

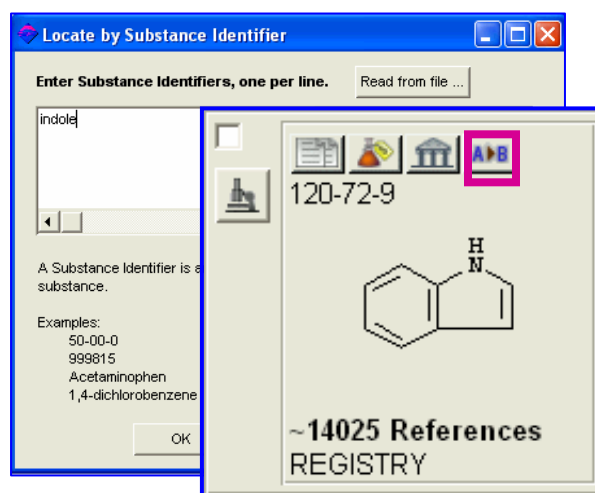
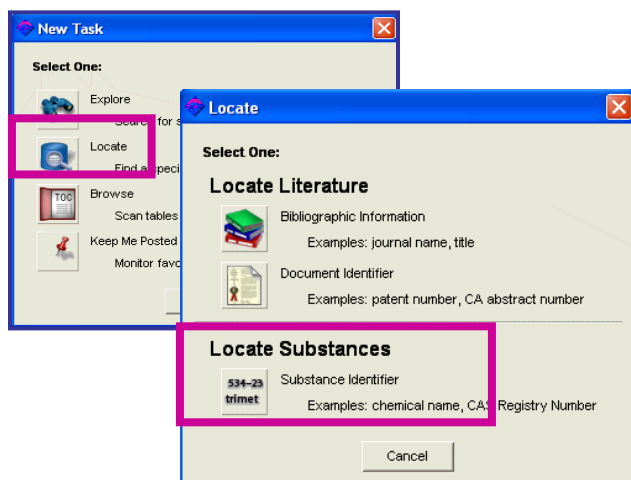
HOW TO

Exploring Reactions: Beginning with Chemical Names

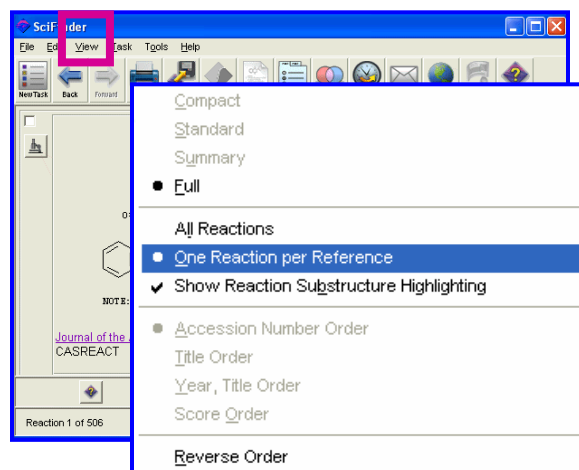
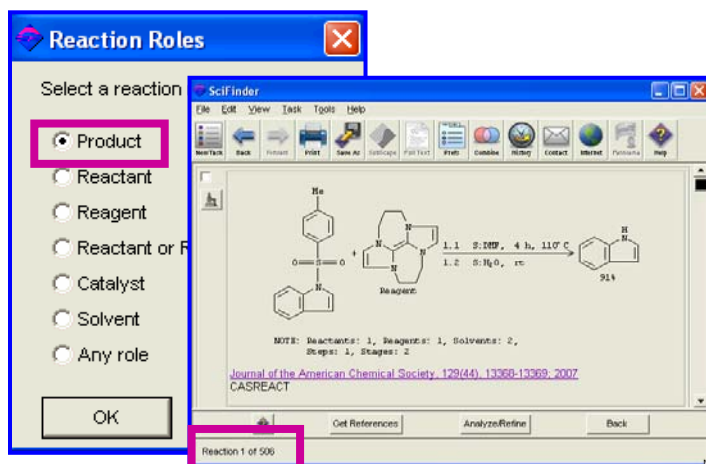


The CAS CASREACT[®] database offers more than 14 million single- and multi-step reactions making it the largest collection of reaction information in the world. Updated once a week with an average of 950 reactions, CASREACT provides information on synthetic organic research, including organometallics, natural products, and biocatalyzed reactions. SciFinder has so many built-in links to reaction information that you can start exploring almost anywhere and quickly find the information you need. Let's begin with a chemical name.

1. The aromatic heterocycle indole functions as a building block in many substances such as alkaloids, amino acids, and proteins used in medicine, pigments, and dyes. Suppose you are researching bacterial production of indole intermediaries. Let's start by *Locating the substance* in the published literature.
2. When you enter the chemical name *indole*, SciFinder locates the CAS RegistrySM record for this substance. From the Registry record, you can link to the document references, commercial sources, regulatory, and reaction information. To view reactions involving *indole*, click the A→B button.



3. SciFinder provides a list of reaction roles from which to choose. When you select *Product*, SciFinder locates 506 reactions in which *indole* is the *product*.
4. The drag-down View menu offers you a choice of display format. You can view *All Reactions* or *One Reaction per Reference*.



5. The *One Reaction per Reference* display produces an answer set of 254 reactions. We can apply SciFinder's powerful Refine tool to better focus the answers.

The screenshot shows the SciFinder main window with a chemical reaction scheme. An 'Analyze or Refine' dialog box is open, with the 'Refine' option selected. The 'Refine' option is highlighted with a pink box. At the bottom of the main window, the text 'One reaction from reference 1 of 254' is highlighted with a pink box.

6. SciFinder offers four ways to *Refine Reactions*. When you select *Reaction Classification*, you have an additional set of choices to make to determine the type of reaction you want. Select *Biotransformation* to view reactions involving *indole* production by microorganisms.

The screenshot shows the 'Refine Reactions' dialog box. The 'Reaction Classification' option is selected and highlighted with a pink box. In the 'Refine by Reaction Classification' sub-dialog, the 'Biotransformation' checkbox is checked, and the 'Include the following classification(s)' radio button is selected.

7. SciFinder locates 7 reactions in which indole is a product of microorganisms. Click the title of the Japanese patent below to view the abstract and additional details. This patent describes a process for making synthetic indole intermediaries that can be used as pharmaceuticals and agrochemicals.

The screenshot shows the SciFinder main window with a chemical reaction scheme. A 'Detail of Reference for Reaction 1' dialog box is open, displaying bibliographic information, patent family information, and an abstract for a Japanese patent.

Bibliographic Information
 Microbial or enzymic manufacture of indoles. Nagasawa, Toru; Yoshida, Toyokazu; Sato, Eiji; Nakamura, Tetsuji. (Mitsubishi Rayon Co., Ltd., Japan). Jpn. Kokai Tokkyo Koho (2002), 5 pp. CODEN: JKKXAF JP 2002017387 A 20020122 Patent written in Japanese. Application: JP 2000-205072 20000706 Priority: CAN 136/84798 AN 2002-56573 CAPLUS

Patent Family Information

Patent No.	Kind	Date	Application No.
JP 2002017387	A	20020122	JP 2000-205072
20000706			
Priority Application			
JP 2000-205072		20000706	

Abstract
 Indole-3-carboxylic acid (I) or its derivs, which may have substituents at positions except 3-position are treated with enzymes, immobilized enzymes, microorganisms, microbial cell cultures, or cell preps. to give (substituted) indole-3-carboxylic acids, useful as synthetic intermediates for pharmaceuticals and agrochems. Reaction of I (at 80 μmol/2 mL) with *Arthrobacter nictotianae* FI 1612 cells in a phosphate buffer at 30° for 3 h gave indole at 29 mmol/L.

It is easy to obtain reaction information!

As you can see, you don't need to be an expert in structure searching to locate the reaction information you need. Begin with a chemical name, and you will have many pathways and built-in links to explore as you locate reaction information.

When you want to . . .

- Locate a specific substance **Click**
- Locate a substance by chemical name or CAS Registry Number® **Click**
- Get reaction information **Click**
- View all reactions or one reaction per reference **Click**
- Focus answer sets **Click**
- Focus answer sets according to reaction classification **Click**

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