COMPUTER SOFTWARE REVIEWS

The Merck Index 13.2 CD-ROM Edition from CambridgeSoft

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Received July 7, 2004

In print, *The Merck Index* is a one-volume encyclopedia of chemicals, drugs, and biologicals that contains more than 10 000 monographs. Each monograph in this authoritative reference source is a concise description of a single substance or a small group of closely related compounds. Since it was first published in 1889, *The Merck Index* has become a standard reference for chemists, biochemists, pharmacologists, pharmacists, and related professionals.

Compounds included are as follows:

- human and veterinary drugs
- biotech drugs and monoclonal antibodies
- substances used for medical imaging
- biologicals and natural products
- plants and herbal medicines
- nutraceuticals and cosmeceuticals
- agricultural chemicals
- industrial chemicals
- laboratory reagents and catalysts
- dyes, colors, and indicators
- environmentally significant substances

Information provided in each monograph includes the following:

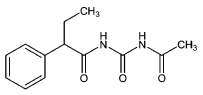
- chemical, common, and generic names
- trademarks and associated companies
- CAS Registry Numbers
- chemical structures
- molecular formulas, weights and percentage composition
- capsule statements identifying compound classes and scientific significance
- scientific and patent literature references
- physical and toxicity data
- therapeutic and commercial uses
- caution and hazard information

The extensively revised 13th edition contains more than 10 000 entries on chemicals, drugs, and natural substances. Coverage of traditional medicines, nutraceuticals, and cosmeceuticals has been enhanced. Other important new features include monographs on new classes of reagents such as fluorescent dyes and chiral catalysts and an increased emphasis on monoclonal antibody therapies and recombinant products, and monographs have been redesigned. Features of the 13th edition include the following:

- over 50% of the material revised, including 500 new monographs
- enhanced capsule statements identifying classes of compounds and their scientific and commercial significance
- focus on novel structural features and new mechanisms of action associated with specific targets
- updated company and trademark information reflects the mergers and changes that have occurred in the chemical, pharmaceutical, and agricultural industries
- molecular weights recalculated using the 1999 IUPAC Table of Standard Atomic Weights
- molecular weights included for derivative compounds
- chemical elements for atomic numbers 109−118
- an expanded therapeutic category index with more than 40 new categories and cross-references
- revised and updated Organic Name Reactions, including 21 new reactions

The stand-alone CD-ROM product contains all of the information in the print version of The Merck Index 13th Edition combined with CambridgeSoft's ChemOffice Net software. It uses ChemFinder software to search and browse over 10 000 monographs. Chemical structures and stereochemistry can be viewed with ChemDraw. There is also a 13.3 Personal Internet Edition of The Merck Index (not reviewed here). Exclusive to CD & Internet Editions are 100 New Monographs and 540 Monographs archived from the 12th edition plus updates which do not appear in the print edition.

A typical monograph from the CD-ROM edition follows:



Monograph Number: 0000101
Title: Acetylpheneturide
CAS Registry Number: 13402-08-9
CAS Name: *N*-[(Acetylamino)carbonyl]-α-ethylbenzeneacetamide
Additional Names: 1-acetyl-3-(2-phenylbutyryl)urea; *N*-(α-ethylphenylacetyl)-*N*′-acetylurea
Trademarks: Crampol (Dainippon)
Molecular Formula: $C_{13}H_{16}N_2O_3$
Molecular Weight: 248.28.
Percent Composition: C 62.89%, H 6.50%, N 11.28%, O 19.33%
Literature References: Synthesis: Umemoto *et al., Yakugaku Zasshi* **83,** 753 (1963), *C.A.* **59,** 13849d (1963); Takamatsu *et al.,* **US 3110728** (1963 to Dainippon). Pharmacology and toxicology: Nakamura *et al., Arzneim.-Forsch.* **18,** 524 (1968).
Properties: Crystals from dil alcohol, mp 100-101°. LD_{50} orally in mice: 4.73 mMole/kg (1.17 g/kg) (Nakamura).
Melting point: mp 100-101°
Toxicity data: LD_{50} orally in mice: 4.73 mMole/kg (1.17 g/kg) (Nakamura)
Therap-Cat: Anticonvulsant.

To start working with The Merck Index, the user double-clicks on The Merck Index icon on the desktop. The Merck Index Autorun screen appears and provides the user with access to the database as well as links to the readme, tech-

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10.1021/ci0400462 CCC: $27.50
Published on Web 08/24/2004

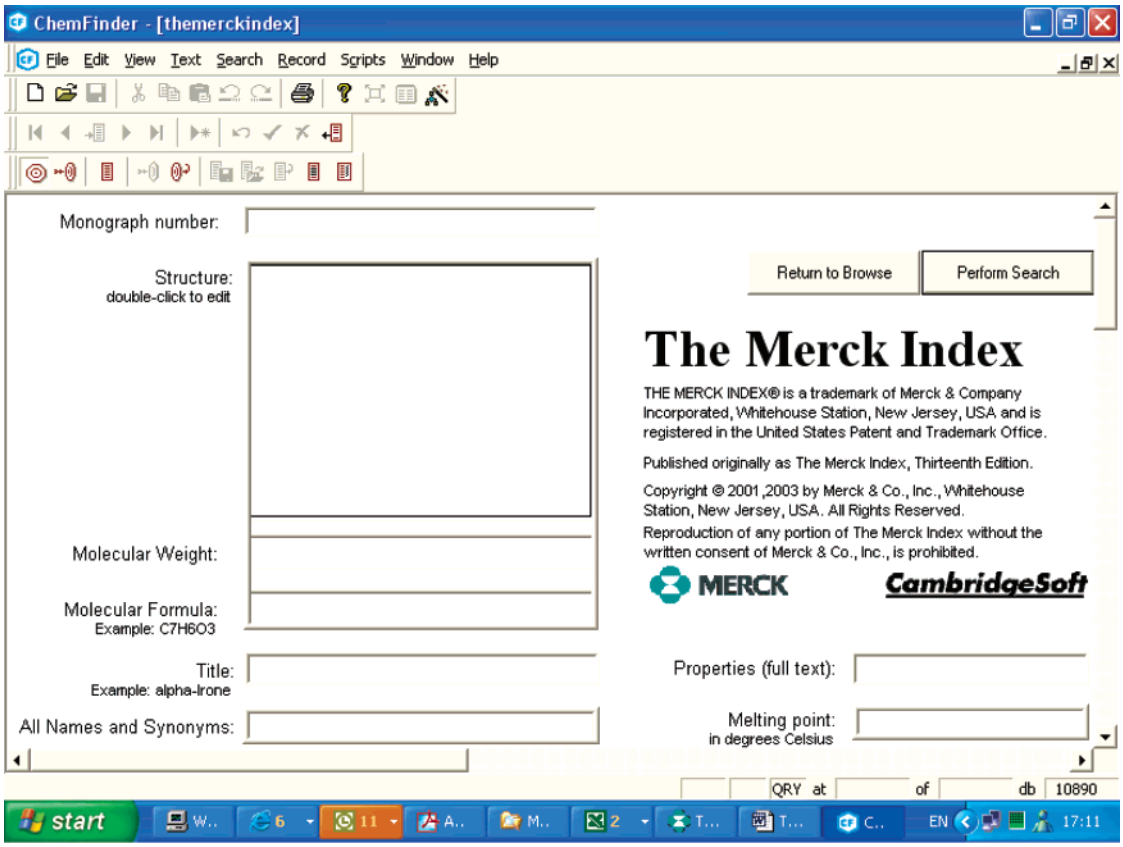


Figure 1.

nical support contact information, and technical documentation that can be helpful when navigating through the software.

In addition to browse mode, there are three major areas of The Merck Index CD-ROM:

- Compound Search
- Name Reactions
- Additional Tables

Browsing a Database. One option in viewing a ChemFinder database is to browse through the database one record at a time as one would turn the pages in a book. The Record Toolbar contains the tools for browsing through the database. By default, the toolbar is docked. However, users can grab it with the mouse and drag it anywhere on the screen that is convenient.

In addition to browsing through the records, you can also go directly to a specific record by using the **Go To Record** button

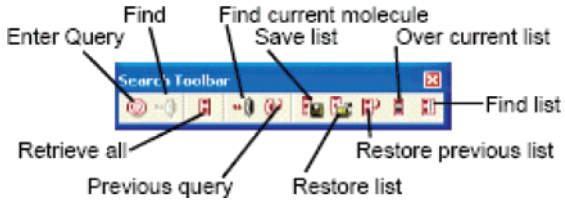
Browsing a database with ChemFinder requires only two basic steps:

1. Opening a Form (which can be thought of as a viewer for the database)
2. Browsing the database.

As users browse through records, counters in the lower right corner of the ChemFinder window change to indicate the current record, the current list size, and the total number of records in the database. The lower left corner of the same window displays help for menu items and other information. When a form is first opened, the current list size will equal the total database record count. If one does a search to find a subset of the entries in the database, the current list size will change to indicate the number of hits in the search.

Searching the Database. Browsing is often a less efficient way to locate specific information when databases are large. In such cases it is better to search the database for a record or data item. Searching a database is like using the index of a book. It is easy to quickly focus on the few pages of interest in when using an index. Similarly, when searching a database, search parameters are entered, and only those records that match the criteria are returned. Once this smaller collection (often called a hit list with each record found termed a hit) is made available, browsing it becomes much more efficient than browsing the whole database.

Searching by Text. The Search toolbar contains a number of functions for performing searches, managing hit lists, etc.



The search form contains a number of search fields as shown in Figure 1 for text and chemical structure searching.

Performing a Structure Search. To perform a structure search of a ChemFinder database, a query is entered by drawing the target structure using the ChemDraw ActiveX control. Structure searches may be used to find compounds which

- contain the drawn structure as a substructure (the default setting)
- are identical to the drawn structure
- are similar to the drawn structure

Using the ChemDraw ActiveX Control. Double-click in the **Structure** box. A blue outline appears around the structure box, and the ChemDraw ActiveX control appears.

The familiar ChemDraw tools are available for structure drawing. Once you have drawn your structure in the structure box, you are ready to perform a search.

Searching for a Structure in ChemFinder. The **Search** menu offers two search options. To view all records in The Merck Index database that contain molecules that have a particular substructure, it is necessary to ensure that the **Substructure** option is selected in the Search menu, and the **Similarity** option is not selected. These menu items are toggles. To start the search for structures containing the query structure, it is necessary to **select Find** from the **Search** menu or click the **Find** tool icon

or the

button.

In some cases, you may wish to combine more than one type of search to find a specific class of compounds. For example, you may want to find all compounds in the database that have a benzene substructure and that have a molecular weight greater than 400. This is achieved by drawing the structure and entering the text search parameter '>400' in the molecular weight field before initiating the search.

Conclusions. The Merck Index 13.2 CD-ROM Edition is a very professional integrated software and database product. It installed on my computer without any problems, has an intuitive user interface based on the well-known ChemOffice suite from CambridgeSoft, and was very easy to learn and use. The system requirements are as follows: Windows 98, Me, NT 4 SP6, 2000, or XP. The list price of the CD-ROM edition is $690, but this is currently reduced to $590 for commercial users and $190 for academic users. It represents good value for money, and I have no hesitation in recommending the product.

CI0400462