SciFinder® Scholar

- **The only resource that gives you :**

  - The world's most comprehensive collection of published scientific research.
  - Both Chemical Literature AND Patents in one source — CAplus
  - The largest substance database in the world — CAS Registry.
  - The most current information updated daily.

SciFinder® Scholar

- ***SIX Main Databases***

CAplus -

Chemistry references

8,000 Journals + 40 Patent issuing organizations

Coverage since 1967 -> 1907

 # Records 16,600,000 -> 21,000,000

MEDLINE -

Life Science references

Coverage since 1958

 # Records 11,500,000

SciFinder® Scholar

CAS Registry -

Chemical substances

Coverage since 1957

Records 28,500,000

CAS REACT -

Organic reactions

Coverage since 1985

Records 4,000,000

SciFinder® Scholar

CHEMLIST -

Inventory Information (Regulated Chemicals)

 # Records 223,000

CHEMCAT -

Chemical Catalog Information

 # Records 11,000,000

Optional Module

SubStructure Module (SSM)

SciFinder® Scholar

CAplus

Content by Document Source

 # Records 20,000,000

Journals	**-**	**74%**
Patent	**-**	**16%**
Conference	**-**	**5%**
Reports	**-**	**2%**
Dissertation	**-**	**2%**
Book	**-**	**1%**

SciFinder® Scholar

CAS Registry

Substance Database

 # Records 28,500,000

Organic	**-**	**60%**
Bio Sequences	**-**	**26%**
Coordination	**-**	**5%**
Polymer	**-**	**4%**
Alloys	**-**	**3%**
Tabular InOrganics	**-**	**2%**

SciFinder® Scholar

CHEMISTRY

+

A LOT MORE

SciFinder® Scholar

BASIC CHEMISTRY ??

4.2 million references (27%)

- General chemistry
- General organic chemistry
- Benzene & its derivatives
- Organometallic compounds
- Biochemical methods
- Aliphatic compounds
- Heterocyclic compounds
- Electrochemistry

SciFinder® Scholar

ENGINEERING ??
5.7 million references (36%)

- Nuclear technology
- Textiles & fibers
- Apparatus & plant equipment
- Waste treatment & disposal
- Geological chemistry
- Propellants & explosives
- Coatings & inks
- Plastic manufacturing

SciFinder® Scholar

PHYSICS ??

4.0 million references (25%)

- Surface chemistry & colloids
- Electric phenomena
- Mass spectroscopy
- Crystallography & liquid crystals
- Thermodynamics
- Thermal properties
- Nuclear phenomena
- Magnetic phenomena

SciFinder® Scholar

BIOLOGY & LIFE SCIENCES ??
3.4 million references (21%)

- Agriculture
- Molecular biology
- Food engineering & biotechnology
- Microbes, algae & fungi
- Fermentation
- Bioindustrial methods
- Animal science
- Plant science

SciFinder® Scholar

MEDICAL SCIENCES ??
3.1 million references (19%)

- Pharmaceutical sciences
- Physiological chemistry
- Toxicology
- Pathological biochemistry
- Veterinary medicine
- Nutirtion
- Immunochemistry
- Radiation biochemistry

SciFinder® Scholar

A WHOLE LOT MORE —

- Education
- Mathematics
- Biotechnology
- Archaeology
- Geoscience
- History
- Astronomy
- Materials
- Economics
- Metallurgy

SciFinder® Scholar

Special features

- Analyze Substances & References
- Refine Substances & References
- Linking to F/T Journal
- Linking to F/T Patents

Citation Linking

- Cited References
- Citing References

- eScience

- CAplus + MEDLINE + OLDMEDLINE (-1966)

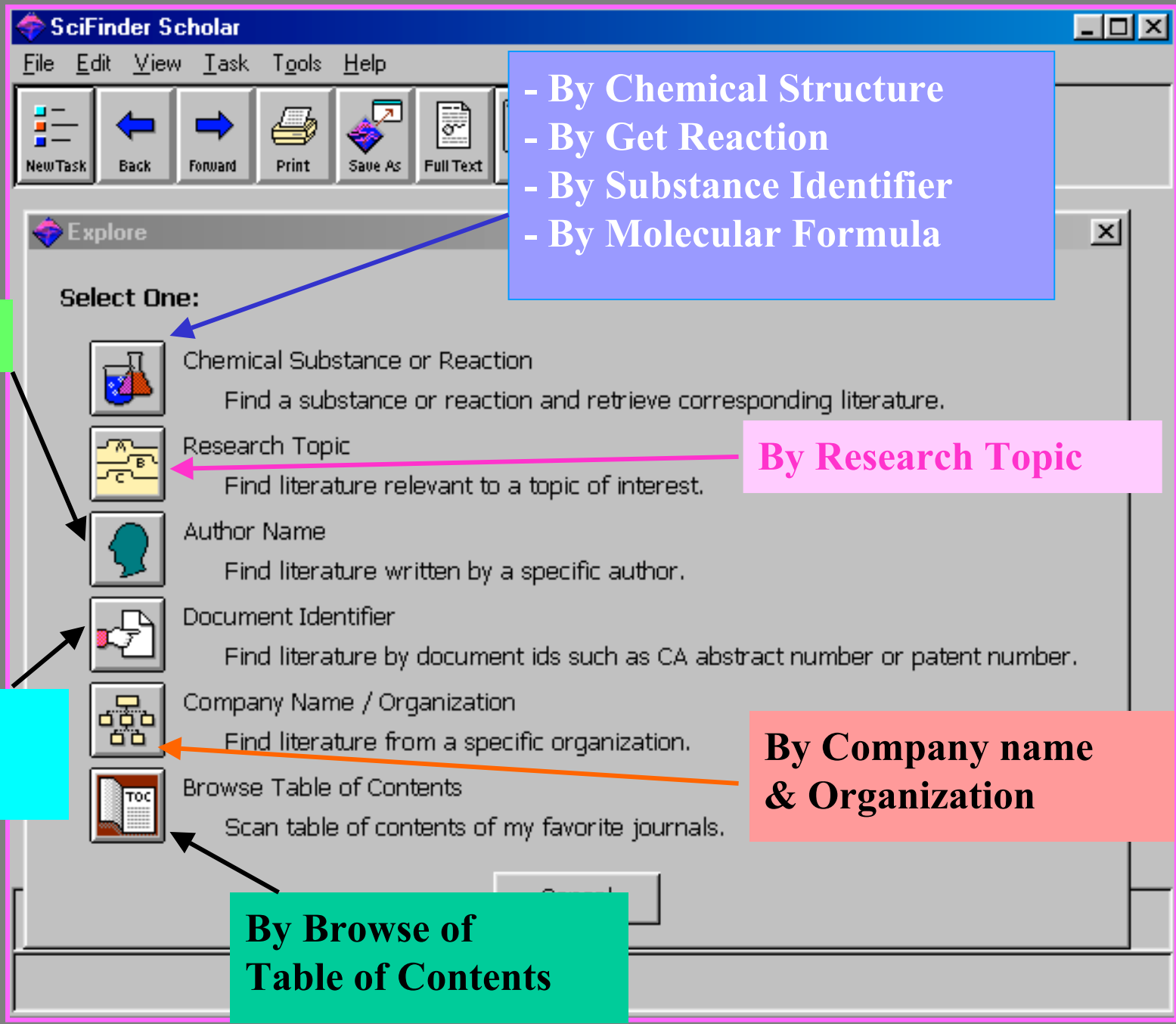
SciFinder® Scholar

Conclusion

# of Substances	21,000,000 + 11,500,000
Abstracts since	1907
# of journals	8,000 + 3,900
Patents (Fulltext)	Yes
# Substances	4,000,000
Full text linking	Yes
CITATION linking	Yes

SciFinder Scholar

The world's leading scientific information resource


SciFinder Scholar
File Edit View Task Tools Help
New Task
Back
Forward
Print
Save As
Full Text
- By Chemical Structure
- By Get Reaction
- By Substance Identifier
- By Molecular Formula
Explore
Select One:
Chemical Substance or Reaction
Find a substance or reaction and retrieve corresponding literature.
Research Topic
Find literature relevant to a topic of interest.
Author Name
Find literature written by a specific author.
Document Identifier
Find literature by document ids such as CA abstract number or patent number.
Company Name / Organization
Find literature from a specific organization.
Browse Table of Contents
Scan table of contents of my favorite journals.
TOC
By Author
By Research Topic
By Document Identifier
By Company name & Organization
By Browse of Table of Contents

Explore by Research Topic

Explore By Research Topic

-ใช้วลีหรือประโยคภาษาอังกฤษแบบง่ายๆ โดยอาจใช้คำ บุพบท (preposition),คำสันธาน (conjunctions) แต่ Sci Finder ไม่รู้จักคำสั่งภาษา computer เช่น พวก Boolean ต่างๆ

-ให้เน้น 2 หรือ 3 concept เชื่อมด้วย preposition เช่น

I am interested in wastewater treatment at Walt Disney world

-ให้ใช้ preposition แทน or และ and จะแน่นอนกว่าเช่น

I am interested in the effects of human growth homone on fetal development ซึ่งดีกว่าใช้

I am interested in the effects of human growth homone and fetal development

ให้กระจายคำที่ต้องการ Modifies เช่น

ใช้ black dragons and black magic แทนที่จะใช้คำว่า

black dragons and magic

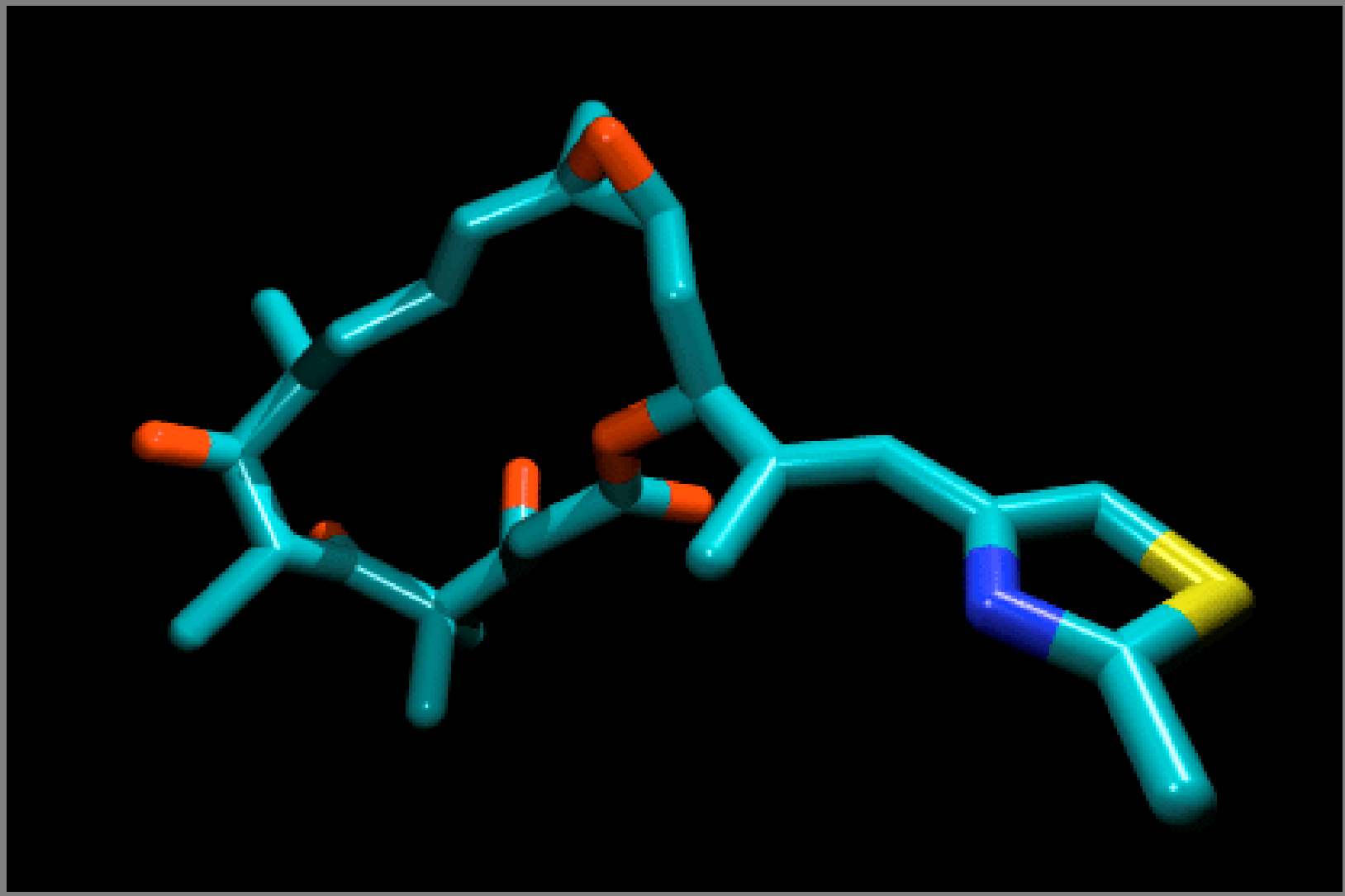
-Sci Finder จะไม่เข้าใจคำที่เป็น negative เช่น not and except แต่คำที่ไม่ต้องการให้ใส่ภายใต้เครื่องหมาย “ junk”

-ใช้คำเหมือน(synonym)ของคุณเองถ้ามี เพื่อโยง concept ที่สัมพันธ์กันเช่น

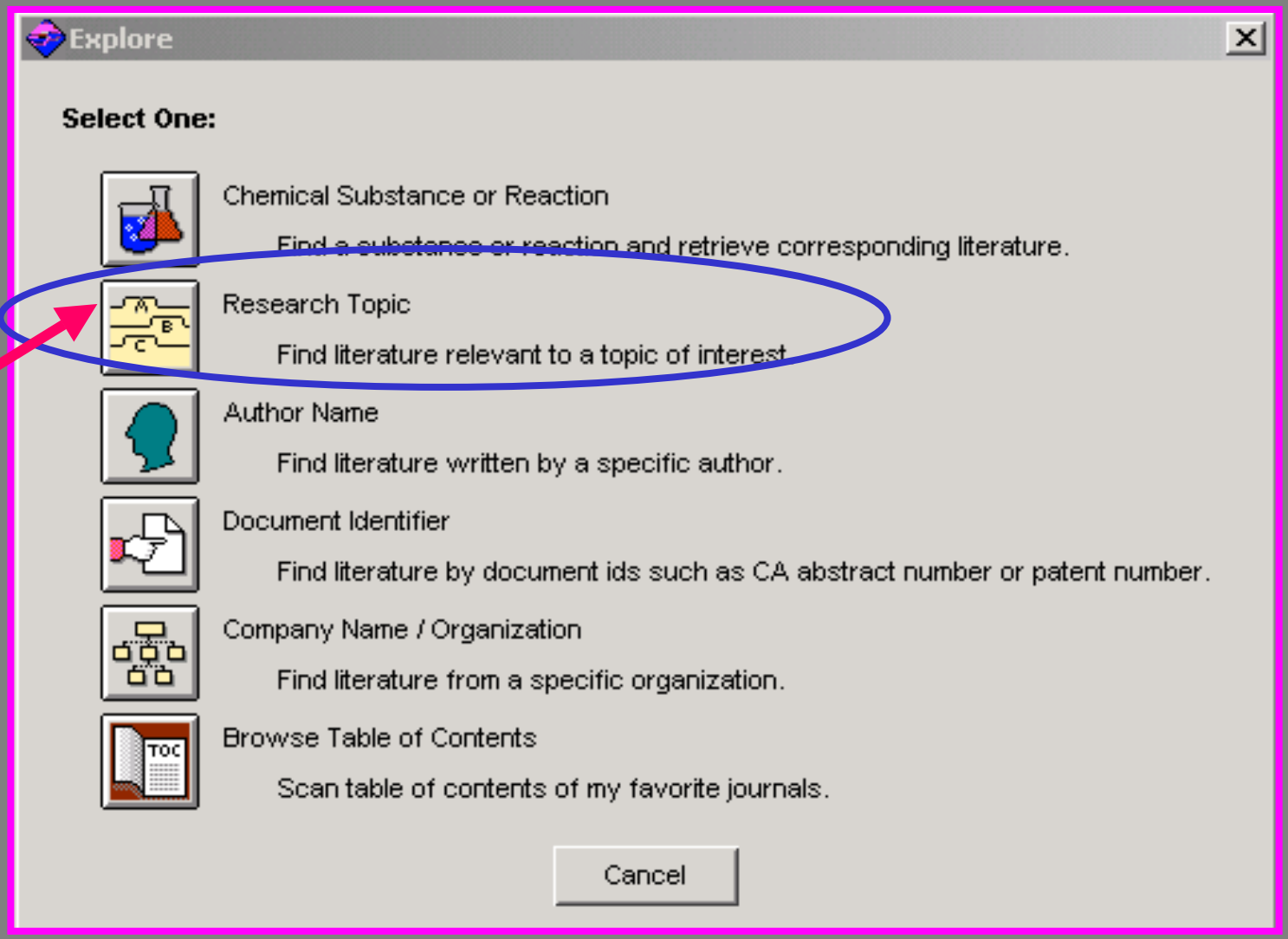
I am interested in topical treatments for poison ivy (Rhus radiacans)

-พยายามใช้วลีที่ต่างๆกันหลายๆทางในการค้น

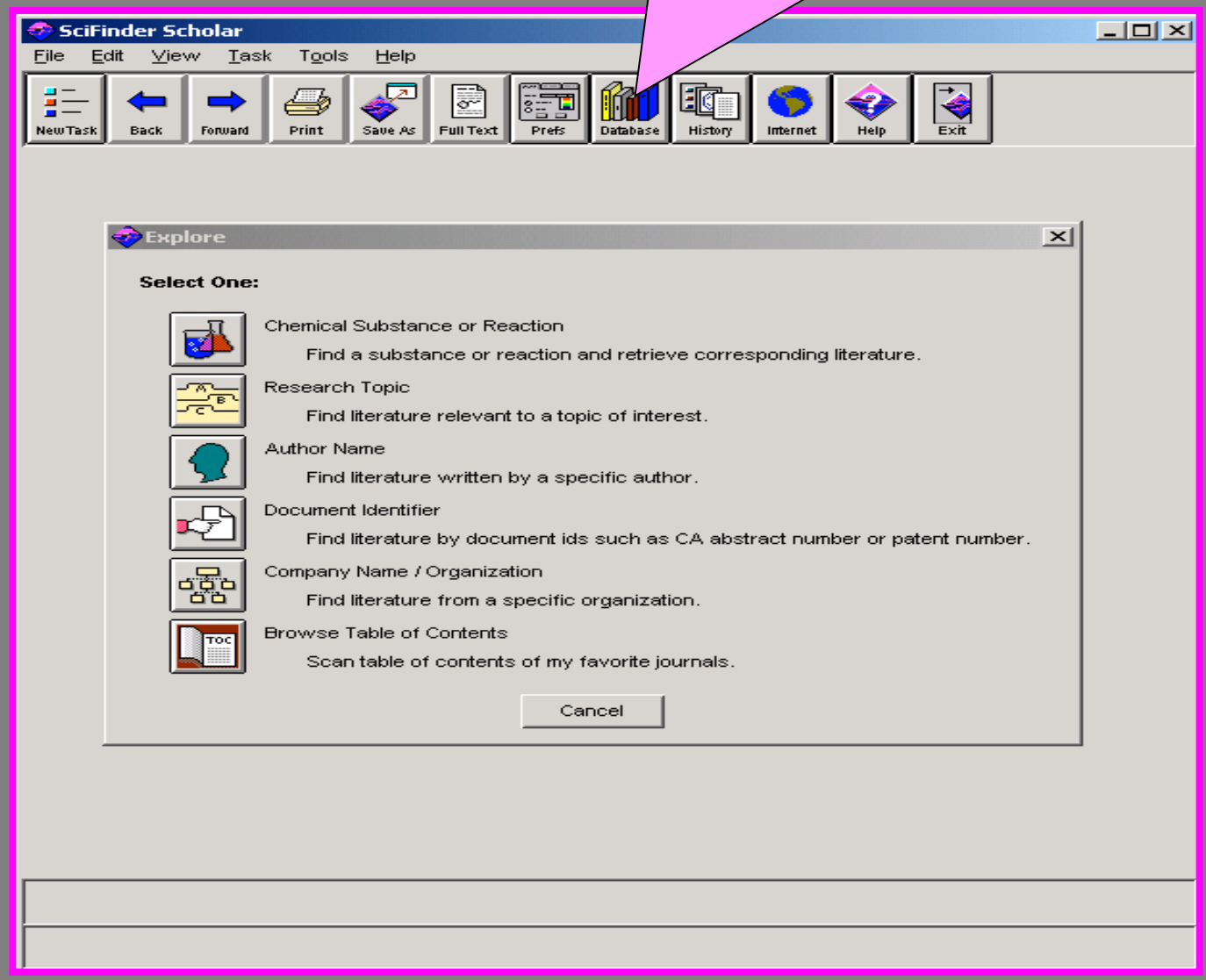
Cancer Fighter "Epothilone B"



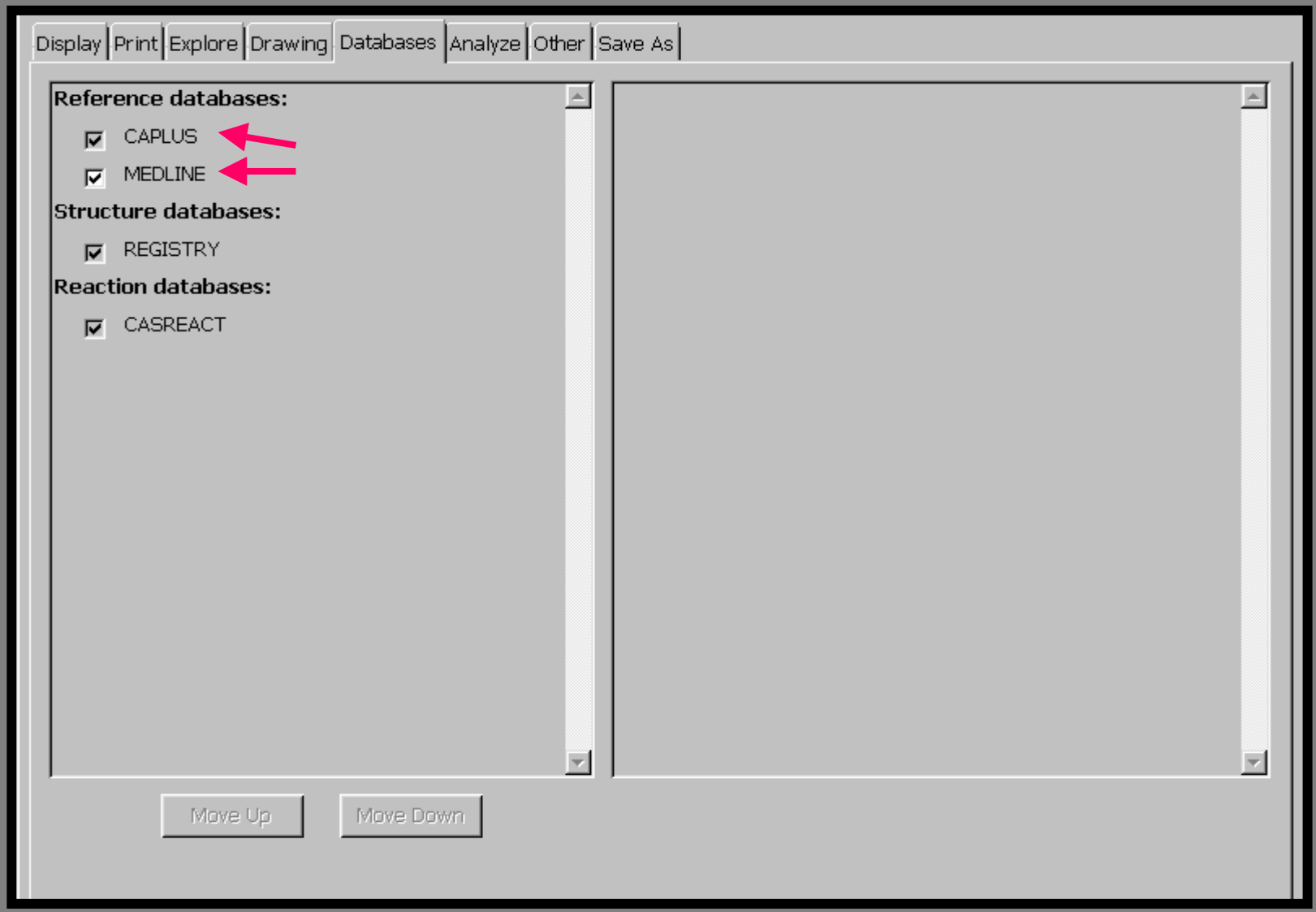
Explore by Research Topic



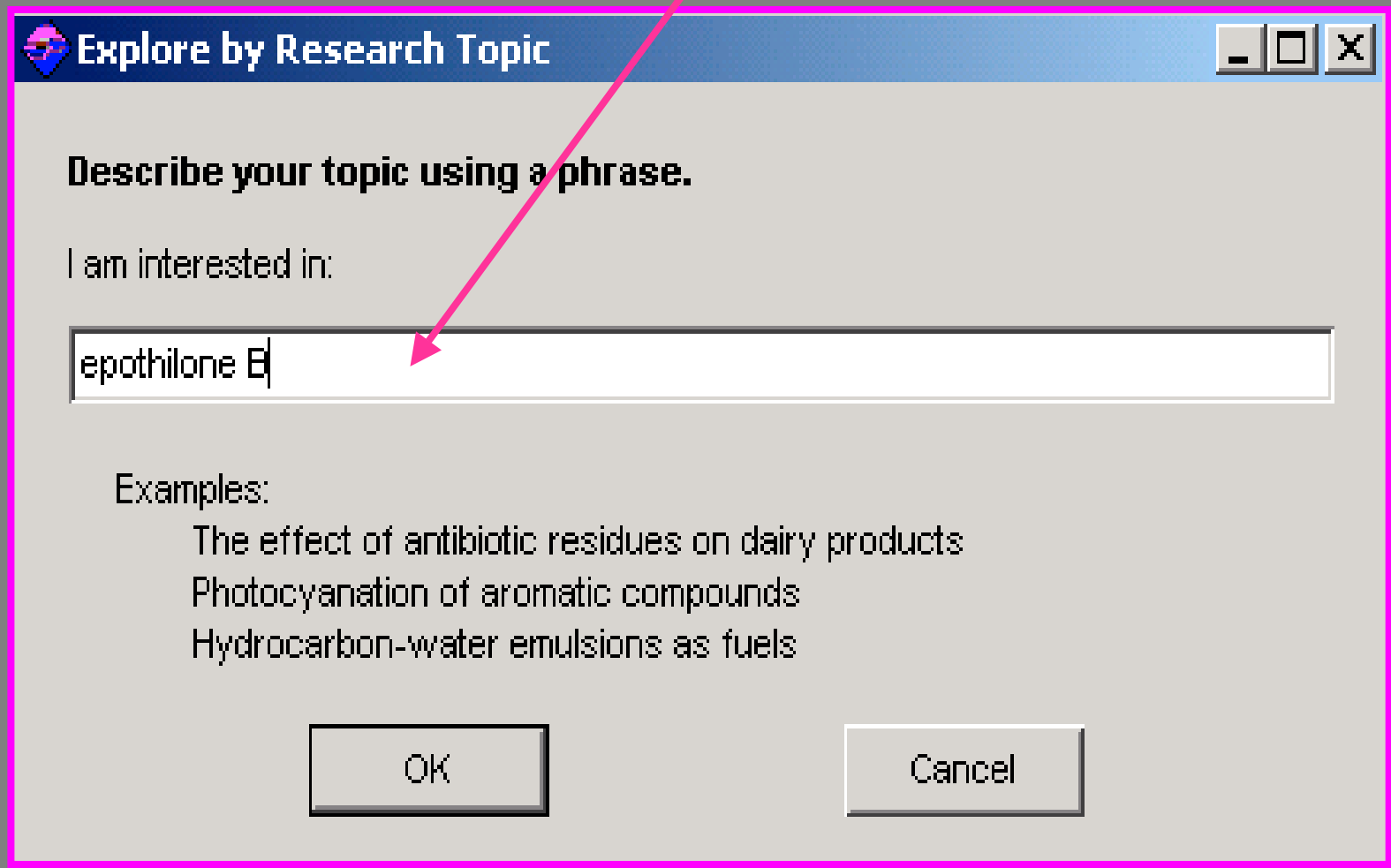
Click at Database



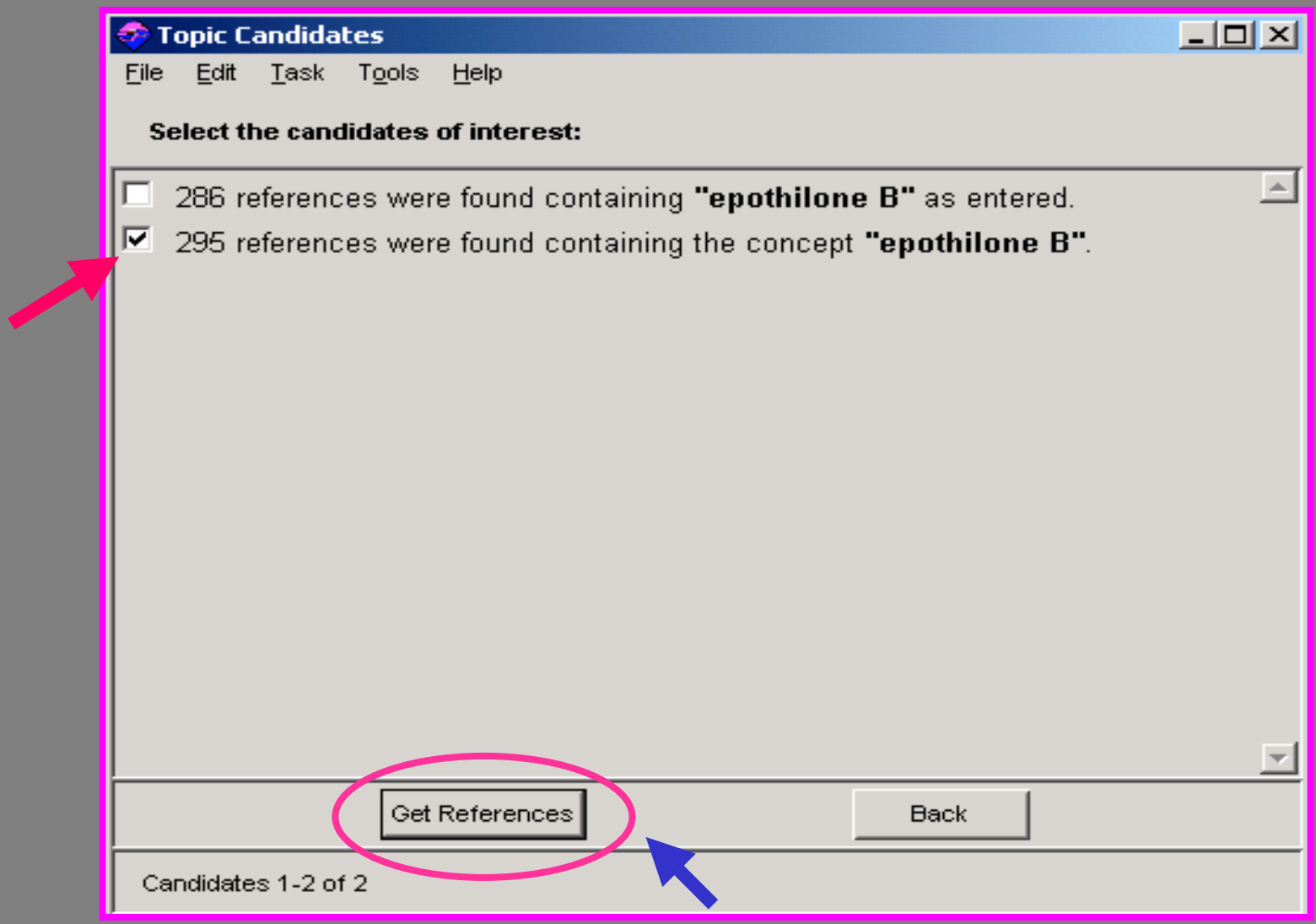
Select the database of interest



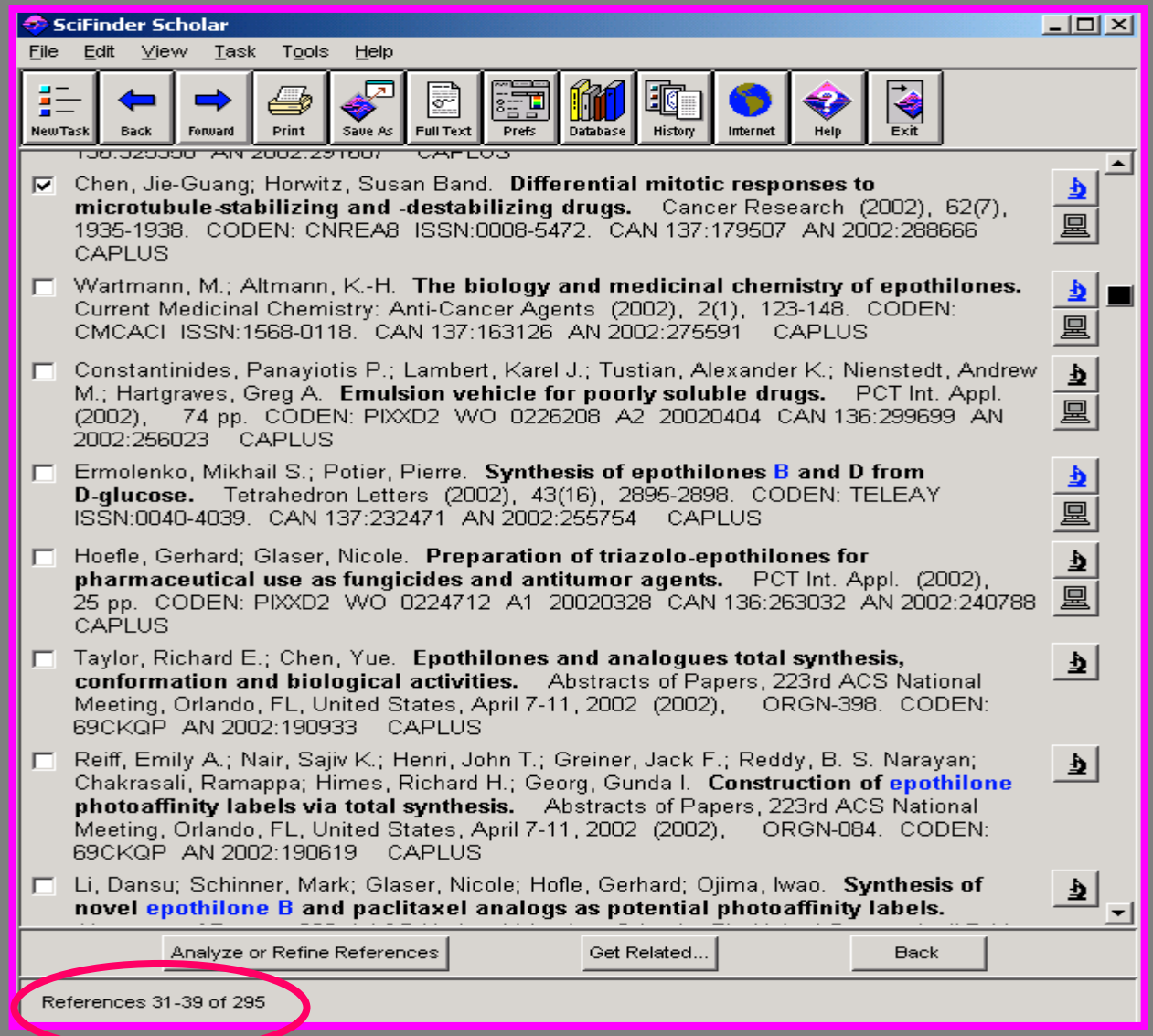
Enter the topic of interest



Select candidates of interest

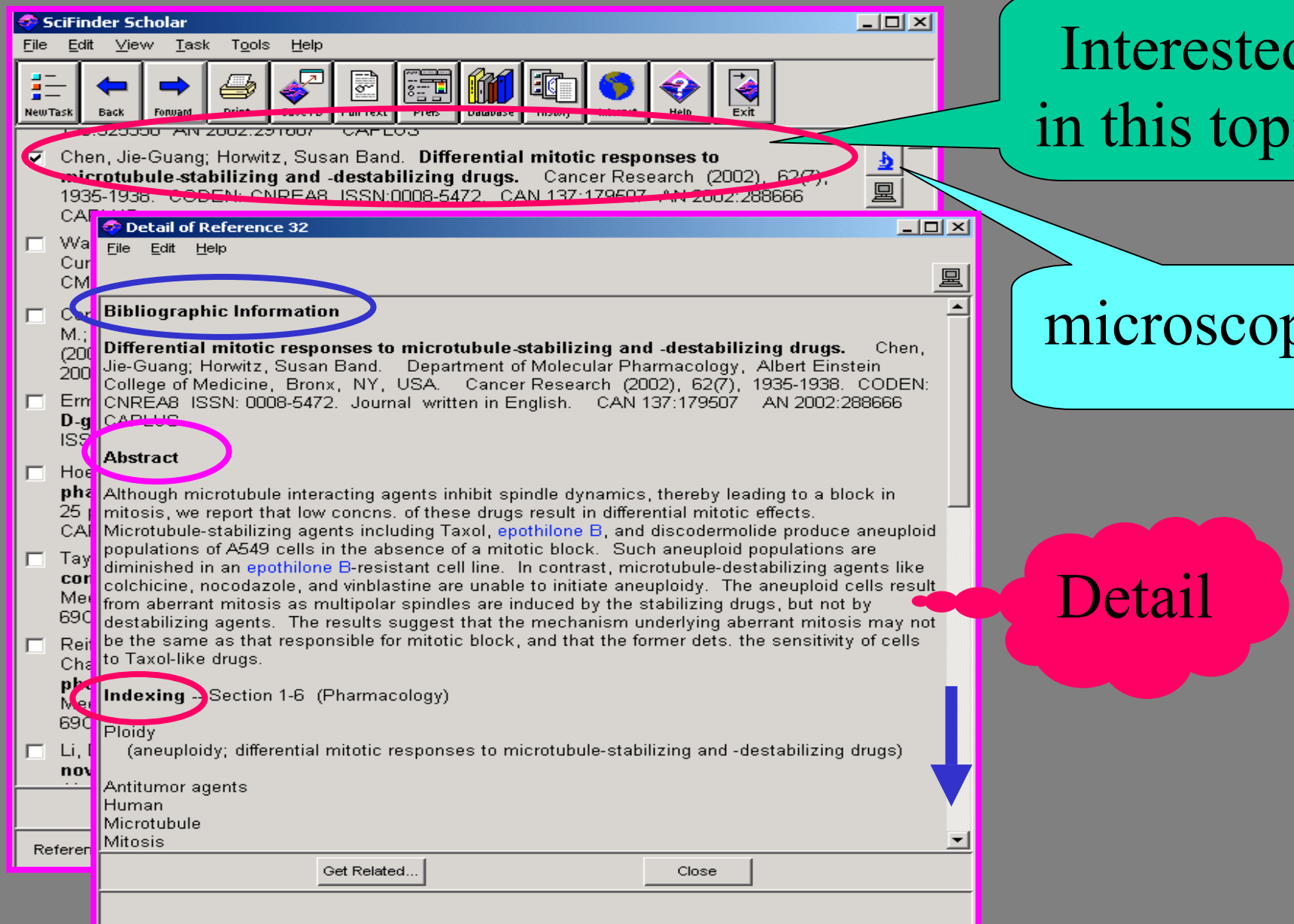


Here are the references!



295 references

Let's view the detail of reference of interest

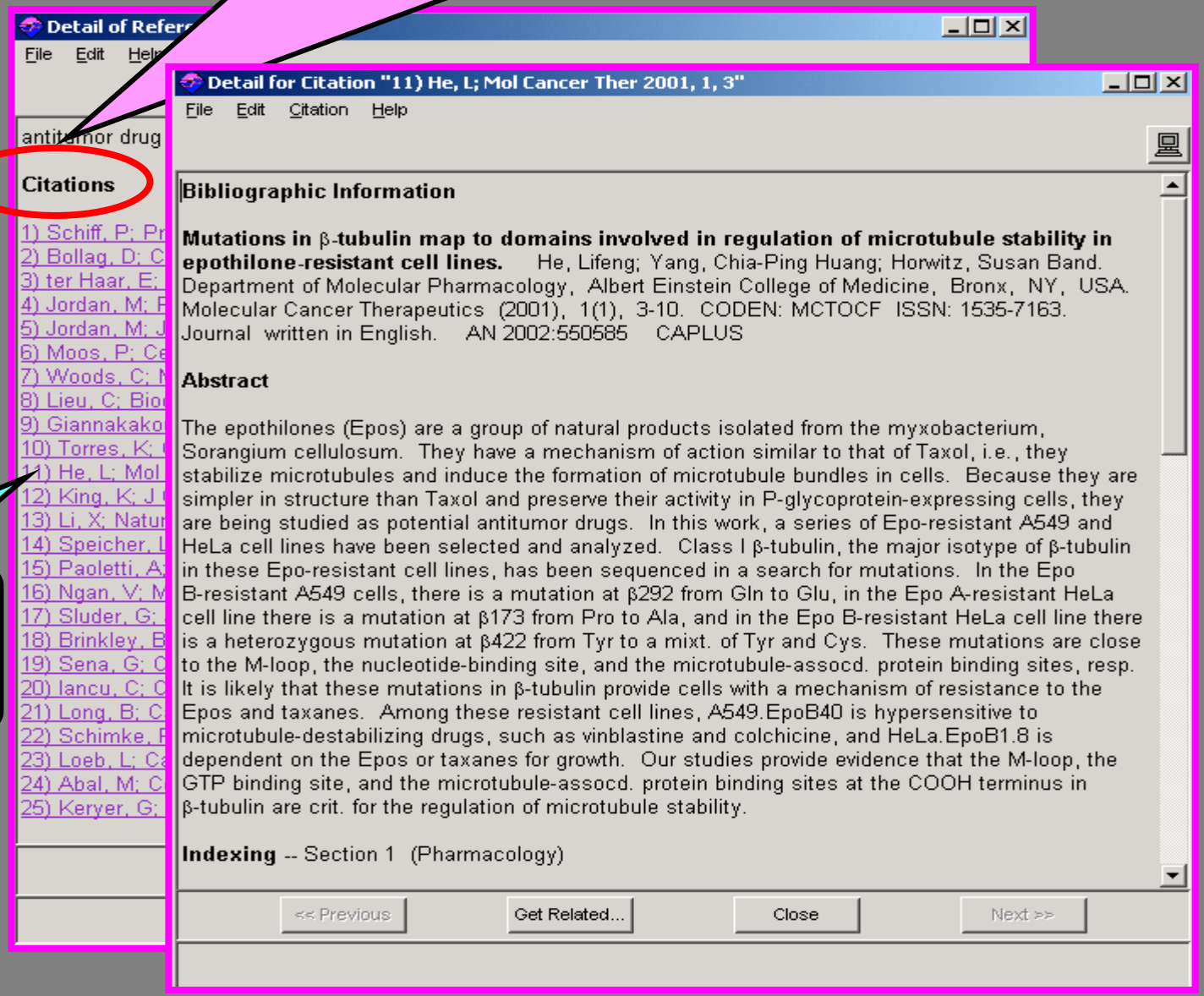


Interested in this topic

microscope

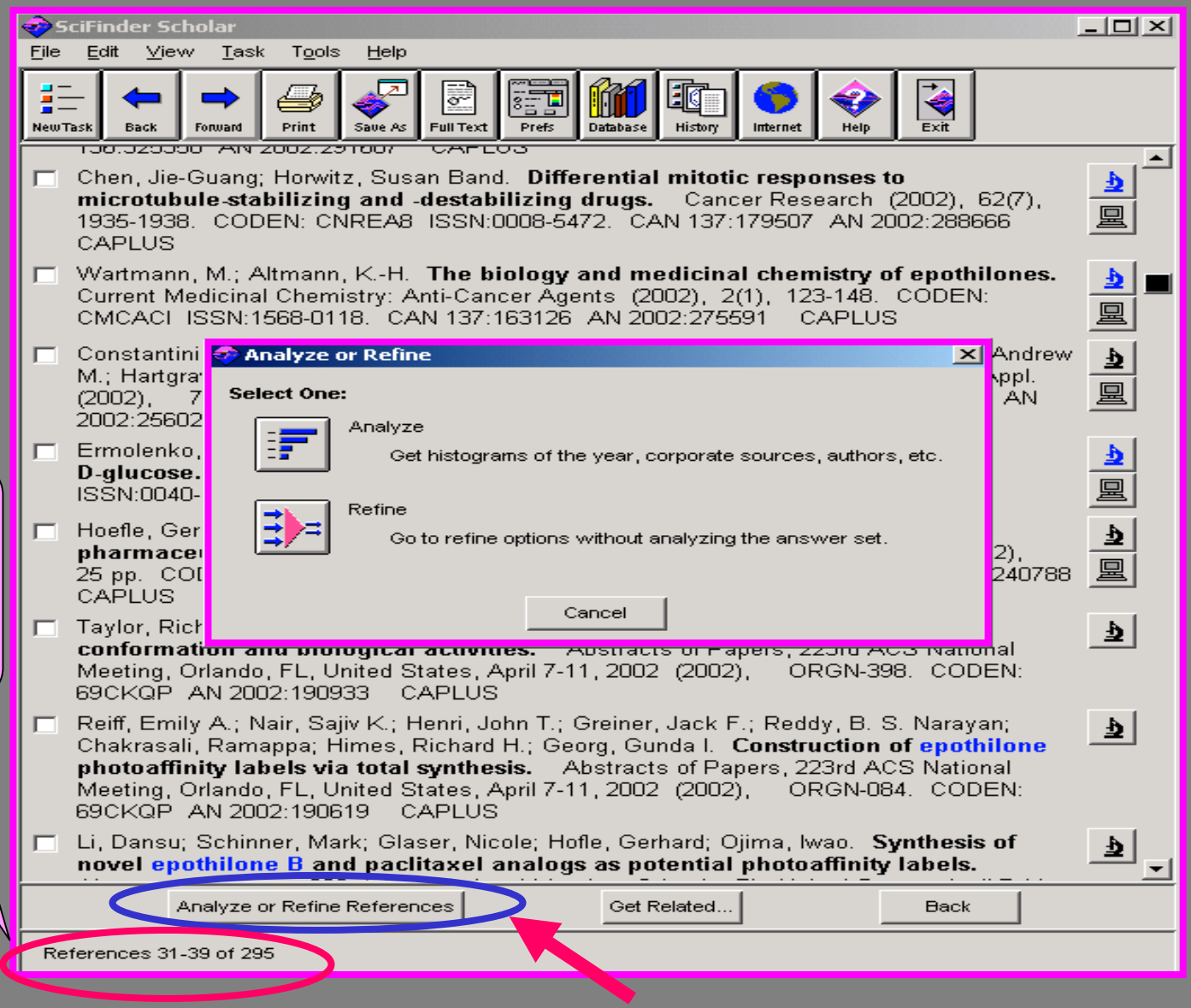
Detail

Here are the Citations!



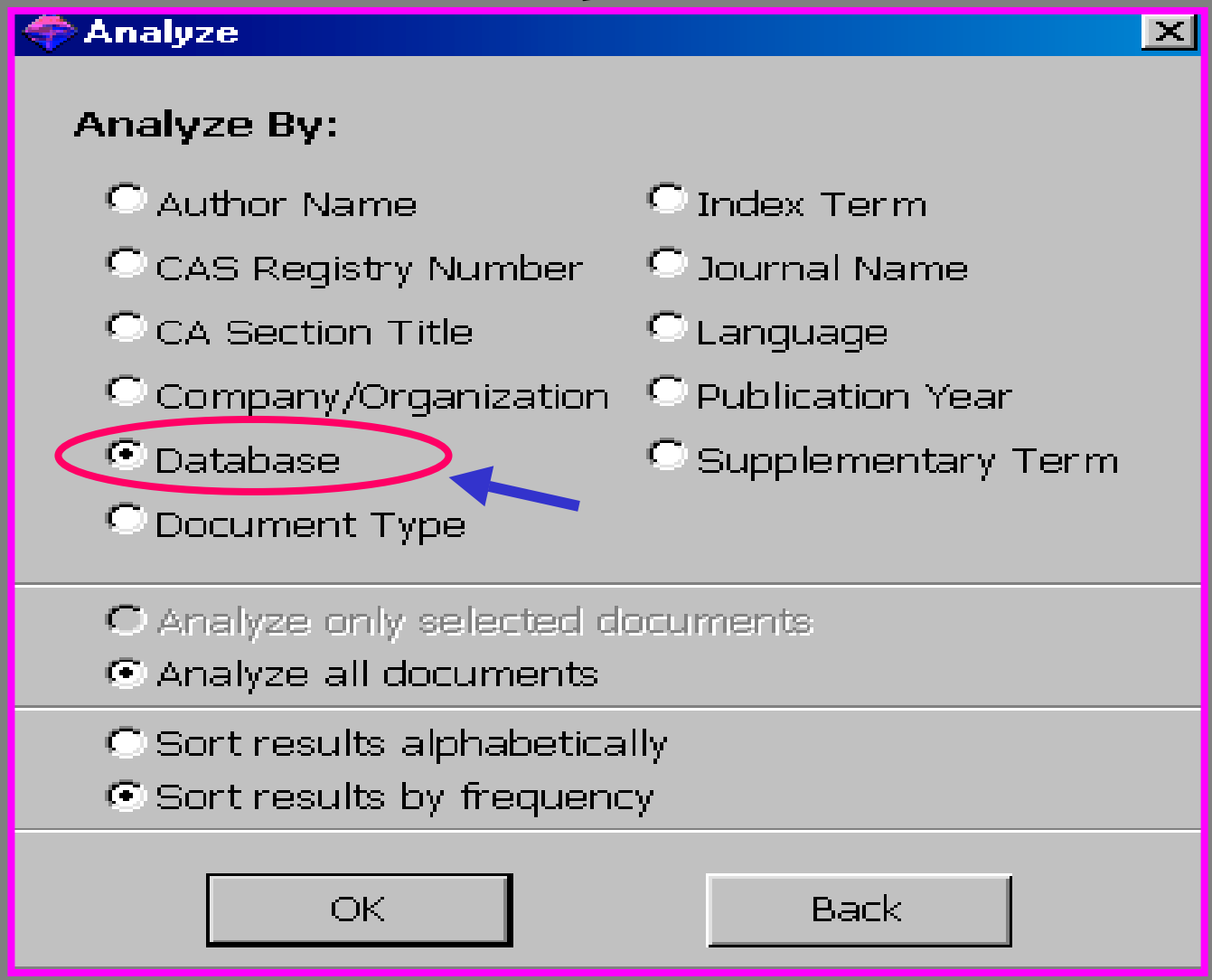
Interested in this reference?

Narrow down the answer set

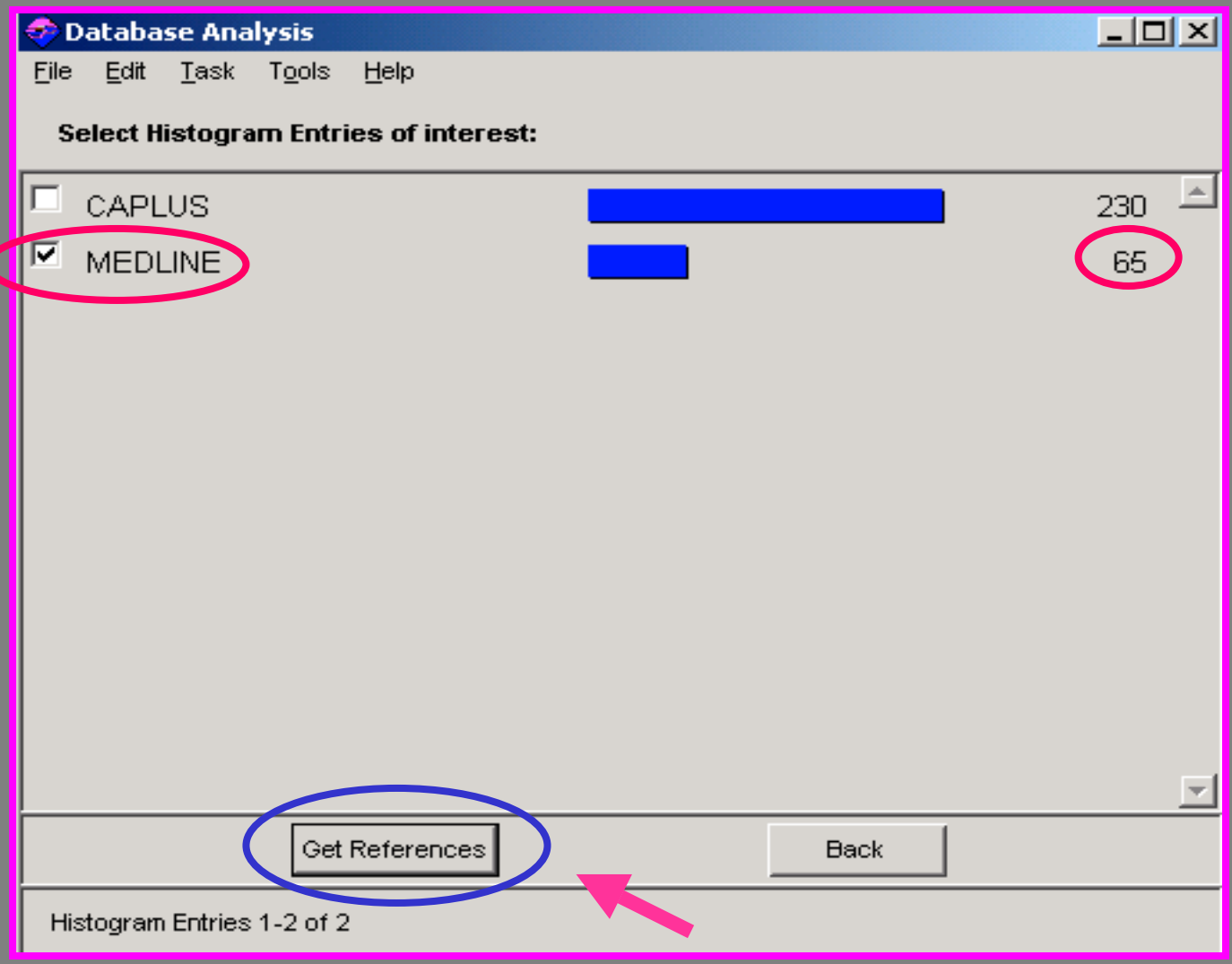


Too large answer set?

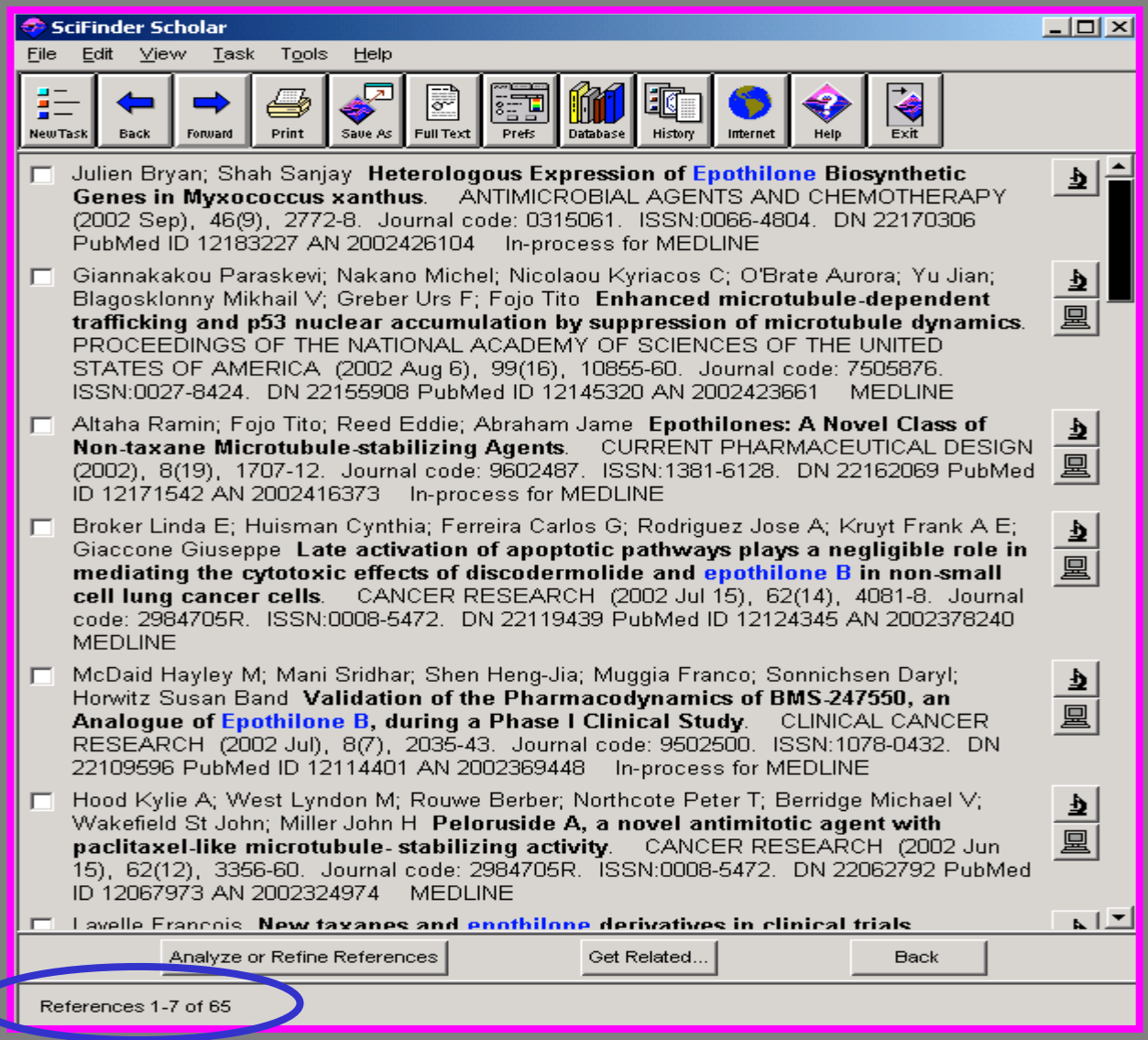
11 options to analyze the answer sets



Select the database of interest

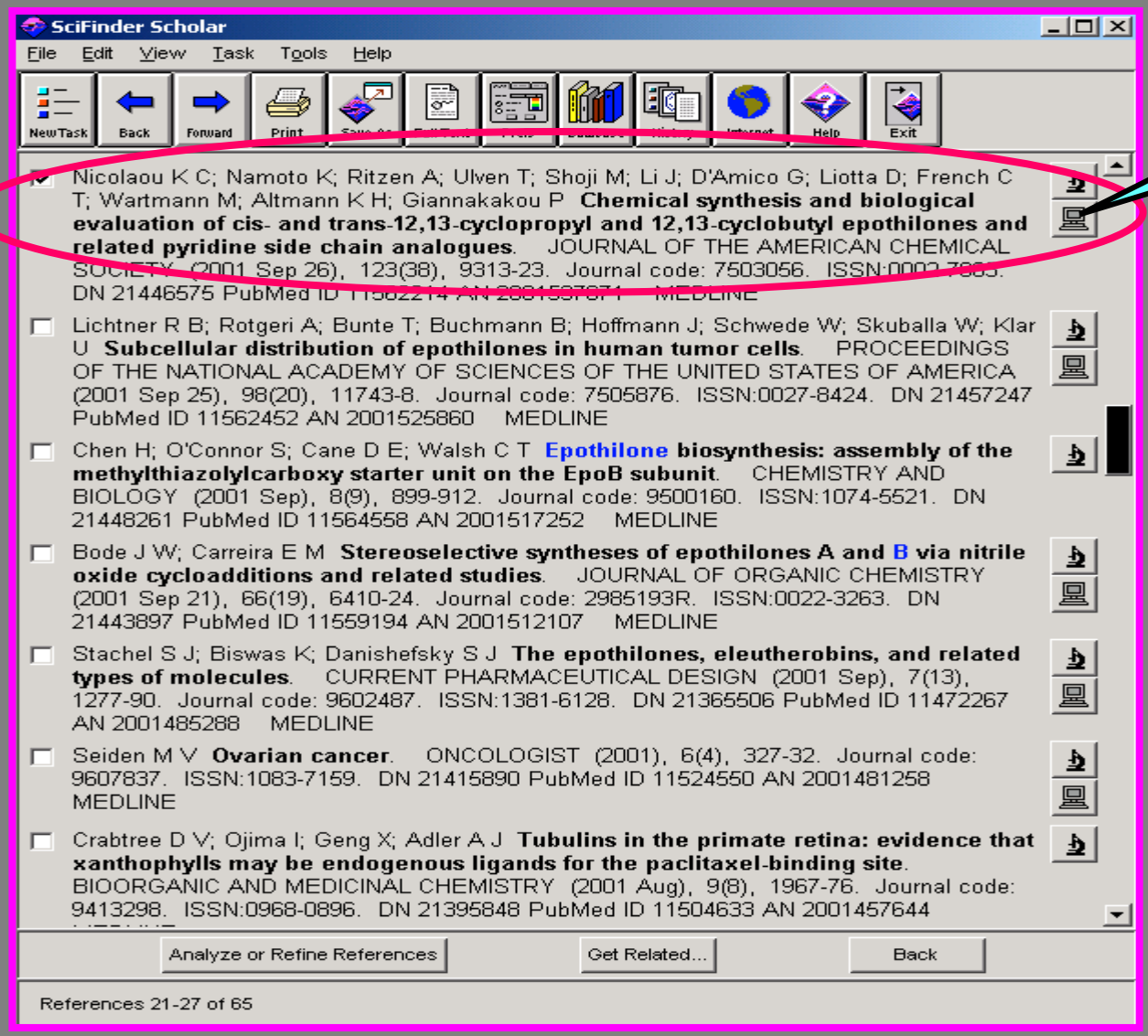


The references retrieved from Medline

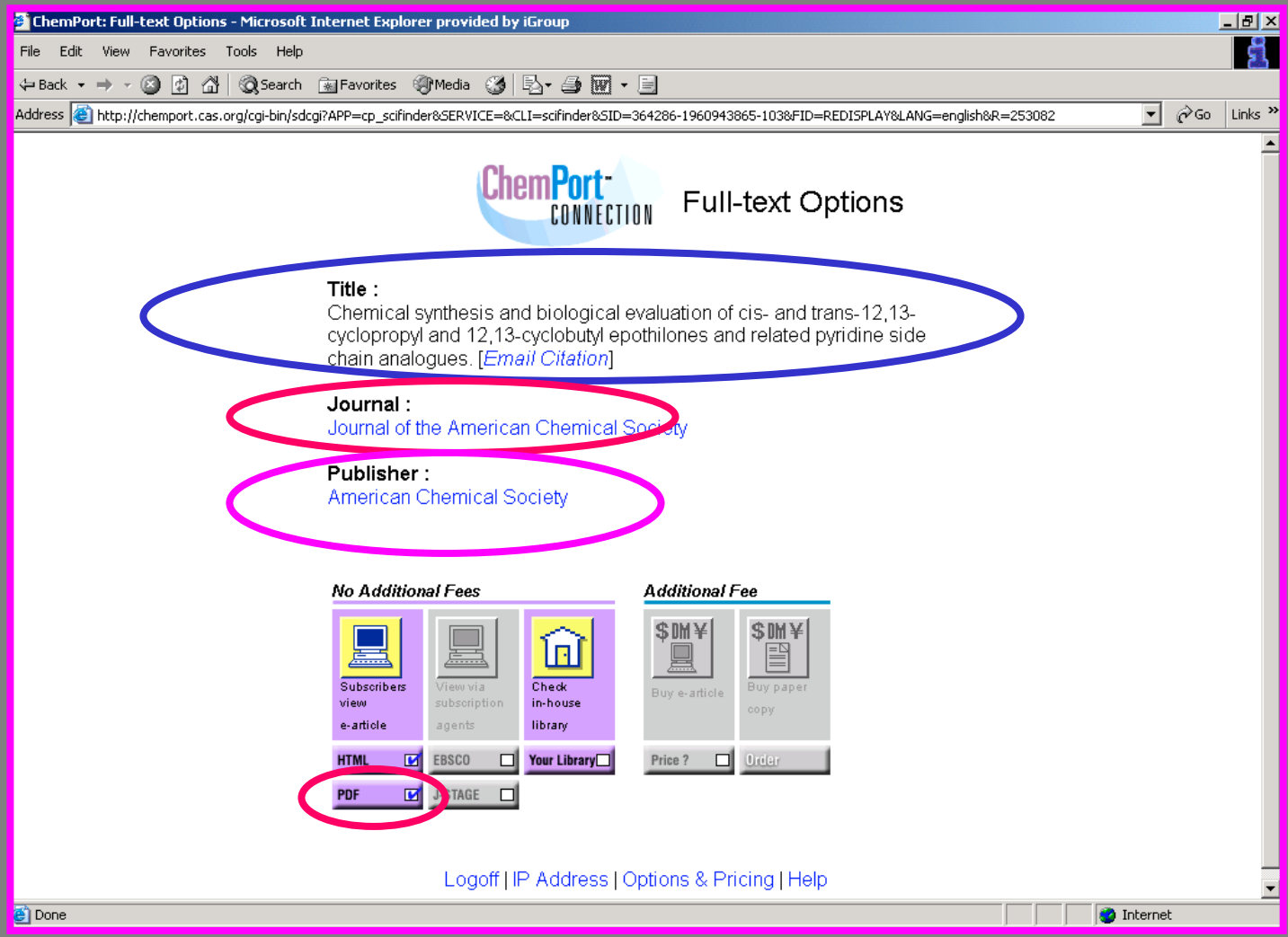


65 references

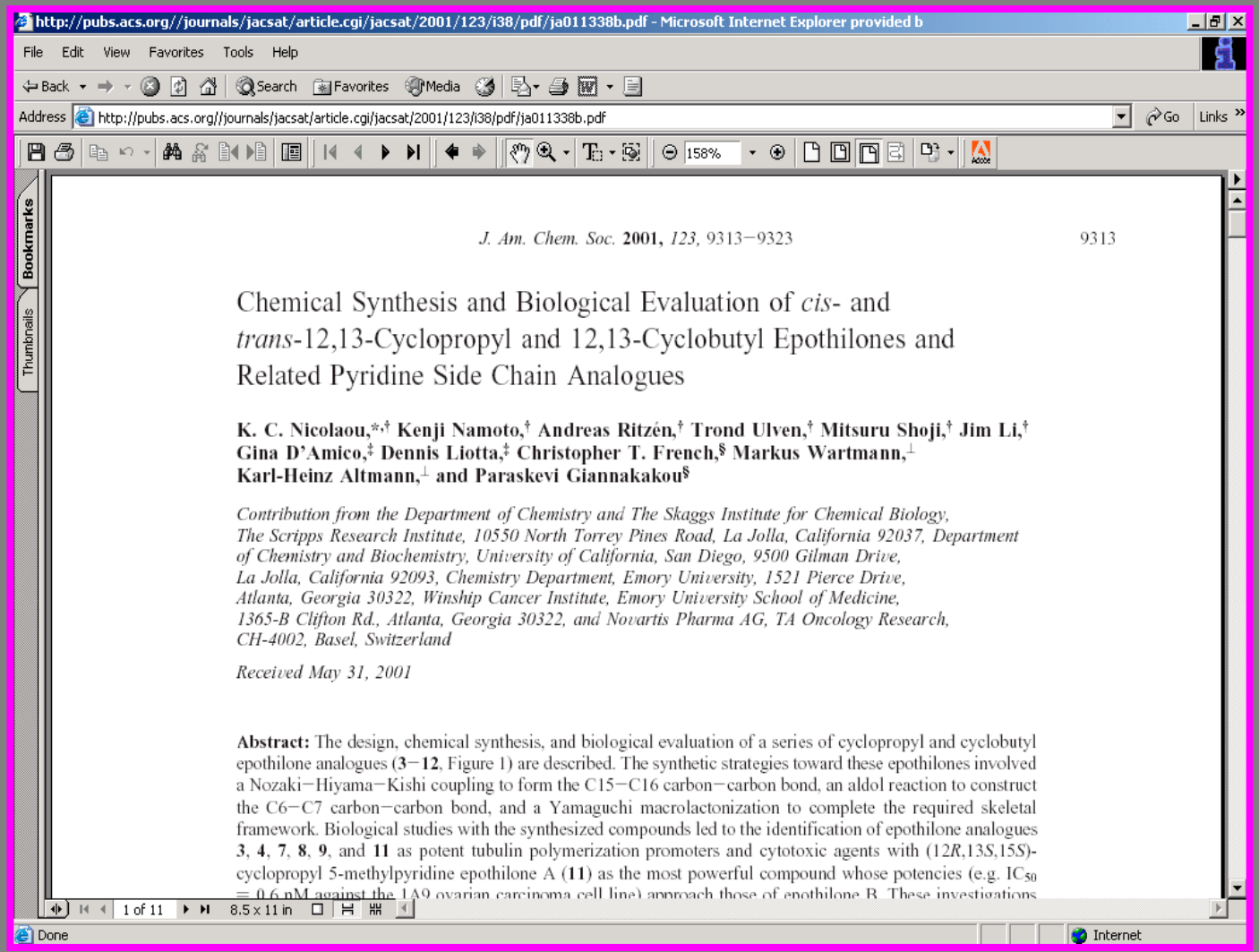
Link to ChemPort to see full-text



Link to see full text if we are a subscriber



Here is the desired full-text!



http://pubs.acs.org//journals/jacsat/article.cgi/jacsat/2001/123/i38/pdf/ja011338b.pdf - Microsoft Internet Explorer provided b

File Edit View Favorites Tools Help

Back Search Favorites Media

Address http://pubs.acs.org//journals/jacsat/article.cgi/jacsat/2001/123/i38/pdf/ja011338b.pdf

Go Links

158%

Bookmarks Thumbnails

Chemical Synthesis and Biological Evaluation of *cis*- and *trans*-12,13-Cyclopropyl and 12,13-Cyclobutyl Epothilones and Related Pyridine Side Chain Analogues

K. C. Nicolaou,*,† Kenji Namoto,† Andreas Ritzén,† Trond Ulven,† Mitsuru Shoji,† Jim Li,† Gina D'Amico,‡ Dennis Liotta,‡ Christopher T. French,§ Markus Wartmann,⊥ Karl-Heinz Altmann,⊥ and Paraskevi Giannakakou§

Contribution from the Department of Chemistry and The Skaggs Institute for Chemical Biology, The Scripps Research Institute, 10550 North Torrey Pines Road, La Jolla, California 92037, Department of Chemistry and Biochemistry, University of California, San Diego, 9500 Gilman Drive, La Jolla, California 92093, Chemistry Department, Emory University, 1521 Pierce Drive, Atlanta, Georgia 30322, Winship Cancer Institute, Emory University School of Medicine, 1365-B Clifton Rd., Atlanta, Georgia 30322, and Novartis Pharma AG, TA Oncology Research, CH-4002, Basel, Switzerland

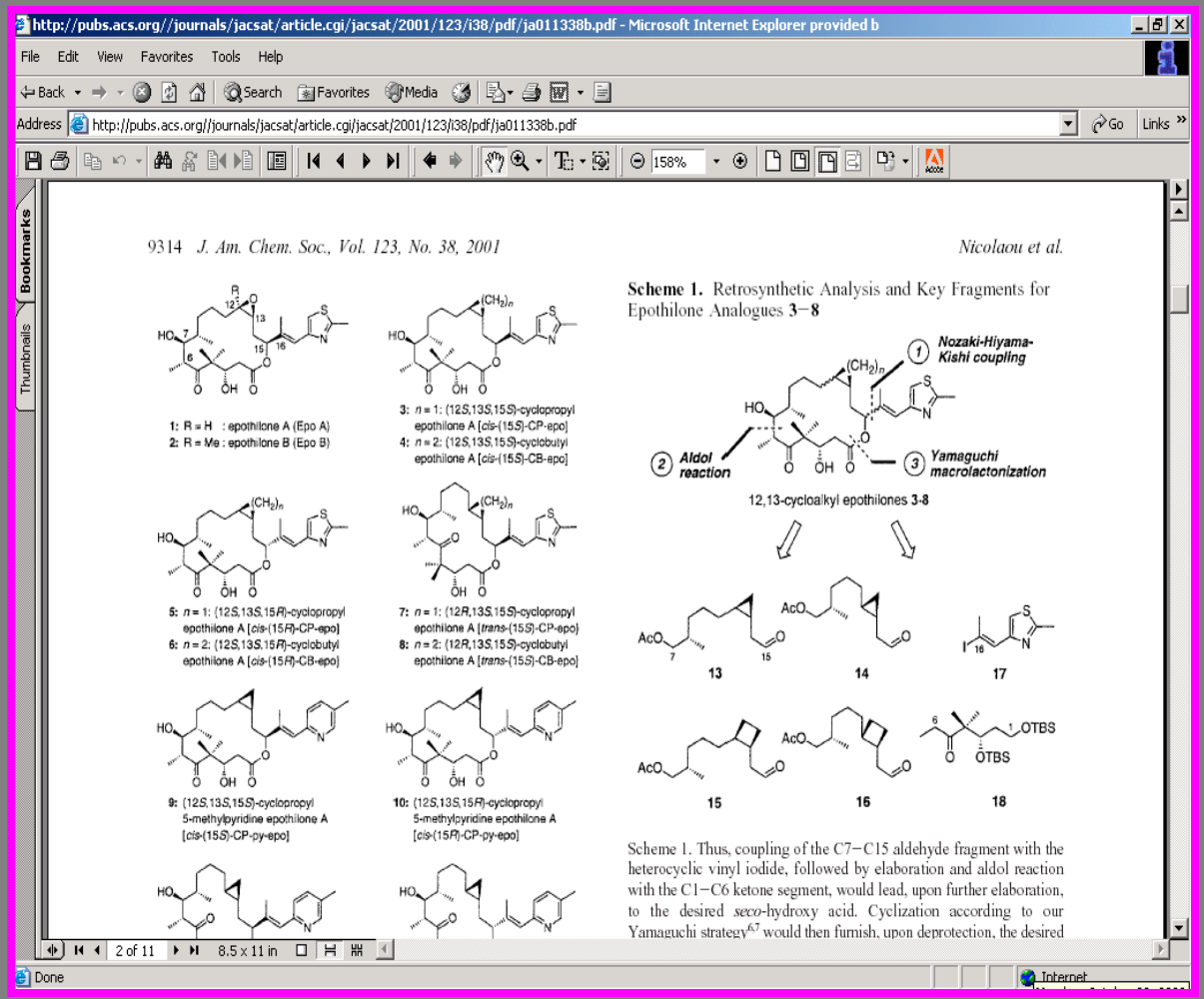
Received May 31, 2001

Abstract: The design, chemical synthesis, and biological evaluation of a series of cyclopropyl and cyclobutyl epothilone analogues (**3**−**12**, Figure 1) are described. The synthetic strategies toward these epothilones involved a Nozaki−Hiyama−Kishi coupling to form the C15−C16 carbon−carbon bond, an aldol reaction to construct the C6−C7 carbon−carbon bond, and a Yamaguchi macrolactonization to complete the required skeletal framework. Biological studies with the synthesized compounds led to the identification of epothilone analogues **3**, **4**, **7**, **8**, **9**, and **11** as potent tubulin polymerization promoters and cytotoxic agents with (12*R*,13*S*,15*S*)-cyclopropyl 5-methylpyridine epothilone A (**11**) as the most powerful compound whose potencies (e.g. IC_{50} = 0.6 nM against the LA9 ovarian carcinoma cell line) approach those of epothilone B. These investigations

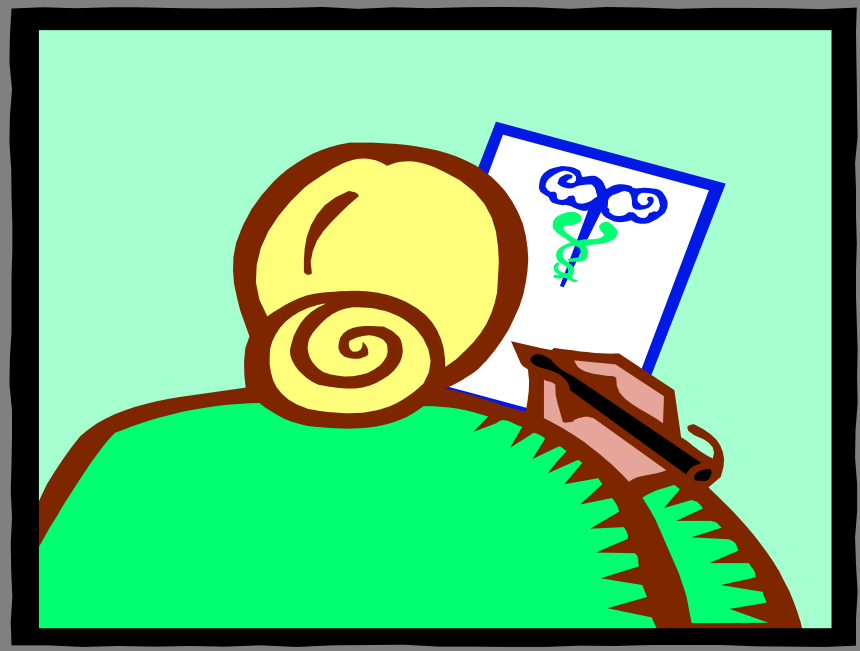
1 of 11 8.5 x 11 in

Done Internet

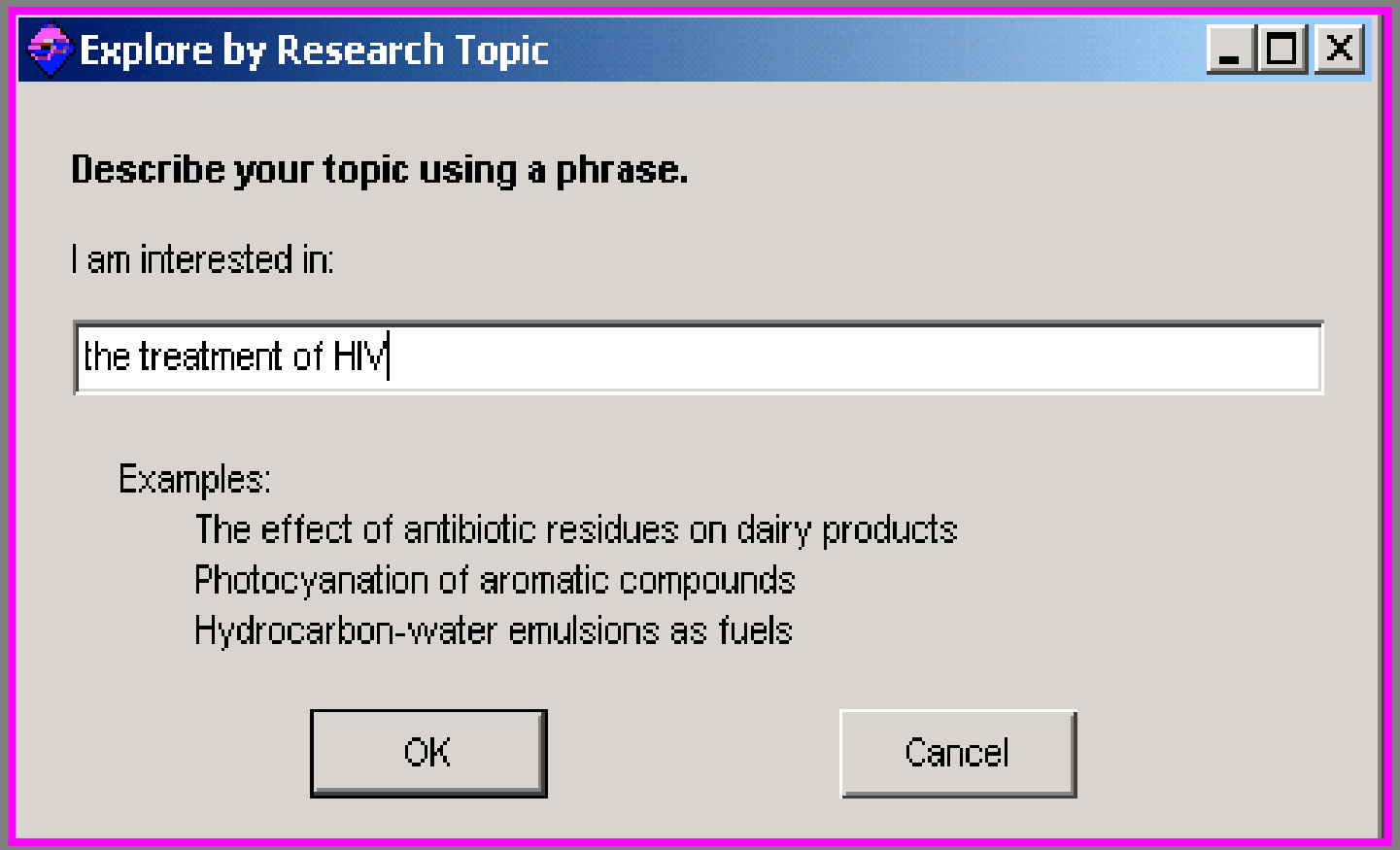
The desired full-text (continued)



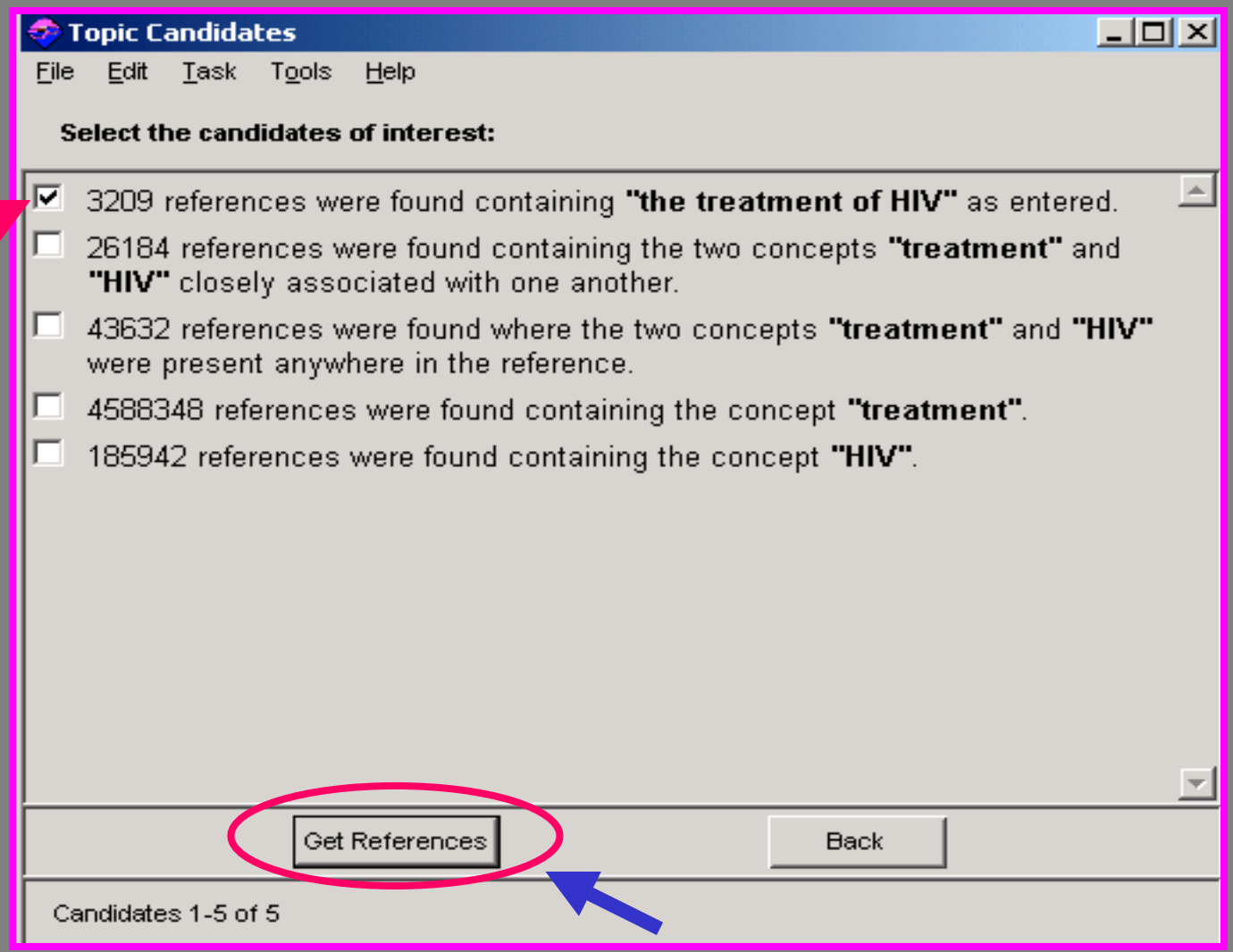
Interested in “The treatment of HIV”?



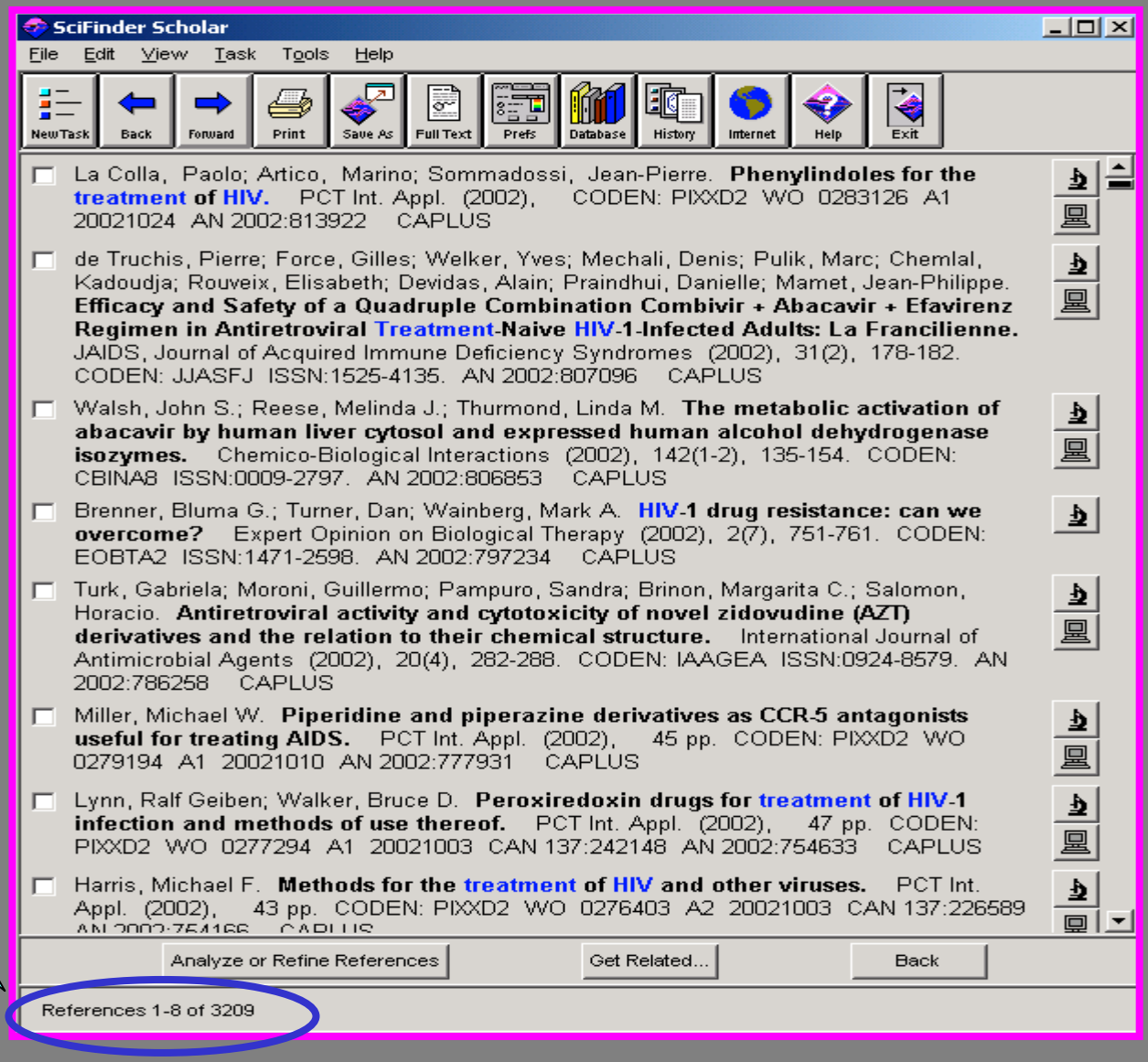
Enter the topic of interest



Select candidates of interest

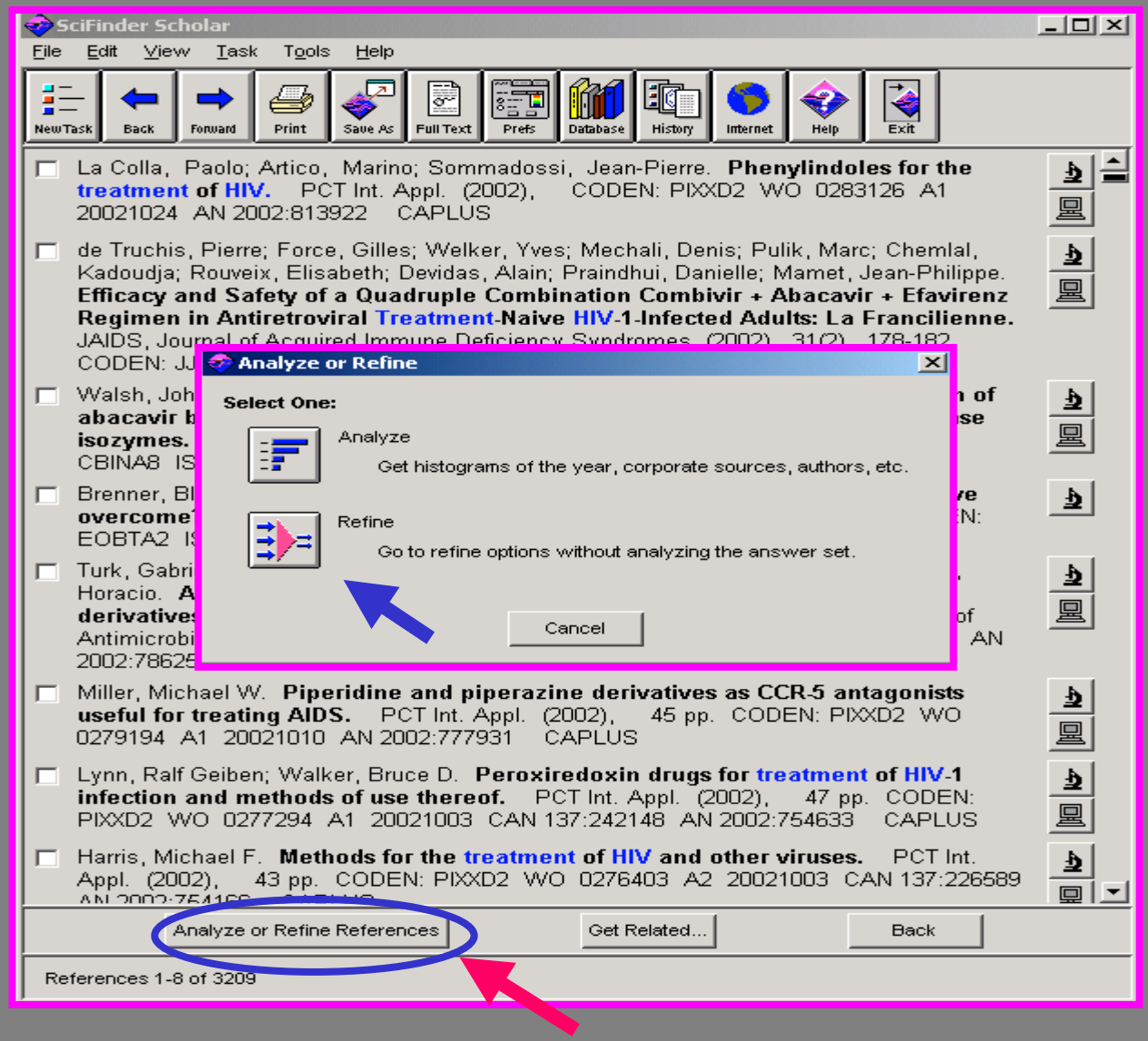


Here are the references!

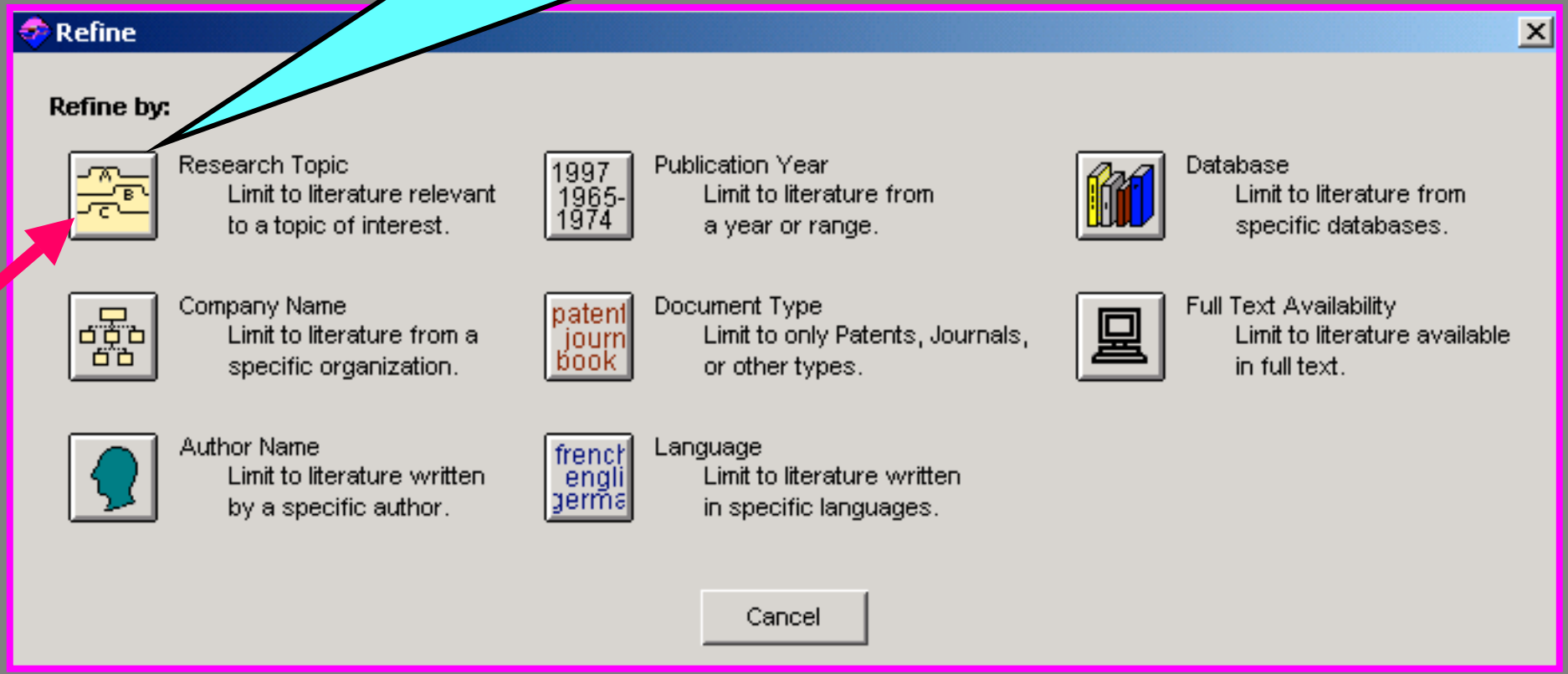


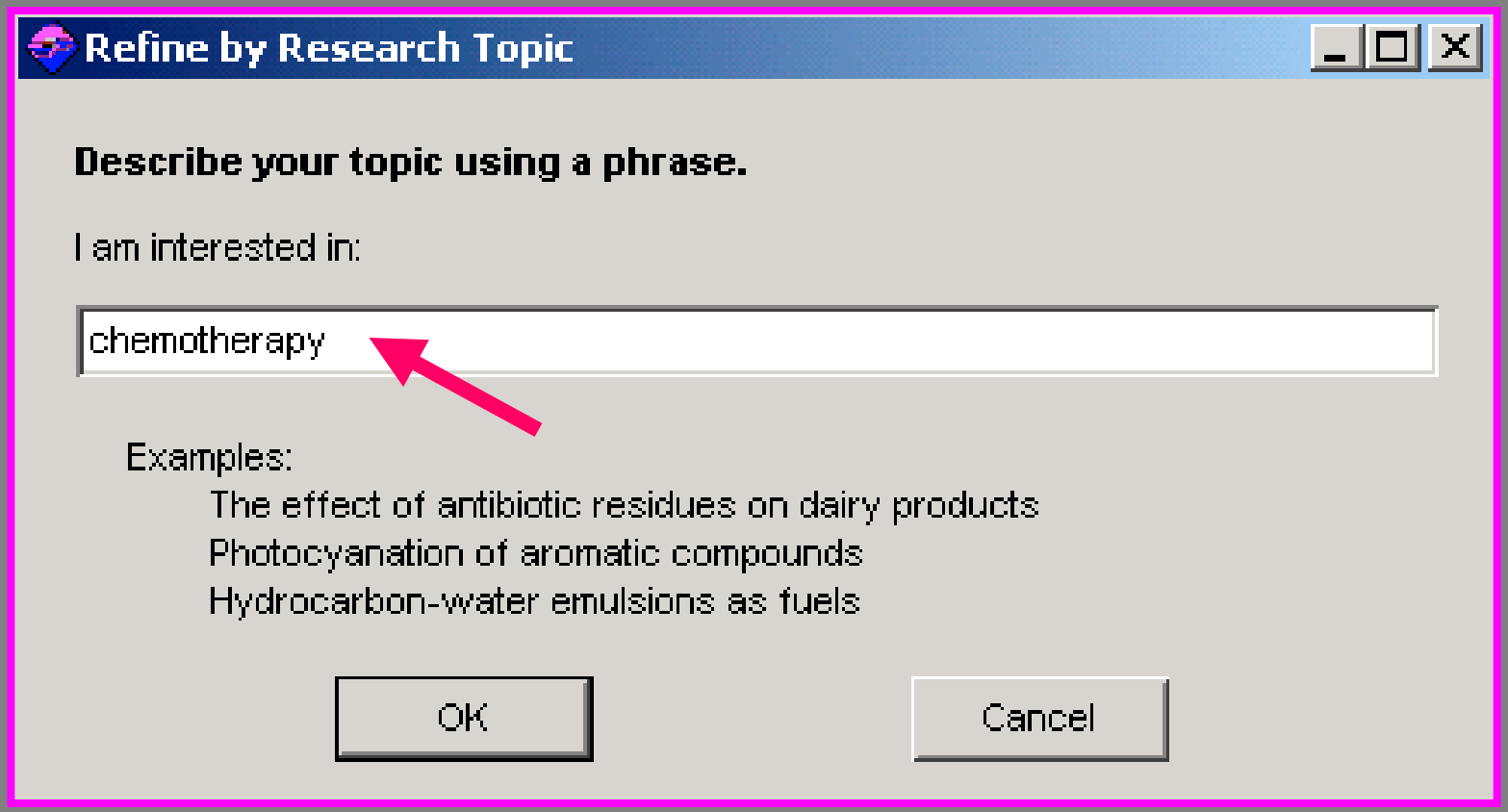
3209 references

Narrow down the answer set

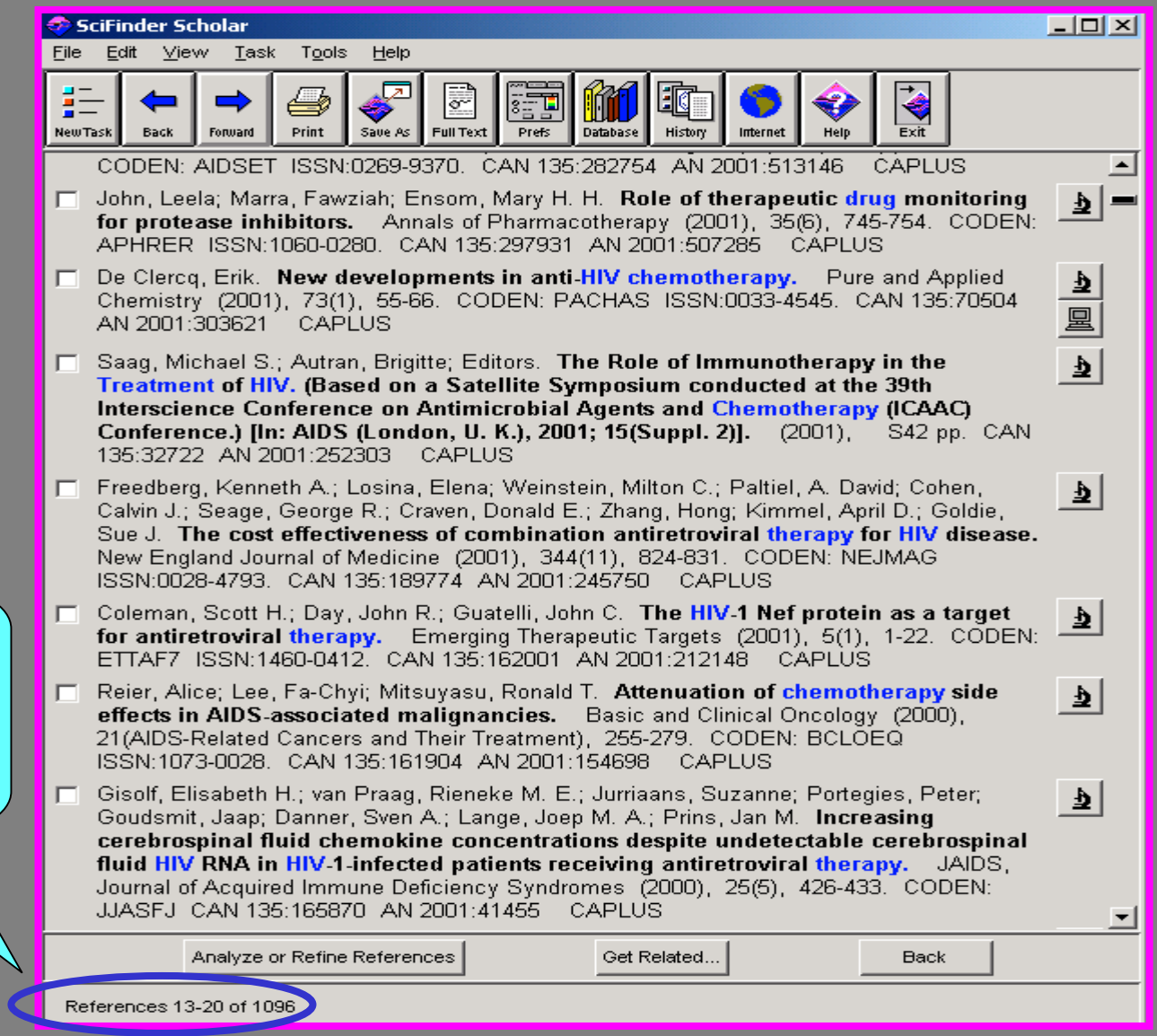


Refine by research topic



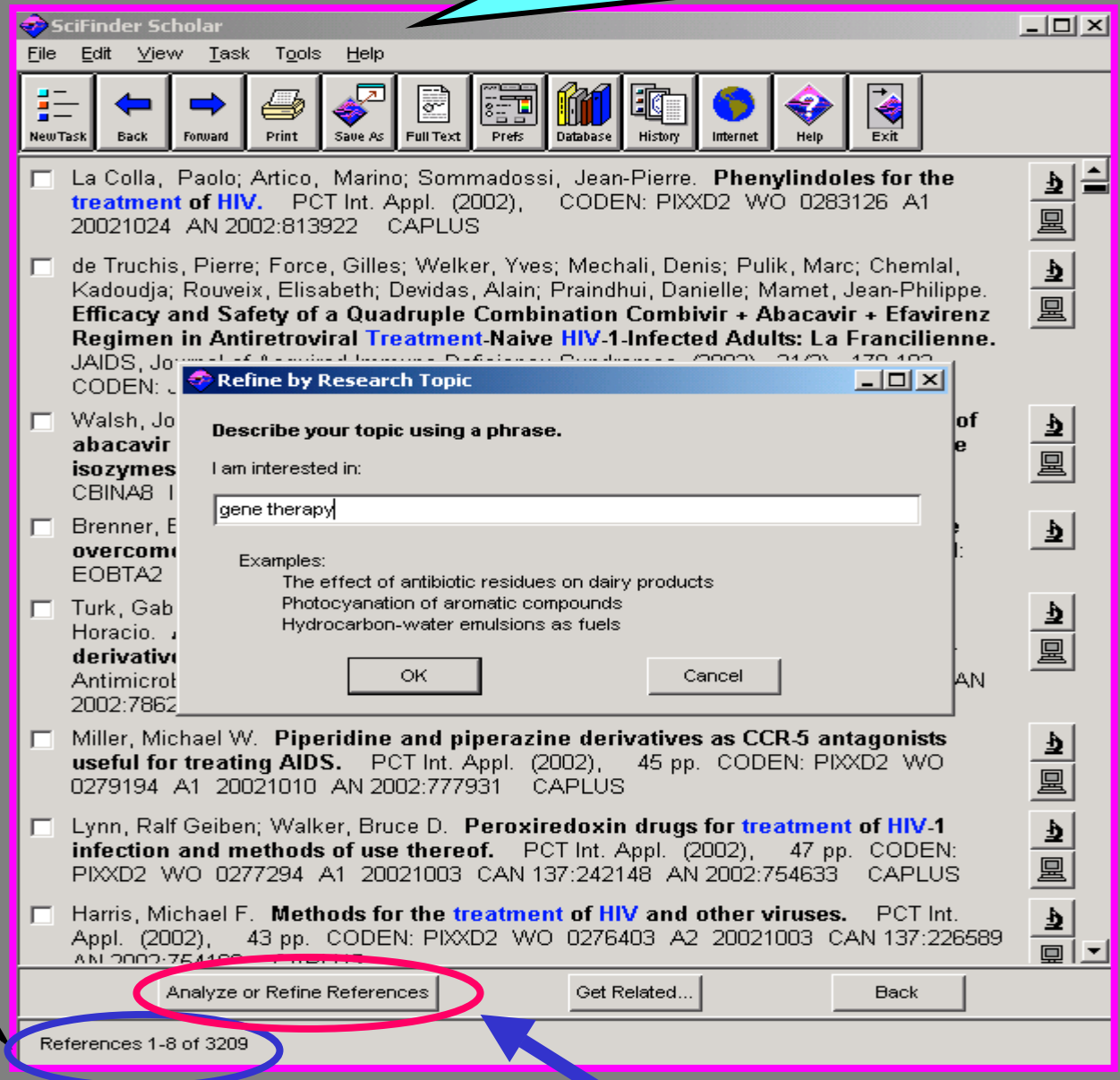

Refine by Research Topic
Describe your topic using a phrase.
I am interested in:
chemotherapy
Examples:
The effect of antibiotic residues on dairy products
Photocyanation of aromatic compounds
Hydrocarbon-water emulsions as fuels
OK
Cancel

Here are the references!



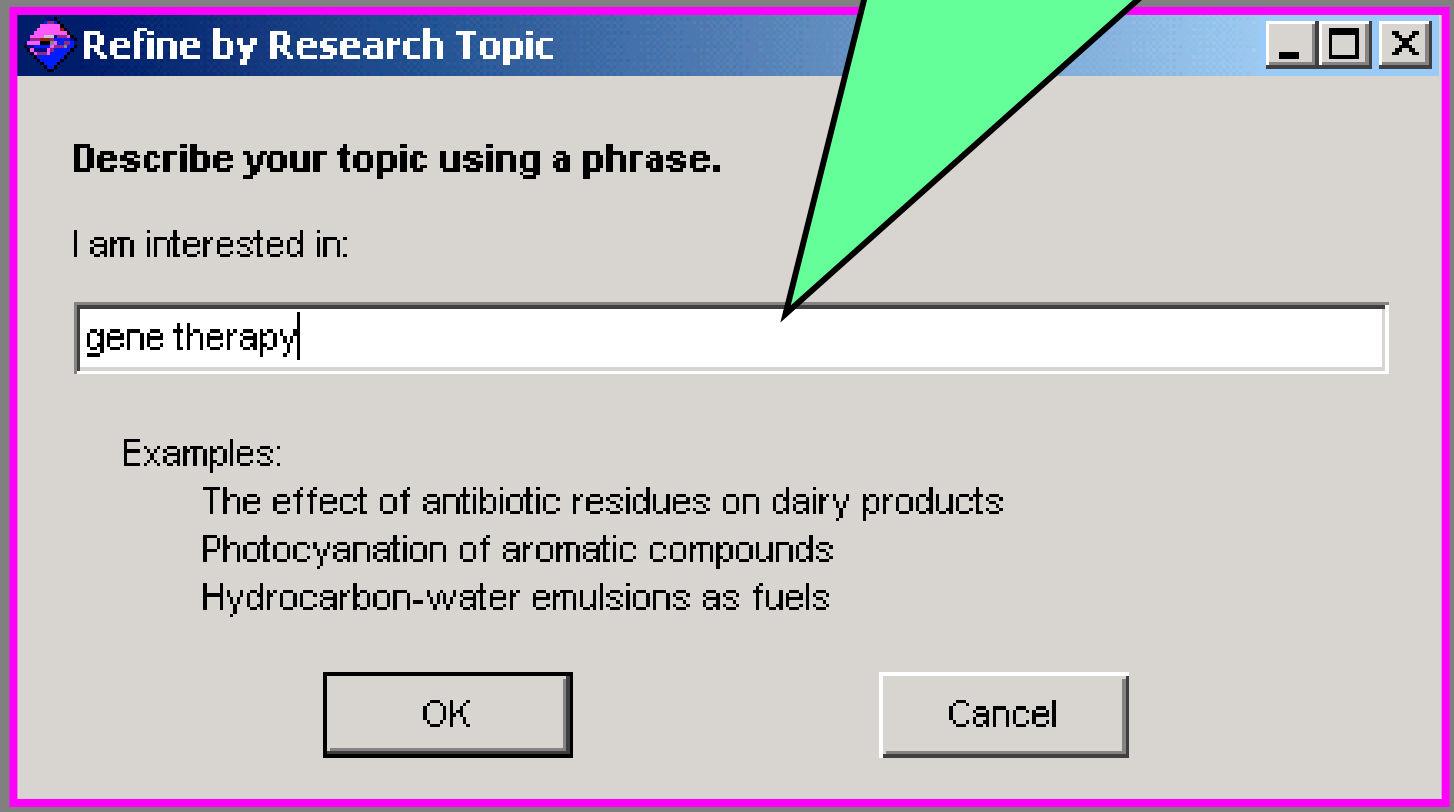
1096 references

Let's narrow down to other area of interest

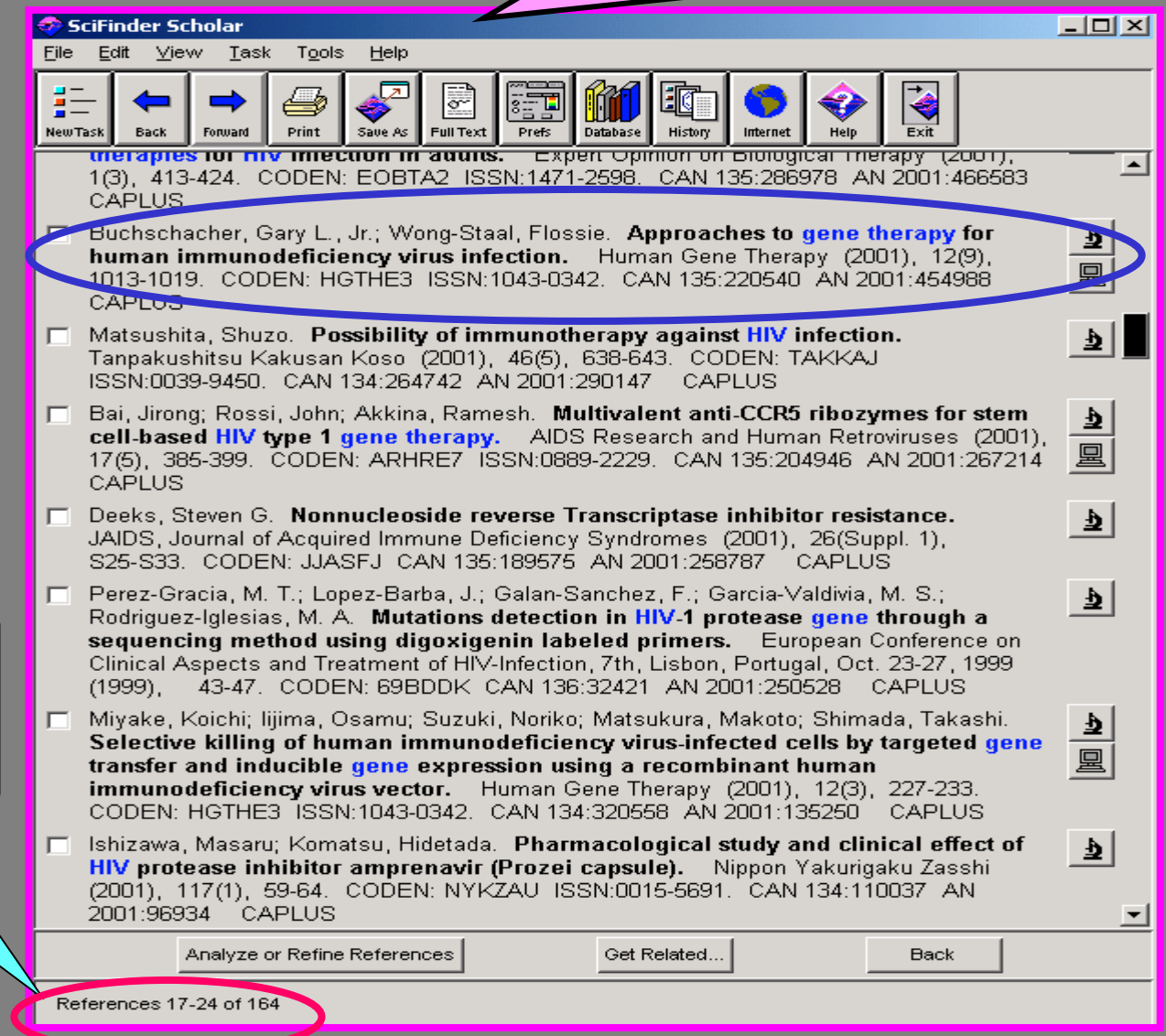


3209 references

Enter topic of interest

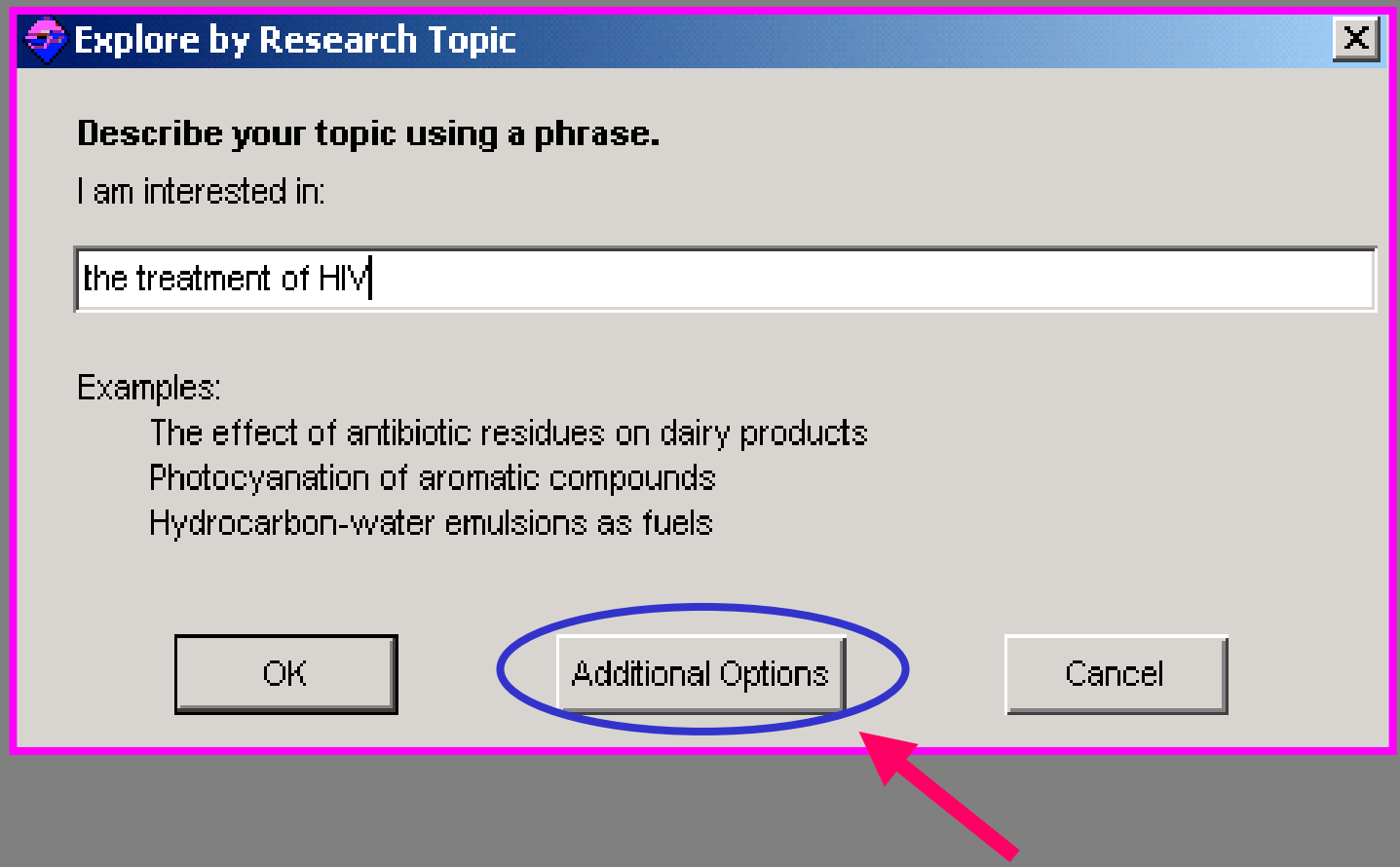


Here are the references about gene therapy!

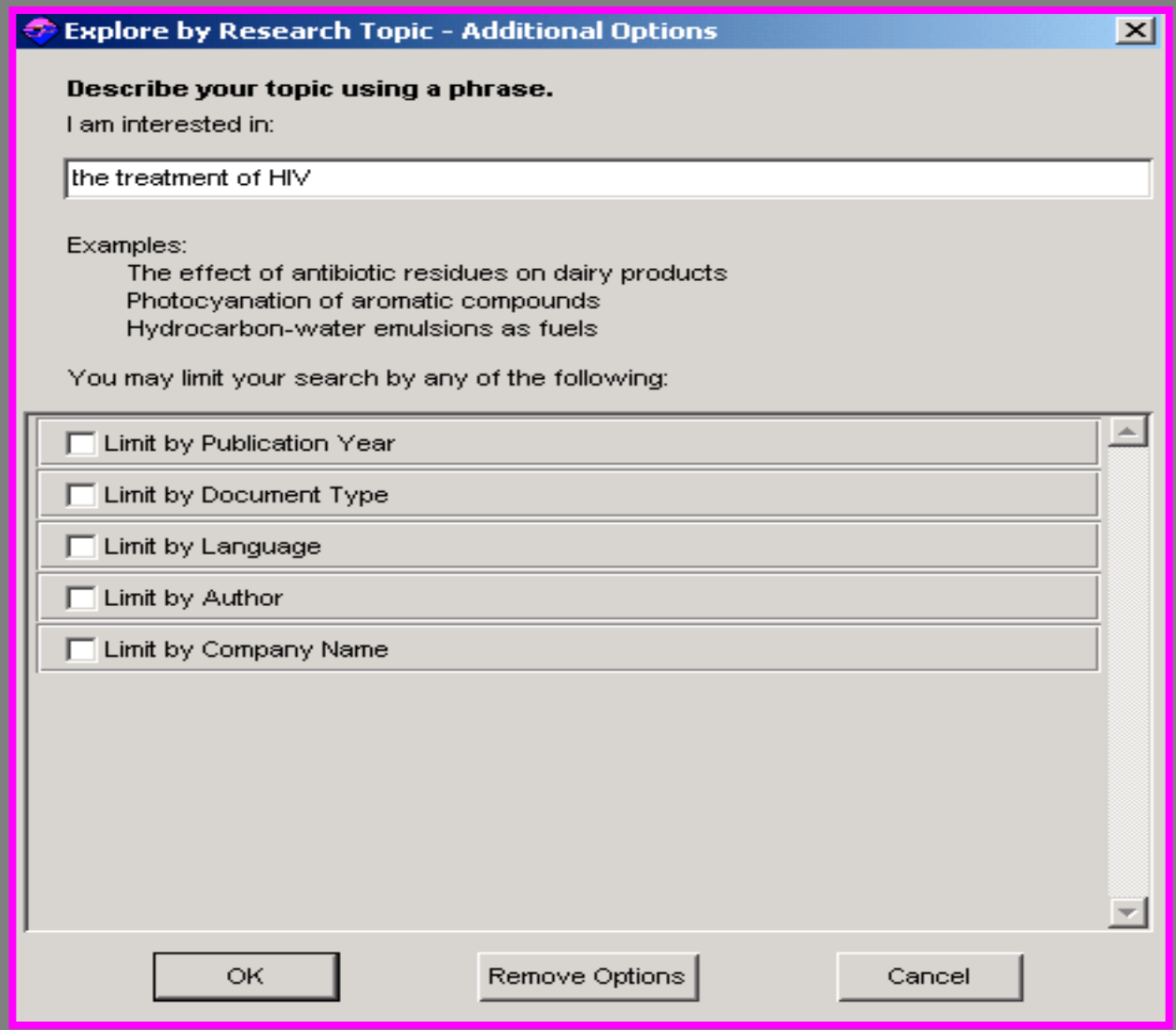


164 references

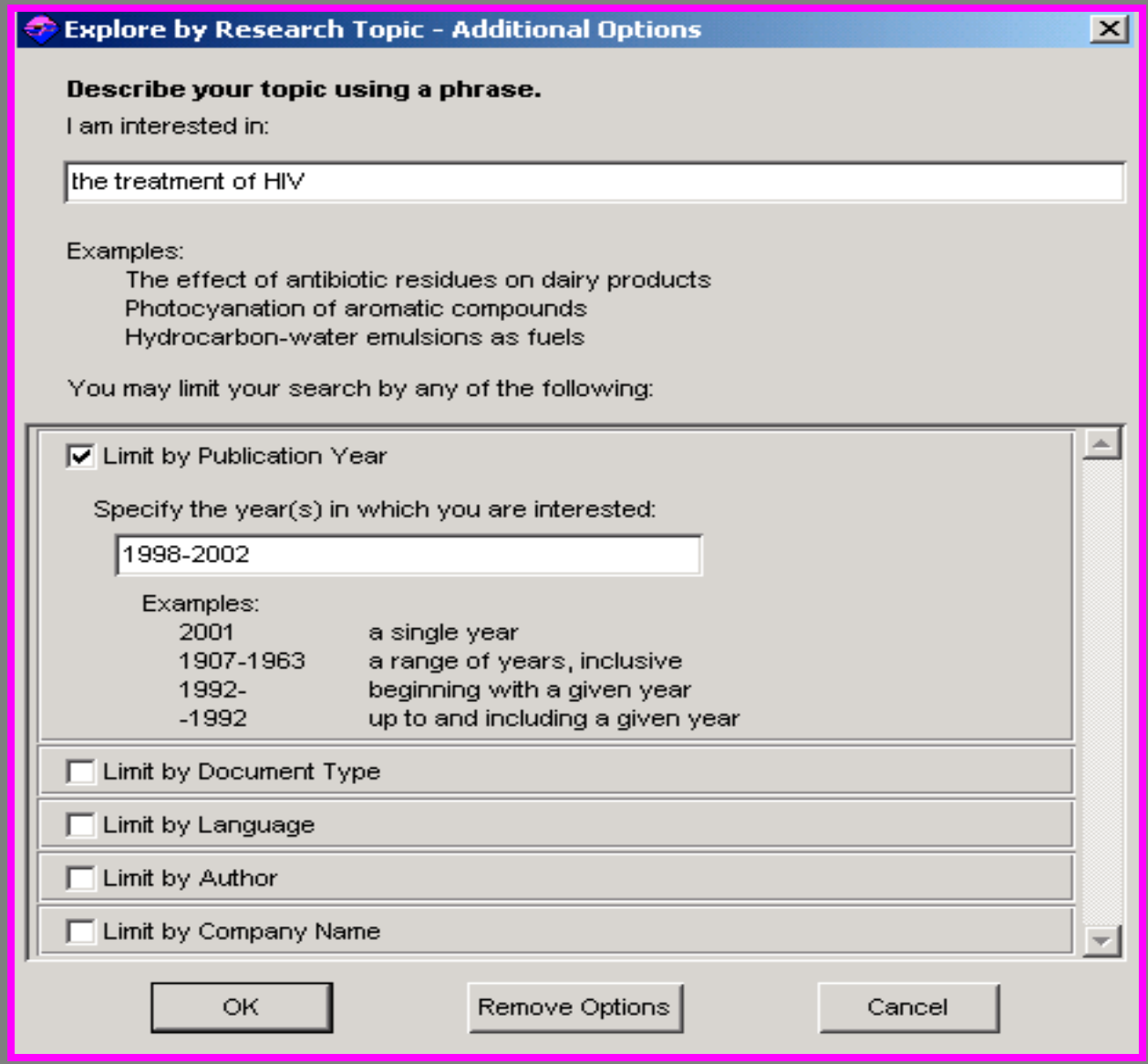
Select Additional Options



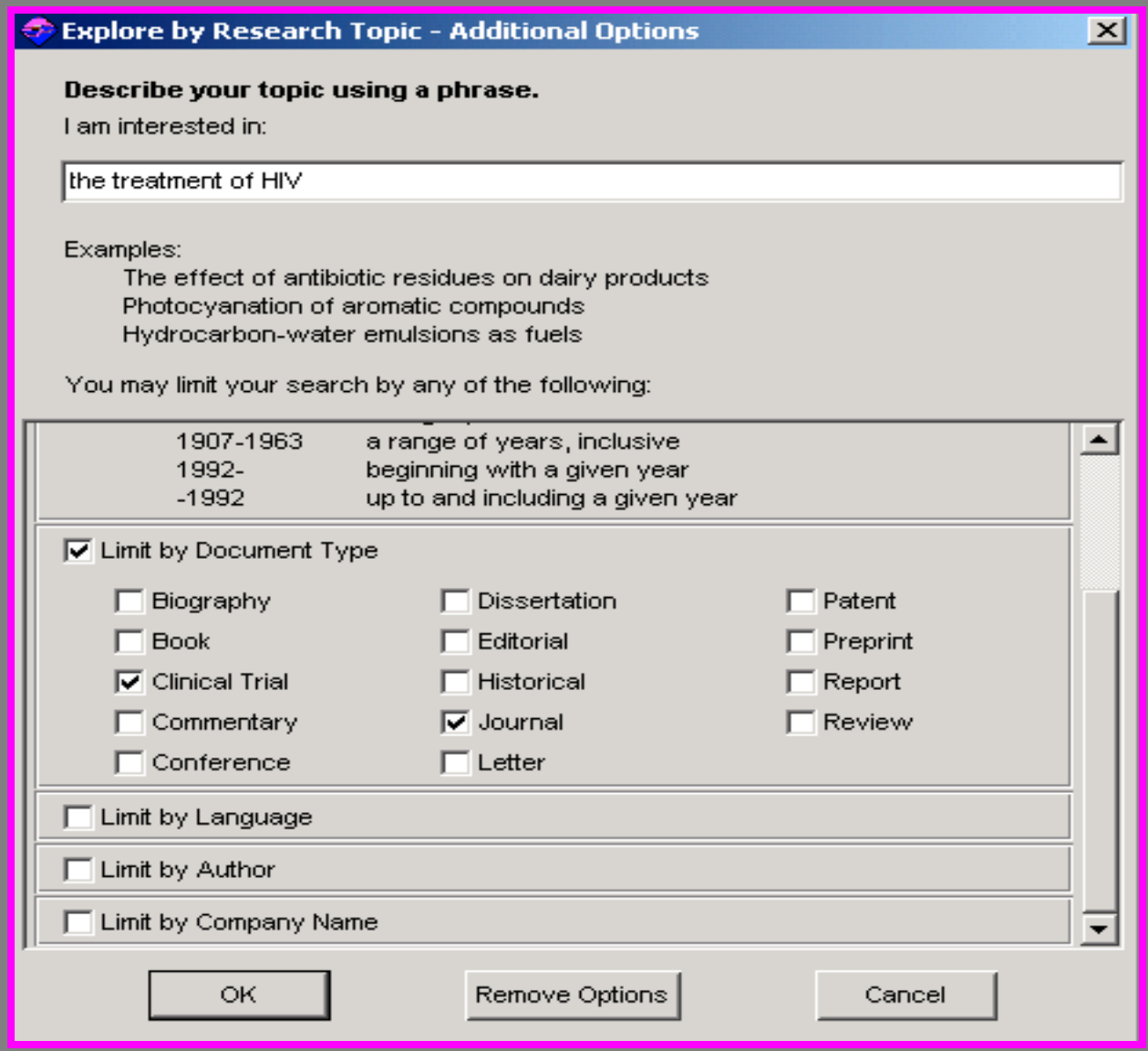
Limit your search



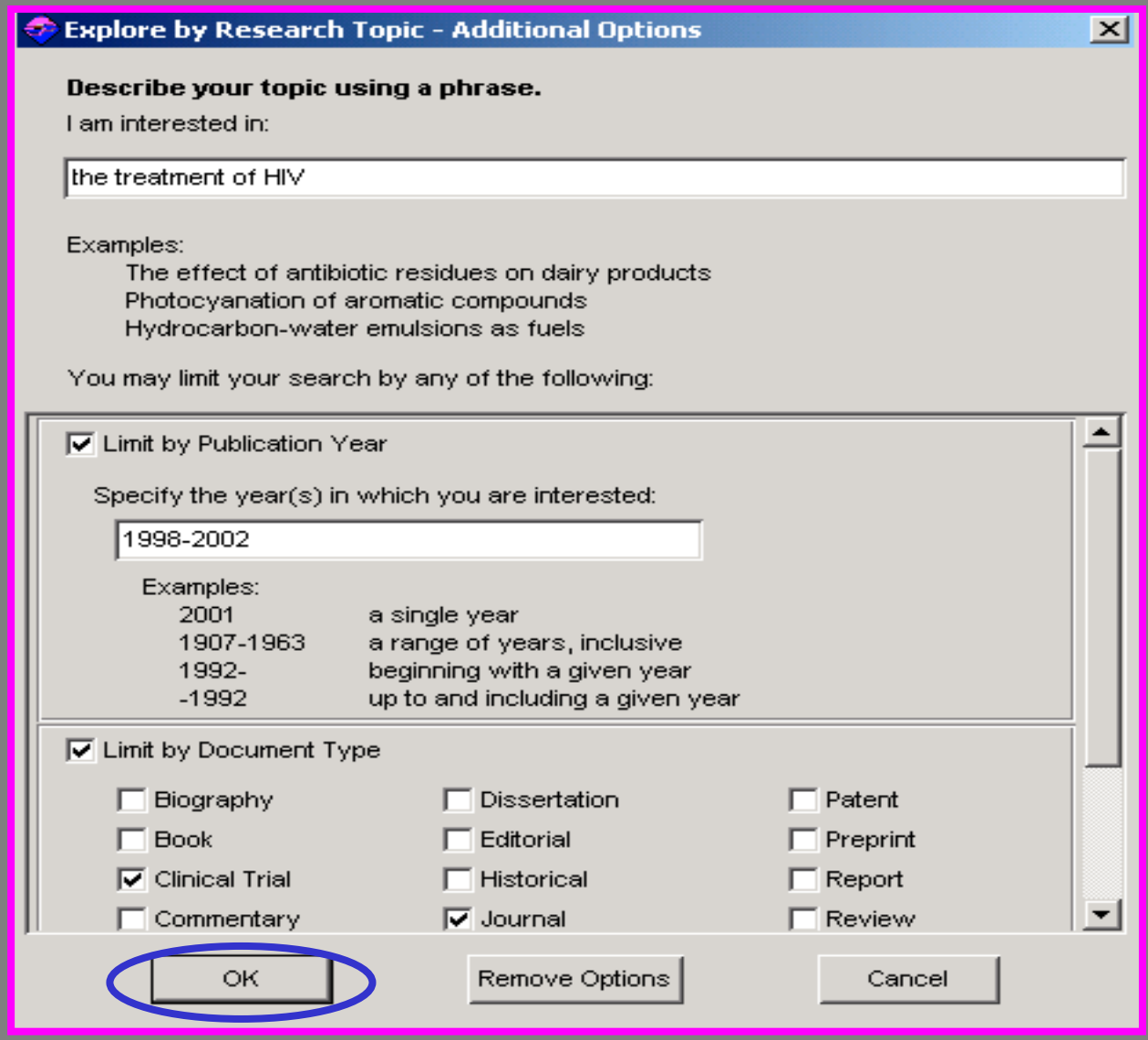
Limit by Publication Year



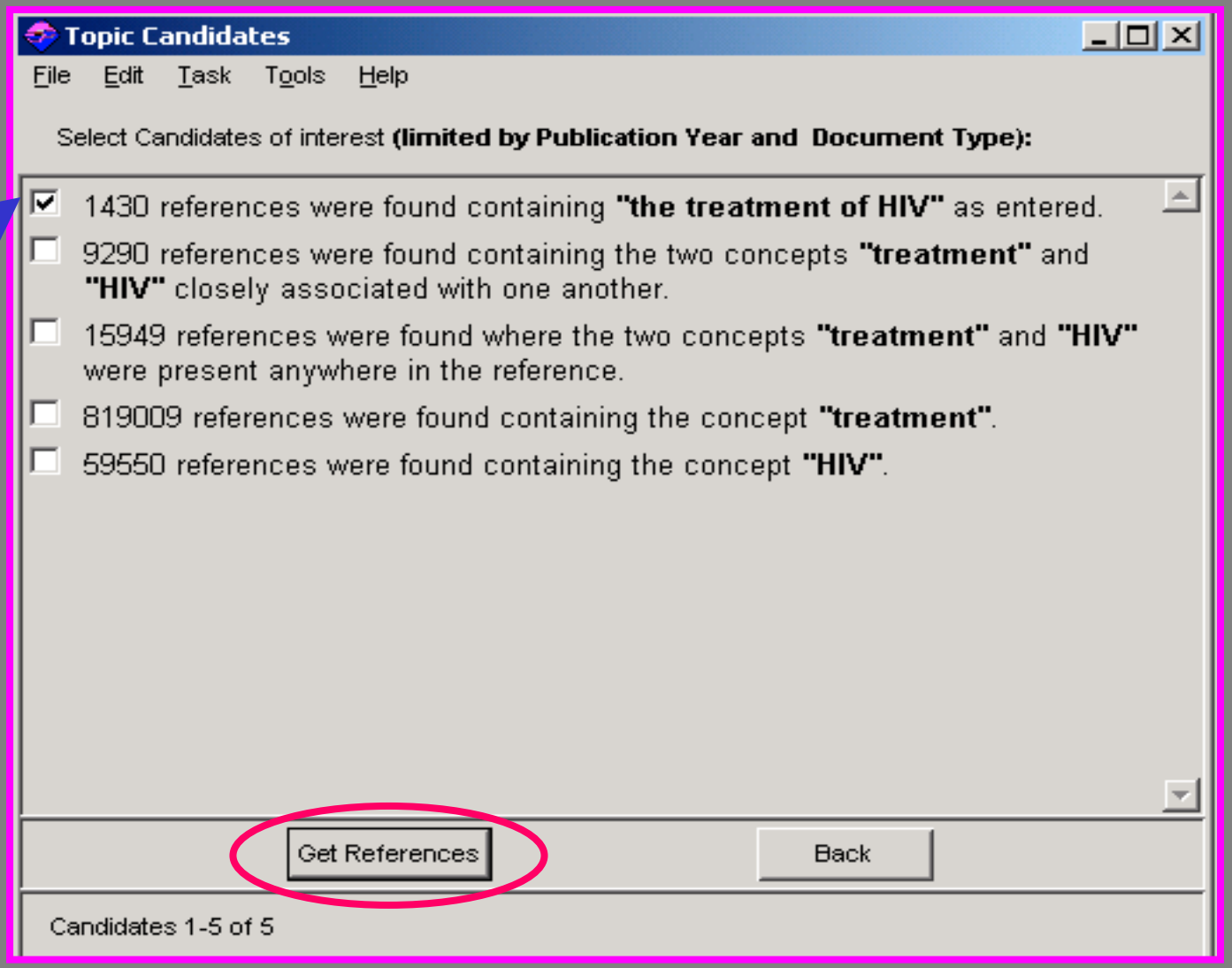
Limit by Document Type



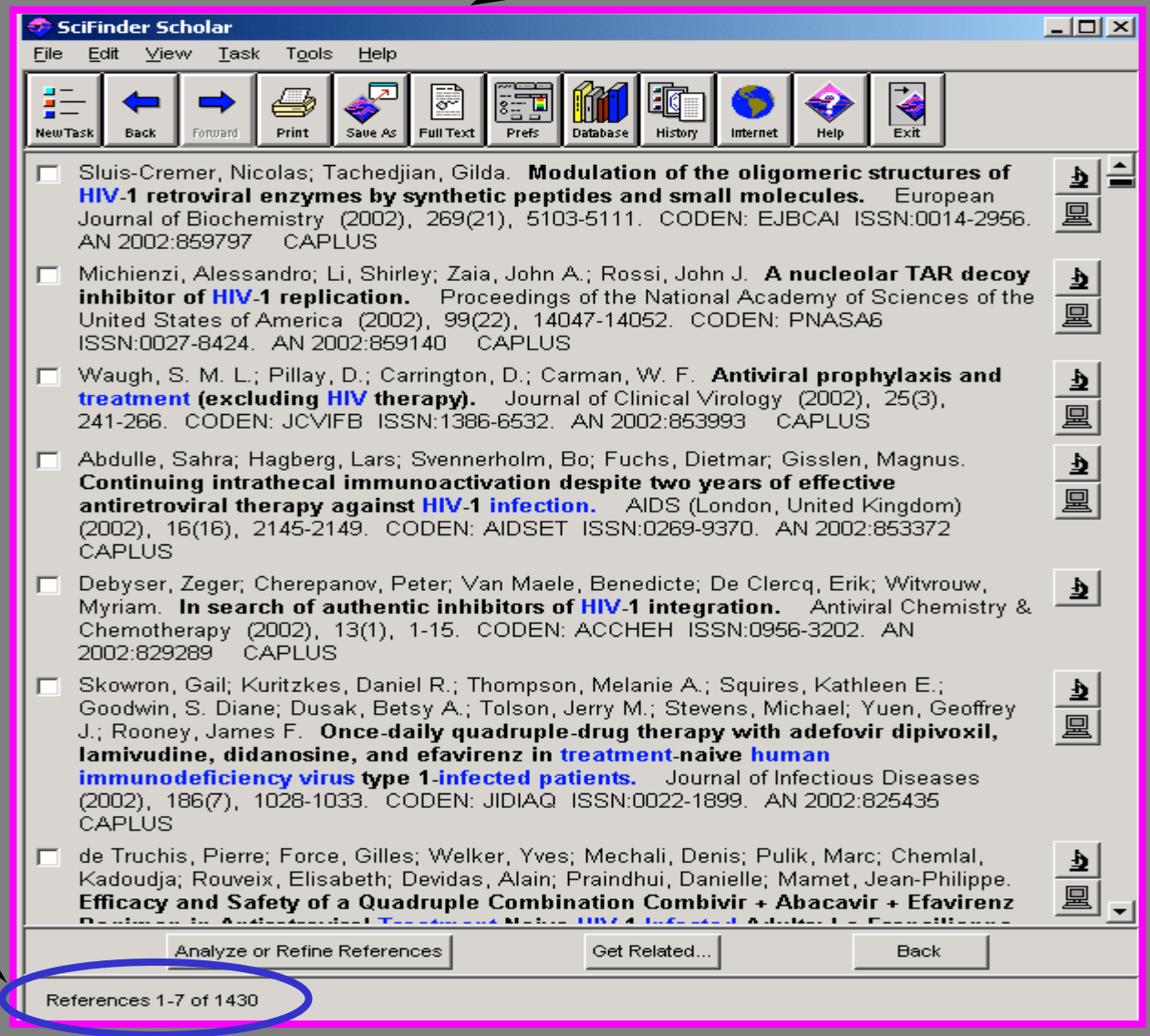
Limit by Publication Year and Document Type



Select candidates of interest



Here are the references after limiting the search!

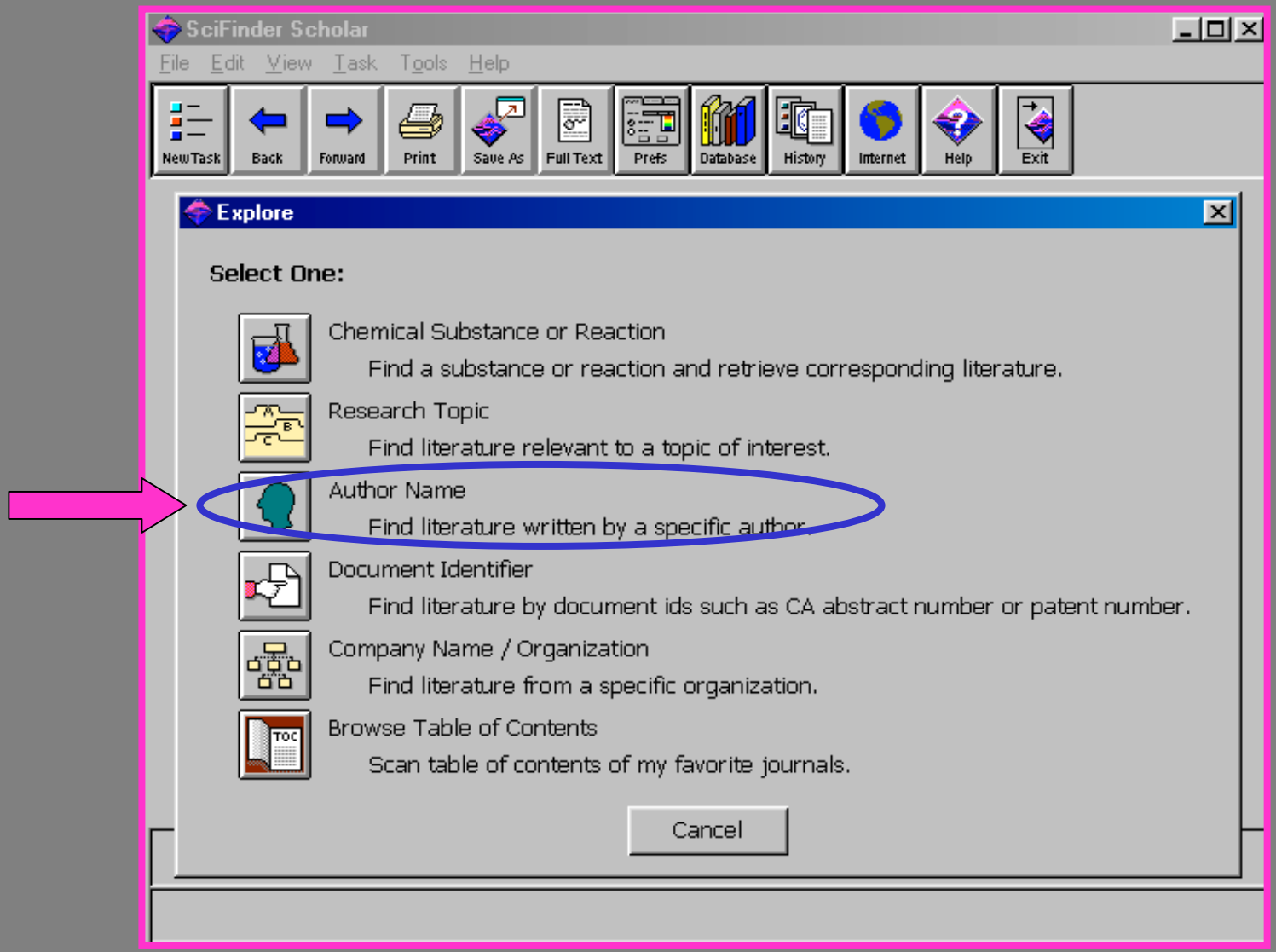


1430 references

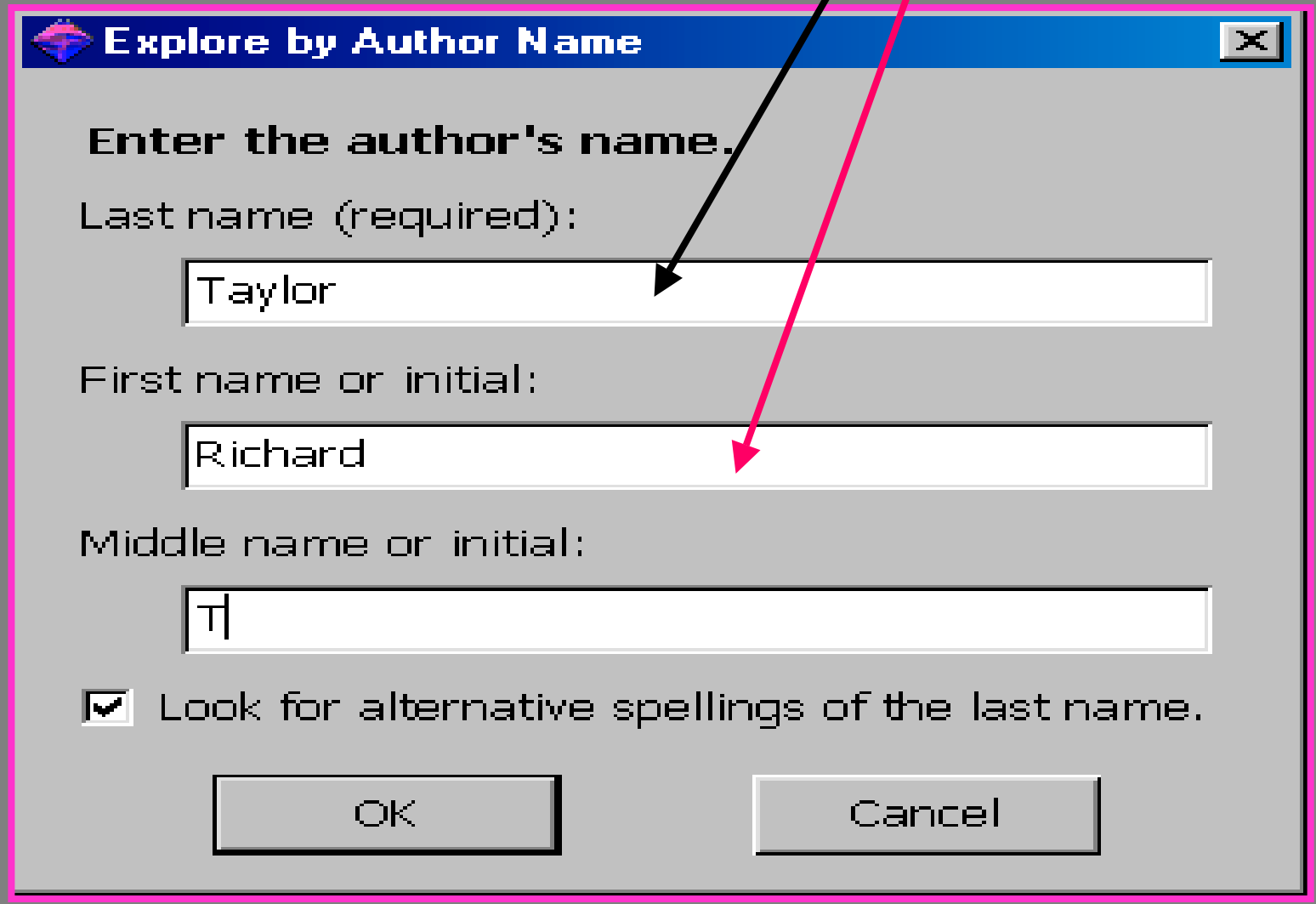
Next

Explore by Author Name

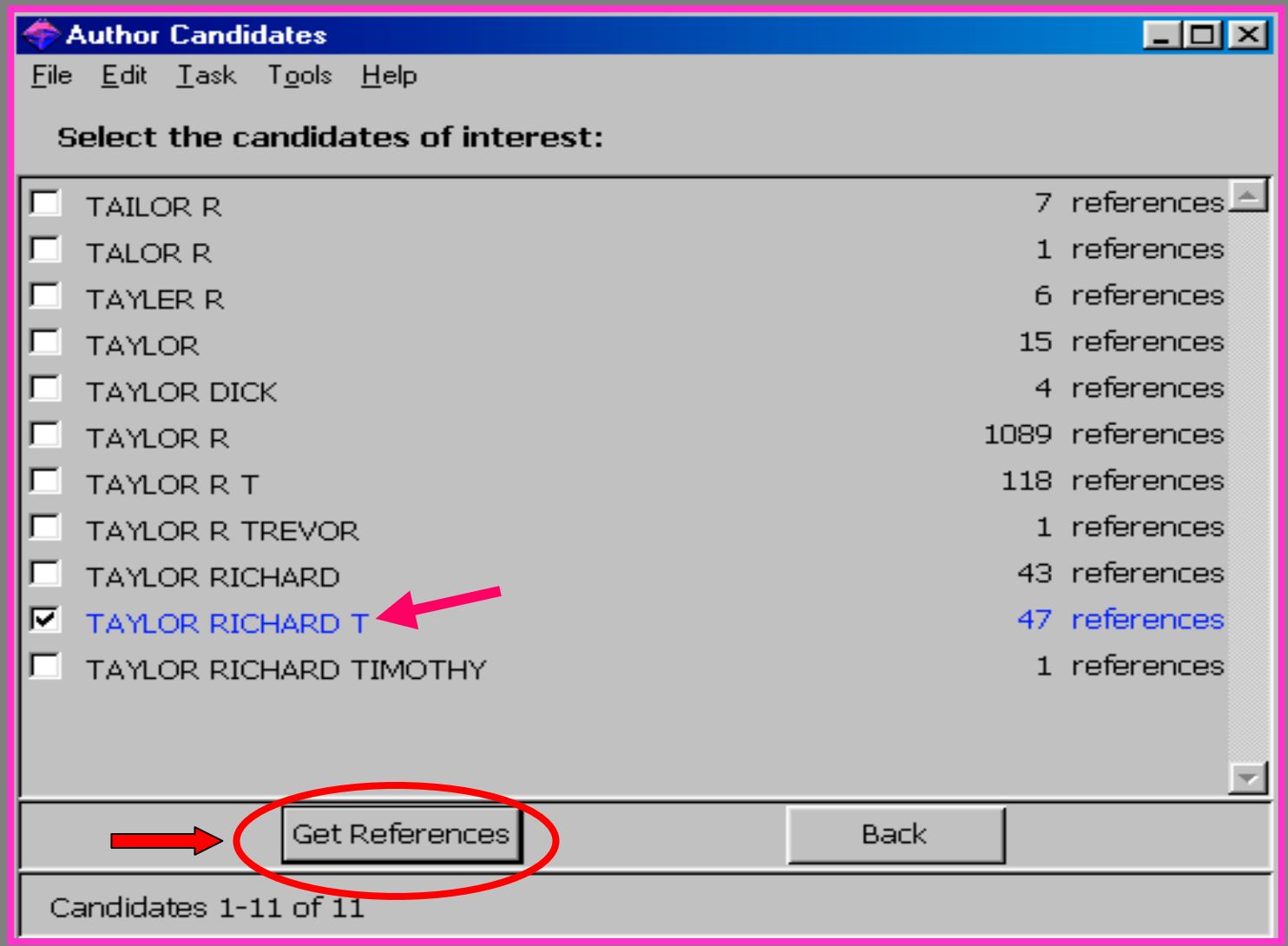
Explore by Author Name



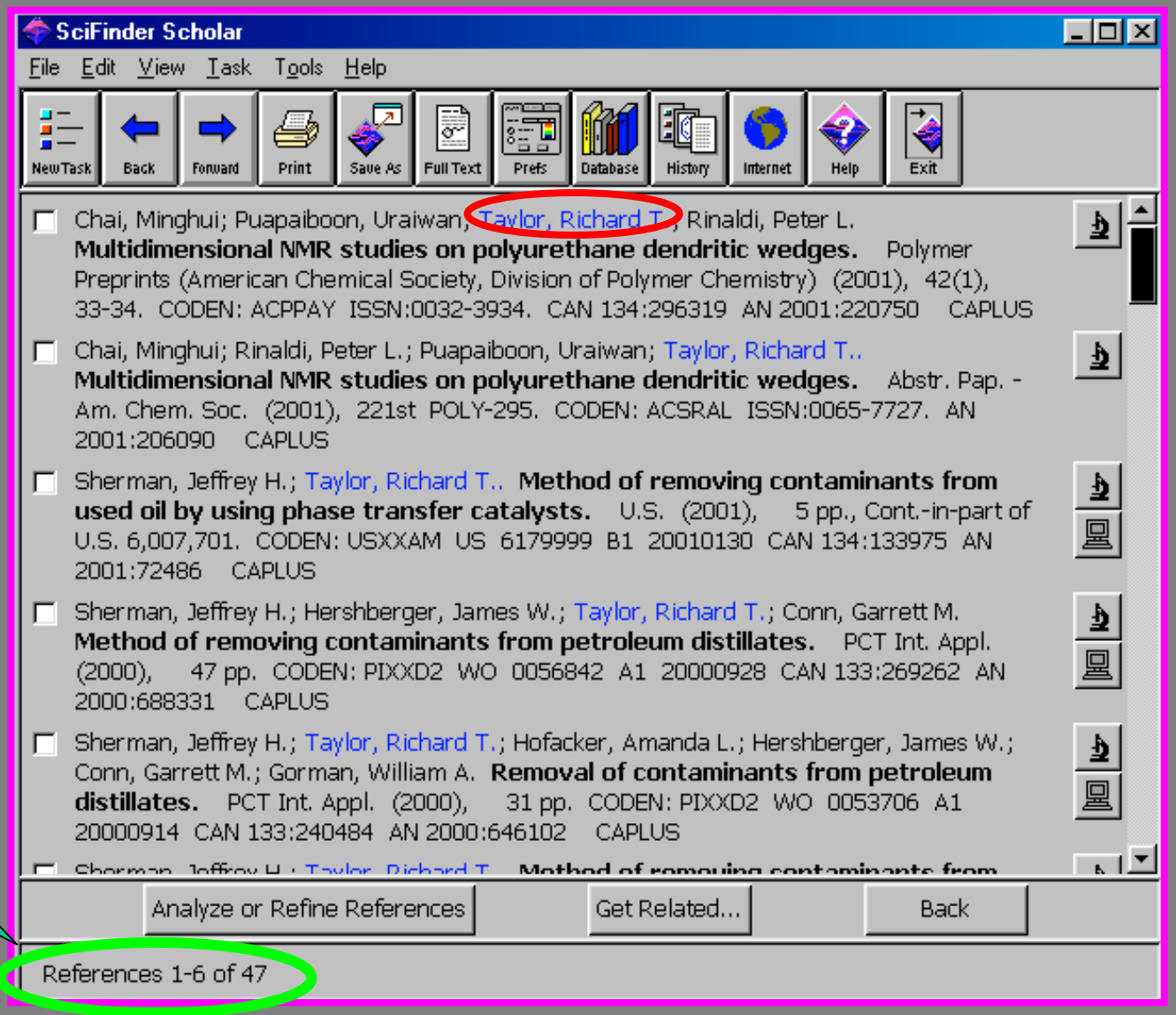
Enter the author’s name



Select the candidates of interest

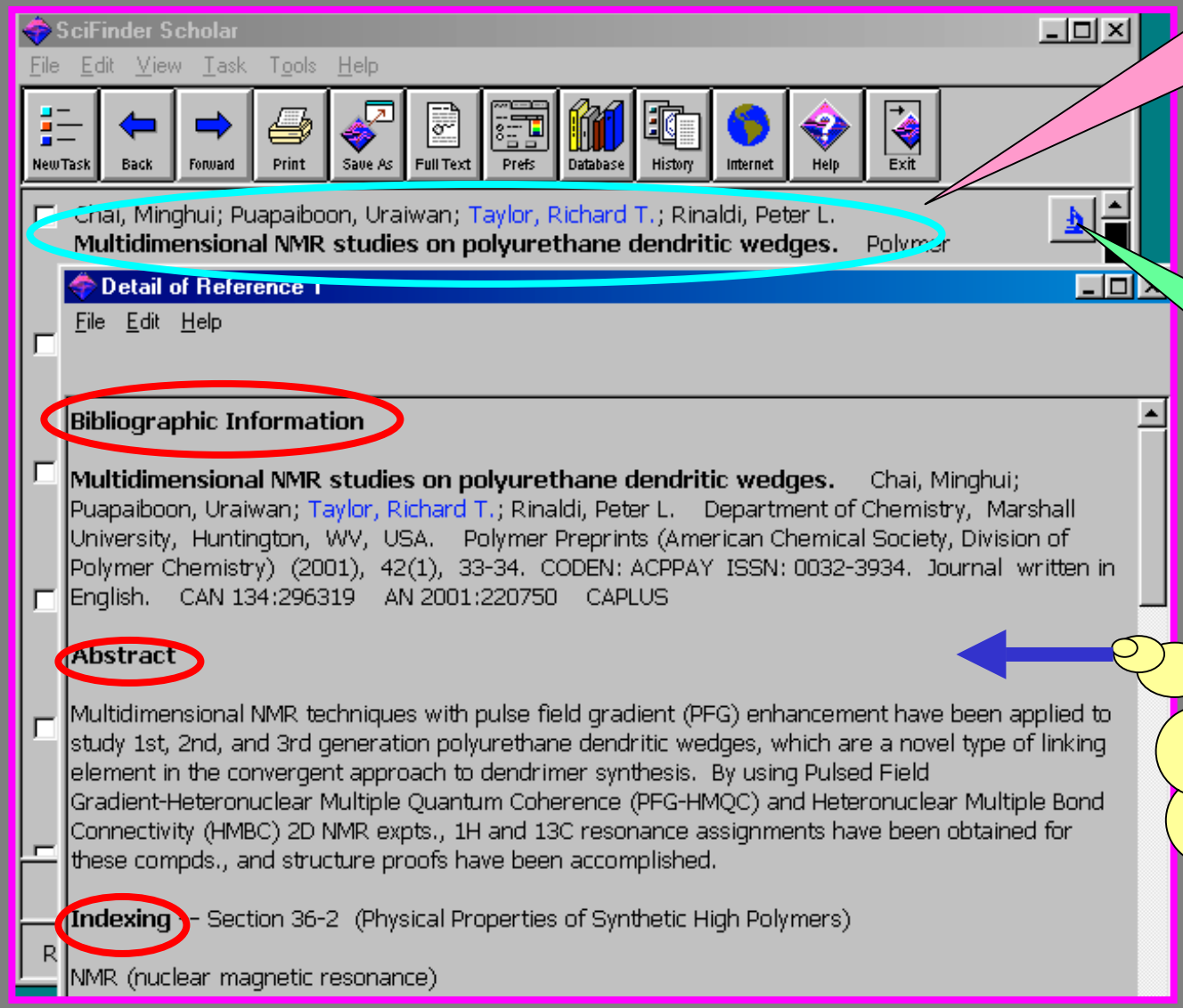


Here are the author's work!



Number of references retrieved

View Detail of Reference



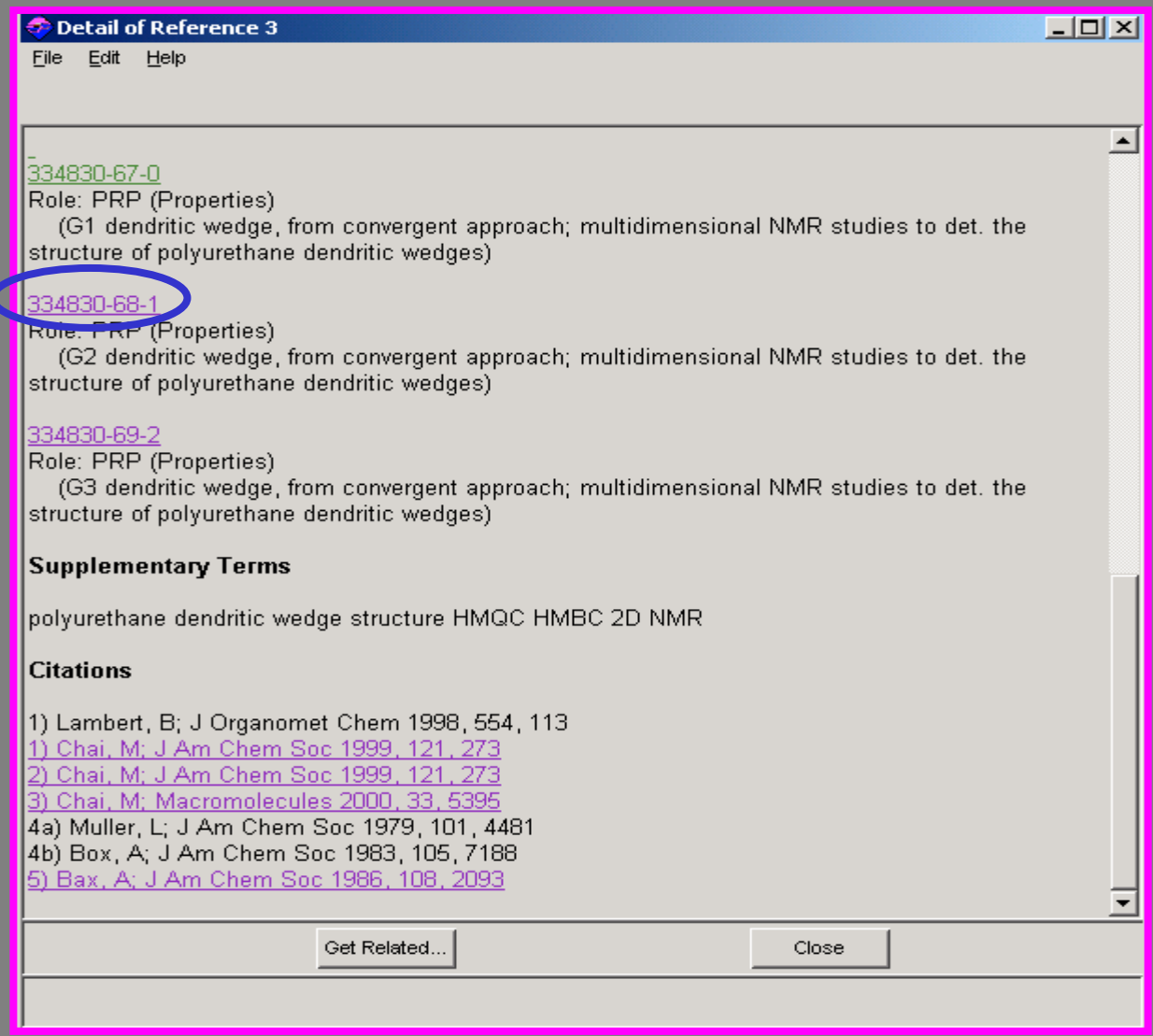
Interested in this reference?

microscope

Here is the detail !

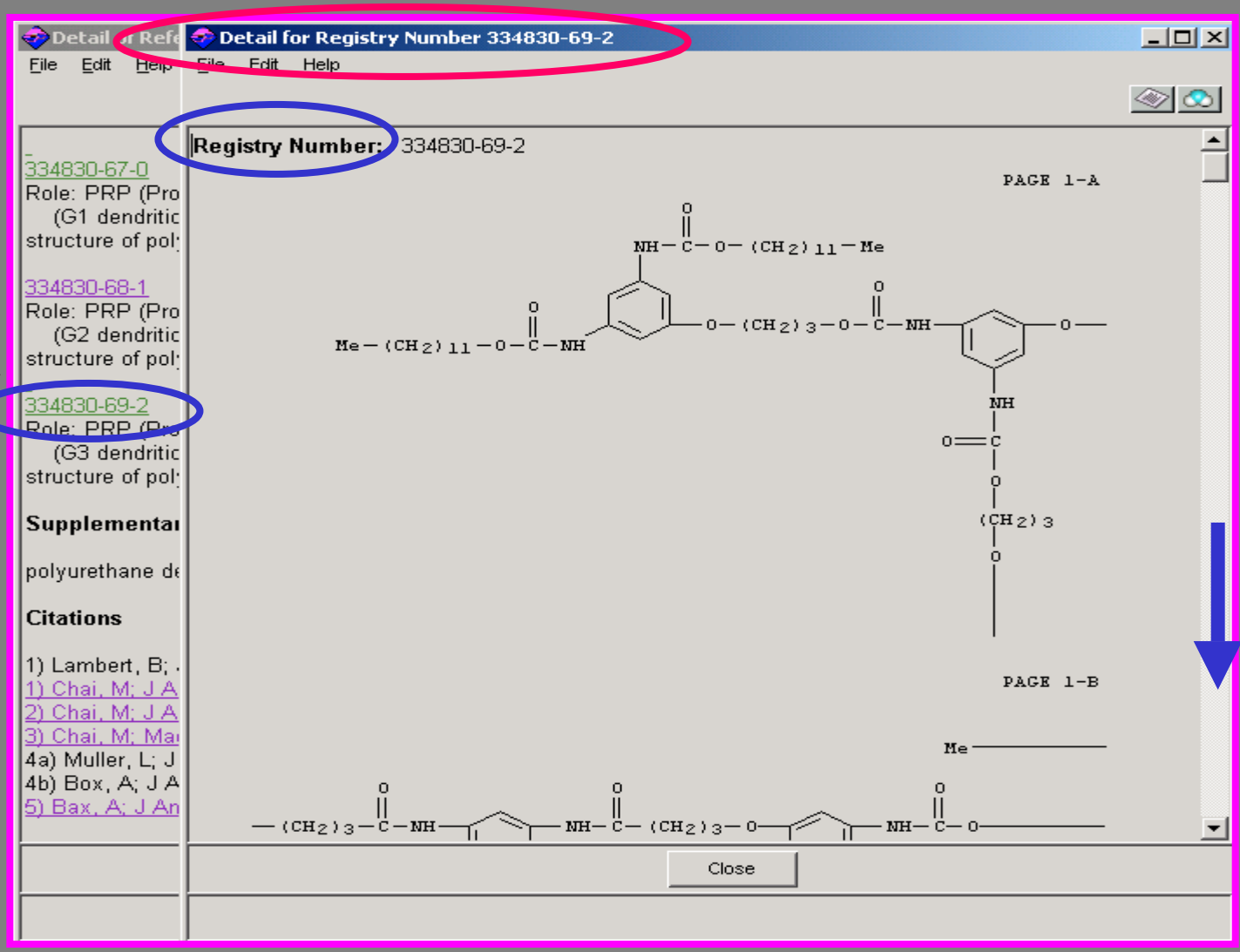
Detail of Reference 1 (continued)

Registry number



View detail of substance in the reference of interest

Hyperlink

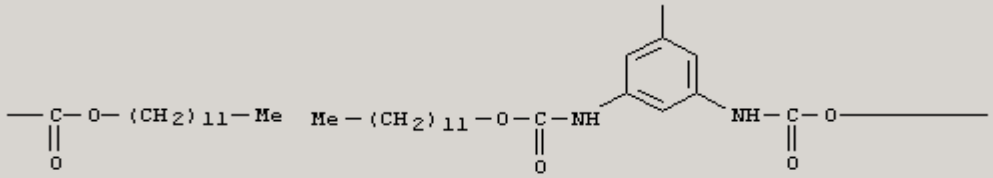


Hyperlink
To view
3D Structure

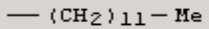
Detail for Registry Number 334830-69-2

File Edit Help

PAGE 2-B



PAGE 2-C



Formula: C173 H278 N14 O34

CA Index Name: Carbamic acid, [[5-(3-hydroxypropoxy)-1,3-phenylene]bis[imino(4-oxo-4,1-butanediyl)oxy-5,1,3-benzenetriyl]]tetrakis-, tetrakis[3-[3,5-bis[[(dodecyloxy)carbonyl]amino]phenoxy]propyl] ester (9CI)

-- **Resources** --

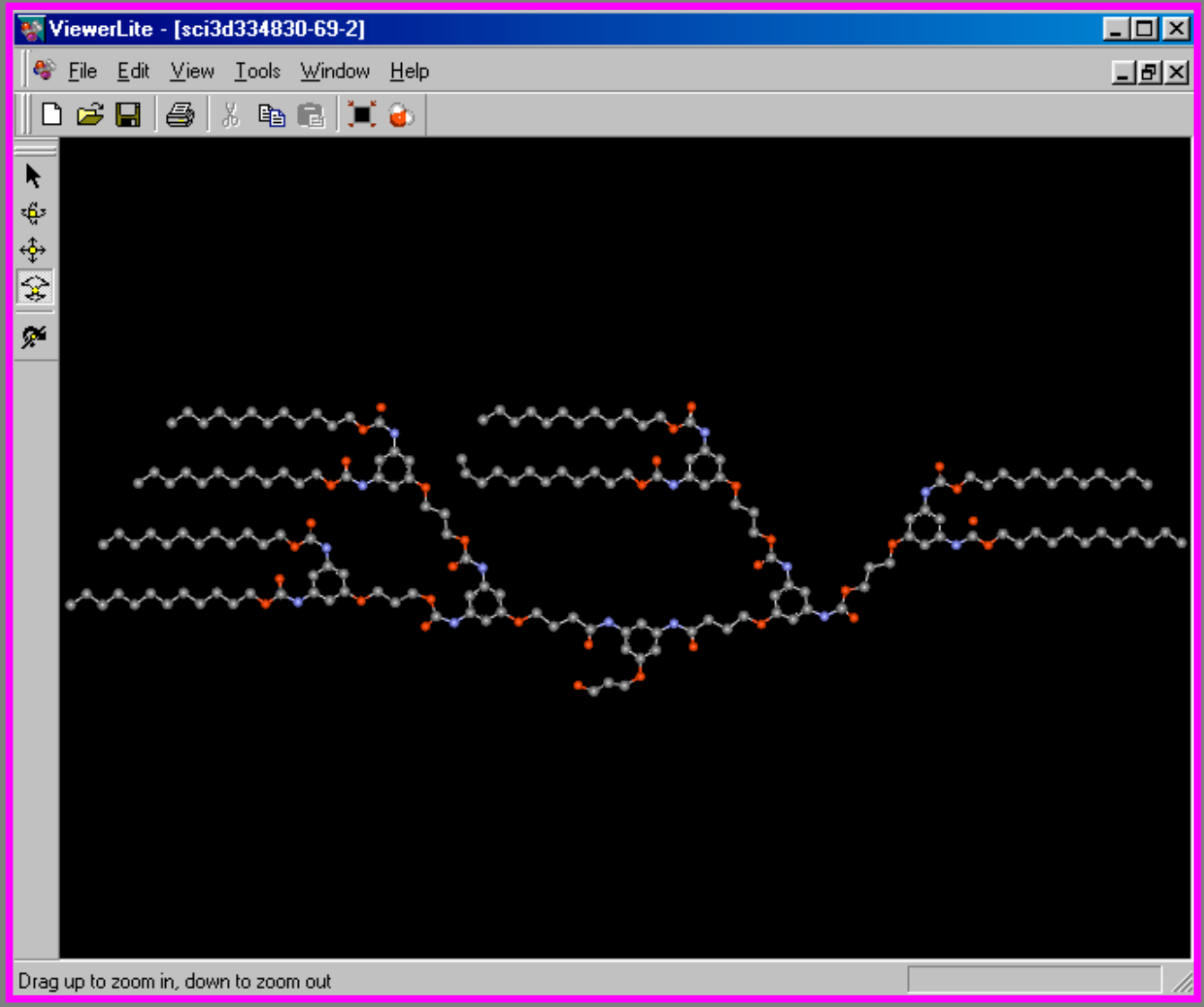
References: ~1

STN Files: CAPLUS, CA

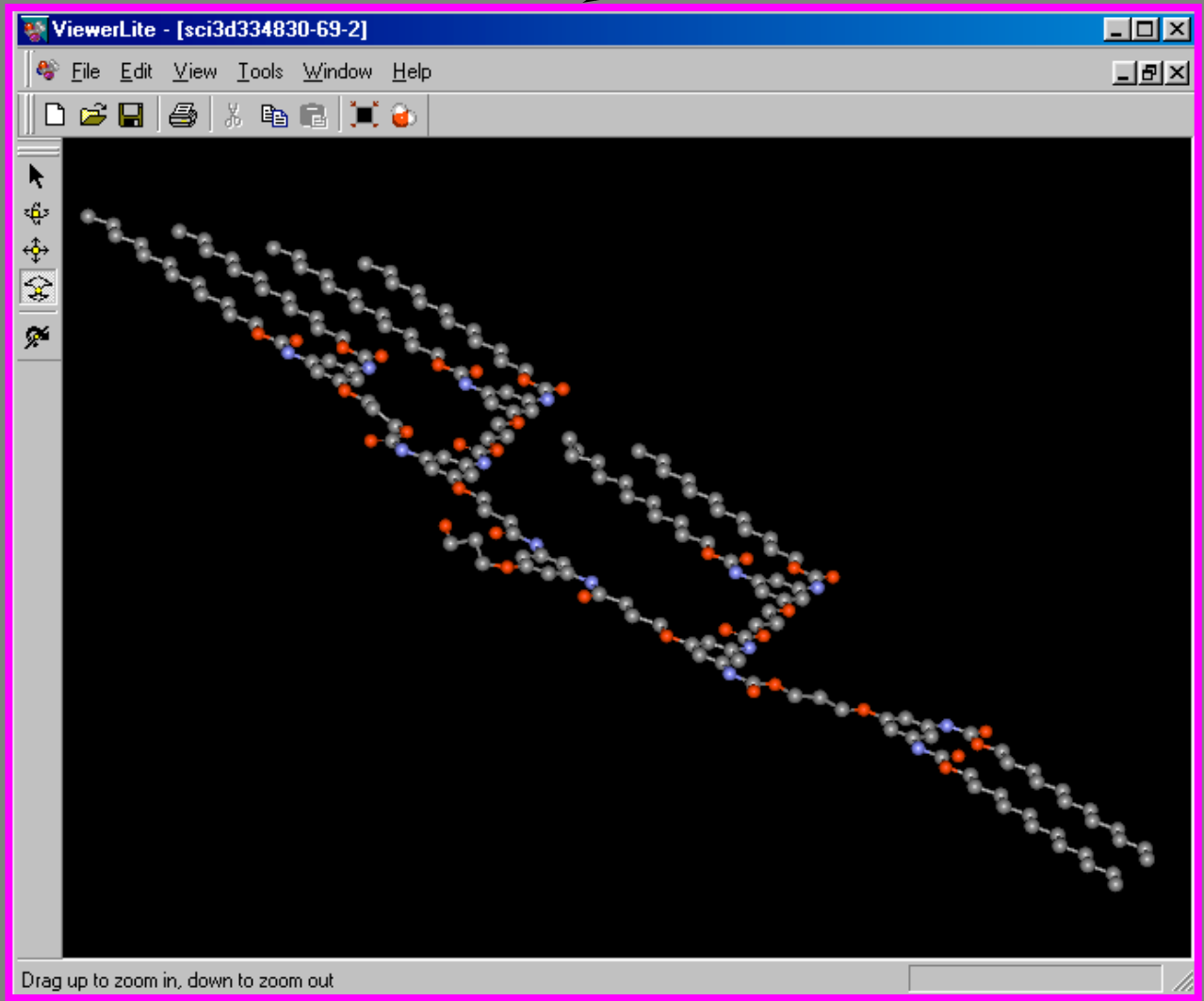
Database: REGISTRY

Close

View 3D structure !

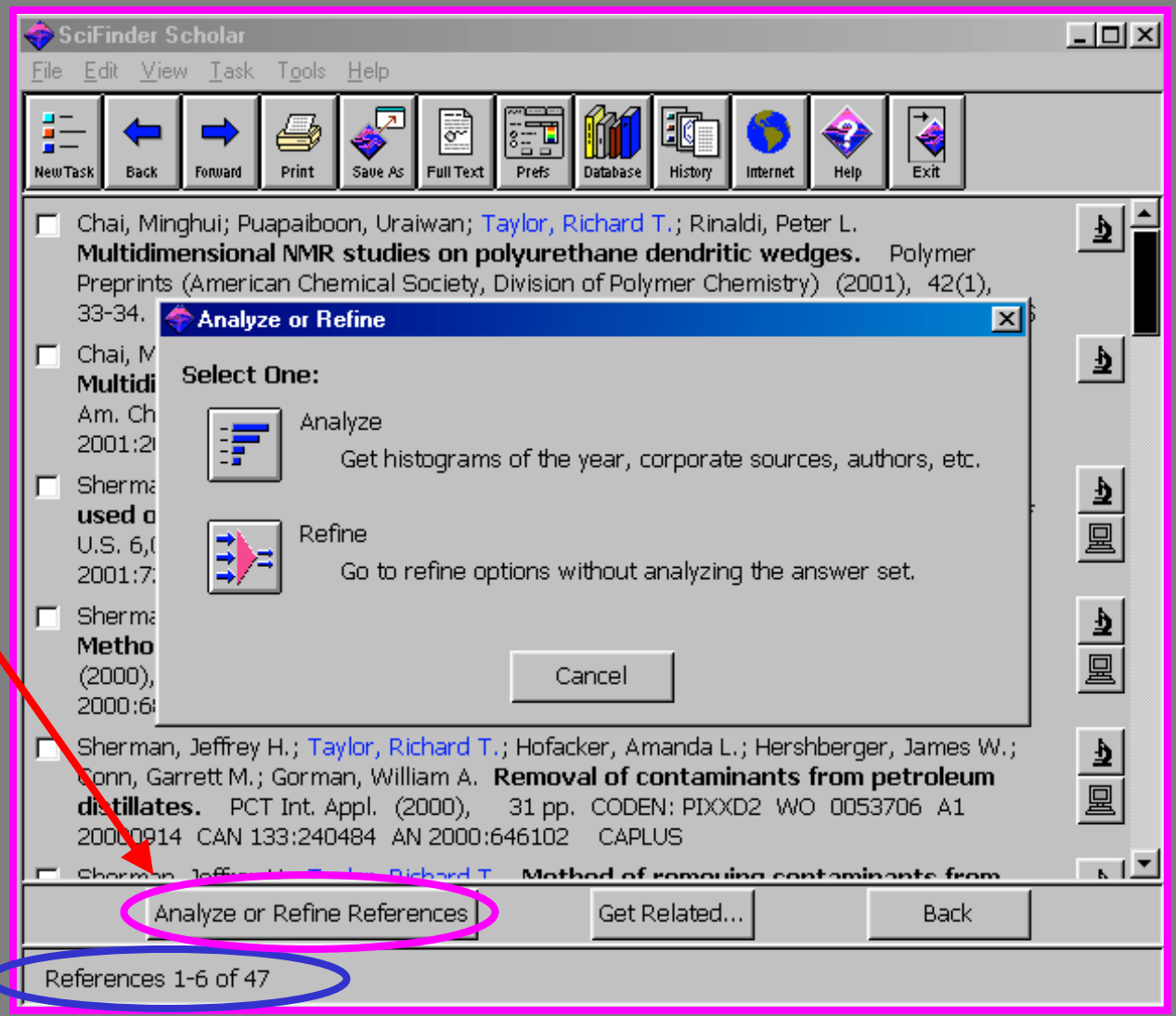


Let’s rotate 3D structure

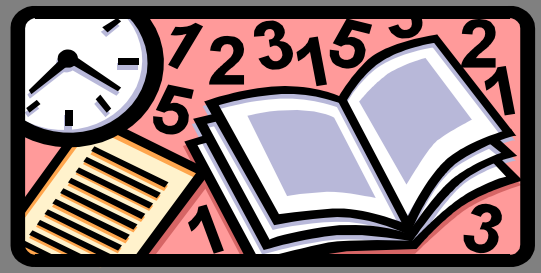


Narrow down answer sets

Too many?

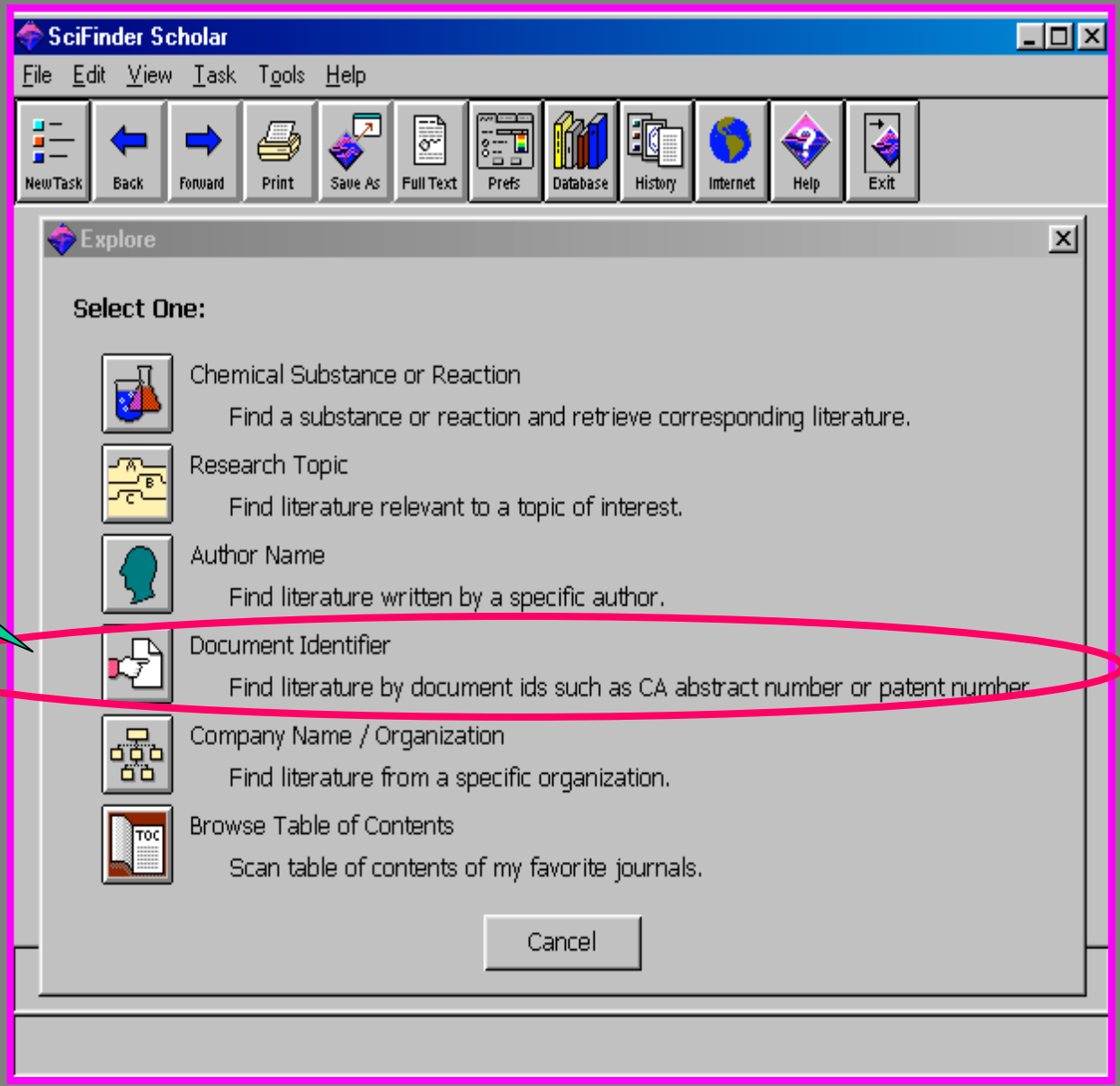


Next

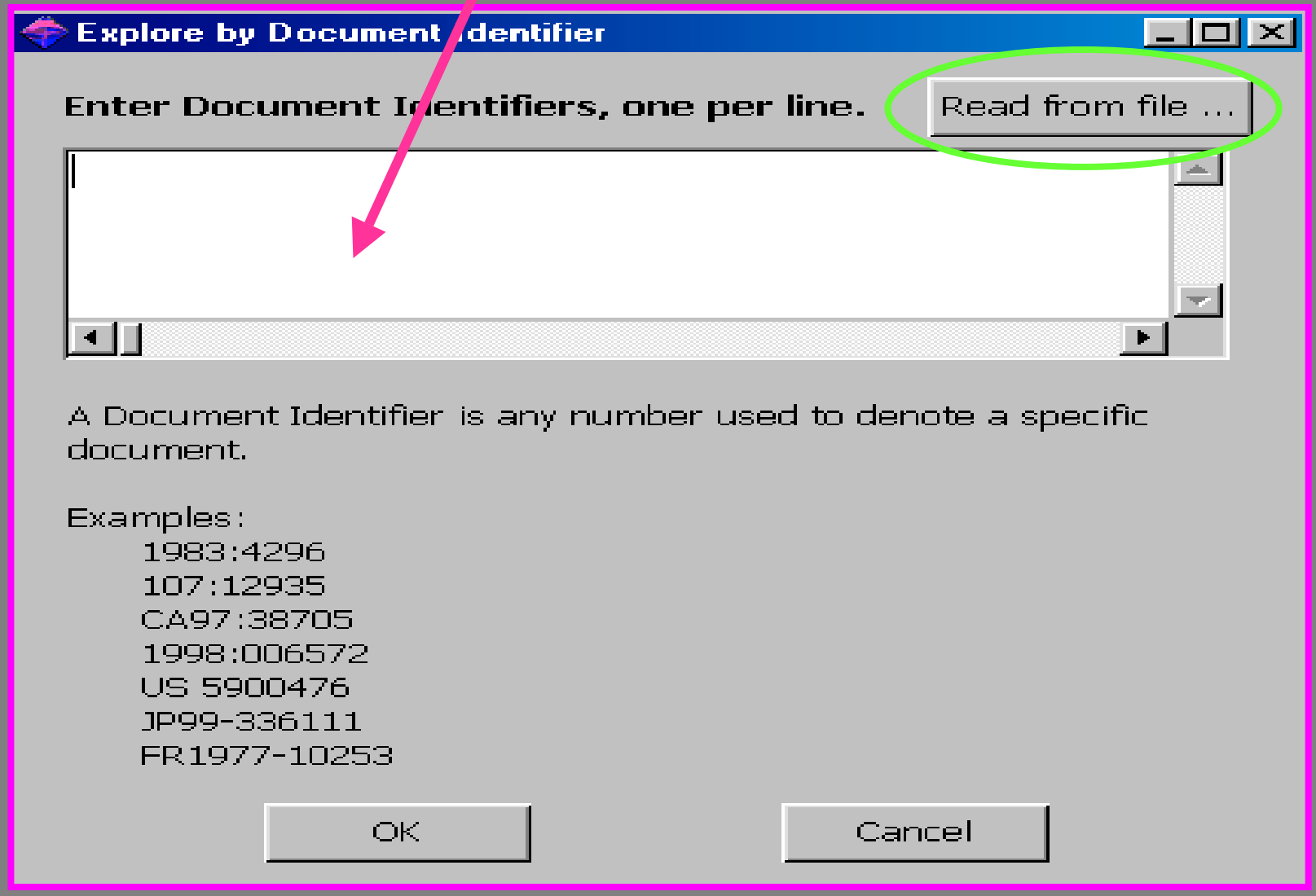


Explore by Document Identifier

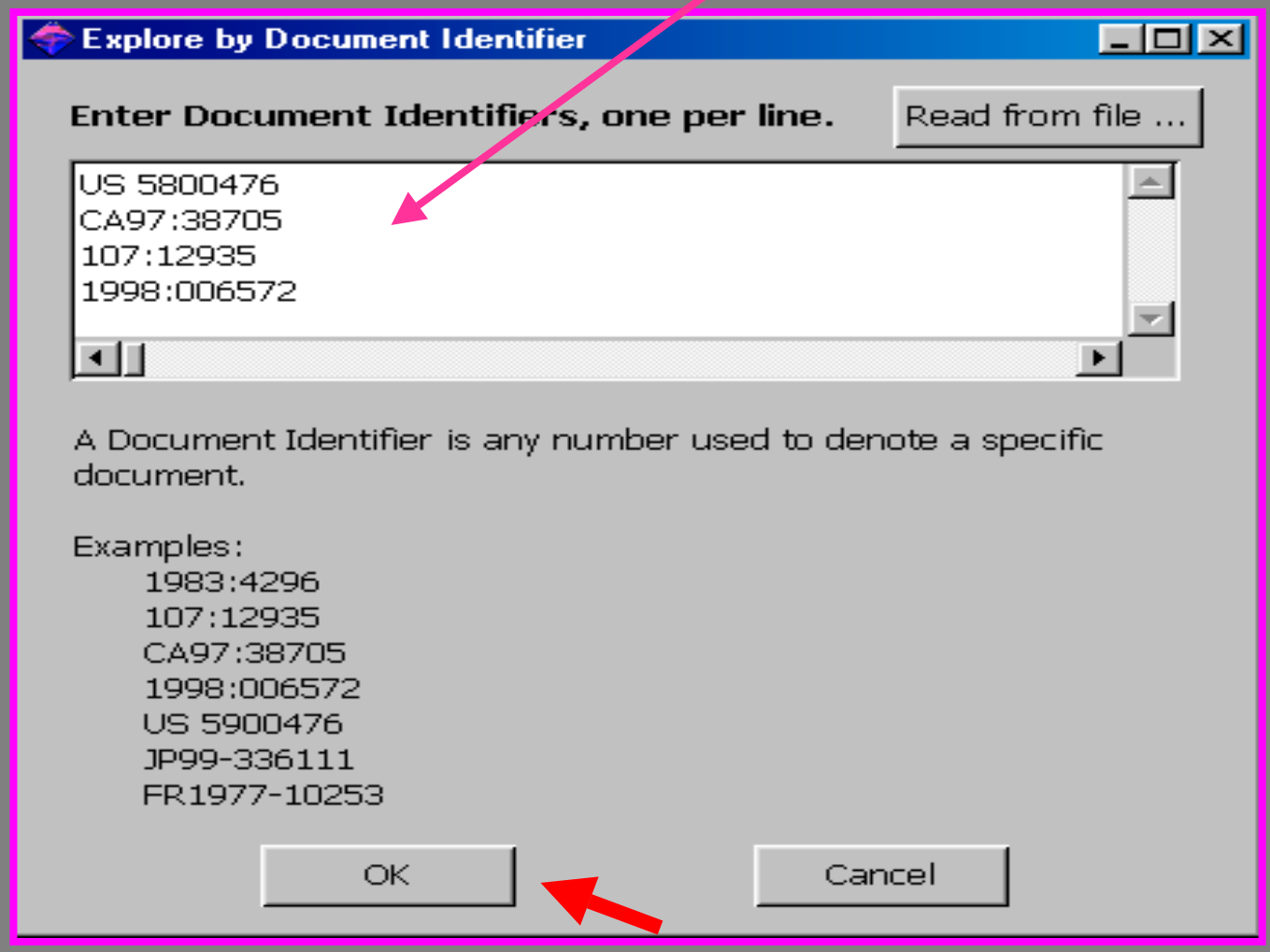
Search by Document Identifier



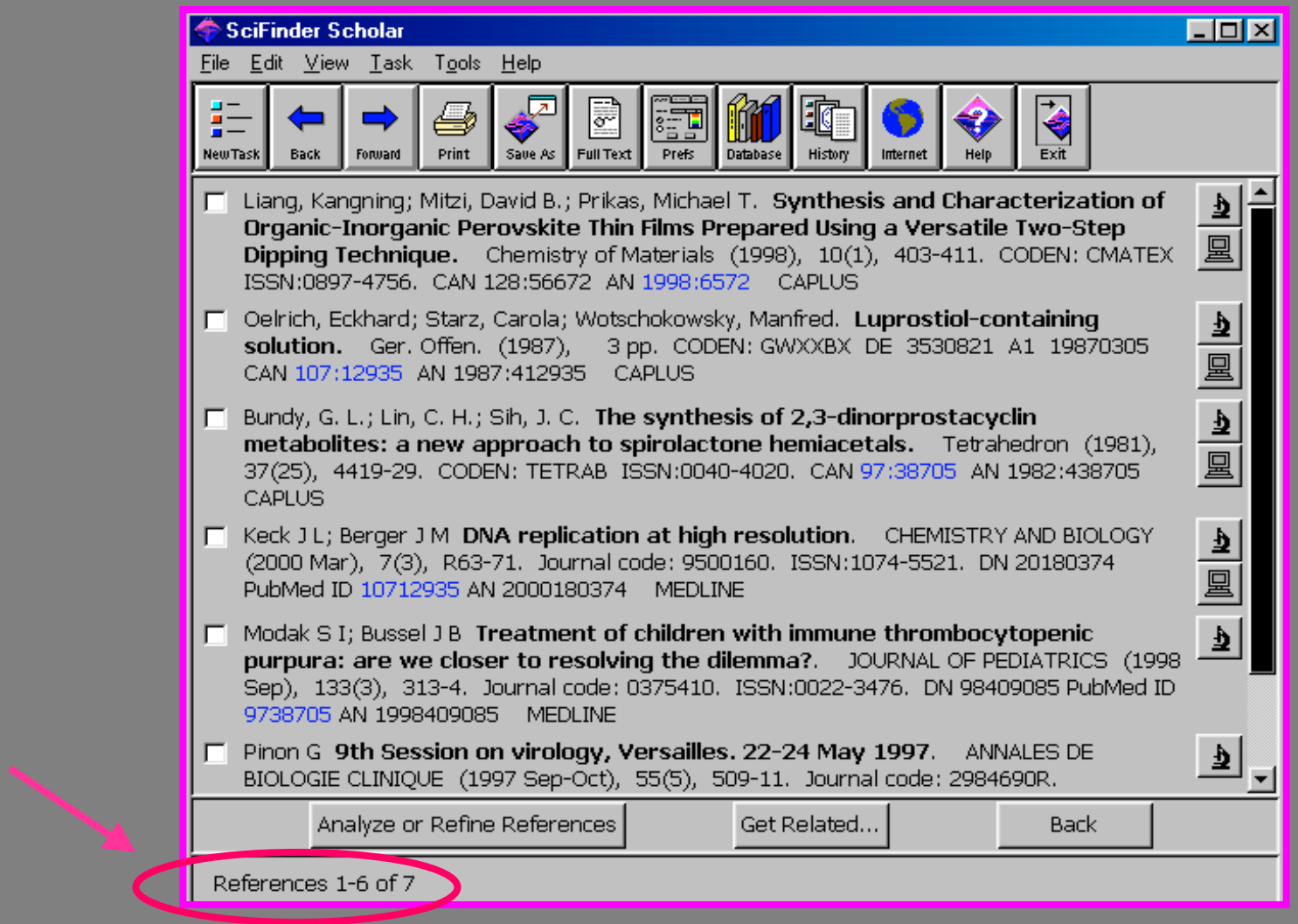
Enter Document Identifiers



Document Identifiers of interest

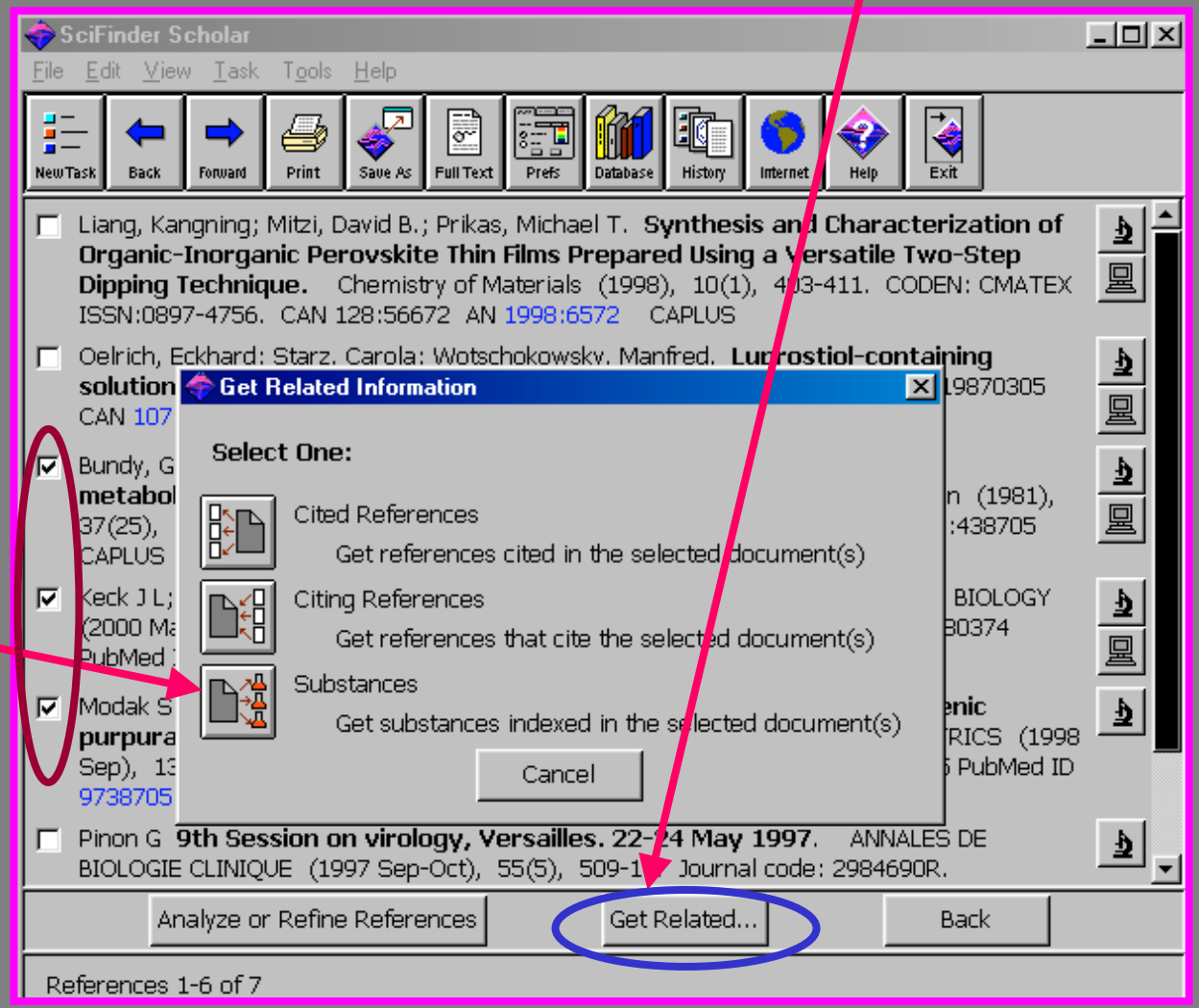


Here are what we want!

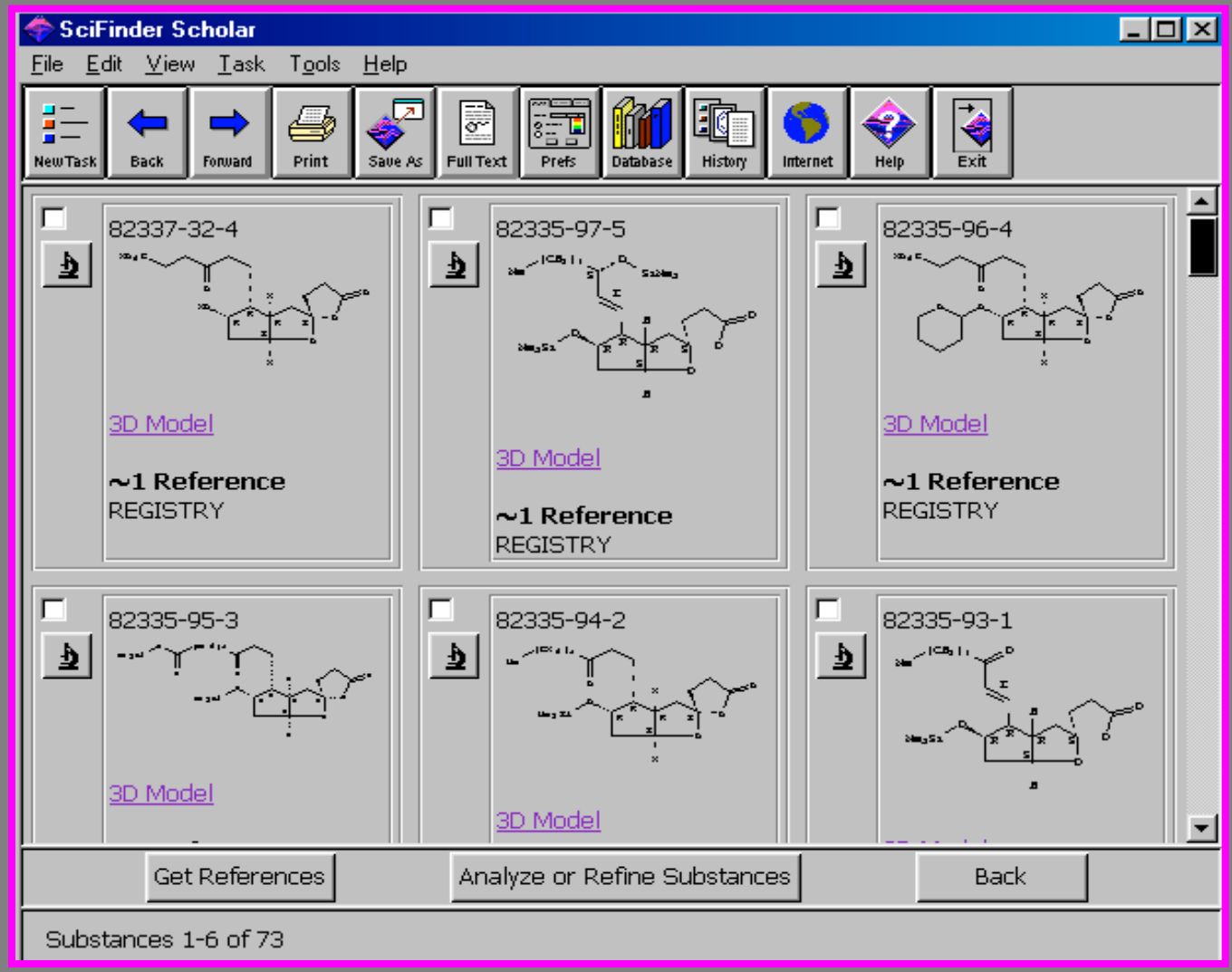


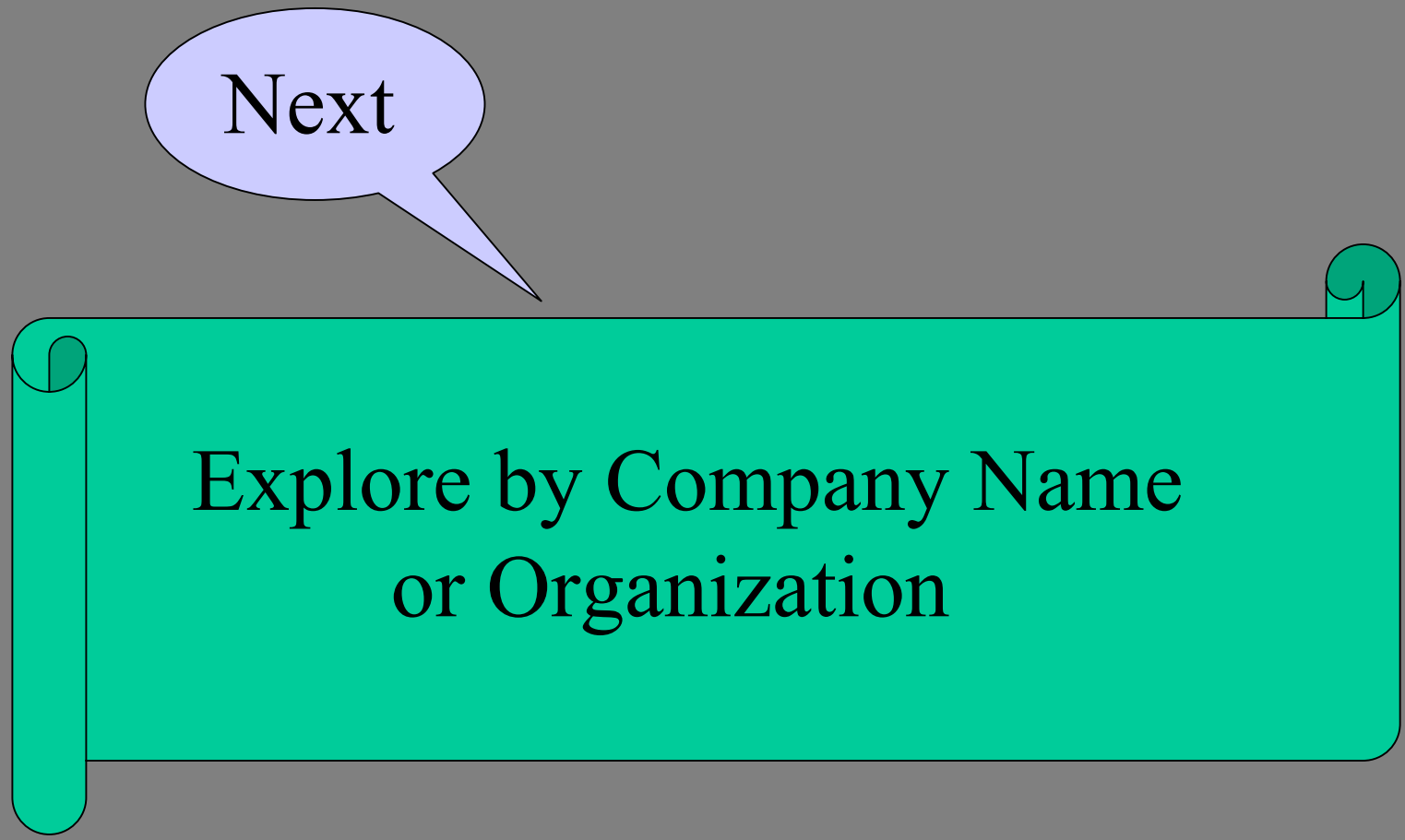
View Related information

View substances in the reference of interest

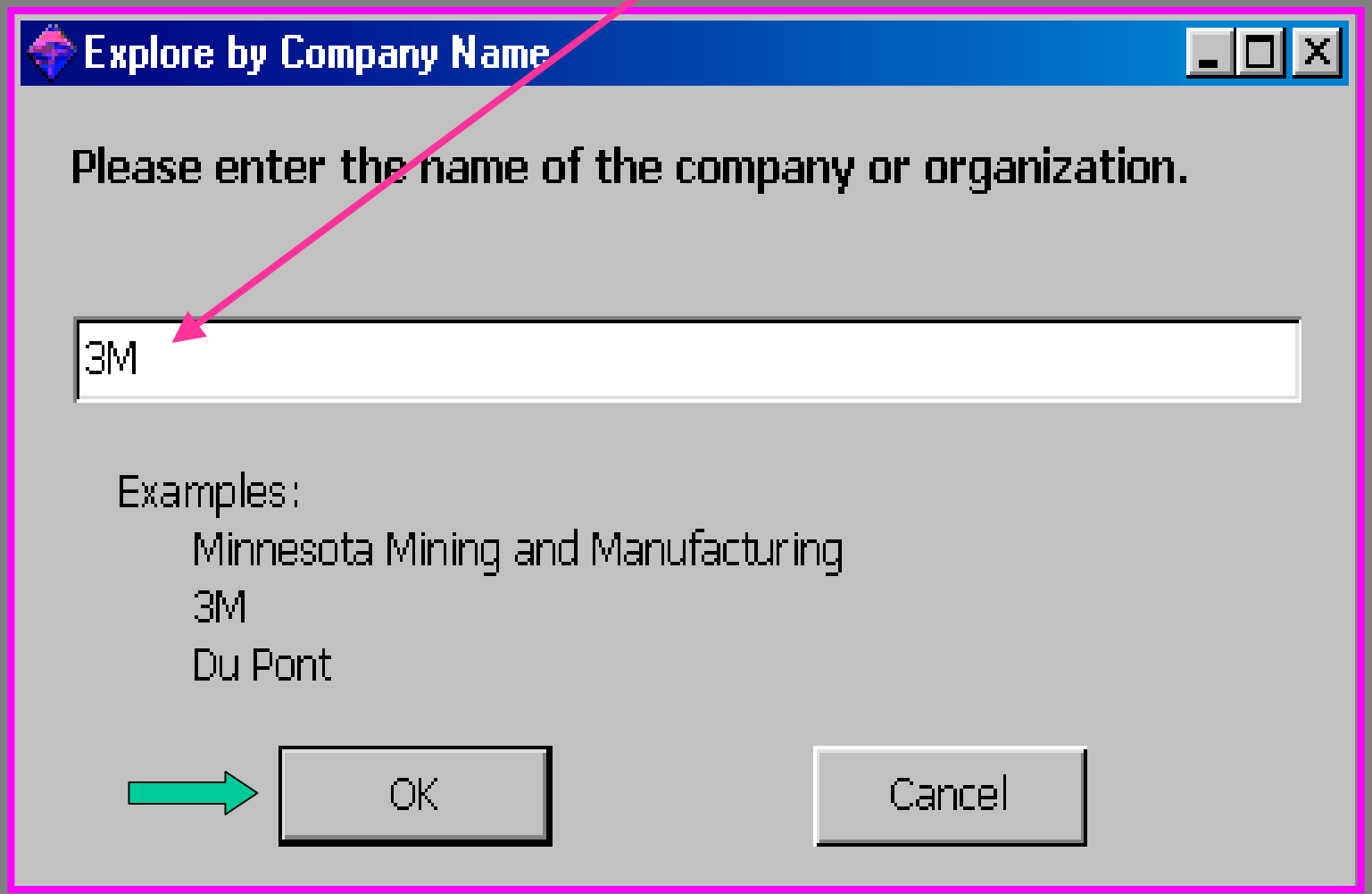


Substances appeared in the literature of interest

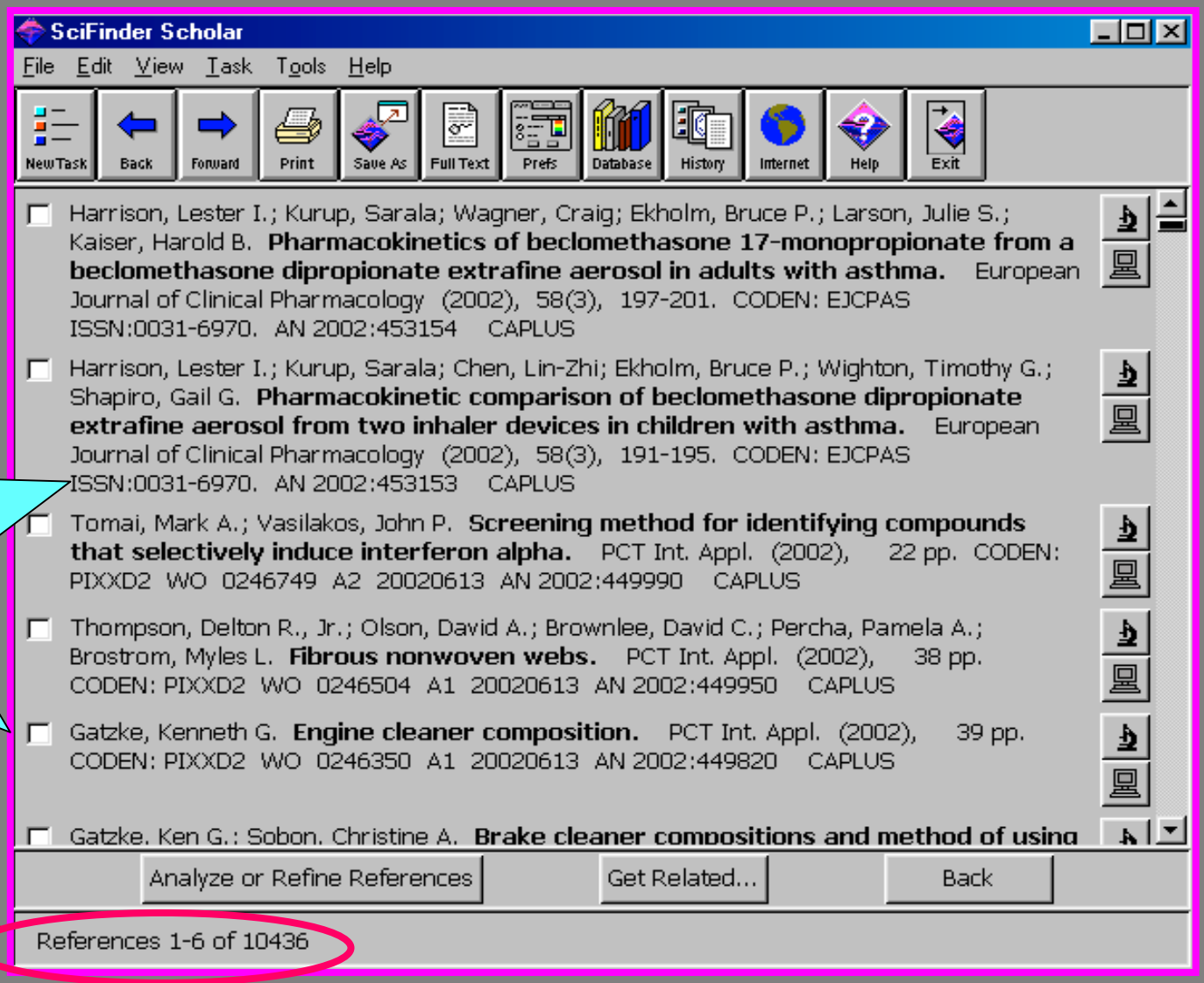



Next
Explore by Company Name
or Organization

Enter the name of the company that we are interested in?

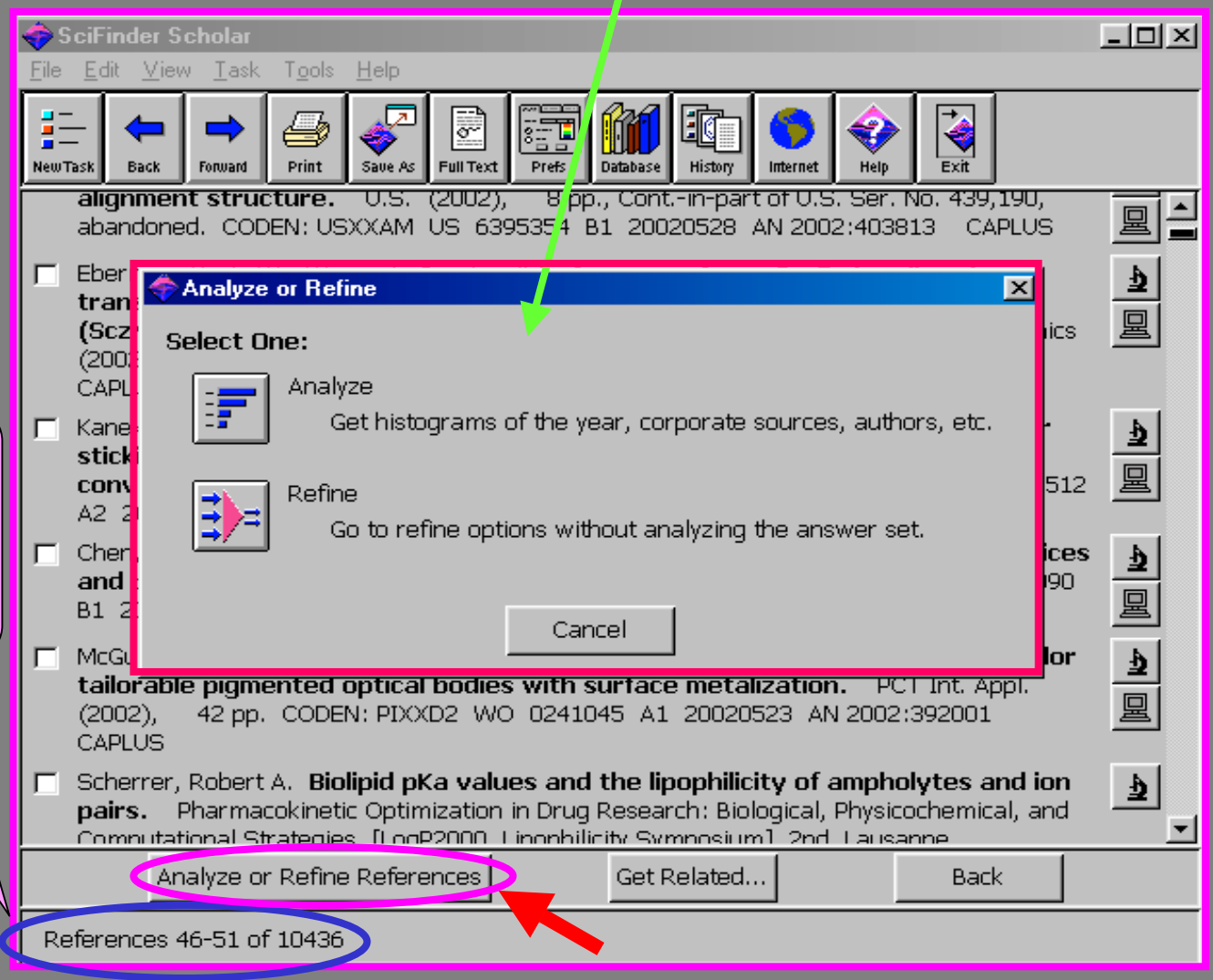


3M's Literatures



Wow!
so many
(10436)

Let's narrow them down

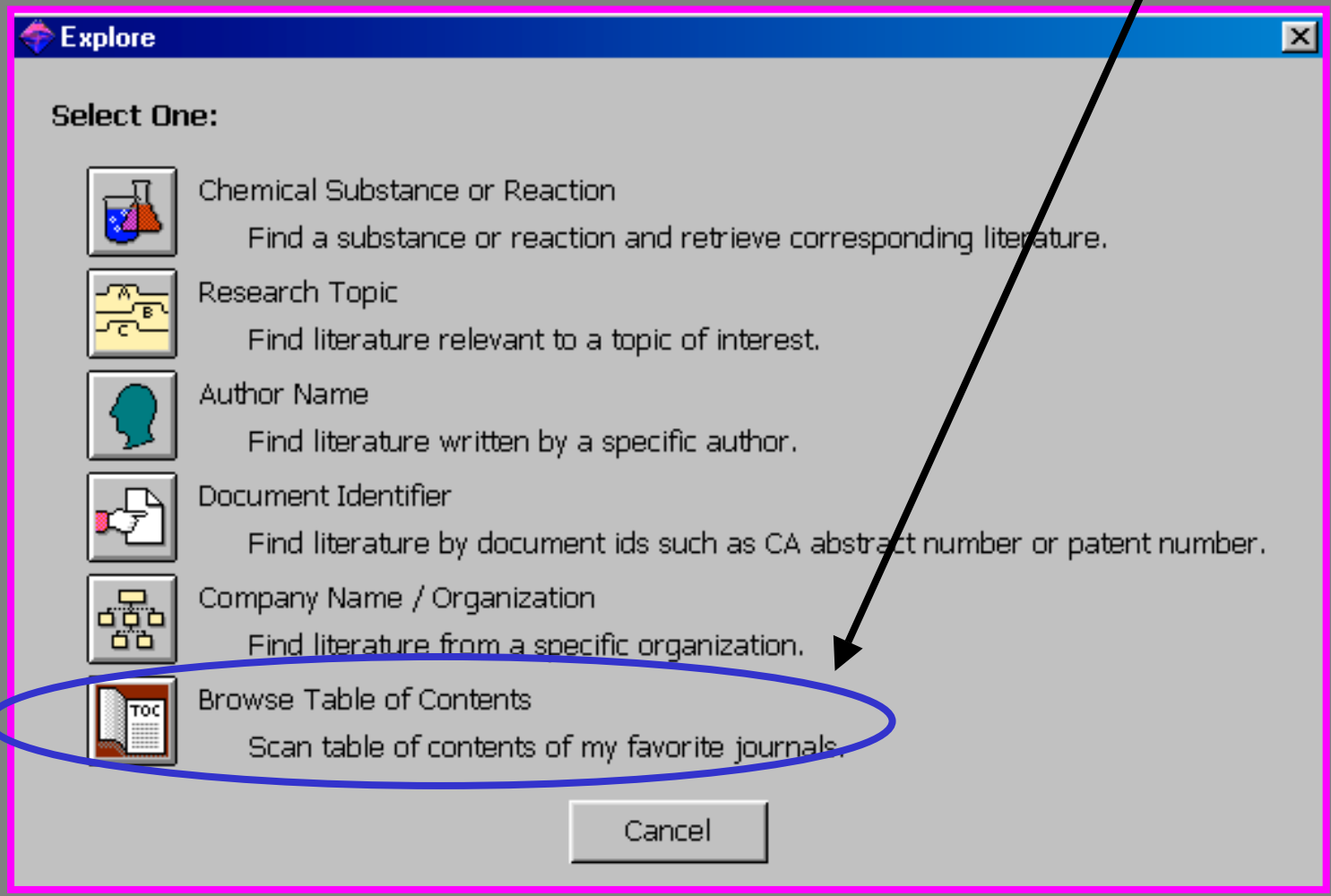


Too large answer set !

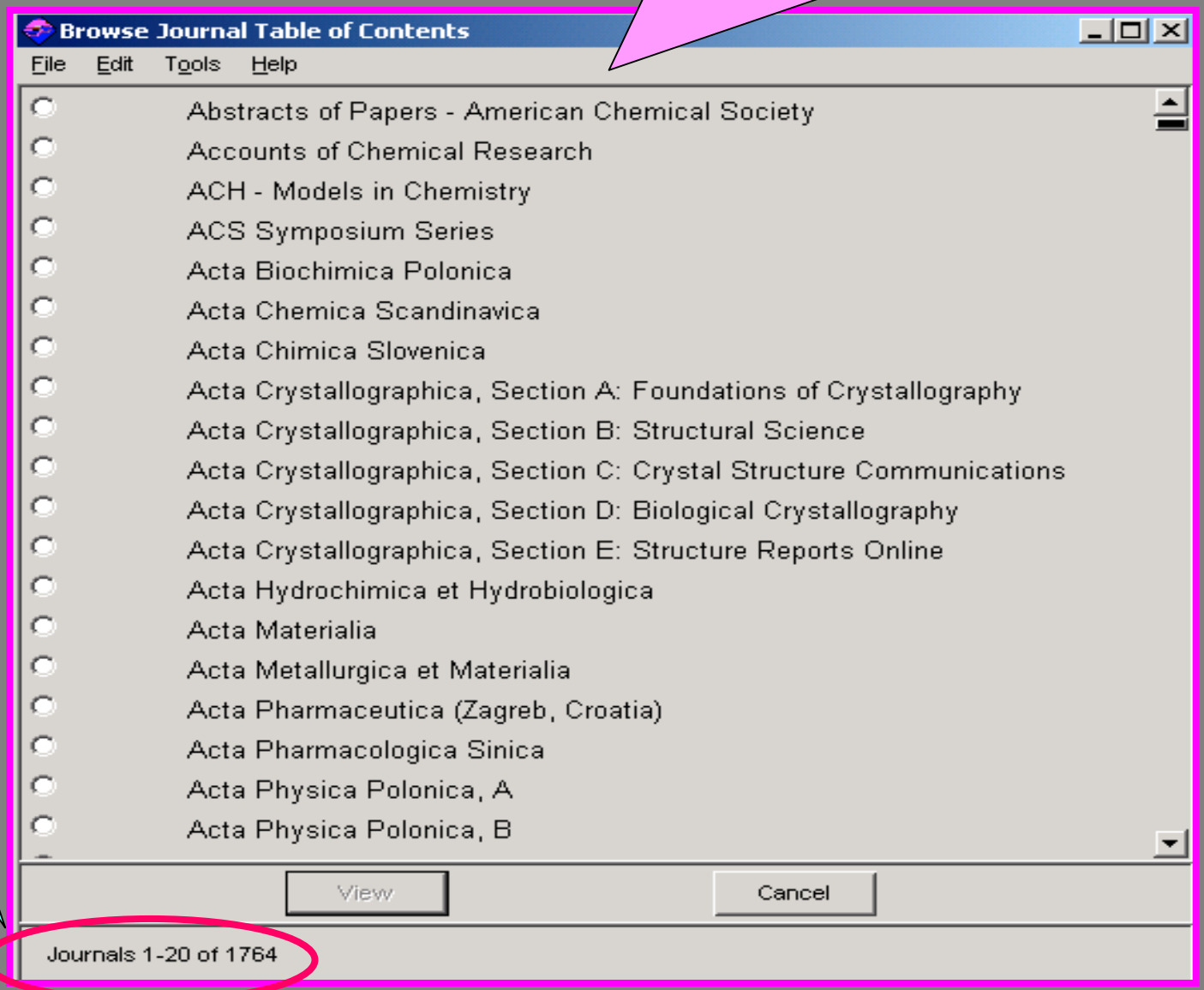
Next

Explore by browse
Table of contents

Search by Browse Table of Contents

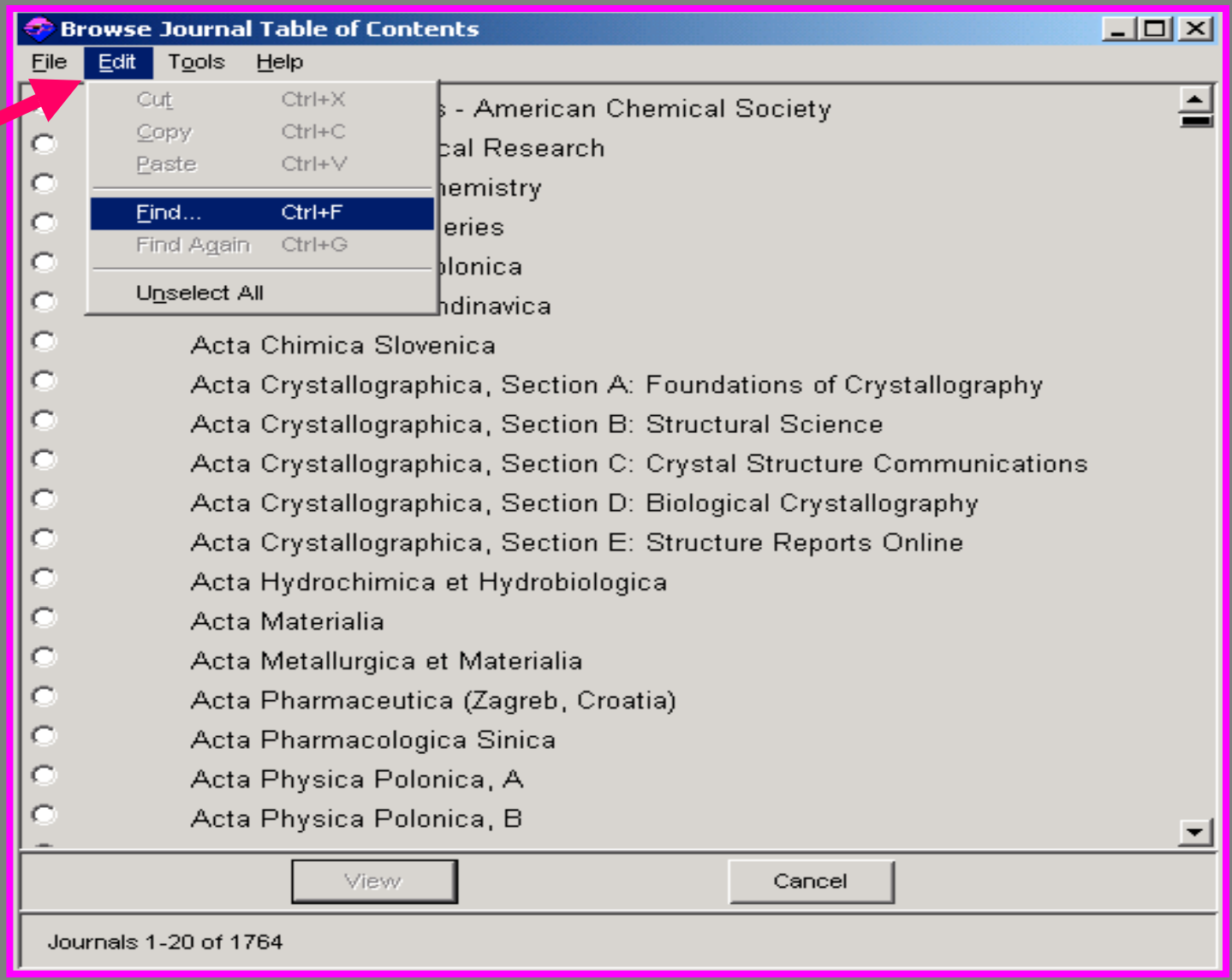


The List of journals!

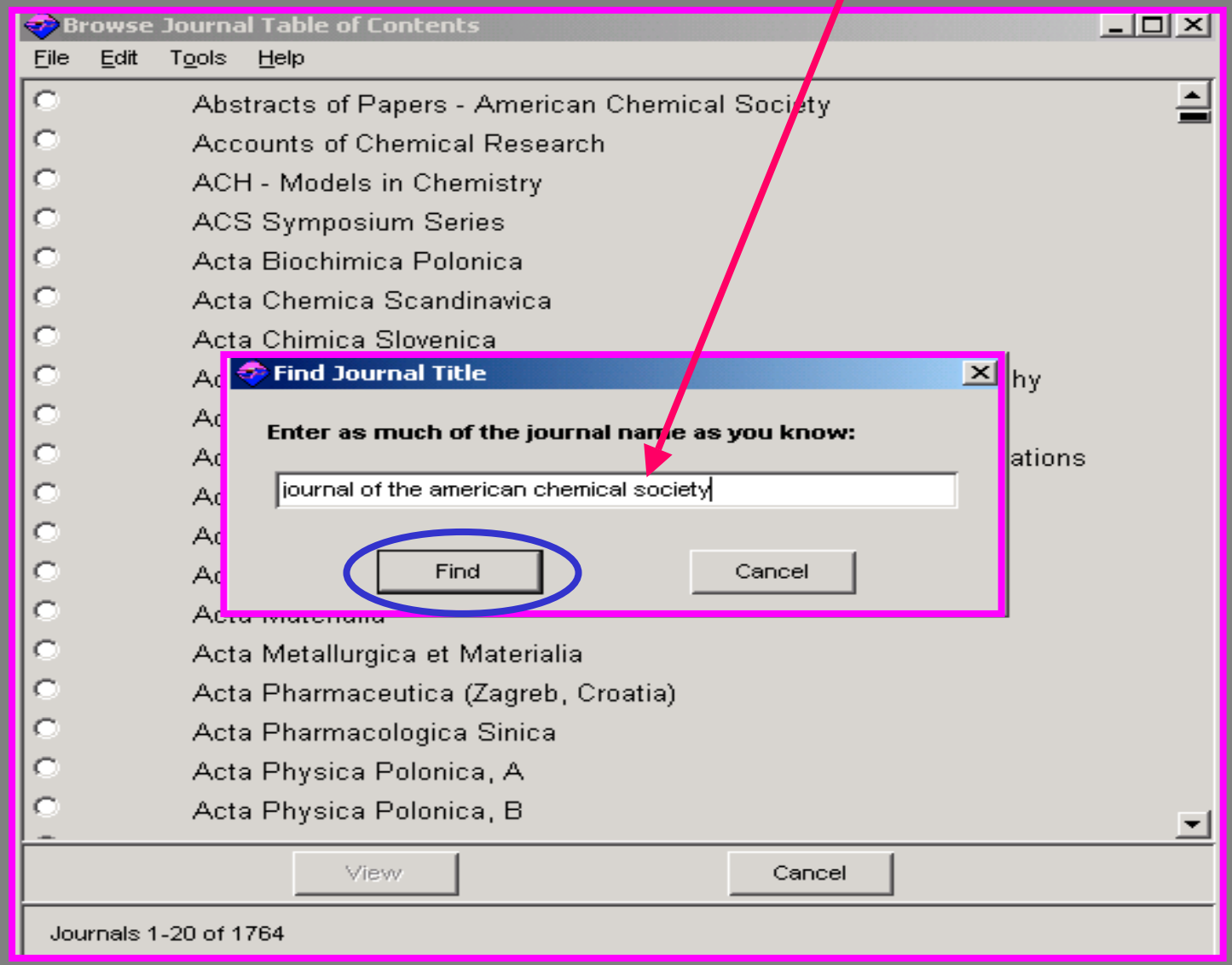


Look at This!

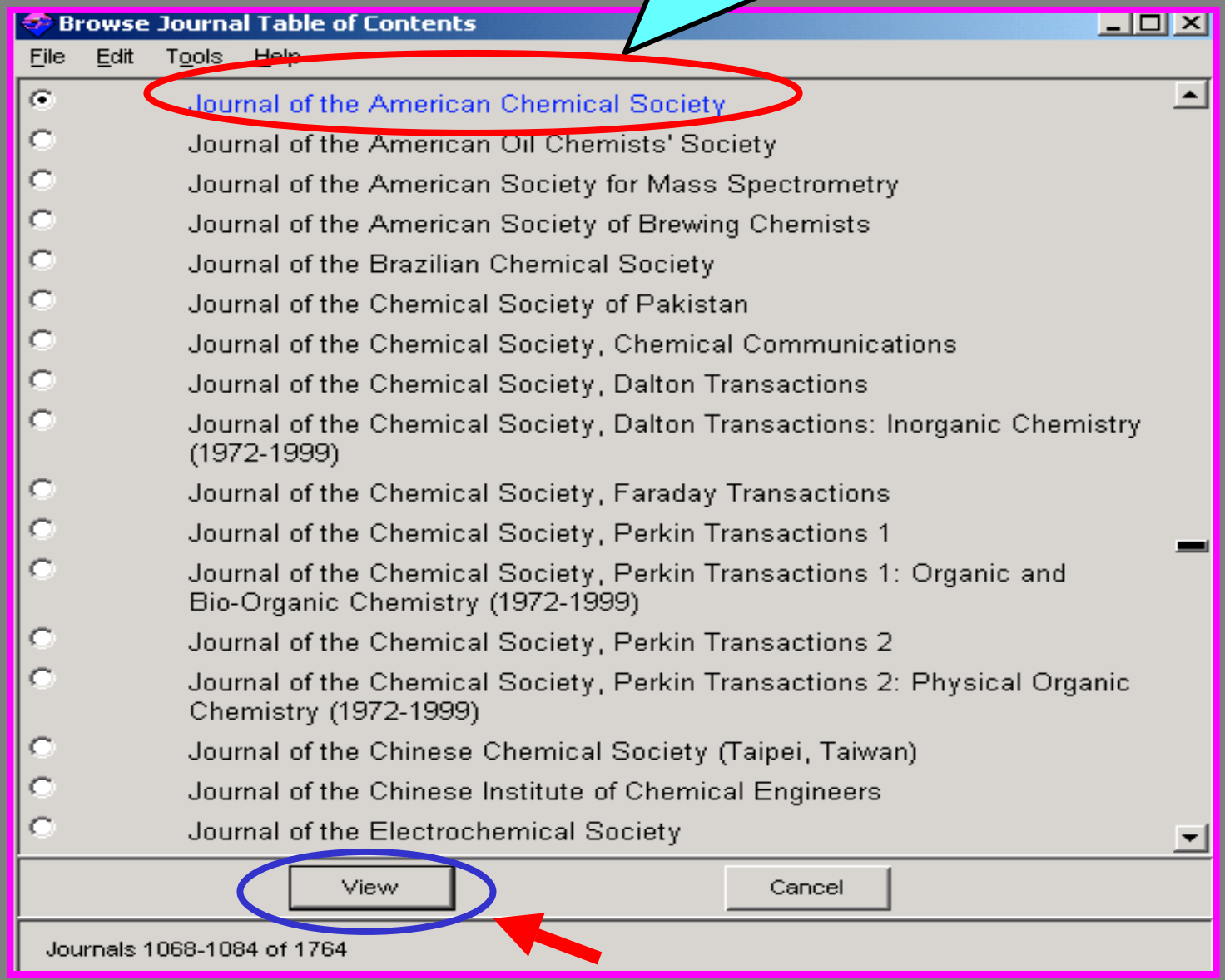
Let's find journal of interest



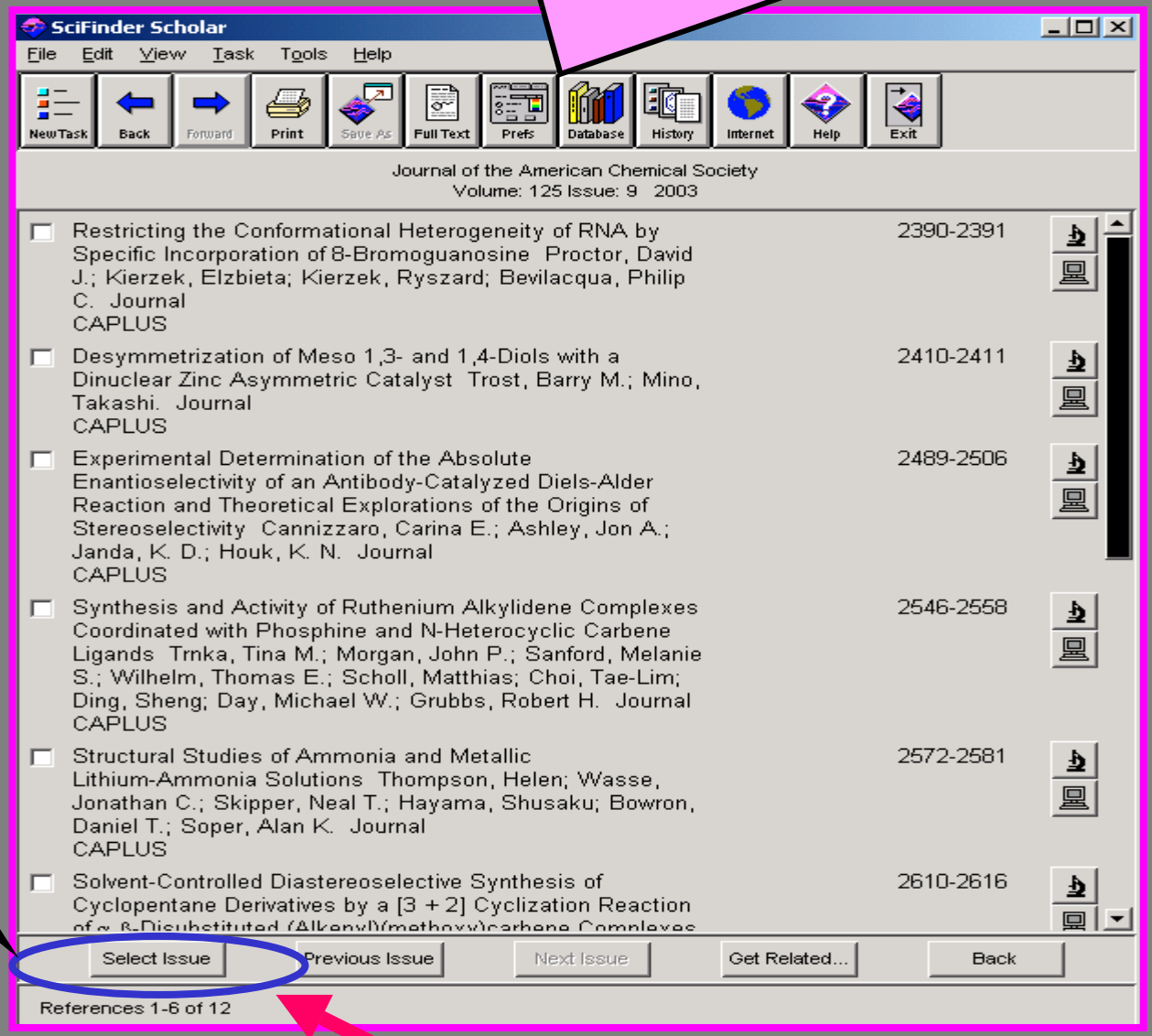
Type journal of interest



Here it is!

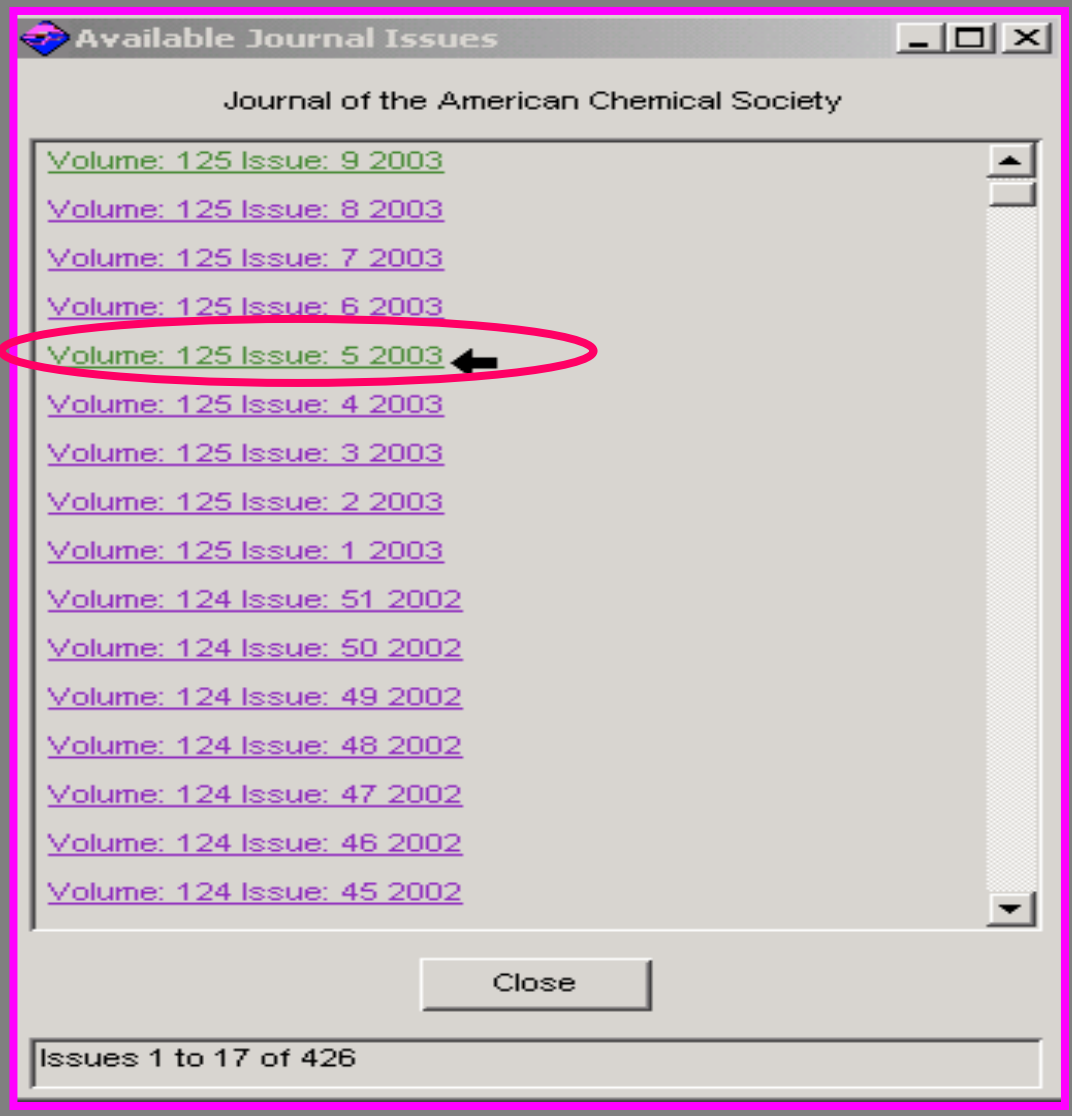

Browse Journal Table of Contents
File
Edit
Tools
Help
Journal of the American Chemical Society
Journal of the American Oil Chemists' Society
Journal of the American Society for Mass Spectrometry
Journal of the American Society of Brewing Chemists
Journal of the Brazilian Chemical Society
Journal of the Chemical Society of Pakistan
Journal of the Chemical Society, Chemical Communications
Journal of the Chemical Society, Dalton Transactions
Journal of the Chemical Society, Dalton Transactions: Inorganic Chemistry (1972-1999)
Journal of the Chemical Society, Faraday Transactions
Journal of the Chemical Society, Perkin Transactions 1
Journal of the Chemical Society, Perkin Transactions 1: Organic and Bio-Organic Chemistry (1972-1999)
Journal of the Chemical Society, Perkin Transactions 2
Journal of the Chemical Society, Perkin Transactions 2: Physical Organic Chemistry (1972-1999)
Journal of the Chinese Chemical Society (Taipei, Taiwan)
Journal of the Chinese Institute of Chemical Engineers
Journal of the Electrochemical Society
View
Cancel
Journals 1068-1084 of 1764

Latest issue of Table of Content

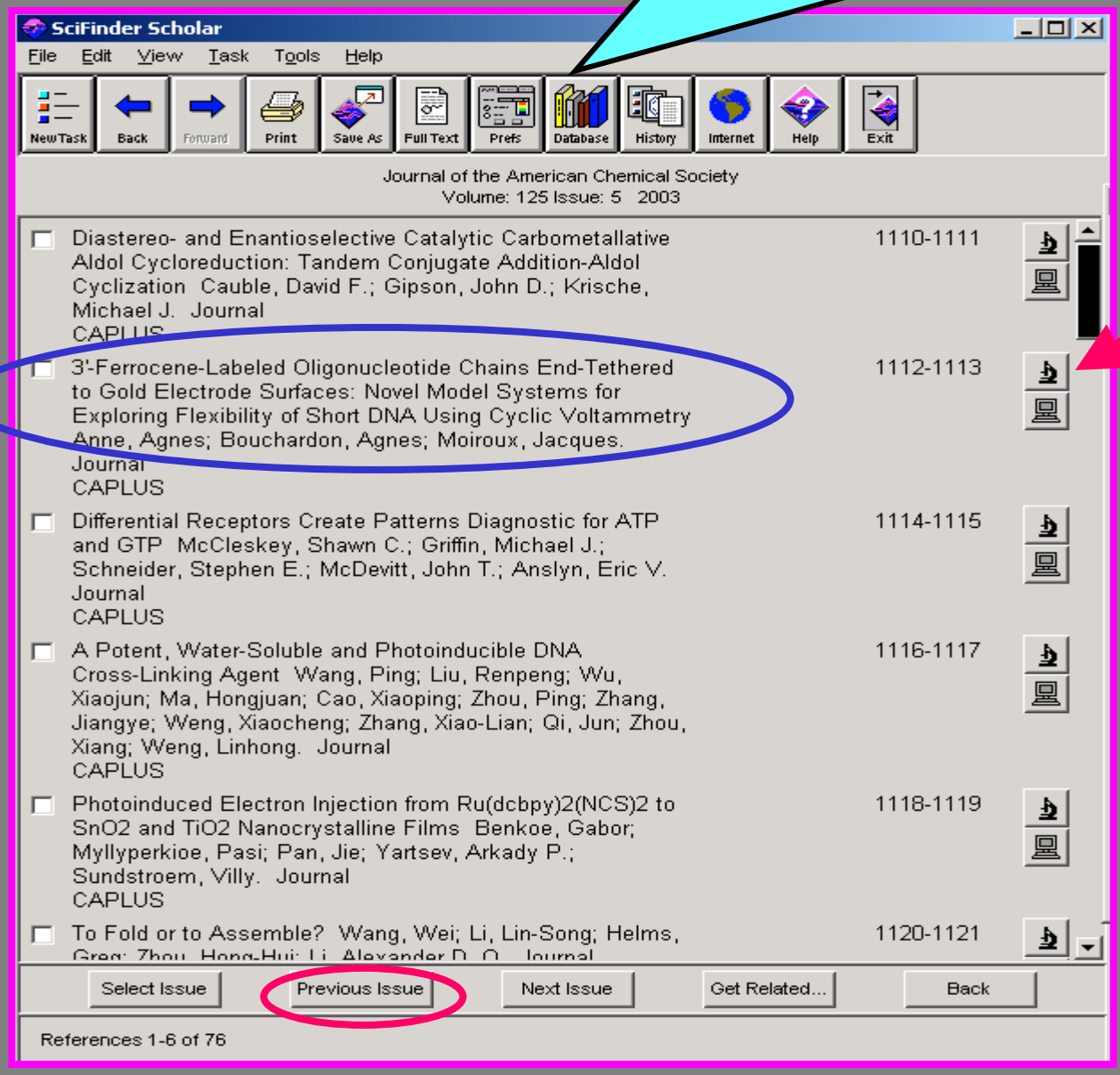


Select issue

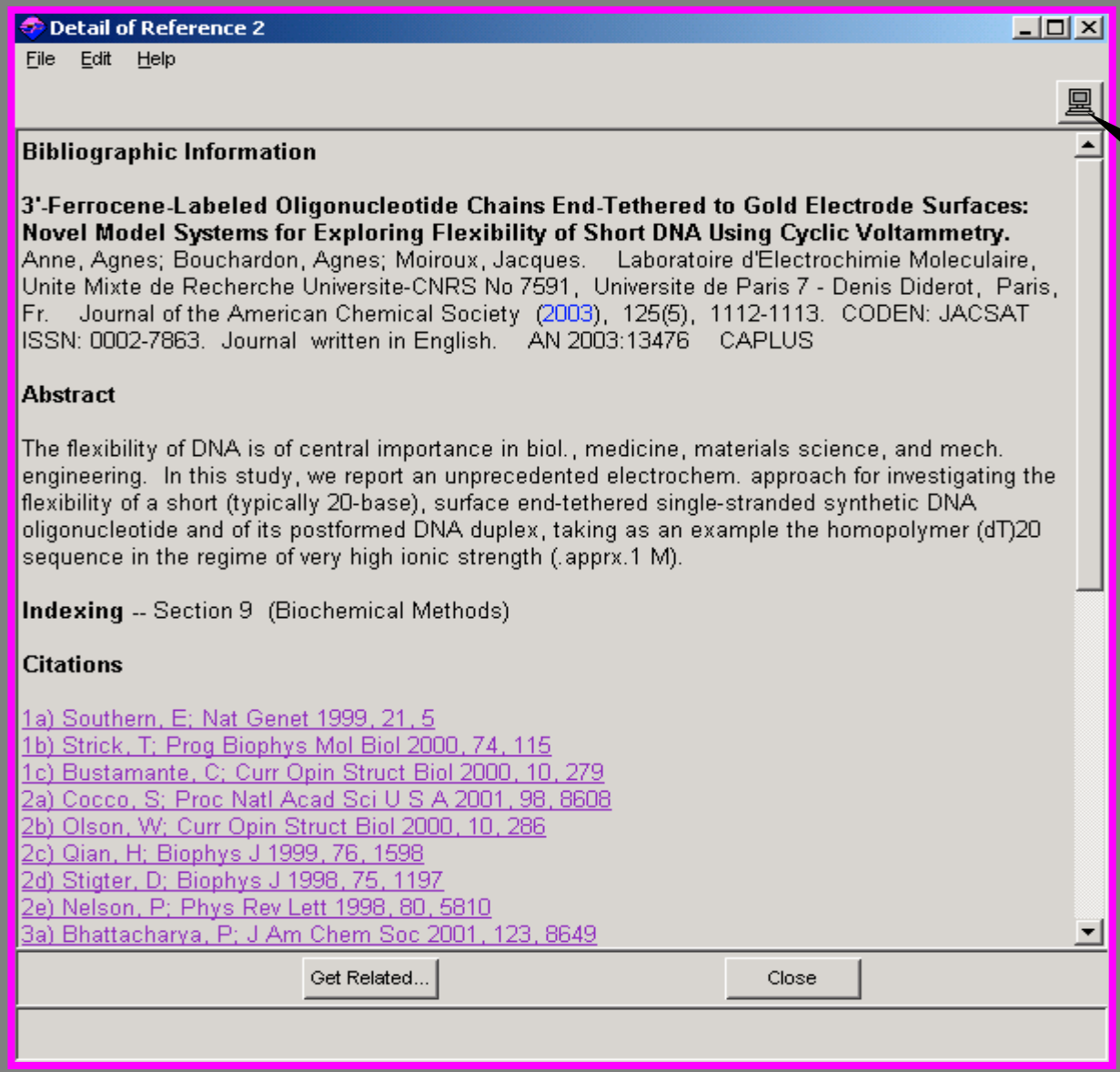
Select issue of interest



Here are the desired issue!

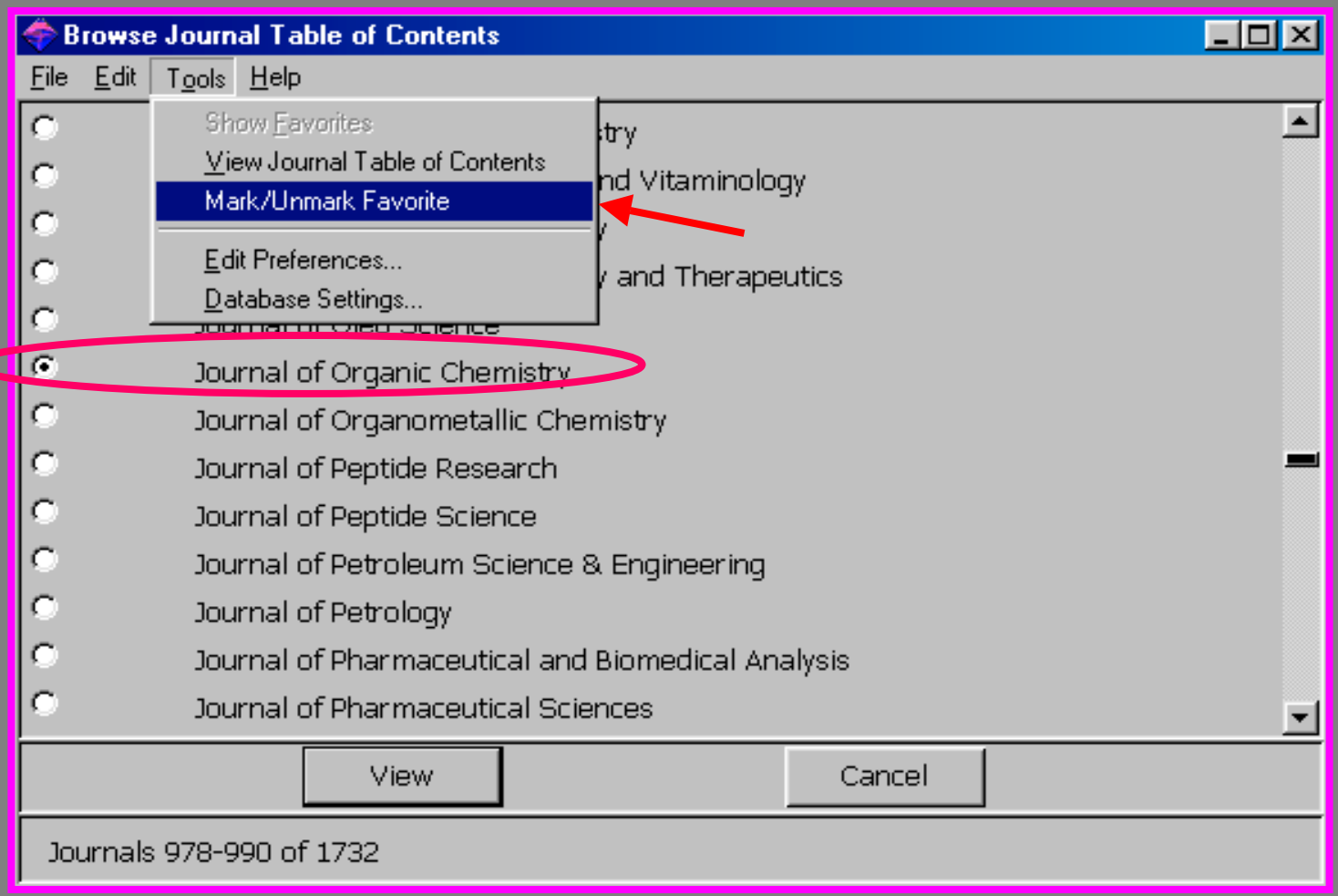


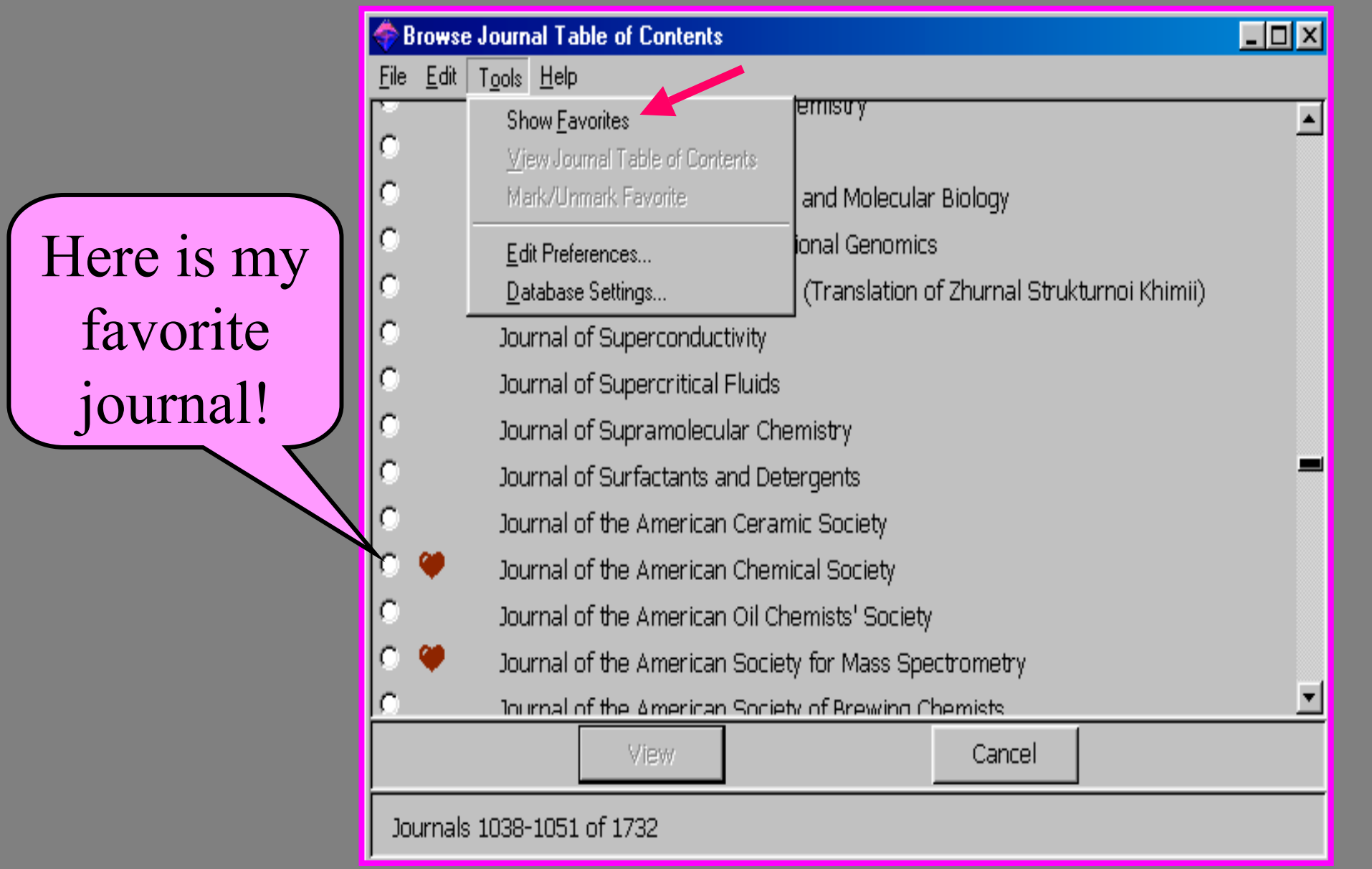
Detail of reference 2



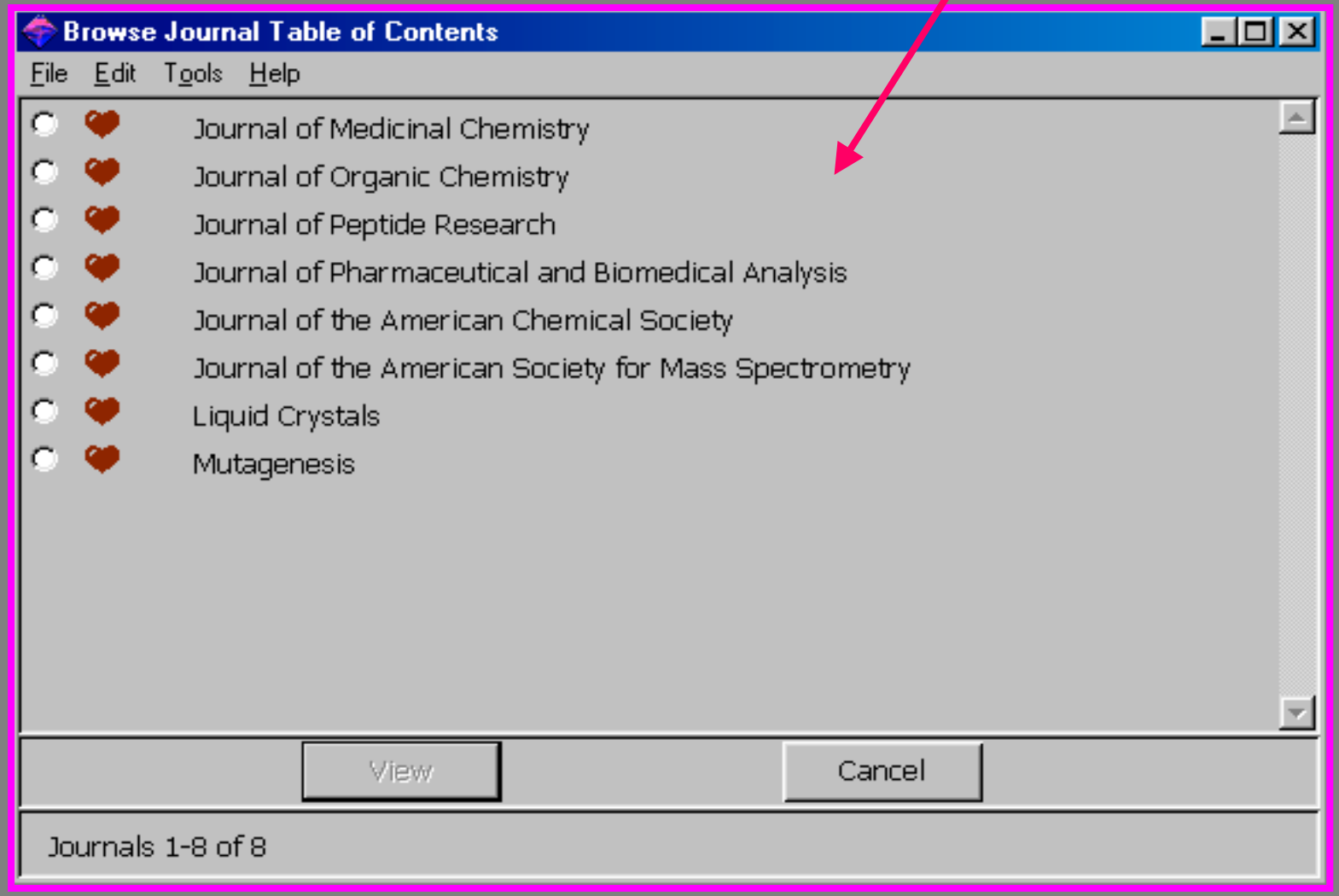
Link to Full text

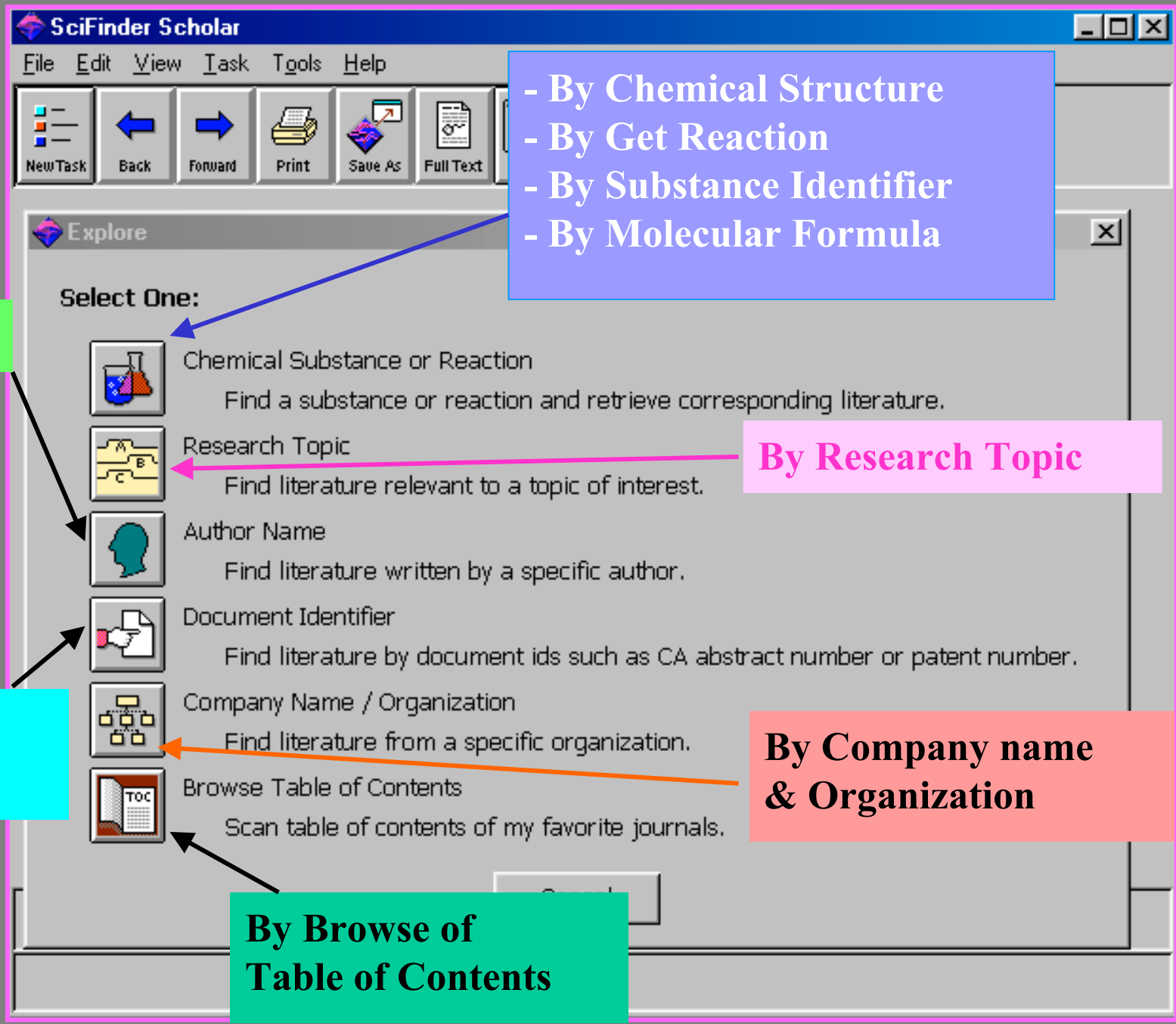
Mark to see only my favorite journal




Here is my favorite journal!
Browse Journal Table of Contents
File
Edit
Tools
Help
Show Favorites
View Journal Table of Contents
Mark/Unmark Favorite
Edit Preferences...
Database Settings...
and Molecular Biology
(Translation of Zhurnal Strukturnoi Khimii)
Journal of Superconductivity
Journal of Supercritical Fluids
Journal of Supramolecular Chemistry
Journal of Surfactants and Detergents
Journal of the American Ceramic Society
Journal of the American Chemical Society
Journal of the American Oil Chemists' Society
Journal of the American Society for Mass Spectrometry
View
Cancel
Journals 1038-1051 of 1732

View all my favorite journals!

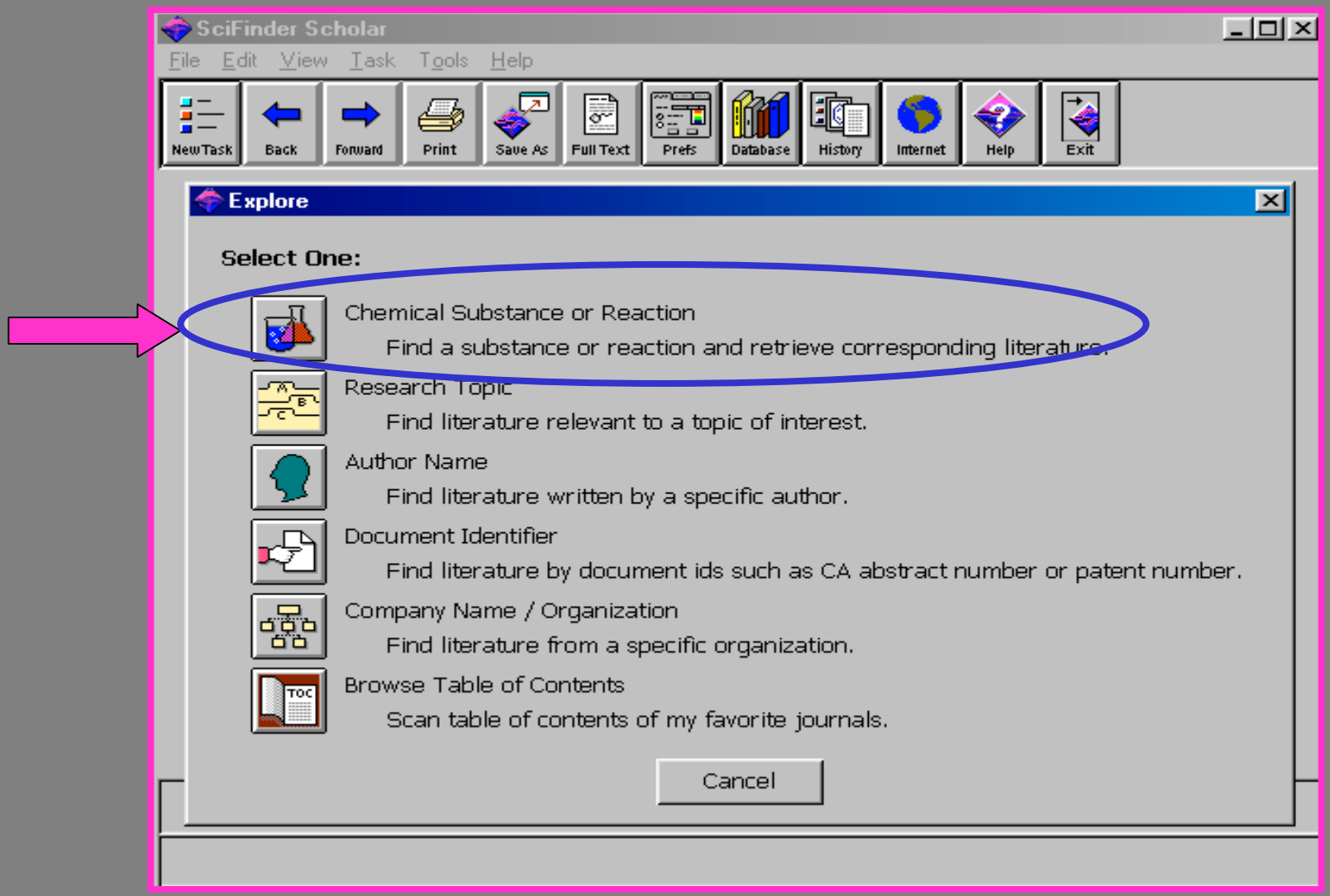



SciFinder Scholar
File Edit View Task Tools Help
New Task
Back
Forward
Print
Save As
Full Text
- By Chemical Structure
- By Get Reaction
- By Substance Identifier
- By Molecular Formula
Explore
Select One:
Chemical Substance or Reaction
Find a substance or reaction and retrieve corresponding literature.
Research Topic
Find literature relevant to a topic of interest.
Author Name
Find literature written by a specific author.
Document Identifier
Find literature by document ids such as CA abstract number or patent number.
Company Name / Organization
Find literature from a specific organization.
Browse Table of Contents
Scan table of contents of my favorite journals.
TOC
By Author
By Research Topic
By Document Identifier
By Company name & Organization
By Browse of Table of Contents

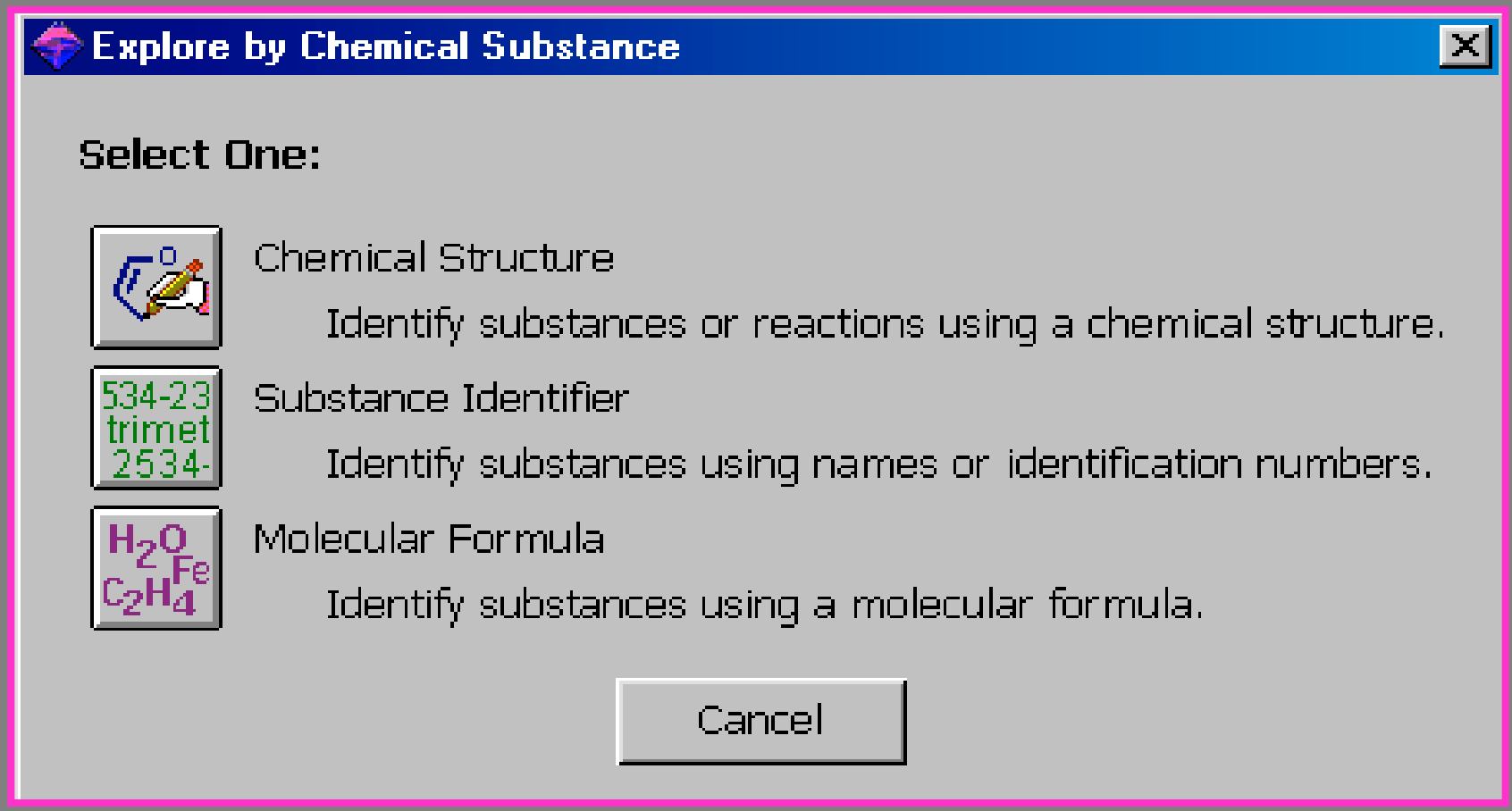
Next

Explore
by
chemical substances and reaction

Search by chemical substance and reaction

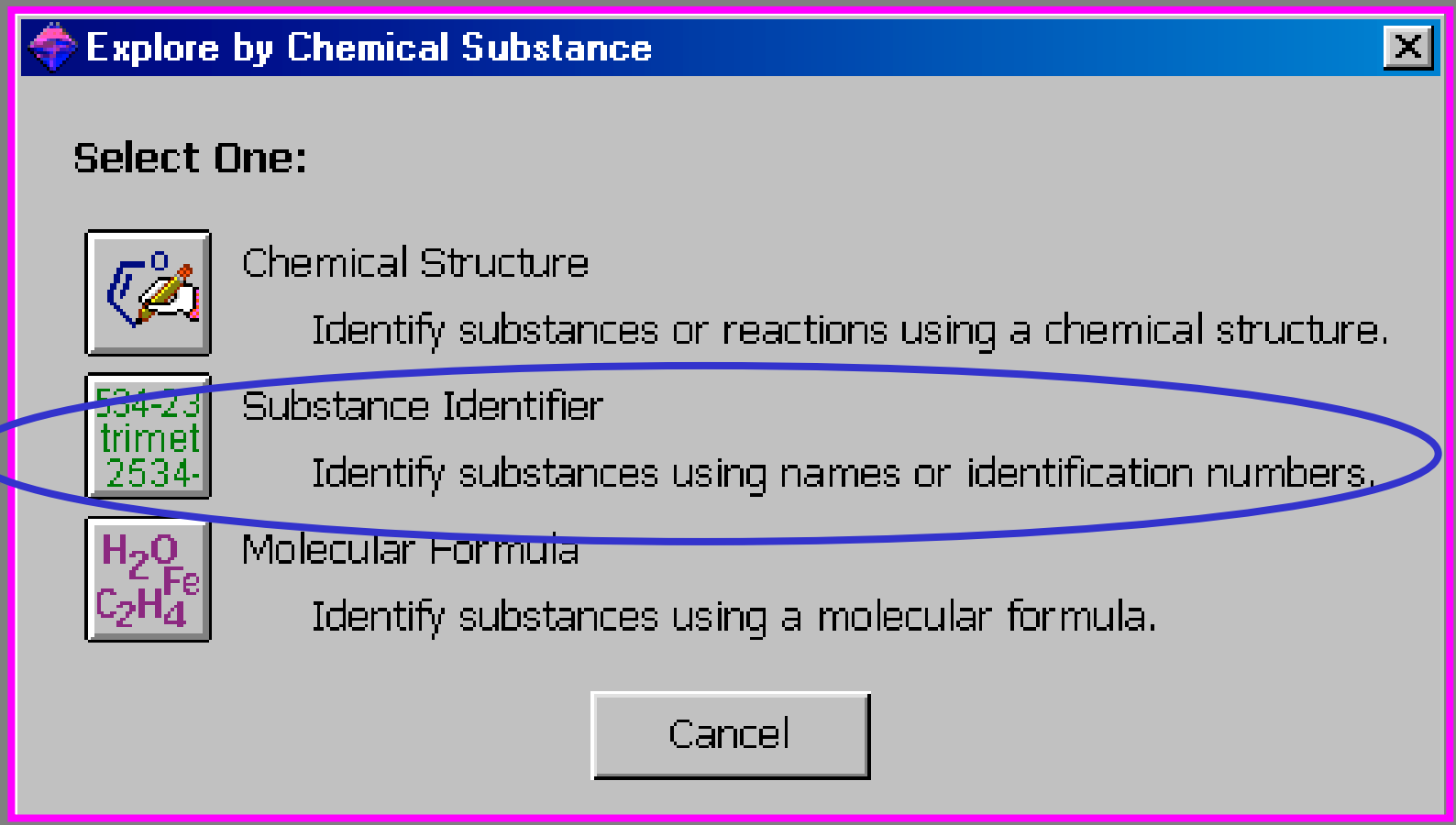


Three options to explore by chemical substance

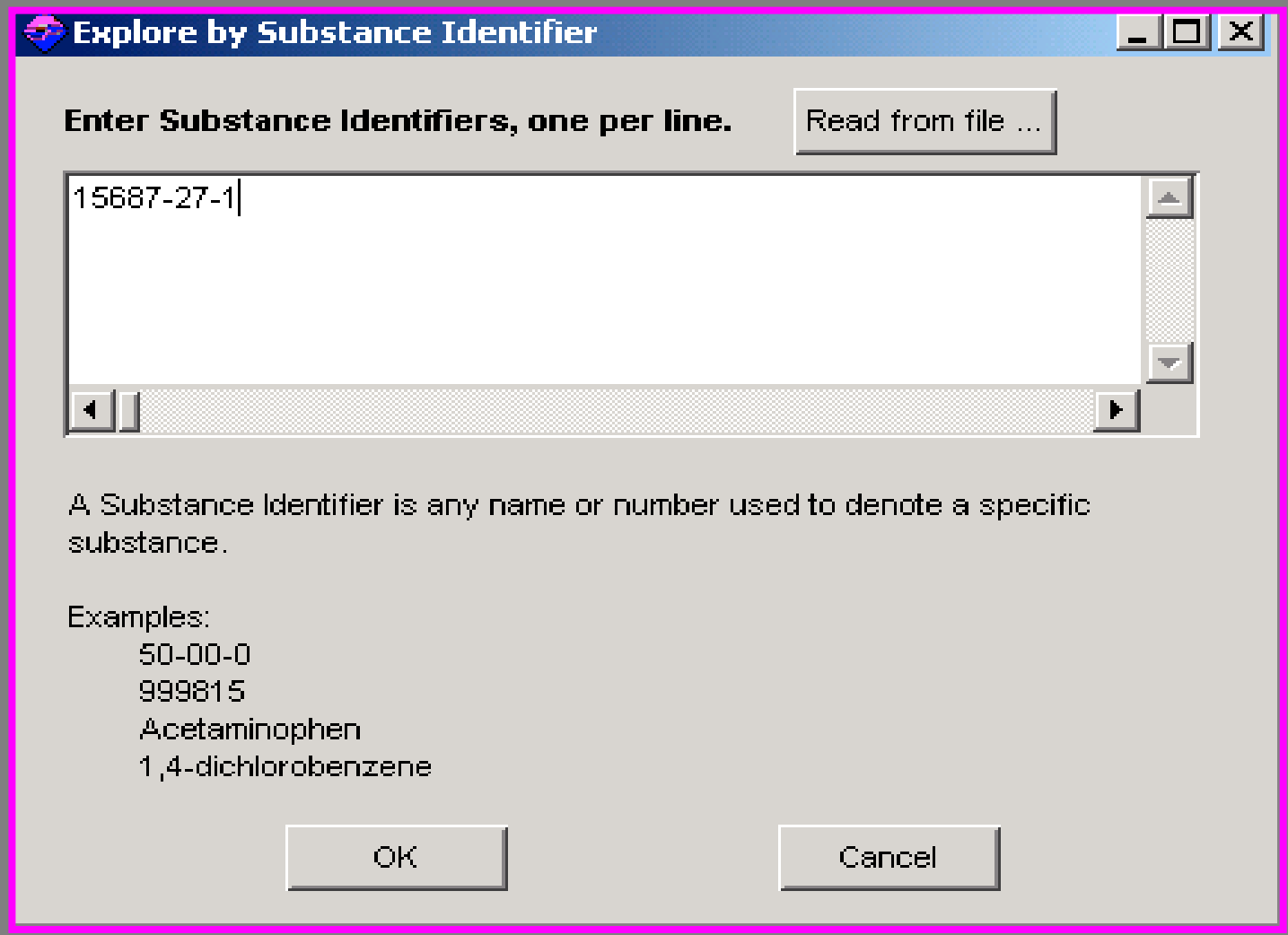


Explore by Substance identifier

Explore by Substance Identifier



Enter Substance Identifier

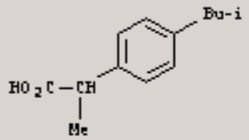


SciFinder Scholar

File Edit View Task Tools Help

New Task | Back | Forward | Print | Save As | Full Text | Prefs | Database | History | Internet | Help | Exit

15687-27-1



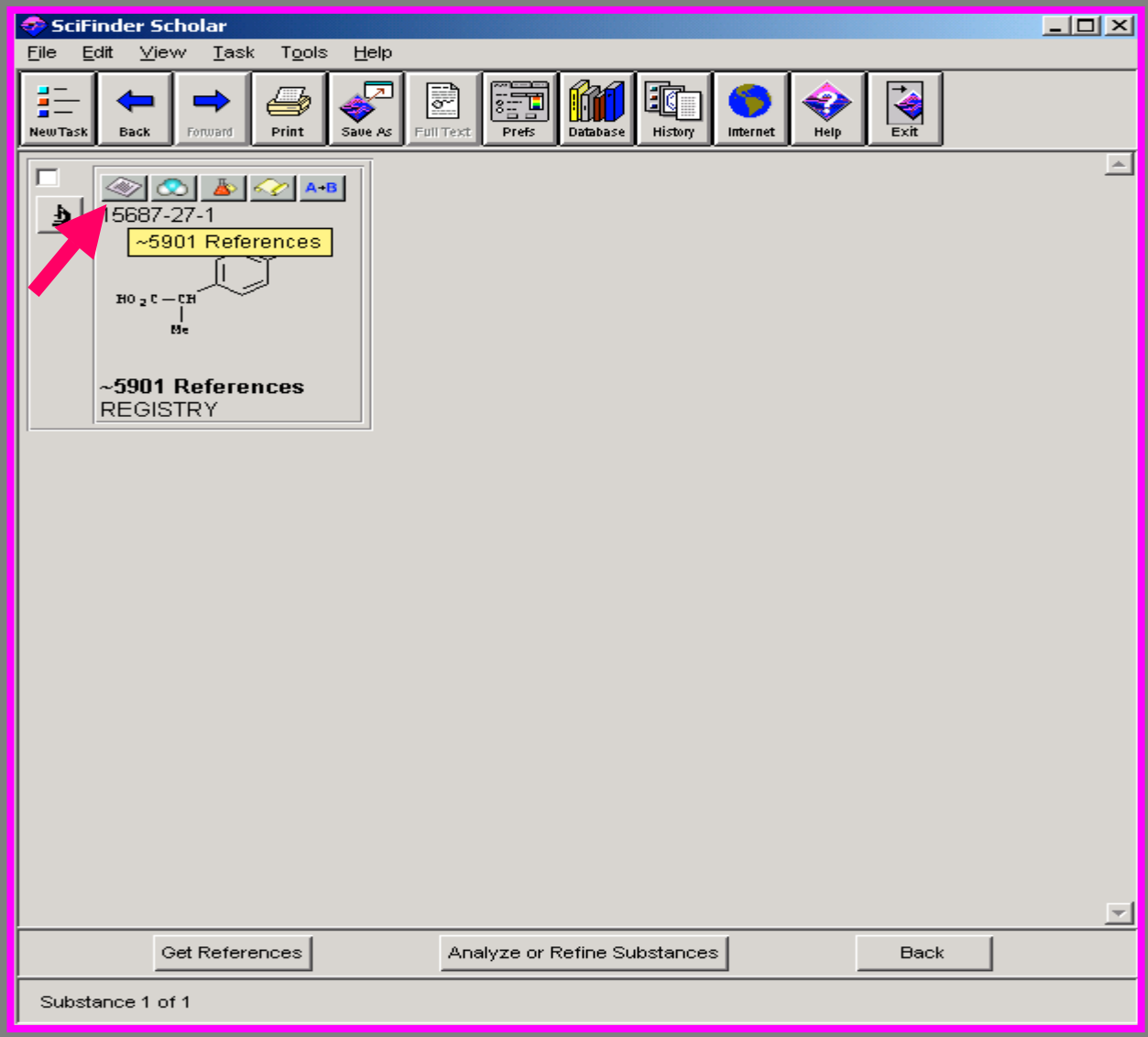
~5901 References

REGISTRY

Get References | Analyze or Refine Substances | Back

Substance 1 of 1

View References

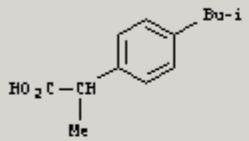


SciFinder Scholar

File Edit View Task Tools Help

New Task | Back | Forward | Print | Save As | Full Text | Prefs | Database | History | Internet | Help | Exit

15687-27-1



~5901 References
REGISTRY

Get References

For this substance, retrieve:

(•) All references ( ) References associated with:

- [ ] Adverse Effect, including Toxicity
- [ ] Analytical Study
- [ ] Biological Study
- [ ] Combinatorial Study
- [ ] Crystal Structure
- [ ] Formation, nonpreparative
- [ ] Miscellaneous
- [ ] Occurrence
- [ ] Preparation
- [ ] Process
- [ ] Properties
- [ ] Reactant or Reagent
- [ ] Spectral Properties
- [ ] Uses

For each **sequence**, retrieve:

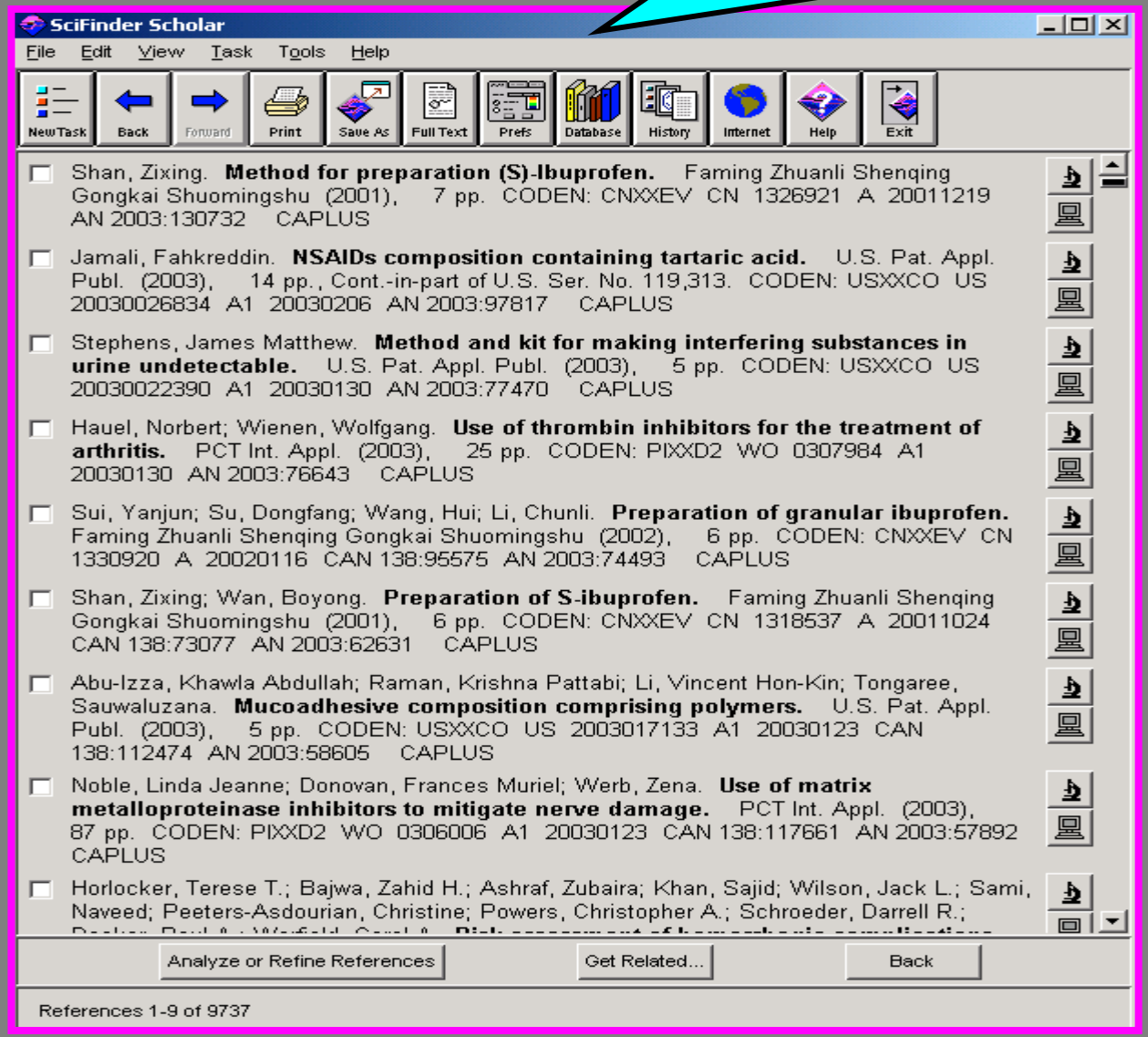
[ ] Additional related references, e.g., activity studies, disease studies. For more detail, click here.

OK Back

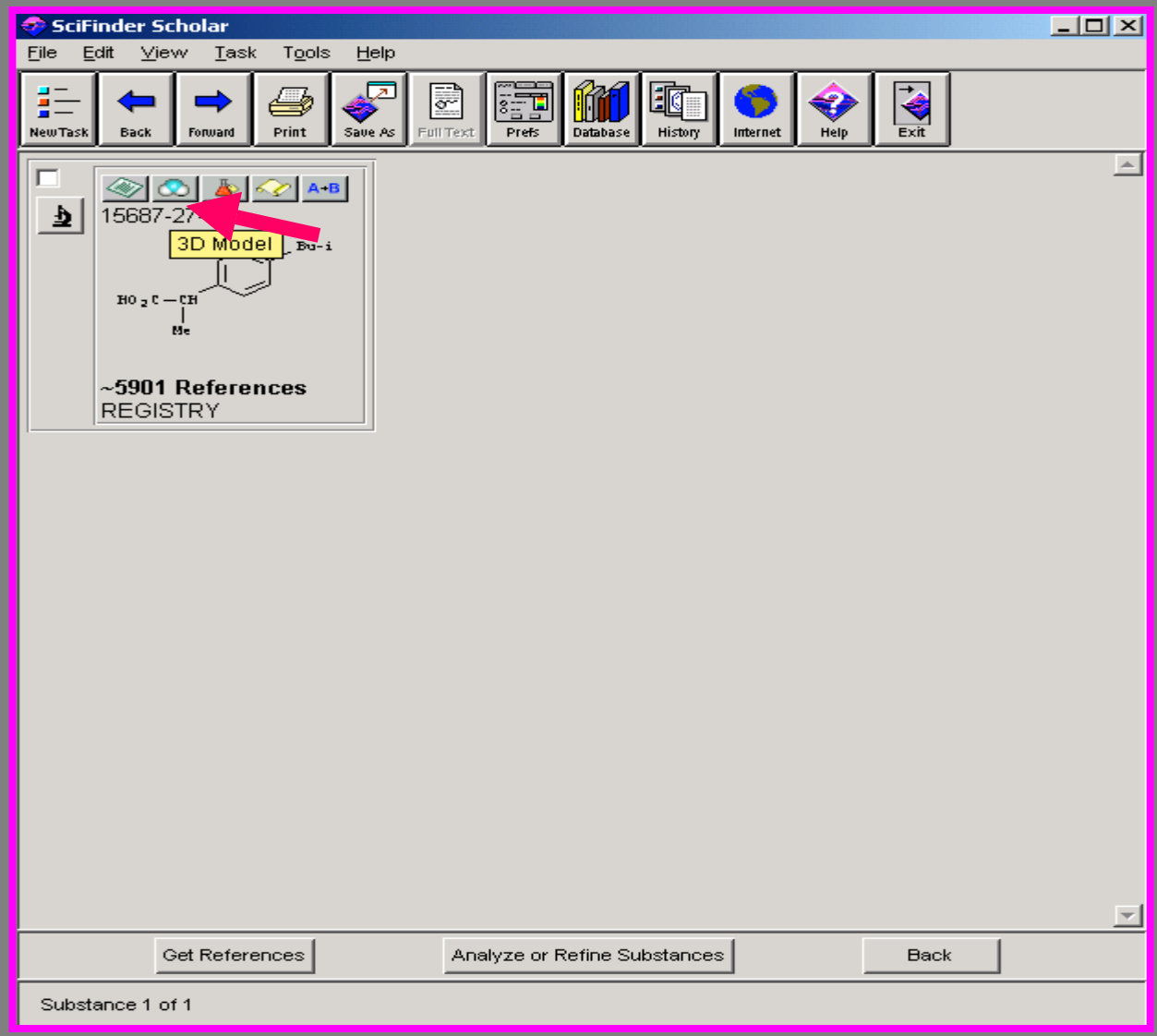
Get References | Analyze or Refine Substances | Back

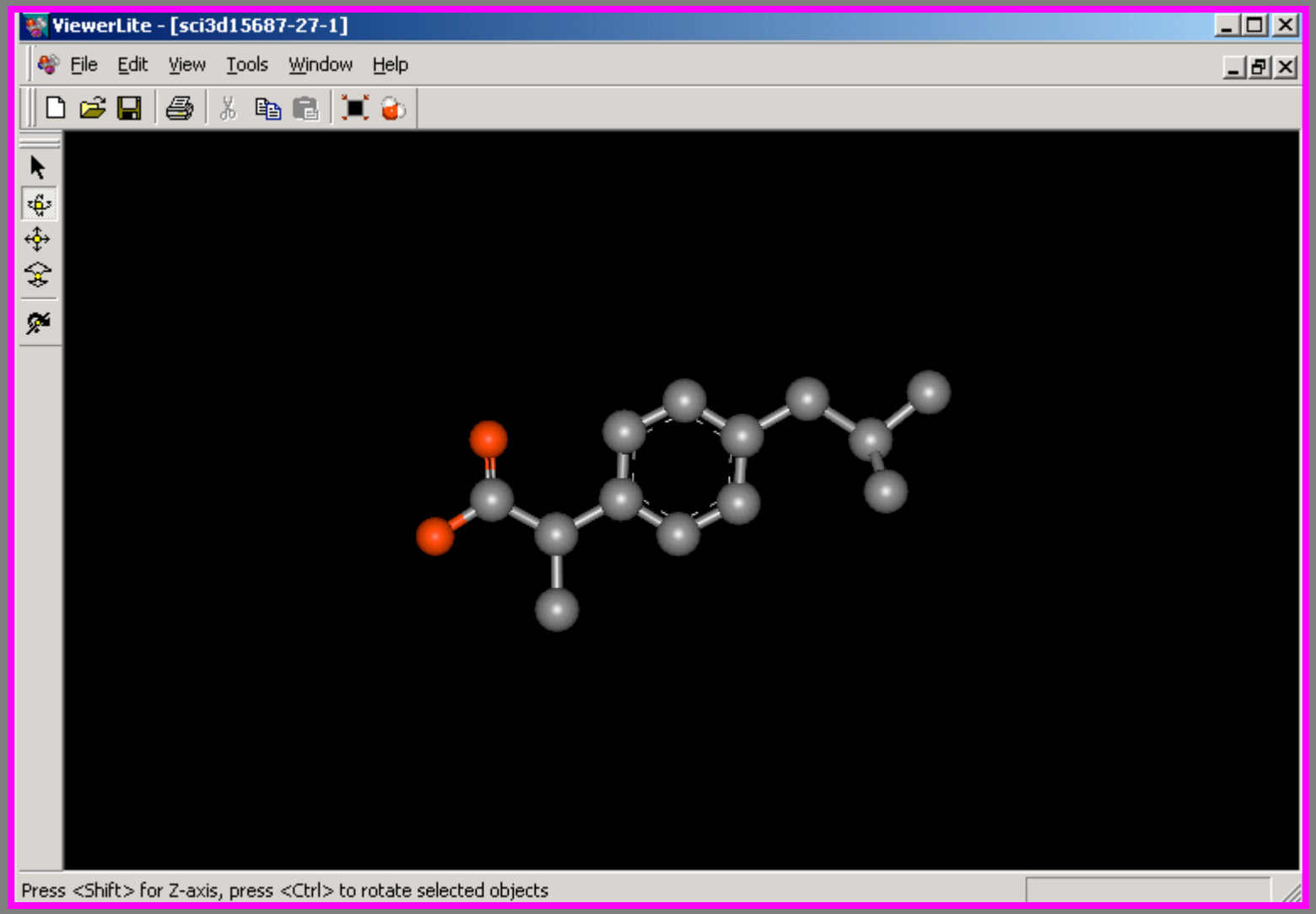
Substance 1 of 1

Here are the desired references

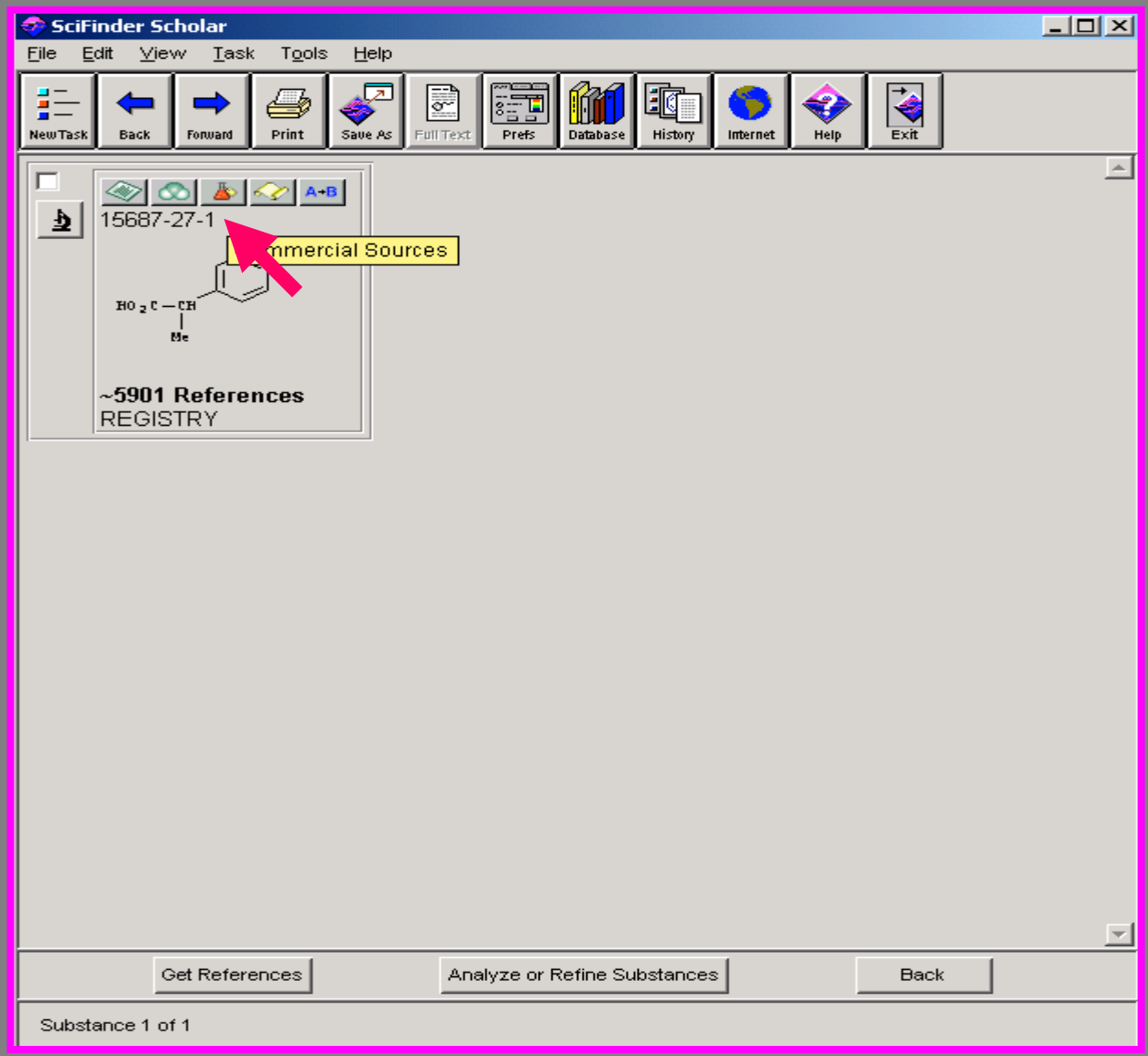


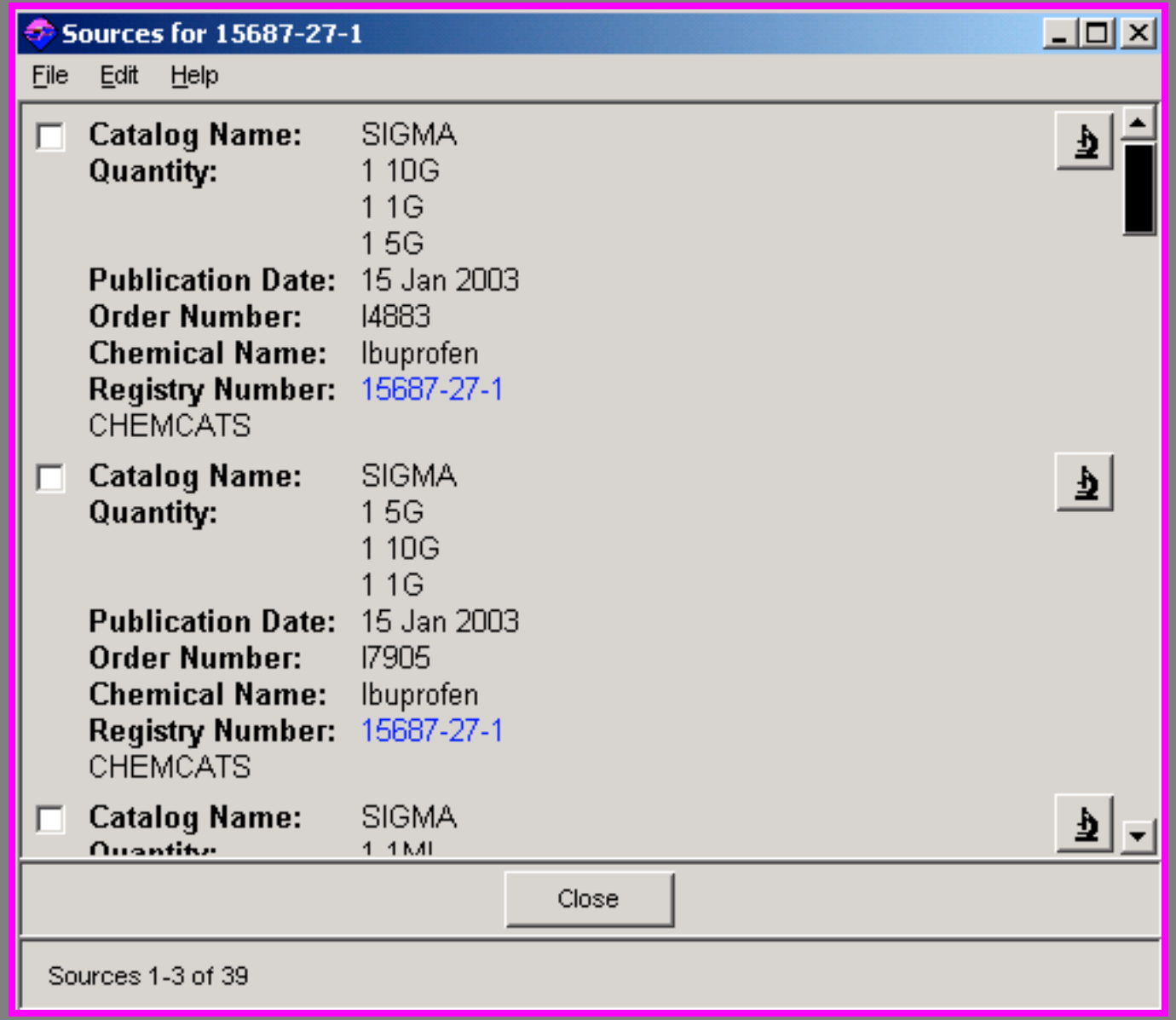
View 3D Structure




ViewerLite - [sci3d15687-27-1]
File Edit View Tools Window Help
Press <Shift> for Z-axis, press <Ctrl> to rotate selected objects

View Commercial Sources




Sources for 15687-27-1
File
Edit
Help
Catalog Name: SIGMA
Quantity: 1 10G
1 1G
1 5G
Publication Date: 15 Jan 2003
Order Number: I4883
Chemical Name: Ibuprofen
Registry Number: 15687-27-1
CHEMCATS
Catalog Name: SIGMA
Quantity: 1 5G
1 10G
1 1G
Publication Date: 15 Jan 2003
Order Number: I7905
Chemical Name: Ibuprofen
Registry Number: 15687-27-1
CHEMCATS
Catalog Name: SIGMA
Close
Sources 1-3 of 39

Detail of Source 1

File Edit Help

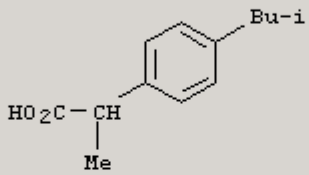
Catalog Name: SIGMA

Publication Date: 15 Jan 2003

Order Number: I4883

Chemical Name: Ibuprofen

Registry Number: 15687-27-1

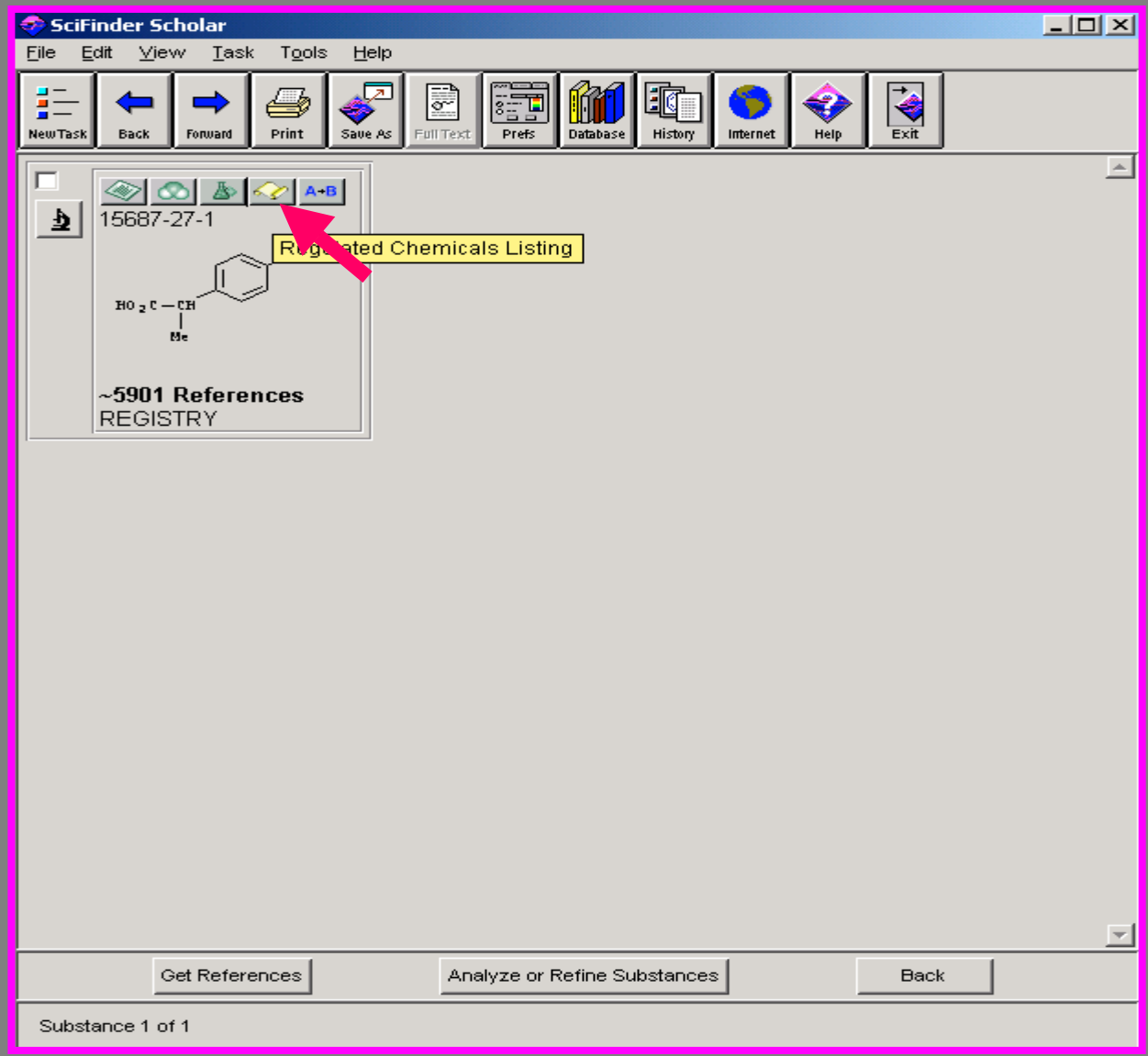


Pricing:
Quantity : 1 10G, Price: inquire:I4883-10G
Quantity : 1 1G, Price: inquire:I4883-1G
Quantity : 1 5G, Price: inquire:I4883-5G
Notes :2003

Company Info:
SIGMA
P O Box 14508
St. Louis, MO, 63178-9916
USA
Phone: 1 800 325 3010
314 771 5750
Fax: 1 800 325 5052
314 771 5757

Close

View Regulated Chemicals Listing



Regulated Chemicals Listing for 15687-27-1

File Edit Help

Accession Number: 18983 CHEMLIST

CAS Registry Number: 15687-27-1

Chemical Name

Benzeneacetic acid, α-methyl-4-(2-methylpropyl)- (TSCA, DSL, AICS, PICCS)
Ibuprofene (French) (DSL)
ibuprofen (English, German) (EINECS, PICCS)
ibuprofene (French) (EINECS)
ibuprofeno (Spanish) (EINECS)
p-(2-Methylpropyl)-α-methylphenylacetic acid (ENCS)
2-(4-Isobutylphenyl)propionic acid (ECL, PICCS)
PHENYLACETIC ACID, 2-METHYL-4-(2-METHYLPROPYL)- (PICCS)
(±)-α-Methyl-4-(2-methylpropyl)benzeneacetic acid
(±)-2-(p-Isobutylphenyl)propionic acid
(±)-Ibuprofen
(±)-Ibuprophen
(4-Isobutylphenyl)-α-methylacetic acid
(RS)-Ibuprofen
(S)-4-Isobutyl-α-methylphenylacetic acid
α-(4-Isobutylphenyl)propionic acid
α-Methyl-4-(2-methylpropyl)benzeneacetic acid
2-(4'-Isobutylphenyl)propionic acid
2-(4-Isobutylphenyl)propanoic acid
2-(p-Isobutylphenyl)propionic acid
4-Isobutyl-α-methylphenylacetic acid
4-Isobutylhydratropic acid
Advil
Brufen
dl-Ibuprofen
Dolgit
Hydratropic acid, p-isobutyl-

Close

Regulated Chemicals Listing 1 of 1

Regulated Chemicals Listing for 15687-27-1

File Edit Help

Unipron

File Segment
AUSTRALIA: AICS; CANADA: DSL; EEC: EINECS; JAPAN: ENCS; KOREA: ECL; PHILIPPINES: PICCS; USA: TSCA

Confidentiality Status
Public

Regulatory List Number
EINECS No.: 239-784-6
ENCS No.: 9-183
ECL Serial No.: KE-21458

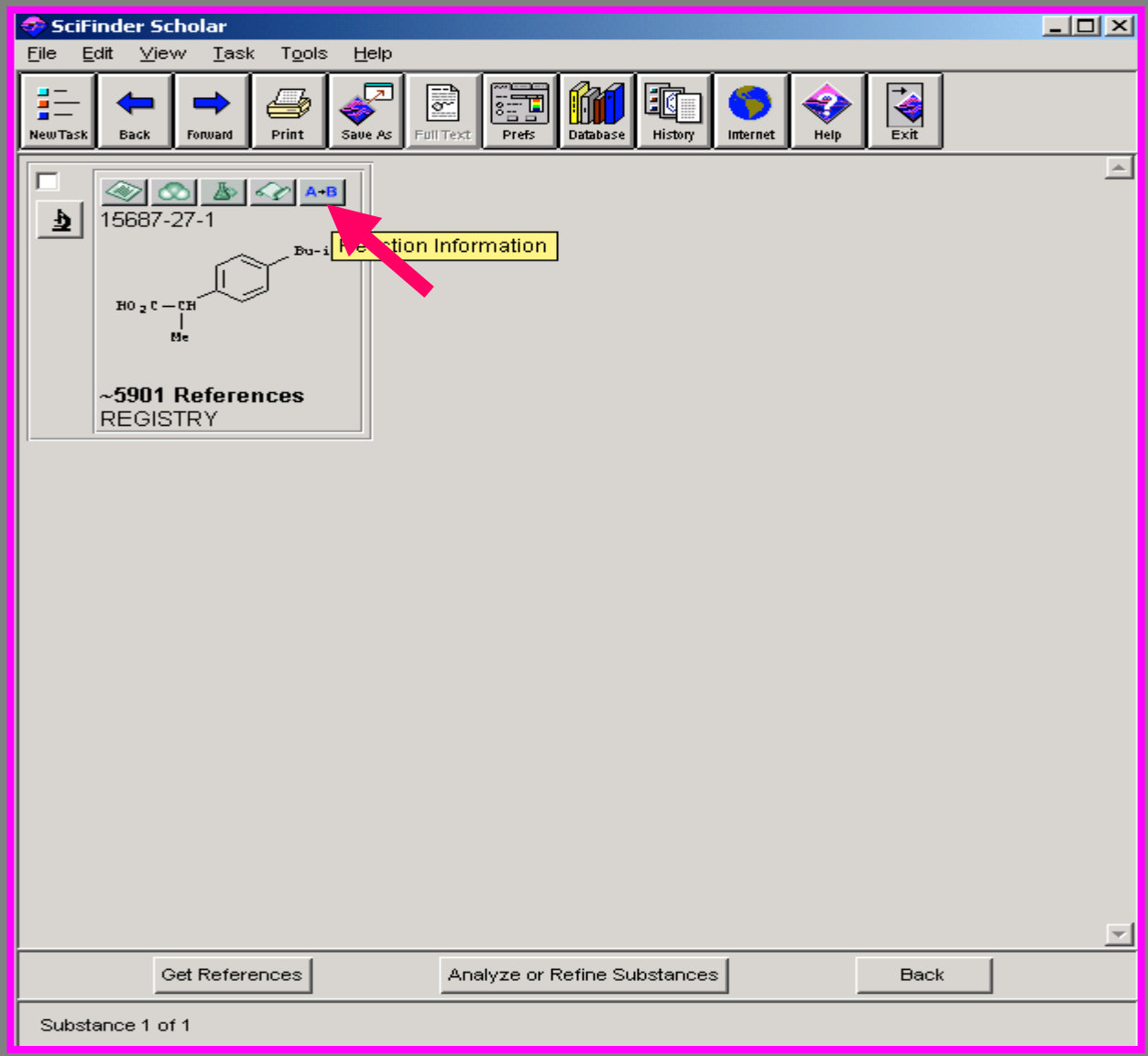
Inventory Status
On TSCA Inventory
May 2002 Inventory Tape.
On DSL
Supplement to Canada Gazette, Part I, January 26, 1991.
On EINECS
Annex to Official Journal of the European Communities, 15 June 1990.
On ENCS
Japanese Gazette. Contained within class: Low Molecular Carbo-monocyclic Organic Compounds.
On AICS
Australian Inventory of Chemical Substances, June 1996 Ed.
On ECL
Korean Existing Chemicals List, January 1997.
On PICCS
Philippines Inventory of Chemicals and Chemical Substances, 2000.

Database: CHEMLIST

Close

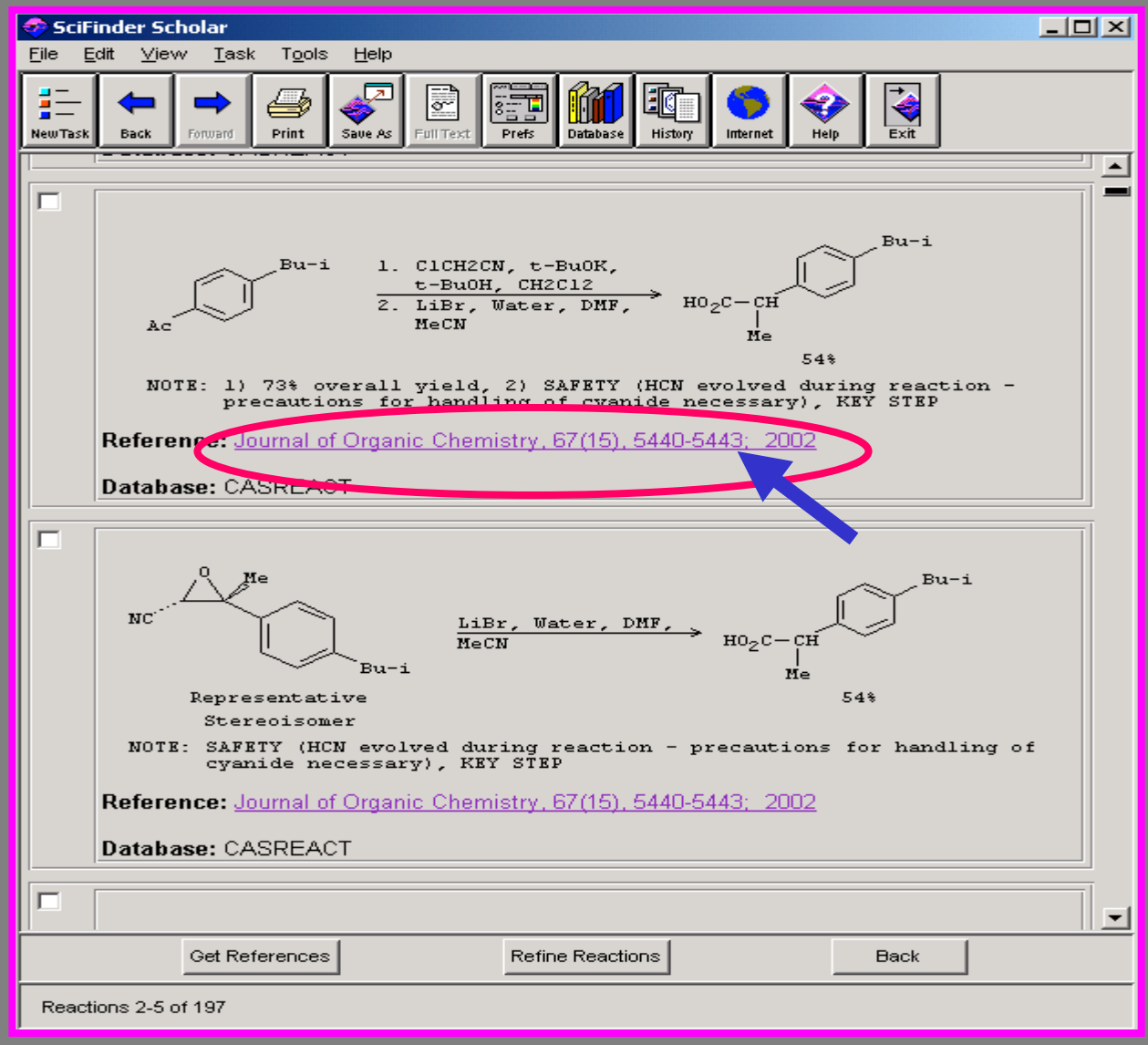
Regulated Chemicals Listing 1 of 1

View Reaction Information



Select a reaction role

Link to view reference of desired reaction



Detail of Reference for Reaction 3

File Edit Help

Bibliographic Information

Rearrangement of Epoxynitriles: A Convenient Homologation of Acyclic and Cyclic Ketones to Carboxylic Acids. Badham, Neil F.; Mendelson, Wilford L.; Allen, Andrew; Diederich, Ann M.; Eggleston, Drake S.; Filan, John J.; Freyer, Alan J.; Killmer, Lewis B., Jr.; Kowalski, Conrad J.; Liu, Li; Novack, Vance J.; Vogt, Frederick G.; Webb, Kevin S.; Yang, Jennifer. GlaxoSmithKline Pharmaceuticals, King of Prussia, PA, USA. Journal of Organic Chemistry (2002), 67(15), 5440-5443. CODEN: JOCEAH ISSN: 0022-3263. Journal written in English. CAN 137:185367 AN 2002:462943 CAPLUS

Abstract

Epoxynitriles, prepd. from aliph. and arom. ketones by Darzens condensation reactions with chloroacetonitrile, undergo rearrangement in the presence of either lithium or magnesium bromide and water to give carboxylic acids. E.g., a soln. of arylcyanocyclohexanone I and chloroacetonitrile in THF is added slowly to a soln. of KOH and benzyltriethylammonium chloride in THF/H2O at 0° and stirred for 1 h to give the spiroepoxynitrile II stereoselectively in 73% yield. E.g., II is added to a soln. of acetonitrile, lithium bromide, and water in DMF and the mixt. is heated at 90-95° for 16 h to give, after a workup to destroy remaining HCN present in the reaction mixt. and sepn. of the stereoisomers, the desired cis-arylcyanocyclohexanecarboxylic acid SB-207499 (a potential agent in the treatment of chromic obstructive pulmonary disease) is isolated in 69% yield. Aryl and aliph. epoxynitriles both rearrange to give carboxylic acids; epoxynitriles with secondary and tertiary alkyl groups on the epoxide do not rearrange. In the absence of water, epoxynitriles yield acylnitrile-derived dimers; water hydrolyzes acylnitrile intermediates to give the isolated carboxylic acids. A mechanism for the rearrangement is proposed in which lithium bromide acts as a simple nucleophile to open epoxides; elimination of hydrogen bromide, protonation or tautomerization of the acylnitrile enols or lithium enolates, and hydrolysis of the acylnitriles yields the obsd. carboxylic acids. This method constitutes a two-step homologation of ketones to secondary carboxylic acids.

Get Related... Close

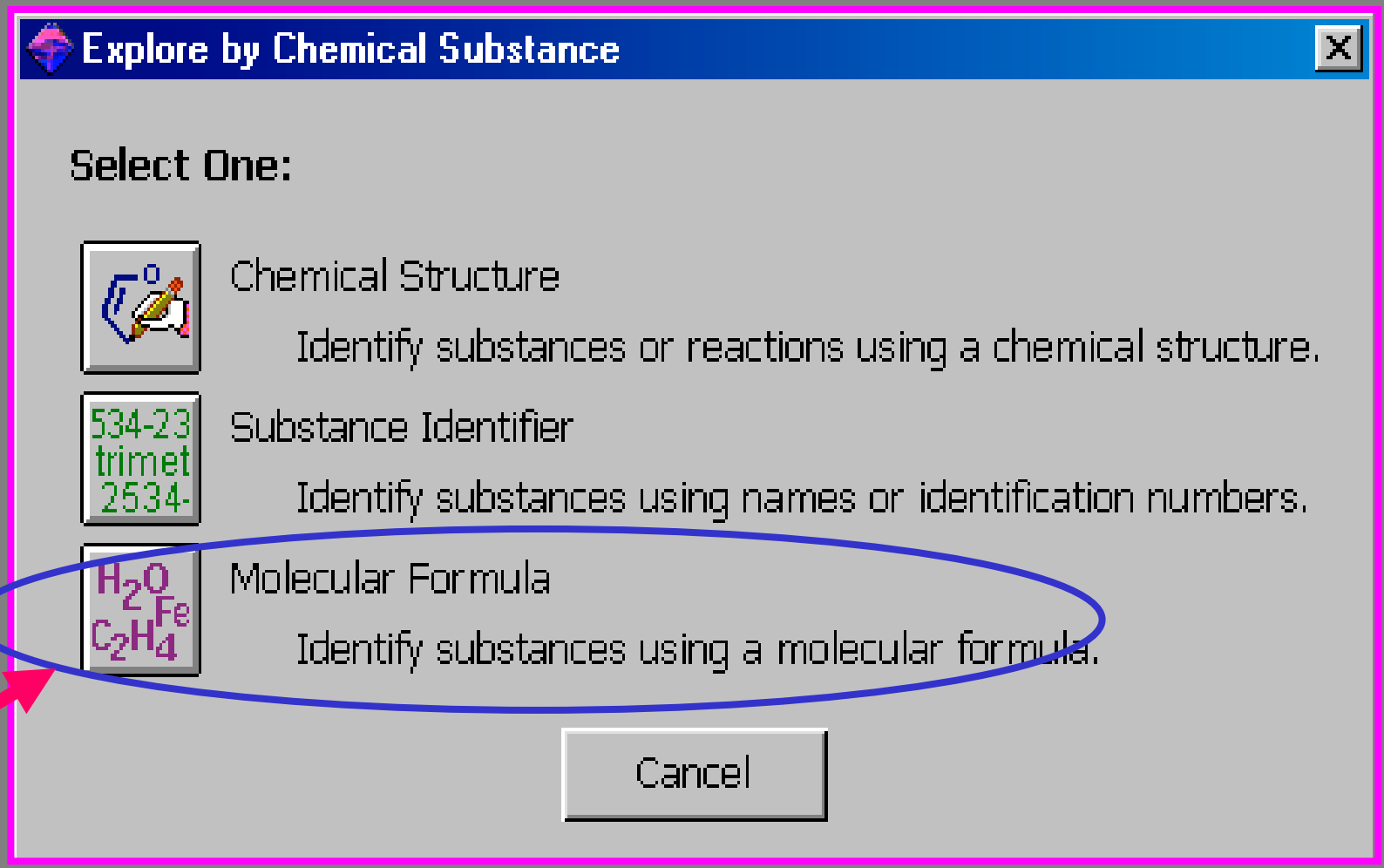
Explore
By
Molecular formula

Explore by Molecular Formula

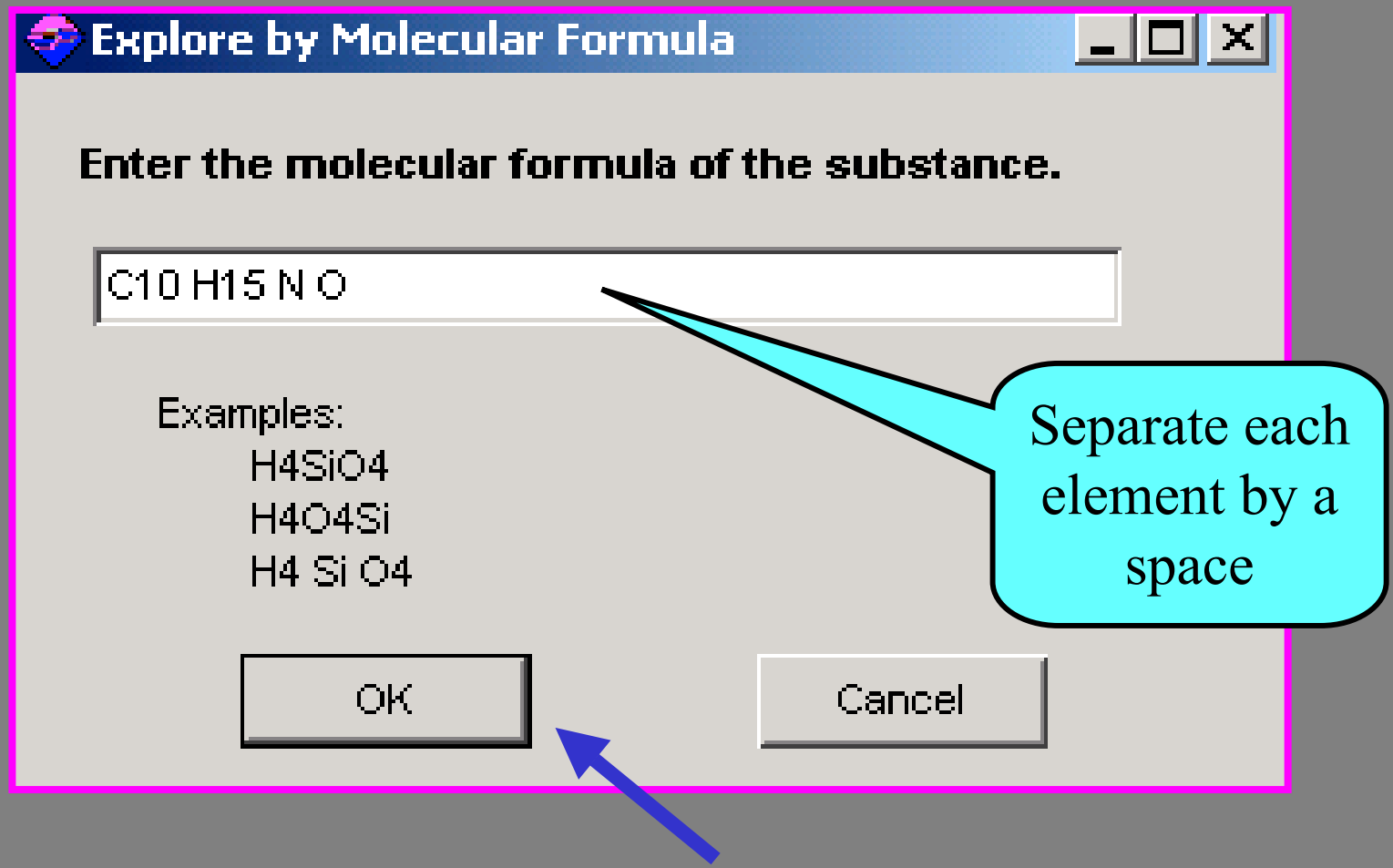
- An unknown compound is known to be involved in barley growth.

- MS and NMR spectra indicate the following:
  - Molecular formula of **C10 H15 N O**
  - A hydroxyphenyl group
  - A tertiary amine
  - A 1,4-disubstituted phenyl ring

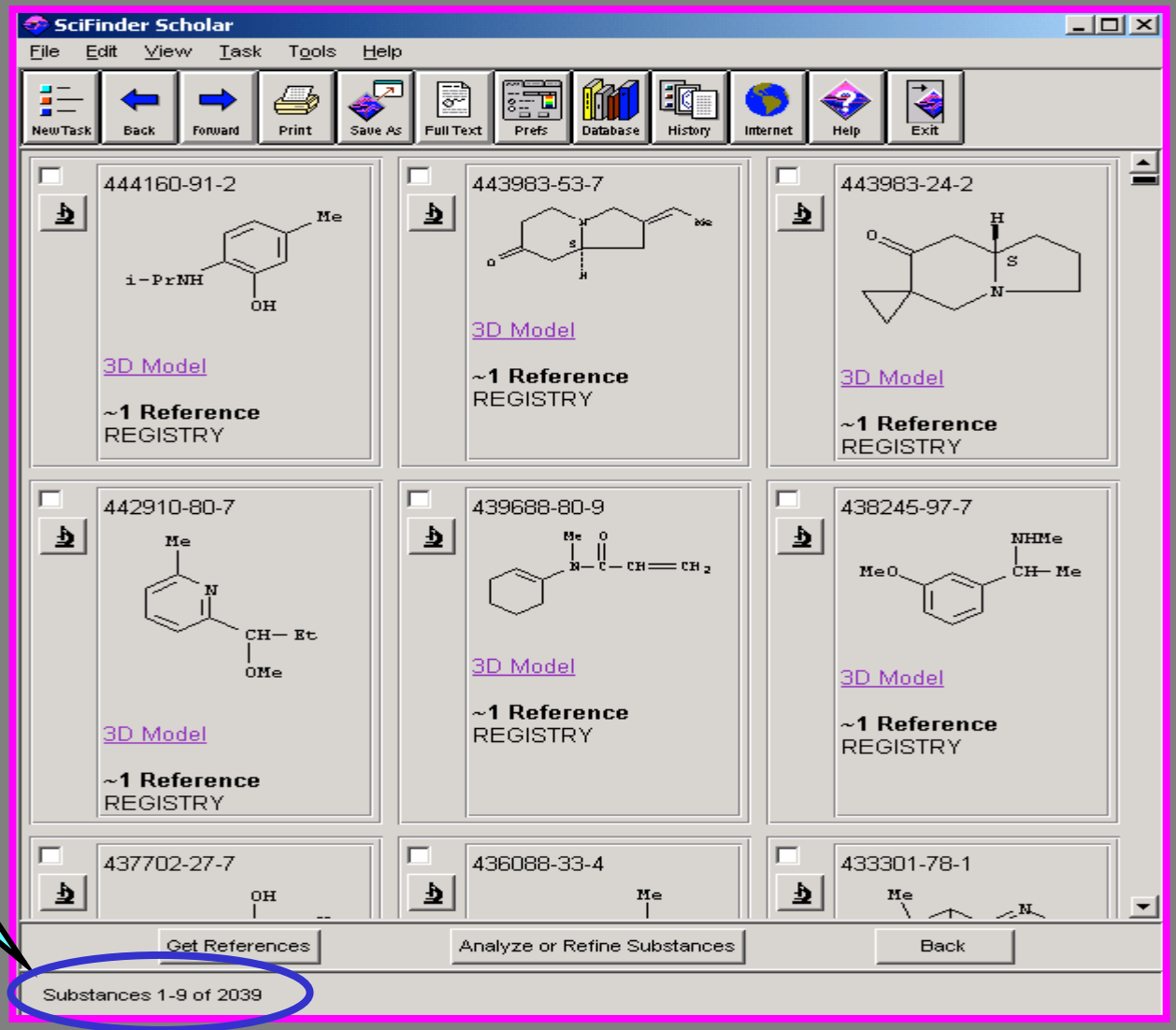
Explore by molecular formula



Enter the molecular formula of the substance

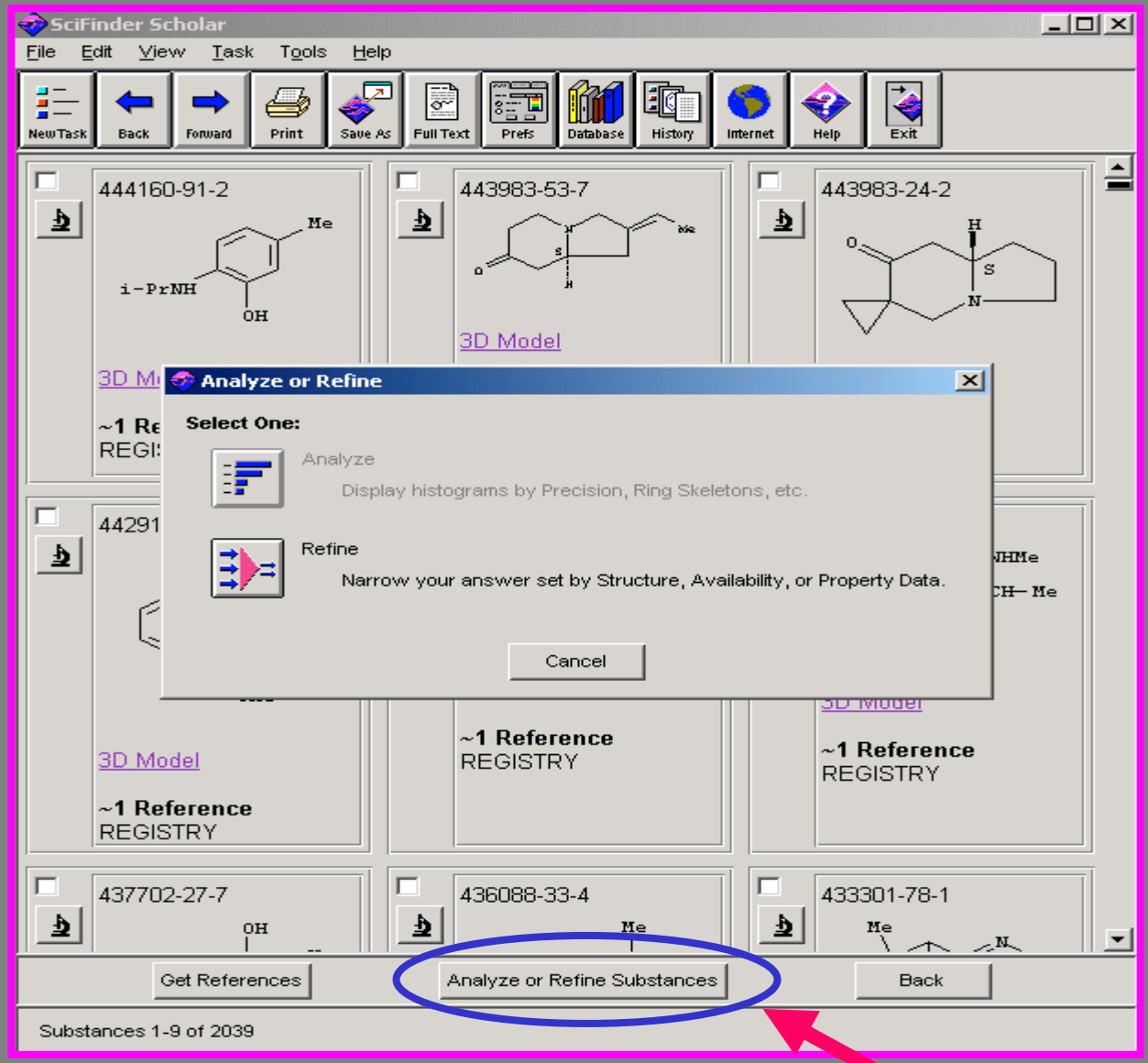


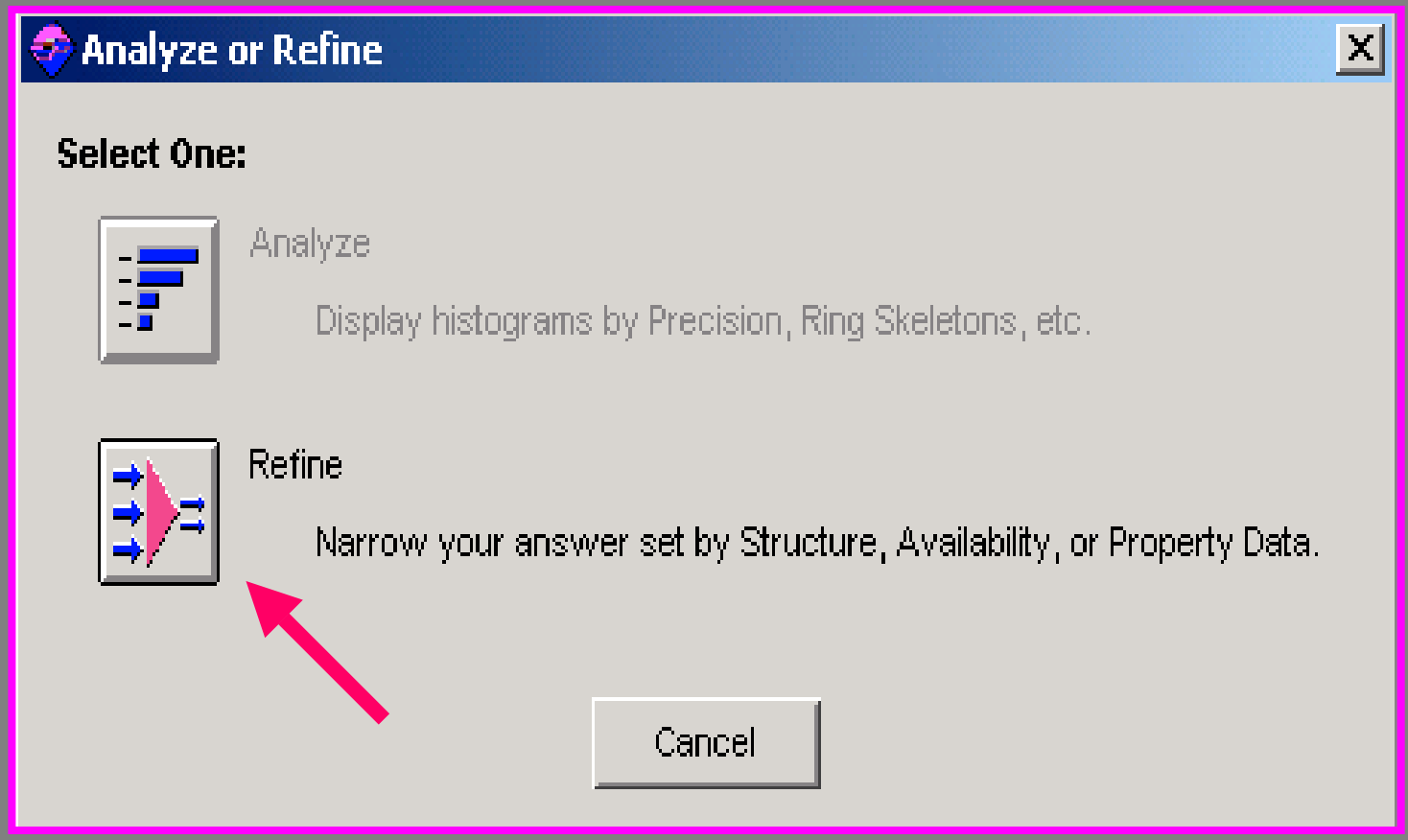
Here are the substances retrieved!



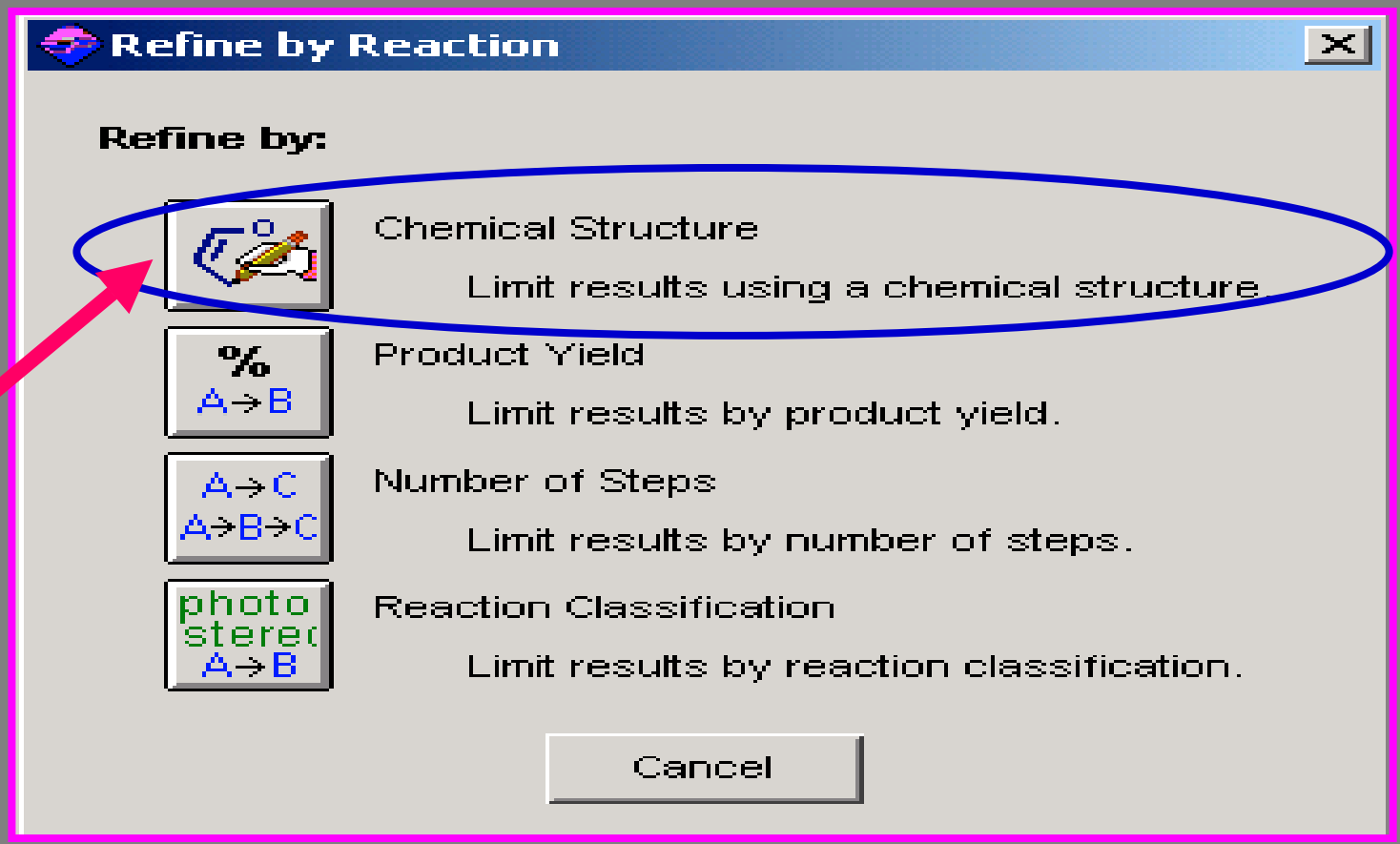
2039 substances

Narrow down answer set

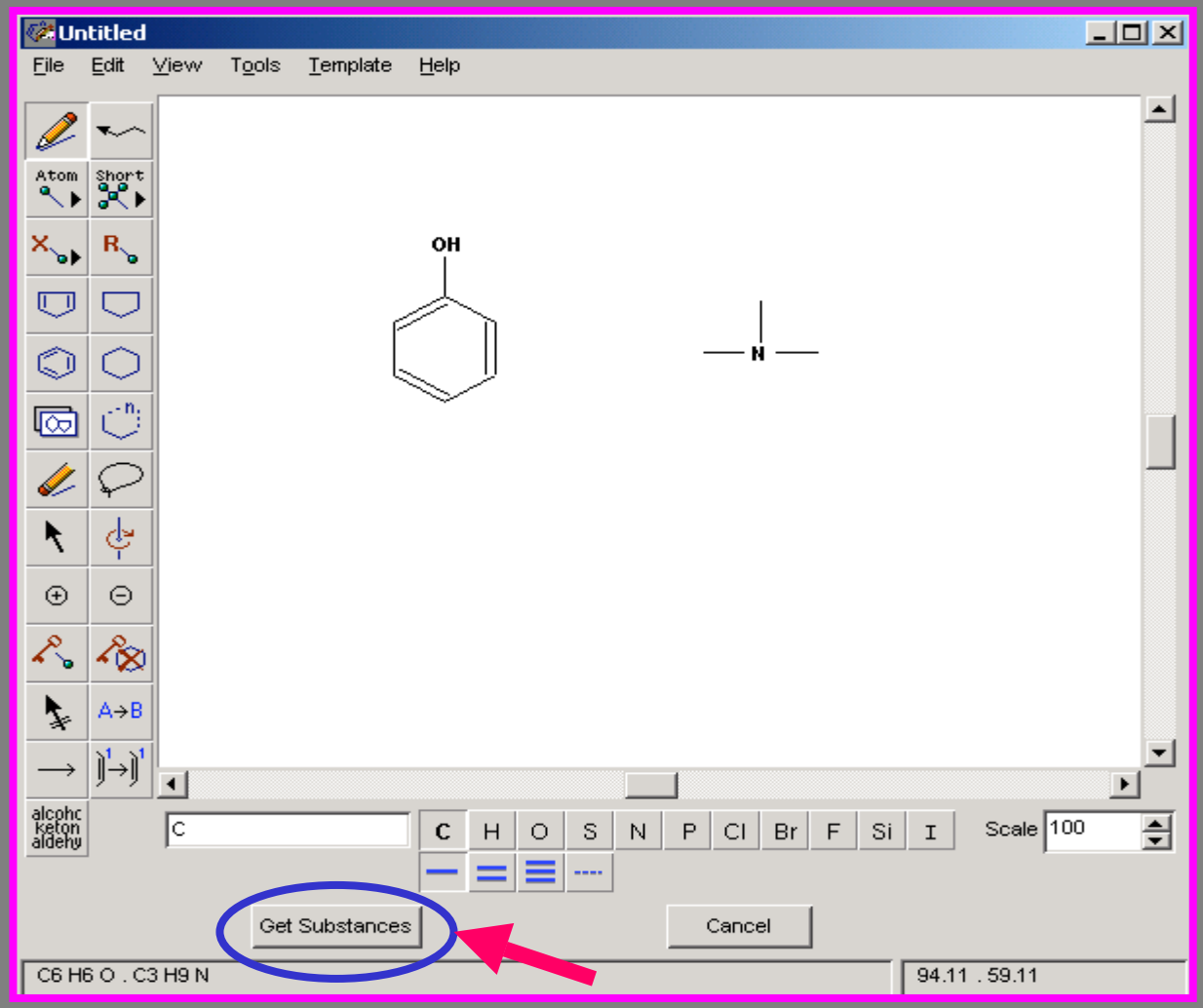



Analyze or Refine
Select One:
Analyze
Display histograms by Precision, Ring Skeletons, etc.
Refine
Narrow your answer set by Structure, Availability, or Property Data.
Cancel

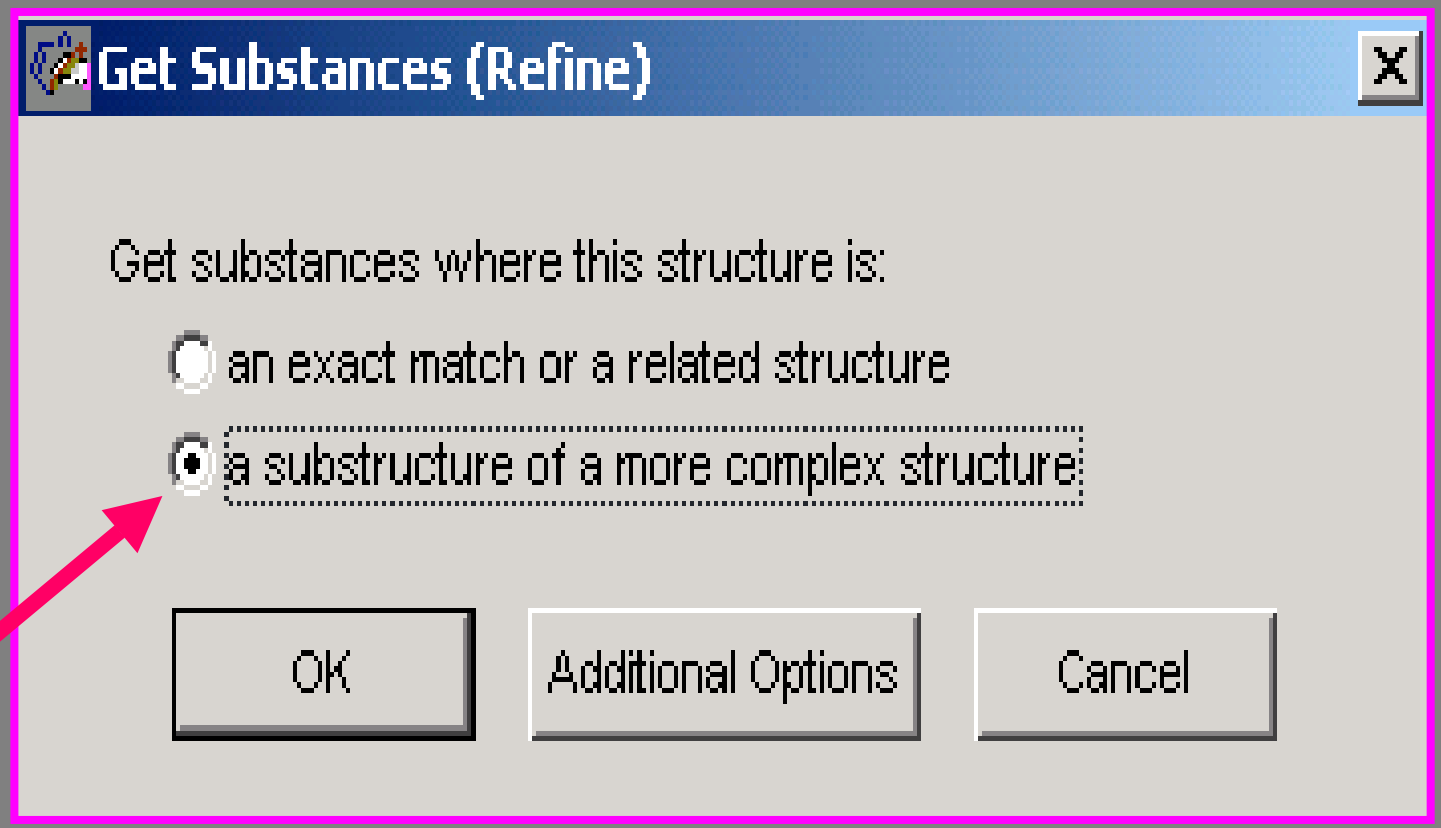
Let's refine reaction by chemical structure



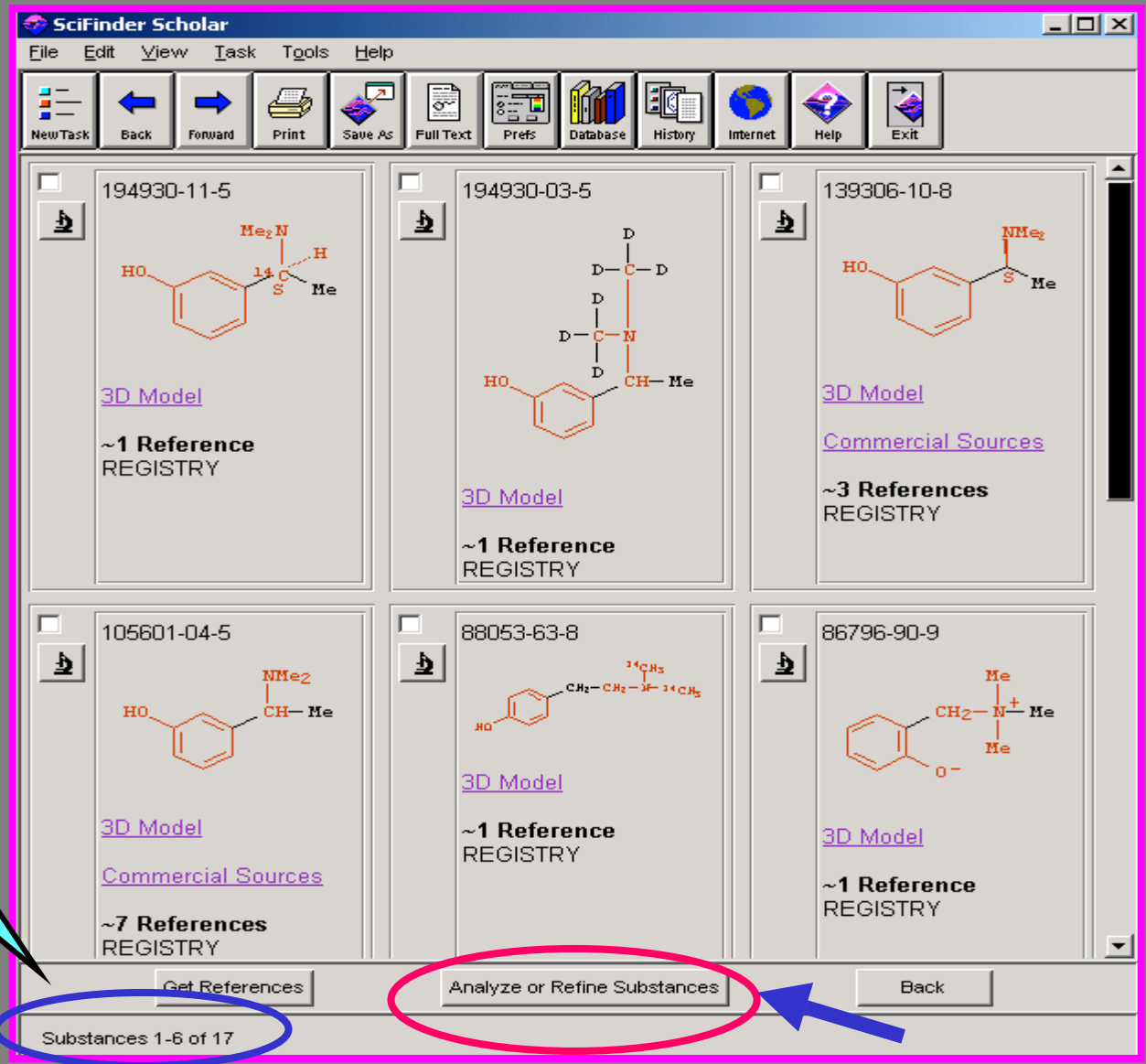
Refine by a hydroxyphenyl group and a tertiary amine



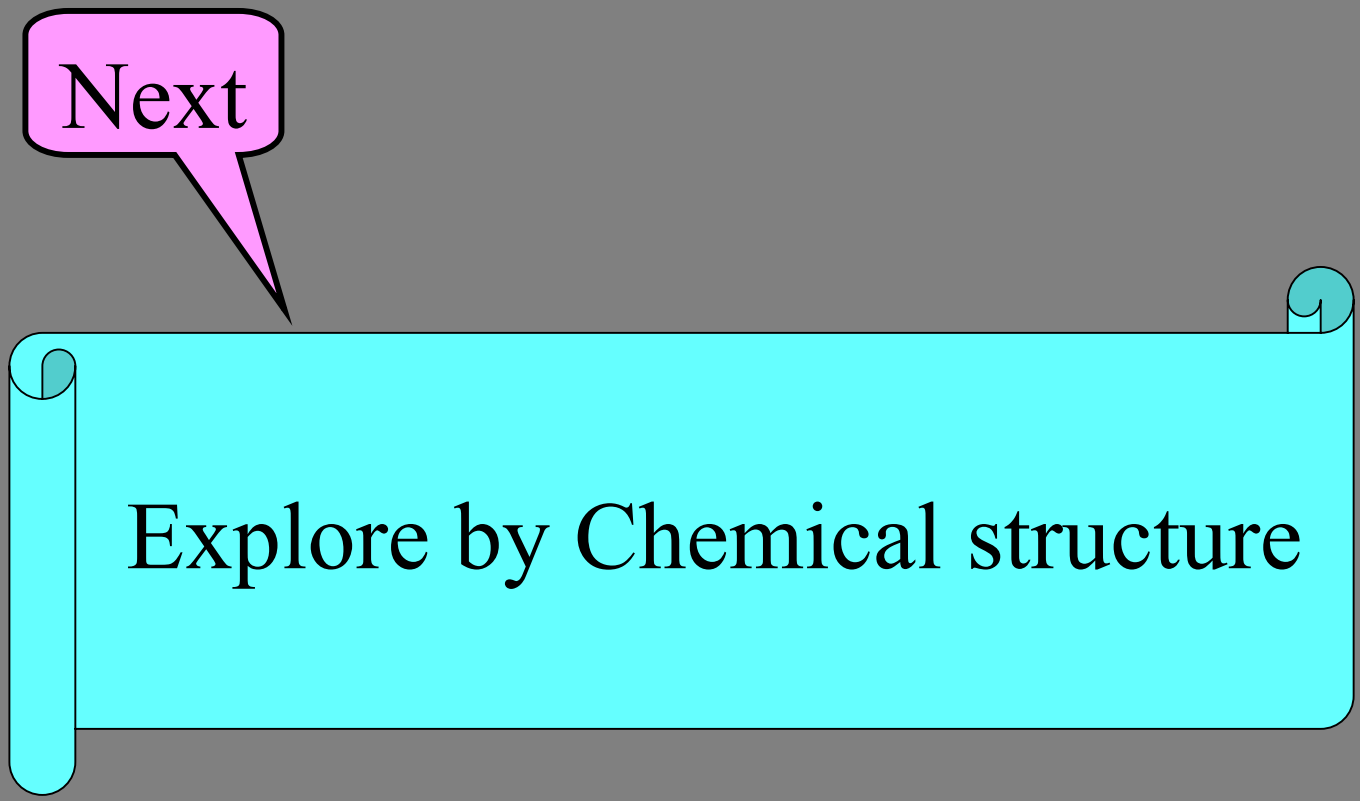
Select a substructure of a more complex structure



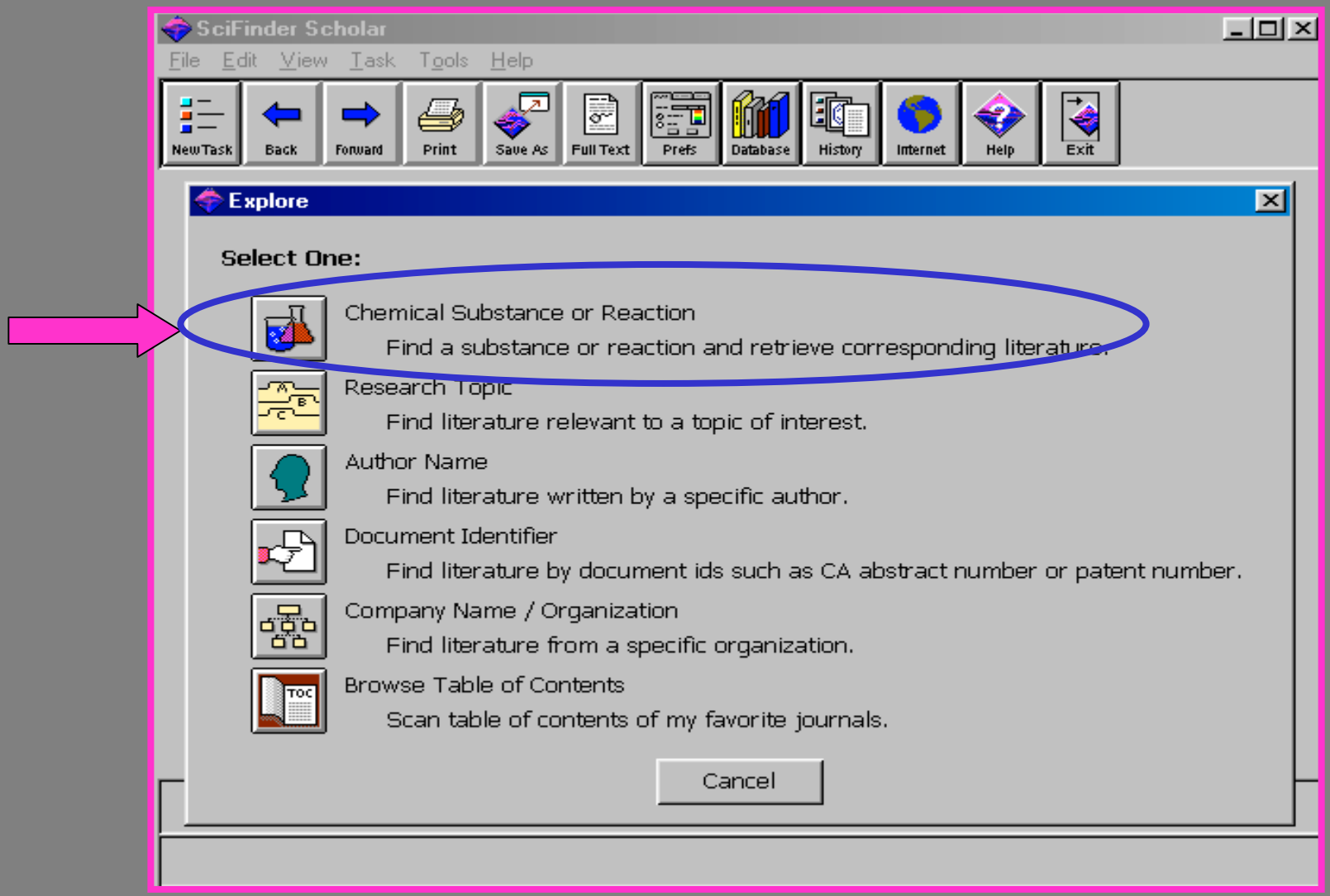
Refine further to isolate 1,4- disubstituted compounds



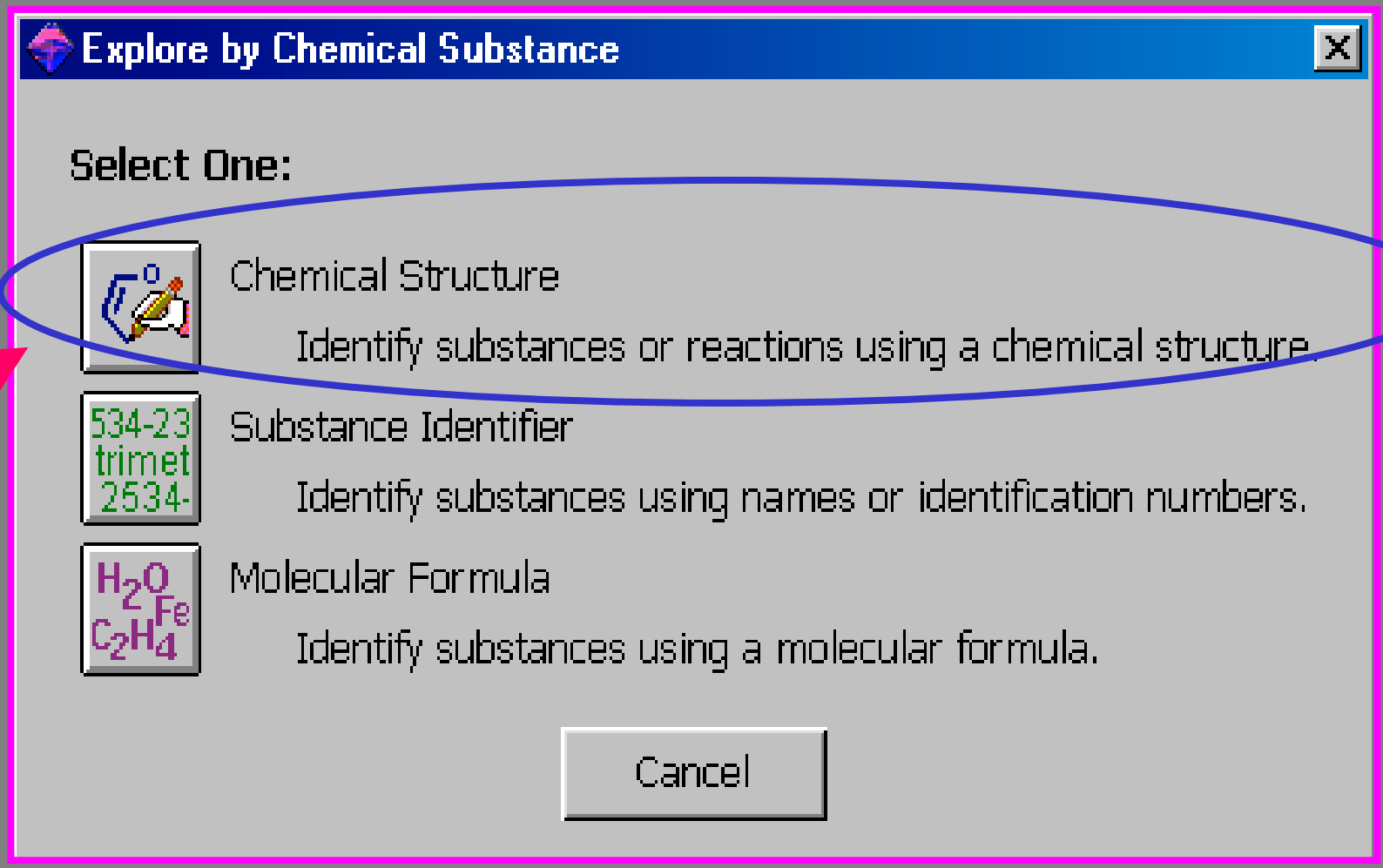
17 substances


Next
Explore by Chemical structure

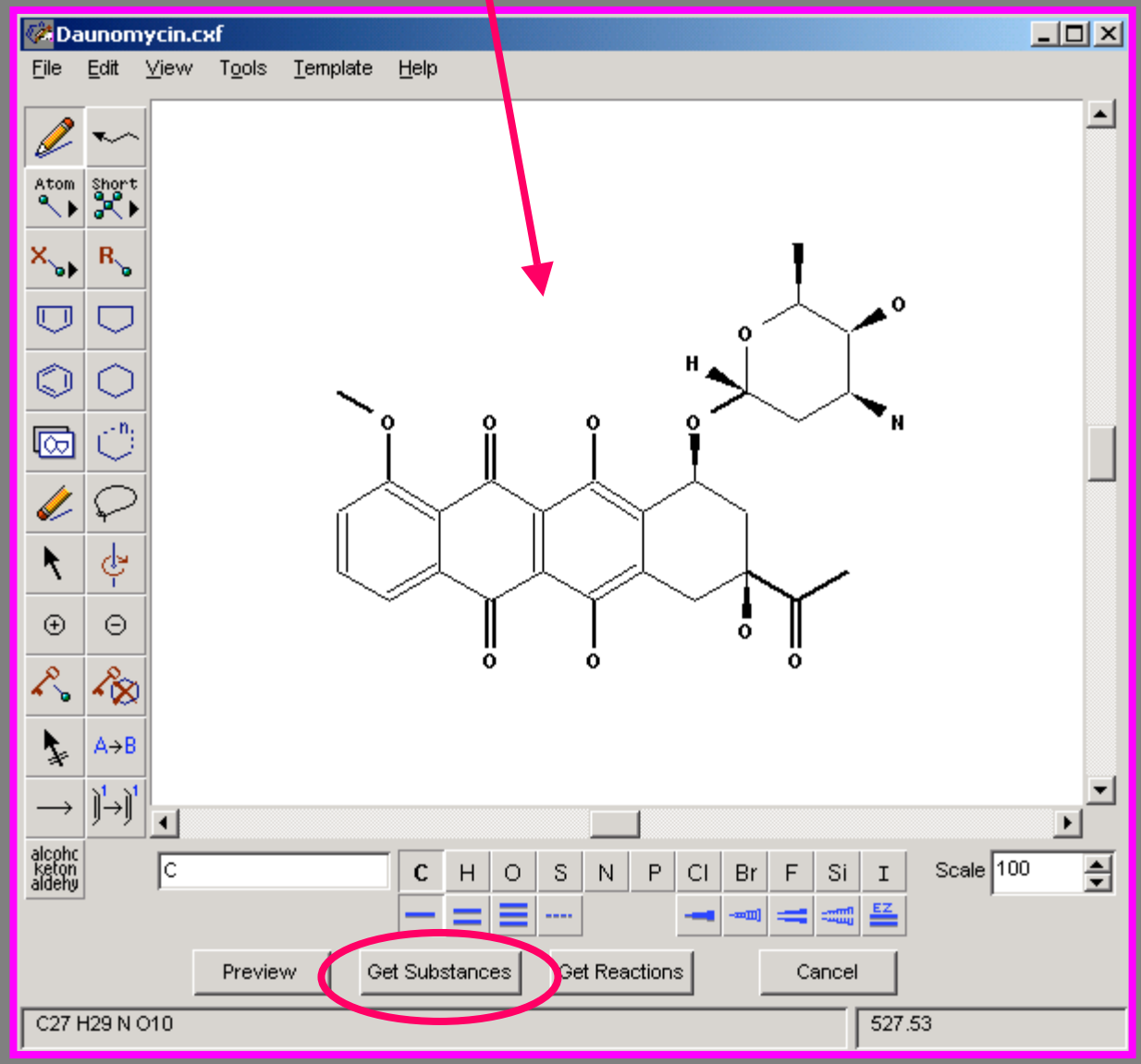
Search by chemical substance and reaction

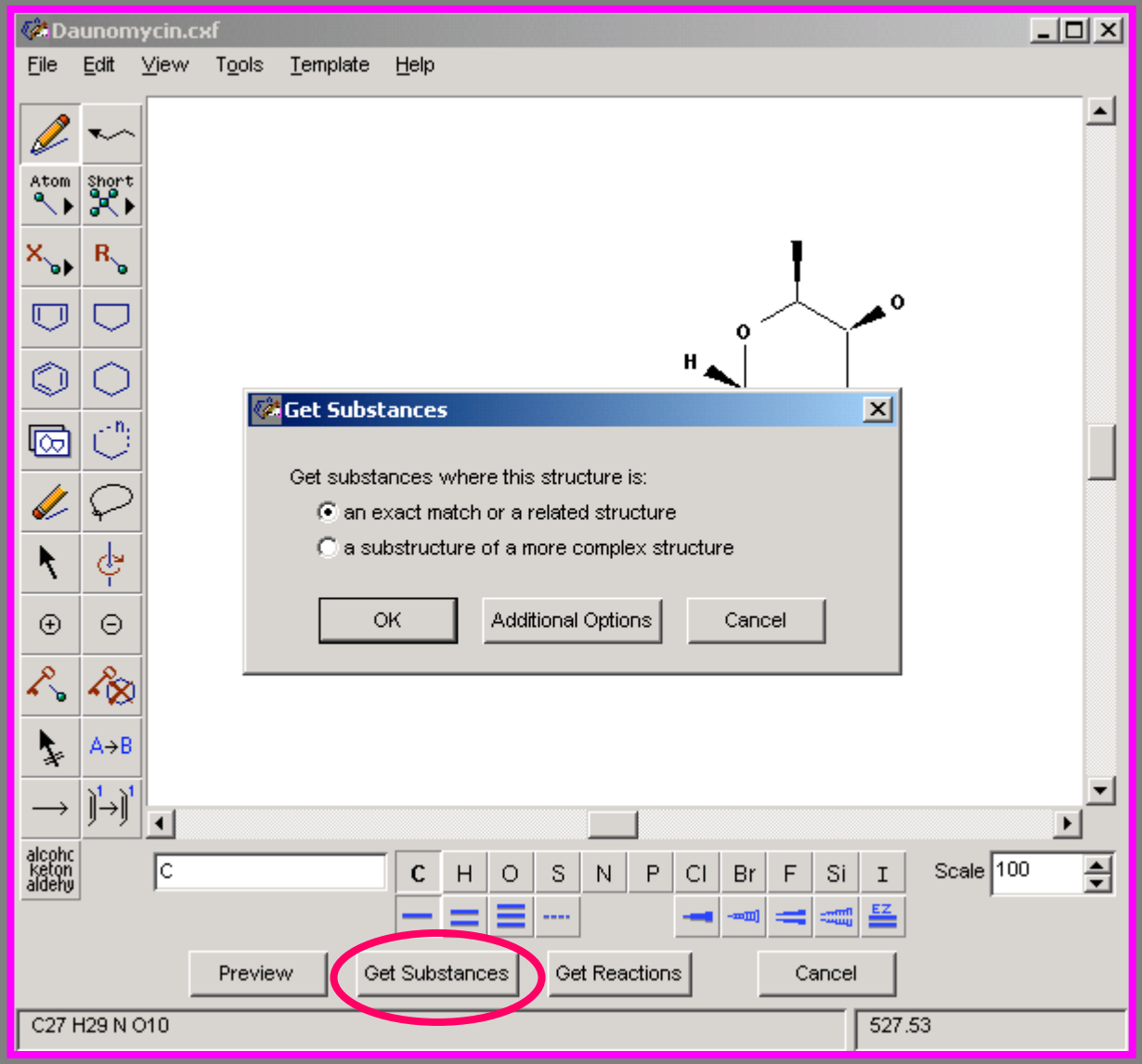


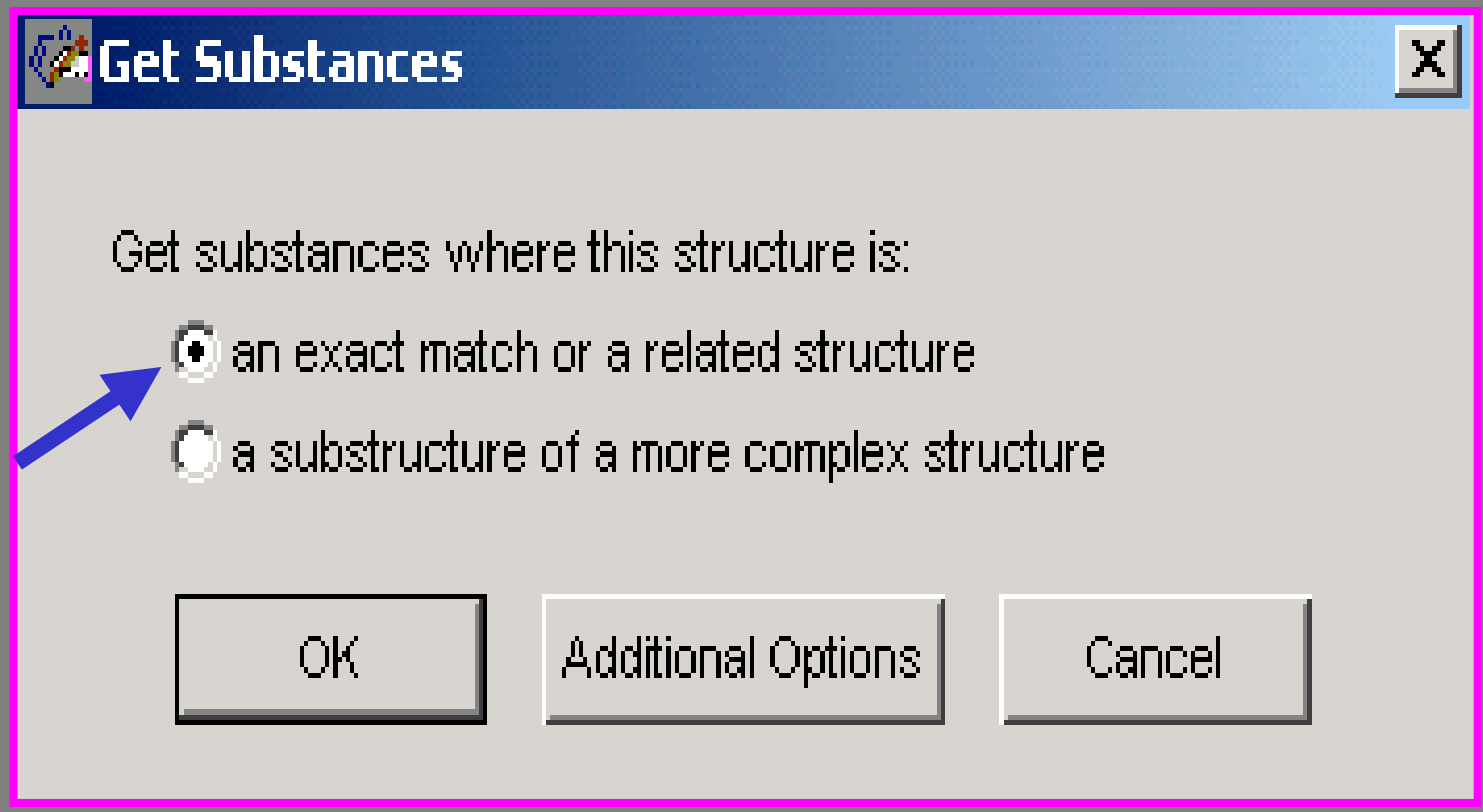
Explore by Chemical Structure



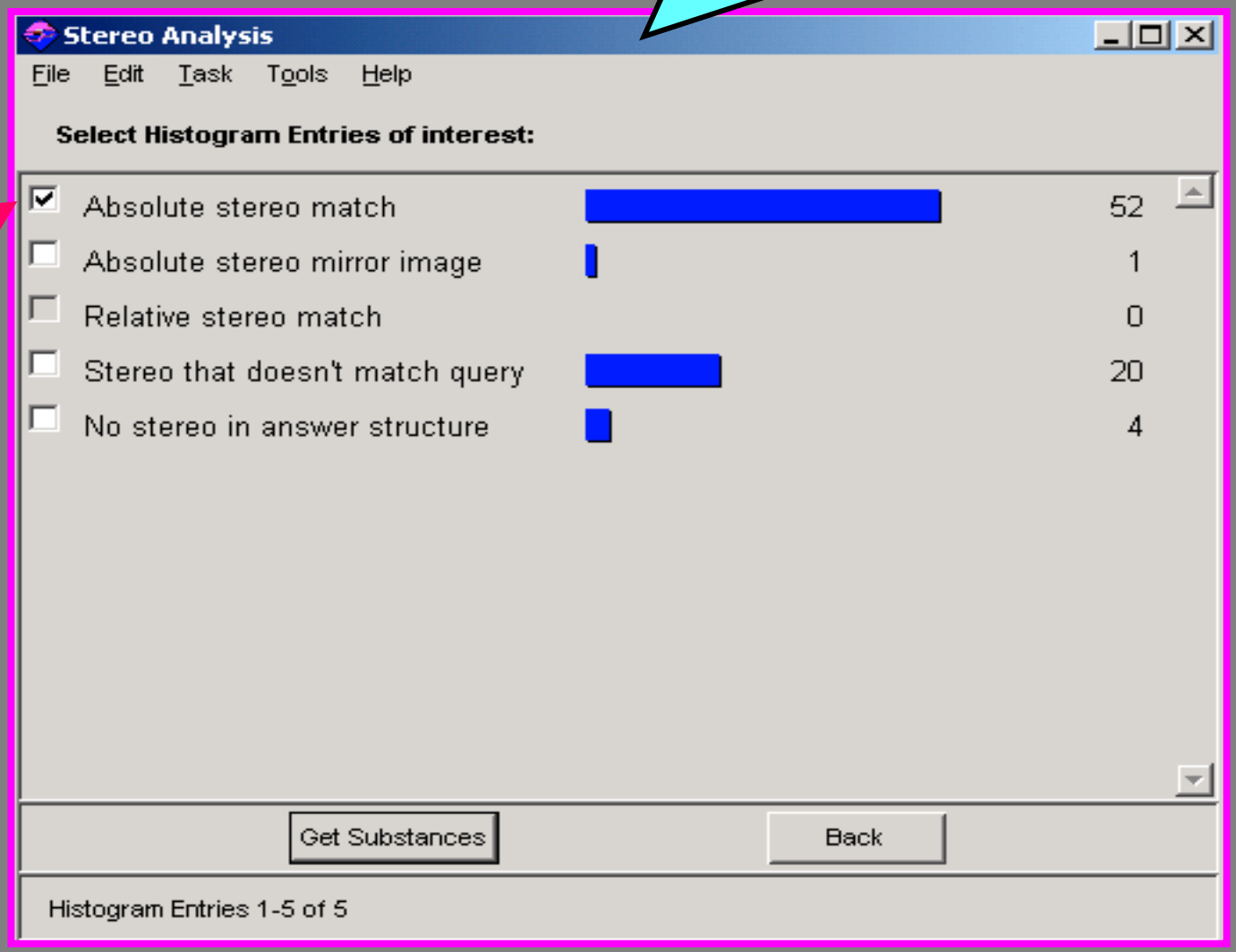
Draw chemical structure of interest




Daunomycin.cxf
File
Edit
View
Tools
Template
Help
Atom
Short
alcohc
keton
aldehy
A→B
O
O
H
Get Substances
Get substances where this structure is:
an exact match or a related structure
a substructure of a more complex structure
OK
Additional Options
Cancel
C
C
H
O
S
N
P
Cl
Br
F
Si
I
Scale
100
Preview
Get Substances
Get Reactions
Cancel
C27 H29 N O10
527.53


Get Substances
Get substances where this structure is:
an exact match or a related structure
a substructure of a more complex structure
OK
Additional Options
Cancel

Stereo Analysis



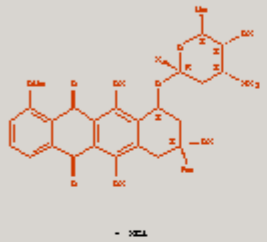
SciFinder Scholar

File Edit View Task Tools Help

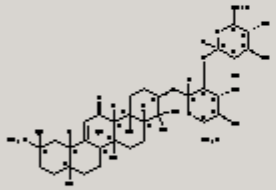
New Task | Back | Forward | Print | Save As | Full Text | Prefs | Database | History | Internet | Help | Exit

495400-71-0

Component Number 1



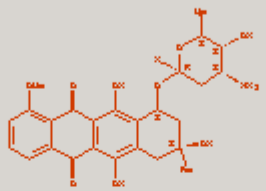
Component Number 2



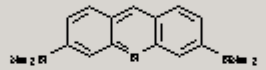
~1 Reference
REGISTRY

476360-24-4

Component Number 1



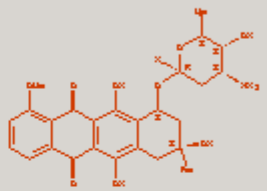
Component Number 2



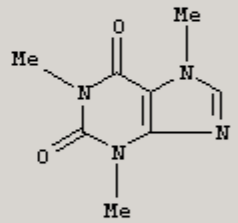
~1 Reference
REGISTRY

439668-52-7

Component Number 1



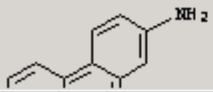
Component Number 2



~1 Reference
REGISTRY

439665-99-3

Component Number 1



390755-64-3

Component Number 1

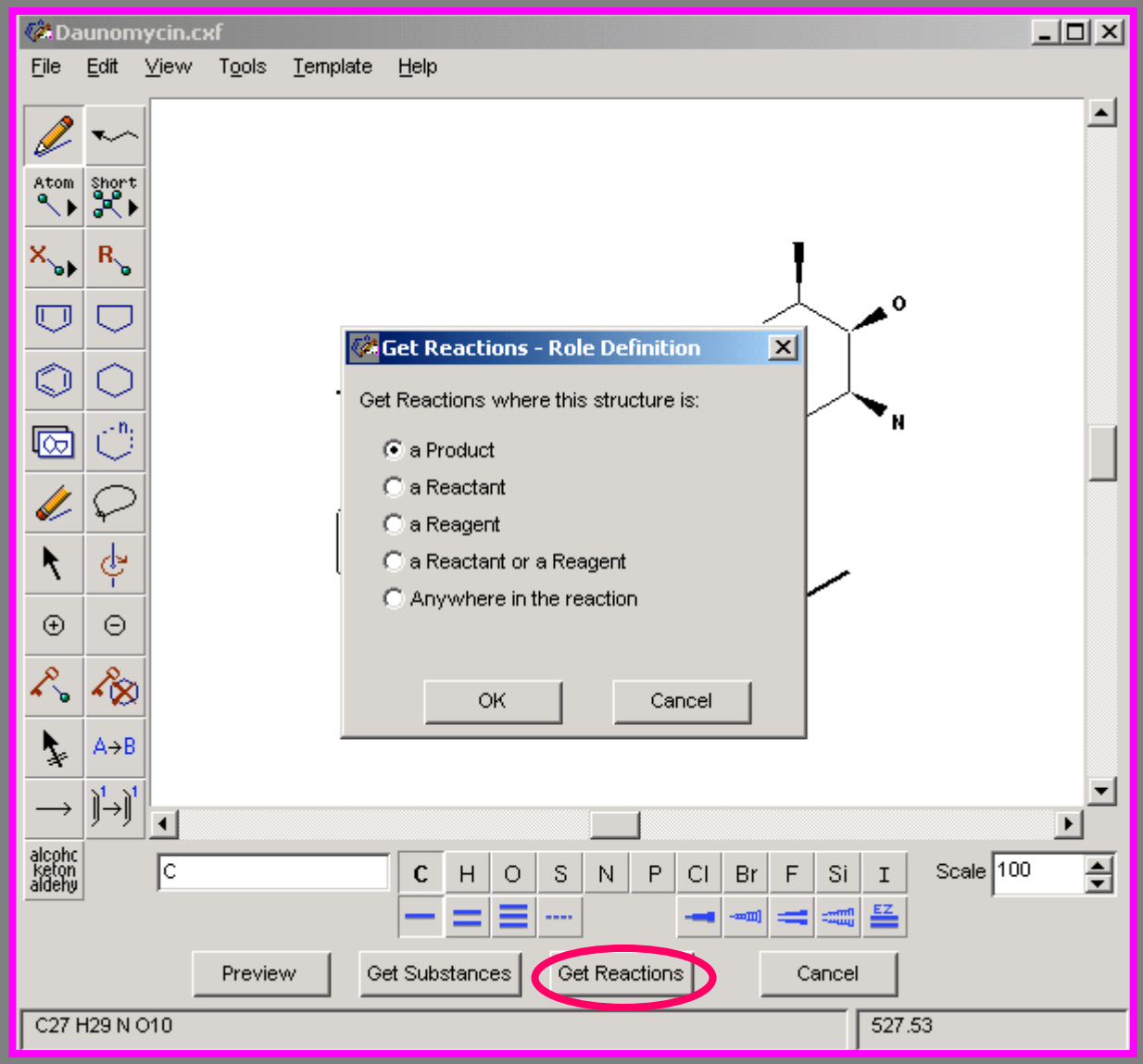
390755-63-2

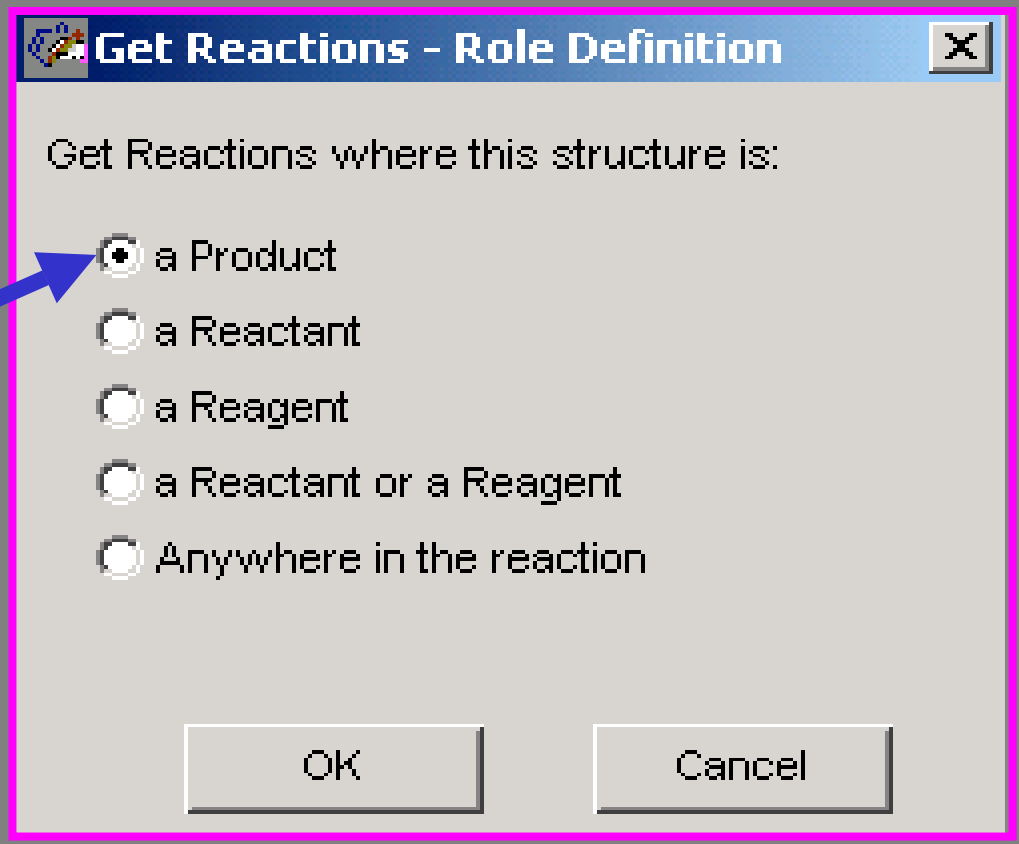
Component Number 1

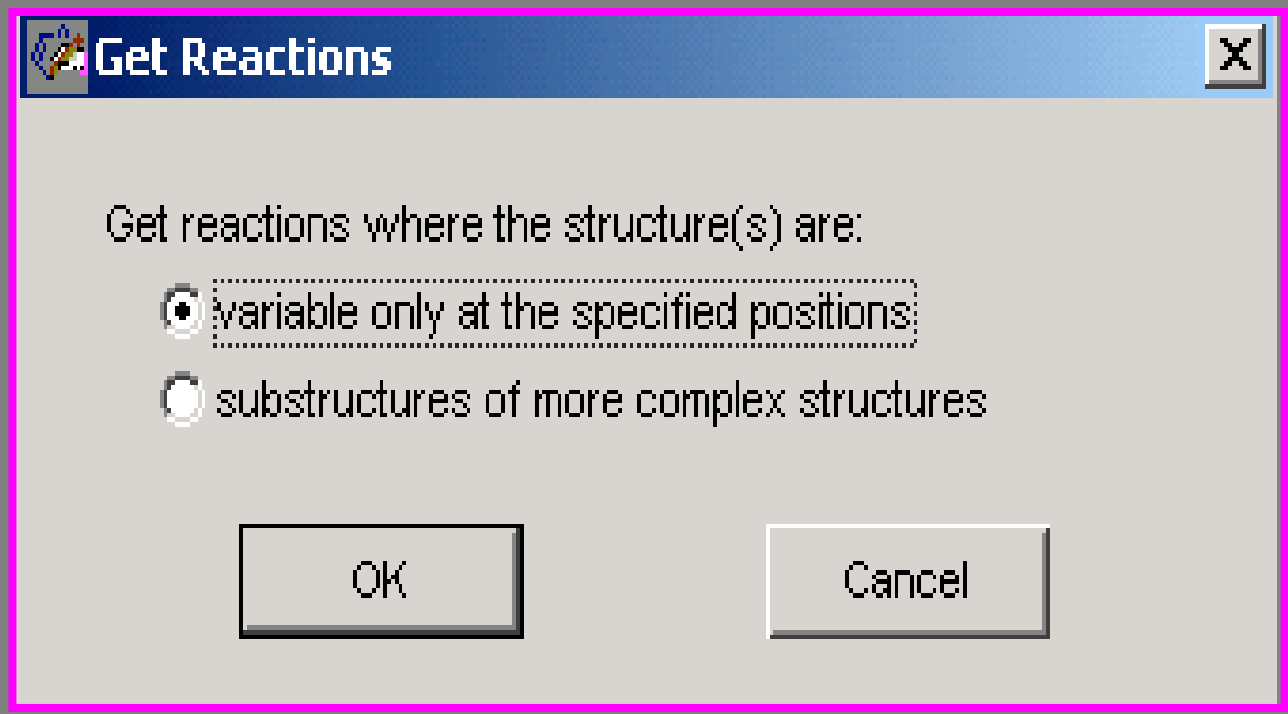
Get References | Analyze or Refine Substances | Back

Substances 1-6 of 52

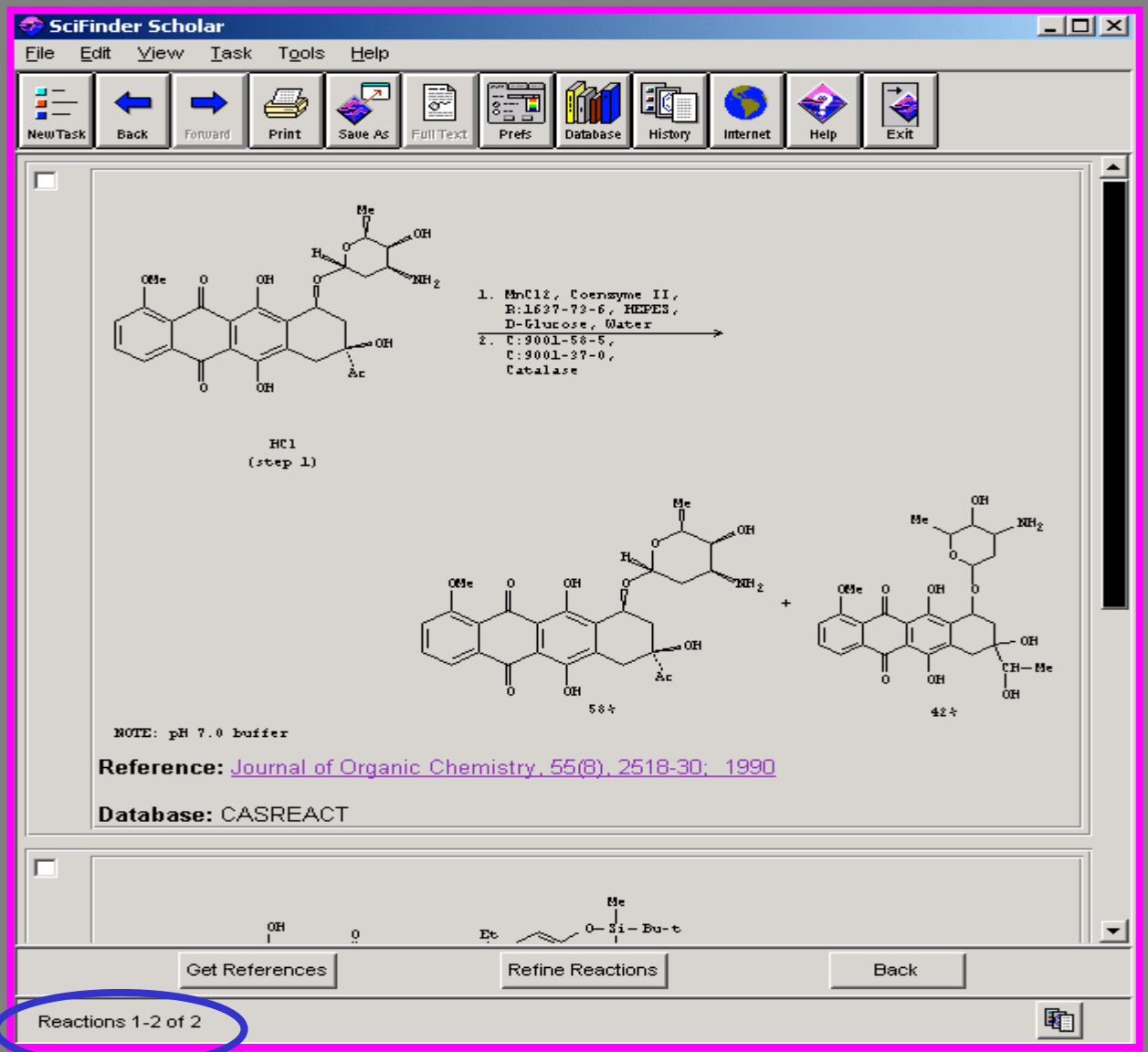
Get reaction containing this substance




Get Reactions - Role Definition
Get Reactions where this structure is:
a Product
a Reactant
a Reagent
a Reactant or a Reagent
Anywhere in the reaction
OK
Cancel


Get Reactions
Get reactions where the structure(s) are:
variable only at the specified positions
substructures of more complex structures
OK
Cancel

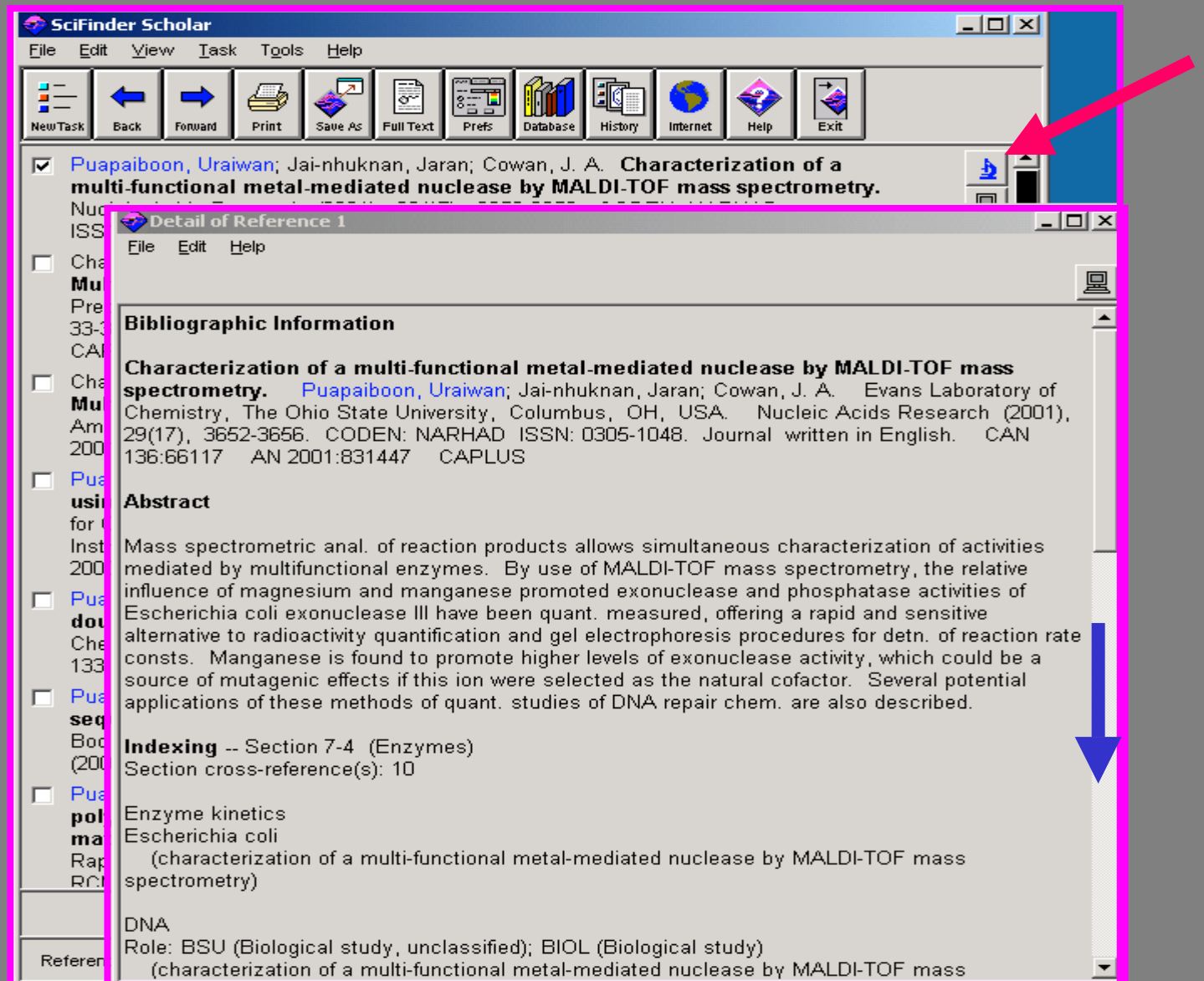
Reactions retrieved



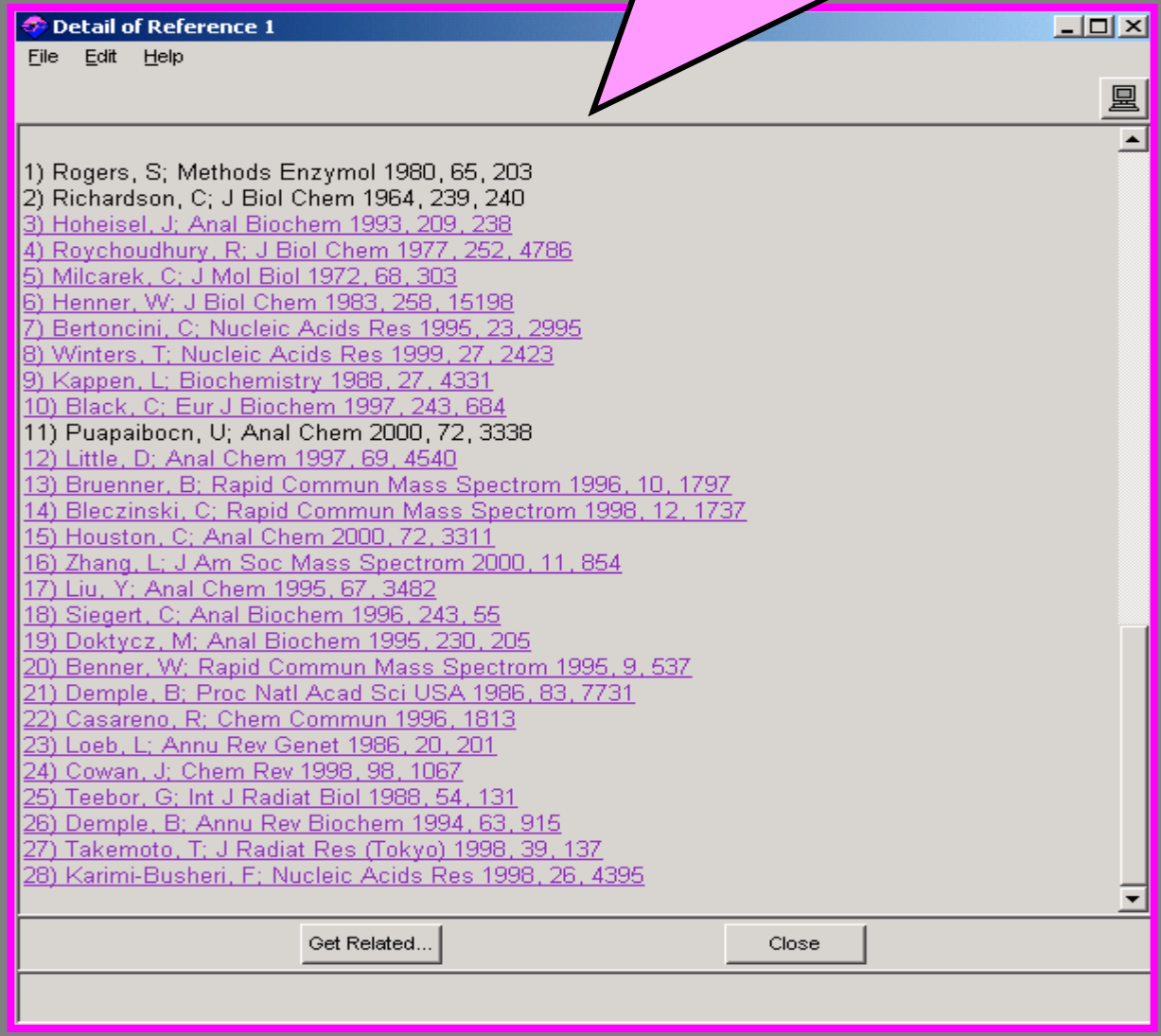
2 reactions

Citation Linking

Link to view detail of literature of interest

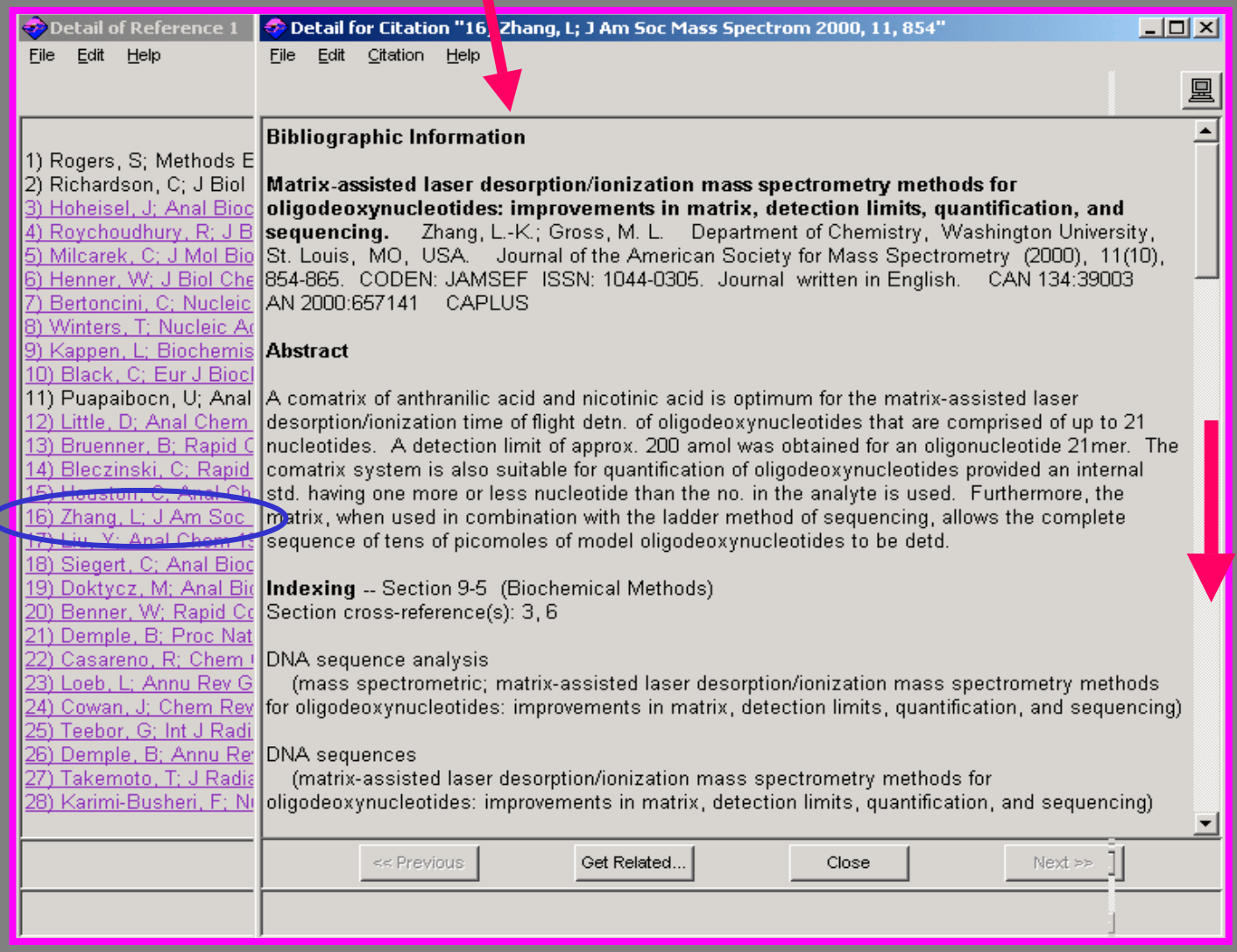


Citation of reference 1

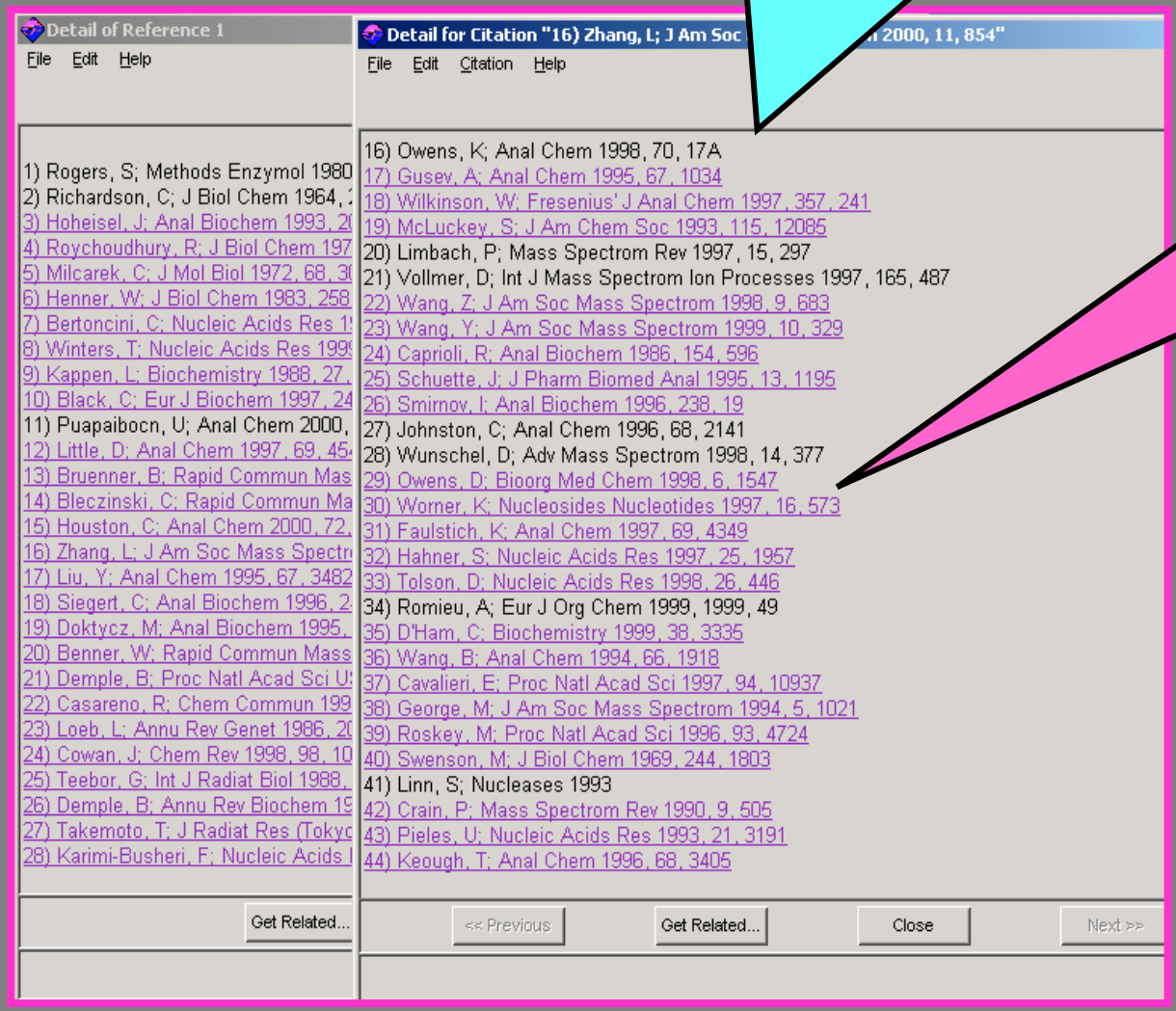


Link to see detail of citation 16

Hyperlink

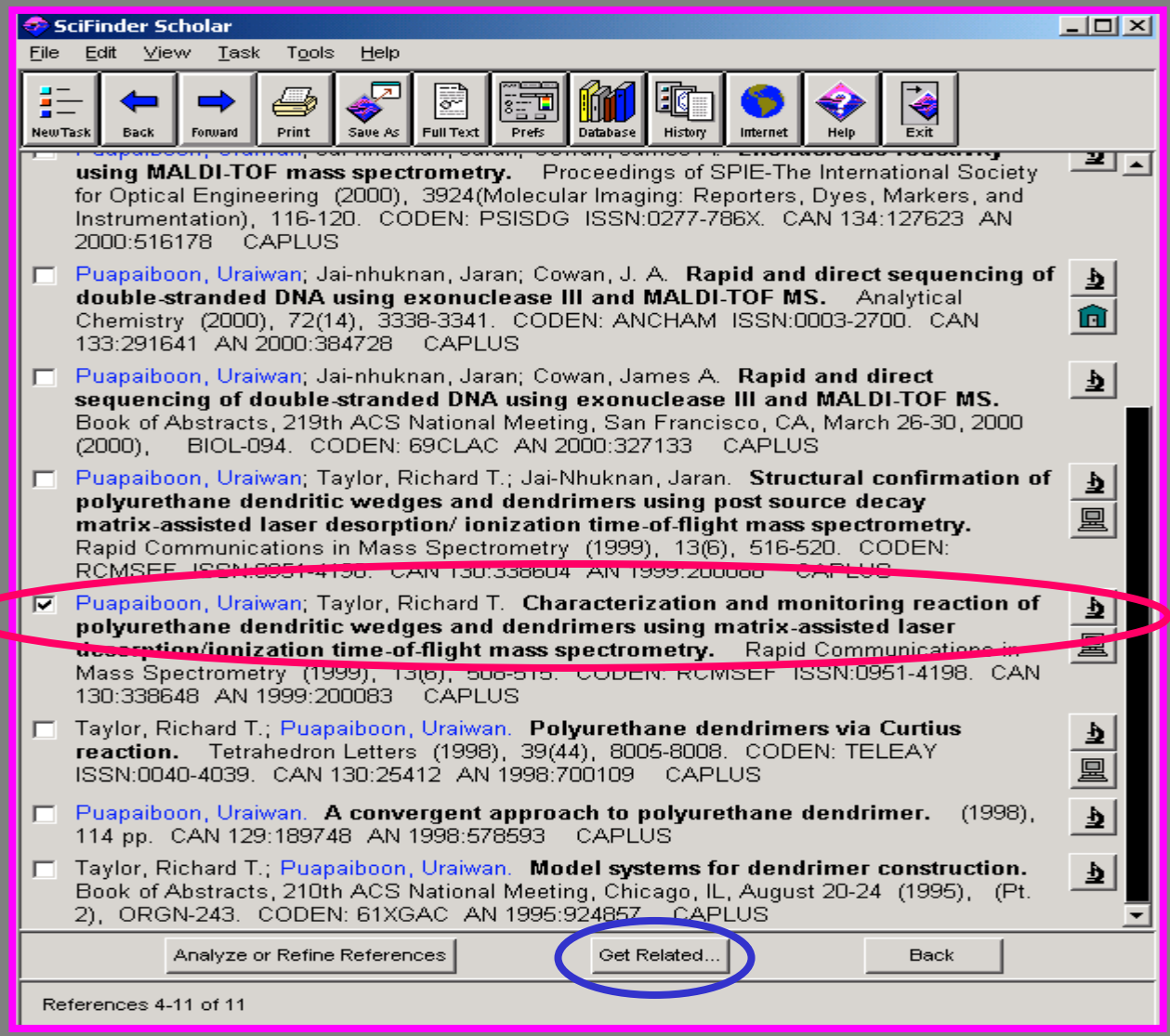


Citation of reference 16

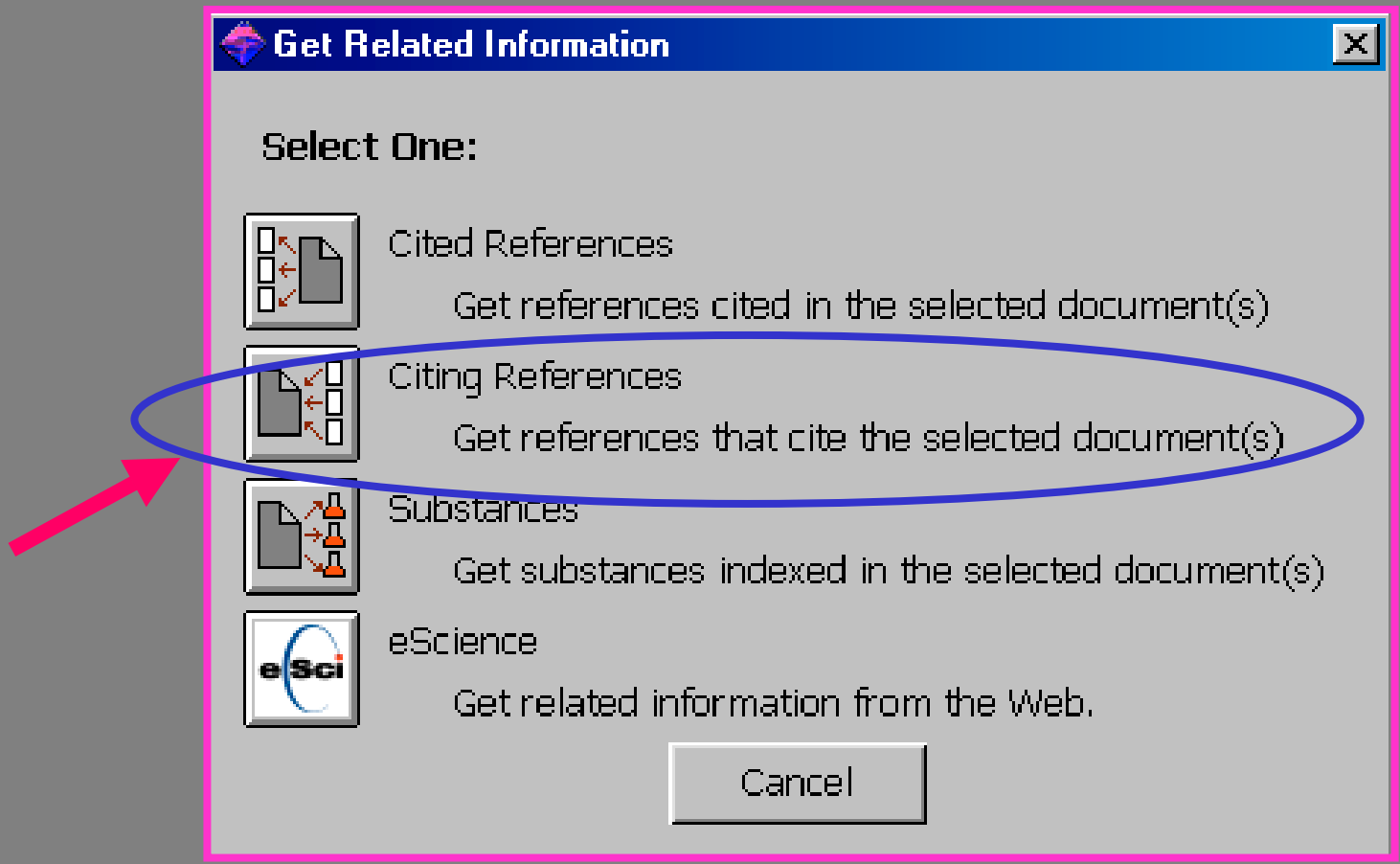


Link to view detail of reference of interest

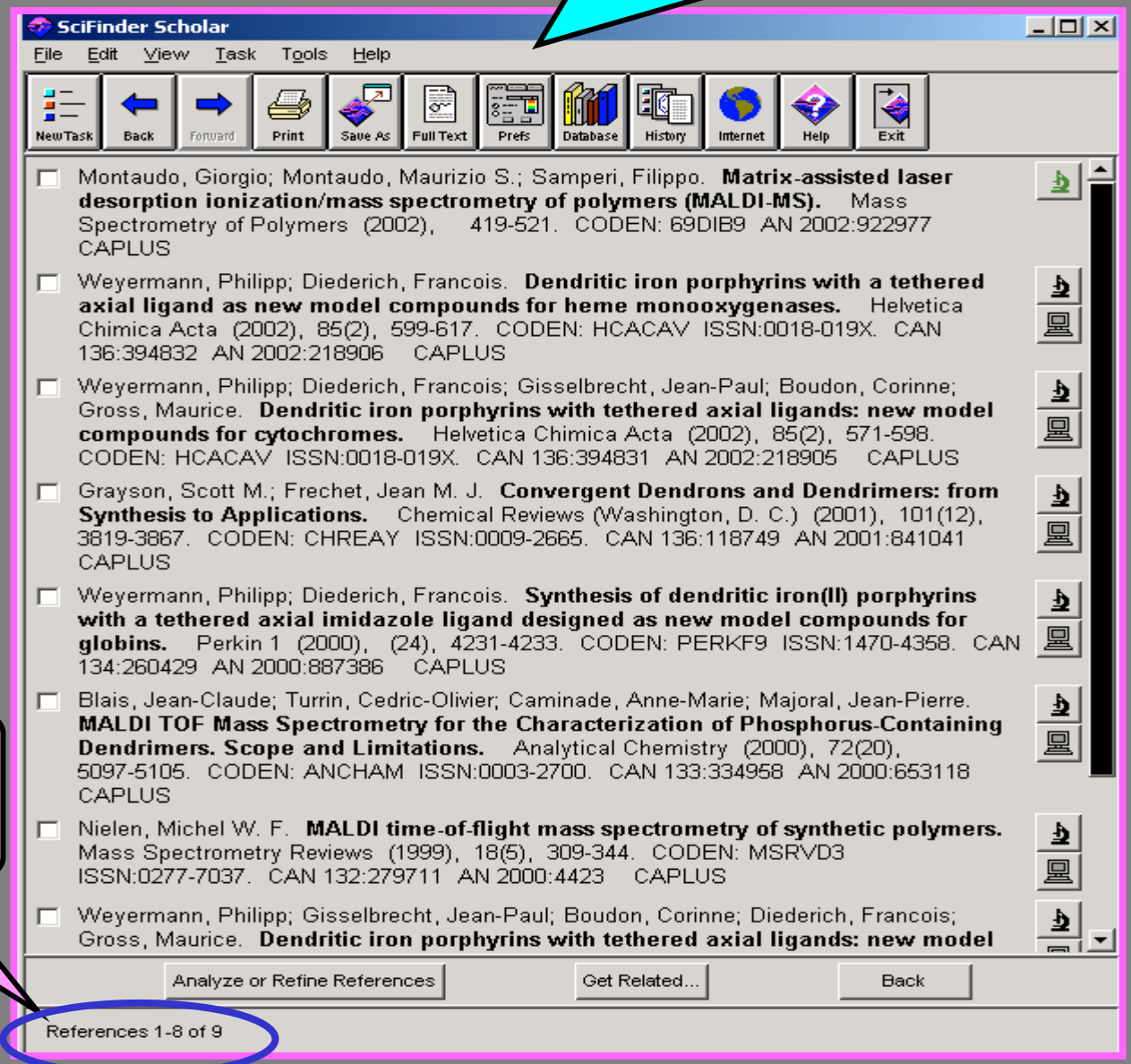
Select the reference of interest



Select one of these options

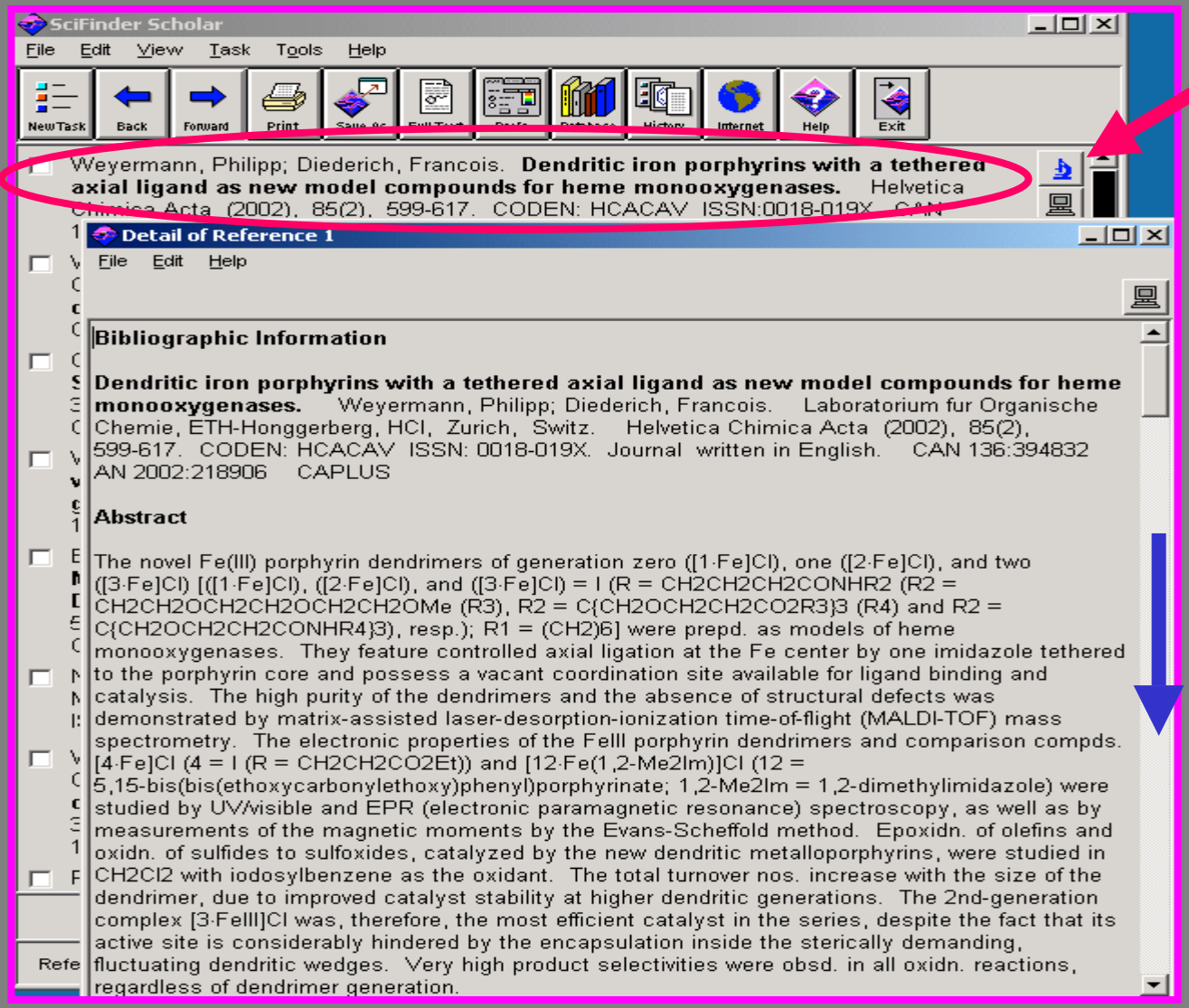


Citing References



9 references

View detail of the literature that are citing the selected document



Wow!

They are really citing my work!

Here it is!