# The Chapman and Hall Dictionary of Drugs on CD-ROM

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A recent addition to the Chapman and Hall Chemical Dictionary series on CD-ROM is the *Dictionary of Drugs*.[2] The *Dictionary of Drugs* is very similar in implementation to the *Dictionary of Natural Products* and the *Dictionary of Organic Compounds*, which have been reviewed in this journal.[3] As in these other products, there is both a text based search engine, Headfast, and a chemical structure search capability employing Hampden's Psibase software, the same interface used in *STN Express*. The *Dictionary of Drugs* on CD-ROM supplants updates to the printed *Dictionary of Drugs* (1990), and annual updates of the CD-ROM are planned, although pricing for the updates has not been established.

The application requires an IBM compatible PC with an Intel 80386 or better processor, 4 MB RAM, 7 MB space on a hard disk, CD-ROM drive, Microsoft Windows 3.1, and MSCDEX 2.1 or higher. Installation from the CD is uncomplicated and requires a floppy "key disk". The software supports postscript or Hewlett-Packard compatible printers. The *Dictionary of Drugs* was tested on 50 MHz and 33 MHz Dell computers connected to an HP LaserJet II, and searching and printing were quick and efficient, with printing requiring about 5 s per page. The *Dictionary of Drugs* was also tested on a Power Macintosh under Insignia's SoftWindows, and it installed normally and both the Headfast and PsiBase modules could be searched and displayed, but its performance was slower than on a 33 Mhz 486 compatible computer. However, when printing in SoftWindows, the SoftWindows usually crashed, quitting to the Mac desktop. When it did not crash, printing required about 5 min per page. This review will not discuss the mechanical details of the use of *Dictionary of Drugs*, since these were discussed in the earlier reviews in this journal and have not changed. The documentation, which is thorough and well written, consists of a three ring minibinder of about 160 pages including an index. No mention is made in the documentation regarding network operation, and no attempt was made here to run *Dictionary of Drugs* over a network.

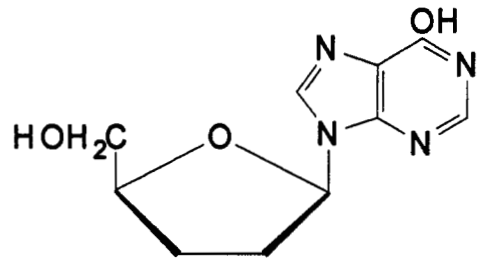
The database consists of about 20 000 structures, searchable and displayable on the PsiBase segment, and 6700 text records, searchable and displayable on the Headfast segment, or about three structures per text record on average. Related compounds are grouped together into a single record, such as salts, stereoisomers, etc. An attractive structure diagram is available for each text record (see Figure 1). There is no statement of policy regarding selection of entries for inclusion. The *Dictionary of Drugs* does not have every drug listed in the 1994 *USP Dictionary of USAN and International Drug Names*, but every marketed drug searched was present.

Considering the array of drug information products on the market today, the overall content of the *Dictionary of Drugs* is most similar to the Merck Index. A typical record (with the structure diagram) is shown in Figure 1 and consists of the following: chemical identifying data, including systematic names, laboratory codes, generic names, and proprietary names; a brief description of physiological activity and a therapeutic classification code (discussed below); physical data, such as molecular weight and formula, melting point, solubilities, optical rotation, morphological descriptor (i.e., "crystalline"); and references with a descriptor word on the content, such as synthesis, spectral data, toxicity, etc. In contrast, PharmaProjects and IMSWorld provide few literature references and no chemical data except identifying information and concentrate on commercial summaries, licensing agreements, and clinical development status. The classification of therapeutic utility is the major feature common to the *Dictionary of Drugs* and Pharmaprojects or IMSWorld. PharmaProjects has a system of about 400 therapeutic classes, and the *Dictionary of Drugs* has a system of approximately 320 classes. Unfortunately, the *Dictionary of Drugs* does not display or print the meaning of its therapeutic classifications in the output (the meanings are provided in a table in the documentation); including a full description of the classification codes would substantially facilitate interpretation of the results, especially since these are a major value added feature of the package.

In addition to journal and monograph citations, references to recent editions of *Martindale, The Extra Pharmacopoeia*, and to Sax's *Dangerous Properties of Industrial Materials* as well as other compendia are common in the *Dictionary of Drugs* HeadFast records. The *Dictionary of Drugs* includes patent references gleaned from Chemical Abstracts, but for many obvious cases of commercially successful drugs, under patent or recently under patent, no patent information is included. Most patents listed have a descriptor word about content, as do most nonpatent references, so patents seem to be intended as ordinary references containing useful technical data, rather than as a source of intellectual property information. This is consistent with the *Dictionary of Drugs* overall goal of providing scientific, rather than commerical, data on drugs and potential drugs.

The greatest deficiency with the *Dictionary of Drugs* is the absence of stereosearch capabilities in the PsiBase structure searching module. All of the searchable structures in the PsiBase module are flat—none of the structures retrieved had any three-dimensional attributes. Instead, for stereoisomeric structures, identical structures are drawn for each isomer, but each stereoisomer has a different name containing stereochemical descriptors. In general, this is not a significant drawback, particularly for most drug substances with only one or two stereocenters, that are probably grouped into the same text record anyway. However, in certain circumstances this can be important, for example, when searching sugars. A search on a generic hexapyranose, such as glucose, gave 540 answers, with all possible stereochemical configurations. Limiting the search to gluco sugars, for

**Didanosine, INN, USAN, BAN**




2,3′-Dideoxyinosine. 2′,3′-Dideoxy-1,9-dihydro-9-β-D-ribofuranosyl-6*H*-purin-6-one. DDI. NSC 612049. BMY 40900. Videx

GXN76-E
[69655-05-6]
Classification: KA2400.

$C_{10}H_{12}N_4O_3$ M 236.230.
Antiviral agent. Potentially of use against HIV infection. Cryst. (EtOH aq. or $CH_2Cl_2/Me_2CO$). Softens at 184-186°, does not melt <300°.

Mitsuya, H *et al.*,*Proc. Natl. Acad. Sci. U.S.A.*,1986, **83**, 1911 (*pharmacol*)
Ray, G *et al.*,*Anal. Lett.*,1987, **20**, 1815 (*hplc*)
Ahluwalia, G *et al.*,*Biochem. Pharmacol.*,1987, **36**, 3797
Hao, Z *et al.*,*Mol. Pharmacol.*,1988, **34**, 431 (*pharmacol*)
Chu, CK *et al.*,*J. Org. Chem.*,1989, **54**, 2217 (*synth, pmr*)
McGowan, JJ *et al.*,*Rev. Infect. Dis.*,1990, **12**, S513 (*rev, antiretroviral props*)
Shelton, MJ *et al.*,*Ann. Pharmacother.*,1992, **26**, 660 (*rev*)
Nassar, MN *et al.*,*Anal. Profiles Drug Subst.*,1993, **22**, 185 (*rev*)

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**Figure 1.** Typical entry in the Chapman and Hall *Dictionary of Drugs* on CD-ROM.

example, cannot be done directly from a PsiBase structure search query but would require manipulation of the list of chemical names. Another weakness is the lack of a copyright notice or identifying mark on the printed output, so identification of the source of the output is not obvious. A method of directly exporting a formatted report with graphics to popular word processing software would also be a great convenience. The clipboard is available for this purpose but cannot export the graphic and text simultaneously.

Despite being a little rough around the edges, *Dictionary of Drugs* provides a rapid and generally easy to use access point to the scientific literature on major aspects of drug development. The size of the database is appropriate, and the organization and content are logical. It is a valuable reference that can be recommended for use by biomedical research organizations.

## REFERENCES AND NOTES

(1) American Cyanamid is now part of the American Home Products Corporation. Author e-mail address: andrew-berks@internetmail.pr.cyanamid.com.
(2) Order from Chapman and Hall, 2-6 Boundary Row, London SE1 8HN, UK, Tel. +44-71-410-6929, or 115 Fifth Ave, New York, NY 10003, tel. 301-699-7777; fax 301-699-1110. Cost is U.S. $1995, or $1695 if the printed work is owned.
(3) (a) *Dictionary of Natural Products.* Running, W. E. *J. Chem. Inf. Comput. Sci.* **1993**, *33*, 934−935. (b) *Dictionary of Organic Compounds.* Mendelsohn, L. D. *J. Chem. Inf. Comput. Sci.* **1993**, *33*, 790−792.

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