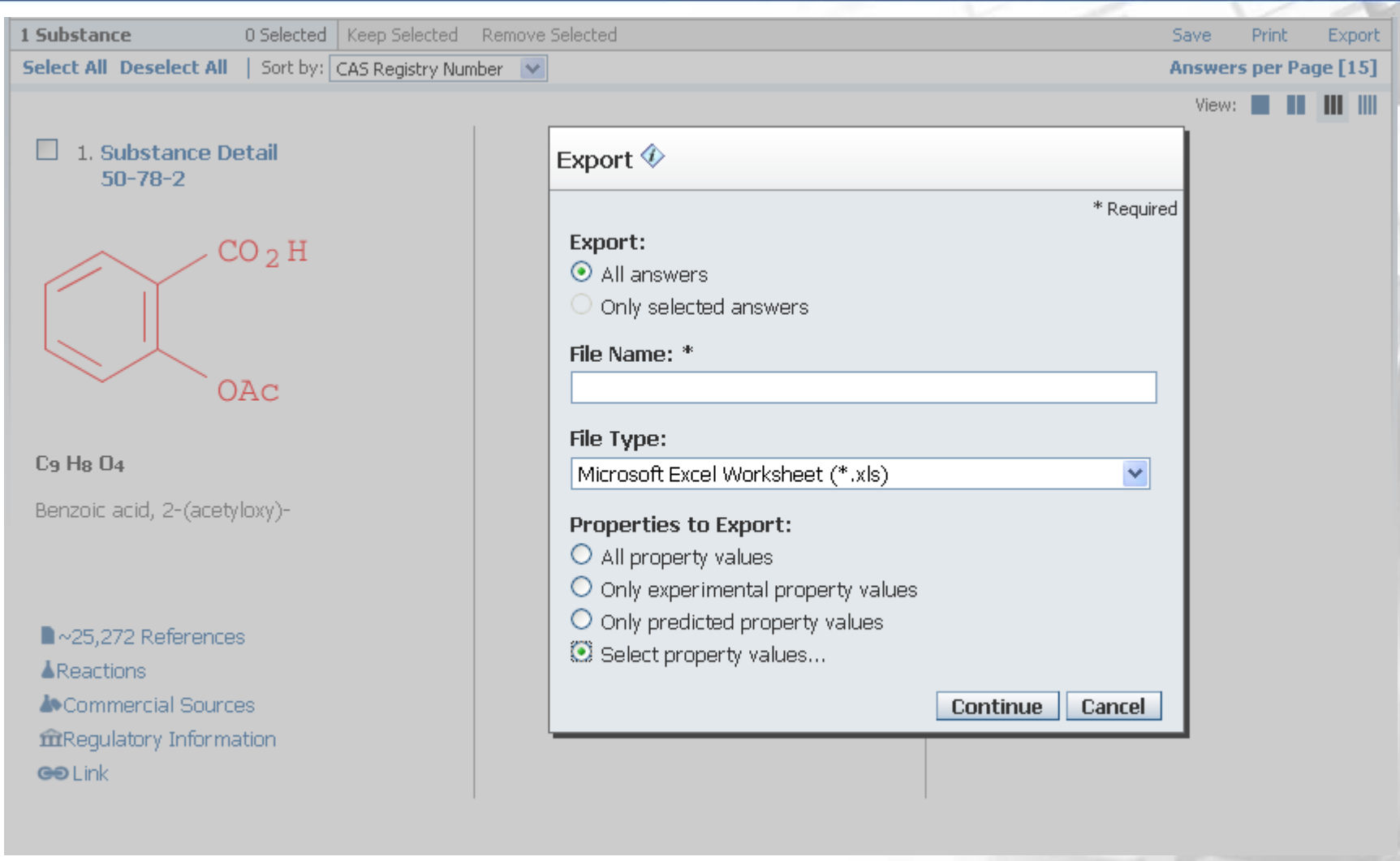
Refine by Property Value (Step 2.1)



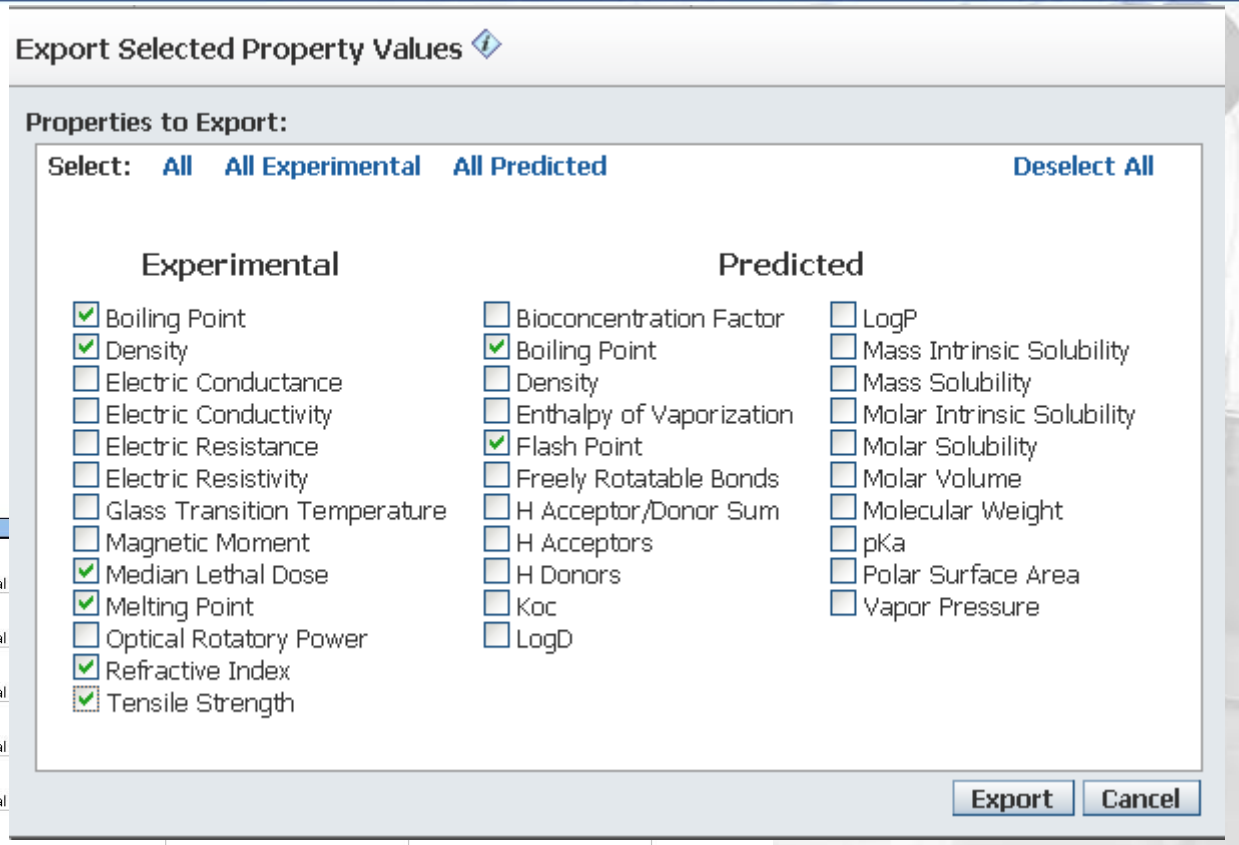
Refine by Property Value (Step 2.2)



Export Substance Property Data (Step 3.1)



Export Substance Property Data (Step 3.2)



SciFinder®

CAS Registry Number	CAS Index Name	Type			
50-78-2	Benzoic acid, 2-(acetyloxy)-	experimental			
50-78-2	Benzoic acid, 2-(acetyloxy)-	experimental			
50-78-2	Benzoic acid, 2-(acetyloxy)-	experimental			
50-78-2	Benzoic acid, 2-(acetyloxy)-	experimental			
50-78-2	Benzoic acid, 2-(acetyloxy)-	experimental			
50-78-2	Benzoic acid, 2-(acetyloxy)-	experimental	Density	Density	1.4 g/cm3
50-78-2	Benzoic acid, 2-(acetyloxy)-	experimental	Density	Density	1.396 g/cm3
50-78-2	Benzoic acid, 2-(acetyloxy)-	experimental	Biological	Median Lethal Dose(LD50)	1216 mg/kg
50-78-2	Benzoic acid, 2-(acetyloxy)-	experimental	Biological	Median Lethal Dose(LD50)	1100 mg/kg
50-78-2	Benzoic acid, 2-(acetyloxy)-	experimental	Biological	Median Lethal Dose(LD50)	880 mg/kg

Carbon-13 NMR Spectrum (new)

Molar Volume	139.5±3.0 cm3/mol	Temp: 20 °C Press: 760 Torr	(80)

Lipinski and Related Properties	Value	Conditions	Notes	Top
Freely Rotatable Bonds	3		(80)	
H Acceptors	4		(80)	
H Donors	1		(80)	
H Donor/Acceptor Sum	5		(80)	
logP	1.190±0.226	Temp: 25 °C	(80)	
Molecular Weight	180.16		(80)	

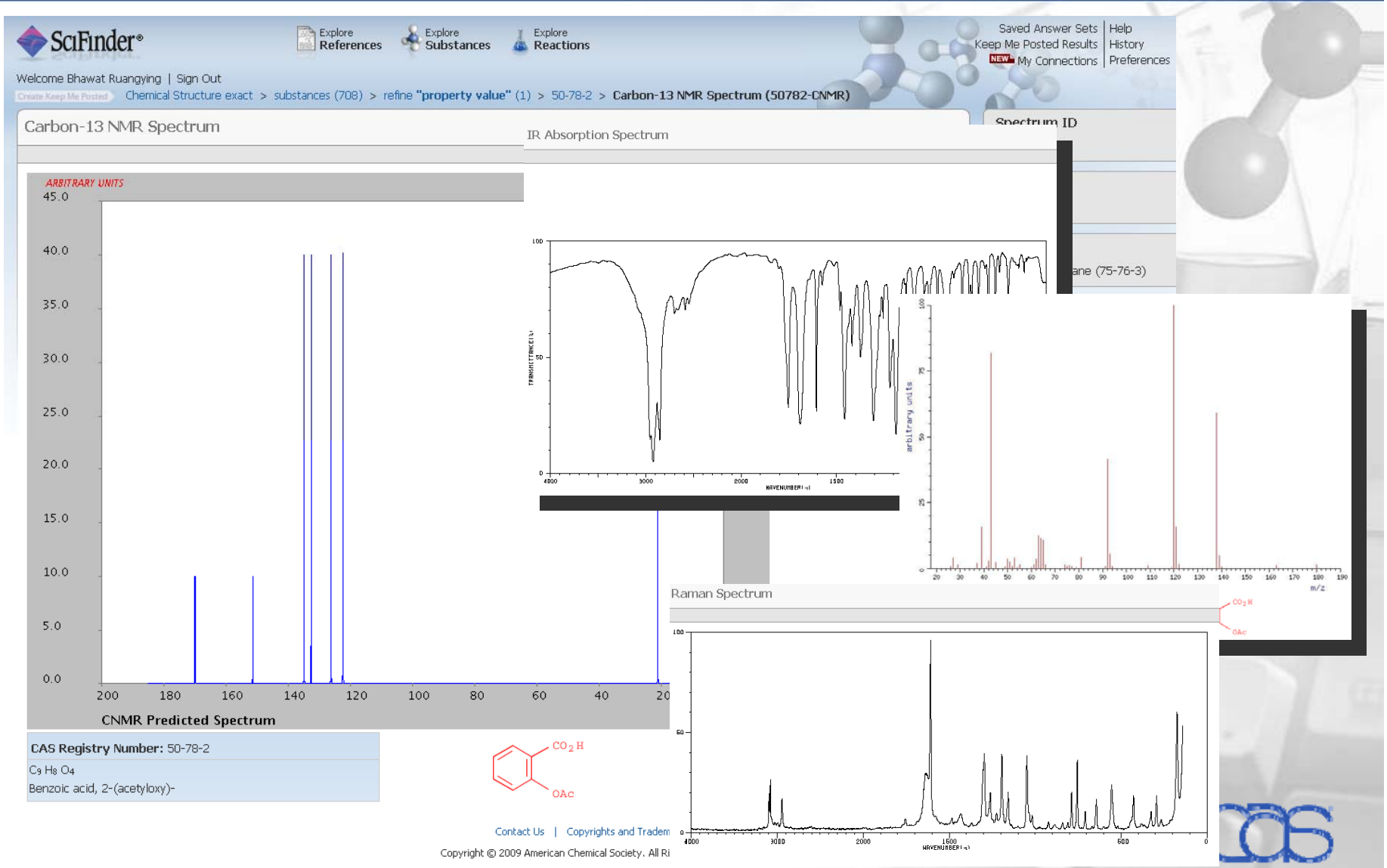
Spectra Properties	Value	Conditions	Notes	Top
Carbon-13 NMR Spectrum NEW	See spectrum		(81)	
Proton NMR Spectrum	See spectrum		(81)	

Structure-related Properties	Value	Conditions	Notes	Top
Polar Surface Area	63.6 A2		(80)	

Thermal Properties	Value	Conditions	Notes	Top
Boiling Point	321.4±25.0 °C	Press: 760 Torr	(80)	
Enthalpy of Vaporization	59.45±3.0 kJ/mol	Press: 760 Torr	(80)	
Flash Point	131.1±16.7 °C		(80)	

(80) Calculated using Advanced Chemistry Development (ACD/Labs) Software V8.14 for Solaris (© 1994-2009 ACD/Labs)
(81) Predicted NMR data calculated using Advanced Chemistry Development, Inc. (ACD/Labs) Software V9.07 (© 1994-2009 ACD/Labs)

C-13 NMR and other spectra



Summary of Scifinder Web

- Provide quick access and user friendly interface to search for scientific information
- New features that are tailor made for the needs of researchers
- Enhanced content for properties, spectra, registration, reaction information and etc
- Personalization features (keep me posted and save as)

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