Chapman and Hall Dictionary of Natural Products on CD-ROM

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The Chapman–Hall *Dictionary of Natural Products on CD-ROM* is the electronic version of the newest addition to the Chapman–Hall Chemical Dictionary Series. It includes all natural products contained in the previous volumes of the series, plus new additions selected by an expert editorial review board. Chapman–Hall plans to release cumulative biennial updates to the database.[1] In the copy provided for review, 20% of the references in the database records had publication dates of 1990 or later. Many of the records retrieved in text searches were marked "Entry Under Review", as were several of the structures retrieved, indicating the publisher's ongoing commitment to this product.

In addition to three levels of text searching provided by the HeadFast/CD search software, there is a structure drawing and search program, PsiBase for Windows. Both programs are produced by Hampton Data Services, Ltd. PsiBase uses the same structure drawing routines as STN Express. Users can draw structures from scratch or from templates included with the program. Structures can be saved and used for future searches. The program can also import structures drawn in a variety of formats. Chapman and Hall's customer support staff were very responsive to requests for more information on the *Dictionary*'s search software, despite the difficulties imposed by time zone differences.

The database was first installed on a public access CD-ROM workstation, a computer which barely meets Chapman–Hall's minimum requirements: MS-DOS version 3.3 or higher (version 4.0 for the computer used), MSCDEX version 2.1, Windows 3.0 or 3.1 (version 3.0), and an 80386SX processor. Installation of the search software proceeded with no difficulties. Nine of the twelve available slots in the two CD changers were occupied by SilverPlatter databases. No compatibility problems were observed between the Chapman–Hall and SilverPlatter databases. The *Dictionary of Natural Products* database is installed in a specific drive in the CD changer, so the other drives were ignored completely during start up. The SPIRS software, which checks each disk in the drives when starting, was unaffected by the presence of the Chapman–Hall disk. Some minor changes were needed to reconfigure the Hewlett-Packard ThinkJet printer to produce the structure diagrams and multiple fonts in a dictionary entry. This change had no effect on output from the SilverPlatter databases. The CD-ROM drive was a Pioneer DRM-600 multidisk changer, one of two connected in series to the terminal. Although the computer was equipped with only 2 MB of RAM, there were no difficulties encountered in running text searches. There were several unrecoverable application errors when the atom by atom portion of structure searches was run, due to the lack of RAM memory. The database was also tested on a Northgate 386DX computer with 4 MB of RAM, MS-DOS 6.0, Windows 3.1, and a Multimedia PC single-disk CD-ROM drive. The structure searches that caused difficulties on the first computer were no longer a problem; atom by atom searches took 20 min instead of 30.

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The general layout of the program is similar to most other Windows-based applications and includes an on-line help system that duplicates much of the printed manual and contains point and click links between related subjects. Commands can be activated with the mouse or through keyboard shortcuts. This familiar layout makes it very easy for new users to learn the Quick and Form search modes.

The Quick search mode most closely resembles the printed source. Records can be searched by specific field or by browsing through the index for that field to select search terms. Terms can also be combined in any of the fields using Boolean operators, proximity operators, or comparisons. The Form search mode extends searching to combinations of fields by presenting a form with blanks corresponding to 16 of the fields or groups of fields in a record. Search terms in the different fields are linked with Boolean operators. A Form search can be made at the compound level or the entry level. The former type of search considers all of the different derivatives and variants in a record as searchable and returns a list of all the variants of a compound that match the search terms. The latter returns only records for which the main entry matches the search request. In both Quick and Form searches, pop-up toolboxes allow Greek letters, Boolean and proximity operator symbols, and range symbols to be entered into a search request.

The command level search is similar to searching an on-line database. However, one has to pay more attention to the layout of records when doing Command searches. The fields in a record are indexed two different ways. Physical constants, molecular formulas, compound classification codes, and the descriptors that correspond to those codes are given separate indexes. Textural fields are combined into Index Groups; for example, all of the names associated with a compound are listed in the same index. Commands can be entered from the keyboard or from a pull-down menu, and search terms can be selected by browsing the index for a particular index group or field. A search using a term which has its own separate index need only be qualified by the field tag: "C47H51NO14". MOLF. Fields that are part of Index Groups (except the TEXT group) cannot be specifically searched unless the field is further qualified by its Index Group. For example, a search for papers with J. L. McLaughlin as the lead author needs to be qualified both by the field and the reference index group and is entered as: "AUTH=MCLAUGHLIN". REFS. Entering terms by selecting them from the index saves the trouble of remembering how different fields are qualified.

The end result of any of the three levels of a search is a list of chemical name entries. Records can be viewed by moving the highlight bar to the record and pressing enter or by clicking on the entry (Figure 1). Once inside the record, a structure can be displayed by clicking on the structure button. Previous or succeeding records can be viewed by using the appropriate controls. Included in the text of an entry are "hot" cross-references to related entries, represented as green keyhole icons. Clicking on the icon transfers one to the related entry. The on-screen and printer output from a record look almost exactly like an entry in a printed Chapman–Hall dictionary

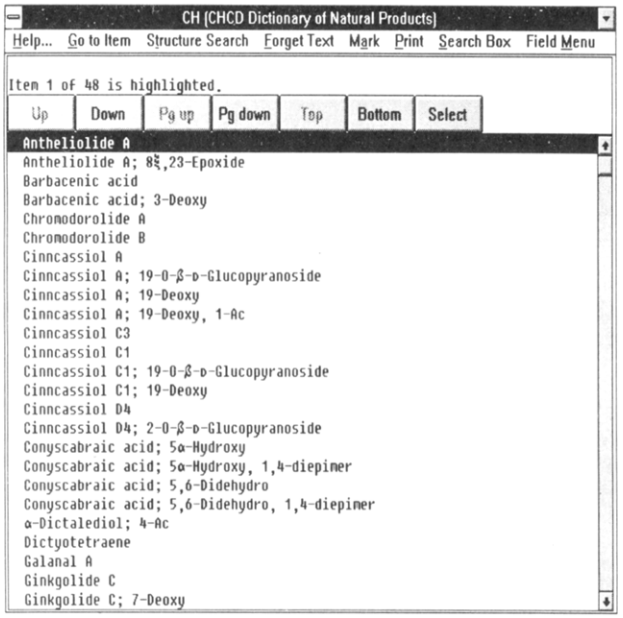


Figure 1. Summary of hit lists.

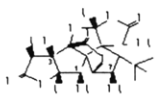
Ginkgolide C

ENTRY UNDER REVIEW

CHKJN05

[15291-76-6]

Classification: L733



$C_{20}H_{24}O_{11}$ M 440.403

Bitter principle from *Ginkgo biloba*. Cryst. (EtOH). Mp > 280° (dec.). $[\alpha]_D$ -19° (c, 1 in dioxan)

7-Deoxy. **Ginkgolide B.** CHKJN06 [15291-77-7] Classification: L733. $C_{20}H_{24}O_{10}$ M 424.404. Isol. from *Ginkgo biloba*. Cryst. (EtOH). Mp > 280° (dec.). $[\alpha]_D$ -63° (c, 1 in dioxan).

1,7-Dideoxy. **Ginkgolide A.** CHKJN07 [15291-75-5] Classification: L733. $C_{20}H_{24}O_9$ M 408.404. Bitter principle from *Ginkgo biloba*. Cryst. (EtOH). Mp > 280° (dec.). $[\alpha]_D$ -39° (c, 1 in dioxan)

Sakabe, N *et al*, *J. Chem. Soc., Chem. Commun.*, 1967, 259, (*cryst struct*)
Maruyama, M *et al*, *Tetrahedron Lett.*, 1967, 299, (*struct*)
Nakanishi, K, *J. Am. Chem. Soc.*, 1971, **93**, 3546, (*biosynth*)
Weinges, K *et al*, *Justus Liebigs Ann. Chem.*, 1986, 1057, (*cryst struct*)
Weinges, K, *Justus Liebigs Ann. Chem.*, 1991, 81, (*synth*)

[0000447]

Figure 2. Entry from the *Dictionary of Natural Products*.

(Figure 2). Users can select portions of the record to print with the mouse. Structure and text can also be exported individually to the Windows Clipboard (with the loss of the entry's typography) for further manipulation or saving to a disk.

The structure search option is versatile and user friendly. Structures can be drawn freehand or built from one of the supplied templates (Figure 3). It is also possible to use other drawing programs to create a structure and then import it into the *Dictionary*. Before actually starting a search, the software confirms the bond and node specifications set by the user by stepping through a list of specifications and highlighting relevant parts of the structure. The results of a structure search can be used to retrieve a list of entries which can then be scanned one at a time or used as the starting point for a text search. Likewise, the structures associated with the results of a text search can be browsed through without opening any of the text entries or used as the starting point for a refined structure search (Figure 3 was generated by going to the structure search option after performing the text search that generated Figures 1 and 2). The ability to save a structure for access by another Chapman–Hall database is also a useful feature. Users can find a reference on the biosynthesis of a natural product in the *Dictionary of Natural Products* and then look for information on possible synthetic intermediates. This was not possible because of the scope of the *Dictionary of Natural Products*' coverage, but would have been possible had the *Dictionary of Organic Compounds* CD been available.

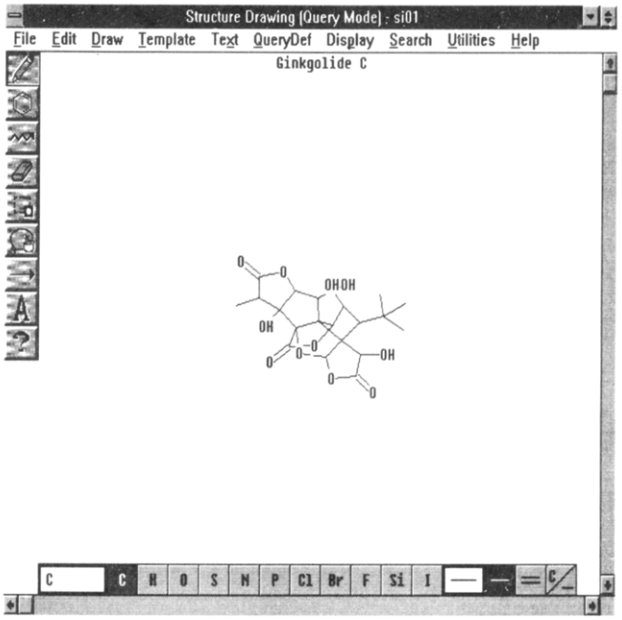


Figure 3. Structure drawing option.

This database would be ideal for a library or information center that supports active research in natural products chemistry and has made a substantial commitment to electronic reference sources. It is relatively easy to learn and use this electronic dictionary to answer the same types of questions the printed version answers. The added capacity to search for any text entry and especially for structures or structural fragments enhances the *Dictionary of Natural Products*' usefulness as a reference tool. In addition, the ability to search for a particular structure or substructure and then combine the results with a text search for a molecular formula, physical constant, or chemical name makes this a very versatile database.

REFERENCES AND NOTES

(1) The Chapman and Hall *Dictionary of Natural Products on CD-ROM* is available from Chapman and Hall, 2–6 Boundary Row, London SE1 8HN, for $4995. This price is for the first year's subscription plus a 6 month update. The annual renewal price is $2975, including a 6 month update.