

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
- Nutrition
- Immunochemistry
- Radiation biochemistry





SciFinder® Scholar

A WHOLE LOT MORE —

- Education [Education](#) [History](#)
- Mathematics [Mathematics](#) [Astronomy](#)
- Biotechnology [Biotechnology](#) [Materials](#)
- Archaeology [Archaeology](#) [Economics](#)
- Geoscience [Geoscience](#) [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**

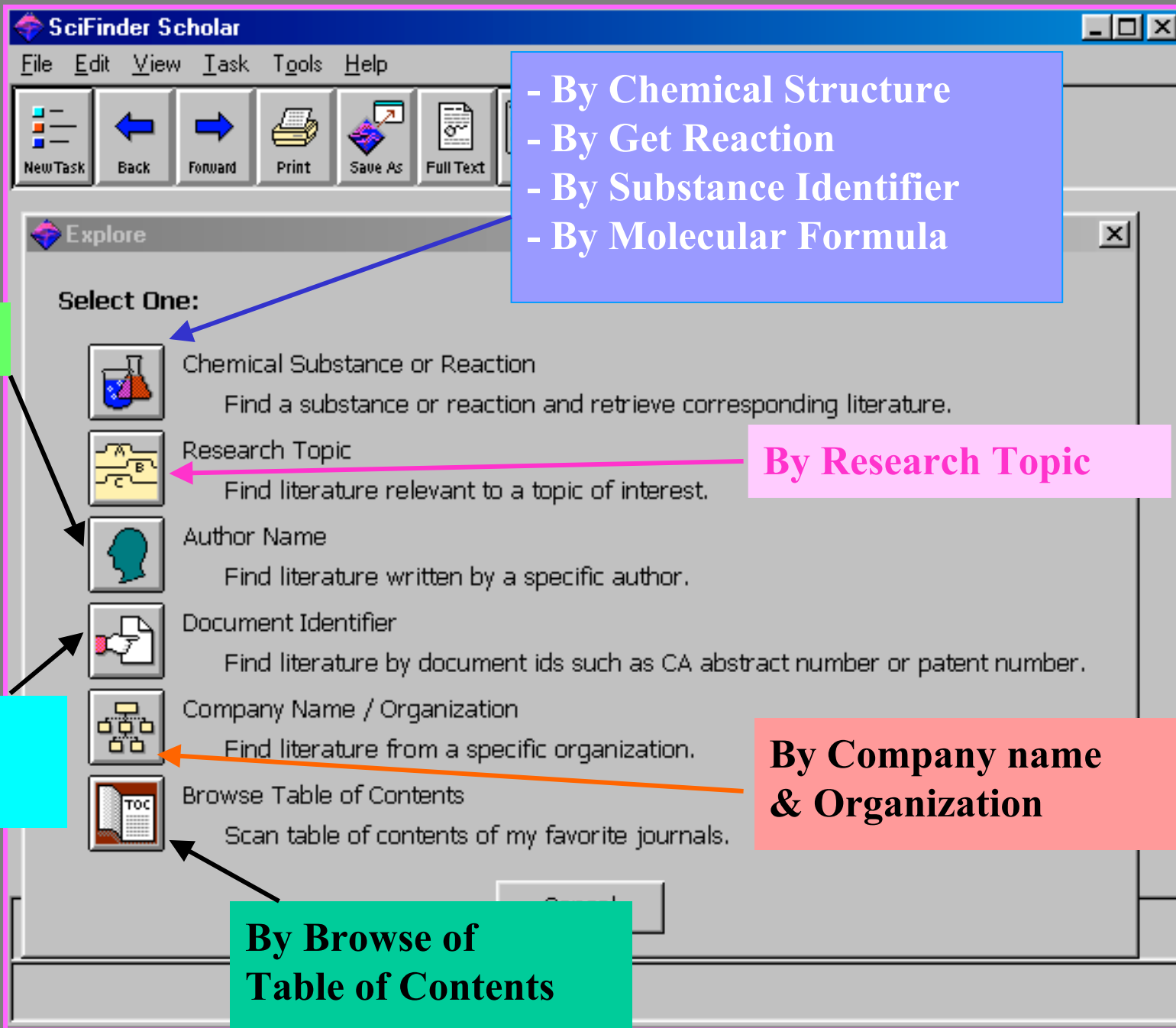
Substances **4,000,000**

Full text linking **Yes**

CITATION linking **Yes**

SciFinder Scholar

*The world's leading scientific
information resource*



Explore by Research Topic

Explore By Research Topic

-ใช้วลีหรือประโยคภาษาอังกฤษแบบง่ายๆ โดยอาจใช้คำ บุพบท (preposition), คำสันธาน (conjunctions) แต่ Sci Finder ไม่รู้จัก คำสั่งภาษา computer เช่น พวง 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 hormone on fetal development ซึ่งดีกว่าใช้

I am interested in the effects of human growth hormone 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”

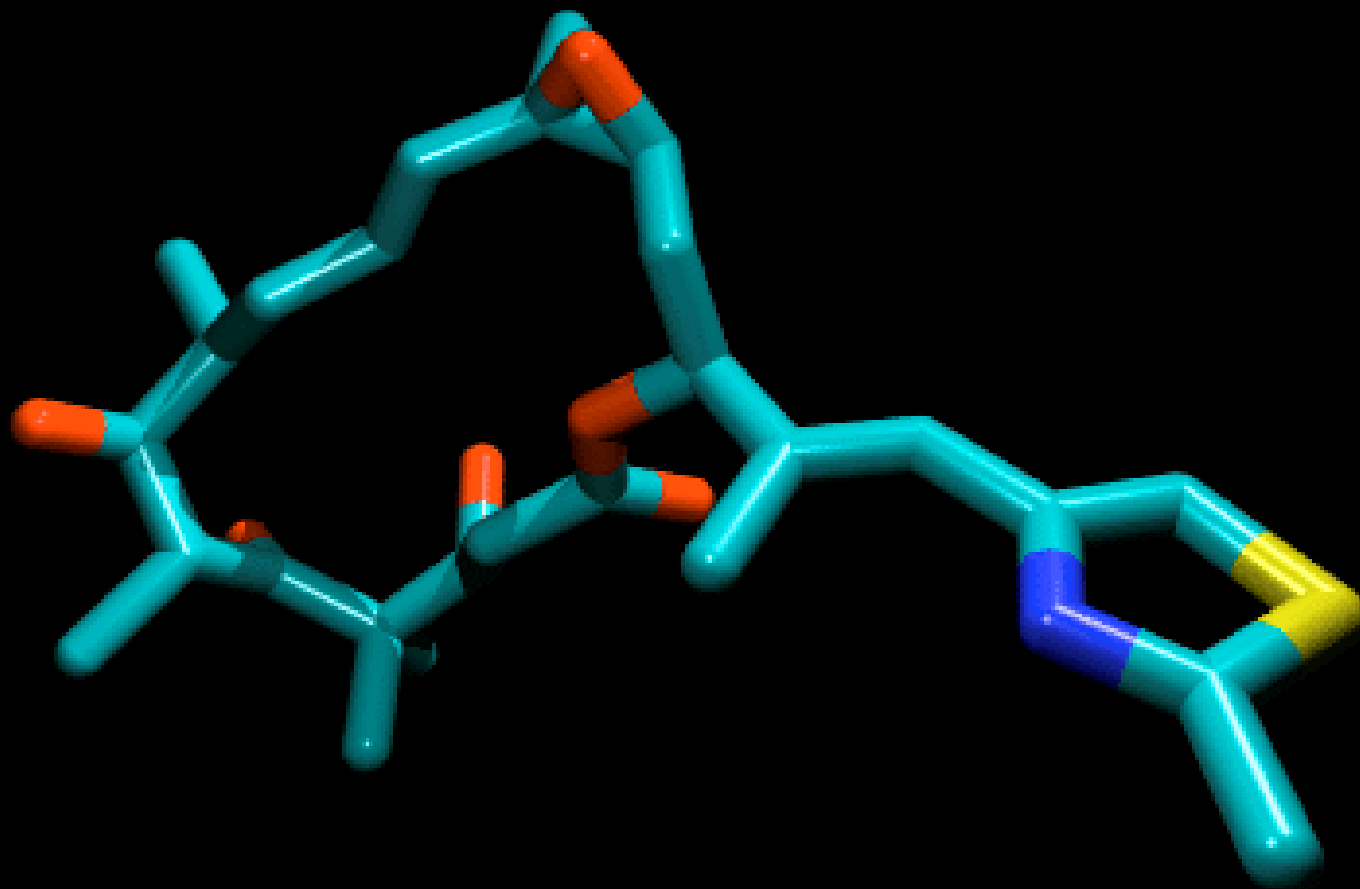
-ใช้คำเหมือน(synonym)ของคุณเองถ้ามี เพื่อโยง concept

ที่สัมพันธ์กันเช่น

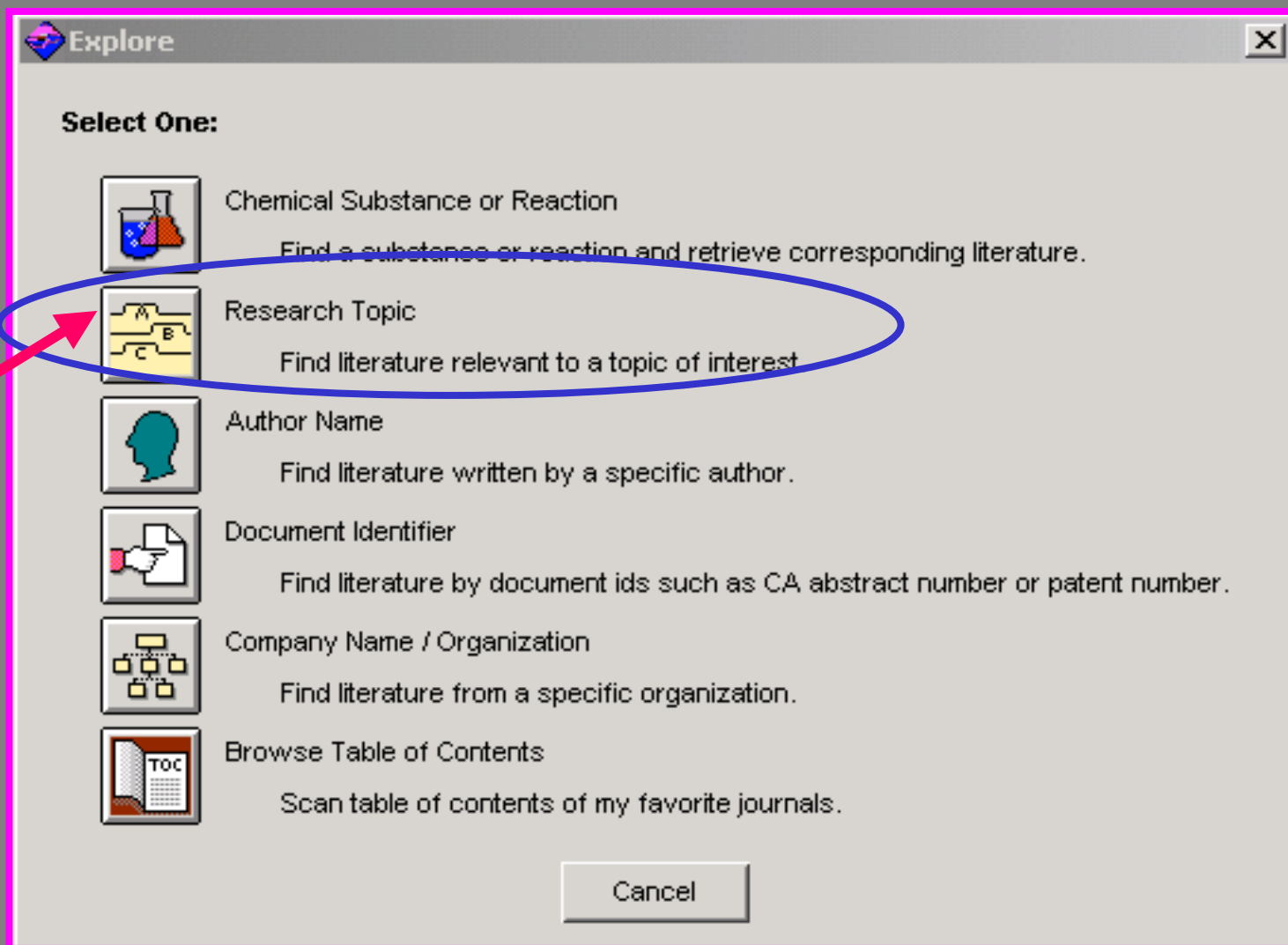
I am interested in topical treatments for poison ivy (Rhus radiacans)

-พยายามใช้วลีที่ต่างๆกันหลายๆทางในการค้น

Cancer Fighter “Epothilone B”








Explore by Research Topic



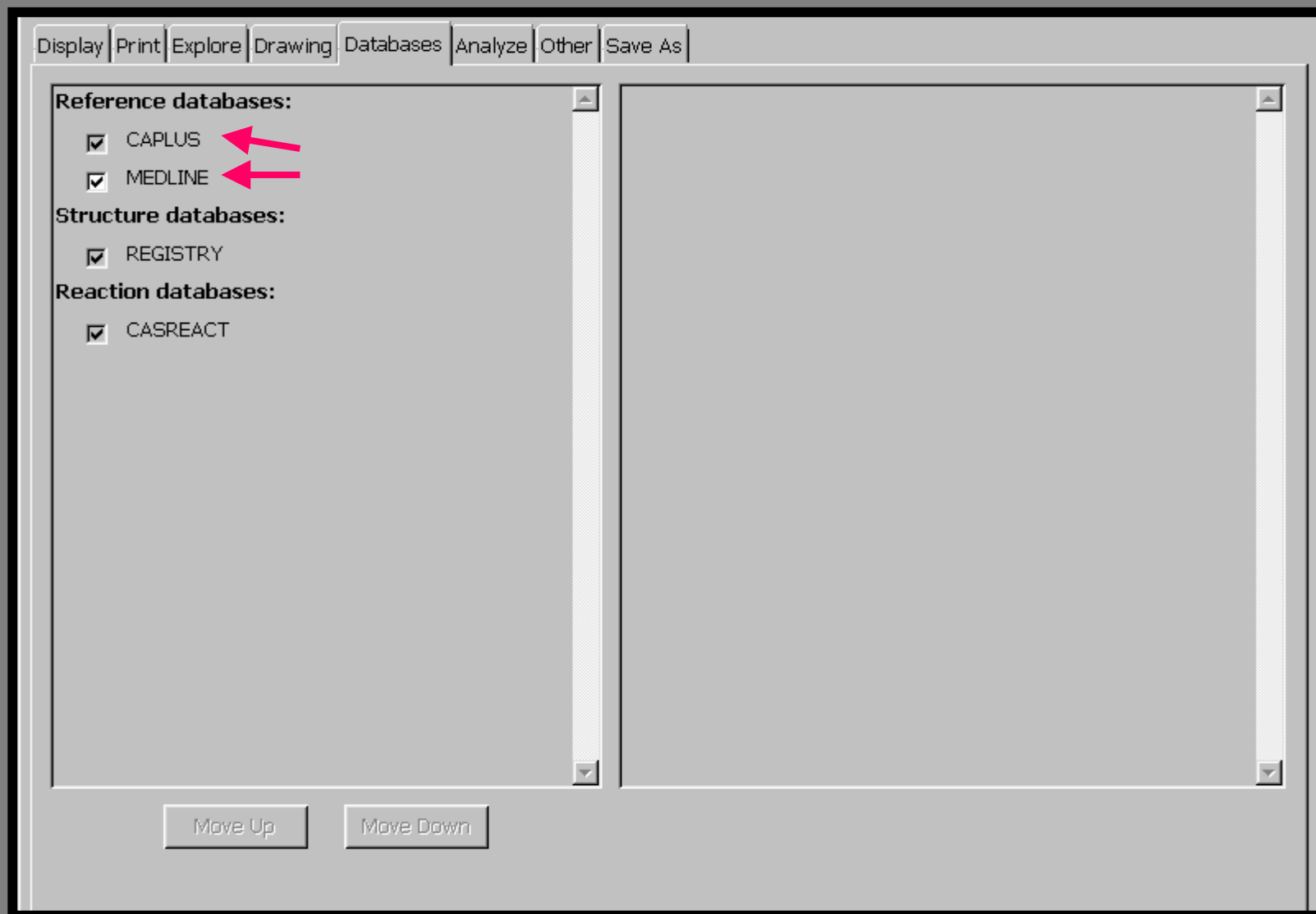
Click at Database

The image shows the SciFinder Scholar software interface. The main window has a menu bar with 'File', 'Edit', 'View', 'Task', 'Tools', and 'Help'. Below the menu bar is a toolbar with buttons for 'NewTask', 'Back', 'Forward', 'Print', 'Save As', 'Full Text', 'Prefs', 'Database', 'History', 'Internet', 'Help', and 'Exit'. A pink speech bubble points to the 'Database' button. An 'Explore' dialog box is open in the foreground, titled 'Explore' with a close button. It contains a 'Select One:' section with six options, each with an icon and a description:

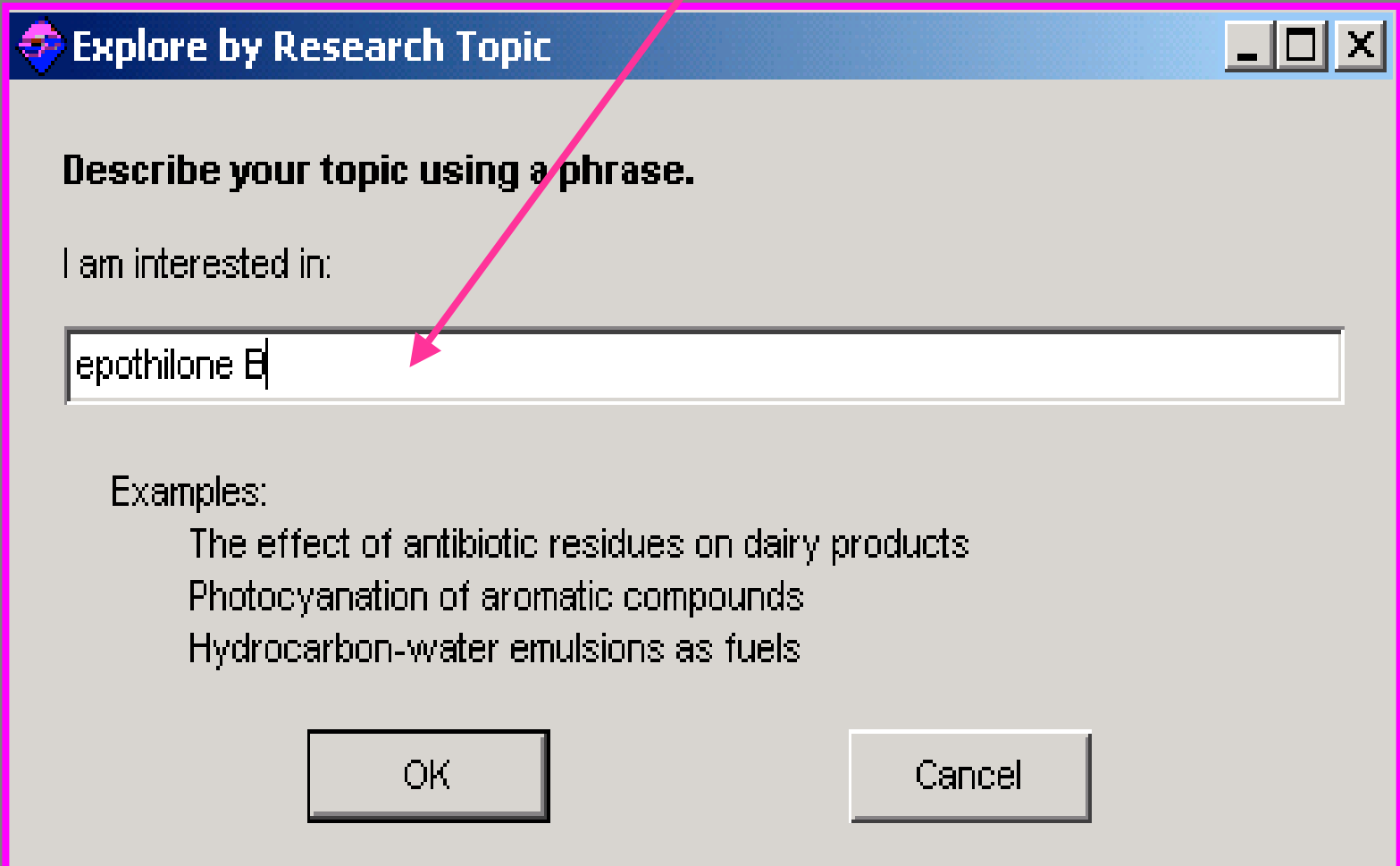
-  **Chemical Substance or Reaction**
Find a substance or reaction and retrieve corresponding literature.
-  **Research Topic**
Find literature relevant to a topic of interest.
-  **Author Name**
Find literature written by a specific author.
-  **Document Identifier**
Find literature by document ids 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.

At the bottom of the dialog box is a 'Cancel' button.

Select the database of interest



Enter the topic of interest



Explore by Research Topic

Describe your topic using a phrase.

I am interested in:

Examples:

- The effect of antibiotic residues on dairy products
- Photocyanation of aromatic compounds
- Hydrocarbon-water emulsions as fuels

OK Cancel

Select candidates of interest

Topic Candidates

File Edit Task Tools Help

Select the candidates of interest:

- 286 references were found containing **"epothilone B"** as entered.
- 295 references were found containing the concept **"epothilone B"**.

Get References Back

Candidates 1-2 of 2

Here are the references!

SciFinder Scholar

File Edit View Task Tools Help

NewTask Back Forward Print Save As Full Text Prefs Database History Internet Help Exit

136.325500 AN 2002.251007 CAPLUS

- Chen, Jie-Guang; Horwitz, Susan Band. **Differential mitotic responses to microtubule-stabilizing and -destabilizing drugs.** Cancer Research (2002), 62(7), 1935-1938. CODEN: CNREA8 ISSN:0008-5472. CAN 137:179507 AN 2002:288666 CAPLUS
- Wartmann, M.; Altmann, K.-H. **The biology and medicinal chemistry of epothilones.** Current Medicinal Chemistry: Anti-Cancer Agents (2002), 2(1), 123-148. CODEN: CMCACI ISSN:1568-0118. CAN 137:163126 AN 2002:275591 CAPLUS
- Constantinides, Panayiotis P.; Lambert, Karel J.; Tustian, Alexander K.; Nienstedt, Andrew M.; Hartgraves, Greg A. **Emulsion vehicle for poorly soluble drugs.** PCT Int. Appl. (2002), 74 pp. CODEN: PIXXD2 WO 0226208 A2 20020404 CAN 136:299699 AN 2002:256023 CAPLUS
- Ermolenko, Mikhail S.; Potier, Pierre. **Synthesis of epothilones B and D from D-glucose.** Tetrahedron Letters (2002), 43(16), 2895-2898. CODEN: TELEAY ISSN:0040-4039. CAN 137:232471 AN 2002:255754 CAPLUS
- Hoefle, Gerhard; Glaser, Nicole. **Preparation of triazolo-epothilones for pharmaceutical use as fungicides and antitumor agents.** PCT Int. Appl. (2002), 25 pp. CODEN: PIXXD2 WO 0224712 A1 20020328 CAN 136:263032 AN 2002:240788 CAPLUS
- Taylor, Richard E.; Chen, Yue. **Epothilones and analogues total synthesis, conformation and biological activities.** Abstracts of Papers, 223rd ACS National Meeting, Orlando, FL, United States, April 7-11, 2002 (2002), ORGN-398. CODEN: 69CKQP AN 2002:190933 CAPLUS
- Reiff, Emily A.; Nair, Sajiv K.; Henri, John T.; Greiner, Jack F.; Reddy, B. S. Narayan; Chakrasali, Ramappa; Himes, Richard H.; Georg, Gunda I. **Construction of epothilone photoaffinity labels via total synthesis.** Abstracts of Papers, 223rd ACS National Meeting, Orlando, FL, United States, April 7-11, 2002 (2002), ORGN-084. CODEN: 69CKQP AN 2002:190619 CAPLUS
- Li, Dansu; Schinner, Mark; Glaser, Nicole; Hofle, Gerhard; Ojima, Iwao. **Synthesis of novel epothilone B and paclitaxel analogs as potential photoaffinity labels.**

Analyze or Refine References Get Related... Back

References 31-39 of 295

295
references

Let's view the detail of reference of interest

The screenshot shows the SciFinder Scholar application window. The main window displays a search result for a paper by Chen, Jie-Guang; Horwitz, Susan Band. The title is "Differential mitotic responses to microtubule-stabilizing and -destabilizing drugs." The journal is Cancer Research (2002), 62(7), 1935-1938. The interface includes a menu bar (File, Edit, View, Task, Tools, Help) and a toolbar with icons for New Task, Back, Forward, Print, Full Text, Print, Database, History, Help, and Exit. A red oval highlights the search result title and authors. A blue oval highlights the "Detail of Reference 32" window title. A pink oval highlights the "Abstract" section. A red oval highlights the "Indexing" section. A blue arrow points to the "Detail" cloud.

Detail of Reference 32

Bibliographic Information

Differential mitotic responses to microtubule-stabilizing and -destabilizing drugs. Chen, Jie-Guang; Horwitz, Susan Band. Department of Molecular Pharmacology, Albert Einstein College of Medicine, Bronx, NY, USA. Cancer Research (2002), 62(7), 1935-1938. CODEN: CNREA8 ISSN: 0008-5472. Journal written in English. CAN 137:179507 AN 2002:288666

Abstract

Although microtubule interacting agents inhibit spindle dynamics, thereby leading to a block in mitosis, we report that low concns. of these drugs result in differential mitotic effects. Microtubule-stabilizing agents including Taxol, **epothilone B**, and discodermolide produce aneuploid populations of A549 cells in the absence of a mitotic block. Such aneuploid populations are diminished in an **epothilone B**-resistant cell line. In contrast, microtubule-destabilizing agents like colchicine, nocodazole, and vinblastine are unable to initiate aneuploidy. The aneuploid cells result from aberrant mitosis as multipolar spindles are induced by the stabilizing drugs, but not by destabilizing agents. The results suggest that the mechanism underlying aberrant mitosis may not be the same as that responsible for mitotic block, and that the former detcs. the sensitivity of cells to Taxol-like drugs.

Indexing -- Section 1-6 (Pharmacology)

Ploidy
(aneuploidy; differential mitotic responses to microtubule-stabilizing and -destabilizing drugs)

Antitumor agents
Human
Microtubule
Mitosis

Interested in this topic

microscope

Detail

Here are the Citations!

The image shows a screenshot of a web browser interface. On the left, a window titled "Detail of Referr" displays a list of citations. The word "Citations" is circled in red. On the right, a larger window titled "Detail for Citation '11' He, L; Mol Cancer Ther 2001, 1, 3" is open, showing the full text of the citation, including the title, authors, journal information, and an abstract. The citation title is "Mutations in β -tubulin map to domains involved in regulation of microtubule stability in epothilone-resistant cell lines." The authors are He, Lifeng; Yang, Chia-Ping Huang; Horwitz, Susan Band. The journal is Molecular Cancer Therapeutics (2001), 1(1), 3-10. The abstract discusses the mechanism of action of epothilones and their resistance in HeLa cell lines.

antitumor drug

Citations

- 1) Schiff, P; Pr
- 2) Bollag, D; C
- 3) ter Haar, E;
- 4) Jordan, M; F
- 5) Jordan, M; J
- 6) Moos, P; Ce
- 7) Woods, C; M
- 8) Lieu, C; Bio
- 9) Giannakako
- 10) Torres, K;
- 11) He, L; Mol
- 12) King, K; J
- 13) Li, X; Natur
- 14) Speicher, L
- 15) Paoletti, A
- 16) Ngan, V; M
- 17) Sluder, G;
- 18) Brinkley, B
- 19) Sena, G; C
- 20) Iancu, C; C
- 21) Long, B; C
- 22) Schimke, P
- 23) Loeb, L; C
- 24) Abal, M; C
- 25) Keryer, G;

Detail for Citation "11" He, L; Mol Cancer Ther 2001, 1, 3"

File Edit Citation Help

Bibliographic Information

Mutations in β -tubulin map to domains involved in regulation of microtubule stability in epothilone-resistant cell lines. He, Lifeng; Yang, Chia-Ping Huang; Horwitz, Susan Band. Department of Molecular Pharmacology, Albert Einstein College of Medicine, Bronx, NY, USA. Molecular Cancer Therapeutics (2001), 1(1), 3-10. CODEN: MCTOCF ISSN: 1535-7163. Journal written in English. AN 2002:550585 CAPLUS

Abstract

The epothilones (Epos) are a group of natural products isolated from the myxobacterium, *Sorangium cellulosum*. They have a mechanism of action similar to that of Taxol, i.e., they stabilize microtubules and induce the formation of microtubule bundles in cells. Because they are simpler in structure than Taxol and preserve their activity in P-glycoprotein-expressing cells, they are being studied as potential antitumor drugs. In this work, a series of Epo-resistant A549 and HeLa cell lines have been selected and analyzed. Class I β -tubulin, the major isotype of β -tubulin in these Epo-resistant cell lines, has been sequenced in a search for mutations. In the Epo B-resistant A549 cells, there is a mutation at β 292 from Gln to Glu, in the Epo A-resistant HeLa cell line there is a mutation at β 173 from Pro to Ala, and in the Epo B-resistant HeLa cell line there is a heterozygous mutation at β 422 from Tyr to a mixt. of Tyr and Cys. These mutations are close to the M-loop, the nucleotide-binding site, and the microtubule-assocd. protein binding sites, resp. It is likely that these mutations in β -tubulin provide cells with a mechanism of resistance to the Epos and taxanes. Among these resistant cell lines, A549.EpoB40 is hypersensitive to microtubule-destabilizing drugs, such as vinblastine and colchicine, and HeLa.EpoB1.8 is dependent on the Epos or taxanes for growth. Our studies provide evidence that the M-loop, the GTP binding site, and the microtubule-assocd. protein binding sites at the COOH terminus in β -tubulin are crit. for the regulation of microtubule stability.

Indexing -- Section 1 (Pharmacology)

<< Previous Get Related... Close Next >>

Interested in this reference?

Narrow down the answer set

The screenshot shows the SciFinder Scholar web interface. At the top, there is a menu bar with 'File', 'Edit', 'View', 'Task', 'Tools', and 'Help'. Below the menu is a toolbar with icons for 'NewTask', 'Back', 'Forward', 'Print', 'Save As', 'Full Text', 'Prefs', 'Database', 'History', 'Internet', 'Help', and 'Exit'. The main content area displays a list of search results, each with a checkbox and a brief description of the article. A dialog box titled 'Analyze or Refine' is open in the center, with a 'Select One:' section containing two options: 'Analyze' (with a bar chart icon) and 'Refine' (with a funnel icon). The 'Analyze' option is selected. Below the dialog box, there are buttons for 'Analyze or Refine References', 'Get Related...', and 'Back'. At the bottom of the page, the text 'References 31-39 of 295' is displayed. A pink speech bubble on the left side of the image contains the text 'Too large answer set?'. A red arrow points from the 'Analyze or Refine References' button to the 'References 31-39 of 295' text.

SciFinder Scholar

File Edit View Task Tools Help

NewTask Back Forward Print Save As Full Text Prefs Database History Internet Help Exit

106.329330 AN 2002.251007 CAPLUS

- Chen, Jie-Guang; Horwitz, Susan Band. **Differential mitotic responses to microtubule-stabilizing and -destabilizing drugs.** Cancer Research (2002), 62(7), 1935-1938. CODEN: CNREA8 ISSN:0008-5472. CAN 137:179507 AN 2002:288666 CAPLUS
- Wartmann, M.; Altmann, K.-H. **The biology and medicinal chemistry of epothilones.** Current Medicinal Chemistry: Anti-Cancer Agents (2002), 2(1), 123-148. CODEN: CMCACI ISSN:1568-0118. CAN 137:163126 AN 2002:275591 CAPLUS
- Constantini M.; Hartgra M.; Hartgra M. (2002), 7 2002:25602
- Ermolenko, **D-glucose.** ISSN:0040-
- Hoefle, Ger **pharmacei** 25 pp. COI CAPLUS
- Taylor, Rich **conformation and biological activities.** Abstracts of Papers, 223rd ACS National Meeting, Orlando, FL, United States, April 7-11, 2002 (2002), ORGN-398. CODEN: 69CKQP AN 2002:190933 CAPLUS
- Reiff, Emily A.; Nair, Sajiv K.; Henri, John T.; Greiner, Jack F.; Reddy, B. S. Narayan; Chakrasali, Ramappa; Himes, Richard H.; Georg, Gunda I. **Construction of epothilone photoaffinity labels via total synthesis.** Abstracts of Papers, 223rd ACS National Meeting, Orlando, FL, United States, April 7-11, 2002 (2002), ORGN-084. CODEN: 69CKQP AN 2002:190619 CAPLUS
- Li, Dansu; Schinner, Mark; Glaser, Nicole; Hofle, Gerhard; Ojima, Iwao. **Synthesis of novel epothilone B and paclitaxel analogs as potential photoaffinity labels.**

Andrew Appl. AN

2), 240788

Analyze or Refine

Select One:

Analyze
Get histograms of the year, corporate sources, authors, etc.

Refine
Go to refine options without analyzing the answer set.

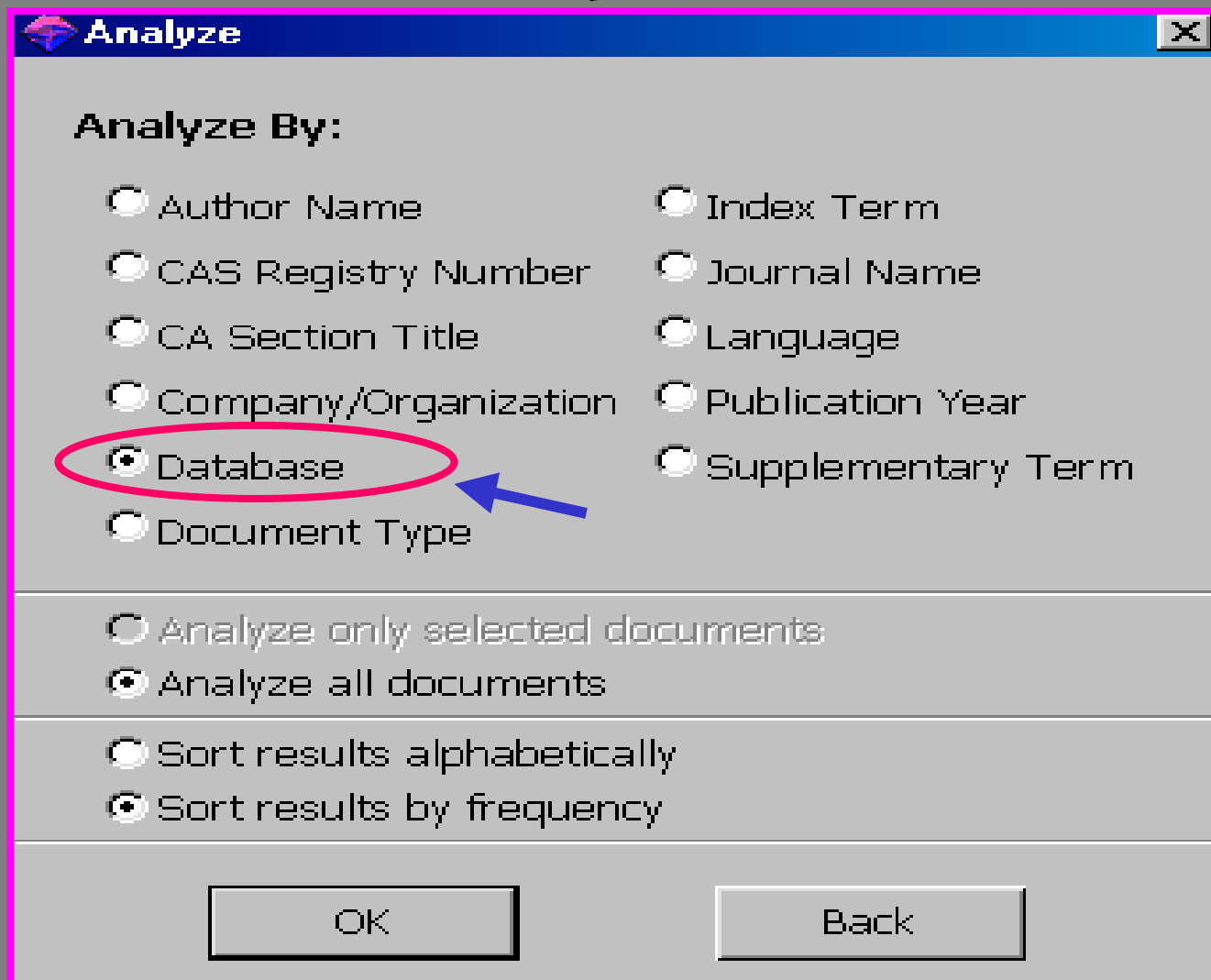
Cancel

Analyze or Refine References Get Related... Back

References 31-39 of 295

Too large answer set?

11 options to analyze the answer sets



Analyze

Analyze By:

- Author Name
- CAS Registry Number
- CA Section Title
- Company/Organization
- Database
- Document Type
- Index Term
- Journal Name
- Language
- Publication Year
- Supplementary Term

Analyze only selected documents

Analyze all documents

Sort results alphabetically

Sort results by frequency

OK Back

Select the database of interest

The screenshot shows a software window titled "Database Analysis" with a menu bar (File, Edit, Task, Tools, Help). The main area is titled "Select Histogram Entries of interest:" and contains a list of two entries:

Database	Count
<input type="checkbox"/> CAPLUS	230
<input checked="" type="checkbox"/> MEDLINE	65

At the bottom of the window, there are two buttons: "Get References" and "Back". The "Get References" button is circled in blue, and a red arrow points to it. The status bar at the bottom left indicates "Histogram Entries 1-2 of 2".

The references retrieved from Medline

SciFinder Scholar

File Edit View Task Tools Help

NewTask Back Forward Print Save As Full Text Prefs Database History Internet Help Exit

- Julien Bryan; Shah Sanjay **Heterologous Expression of Epothilone Biosynthetic Genes in Myxococcus xanthus.** ANTIMICROBIAL AGENTS AND CHEMOTHERAPY (2002 Sep), 46(9), 2772-8. Journal code: 0315061. ISSN:0066-4804. DN 22170306 PubMed ID 12183227 AN 2002426104 In-process for MEDLINE
- Giannakakou Paraskevi; Nakano Michel; Nicolaou Kyriacos C; O'Brate Aurora; Yu Jian; Blagosklonny Mikhail V; Greber Urs F; Fojo Tito **Enhanced microtubule-dependent trafficking and p53 nuclear accumulation by suppression of microtubule dynamics.** PROCEEDINGS OF THE NATIONAL ACADEMY OF SCIENCES OF THE UNITED STATES OF AMERICA (2002 Aug 6), 99(16), 10855-60. Journal code: 7505876. ISSN:0027-8424. DN 22155908 PubMed ID 12145320 AN 2002423661 MEDLINE
- Altafa Ramin; Fojo Tito; Reed Eddie; Abraham Jame **Epothilones: A Novel Class of Non-taxane Microtubule-stabilizing Agents.** CURRENT PHARMACEUTICAL DESIGN (2002), 8(19), 1707-12. Journal code: 9602487. ISSN:1381-6128. DN 22162069 PubMed ID 12171542 AN 2002416373 In-process for MEDLINE
- Broker Linda E; Huisman Cynthia; Ferreira Carlos G; Rodriguez Jose A; Kruyt Frank A E; Giaccone Giuseppe **Late activation of apoptotic pathways plays a negligible role in mediating the cytotoxic effects of discodermolide and epothilone B in non-small cell lung cancer cells.** CANCER RESEARCH (2002 Jul 15), 62(14), 4081-8. Journal code: 2984705R. ISSN:0008-5472. DN 22119439 PubMed ID 12124345 AN 2002378240 MEDLINE
- McDaid Hayley M; Mani Sridhar; Shen Heng-Jia; Muggia Franco; Sonnichsen Daryl; Horwitz Susan Band **Validation of the Pharmacodynamics of BMS-247550, an Analogue of Epothilone B, during a Phase I Clinical Study.** CLINICAL CANCER RESEARCH (2002 Jul), 8(7), 2035-43. Journal code: 9502500. ISSN:1078-0432. DN 22109596 PubMed ID 12114401 AN 2002369448 In-process for MEDLINE
- Hood Kylie A; West Lyndon M; Rouwe Berber; Northcote Peter T; Berridge Michael V; Wakefield St John; Miller John H **Peloruside A, a novel antimetabolic agent with paclitaxel-like microtubule-stabilizing activity.** CANCER RESEARCH (2002 Jun 15), 62(12), 3356-60. Journal code: 2984705R. ISSN:0008-5472. DN 22062792 PubMed ID 12067973 AN 2002324974 MEDLINE
- Lavelle Francois **New taxanes and epothilone derivatives in clinical trials**

Analyze or Refine References Get Related... Back

References 1-7 of 65

65
references








Link to ChemPort to see full-text

Computer icon

SciFinder Scholar

File Edit View Task Tools Help

NewTask Back Forward Print Save As Print Preview Print All Print Settings Internet Help Exit

- Nicolaou K C; Namoto K; Ritzen A; Ulven T; Shoji M; Li J; D'Amico G; Liotta D; French C T; Wartmann M; Altmann K H; Giannakakou P **Chemical synthesis and biological evaluation of cis- and trans-12,13-cyclopropyl and 12,13-cyclobutyl epothilones and related pyridine side chain analogues.** JOURNAL OF THE AMERICAN CHEMICAL SOCIETY (2001 Sep 26), 123(38), 9313-23. Journal code: 7503056. ISSN:0002-7885. DN 21446575 PubMed ID 11562214 AN 2001537671 MEDLINE 
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- Chen H; O'Connor S; Cane D E; Walsh C T **Epothilone biosynthesis: assembly of the methylthiazolylcarboxy starter unit on the EpoB subunit.** CHEMISTRY AND BIOLOGY (2001 Sep), 8(9), 899-912. Journal code: 9500160. ISSN:1074-5521. DN 21448261 PubMed ID 11564558 AN 2001517252 MEDLINE 
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References 21-27 of 65

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J. Am. Chem. Soc. **2001**, *123*, 9313–9323 9313

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. IC₅₀ = 0.6 nM against the 1A9 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)

9314 *J. Am. Chem. Soc.*, Vol. 123, No. 38, 2001

Nicolaou et al.

Scheme 1. Retrosynthetic Analysis and Key Fragments for Epothilone Analogues 3–8

1: R = H : epothilone A (Epo A)
2: R = Me : epothilone B (Epo B)

3: n = 1: (12*S*,13*S*,15*S*)-cyclopropyl epothilone A [*cis*-(15*S*)-CP-epo]
4: n = 2: (12*S*,13*S*,15*S*)-cyclobutyl epothilone A [*cis*-(15*S*)-CB-epo]

5: n = 1: (12*S*,13*S*,15*R*)-cyclopropyl epothilone A [*cis*-(15*R*)-CP-epo]
6: n = 2: (12*S*,13*S*,15*R*)-cyclobutyl epothilone A [*cis*-(15*R*)-CB-epo]

7: n = 1: (12*R*,13*S*,15*S*)-cyclopropyl epothilone A [*trans*-(15*S*)-CP-epo]
8: n = 2: (12*R*,13*S*,15*S*)-cyclobutyl epothilone A [*trans*-(15*S*)-CB-epo]

9: (12*S*,13*S*,15*S*)-cyclopropyl 5-methylpyridine epothilone A [*cis*-(15*S*)-CP-py-epo]
10: (12*S*,13*S*,15*R*)-cyclopropyl 5-methylpyridine epothilone A [*cis*-(15*R*)-CP-py-epo]

11: (12*S*,13*S*,15*S*)-cyclobutyl 5-methylpyridine epothilone A [*cis*-(15*S*)-CB-py-epo]
12: (12*S*,13*S*,15*R*)-cyclobutyl 5-methylpyridine epothilone A [*cis*-(15*R*)-CB-py-epo]

13, 14, 15, 16, 17

18

1) Nozaki-Hiyama-Kishi coupling
2) Aldol reaction
3) Yamaguchi macrolactonization

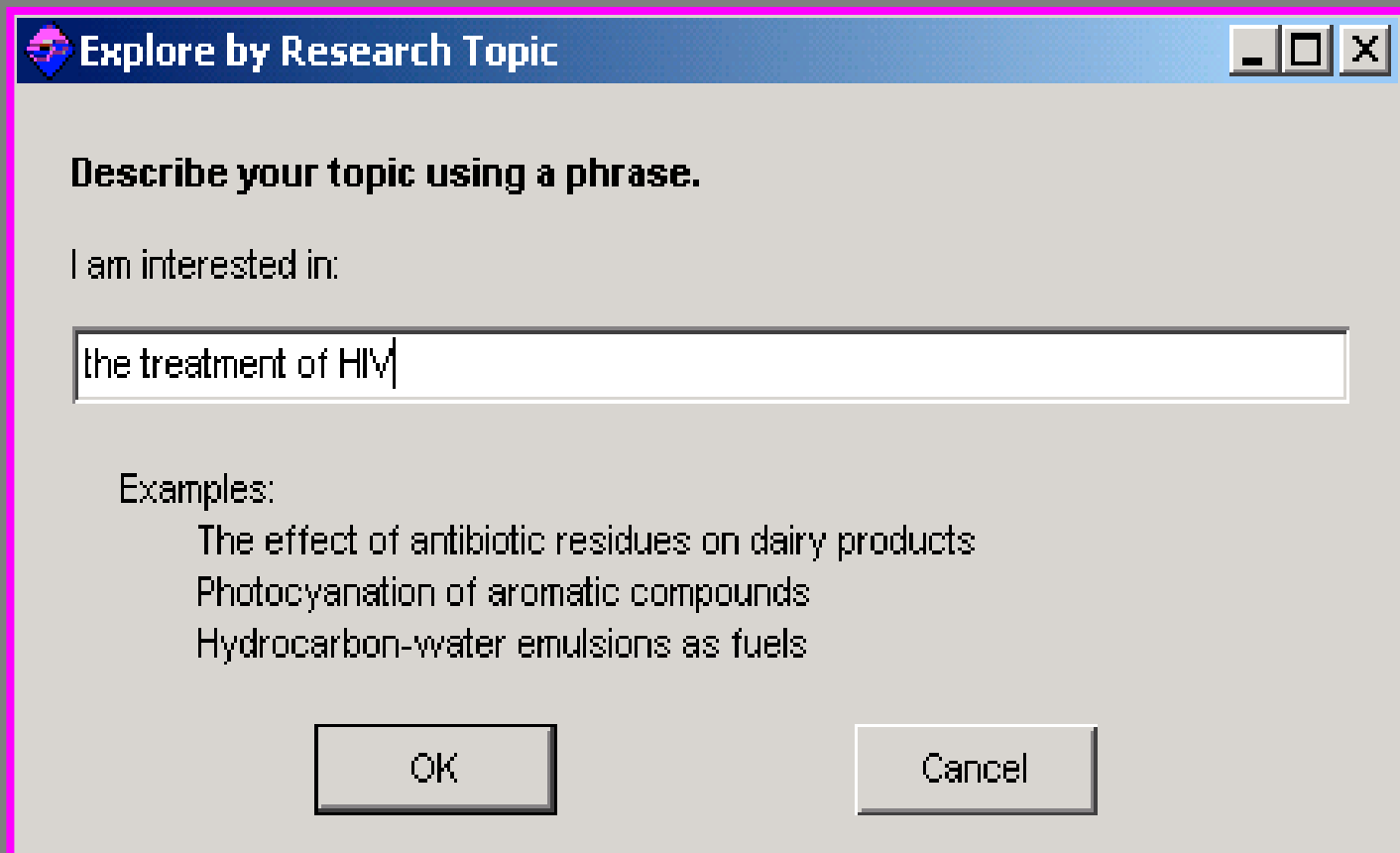
12,13-cycloalkyl epothilones 3-8

Scheme 1. Thus, coupling of the C7–C15 aldehyde fragment with the heterocyclic vinyl iodide, followed by elaboration and aldol reaction with the C1–C6 ketone segment, would lead, upon further elaboration, to the desired *seco*-hydroxy acid. Cyclization according to our Yamaguchi strategy⁶⁷ would then furnish, upon deprotection, the desired

Interested in “The treatment of HIV”?



Enter the topic of interest



Explore by Research Topic

Describe your topic using a phrase.

I am interested in:

Examples:

- The effect of antibiotic residues on dairy products
- Photocyanation of aromatic compounds
- Hydrocarbon-water emulsions as fuels

OK Cancel

Select candidates of interest

The screenshot shows a window titled "Topic Candidates" with a menu bar (File, Edit, Task, Tools, Help) and a list of five candidates. The first candidate is selected. A red arrow points to the first checkbox, and a blue arrow points to the "Get References" button. The "Get References" button is circled in red.

Topic Candidates

File Edit Task Tools Help

Select the candidates of interest:

- 3209 references were found containing **"the treatment of HIV"** as entered.
- 26184 references were found containing the two concepts **"treatment"** and **"HIV"** closely associated with one another.
- 43632 references were found where the two concepts **"treatment"** and **"HIV"** were present anywhere in the reference.
- 4588348 references were found containing the concept **"treatment"**.
- 185942 references were found containing the concept **"HIV"**.

Get References Back

Candidates 1-5 of 5

Here are the references!

SciFinder Scholar

File Edit View Task Tools Help

NewTask Back Forward Print Save As Full Text Prefs Database History Internet Help Exit

- La Colla, Paolo; Artico, Marino; Sommadossi, Jean-Pierre. **Phenylindoles for the treatment of HIV.** PCT Int. Appl. (2002), CODEN: PIXXD2 WO 0283126 A1 20021024 AN 2002:813922 CAPLUS
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- Harris, Michael F. **Methods for the treatment of HIV and other viruses.** PCT Int. Appl. (2002), 43 pp. CODEN: PIXXD2 WO 0276403 A2 20021003 CAN 137:226589 AN 2002:754166 CAPLUS

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References 1-8 of 3209

3209
references

Narrow down the answer set

The screenshot shows the SciFinder Scholar application window. The main area displays a list of search results. A dialog box titled "Analyze or Refine" is open, allowing the user to select an action:

- Analyze:** Get histograms of the year, corporate sources, authors, etc.
- Refine:** Go to refine options without analyzing the answer set.

A blue arrow points to the "Refine" option in the dialog box. At the bottom of the main window, the "Analyze or Refine References" button is circled in blue, with a red arrow pointing to it. The status bar at the bottom indicates "References 1-8 of 3209".









References listed in the background:

- La Colla, Paolo; Artico, Marino; Sommadossi, Jean-Pierre. **Phenylindoles for the treatment of HIV.** PCT Int. Appl. (2002), CODEN: PIXXD2 WO 0283126 A1 20021024 AN 2002:813922 CAPLUS
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- Turk, Gabriella; Horacio. **A derivative:** Antimicrobi 2002:78625
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- Lynn, Ralf Geiben; Walker, Bruce D. **Peroxiredoxin drugs for treatment of HIV-1 infection and methods of use thereof.** PCT Int. Appl. (2002), 47 pp. CODEN: PIXXD2 WO 0277294 A1 20021003 CAN 137:242148 AN 2002:754633 CAPLUS
- Harris, Michael F. **Methods for the treatment of HIV and other viruses.** PCT Int. Appl. (2002), 43 pp. CODEN: PIXXD2 WO 0276403 A2 20021003 CAN 137:226589 AN 2002:754166 CAPLUS

Refine by research topic

Refine

Refine by:

	Research Topic Limit to literature relevant to a topic of interest.		Publication Year Limit to literature from a year or range.		Database Limit to literature from specific databases.
	Company Name Limit to literature from a specific organization.		Document Type Limit to only Patents, Journals, or other types.		Full Text Availability Limit to literature available in full text.
	Author Name Limit to literature written by a specific author.		Language Limit to literature written in specific languages.		

Cancel



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!

SciFinder Scholar

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CODEN: AIDSET ISSN:0269-9370. CAN 135:282754 AN 2001:513146 CAPLUS

- John, Leela; Marra, Fawziah; Ensom, Mary H. H. **Role of therapeutic drug monitoring for protease inhibitors.** *Annals of Pharmacotherapy* (2001), 35(6), 745-754. CODEN: APHRER ISSN:1060-0280. CAN 135:297931 AN 2001:507285 CAPLUS
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References 13-20 of 1096

1096
references

Let's narrow down to other area of interest

The screenshot shows the SciFinder Scholar web application interface. At the top, there is a menu bar with 'File', 'Edit', 'View', 'Task', 'Tools', and 'Help'. Below the menu is a toolbar with icons for 'NewTask', 'Back', 'Forward', 'Print', 'Save As', 'Full Text', 'Prefs', 'Database', 'History', 'Internet', 'Help', and 'Exit'. The main content area displays a list of search results, each with a checkbox and a brief description of the article. A dialog box titled 'Refine by Research Topic' is open in the foreground, prompting the user to 'Describe your topic using a phrase.' The input field contains the text 'gene therapy'. Below the input field, there are 'Examples:' such as 'The effect of antibiotic residues on dairy products', 'Photocyanation of aromatic compounds', and 'Hydrocarbon-water emulsions as fuels'. The dialog box has 'OK' and 'Cancel' buttons. At the bottom of the interface, there are buttons for 'Analyze or Refine References', 'Get Related...', and 'Back'. The status bar at the very bottom indicates 'References 1-8 of 3209'.

SciFinder Scholar

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de Truchis, Pierre; Force, Gilles; Welker, Yves; Mechali, Denis; Pulik, Marc; Chemlal, Kadoudja; Rouveix, Elisabeth; Devidas, Alain; Praindhui, Danielle; Mamet, Jean-Philippe. **Efficacy and Safety of a Quadruple Combination Combivir + Abacavir + Efavirenz Regimen in Antiretroviral Treatment-Naive HIV-1-Infected Adults: La Francilienne.** JAIDS, Journal of Acquired Immune Deficiency Syndromes (2002), 31(2), 179-189. CODEN: J

Walsh, Jo **abacavir isozymes** CBINA8 I

Brenner, E **overcome** EOBT2

Turk, Gab Horacio. **derivative** Antimicrob 2002:7862

Miller, Michael W. **Piperidine and piperazine derivatives as CCR-5 antagonists useful for treating AIDS.** PCT Int. Appl. (2002), 45 pp. CODEN: PIXXD2 WO 0279194 A1 20021010 AN 2002:777931 CAPLUS

Lynn, Ralf Geiben; Walker, Bruce D. **Peroxioredoxin drugs for treatment of HIV-1 infection and methods of use thereof.** PCT Int. Appl. (2002), 47 pp. CODEN: PIXXD2 WO 0277294 A1 20021003 CAN 137:242148 AN 2002:754633 CAPLUS

Harris, Michael F. **Methods for the treatment of HIV and other viruses.** PCT Int. Appl. (2002), 43 pp. CODEN: PIXXD2 WO 0276403 A2 20021003 CAN 137:226589 AN 2002:754400 CAPLUS

Refine by Research Topic

Describe your topic using a phrase.

I am interested in:

gene therapy

Examples:

The effect of antibiotic residues on dairy products
Photocyanation of aromatic compounds
Hydrocarbon-water emulsions as fuels

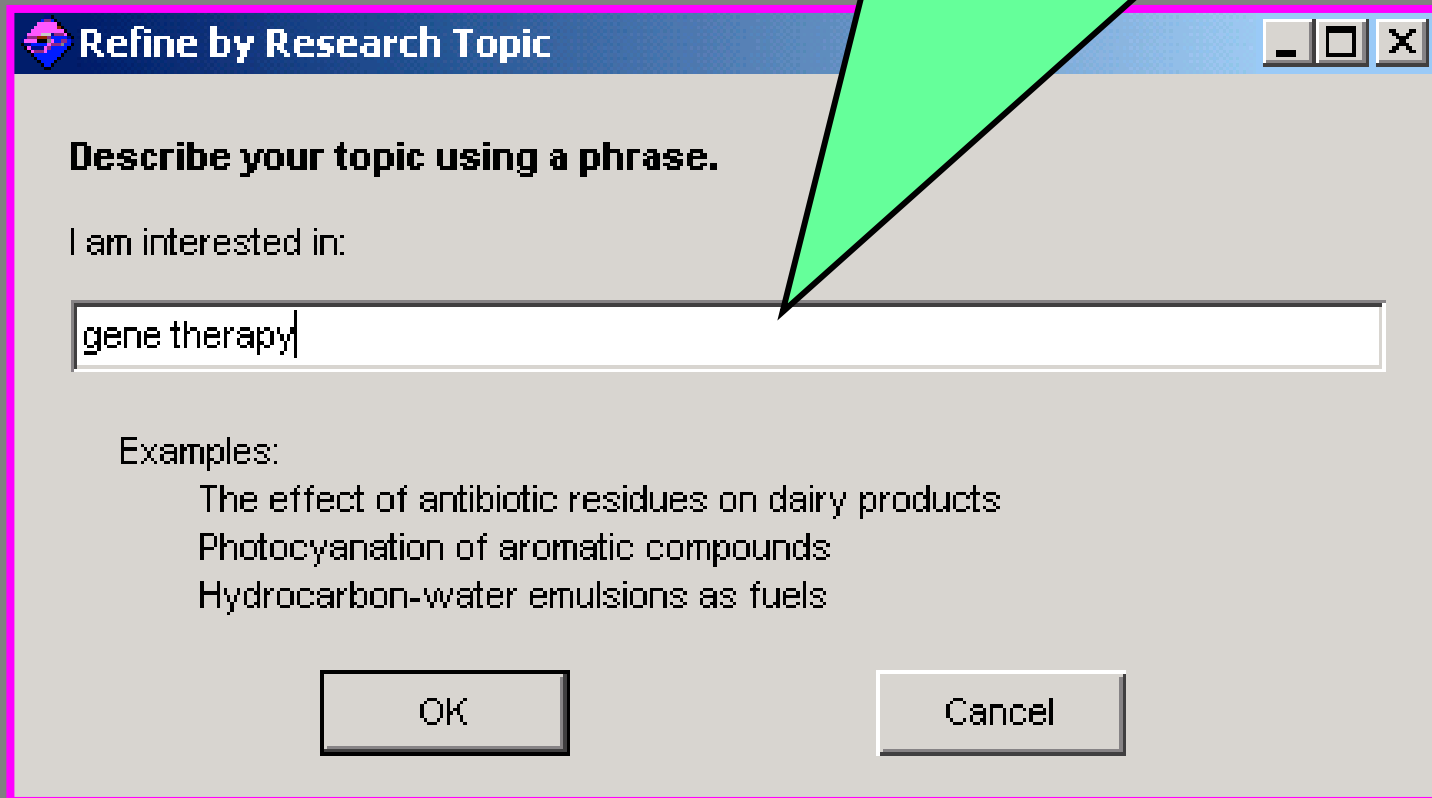
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References 1-8 of 3209

3209
references

Enter topic of interest



Refine by Research Topic

Describe your topic using a phrase.

I am interested in:

Examples:

- The effect of antibiotic residues on dairy products
- Photocyanation of aromatic compounds
- Hydrocarbon-water emulsions as fuels

OK Cancel

Here are the references about gene therapy!

SciFinder Scholar

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References 17-24 of 164

164
references

Select Additional Options

 **Explore by Research Topic** 

Describe your topic using a phrase.

I am interested in:

Examples:

- The effect of antibiotic residues on dairy products
- Photocyanation of aromatic compounds
- Hydrocarbon-water emulsions as fuels

Limit your search

Explore by Research Topic - Additional Options [X]

Describe your topic using a phrase.
I am interested in:

the treatment of HIV

Examples:
The effect of antibiotic residues on dairy products
Photocyanation of aromatic compounds
Hydrocarbon-water emulsions as fuels

You may limit your search by any of the following:

- Limit by Publication Year
- Limit by Document Type
- Limit by Language
- Limit by Author
- Limit by Company Name

OK Remove Options Cancel

Limit by Publication Year

Explore by Research Topic - Additional Options

Describe your topic using a phrase.
I am interested in:

the treatment of HIV

Examples:
The effect of antibiotic residues on dairy products
Photocyanation of aromatic compounds
Hydrocarbon-water emulsions as fuels

You may limit your search by any of the following:

Limit by Publication Year

Specify the year(s) in which you are interested:

1998-2002

Examples:

2001	a single year
1907-1963	a range of years, inclusive
1992-	beginning with a given year
-1992	up to and including a given year

Limit by Document Type

Limit by Language

Limit by Author

Limit by Company Name

OK Remove Options Cancel

Limit by Document Type

Explore by Research Topic - Additional Options

Describe your topic using a phrase.
I am interested in:

Examples:
The effect of antibiotic residues on dairy products
Photocyanation of aromatic compounds
Hydrocarbon-water emulsions as fuels

You may limit your search by any of the following:

1907-1963	a range of years, inclusive
1992-	beginning with a given year
-1992	up to and including a given year

Limit by Document Type

<input type="checkbox"/> Biography	<input type="checkbox"/> Dissertation	<input type="checkbox"/> Patent
<input type="checkbox"/> Book	<input type="checkbox"/> Editorial	<input type="checkbox"/> Preprint
<input checked="" type="checkbox"/> Clinical Trial	<input type="checkbox"/> Historical	<input type="checkbox"/> Report
<input type="checkbox"/> Commentary	<input checked="" type="checkbox"/> Journal	<input type="checkbox"/> Review
<input type="checkbox"/> Conference	<input type="checkbox"/> Letter	

Limit by Language

Limit by Author

Limit by Company Name

OK Remove Options Cancel

Limit by Publication Year and Document Type

Explore by Research Topic - Additional Options

Describe your topic using a phrase.
I am interested in:

Examples:
The effect of antibiotic residues on dairy products
Photocyanation of aromatic compounds
Hydrocarbon-water emulsions as fuels

You may limit your search by any of the following:

Limit by Publication Year

Specify the year(s) in which you are interested:

Examples:
2001 a single year
1907-1963 a range of years, inclusive
1992- beginning with a given year
-1992 up to and including a given year

Limit by Document Type

<input type="checkbox"/> Biography	<input type="checkbox"/> Dissertation	<input type="checkbox"/> Patent
<input type="checkbox"/> Book	<input type="checkbox"/> Editorial	<input type="checkbox"/> Preprint
<input checked="" type="checkbox"/> Clinical Trial	<input type="checkbox"/> Historical	<input type="checkbox"/> Report
<input type="checkbox"/> Commentary	<input checked="" type="checkbox"/> Journal	<input type="checkbox"/> Review

Select candidates of interest

Topic Candidates

File Edit Task Tools Help

Select Candidates of interest (**limited by Publication Year and Document Type**):

- 1430 references were found containing **"the treatment of HIV"** as entered.
- 9290 references were found containing the two concepts **"treatment"** and **"HIV"** closely associated with one another.
- 15949 references were found where the two concepts **"treatment"** and **"HIV"** were present anywhere in the reference.
- 819009 references were found containing the concept **"treatment"**.
- 59550 references were found containing the concept **"HIV"**.

Get References Back

Candidates 1-5 of 5

Here are the references after limiting the search!

SciFinder Scholar

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NewTask Back Forward Print Save As Full Text Prefs Database History Internet Help Exit

- Sluis-Cremer, Nicolas; Tachedjian, Gilda. **Modulation of the oligomeric structures of HIV-1 retroviral enzymes by synthetic peptides and small molecules.** European Journal of Biochemistry (2002), 269(21), 5103-5111. CODEN: EJBCAI ISSN:0014-2956. AN 2002:859797 CAPLUS
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Analyze or Refine References Get Related... Back

References 1-7 of 1430

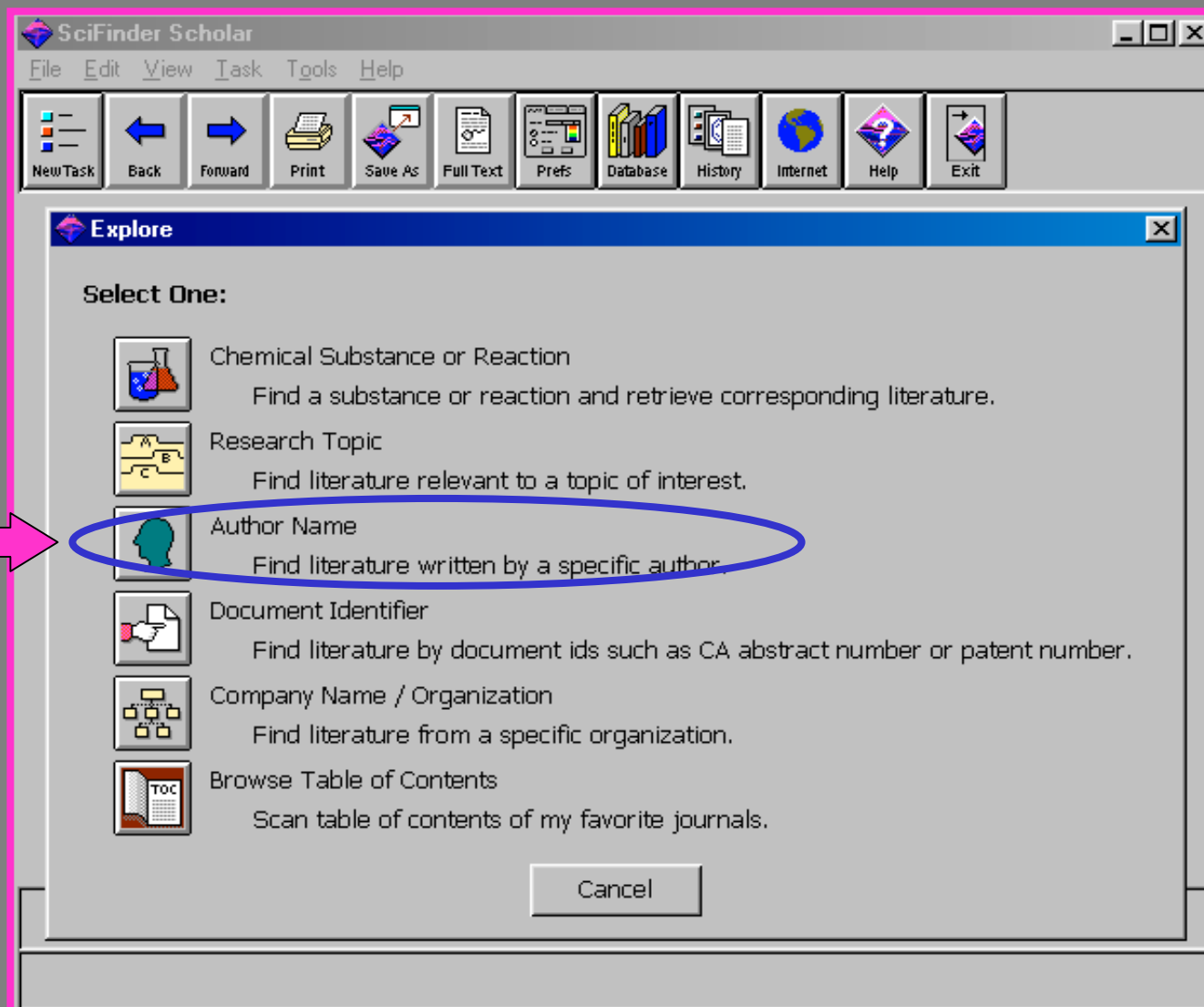
1430
references

Next



Explore by Author Name

Explore by Author Name



Enter the author's name

Explore by Author Name [X]

Enter the author's name.

Last name (required):

Taylor

First name or initial:

Richard

Middle name or initial:

T

Look for alternative spellings of the last name.

OK Cancel

The image shows a dialog box with a blue title bar containing a small icon and the text 'Explore by Author Name' followed by a close button (X). The main area is light gray. It contains the instruction 'Enter the author's name.' followed by three text input fields. The first field is labeled 'Last name (required):' and contains the text 'Taylor'. The second field is labeled 'First name or initial:' and contains 'Richard'. The third field is labeled 'Middle name or initial:' and contains 'T'. Below the fields is a checked checkbox with the text 'Look for alternative spellings of the last name.'. At the bottom are two buttons: 'OK' and 'Cancel'. Two arrows originate from the top text box: a black arrow points to the 'Taylor' text in the first input field, and a red arrow points to the 'Richard' text in the second input field.


Select the candidates of interest

Author Candidates

File Edit Task Tools Help

Select the candidates of interest:

<input type="checkbox"/>	TAILOR R	7 references
<input type="checkbox"/>	TALOR R	1 references
<input type="checkbox"/>	TAYLER R	6 references
<input type="checkbox"/>	TAYLOR	15 references
<input type="checkbox"/>	TAYLOR DICK	4 references
<input type="checkbox"/>	TAYLOR R	1089 references
<input type="checkbox"/>	TAYLOR R T	118 references
<input type="checkbox"/>	TAYLOR R TREVOR	1 references
<input type="checkbox"/>	TAYLOR RICHARD	43 references
<input checked="" type="checkbox"/>	TAYLOR RICHARD T	47 references
<input type="checkbox"/>	TAYLOR RICHARD TIMOTHY	1 references

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Candidates 1-11 of 11

Here are the author's work!

SciFinder Scholar

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- Chai, Minghui; Puapaiboon, Uraiwan; **Taylor, Richard T.**; Rinaldi, Peter L. **Multidimensional NMR studies on polyurethane dendritic wedges.** Polymer Preprints (American Chemical Society, Division of Polymer Chemistry) (2001), 42(1), 33-34. CODEN: ACPPAY ISSN:0032-3934. CAN 134:296319 AN 2001:220750 CAPLUS
- Chai, Minghui; Rinaldi, Peter L.; Puapaiboon, Uraiwan; **Taylor, Richard T.** **Multidimensional NMR studies on polyurethane dendritic wedges.** Abstr. Pap. - Am. Chem. Soc. (2001), 221st POLY-295. CODEN: ACSRAL ISSN:0065-7727. AN 2001:206090 CAPLUS
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- Sherman, Jeffrey H.; **Taylor, Richard T.**; Hofacker, Amanda L.; Hershberger, James W.; Conn, Garrett M.; Gorman, William A. **Removal of contaminants from petroleum distillates.** PCT Int. Appl. (2000), 31 pp. CODEN: PIXXD2 WO 0053706 A1 20000914 CAN 133:240484 AN 2000:646102 CAPLUS
- Sherman, Jeffrey H.; **Taylor, Richard T.** **Method of removing contaminants from**

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References 1-6 of 47

Number of
references
retrieved

View Detail of Reference

Interested in this reference?

The screenshot shows the SciFinder Scholar web application. At the top, there is a menu bar with 'File', 'Edit', 'View', 'Task', 'Tools', and 'Help'. Below the menu is a toolbar with icons for 'NewTask', 'Back', 'Forward', 'Print', 'Save As', 'Full Text', 'Prefs', 'Database', 'History', 'Internet', 'Help', and 'Exit'. The main content area displays a search result for 'Multidimensional NMR studies on polyurethane dendritic wedges' by Chai, Minghui; Puapaiboon, Uraiwan; Taylor, Richard T.; and Rinaldi, Peter L. The reference is listed in 'Polymer Preprints'. Below the search result, there is a 'Detail of Reference' window. This window has a menu bar with 'File', 'Edit', and 'Help'. It contains three sections: 'Bibliographic Information', 'Abstract', and 'Indexing'. The 'Bibliographic Information' section provides details about the authors, their affiliation (Department of Chemistry, Marshall University), the journal (Polymer Preprints), volume (42), issue (1), pages (33-34), and ISSN (0032-3934). The 'Abstract' section describes the use of multidimensional NMR techniques with pulse field gradient (PFG) enhancement to study polyurethane dendritic wedges. The 'Indexing' section indicates the reference is in Section 36-2 (Physical Properties of Synthetic High Polymers) and is indexed under 'R' (NMR (nuclear magnetic resonance)).

Chai, Minghui; Puapaiboon, Uraiwan; Taylor, Richard T.; Rinaldi, Peter L.
Multidimensional NMR studies on polyurethane dendritic wedges. Polymer

Detail of Reference

File Edit Help

Bibliographic Information

Multidimensional NMR studies on polyurethane dendritic wedges. Chai, Minghui; Puapaiboon, Uraiwan; Taylor, Richard T.; Rinaldi, Peter L. Department of Chemistry, Marshall University, Huntington, WV, USA. Polymer Preprints (American Chemical Society, Division of Polymer Chemistry) (2001), 42(1), 33-34. CODEN: ACPPAY ISSN: 0032-3934. Journal written in English. CAN 134:296319 AN 2001:220750 CAPLUS

Abstract

Multidimensional NMR techniques with pulse field gradient (PFG) enhancement have been applied to study 1st, 2nd, and 3rd generation polyurethane dendritic wedges, which are a novel type of linking element in the convergent approach to dendrimer synthesis. By using Pulsed Field Gradient-Heteronuclear Multiple Quantum Coherence (PFG-HMQC) and Heteronuclear Multiple Bond Connectivity (HMBC) 2D NMR expts., ¹H and ¹³C resonance assignments have been obtained for these compds., and structure proofs have been accomplished.

Indexing - Section 36-2 (Physical Properties of Synthetic High Polymers)

R
NMR (nuclear magnetic resonance)

microscope

Here is the detail !

Detail of Reference 1 (continued)

Registry
number

Detail of Reference 3
File Edit Help

[334830-67-0](#)
Role: PRP (Properties)
(G1 dendritic wedge, from convergent approach; multidimensional NMR studies to det. the structure of polyurethane dendritic wedges)

[334830-68-1](#)
Role: PRP (Properties)
(G2 dendritic wedge, from convergent approach; multidimensional NMR studies to det. the structure of polyurethane dendritic wedges)

[334830-69-2](#)
Role: PRP (Properties)
(G3 dendritic wedge, from convergent approach; multidimensional NMR studies to det. the structure of polyurethane dendritic wedges)

Supplementary Terms
polyurethane dendritic wedge structure HMQC HMBC 2D NMR

Citations
1) Lambert, B; J Organomet Chem 1998, 554, 113
1) Chai, M; J Am Chem Soc 1999, 121, 273
2) Chai, M; J Am Chem Soc 1999, 121, 273
3) Chai, M; Macromolecules 2000, 33, 5395
4a) Muller, L; J Am Chem Soc 1979, 101, 4481
4b) Box, A; J Am Chem Soc 1983, 105, 7188
5) Bax, A; J Am Chem Soc 1986, 108, 2093

Get Related... Close

View detail of substance in the reference of interest

Hyperlink

Detail for Registry Number 334830-69-2

File Edit Help

Registry Number: 334830-69-2

334830-67-0
Role: PRP (Pro
(G1 dendritic
structure of pol;

334830-68-1
Role: PRP (Pro
(G2 dendritic
structure of pol;

334830-69-2
Role: PRP (Pro
(G3 dendritic
structure of pol;

Supplemental
polyurethane de

Citations
1) Lambert, B; .
1) Chai, M; J A
2) Chai, M; J A
3) Chai, M; Ma
4a) Muller, L; J
4b) Box, A; J A
5) Bax, A; J An

PAGE 1-A

CCOC(=O)Nc1ccc(OCCOC(=O)Nc2ccc(OCCOC(=O)Nc3ccc(OCCOC(=O)N)cc3)cc2)cc1

PAGE 1-B

CCOC(=O)Nc1ccc(OCCOC(=O)Nc2ccc(OCCOC(=O)N)cc2)cc1

Me

CCOC(=O)Nc1ccc(OCCOC(=O)Nc2ccc(OCCOC(=O)N)cc2)cc1

Close

Hyperlink
To view
3D Structure

Detail for Registry Number 334830-69-2

File Edit Help

PAGE 2-B

PAGE 2-C

— (CH₂)₁₁—Me

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 --

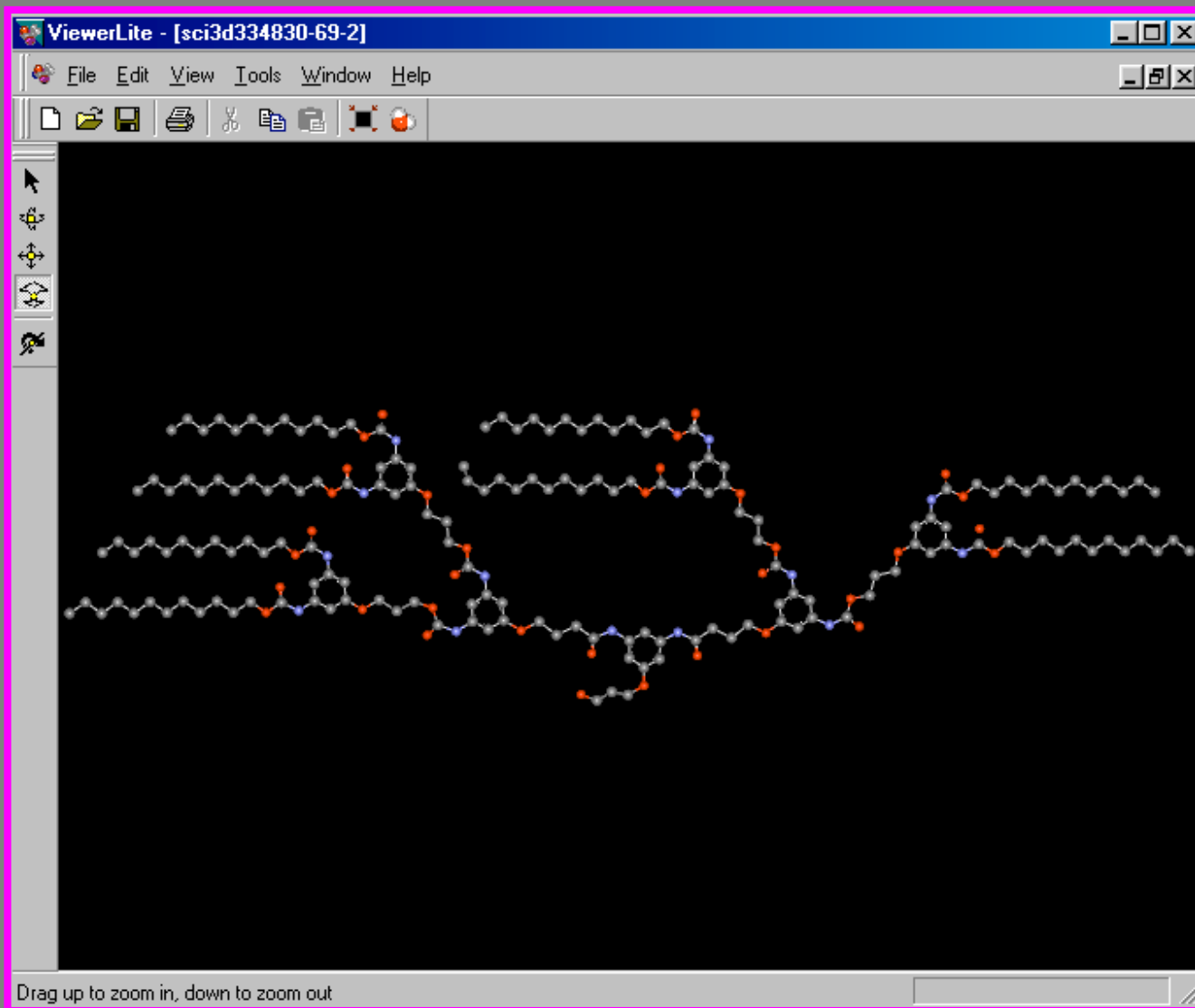
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STN Files: CAPLUS, CA

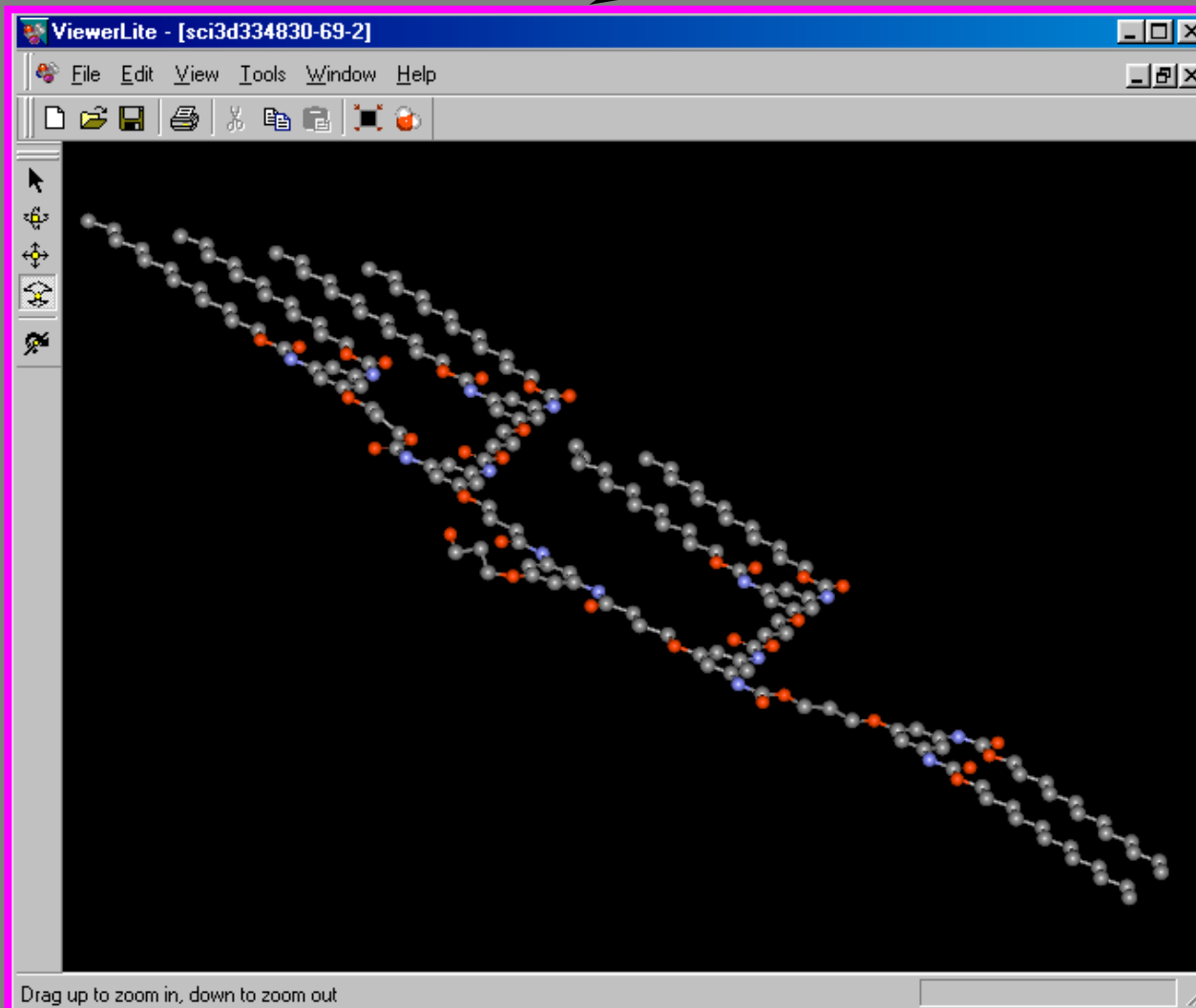
Database: REGISTRY

Close

View 3D structure !



Let's rotate 3D structure



Narrow down
answer sets

Too many?

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- Chai, Minghui; Puapaiboon, Uraiwan; Taylor, Richard T.; Rinaldi, Peter L. **Multidimensional NMR studies on polyurethane dendritic wedges.** Polymer Preprints (American Chemical Society, Division of Polymer Chemistry) (2001), 42(1), 33-34.
- Chai, M **Multidi** Am. Ch 2001:2
- Sherma **used o** U.S. 6, 2001:7
- Sherma **Metho** (2000), 2000:6
- Sherman, Jeffrey H.; Taylor, Richard T.; Hofacker, Amanda L.; Hershberger, James W.; Conn, Garrett M.; Gorman, William A. **Removal of contaminants from petroleum distillates.** PCT Int. Appl. (2000), 31 pp. CODEN: PDXD2 WO 0053706 A1 2000:0914 CAN 133:240484 AN 2000:646102 CAPLUS
- Sherman, Jeffrey H.; Taylor, Richard T. **Method of removing contaminants from**

Analyze or Refine

Select One:

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Get histograms of the year, corporate sources, authors, etc.
- Refine
Go to refine options without analyzing the answer set.

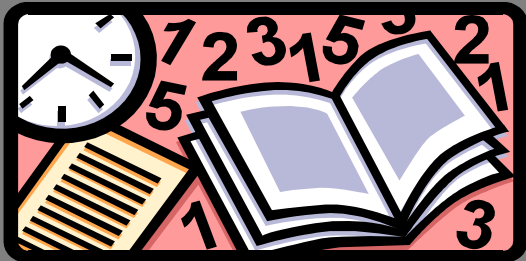
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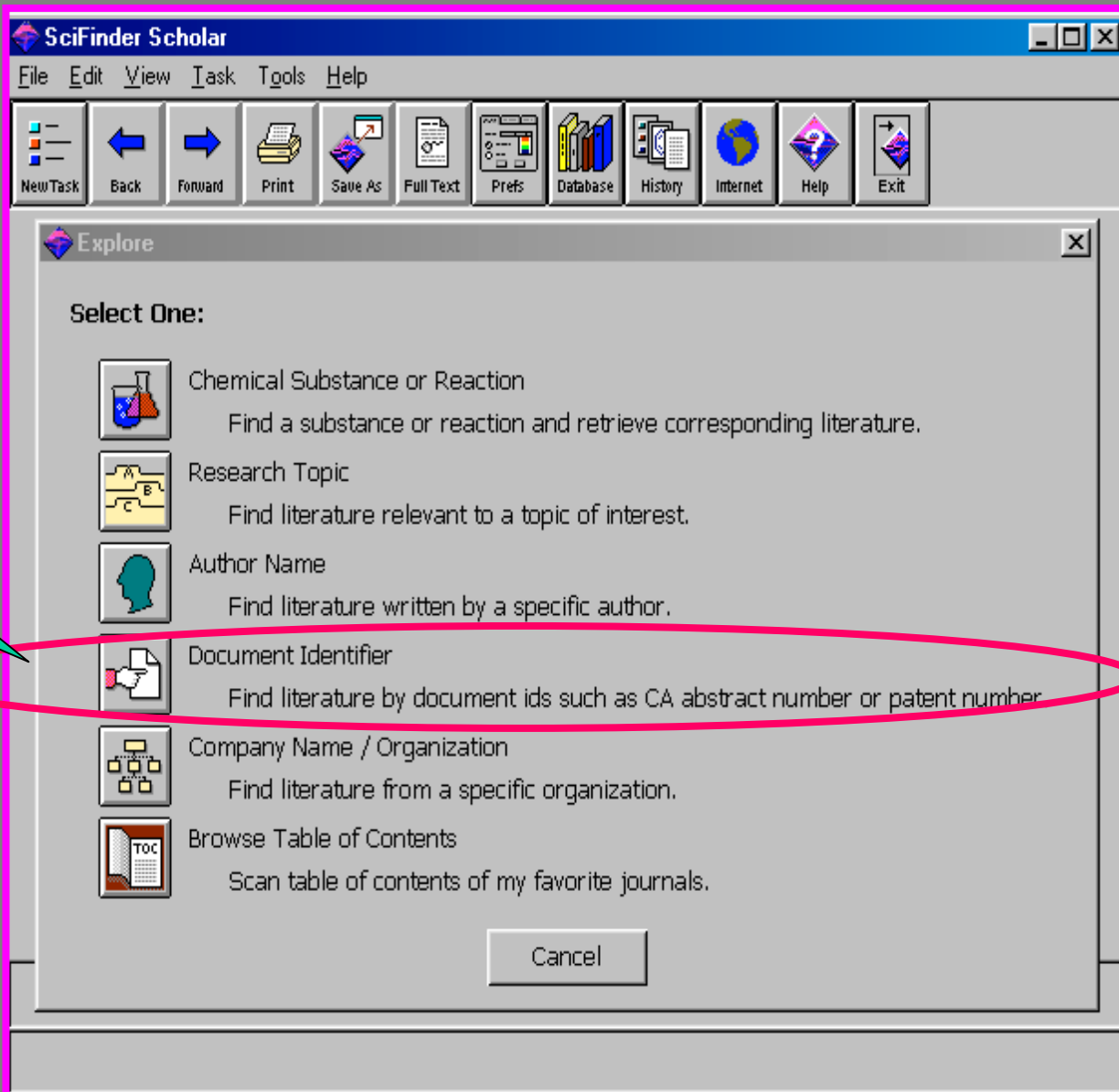
References 1-6 of 47

Next

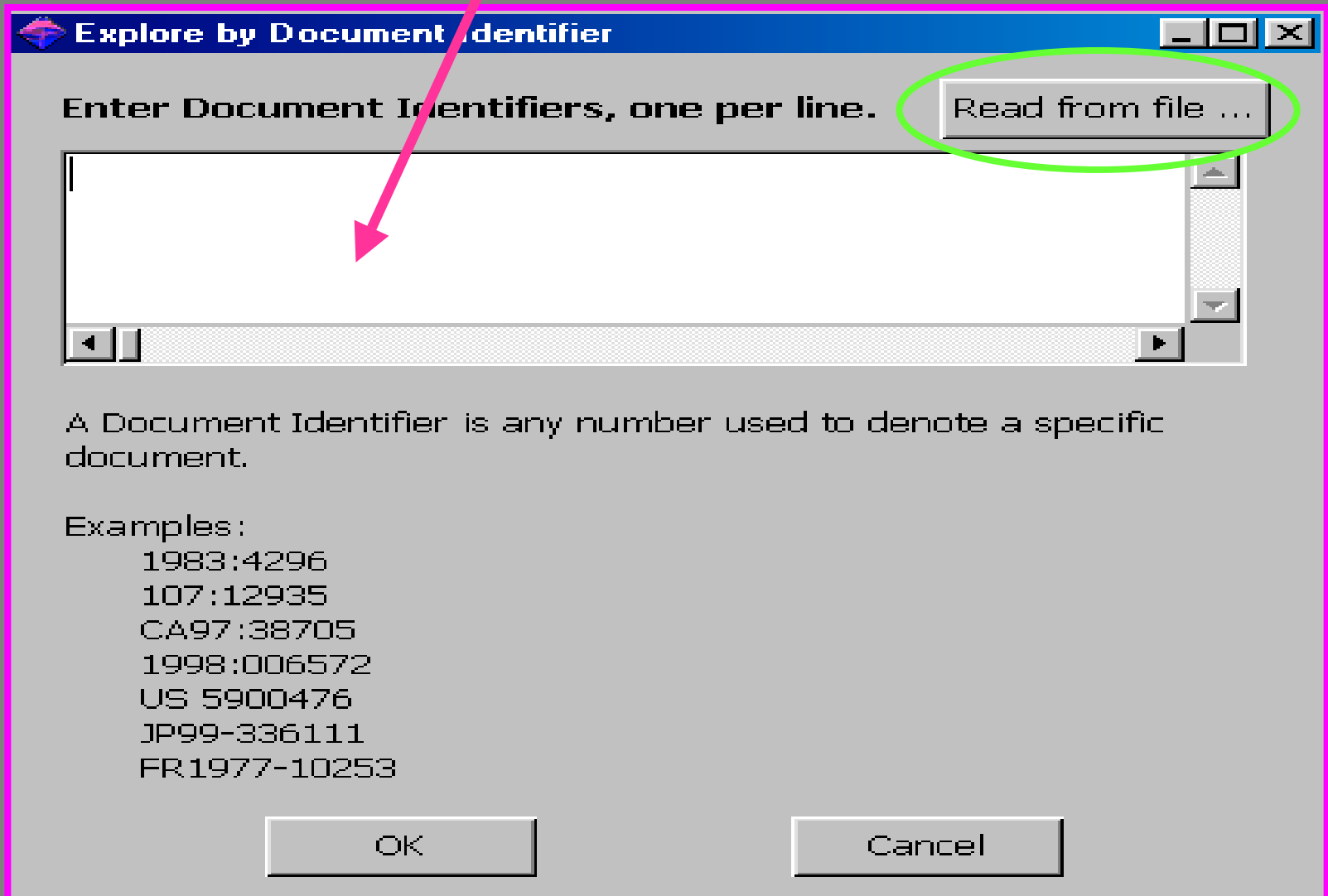


Explore by Document Identifier

Search by
Document
Identifier



Enter Document Identifiers



Explore by Document Identifier

Enter Document Identifiers, one per line.

Read from file ...

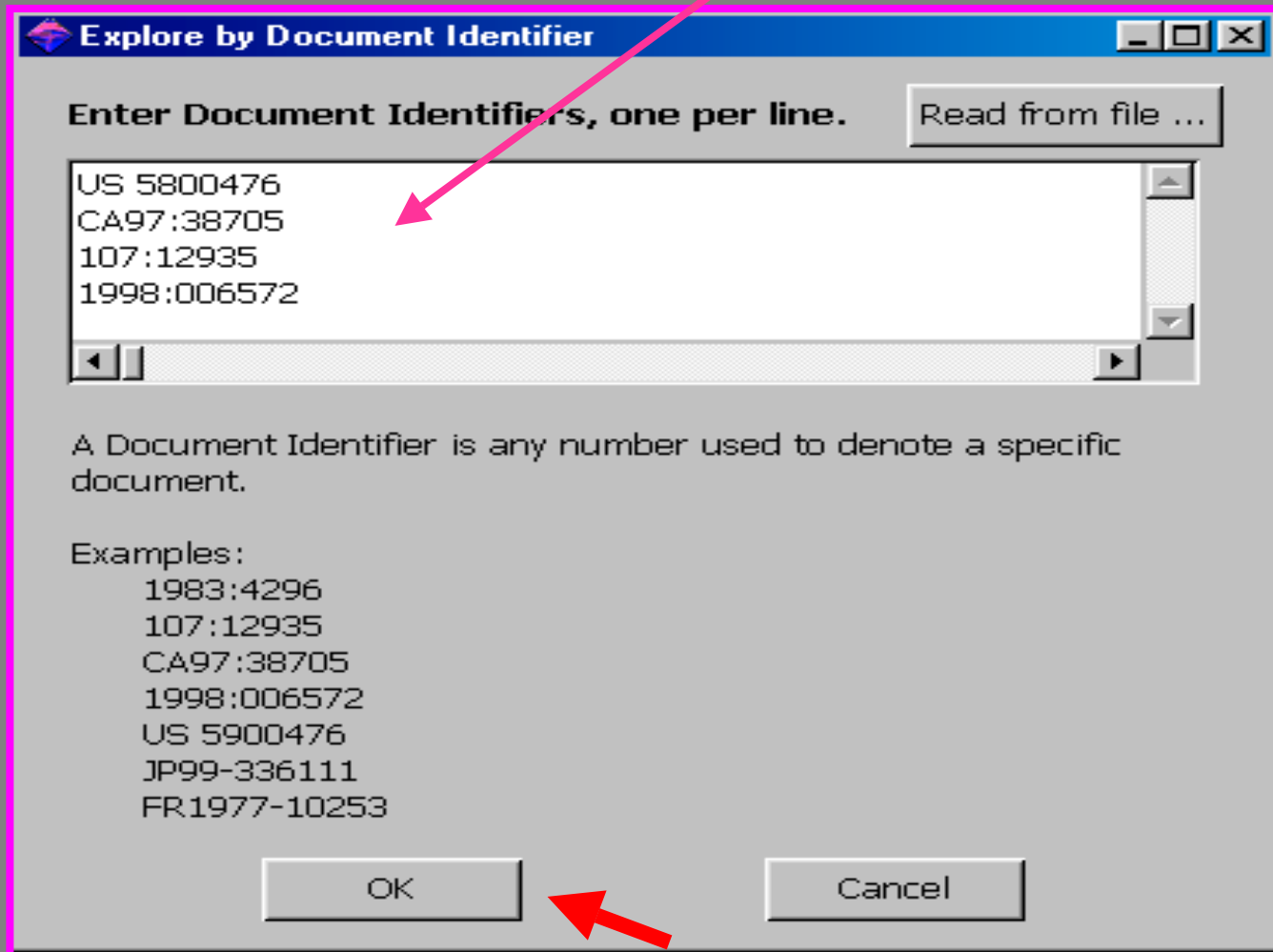
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- Liang, Kangning; Mitzi, David B.; Prikas, Michael T. **Synthesis and Characterization of Organic-Inorganic Perovskite Thin Films Prepared Using a Versatile Two-Step Dipping Technique.** Chemistry of Materials (1998), 10(1), 403-411. CODEN: CMATEX ISSN:0897-4756. CAN 128:56672 AN [1998:6572](#) CAPLUS
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References 1-6 of 7

View Related information

View substances in the reference of interest

The screenshot displays the SciFinder Scholar software interface. At the top, there is a menu bar with 'File', 'Edit', 'View', 'Task', 'Tools', and 'Help'. Below the menu is a toolbar with icons for 'NewTask', 'Back', 'Forward', 'Print', 'Save As', 'Full Text', 'Prefs', 'Database', 'History', 'Internet', 'Help', and 'Exit'. The main window shows a list of search results. A red oval highlights the 'Substances' option in the 'Get Related Information' dialog box, which is also highlighted by a red arrow from the text on the left. The dialog box has a title bar that says 'Get Related Information' and a 'Cancel' button. The 'Substances' option is selected, and its description is 'Get substances indexed in the selected document(s)'. The background shows a list of references, with the first one being 'Liang, Kangning; Mitzi, David B.; Prikas, Michael T. Synthesis and Characterization of Organic-Inorganic Perovskite Thin Films Prepared Using a Versatile Two-Step Dipping Technique. Chemistry of Materials (1998), 10(1), 403-411. CODEN: CMATEX ISSN:0897-4756. CAN 128:56672 AN 1998:6572 CAPLUS'. The 'Get Related...' button at the bottom of the main window is also circled in blue.

SciFinder Scholar

File Edit View Task Tools Help

NewTask Back Forward Print Save As Full Text Prefs Database History Internet Help Exit

Liang, Kangning; Mitzi, David B.; Prikas, Michael T. **Synthesis and Characterization of Organic-Inorganic Perovskite Thin Films Prepared Using a Versatile Two-Step Dipping Technique.** Chemistry of Materials (1998), 10(1), 403-411. CODEN: CMATEX ISSN:0897-4756. CAN 128:56672 AN 1998:6572 CAPLUS

Oelrich, Eckhard; Starz, Carola; Wotschokowsky, Manfred. **Lucrostriol-containing solution** CAN 107

Bundy, G **metabol** 37(25), CAPLUS

Keck J L; (2000 Ma PubMed

Modak S **purpura** Sep), 13 9738705

Pinon G **9th Session on virology, Versailles. 22-24 May 1997.** ANNALES DE BIOLOGIE CLINIQUE (1997 Sep-Oct), 55(5), 509-1 Journal code: 2984690R.

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Select One:

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Substances
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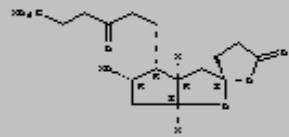

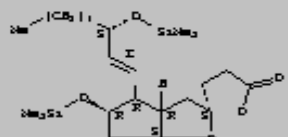

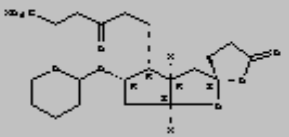

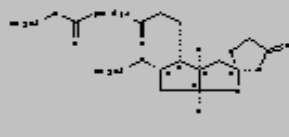

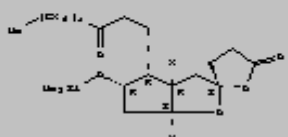

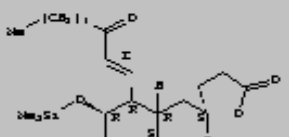
References 1-6 of 7

Substances appeared in the literature of interest

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<input type="checkbox"/>  82337-32-4  3D Model ~1 Reference REGISTRY	<input type="checkbox"/>  82335-97-5  3D Model ~1 Reference REGISTRY	<input type="checkbox"/>  82335-96-4  3D Model ~1 Reference REGISTRY
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Substances 1-6 of 73

Next

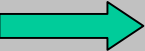
Explore by Company Name
or Organization

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

 Explore by Company Name _ □ X

Please enter the name of the company or organization.

Examples:
Minnesota Mining and Manufacturing
3M
Du Pont



3M's Literatures

SciFinder Scholar

File Edit View Task Tools Help

NewTask Back Forward Print Save As Full Text Prefs Database History Internet Help Exit

- Harrison, Lester I.; Kurup, Sarala; Wagner, Craig; Ekholm, Bruce P.; Larson, Julie S.; Kaiser, Harold B. **Pharmacokinetics of beclomethasone 17-monopropionate from a beclomethasone dipropionate extrafine aerosol in adults with asthma.** European Journal of Clinical Pharmacology (2002), 58(3), 197-201. CODEN: EJCPAS ISSN:0031-6970. AN 2002:453154 CAPLUS
- Harrison, Lester I.; Kurup, Sarala; Chen, Lin-Zhi; Ekholm, Bruce P.; Wighton, Timothy G.; Shapiro, Gail G. **Pharmacokinetic comparison of beclomethasone dipropionate extrafine aerosol from two inhaler devices in children with asthma.** European Journal of Clinical Pharmacology (2002), 58(3), 191-195. CODEN: EJCPAS ISSN:0031-6970. AN 2002:453153 CAPLUS
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References 1-6 of 10436

Wow!
so many
(10436)

Let's narrow them down

The screenshot shows the SciFinder Scholar application window. The title bar reads "SciFinder Scholar" and the menu bar includes "File", "Edit", "View", "Task", "Tools", and "Help". Below the menu bar is a toolbar with icons for "NewTask", "Back", "Forward", "Print", "Save As", "Full Text", "Prefs", "Database", "History", "Internet", "Help", and "Exit".

The main content area displays a list of search results. A dialog box titled "Analyze or Refine" is overlaid on the results. The dialog box has a blue header and contains the following text:

Select One:

- Analyze: Get histograms of the year, corporate sources, authors, etc.
- Refine: Go to refine options without analyzing the answer set.

A "Cancel" button is located at the bottom of the dialog box. A green arrow points from the "Let's narrow them down" text to the "Refine" option in the dialog box.

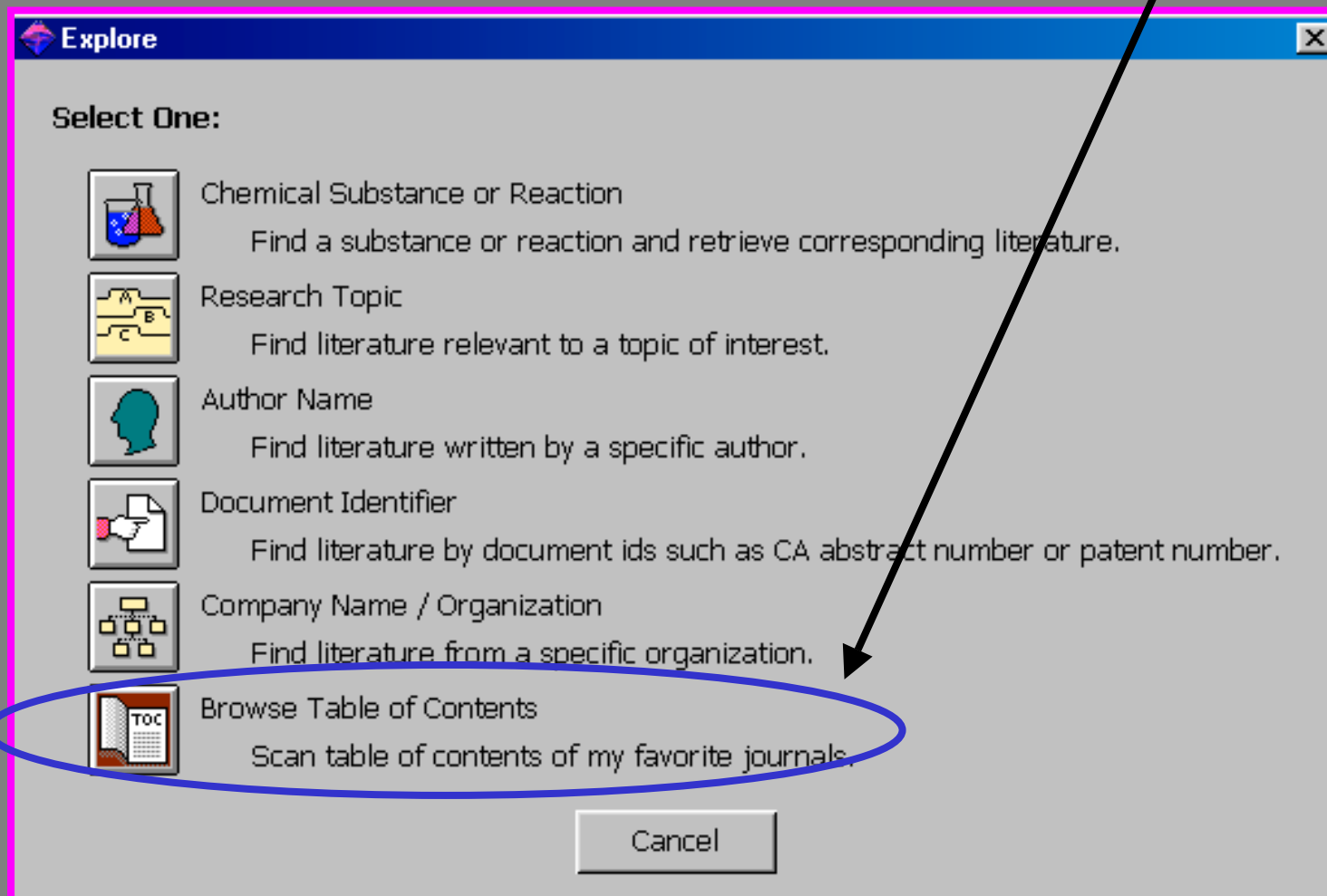
At the bottom of the SciFinder Scholar window, there is a status bar. The text "References 46-51 of 10436" is circled in blue. A red arrow points to the "Analyze or Refine References" button, which is also circled in pink.

Too large answer set !

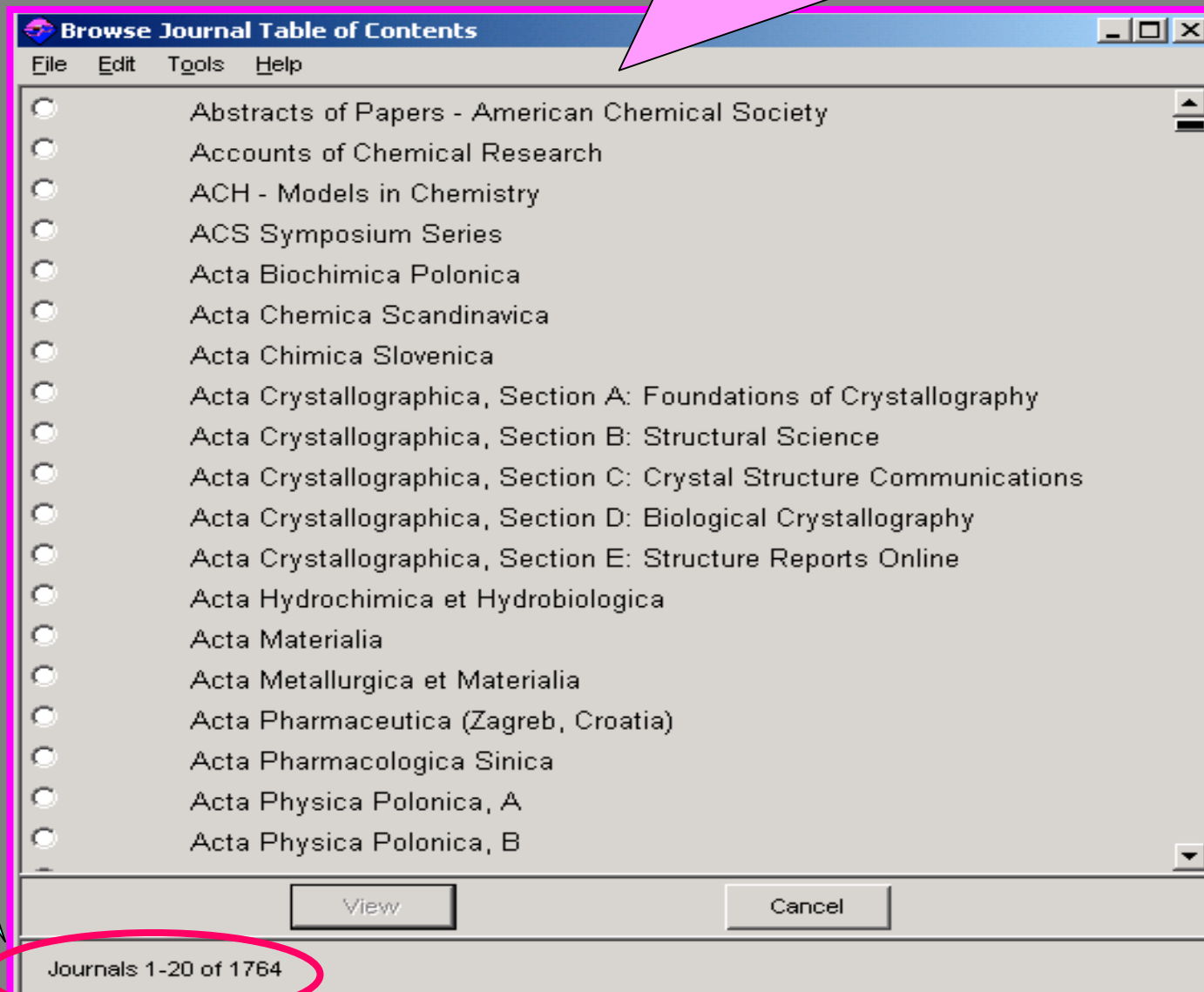
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Explore by browse
Table of contents

Search by Browse Table of Contents



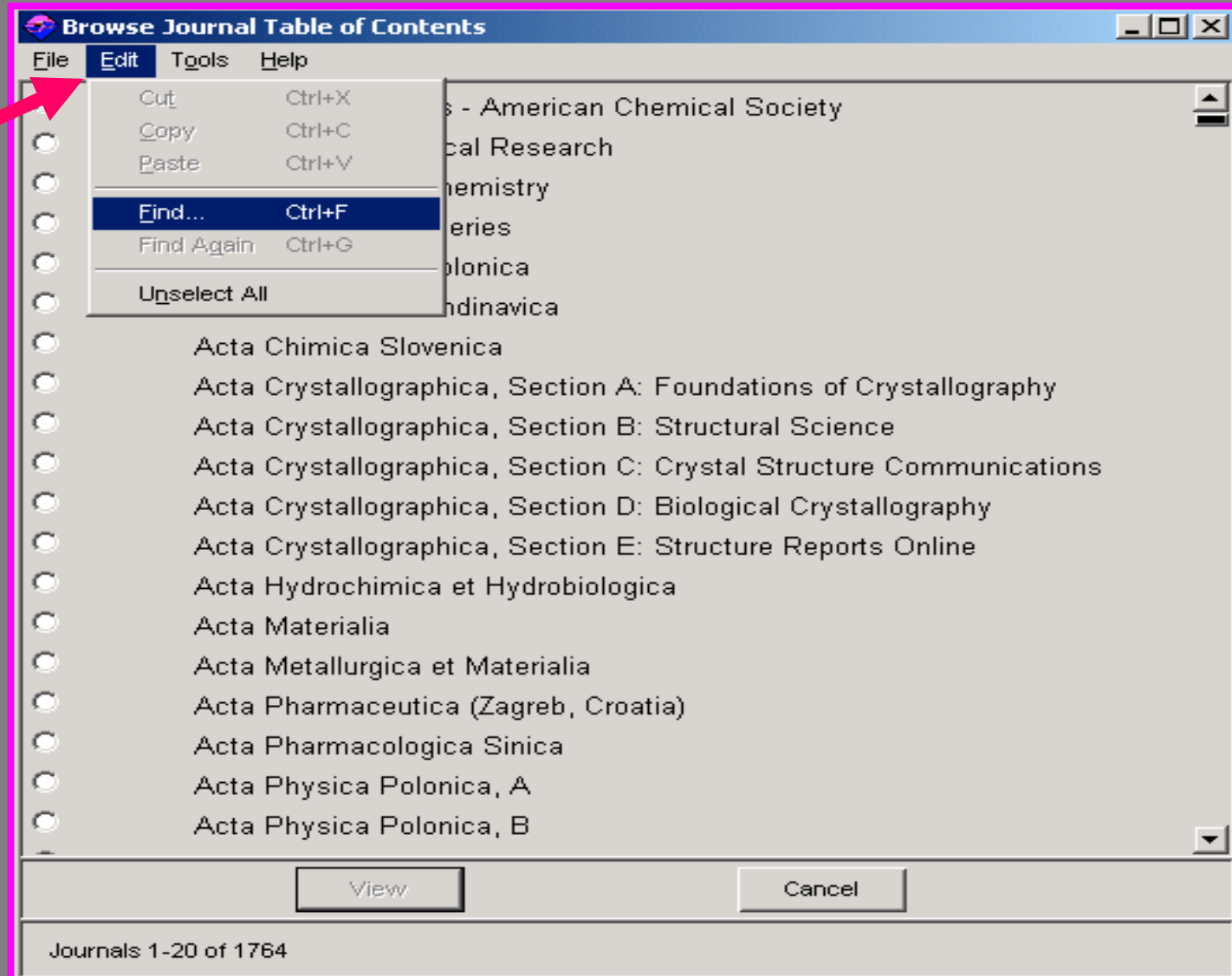
The List of journals!



Look at
This!

Journals 1-20 of 1764

Let's find journal of interest



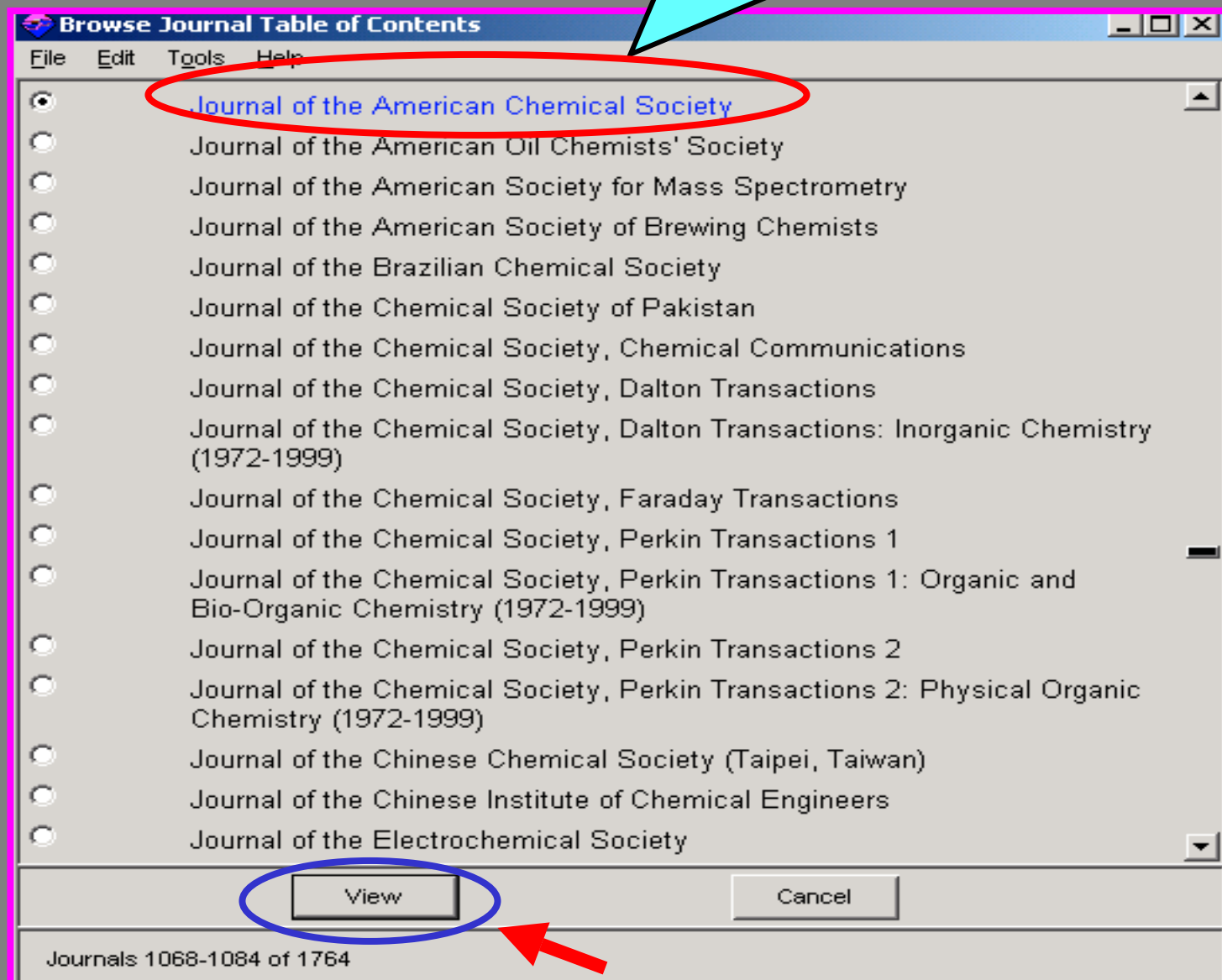
Type journal of interest

The image shows a software interface for browsing journal tables of contents. The main window, titled "Browse Journal Table of Contents", has a menu bar with "File", "Edit", "Tools", and "Help". It displays a list of journals, each preceded by a radio button. The list includes titles such as "Abstracts of Papers - American Chemical Society", "Accounts of Chemical Research", "ACH - Models in Chemistry", "ACS Symposium Series", "Acta Biochimica Polonica", "Acta Chemica Scandinavica", "Acta Chimica Slovenica", "Acta Metallurgica et Materialia", "Acta Pharmaceutica (Zagreb, Croatia)", "Acta Pharmaceutica Sinica", "Acta Physica Polonica, A", and "Acta Physica Polonica, B".

An overlaid dialog box titled "Find Journal Title" prompts the user to "Enter as much of the journal name as you know:". The search input field contains the text "journal of the american chemical society". Below the input field are two buttons: "Find" and "Cancel". The "Find" button is circled in blue. A red arrow points from the text "Type journal of interest" to the search input field.

At the bottom of the main window, there are "View" and "Cancel" buttons, and a status bar indicating "Journals 1-20 of 1764".

Here it is!



Latest issue of Table of Content

Journal of the American Chemical Society
Volume: 125 Issue: 9 2003

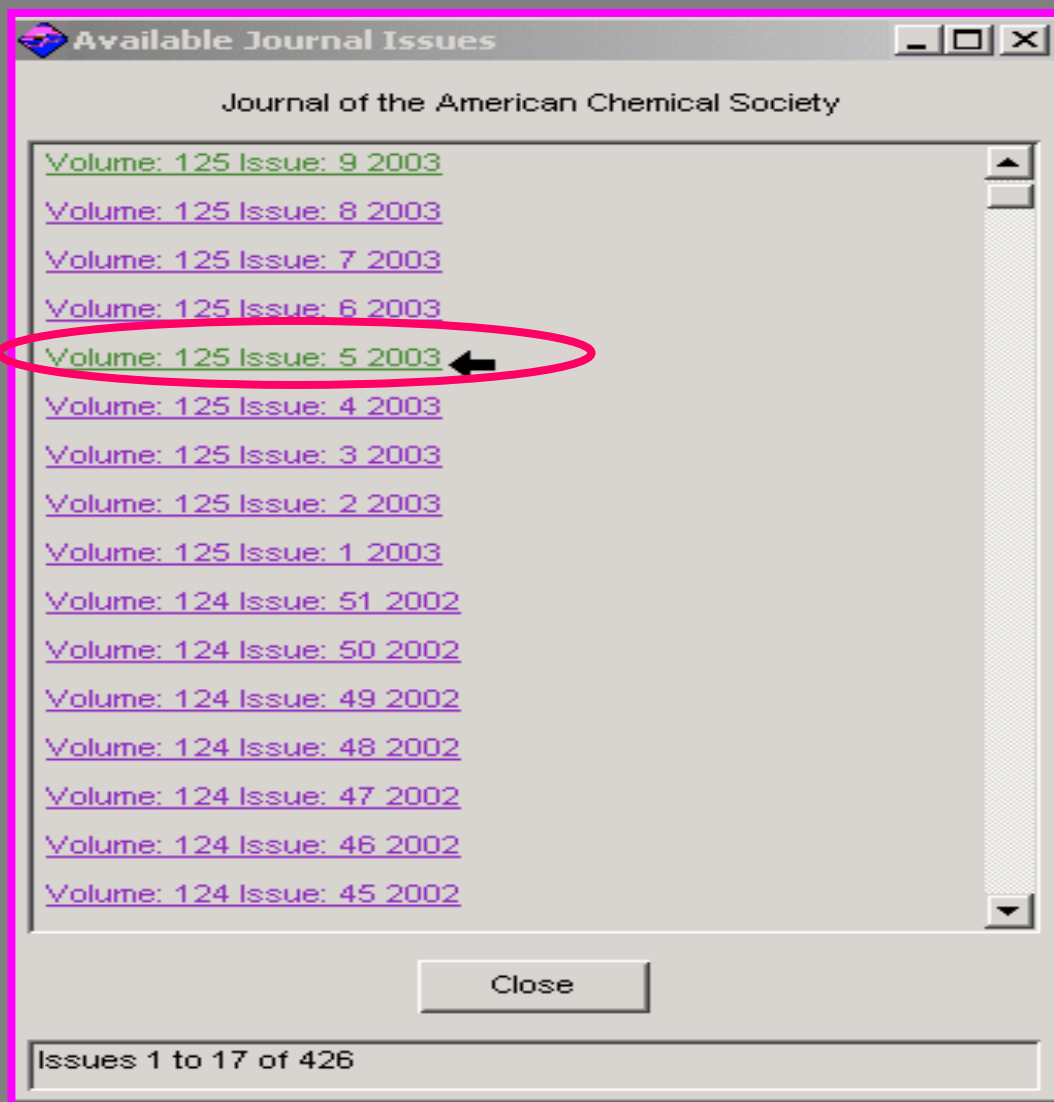
<input type="checkbox"/>	Restricting the Conformational Heterogeneity of RNA by Specific Incorporation of 8-Bromoguanosine Proctor, David J.; Kierzek, Elzbieta; Kierzek, Ryszard; Bevilacqua, Philip C. Journal CAPLUS	2390-2391		
<input type="checkbox"/>	Desymmetrization of Meso 1,3- and 1,4-Diols with a Dinuclear Zinc Asymmetric Catalyst Trost, Barry M.; Mino, Takashi. Journal CAPLUS	2410-2411		
<input type="checkbox"/>	Experimental Determination of the Absolute Enantioselectivity of an Antibody-Catalyzed Diels-Alder Reaction and Theoretical Explorations of the Origins of Stereoselectivity Cannizzaro, Carina E.; Ashley, Jon A.; Janda, K. D.; Houk, K. N. Journal CAPLUS	2489-2506		
<input type="checkbox"/>	Synthesis and Activity of Ruthenium Alkylidene Complexes Coordinated with Phosphine and N-Heterocyclic Carbene Ligands Trnka, Tina M.; Morgan, John P.; Sanford, Melanie S.; Wilhelm, Thomas E.; Scholl, Matthias; Choi, Tae-Lim; Ding, Sheng; Day, Michael W.; Grubbs, Robert H. Journal CAPLUS	2546-2558		
<input type="checkbox"/>	Structural Studies of Ammonia and Metallic Lithium-Ammonia Solutions Thompson, Helen; Wasse, Jonathan C.; Skipper, Neal T.; Hayama, Shusaku; Bowron, Daniel T.; Soper, Alan K. Journal CAPLUS	2572-2581		
<input type="checkbox"/>	Solvent-Controlled Diastereoselective Synthesis of Cyclopentane Derivatives by a [3 + 2] Cyclization Reaction of α , β -Disubstituted (Alkenyl)(methoxy)carbene Complexes	2610-2616		

Select Issue Previous Issue Next Issue Get Related... Back

References 1-6 of 12

Select issue

Select issue of interest



Here are the desired issue!

Journal of the American Chemical Society
Volume: 125 Issue: 5 2003

Article Title	Page Range	Actions
<input type="checkbox"/> Diastereo- and Enantioselective Catalytic Carbometallative Aldol Cycloaddition: Tandem Conjugate Addition-Aldol Cyclization Cauble, David F.; Gipson, John D.; Krische, Michael J. Journal CAPLUS	1110-1111	[Microscope icon] [Laptop icon]
<input type="checkbox"/> 3'-Ferrocene-Labeled Oligonucleotide Chains End-Tethered to Gold Electrode Surfaces: Novel Model Systems for Exploring Flexibility of Short DNA Using Cyclic Voltammetry Anne, Agnes; Bouchardon, Agnes; Moiroux, Jacques. Journal CAPLUS	1112-1113	[Microscope icon] [Laptop icon]
<input type="checkbox"/> Differential Receptors Create Patterns Diagnostic for ATP and GTP McCleskey, Shawn C.; Griffin, Michael J.; Schneider, Stephen E.; McDevitt, John T.; Anslyn, Eric V. Journal CAPLUS	1114-1115	[Microscope icon] [Laptop icon]
<input type="checkbox"/> A Potent, Water-Soluble and Photoinducible DNA Cross-Linking Agent Wang, Ping; Liu, Renpeng; Wu, Xiaojun; Ma, Hongjuan; Cao, Xiaoping; Zhou, Ping; Zhang, Jiangye; Weng, Xiaocheng; Zhang, Xiao-Lian; Qi, Jun; Zhou, Xiang; Weng, Linhong. Journal CAPLUS	1116-1117	[Microscope icon] [Laptop icon]
<input type="checkbox"/> Photoinduced Electron Injection from Ru(dcbpy) ₂ (NCS) ₂ to SnO ₂ and TiO ₂ Nanocrystalline Films Benkoe, Gabor; Myllyperkiö, Pasi; Pan, Jie; Yartsev, Arkady P.; Sundstroem, Villy. Journal CAPLUS	1118-1119	[Microscope icon] [Laptop icon]
<input type="checkbox"/> To Fold or to Assemble? Wang, Wei; Li, Lin-Song; Helms, Greg; Zhou, Hong-Hui; Li, Alexander D. O. Journal	1120-1121	[Microscope icon] [Dropdown arrow]

Select Issue Previous Issue Next Issue Get Related... Back

References 1-6 of 76

Detail of reference 2

Detail of Reference 2

File Edit Help

Bibliographic Information

3'-Ferrocene-Labeled Oligonucleotide Chains End-Tethered to Gold Electrode Surfaces: Novel Model Systems for Exploring Flexibility of Short DNA Using Cyclic Voltammetry.
Anne, Agnes; Bouchardon, Agnes; Moiroux, Jacques. Laboratoire d'Electrochimie Moleculaire, Unite Mixte de Recherche Universite-CNRS No 7591, Universite de Paris 7 - Denis Diderot, Paris, Fr. Journal of the American Chemical Society (2003), 125(5), 1112-1113. CODEN: JACSAT ISSN: 0002-7863. Journal written in English. AN 2003:13476 CAPLUS

Abstract

The flexibility of DNA is of central importance in biol., medicine, materials science, and mech. engineering. In this study, we report an unprecedented electrochem. approach for investigating the flexibility of a short (typically 20-base), surface end-tethered single-stranded synthetic DNA oligonucleotide and of its postformed DNA duplex, taking as an example the homopolymer (dT)20 sequence in the regime of very high ionic strength (.apprx.1 M).

Indexing -- Section 9 (Biochemical Methods)

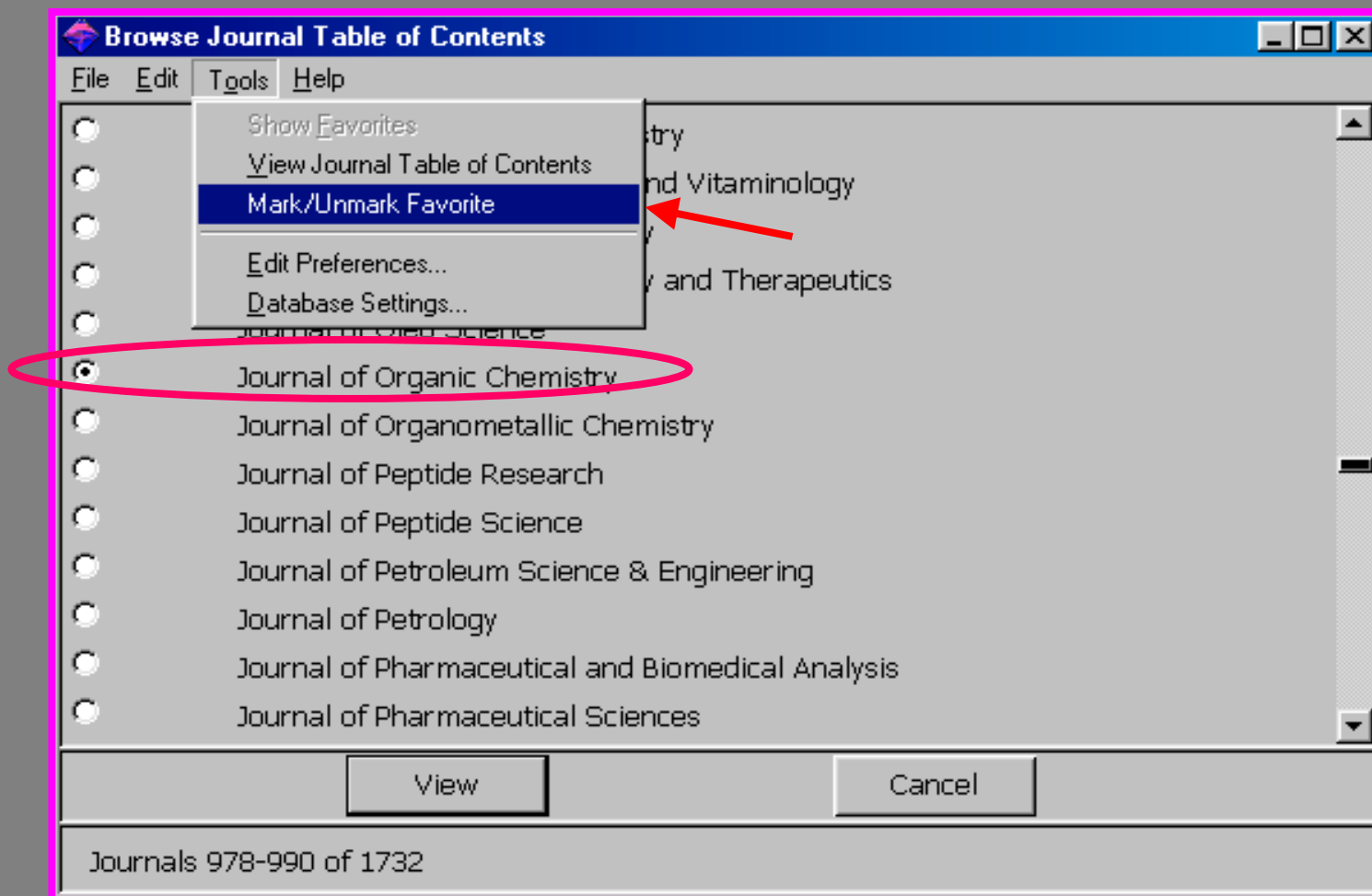
Citations

[1a\) Southern, E; Nat Genet 1999, 21, 5](#)
[1b\) Strick, T; Prog Biophys Mol Biol 2000, 74, 115](#)
[1c\) Bustamante, C; Curr Opin Struct Biol 2000, 10, 279](#)
[2a\) Cocco, S; Proc Natl Acad Sci U S A 2001, 98, 8608](#)
[2b\) Olson, W; Curr Opin Struct Biol 2000, 10, 286](#)
[2c\) Qian, H; Biophys J 1999, 76, 1598](#)
[2d\) Stigter, D; Biophys J 1998, 75, 1197](#)
[2e\) Nelson, P; Phys Rev Lett 1998, 80, 5810](#)
[3a\) Bhattacharya, P; J Am Chem Soc 2001, 123, 8649](#)

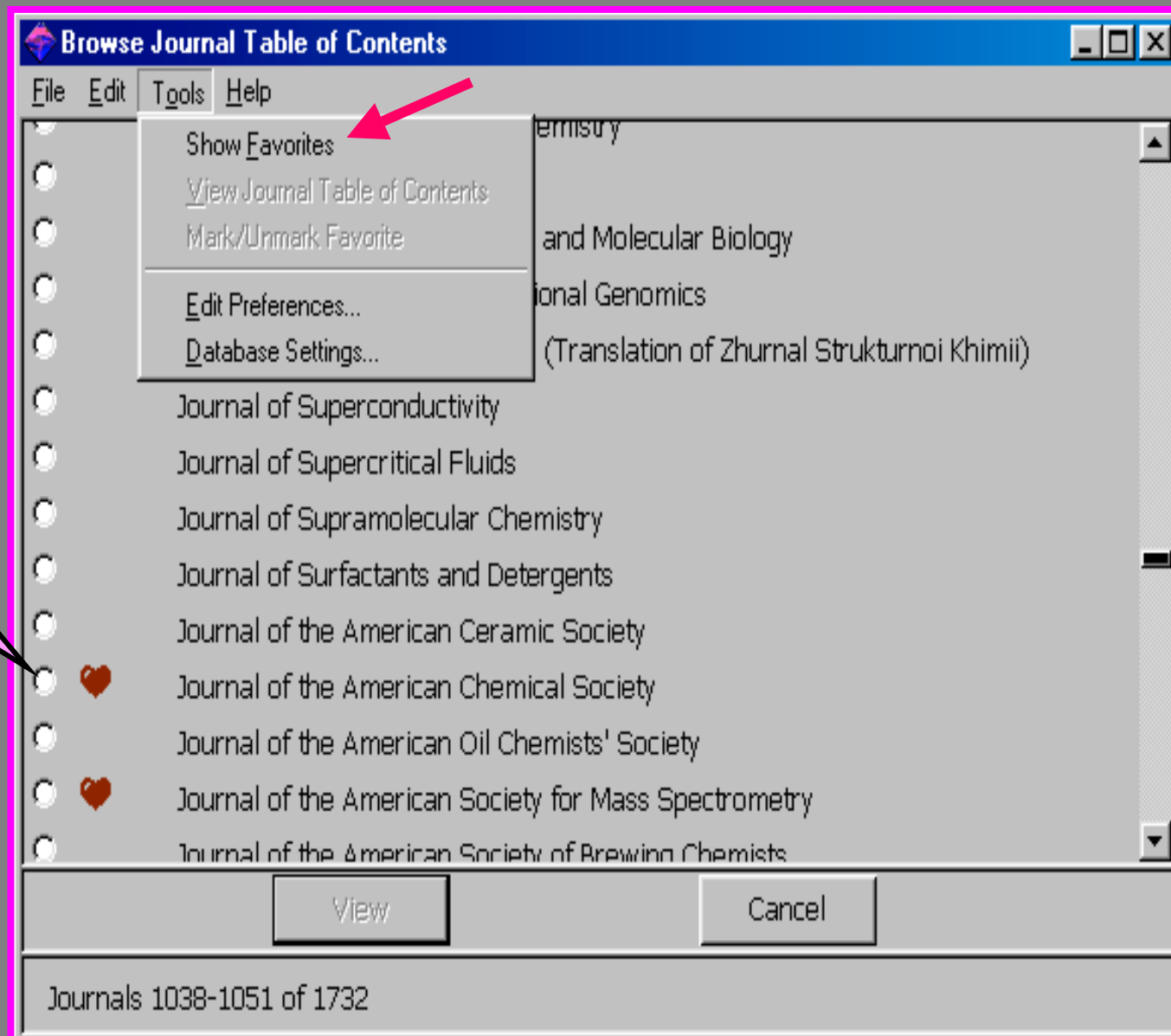
Get Related... Close

Link to
Full text

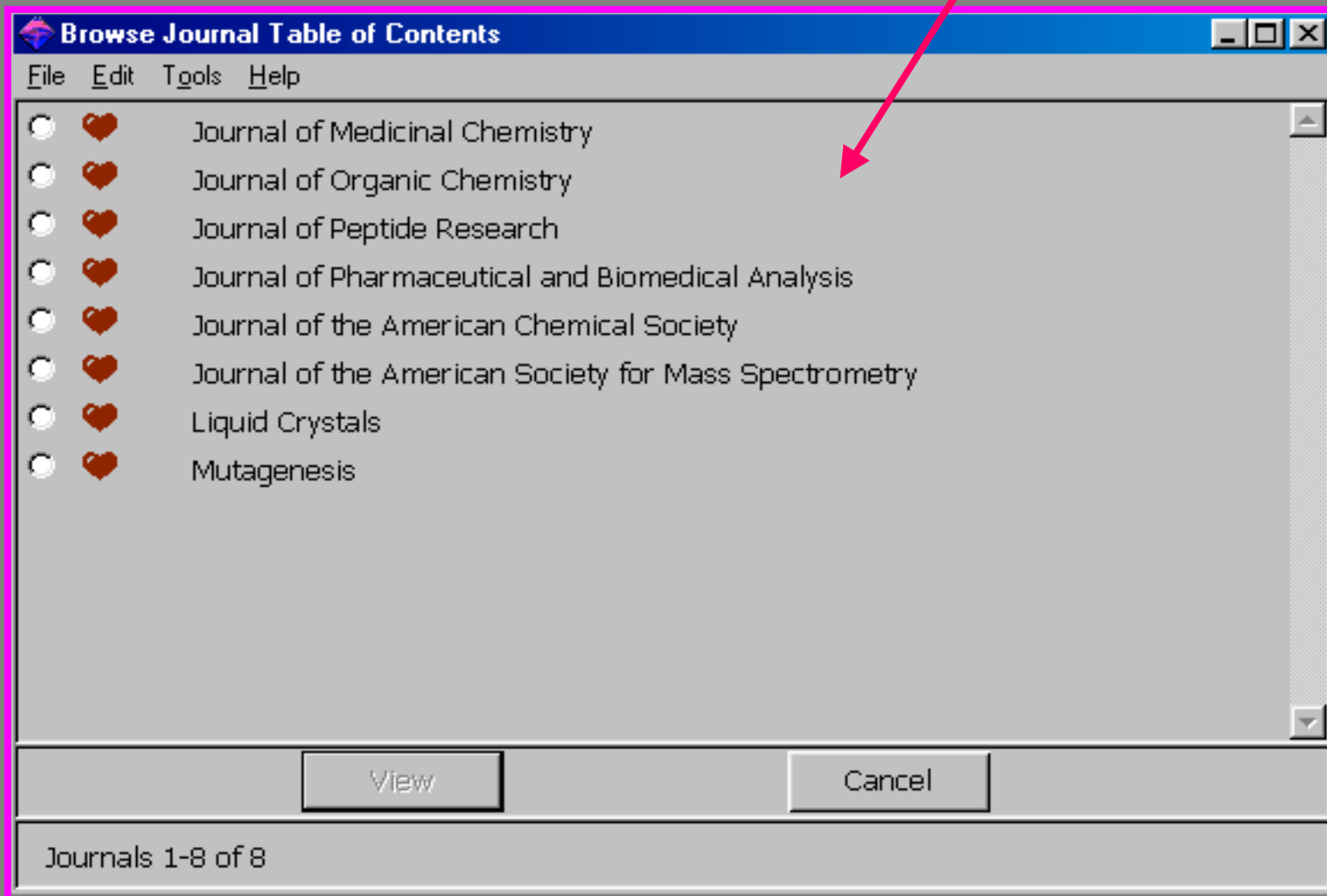
Mark to see only my favorite journal

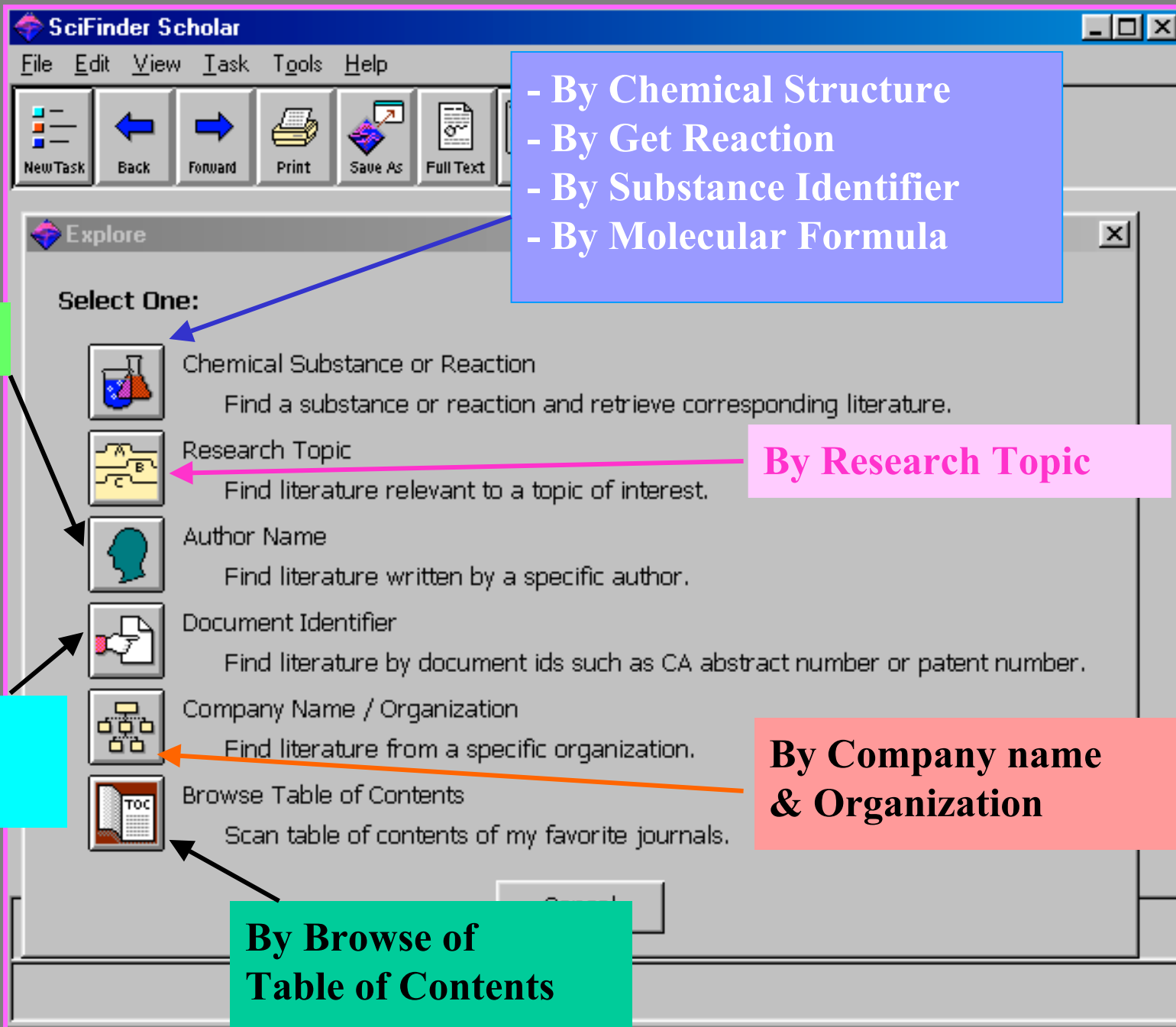


Here is my
favorite
journal!



View all my favorite journals!

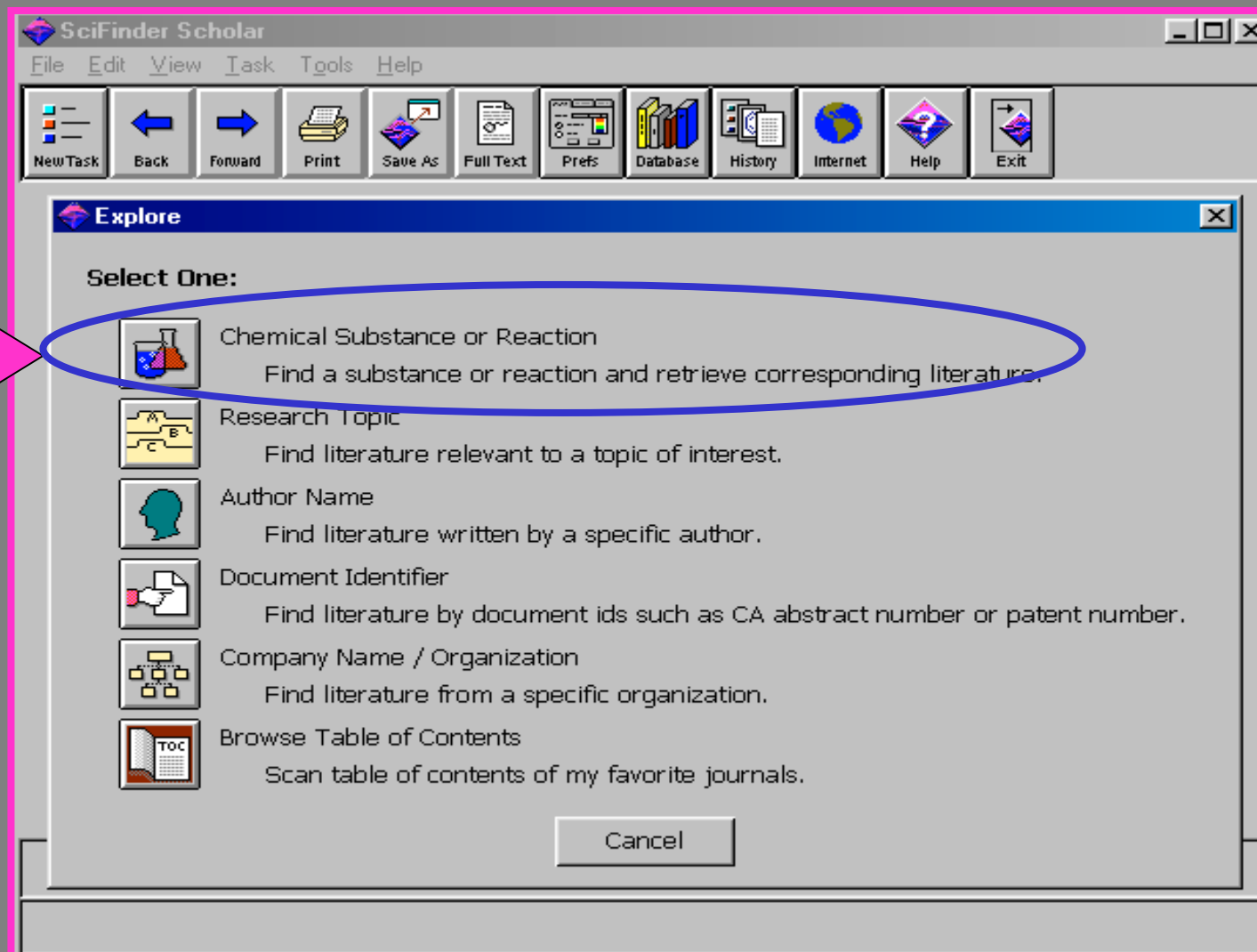




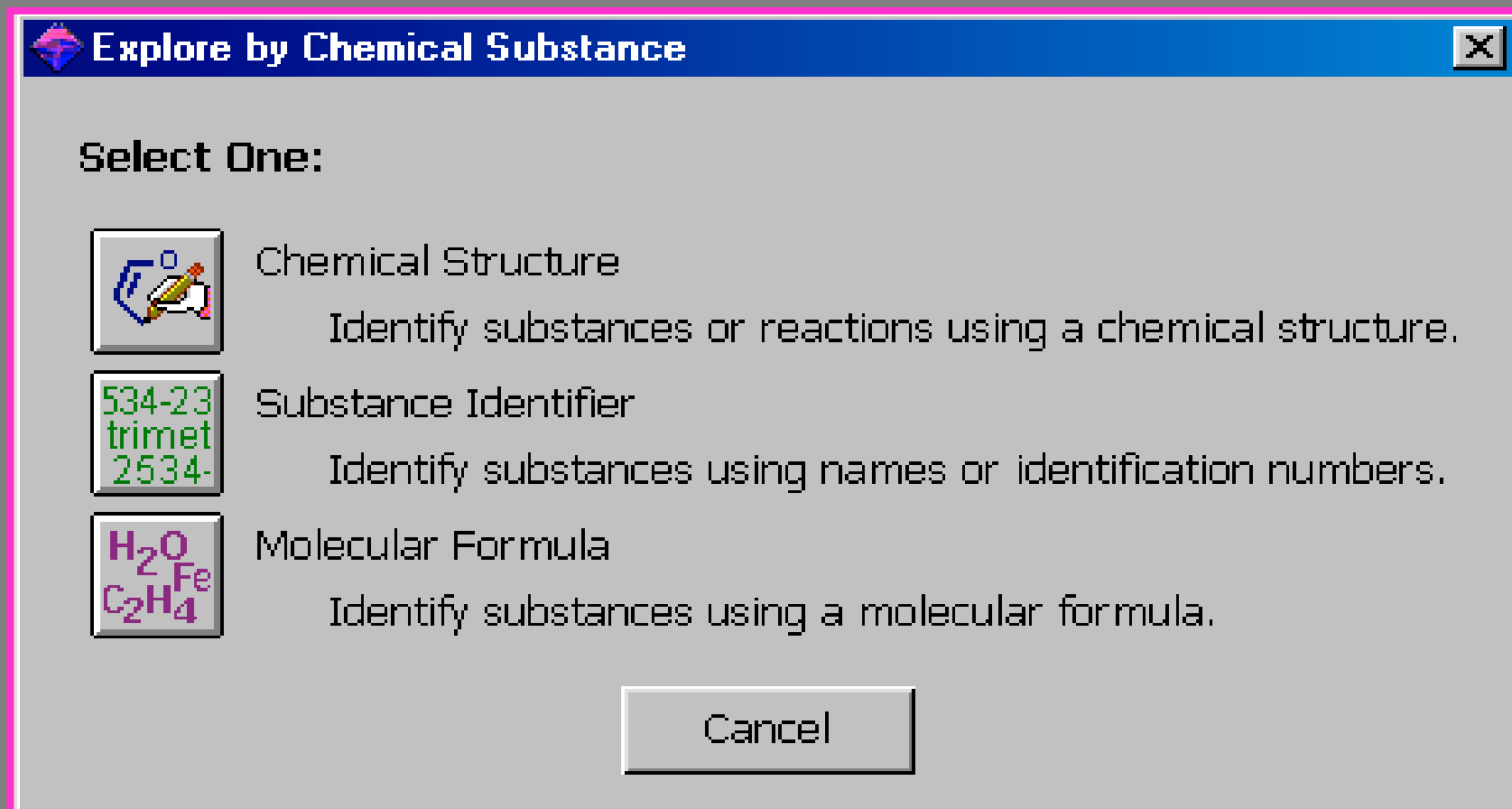
Next

Explore
by
chemical substances and reaction

Search by chemical substance and reaction

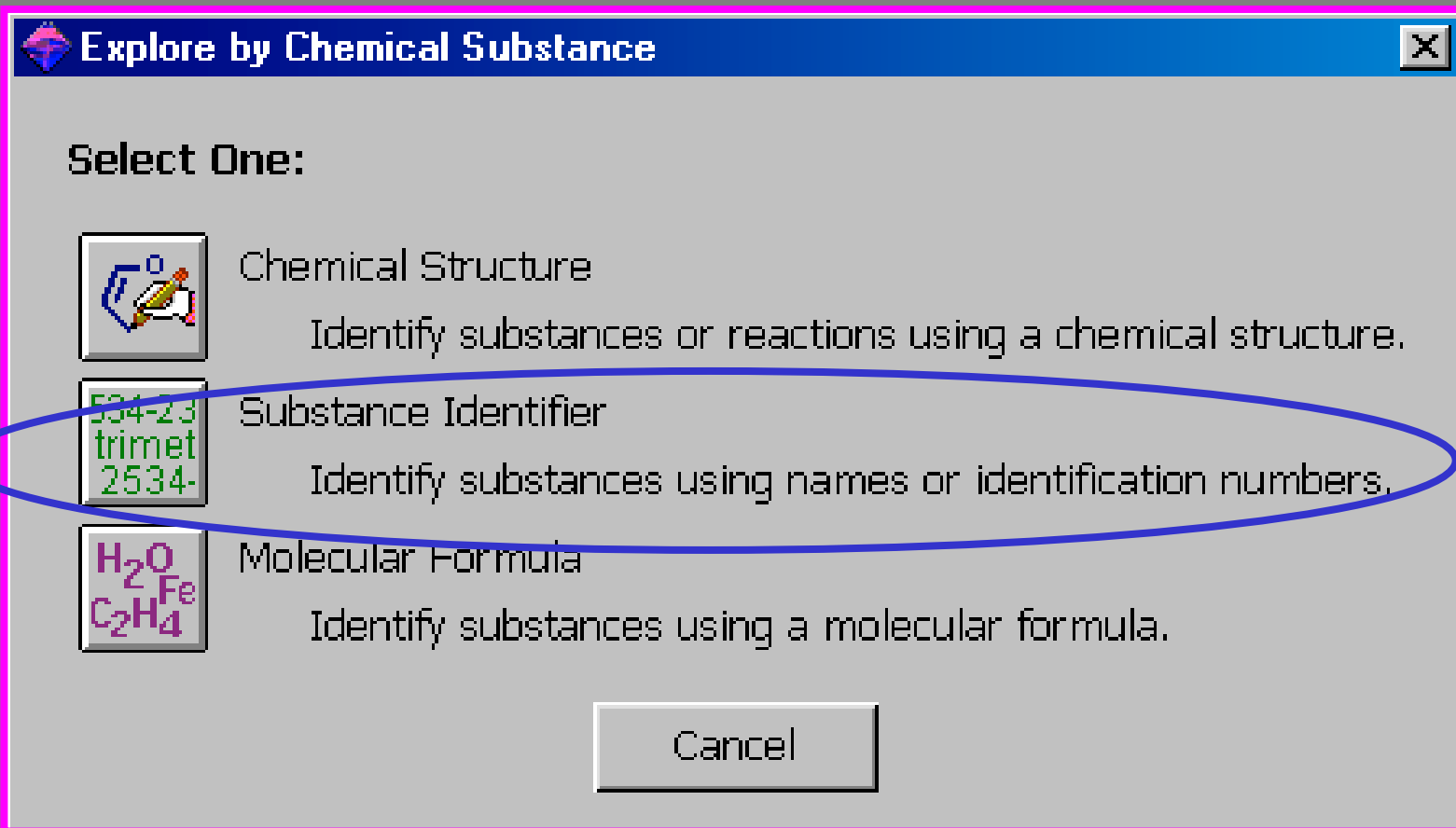


Three options to explore by chemical substance




Explore
by
Substance identifier

Explore by Substance Identifier



Enter Substance Identifier

 **Explore by Substance Identifier** _ □ ×

Enter Substance Identifiers, one per line. Read from file ...

15687-27-1|

A Substance Identifier is any name or number used to denote a specific substance.

Examples:

- 50-00-0
- 999815
- Acetaminophen
- 1,4-dichlorobenzene

OK Cancel



15687-27-1

CC(C)C1=CC=C(C=C1)C(C)C(=O)O

~5901 References
REGISTRY

Get References Analyze or Refine Substances Back

View References

The screenshot displays the SciFinder Scholar web application interface. At the top, there is a menu bar with 'File', 'Edit', 'View', 'Task', 'Tools', and 'Help'. Below the menu is a toolbar with icons for 'New Task', 'Back', 'Forward', 'Print', 'Save As', 'Full Text', 'Prefs', 'Database', 'History', 'Internet', 'Help', and 'Exit'. The main content area shows a search result for the chemical structure of 2-methylbenzoic acid, with the identifier '5687-27-1' and '~5901 References' displayed in a yellow box. A red arrow points to the 'View References' icon (a document with a magnifying glass) in the top-left corner of the result panel. Below the chemical structure, the text '~5901 References' and 'REGISTRY' is visible. At the bottom of the interface, there are three buttons: 'Get References', 'Analyze or Refine Substances', and 'Back'. The status bar at the very bottom indicates 'Substance 1 of 1'.

SciFinder Scholar

File Edit View Task Tools Help

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

5687-27-1
~5901 References

Cc1ccccc1C(=O)O

~5901 References
REGISTRY

Get References Analyze or Refine Substances Back

Substance 1 of 1



15687-27-1

CC(O)C1=CC=C(C=C1)C

~5901 References
REGISTRY

Get References

For this substance, retrieve:

All references References associated with:

<input type="checkbox"/> Adverse Effect, including Toxicity	<input type="checkbox"/> Occurrence
<input type="checkbox"/> Analytical Study	<input type="checkbox"/> Preparation
<input type="checkbox"/> Biological Study	<input type="checkbox"/> Process
<input type="checkbox"/> Combinatorial Study	<input type="checkbox"/> Properties
<input type="checkbox"/> Crystal Structure	<input type="checkbox"/> Reactant or Reagent
<input type="checkbox"/> Formation, nonpreparative	<input type="checkbox"/> Spectral Properties
<input type="checkbox"/> Miscellaneous	<input type="checkbox"/> 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

Here are the desired references

SciFinder Scholar

File Edit View Task Tools Help

NewTask Back Forward Print Save As Full Text Prefs Database History Internet Help Exit

- Shan, Zixing. **Method for preparation (S)-ibuprofen.** Faming Zhuanli Shenqing Gongkai Shuomingshu (2001), 7 pp. CODEN: CNXXEV CN 1326921 A 20011219 AN 2003:130732 CAPLUS
- Jamali, Fahkreddin. **NSAIDs composition containing tartaric acid.** U.S. Pat. Appl. Publ. (2003), 14 pp., Cont.-in-part of U.S. Ser. No. 119,313. CODEN: USXXCO US 20030026834 A1 20030206 AN 2003:97817 CAPLUS
- Stephens, James Matthew. **Method and kit for making interfering substances in urine undetectable.** U.S. Pat. Appl. Publ. (2003), 5 pp. CODEN: USXXCO US 20030022390 A1 20030130 AN 2003:77470 CAPLUS
- Hauer, Norbert; Wienen, Wolfgang. **Use of thrombin inhibitors for the treatment of arthritis.** PCT Int. Appl. (2003), 25 pp. CODEN: PIXXD2 WO 0307984 A1 20030130 AN 2003:76643 CAPLUS
- Sui, Yanjun; Su, Dongfang; Wang, Hui; Li, Chunli. **Preparation of granular ibuprofen.** Faming Zhuanli Shenqing Gongkai Shuomingshu (2002), 6 pp. CODEN: CNXXEV CN 1330920 A 20020116 CAN 138:95575 AN 2003:74493 CAPLUS
- Shan, Zixing; Wan, Boyong. **Preparation of S-ibuprofen.** Faming Zhuanli Shenqing Gongkai Shuomingshu (2001), 6 pp. CODEN: CNXXEV CN 1318537 A 20011024 CAN 138:73077 AN 2003:62631 CAPLUS
- Abu-Izza, Khawla Abdullah; Raman, Krishna Pattabi; Li, Vincent Hon-Kin; Tongaree, Sauwaluzana. **Mucoadhesive composition comprising polymers.** U.S. Pat. Appl. Publ. (2003), 5 pp. CODEN: USXXCO US 2003017133 A1 20030123 CAN 138:112474 AN 2003:58605 CAPLUS
- Noble, Linda Jeanne; Donovan, Frances Muriel; Werb, Zena. **Use of matrix metalloproteinase inhibitors to mitigate nerve damage.** PCT Int. Appl. (2003), 87 pp. CODEN: PIXXD2 WO 0306006 A1 20030123 CAN 138:117661 AN 2003:57892 CAPLUS
- Horlocker, Terese T.; Bajwa, Zahid H.; Ashraf, Zubaira; Khan, Sajid; Wilson, Jack L.; Sami, Naveed; Peeters-Asdourian, Christine; Powers, Christopher A.; Schroeder, Darrell R.; ...

Analyze or Refine References Get Related... Back

References 1-9 of 9737

View 3D Structure

The screenshot displays the SciFinder Scholar web application interface. At the top, there is a menu bar with options: File, Edit, View, Task, Tools, and Help. Below the menu is a toolbar containing icons for New Task, Back, Forward, Print, Save As, Full Text, Prefs, Database, History, Internet, Help, and Exit. The main content area shows a search result for the chemical structure of 2-methylbutanoic acid, with the identifier 15687-27. A yellow box labeled "3D Model" is positioned above the chemical structure, and a red arrow points to it. Below the structure, it indicates "~5901 References" and "REGISTRY". At the bottom of the interface, there are three buttons: "Get References", "Analyze or Refine Substances", and "Back". The status bar at the very bottom shows "Substance 1 of 1".

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

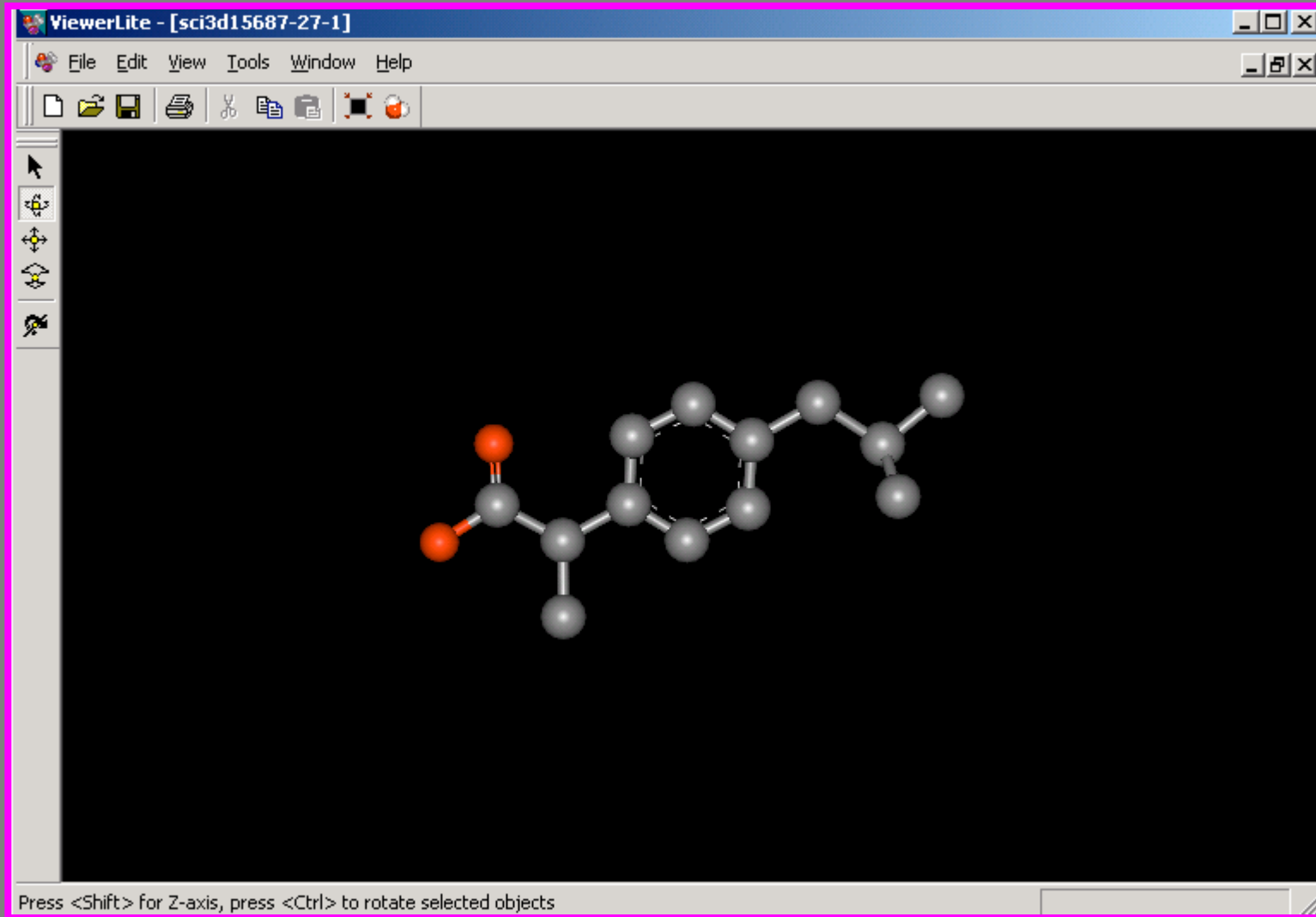
3D Model

CC(C)C(=O)O

~5901 References
REGISTRY

Get References Analyze or Refine Substances Back

Substance 1 of 1



View Commercial Sources

The screenshot displays the SciFinder Scholar web application interface. At the top, the title bar reads "SciFinder Scholar" and the menu bar includes "File", "Edit", "View", "Task", "Tools", and "Help". Below the menu is a toolbar with icons for "NewTask", "Back", "Forward", "Print", "Save As", "Full Text", "Prefs", "Database", "History", "Internet", "Help", and "Exit".

The main content area shows a search result for the chemical structure of 2-methylbenzoic acid. The structure is represented by a benzene ring with a carboxylic acid group ($\text{HO}_2\text{C}-\text{CH}$) and a methyl group (Me) attached. Above the structure is the identifier "15687-27-1". A yellow tooltip labeled "Commercial Sources" is positioned over a yellow folder icon, with a red arrow pointing to it from the right. Below the structure, the text reads "~5901 References" and "REGISTRY".

At the bottom of the interface, there are three buttons: "Get References", "Analyze or Refine Substances", and "Back". The status bar at the very bottom indicates "Substance 1 of 1".

Sources for 15687-27-1

File Edit Help

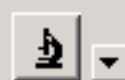
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Quantity: 1 10G
1 1G
1 5G
Publication Date: 15 Jan 2003
Order Number: I4883
Chemical Name: Ibuprofen
Registry Number: 15687-27-1
CHEMCATS



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
Quantity: 1 1MI



Close

Detail of Source 1

File Edit Help

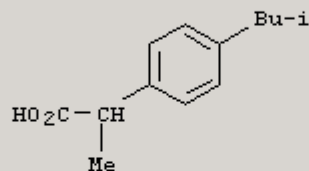
Catalog Name: SIGMA

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

The screenshot displays the SciFinder Scholar web application interface. At the top, there is a menu bar with 'File', 'Edit', 'View', 'Task', 'Tools', and 'Help'. Below the menu is a toolbar with icons for 'NewTask', 'Back', 'Forward', 'Print', 'Save As', 'Full Text', 'Prefs', 'Database', 'History', 'Internet', 'Help', and 'Exit'. The main content area features a search bar with a magnifying glass icon and a dropdown menu with options like 'A+B'. Below the search bar, the identifier '15687-27-1' is displayed. A chemical structure of 4-methylbenzoic acid is shown, with the text '~5901 References' and 'REGISTRY' below it. A red arrow points to the 'Regulated Chemicals Listing' button, which is highlighted in yellow. At the bottom of the interface, there are three buttons: 'Get References', 'Analyze or Refine Substances', and 'Back'. The status bar at the very bottom indicates 'Substance 1 of 1'.

SciFinder Scholar

File Edit View Task Tools Help

NewTask Back Forward Print Save As Full Text Prefs Database History Internet Help Exit

15687-27-1

Regulated Chemicals Listing

CC(C(=O)O)C1=CC=CC=C1

~5901 References
REGISTRY

Get References Analyze or Refine Substances Back

Substance 1 of 1

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)
(\pm)- α -Methyl-4-(2-methylpropyl)benzeneacetic acid
(\pm)-2-(p-Isobutylphenyl)propionic acid
(\pm)-Ibuprofen
(\pm)-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
Hvdratronic acid n-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

The screenshot displays the SciFinder Scholar web application interface. At the top, there is a blue header bar with the SciFinder Scholar logo and a menu bar containing 'File', 'Edit', 'View', 'Task', 'Tools', and 'Help'. Below the menu bar is a toolbar with various icons for navigation and actions: 'NewTask', 'Back', 'Forward', 'Print', 'Save As', 'Full Text', 'Prefs', 'Database', 'History', 'Internet', 'Help', and 'Exit'. The main content area features a search results card for the compound 15687-27-1. The card includes a chemical structure of 2-(4-iodophenyl)acetic acid, the text '15687-27-1', and a yellow callout box with a red arrow pointing to the 'Reaction Information' button. Below the structure, it states '~5901 References' and 'REGISTRY'. At the bottom of the interface, there are three buttons: 'Get References', 'Analyze or Refine Substances', and 'Back'. The status bar at the very bottom indicates 'Substance 1 of 1'.

SciFinder Scholar

File Edit View Task Tools Help

NewTask Back Forward Print Save As Full Text Prefs Database History Internet Help Exit

15687-27-1

Reaction Information

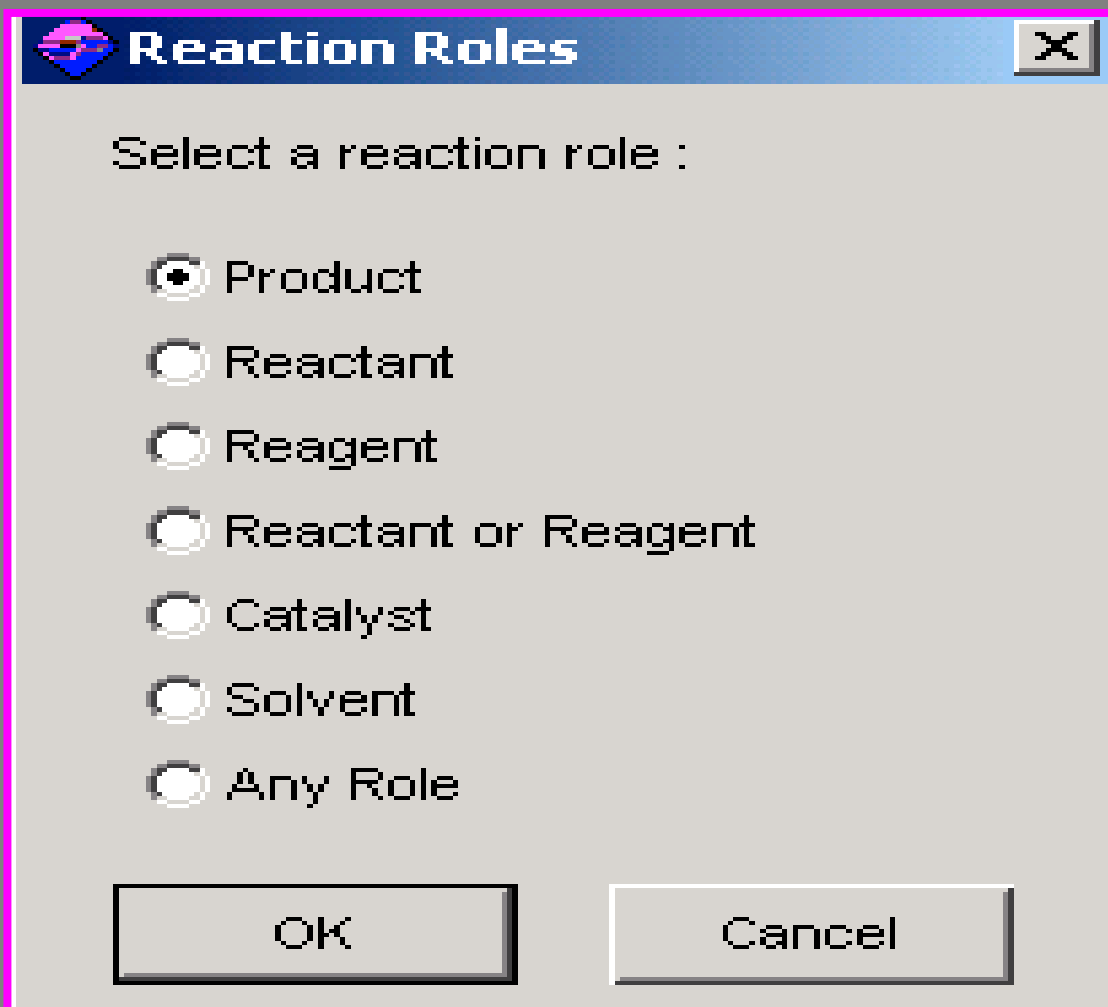
CC(O)Cc1ccc(I)cc1

~5901 References
REGISTRY

Get References Analyze or Refine Substances Back

Substance 1 of 1

Select a reaction role



The image shows a software dialog box titled "Reaction Roles". The title bar is blue with a small icon on the left and a close button (X) on the right. The main area is light gray and contains the text "Select a reaction role :". Below this text is a list of seven radio button options: "Product", "Reactant", "Reagent", "Reactant or Reagent", "Catalyst", "Solvent", and "Any Role". The "Product" option is selected, indicated by a small black dot in the center of the radio button. At the bottom of the dialog are two buttons: "OK" and "Cancel".

Reaction Roles

Select a reaction role :

- Product
- Reactant
- Reagent
- Reactant or Reagent
- Catalyst
- Solvent
- Any Role

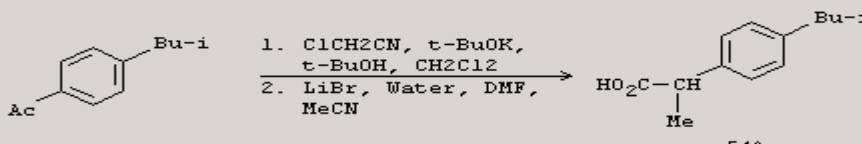
OK Cancel

Link to view reference of desired reaction

SciFinder Scholar

File Edit View Task Tools Help

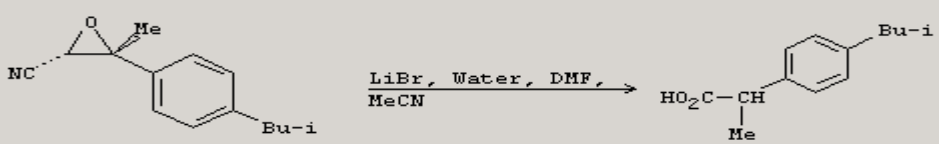
NewTask Back Forward Print Save As Full Text Prefs Database History Internet Help Exit



NOTE: 1) 73% overall yield, 2) SAFETY (HCN evolved during reaction - precautions for handling of cyanide necessary), KEY STEP

Reference: [Journal of Organic Chemistry, 67\(15\), 5440-5443, 2002](#)

Database: CASREACT



Representative Stereoisomer

NOTE: SAFETY (HCN evolved during reaction - precautions for handling of cyanide necessary), KEY STEP

Reference: [Journal of Organic Chemistry, 67\(15\), 5440-5443, 2002](#)

Database: CASREACT

Get References Refine Reactions Back

Reactions 2-5 of 197

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-arylcyano-cyclohexanecarboxylic acid SB-207499 (a potential agent in the treatment of chronic 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

Explore by Chemical Substance

Select One:



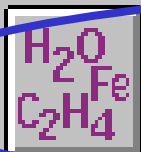
Chemical Structure

Identify substances or reactions using a chemical structure.



Substance Identifier

Identify substances using names or identification numbers.

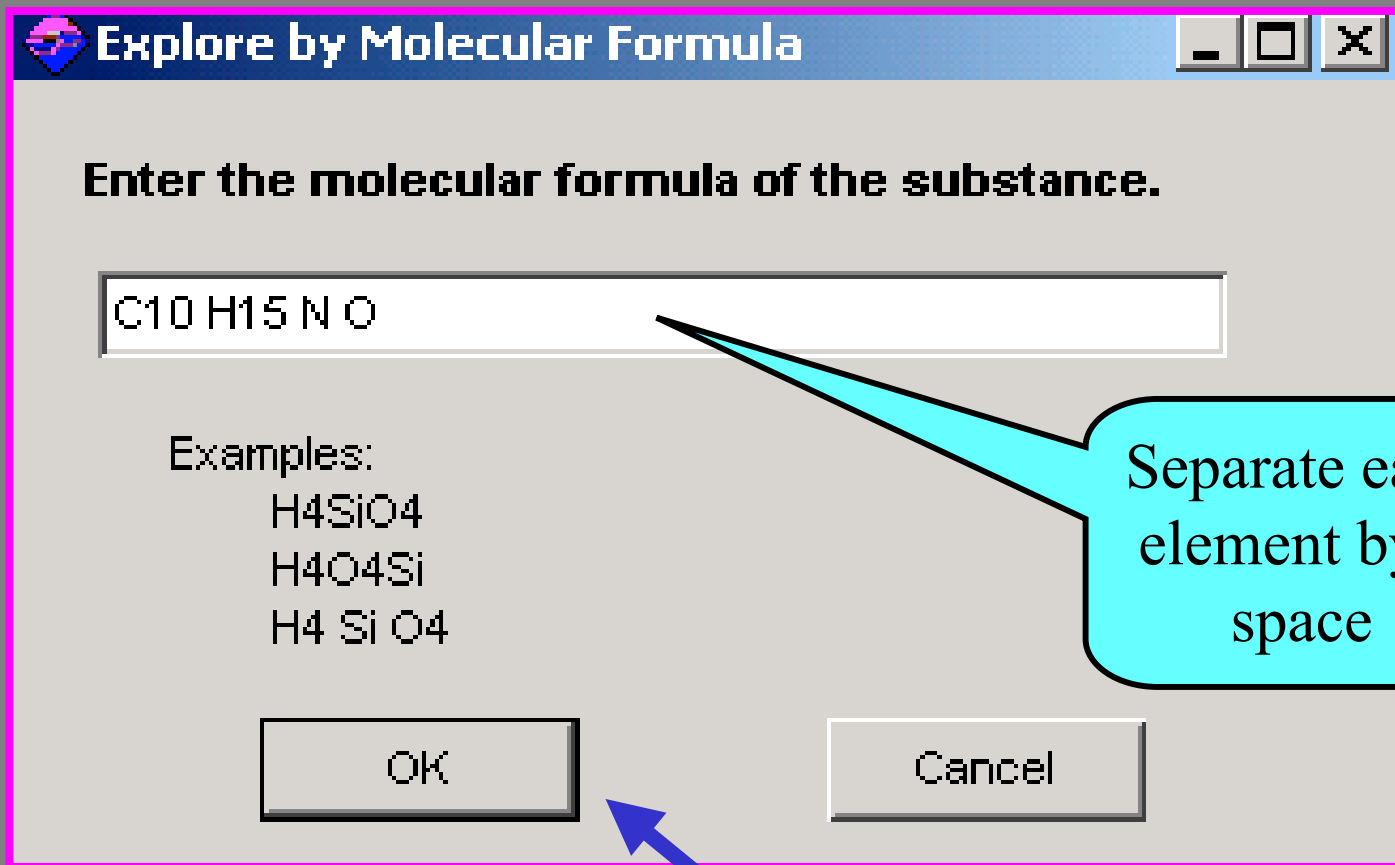


Molecular Formula

Identify substances using a molecular formula.

Cancel

Enter the molecular formula of the substance

A dialog box titled "Explore by Molecular Formula" with a blue header bar. It contains a text input field with "C10 H15 N O", a list of examples, and "OK" and "Cancel" buttons. A cyan callout bubble points to the input field, and a blue arrow points to the "OK" button.

Explore by Molecular Formula

Enter the molecular formula of the substance.

C10 H15 N O

Examples:
H4SiO4
H4O4Si
H4 Si O4

OK Cancel

Separate each element by a space

Here are the substances retrieved!

SciFinder Scholar

File Edit View Task Tools Help

NewTask Back Forward Print Save As Full Text Prefs Database History Internet Help Exit

444160-91-2
CC1=CC=C(C=C1)C(O)CNC(C)C
[3D Model](#)
~1 Reference REGISTRY

443983-53-7
CC1=CC=C(C=C1)C(O)CNC(C)C
[3D Model](#)
~1 Reference REGISTRY

443983-24-2
CC1=CC=C(C=C1)C(O)CNC(C)C
[3D Model](#)
~1 Reference REGISTRY

442910-80-7
CC1=CC=C(C=C1)C(O)CNC(C)C
[3D Model](#)
~1 Reference REGISTRY

439688-80-9
CC1=CC=C(C=C1)C(O)CNC(C)C
[3D Model](#)
~1 Reference REGISTRY

438245-97-7
CC1=CC=C(C=C1)C(O)CNC(C)C
[3D Model](#)
~1 Reference REGISTRY

437702-27-7
CC1=CC=C(C=C1)C(O)CNC(C)C
[3D Model](#)
~1 Reference REGISTRY

436088-33-4
CC1=CC=C(C=C1)C(O)CNC(C)C
[3D Model](#)
~1 Reference REGISTRY

433301-78-1
CC1=CC=C(C=C1)C(O)CNC(C)C
[3D Model](#)
~1 Reference REGISTRY

Get References Analyze or Refine Substances Back

Substances 1-9 of 2039

2039
substances

Narrow down answer set

The screenshot displays the SciFinder Scholar software interface. At the top, there is a menu bar with 'File', 'Edit', 'View', 'Task', 'Tools', and 'Help'. Below the menu is a toolbar with icons for 'New Task', 'Back', 'Forward', 'Print', 'Save As', 'Full Text', 'Prefs', 'Database', 'History', 'Internet', 'Help', and 'Exit'. The main area is a grid of search results, each containing a chemical structure and a reference count. A dialog box titled 'Analyze or Refine' is open in the center, with the following options:

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

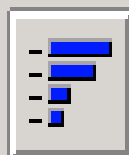
A red arrow points to the 'Analyze or Refine Substances' button at the bottom of the interface. The status bar at the bottom left shows 'Substances 1-9 of 2039'.



Analyze or Refine

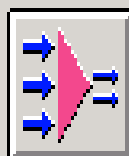


Select One:



Analyze

Display histograms by Precision, Ring Skeletons, etc.



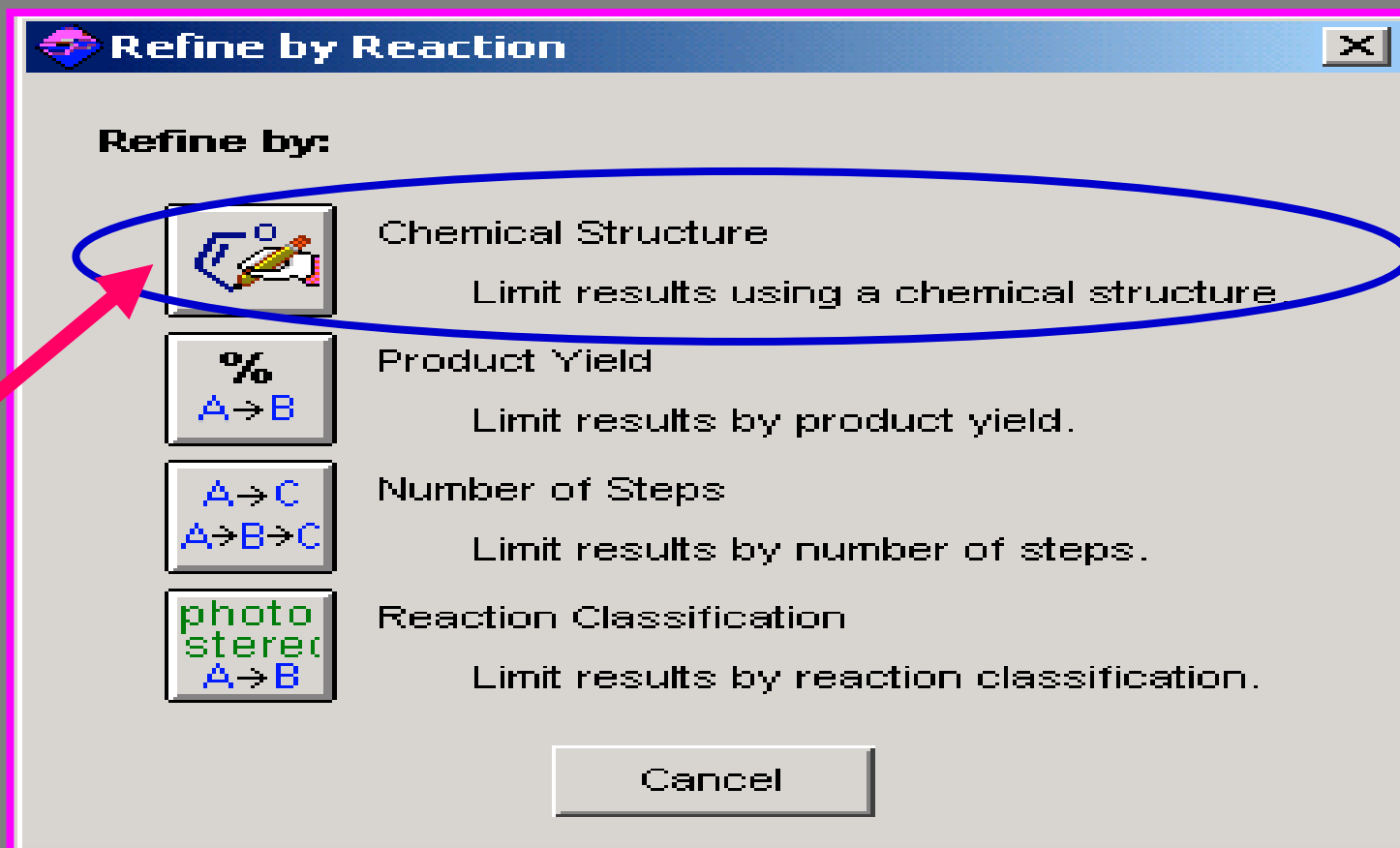
Refine

Narrow your answer set by Structure, Availability, or Property Data.

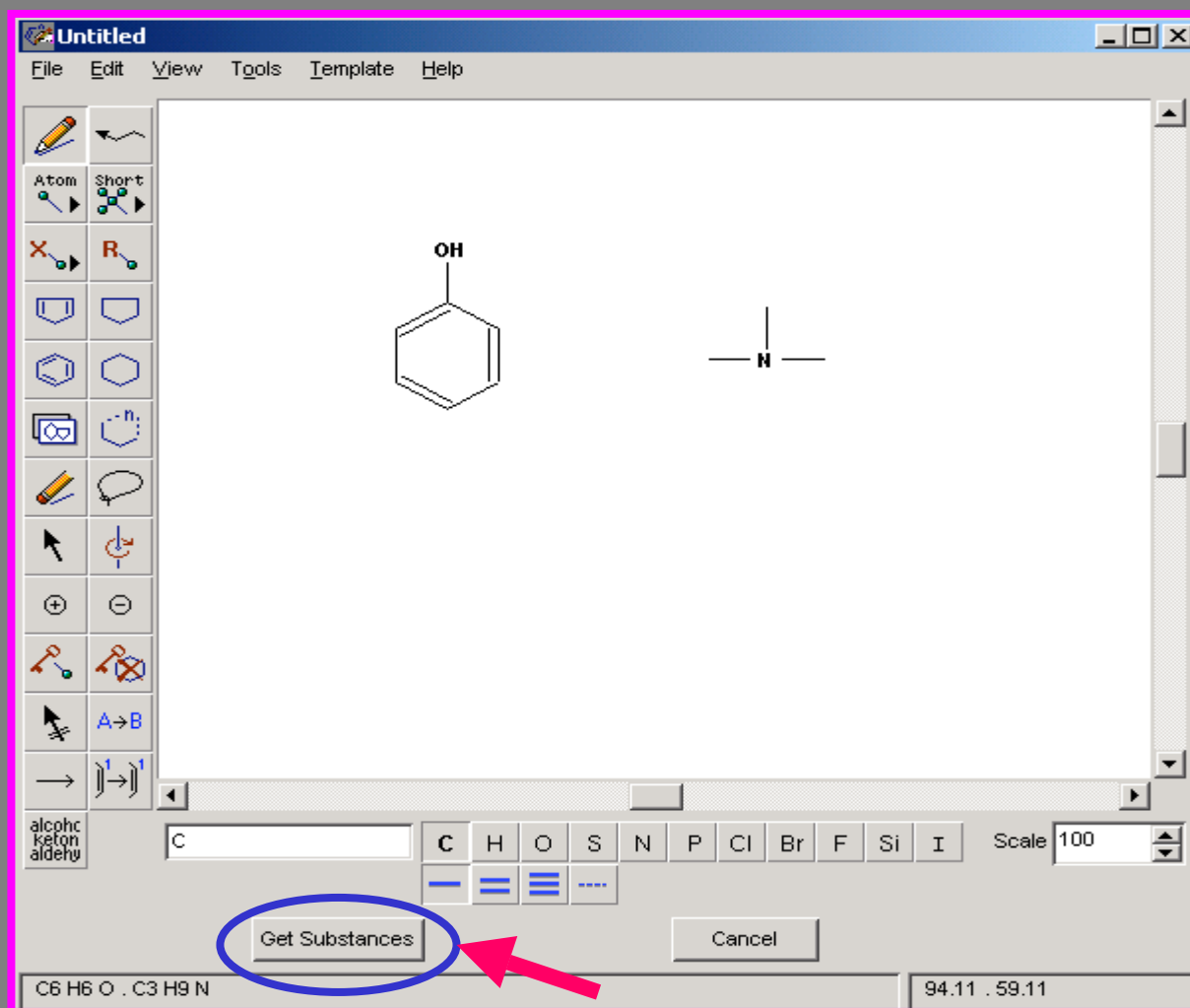


Cancel

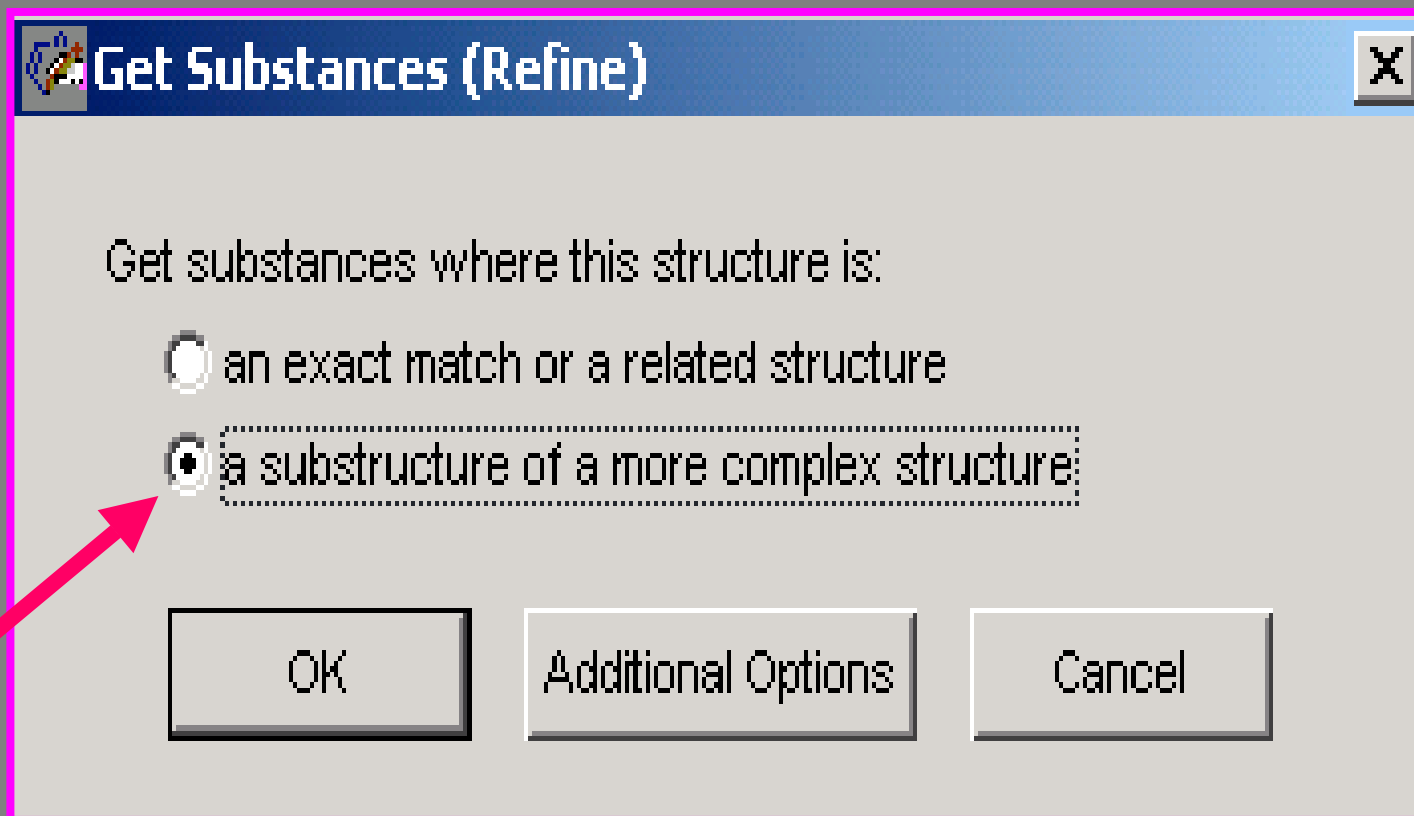
Let's refine reaction by chemical structure



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

SciFinder Scholar

File Edit View Task Tools Help

NewTask Back Forward Print Save As Full Text Prefs Database History Internet Help Exit

194930-11-5
CN(C)c1ccc(O)cc1C(S)C
[3D Model](#)
~1 Reference
REGISTRY

194930-03-5
CN(C)C1=CC=C(O)C=C1C2=CC=CC=C2C3=CC=CC=C3
[3D Model](#)
~1 Reference
REGISTRY

139306-10-8
CN(C)S(C)c1ccc(O)cc1
[3D Model](#)
[Commercial Sources](#)
~3 References
REGISTRY

105601-04-5
CN(C)C(C)C1=CC=C(O)C=C1
[3D Model](#)
[Commercial Sources](#)
~7 References
REGISTRY

88053-63-8
CN(C)C(C)C1=CC=C(O)C=C1
[3D Model](#)
~1 Reference
REGISTRY

86796-90-9
CN(C)C(C)C1=CC=C(O)C=C1
[3D Model](#)
~1 Reference
REGISTRY

Get References Analyze or Refine Substances Back

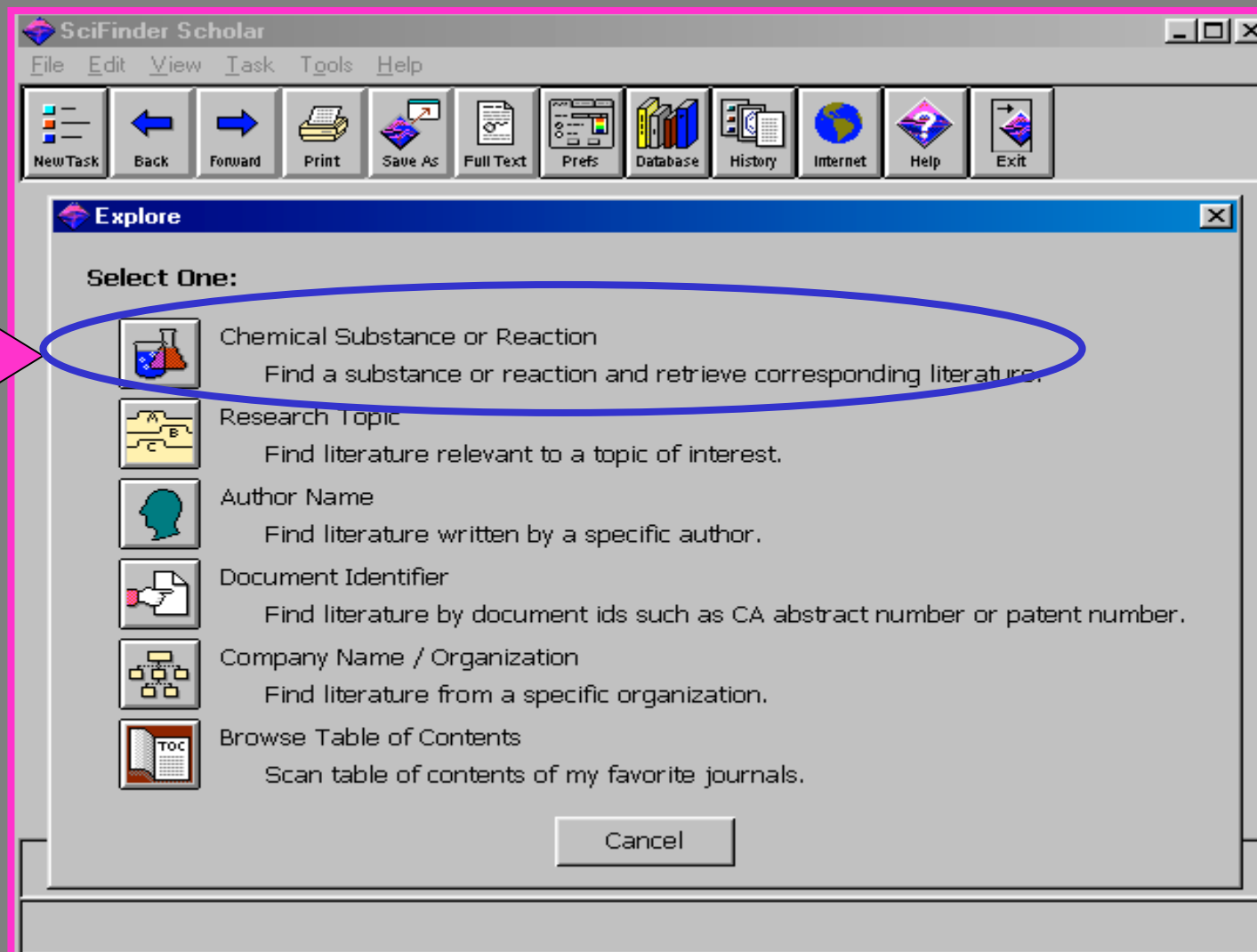
Substances 1-6 of 17

17
substances

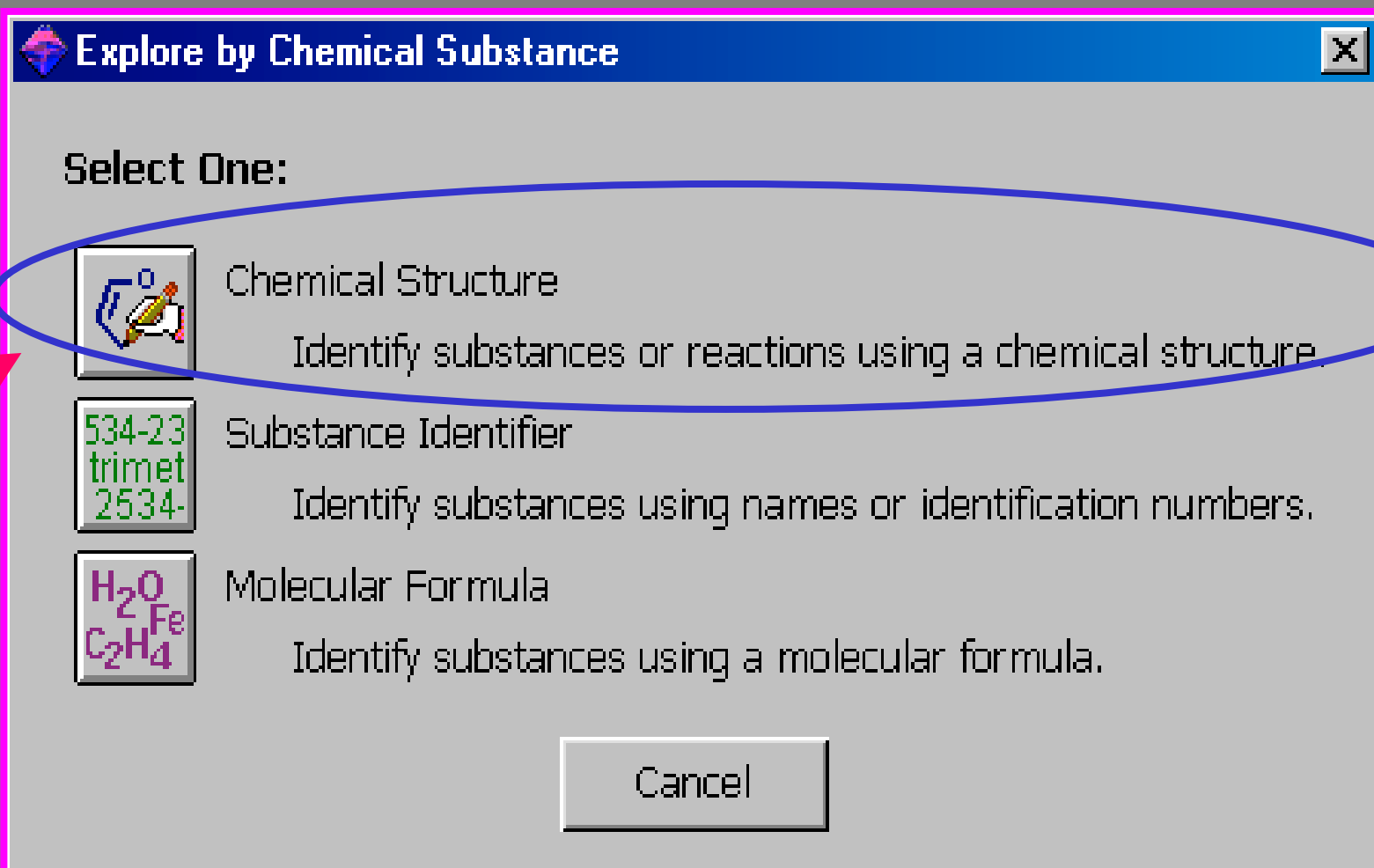
Next

Explore by Chemical structure

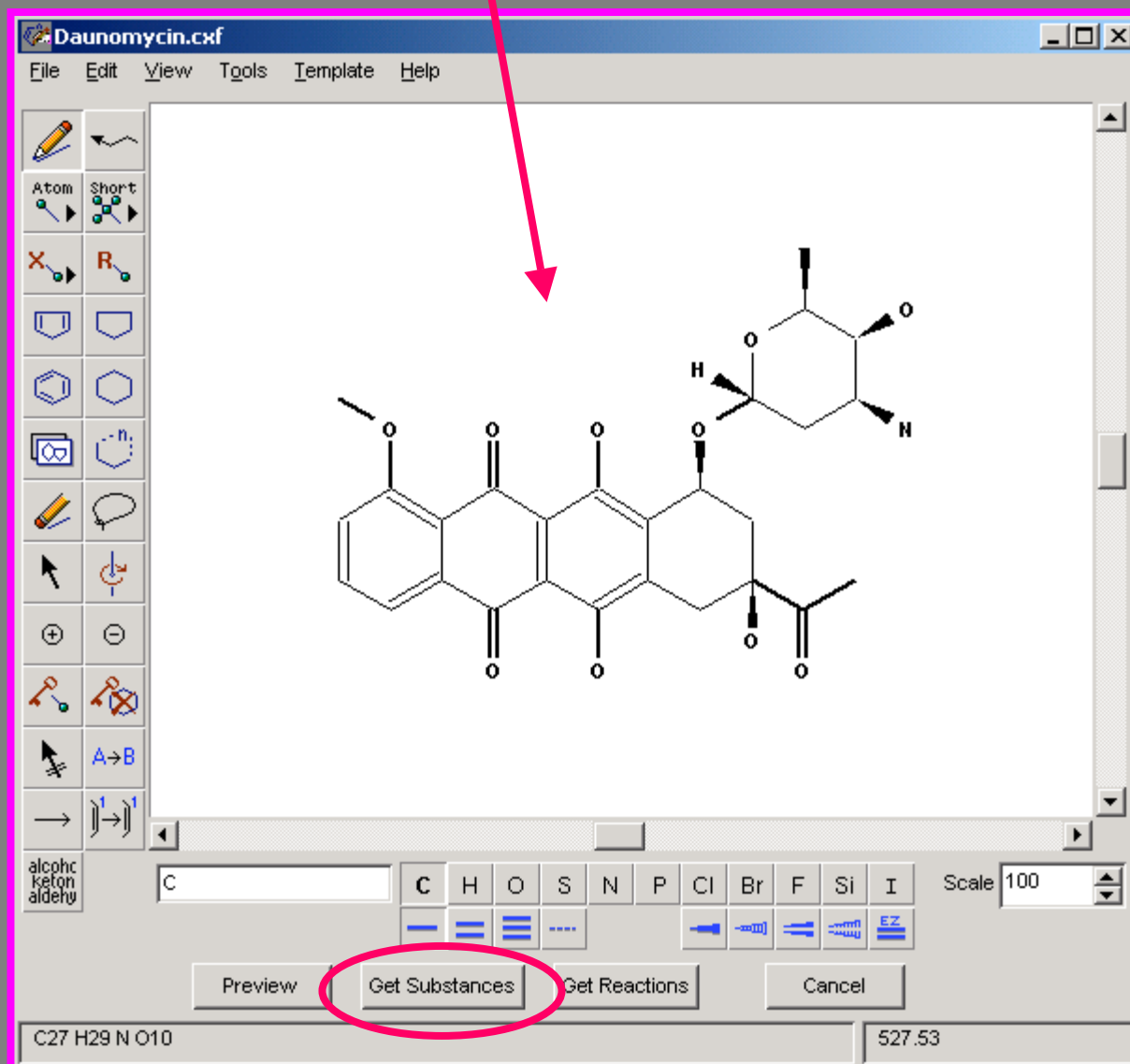
Search by chemical substance and reaction

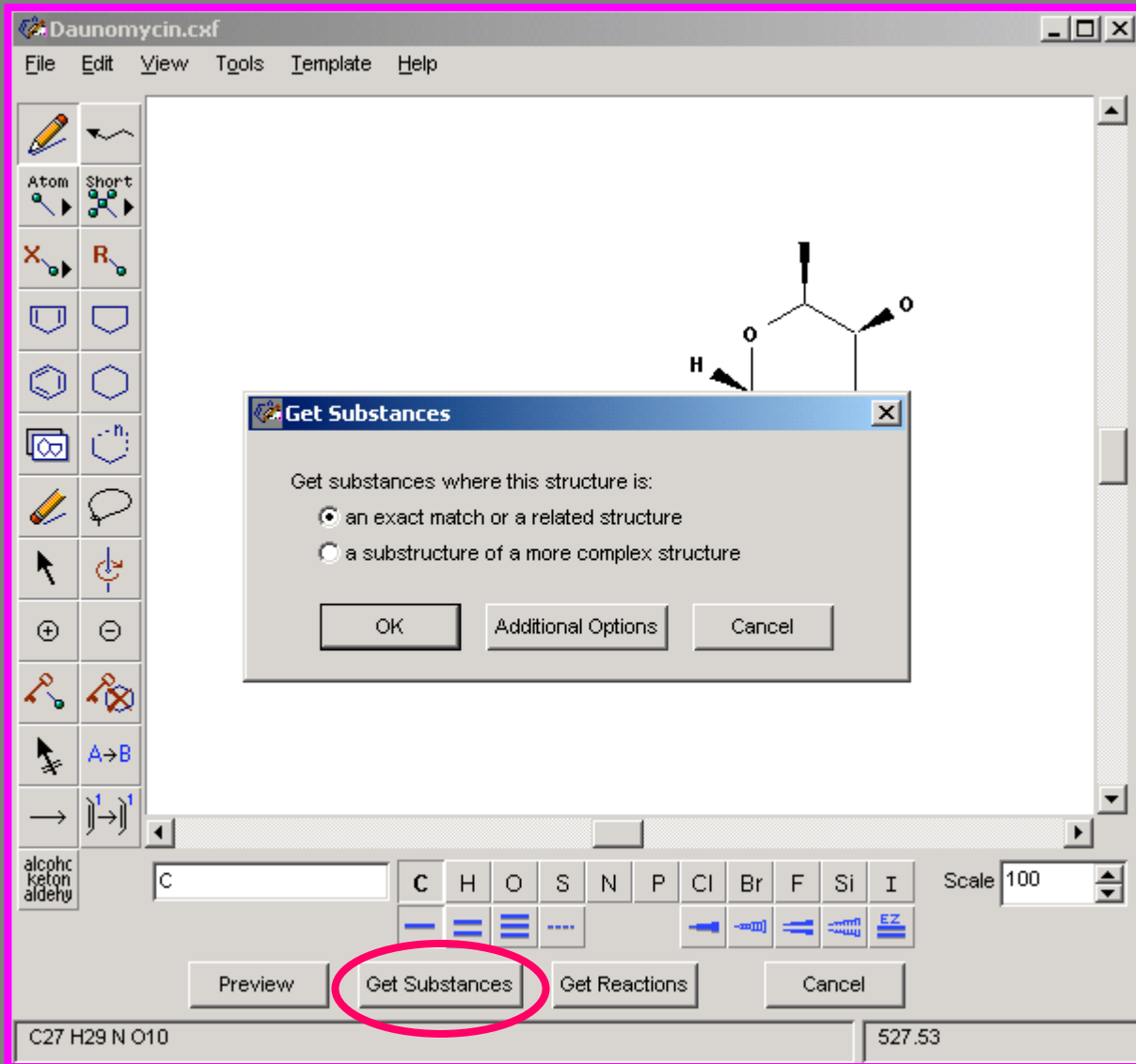


Explore by Chemical Structure



Draw chemical structure of interest







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

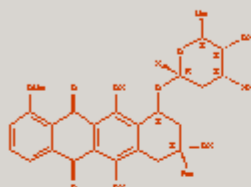
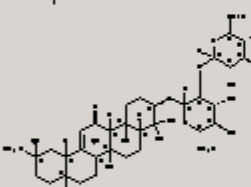
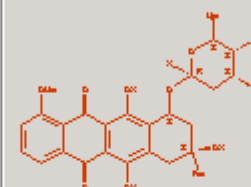

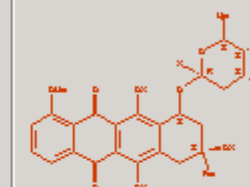
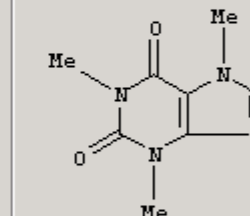
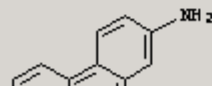


Cancel

Stereo Analysis

The screenshot shows the 'Stereo Analysis' software window. The title bar reads 'Stereo Analysis' and the menu bar includes 'File', 'Edit', 'Task', 'Tools', and 'Help'. The main area is titled 'Select Histogram Entries of interest:' and contains a list of five entries. Each entry has a checkbox, a blue bar chart representing its frequency, and a numerical value. A red arrow points to the first entry, 'Absolute stereo match', which is checked. At the bottom, there are two buttons: 'Get Substances' and 'Back'. A status bar at the very bottom indicates 'Histogram Entries 1-5 of 5'.

Entry	Count
<input checked="" type="checkbox"/> Absolute stereo match	52
<input type="checkbox"/> Absolute stereo mirror image	1
<input type="checkbox"/> Relative stereo match	0
<input type="checkbox"/> Stereo that doesn't match query	20
<input type="checkbox"/> No stereo in answer structure	4



<p> 495400-71-0</p> <p>Component Number 1</p>  <p>Component Number 2</p>  <p>~1 Reference REGISTRY</p>	<p> 476360-24-4</p> <p>Component Number 1</p>  <p>Component Number 2</p>  <p>~1 Reference REGISTRY</p>	<p> 439668-52-7</p> <p>Component Number 1</p>  <p>Component Number 2</p>  <p>~1 Reference REGISTRY</p>
<p> 439665-99-3</p> <p>Component Number 1</p> 	<p> 390755-64-3</p> <p>Component Number 1</p> 	<p> 390755-63-2</p> <p>Component Number 1</p> 
Get References	Analyze or Refine Substances	Back

Get reaction containing this substance

The screenshot shows the ChemDraw software interface with the 'Get Reactions - Role Definition' dialog box open. The dialog box contains the following text and options:

Get Reactions where this structure is:

- a Product
- a Reactant
- a Reagent
- a Reactant or a Reagent
- Anywhere in the reaction

Buttons: OK, Cancel

The main window shows a chemical structure of a substituted piperidine ring. The 'Get Reactions' button at the bottom of the main window is circled in red.

alcoh
keton
aldehy


C

C H O S N P Cl Br F Si I

Scale 100

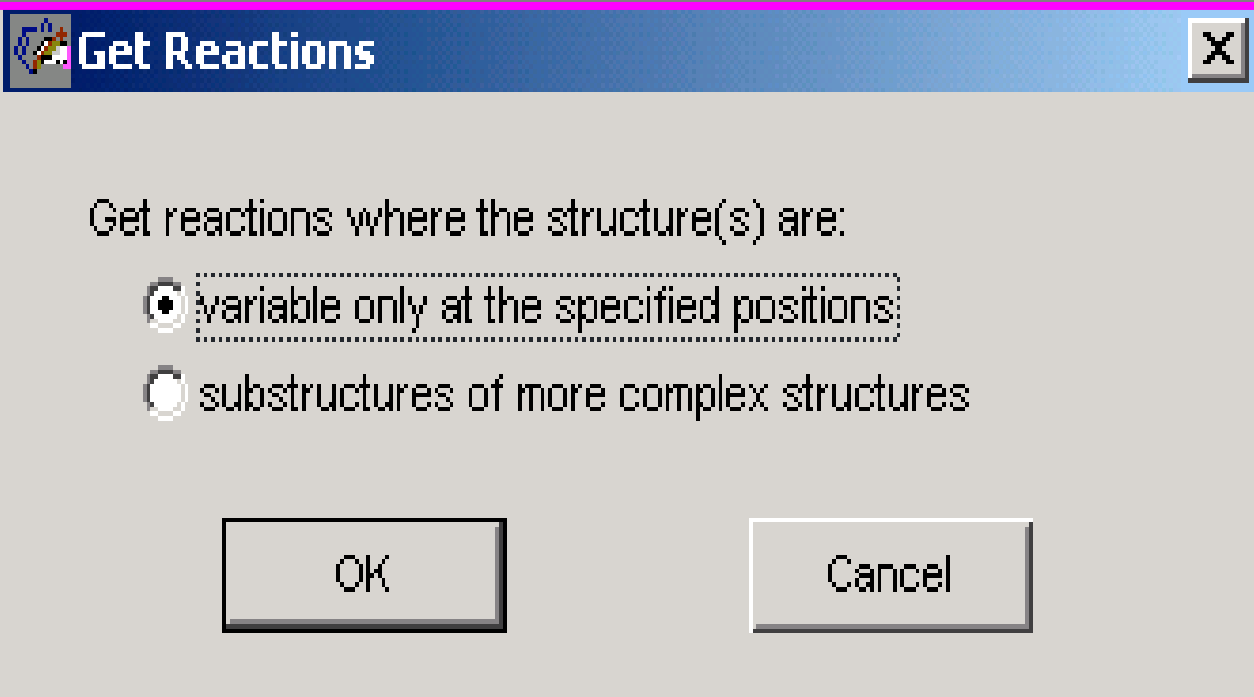
Preview Get Substances **Get Reactions** Cancel

C27 H29 N O10 527.53

 **Get Reactions - Role Definition** ✕

Get Reactions where this structure is:

- a Product
- a Reactant
- a Reagent
- a Reactant or a Reagent
- Anywhere in the reaction

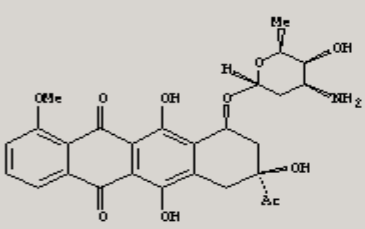


Reactions retrieved

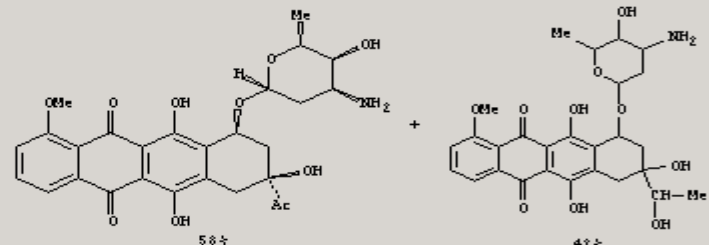
SciFinder Scholar

File Edit View Task Tools Help

NewTask Back Forward Print Save As Full Text Prefs Database History Internet Help Exit


HC1
(step 1)

1. MnCl₂, Coenzyme II,
R:1627-72-6, HEPES,
D-Glucose, Water
2. C:9001-58-5,
C:9001-27-0,
Catalase


58+ 42+

NOTE: pH 7.0 buffer

Reference: [Journal of Organic Chemistry, 55\(8\), 2518-30, 1990](#)

Database: CASREACT

OH O Et Me O-Si-Bu-t

Get References Refine Reactions Back

Reactions 1-2 of 2

2
reactions

Citation Linking

Link to view detail of literature of interest

The screenshot displays the SciFinder Scholar web application. The main window shows a search result for the article: "Characterization of a multi-functional metal-mediated nuclease by MALDI-TOF mass spectrometry." by Puapaiboon, Uraiwan; Jai-nhuknan, Jaran; Cowan, J. A. A red arrow points to a small icon in the top right corner of the search result list, which is used to open the detailed view.

The detailed view window, titled "Detail of Reference 1", contains the following information:

Bibliographic Information

Characterization of a multi-functional metal-mediated nuclease by MALDI-TOF mass spectrometry. Puapaiboon, Uraiwan; Jai-nhuknan, Jaran; Cowan, J. A. Evans Laboratory of Chemistry, The Ohio State University, Columbus, OH, USA. Nucleic Acids Research (2001), 29(17), 3652-3656. CODEN: NARHAD ISSN: 0305-1048. Journal written in English. CAN 136:66117 AN 2001:831447 CAPLUS

Abstract

Mass spectrometric anal. of reaction products allows simultaneous characterization of activities mediated by multifunctional enzymes. By use of MALDI-TOF mass spectrometry, the relative influence of magnesium and manganese promoted exonuclease and phosphatase activities of Escherichia coli exonuclease III have been quant. measured, offering a rapid and sensitive alternative to radioactivity quantification and gel electrophoresis procedures for detn. of reaction rate consts. Manganese is found to promote higher levels of exonuclease activity, which could be a source of mutagenic effects if this ion were selected as the natural cofactor. Several potential applications of these methods of quant. studies of DNA repair chem. are also described.

Indexing -- Section 7-4 (Enzymes)


Section cross-reference(s): 10

Enzyme kinetics
Escherichia coli
(characterization of a multi-functional metal-mediated nuclease by MALDI-TOF mass spectrometry)

DNA
Role: BSU (Biological study, unclassified); BIOL (Biological study)
(characterization of a multi-functional metal-mediated nuclease by MALDI-TOF mass spectrometry)

Referen

Citation of reference 1



Detail of Reference 1

File Edit Help

- 1) Rogers, S; Methods Enzymol 1980, 65, 203
- 2) Richardson, C; J Biol Chem 1964, 239, 240
- 3) Hoheisel, J; [Anal Biochem 1993, 209, 238](#)
- 4) Roychoudhury, R; J Biol Chem 1977, 252, 4786
- 5) Milcarek, C; J Mol Biol 1972, 68, 303
- 6) Henner, W; J Biol Chem 1983, 258, 15198
- 7) Bertoncini, C; Nucleic Acids Res 1995, 23, 2995
- 8) Winters, T; Nucleic Acids Res 1999, 27, 2423
- 9) Kappen, L; Biochemistry 1988, 27, 4331
- 10) Black, C; Eur J Biochem 1997, 243, 684
- 11) Puapaiboch, U; Anal Chem 2000, 72, 3338
- 12) Little, D; [Anal Chem 1997, 69, 4540](#)
- 13) Bruenner, B; [Rapid Commun Mass Spectrom 1996, 10, 1797](#)
- 14) Bleczinski, C; [Rapid Commun Mass Spectrom 1998, 12, 1737](#)
- 15) Houston, C; Anal Chem 2000, 72, 3311
- 16) Zhang, L; J Am Soc Mass Spectrom 2000, 11, 854
- 17) Liu, Y; Anal Chem 1995, 67, 3482
- 18) Siegert, C; Anal Biochem 1996, 243, 55
- 19) Doktycz, M; Anal Biochem 1995, 230, 205
- 20) Benner, W; [Rapid Commun Mass Spectrom 1995, 9, 537](#)
- 21) Demple, B; [Proc Natl Acad Sci USA 1986, 83, 7731](#)
- 22) Casareno, R; Chem Commun 1996, 1813
- 23) Loeb, L; Annu Rev Genet 1986, 20, 201
- 24) Cowan, J; Chem Rev 1998, 98, 1067
- 25) Teebor, G; Int J Radiat Biol 1988, 54, 131
- 26) Demple, B; Annu Rev Biochem 1994, 63, 915
- 27) Takemoto, T; J Radiat Res (Tokyo) 1998, 39, 137
- 28) Karimi-Busheri, F; Nucleic Acids Res 1998, 26, 4395

Get Related... Close

Link to see detail of citation 16

Hyperlink

Detail of Reference 1
File Edit Help

- 1) Rogers, S; Methods E
- 2) Richardson, C; J Biol
- 3) Hoheisel, J; Anal Bioc
- 4) Roychoudhury, R; J B
- 5) Milcarek, C; J Mol Bio
- 6) Henner, W; J Biol Che
- 7) Bertocini, C; Nucleic
- 8) Winters, T; Nucleic A
- 9) Kappen, L; Biochemis
- 10) Black, C; Eur J Biocl
- 11) Puapaibocn, U; Anal
- 12) Little, D; Anal Chem
- 13) Bruenner, B; Rapid C
- 14) Blecziński, C; Rapid
- 15) Houston, C; Anal Ch
- 16) Zhang, L; J Am Soc
- 17) Liu, Y; Anal Chem
- 18) Siegert, C; Anal Bioc
- 19) Doktycz, M; Anal Bi
- 20) Benner, W; Rapid Co
- 21) Demple, B; Proc Nat
- 22) Casareno, R; Chem
- 23) Loeb, L; Annu Rev G
- 24) Cowan, J; Chem Rev
- 25) Teebor, G; Int J Radi
- 26) Demple, B; Annu Re
- 27) Takemoto, T; J Radia
- 28) Karimi-Busheri, F; Ni

Detail for Citation "16: Zhang, L; J Am Soc Mass Spectrom 2000, 11, 854"
File Edit Citation Help

Bibliographic Information

Matrix-assisted laser desorption/ionization mass spectrometry methods for oligodeoxynucleotides: improvements in matrix, detection limits, quantification, and sequencing. Zhang, L.-K.; Gross, M. L. Department of Chemistry, Washington University, St. Louis, MO, USA. Journal of the American Society for Mass Spectrometry (2000), 11(10), 854-865. CODEN: JAMSEF ISSN: 1044-0305. Journal written in English. CAN 134:39003 AN 2000:657141 CAPLUS

Abstract

A comatrix of anthranilic acid and nicotinic acid is optimum for the matrix-assisted laser desorption/ionization time of flight detn. of oligodeoxynucleotides that are comprised of up to 21 nucleotides. A detection limit of approx. 200 amol was obtained for an oligonucleotide 21mer. The comatrix system is also suitable for quantification of oligodeoxynucleotides provided an internal std. having one more or less nucleotide than the no. in the analyte is used. Furthermore, the matrix, when used in combination with the ladder method of sequencing, allows the complete sequence of tens of picomoles of model oligodeoxynucleotides to be detd.

Indexing -- Section 9-5 (Biochemical Methods)
Section cross-reference(s): 3, 6

DNA sequence analysis
(mass spectrometric; matrix-assisted laser desorption/ionization mass spectrometry methods for oligodeoxynucleotides: improvements in matrix, detection limits, quantification, and sequencing)

DNA sequences
(matrix-assisted laser desorption/ionization mass spectrometry methods for oligodeoxynucleotides: improvements in matrix, detection limits, quantification, and sequencing)

<< Previous Get Related... Close Next >>

Citation of reference 16

Detail of Reference 1	Detail for Citation "16) Zhang, L; J Am Soc Mass Spectrom 2000, 11, 854"
File Edit Help	File Edit Citation Help
1) Rogers, S; Methods Enzymol 1980 2) Richardson, C; J Biol Chem 1964, 1 3) Hoheisel, J; Anal Biochem 1993, 21 4) Roychoudhury, R; J Biol Chem 197 5) Milcarek, C; J Mol Biol 1972, 68, 3 6) Henner, W; J Biol Chem 1983, 258 7) Bertoncini, C; Nucleic Acids Res 1 8) Winters, T; Nucleic Acids Res 199 9) Kappen, L; Biochemistry 1988, 27, 10) Black, C; Eur J Biochem 1997, 24 11) Puapaibocn, U; Anal Chem 2000, 12) Little, D; Anal Chem 1997, 69, 45 13) Bruenner, B; Rapid Commun Mas 14) Blecziński, C; Rapid Commun Ma 15) Houston, C; Anal Chem 2000, 72, 16) Zhang, L; J Am Soc Mass Spectr 17) Liu, Y; Anal Chem 1995, 67, 3482 18) Siegert, C; Anal Biochem 1996, 2 19) Doktycz, M; Anal Biochem 1995, 20) Benner, W; Rapid Commun Mass 21) Demple, B; Proc Natl Acad Sci U 22) Casareno, R; Chem Commun 199 23) Loeb, L; Annu Rev Genet 1986, 2 24) Cowan, J; Chem Rev 1998, 98, 10 25) Teebor, G; Int J Radiat Biol 1988, 26) Demple, B; Annu Rev Biochem 19 27) Takemoto, T; J Radiat Res (Tokyo 28) Karimi-Busheri, F; Nucleic Acids	16) Owens, K; Anal Chem 1998, 70, 17A 17) Gusev, A; Anal Chem 1995, 67, 1034 18) Wilkinson, W; Fresenius' J Anal Chem 1997, 357, 241 19) McLuckey, S; J Am Chem Soc 1993, 115, 12085 20) Limbach, P; Mass Spectrom Rev 1997, 15, 297 21) Vollmer, D; Int J Mass Spectrom Ion Processes 1997, 165, 487 22) Wang, Z; J Am Soc Mass Spectrom 1998, 9, 683 23) Wang, Y; J Am Soc Mass Spectrom 1999, 10, 329 24) Caprioli, R; Anal Biochem 1986, 154, 596 25) Schuette, J; J Pharm Biomed Anal 1995, 13, 1195 26) Smirnov, I; Anal Biochem 1996, 238, 19 27) Johnston, C; Anal Chem 1996, 68, 2141 28) Wunschel, D; Adv Mass Spectrom 1998, 14, 377 29) Owens, D; Bioorg Med Chem 1998, 6, 1547 30) Womer, K; Nucleosides Nucleotides 1997, 16, 573 31) Faulstich, K; Anal Chem 1997, 69, 4349 32) Hahner, S; Nucleic Acids Res 1997, 25, 1957 33) Tolson, D; Nucleic Acids Res 1998, 26, 446 34) Romieu, A; Eur J Org Chem 1999, 1999, 49 35) D'Ham, C; Biochemistry 1999, 38, 3335 36) Wang, B; Anal Chem 1994, 66, 1918 37) Cavalieri, E; Proc Natl Acad Sci 1997, 94, 10937 38) George, M; J Am Soc Mass Spectrom 1994, 5, 1021 39) Roskey, M; Proc Natl Acad Sci 1996, 93, 4724 40) Swenson, M; J Biol Chem 1969, 244, 1803 41) Linn, S; Nucleases 1993 42) Crain, P; Mass Spectrom Rev 1990, 9, 505 43) Pieles, U; Nucleic Acids Res 1993, 21, 3191 44) Keough, T; Anal Chem 1996, 68, 3405
Get Related...	<< Previous Get Related... Close Next >>

Link to view
detail of
reference of
interest

Select the reference of interest

SciFinder Scholar

File Edit View Task Tools Help

NewTask Back Forward Print Save As Full Text Prefs Database History Internet Help Exit

Puapaiboon, Uraiwan; Jai-nhuknan, Jaran; Cowan, J. A. **Rapid and direct sequencing of double-stranded DNA using exonuclease III and MALDI-TOF MS.** Analytical Chemistry (2000), 72(14), 3338-3341. CODEN: ANCHAM ISSN:0003-2700. CAN 133:291641 AN 2000:384728 CAPLUS

Puapaiboon, Uraiwan; Jai-nhuknan, Jaran; Cowan, James A. **Rapid and direct sequencing of double-stranded DNA using exonuclease III and MALDI-TOF MS.** Book of Abstracts, 219th ACS National Meeting, San Francisco, CA, March 26-30, 2000 (2000), BIOL-094. CODEN: 69CLAC AN 2000:327133 CAPLUS

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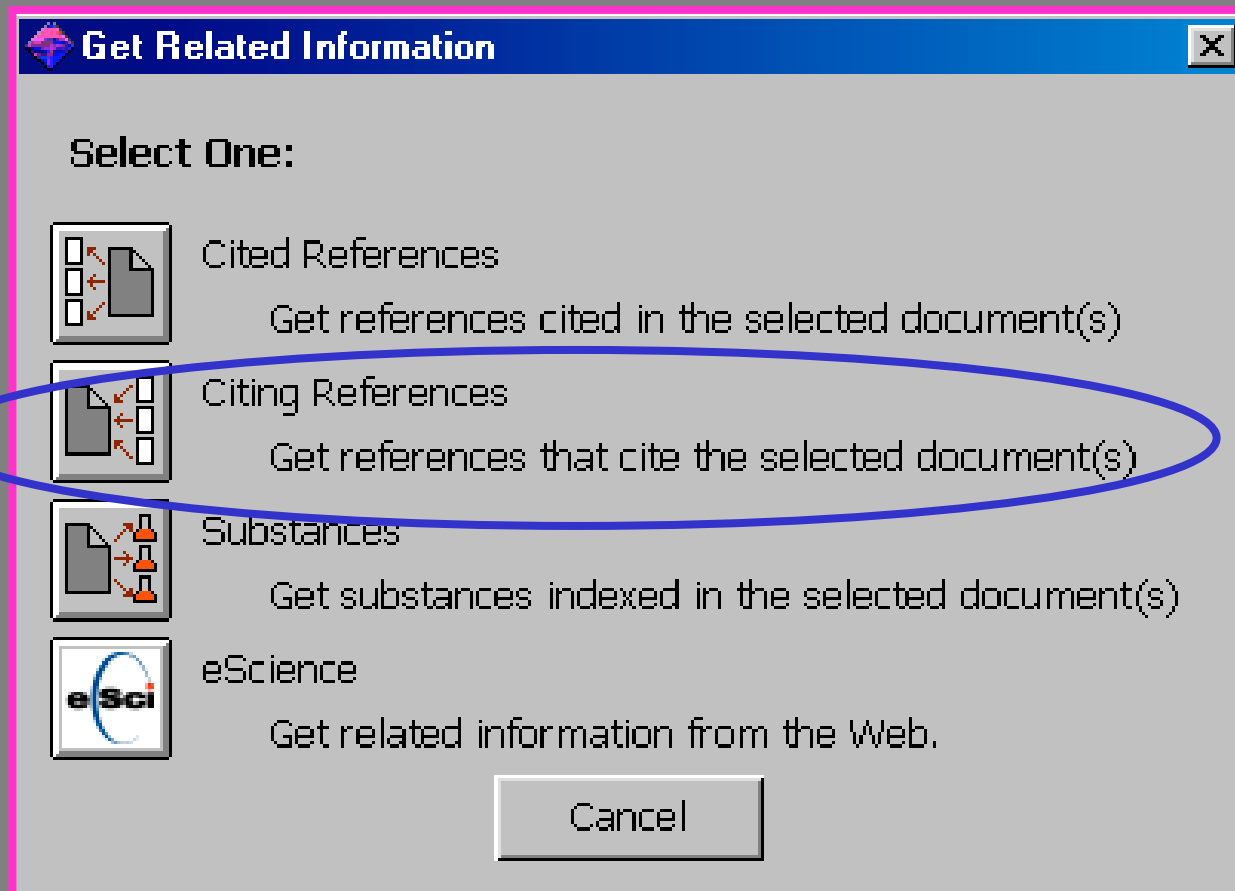
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Abstract

The novel Fe(III) porphyrin dendrimers of generation zero ([1-Fe]Cl), one ([2-Fe]Cl), and two ([3-Fe]Cl) ([1-Fe]Cl), ([2-Fe]Cl), and ([3-Fe]Cl) = 1 (R = CH₂CH₂CH₂CONHR₂ (R₂ = CH₂CH₂OCH₂CH₂OCH₂CH₂OMe (R₃), R₂ = C(CH₂OCH₂CH₂CO₂R₃)₃ (R₄) and R₂ = C(CH₂OCH₂CH₂CONHR₄)₃), resp.); R₁ = (CH₂)₆) were prepd. as models of heme monooxygenases. They feature controlled axial ligation at the Fe center by one imidazole tethered to the porphyrin core and possess a vacant coordination site available for ligand binding and catalysis. The high purity of the dendrimers and the absence of structural defects was demonstrated by matrix-assisted laser-desorption-ionization time-of-flight (MALDI-TOF) mass spectrometry. The electronic properties of the Fe(III) porphyrin dendrimers and comparison compds. [4-Fe]Cl (4 = 1 (R = CH₂CH₂CO₂Et)) and [12-Fe(1,2-Me₂Im)]Cl (12 = 5,15-bis(bis(ethoxycarbonylethoxy)phenyl)porphyrinate; 1,2-Me₂Im = 1,2-dimethylimidazole) were studied by UV/visible and EPR (electronic paramagnetic resonance) spectroscopy, as well as by measurements of the magnetic moments by the Evans-Scheffold method. Epoxidn. of olefins and oxidn. of sulfides to sulfoxides, catalyzed by the new dendritic metalloporphyrins, were studied in CH₂Cl₂ with iodossylbenzene as the oxidant. The total turnover nos. increase with the size of the dendrimer, due to improved catalyst stability at higher dendritic generations. The 2nd-generation complex [3-Fe(III)]Cl was, therefore, the most efficient catalyst in the series, despite the fact that its active site is considerably hindered by the encapsulation inside the sterically demanding, fluctuating dendritic wedges. Very high product selectivities were obsd. in all oxidn. reactions, regardless of dendrimer generation.

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