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[F0005]

Comprehensive Synthetic Organic Chemistry Information

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Abstract: As information, specifically chemical information, has become an increasingly important competitive advantage around the globe, Chemical Abstracts Service (CAS), a division of the American Chemical Society, has gained recognition as the world's largest storehouse of chemistry-related information. CAS products and databases enable chemists to answer their questions easily and quickly. This paper illustrates how modern chemical information tools can be used to address typical organic chemists' questions easily and quickly.

Synthetic chemists often ask the following questions during the course of their work:

- Is this substance known?
- Has anyone worked with this substance before?
- Is the use of this substance regulated by a government body?
- Can I buy this chemical-from whom and how much is it?
- How can I make this substance, or an analog of it, that will further my work?
- What special safety conditions might apply in reactions involving this compound?

As information has become an increasingly important competitive advantage around the globe, Chemical Abstracts Service (CAS), a division of the American Chemical Society, has gained recognition as the world's largest storehouse of chemistry-related information. CAS products and databases enable chemists to answer these questions easily and quickly.

The suite of CAS databases contains references to more than 14 million scientific abstracts; nearly 17 million unique chemical substances, including more than 12 million organic chemical substance records; 3.1 million chemical reactions; and supply information on nearly 400,000 commercial chemical products.

Chemical information is at the center of CAS' mission. The CAS databases, built by more than 400 chemists in Columbus, Ohio, have the largest combined collection of scientific abstracts and patent information in the world. Besides journals and patent literature, CAS monitors conference proceedings, related books, dissertations and electronic-only documents. Every day, chemists and other scientists make more than 10,000 updates to CAS databases, striving to ensure that customers have access to the most current chemical information possible. CAS also monitors and improves the quality of its databases on an ongoing basis according to 15 key quality standards. As a result of this dedication, scientists from around the world can access extremely comprehensive, current and high quality synthetic organic chemical information.

One of CAS' key databases, the CAS Chemical Registry System, is the largest substance identification system in existence, containing nearly 17 million substances records for chemicals reported in patents and chemical literature since 1957 and including the largest collection of organic substances with 12 million records. CAS Registry Numbers((CAS RN) have become the international standard for concise and reliable substance information. This database is a prime source for scientists when they need to identify whether a substance is known to the world or to find a chemical name or CAS Registry Number for reporting purposes. Scientists can then access the CHEMLIST file to determine if specific substances are regulated in certain countries.

The CHEMCATS database is a next logical stop for scientific organic chemists as they seek to determine whether they should make or buy the starting material needed to synthesize the compound under investigation. CHEMCATS offers access to 300 commercial chemical suppliers and 400,000 commercial products including price information.

As part of a project, chemists may decide they should look into synthesizing the compound directly. The CASREACT database gives the chemist the ability to search 3.1 million single and multistep reactions. Depending on the tools needed, chemists can specify certain reactive sites as well as map atoms between reactants and products to ensure they retrieve relevant and targeted reaction information. Several typical queries are shown below as examples.

The CASREACT and Registry databases are extremely useful in addressing combinatorial library questions whether a chemist is looking for new reaction ideas or starting materials to build a library or seeking methods to screen reactions products. CAS databases contain the most current information available; many of these key databases are updated daily with new information from journals and patents published throughout the world.

Collecting and indexing chemical information from around the world and building comprehensive, current databases are critical to CAS' mission. However, CAS must work to ensure that researchers and chemists can extract the specific chemical information they need from this compendium of knowledge.

During the past few years, CAS has introduced products and services designed to help scientists access CAS information more easily. These give today's chemists a myriad of pathways to findthe information they need. Here are a few examples:

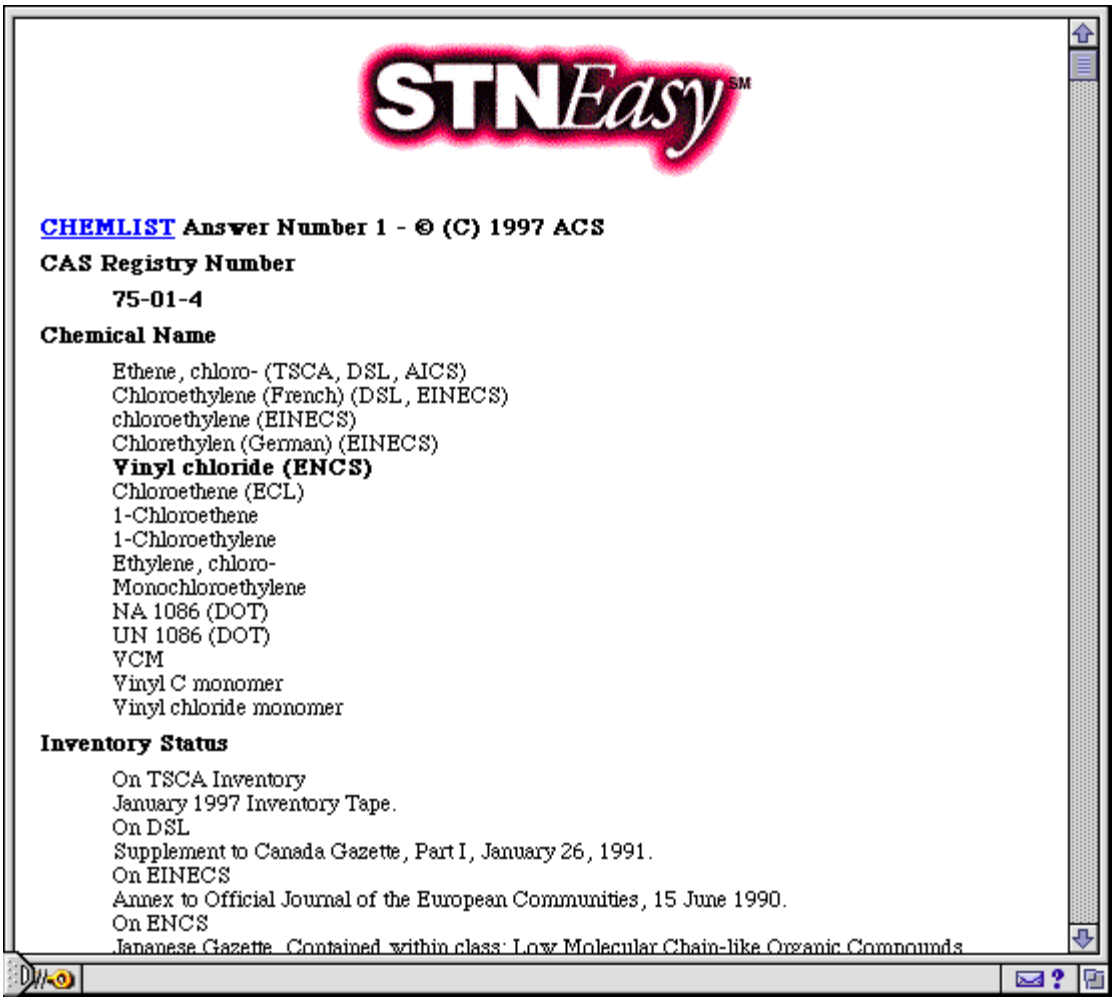
Since STN Easy is a World-Wide-Web-based service, it is an excellent entry point for individuals who are just beginning to search for scientific information online. Without any knowledge of databases or search commands, anyone can use STN Easy to find and display information about chemistry, life sciences, patents, pharmaceuticals, physics, math/computer sciences, engineering, and general science. Material Safety Data Sheets and chemical catalogs are also available.

STN Easy offers two levels of searching: a basic level that requires no experience in scientific searching or with the World Wide Web itself, and an advanced level for those with intermediate skills. A person using basic searching can simply select a subject category or database and enter a few words indicating the topic to be searched. Adding qualifying terms focuses the search more narrowly. Advanced searching allows a person to choose a subject category or database, select Boolean operators, and specify other qualifiers such as the name of the author or company. The results of a search can be organized chronologically or by

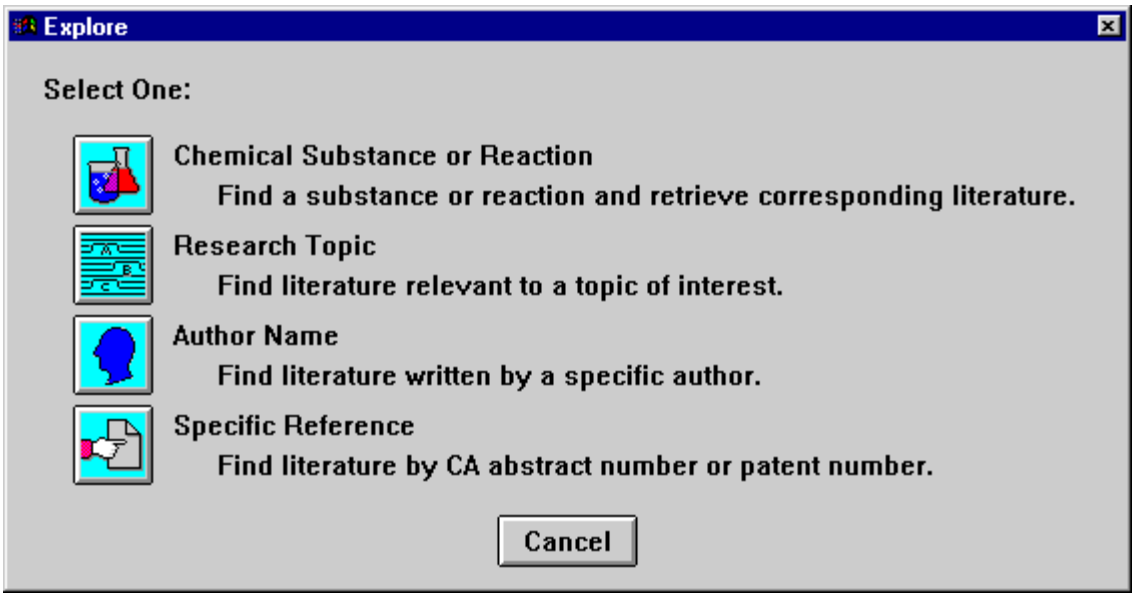
relevance.

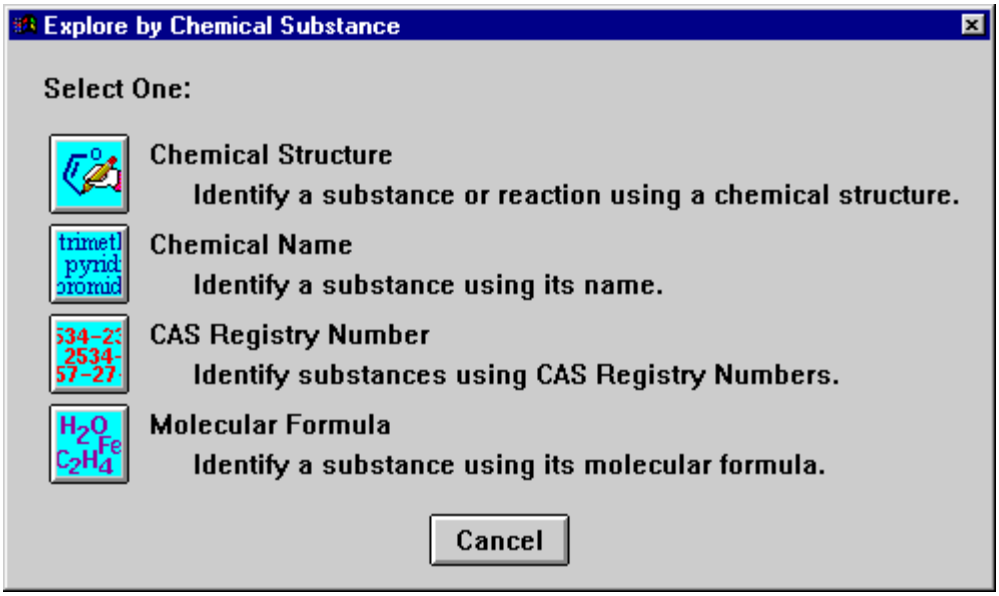
Finding Regulatory Information on STN Easy

CHEMLIST Indicates Relevant Chemical Inventories



SciFinder is geared toward the scientist who needs to access chemical, structure and reaction information at the desktop-and for those researchers who need regular, current information. The vision of providing easy access to chemical information at the desktop inspired the creation of this award-winning client-server application. SciFinder combines CAS' extensive databases with an intelligent, easy-to-use desktop interface. Without any training in information retrieval, scientists can answer most of their routine questions simply by entering a few keywords and clicking an on-screen button.



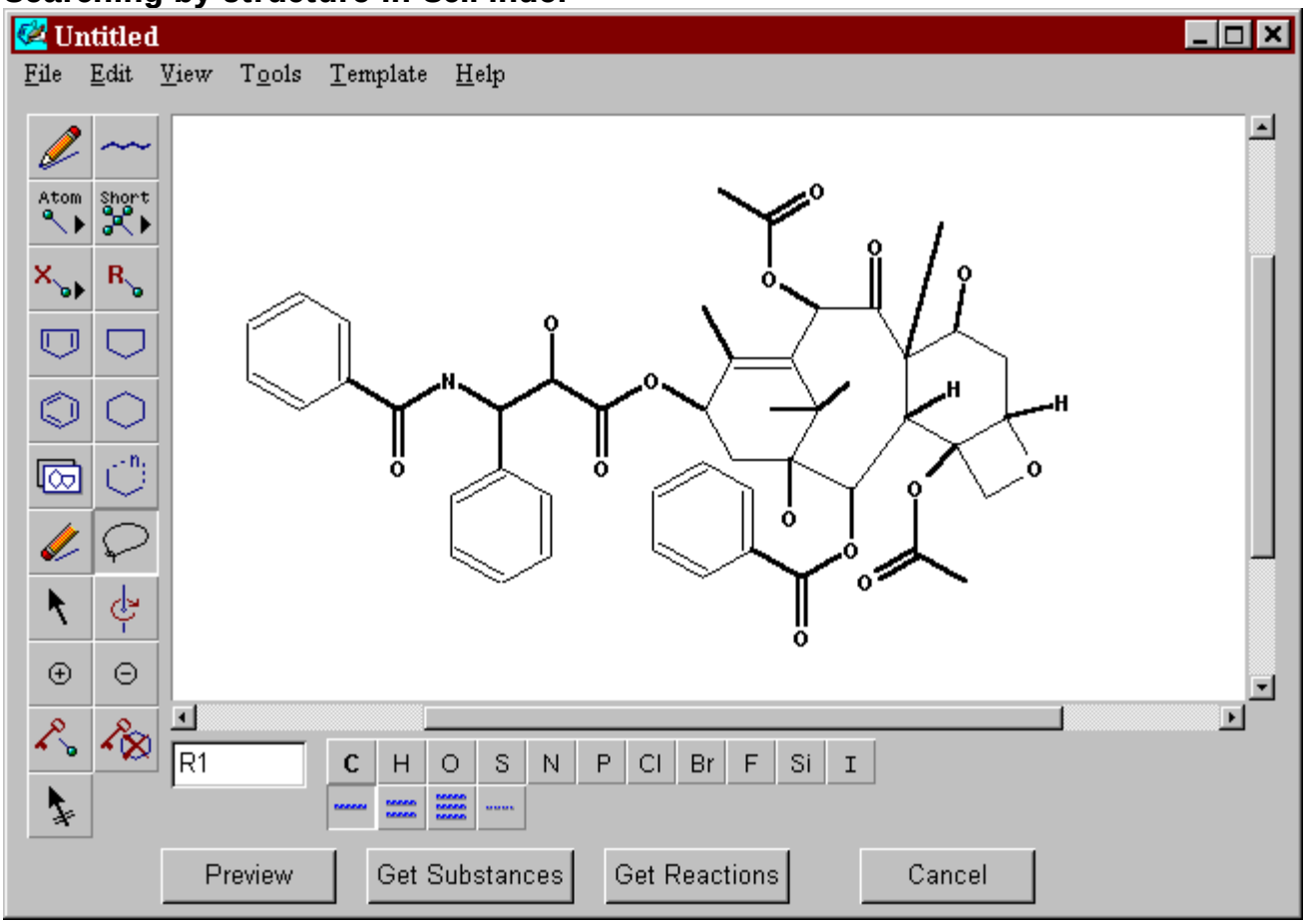


SciFinder provides the user with three pathways to knowledge. Users can search for information using conversational phrases and analyze the resulting references by date, company or other criteria. SciFinder can also locate the molecular structure of a substance, search for reactions, find commercial source information for substances or locate the work of a particular author-even without the correct spelling of his or her name. Second, SciFinder allows the scientist to browse through the table of contents of over 1,400

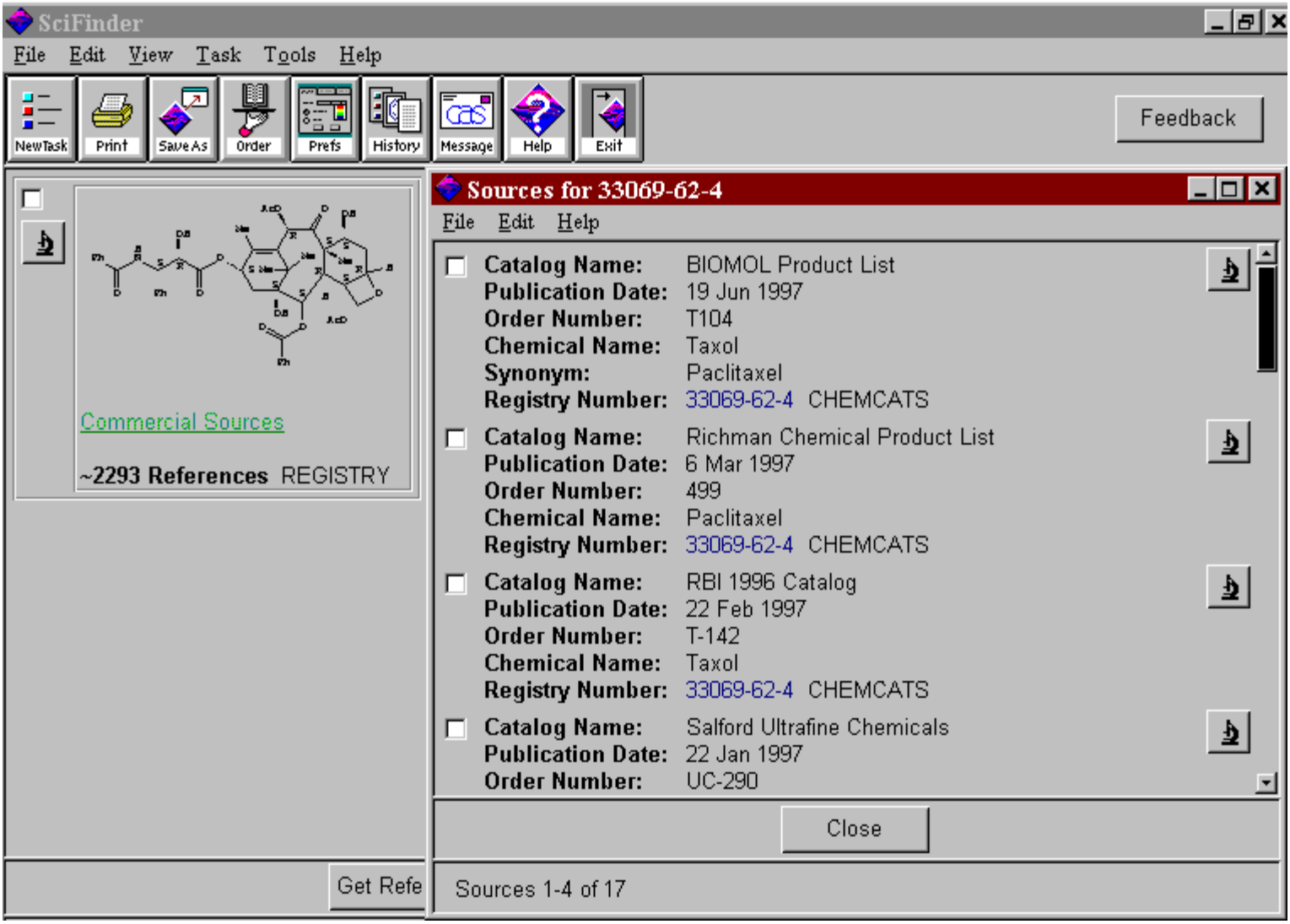
popular scientific journals as soon as they are available as well as order documents from CAS. And finally, users can request that SciFinder monitor new literature on current subjects and alert them to recent developments.

Finding Information on Taxol, a Potential Anti-Cancer Drug

Searching by structure in SciFinder



SciFinder leads you to commercial catalogs



Catalog information in CHEMCATS includes prices for many suppliers

Detail of Source 3

File Edit Help

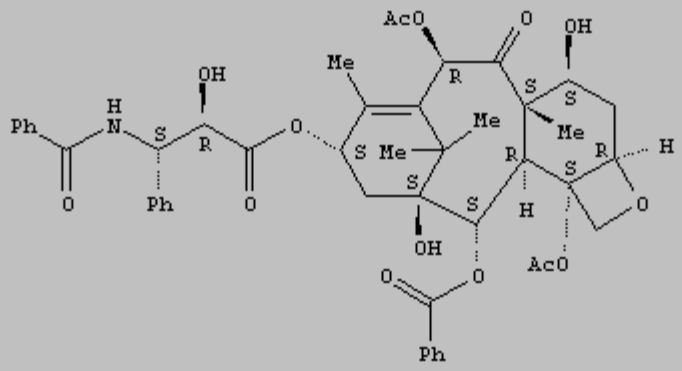
Catalog Name: RBI 1996 Catalog

Publication Date: 22 Feb 1997

Order Number: T-142

Chemical Name: Taxol

Registry Number: 33069-62-4



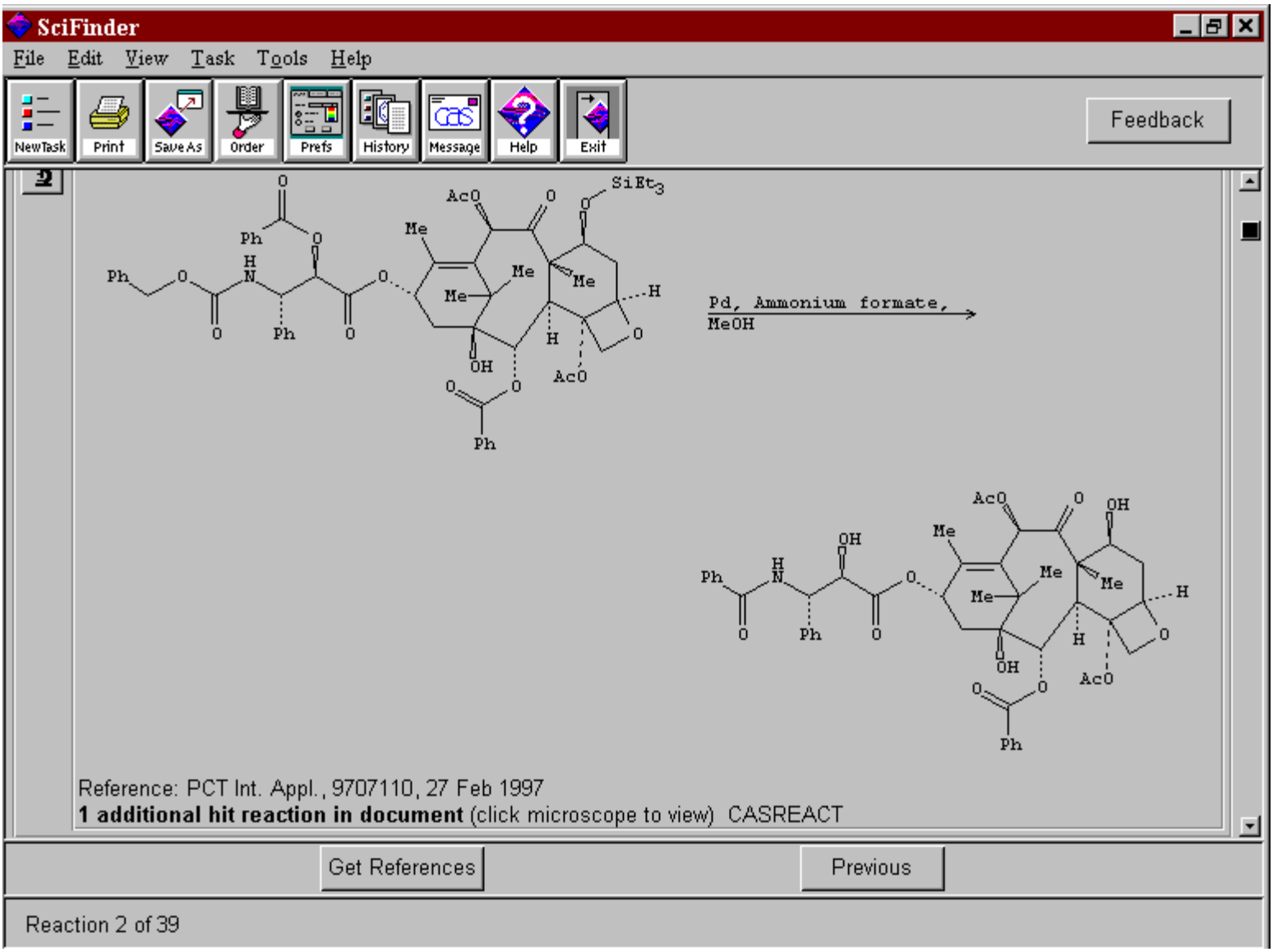
Pricing:

Quantity : 1 mg, Price: 16.00
Quantity : 5 mg, Price: 63.00
Quantity : 25 mg, Price: 236.00

Company Info: Research Biochemicals International
Customer Service Department

Close

Reaction Searching: another powerful SciFinder feature



For those researchers and information professionals who require extremely comprehensive scientific information from multiple technical resources, they can turn to STN International, the scientific and technical information network dedicated to meeting these comprehensive information needs. STN provides a complete collection of in-depth databases in science and technology to offer quick, direct links to the literature, patents and catalogs. For example, the CHEMCATS file contains 400,000 commercially available chemicals. The combined offerings of 300 chemical suppliers are updated weekly on STN.

STN databases cover numerous scientific and technical topics including chemistry, medicine, biotechnology, pharmacology, health and safety, engineering, geology, energy, government regulations, mathematics, physics, materials science, business and petroleum.

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