

The only problem I encountered was with the Bitstream package. In the version I have, dated 10/04/90, there is a bug, which has yet to be fixed. When I used the software with WordPerfect on a Compaq 386 and HP LaserJet II printer, the printout came out in an odd way, and actually printed out the wrong characters. Every letter and number in the output is increased by one. Thus "chemistry" comes out "difnjtusZ" and "<sup>13</sup>C NMR" comes out "<sup>24</sup>D ONS". Whenever this happens, and it did occur regularly, I followed the suggestion in the 12/90 supplement to the manual, which suggests either turning off the printer and turning it back on or exiting WordPerfect, and restarting WordPerfect by typing flwp (the facelift modification to WordPerfect). The latter worked every time I need to do it. Since I first wrote this review, I upgraded my computer system to an AST 486/33 and an HP LaserJet III printer. The bug which occurred often in my old system has never yet appeared in the new system.

The HP Type Director fonts included in the basic Premier Collection package consists of eight typefaces from two of the most popular typeface families: Univers and CG Times. Included in the CG Times typeface are regular, bold, italic and bold italic. The Univers typeface includes medium, medium italic, bold, and bold italic. The other typefaces included on the third disk, called Decorative 1, include the typefaces: Brush, Dom Casual, Park Avenue, and Unical. HP sells many other typefaces.

The Bitstream Facelift Companion Value Pack kit includes the following fonts: Amerigo (Roman, italic, bold, and bold

italic), Charter (Roman, italic, black (like bold), and black italic), Century Schoolbook (Roman, italic, bold, and bold italic), Futura Light (light, light italic, medium condensed, and extra black), Swiss compressed, Swiss extra compressed, Exotic demi-bold, and Exotic bold. Bitstream also sells lots of other fonts.

For both packages I can safely say that after looking at a few different fonts and trying a few different point sizes one can quickly forget what you were printing and why you were printing it in the first place. The variety in either package exceeds most normal needs.

In summary both of these packages work well and provide considerable enhancements to the capabilities of a laser printer. I would recommend either and I keep both loaded in my system. If one had to choose between the two I would favor Bitstream slightly over HP Type Director simply because of its smaller hard-disk space requirements.

## REFERENCES AND NOTES

- (1) The Bitstream Facelift is available from Bitstream Inc., 215 First Street, Cambridge MA 02142-1270 (Phone: 800-522-FONT or 617-497-6222, FAX: 617-868-0784). The price for the basic Bitstream Facelift Companion Value Pack kit is \$195.00. The additional fonts in the Symbols 1 package costs \$195.00. There are various starter kits available for over two dozen different software packages, with price ranging from free to \$95.00, with the median price being \$15.00.
- (2) HP Type Director 2.0 is available from Hewlett-Packard, Boise Division, P.O. Box 15, Boise, ID 83707-9334. (For the nearest dealer phone 800-752-0900). The price for Type Director, Version 2.0 Premier Collection with the basic fonts is \$195.00.

## The Beilstein Current Facts in Chemistry CD ROM

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The latest addition to the computerized activities of the Beilstein Institute is a CD-ROM product of the recent chemical literature. Called *Beilstein Current Facts in Chemistry on CD-ROM*,<sup>1</sup> this CD-ROM contains facts, data, and structure information abstracted from the chemical literature, beginning with January 1990. Currents Facts is to be issued quarterly and will contain data which is at least 5 months old. Each quarterly disk will contain the past 12 months' of literature data. This means the older data on the disk will be deleted as new data from the most recent 3-month period is added. It will be possible to keep one CD-ROM disk which contains a full year's data, from January to December by keeping and storing every fourth disk. It is expected that some 300 000 compounds, found from scanning the chemical literature of some 82 core journals, will be included in this database every year.

The equipment required to use the system is a IBM PC or compatible clone, MS-DOS version 3.1 or higher, with 640K of main memory. The Current Facts system is able to run in about 500 000 bytes of free memory, after the operating

system, mouse and CD-ROM drivers are loaded in the computer. A variety of graphics cards, seven in all, from CGA to VGA, work with the system. A standard internal or external CD-ROM drive, with version 2.10 or higher of Microsoft MSCDEX is also needed. The CD-ROM is not available for an Apple Macintosh system, and there are no current plans to implement such a version. The system also allows one to print out search results with a wide variety of dot-matrix, laser, and color printers.

Installation of the system was simple. I installed the system on an Epson 286 computer with a SONY internal CD-ROM drive and a laser printer. The system loads directly from the CD-ROM by typing "CFINST.EXE". The automatic loading of the system does produce a little overhead on your hard disk, since, for example, all graphics drivers are loaded, not just the one you need. However, it is easy to erase the extra file from the hard disk once the installation is completed. It is that simple, and it works. The system can also be manually loaded, and use of a RAMDISK requires some small modifications. The introductory 17-page short manual is both quite short and

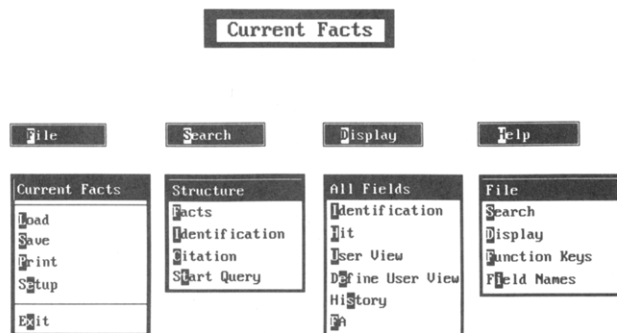


Figure 1. Current facts main menu.

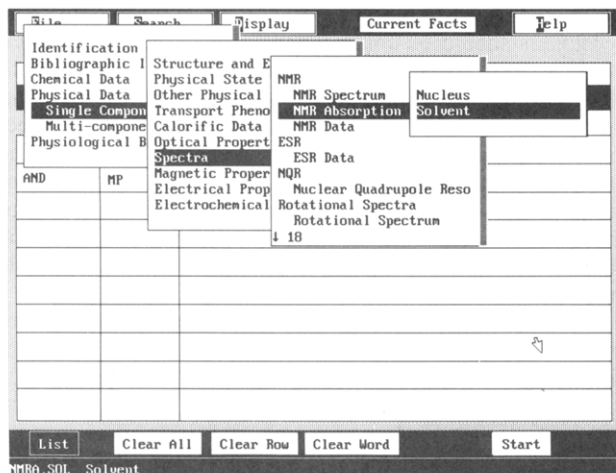


Figure 2. Hierarchical field listing.

easy to read. The more complete 5-chapter User Guide and 4-chapter (plus a few appendices) Reference Manual are both good with many examples and contain good figures of screen dumps.

The CD-ROM disk is searchable in a number of ways, by facts, by identification, by citation, and by structure. The structure search uses the S<sup>4</sup> search system, which same is the structure search system used for the Beilstein Database on the DIALOG system.<sup>2</sup> Help messages abound throughout the system, making it unnecessary to refer back to the manual.

The main menu which is shown on the top of the display screen has four options—File, Search, Display, and Help (see Figure 1). These main menus are then further broken down into submenus as described below. The File or housekeeping menu is broken down into five submenus for Set-up, Load, Save, Print, and to Exit the system. A very nice feature of the system is the ability to store data and query structures for later use via the Load option.

The Search menu consists of five submenus. They support searching by Structure, Facts, Identification, Citation, and to start a Search Query. The citation searching allows one to search by Coden, year, volume, issue number, page number, or author. In the facts option one can search by field name and value, and then use Boolean operators to combine terms. If you are not sure of the searchable "facts" fields, the LIST command or F2 function key provides a useful online display of the formation in hierarchical field ordering, as shown in Figure 2. One gets to the structure searching module by choosing the search option, and you are then transferred into the MOLKICK program for structure drawing. From there to search requires a click of the mouse button; the search starts and finishes in just a few seconds.

The Display menu has seven submenus. These are All Fields, Identification, Hit, User View, Define User View, History, and FA (field availability). The first thing that comes

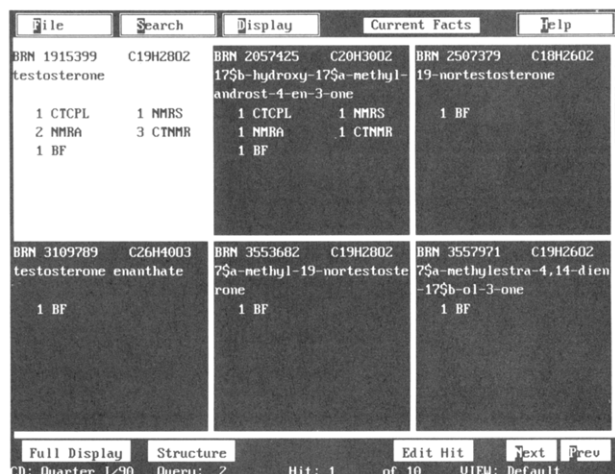


Figure 3. Short display mode.

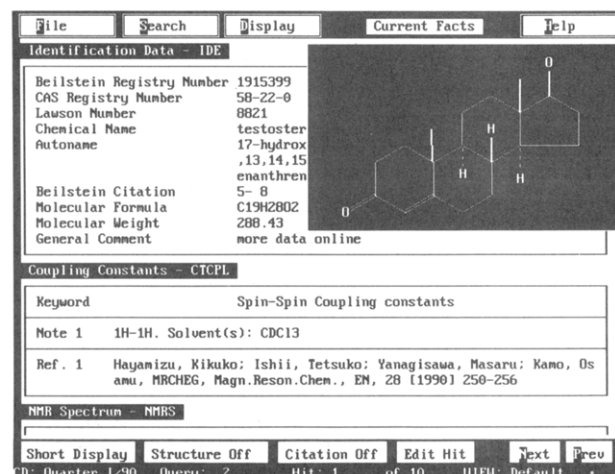


Figure 4. Full display mode.

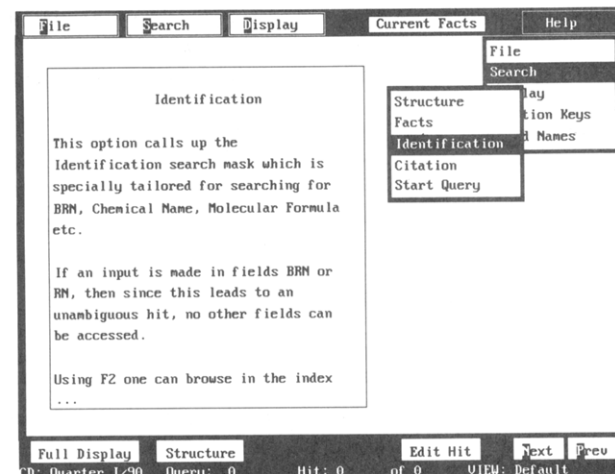


Figure 5. Sample current facts help message.

up on the display option is a short form of the hits, with the screen filled with six boxes (for an example of this see Figure 3). In each box is the Beilstein Registry Number (BRN), molecular formula, name, and list of what data are available (e.g., 1 PRE means one method of preparation is given). One then clicks on another submenu and the entire record, with or without the structure, is displayed (see Figure 4). One can click to the next hit, as well as go back to a previous hit. The next step would then be to go and print out the results on one of the many printers supported by the system. In the print option (one of the submenu options mentioned in the File menu

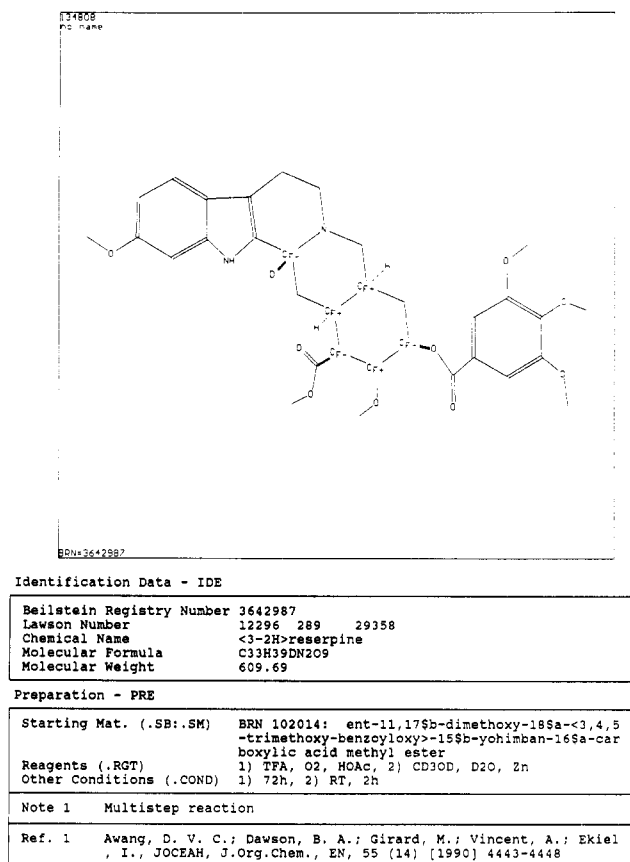


Figure 6. Product from search in which a yohimbane derivative was the starting material.

above), you can choose either structure or data or both, as well as a range of which hits to print out. What is most useful in the display output is the BRN and the Source Field. The former allows you to go online (to STN, DIALOG, or Maxwell/Online—ORBIT) to access the considerable amount of data on a compound which is available online, while the latter allows you to go to the *Beilstein Handbook* to look up additional information on a compound. Thus the online system, *Handbook* and CD-ROM are all well linked and integrated in three useful and complementary products.

The Help menu has five submenus for the areas of help messages. They are **File**, **Search**, **Display**, **Function Keys**, and **Fields Names**. The messages are generally short and clear. For example, Figure 5 shows the help message for the

"Identification" search field. In the case of the field names there are three choices to look at. The first has the field names sorted in Field Code order, the second has them sorted in Field Name order, and the third has a hierarchical sort. The last is perhaps the most useful for someone who is new in using the database.

A number of sample searches were performed, and all seemed to provide appropriate results. One sample search for compounds that have an ionization potential between 7-9 electron volts and contain a Br atom and 2 N atoms gave one hit, 1-vinyl-4-bromopyrazole. A second search, for compounds that are synthesized by using a yohimbane derivative as the starting material, gave three hits. One of the resulting three hits is shown in Figure 6.

All in all this is a nice, easy to use, workable system. The developers should be commended for an excellent product, which makes use of the large capacity of the CD-ROM. With CD-ROM drive prices dropping rapidly and some now selling for about \$400 (including cables and drivers), I would expect to see more CD-ROM products for chemists come to the marketplace in the near future.<sup>3</sup> The current economics of the pricing of this product are surprisingly reasonable<sup>1</sup> and should make it possible for the Beilstein Institute to get the number of users needed for this product to make it a viable product.

To sum it up I would say that Current Facts is a far more useful chemical information product than a collection of bibliographic citations. This CD-ROM deserves serious consideration for a space on every chemist's computer system.

## REFERENCES AND NOTES

- (1) Beilstein Current Facts in Chemistry on CD-ROM is available from Springer-Verlag Publishers, 175 Fifth Avenue, New York, NY 10010 (Phone: 212-460-1622; FAX: 212-533-5781). The pricing depends on whether the CD-ROM you buy is for yourself only (individual) or if you are a *Beilstein Handbook* subscriber and if you are in a university or industry/government. The single unit costs for an individual (either in a university or an industrial company) is \$490.00 per year. The yearly subscriptions for nonsubscribers to the printed *Beilstein Handbook* are \$1490.00 for universities and \$2990.00 for industrial companies. For a current *Beilstein Handbook* subscriber at a university (such as a library) the price is \$490.00 per year, while the price is \$1490.00 per year for a *Handbook* subscriber in industry. The ISSN for this product is 0939-7598. There are also special prices for LAN (local area network) usage for both university and industrial company users. Please contact Springer-Verlag for details on the prices for the LAN version.
- (2) DIALOG Information Services, Inc., 3460 Hillview Ave., Palo Alto, CA 94304. (Phone: 800-334-2564 or 415-858-3785; FAX: 415-858-7069).
- (3) Heller, S. R. NIST/EPA/MSDC Mass Spectral Database, PC Version 3.0 (1): *J. Chem. Inf. Comput. Sci.* **1991**, *31*, 352-354.

## NIST Structures and Properties Database and Estimation Program<sup>1</sup>

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The latest addition to the computerized products of the National Institute of Standards and Technology (NIST) is the NIST Structures and Properties Database and Estimation Program (NIST S&P) written by Stephen Stein, Johannes Rukkers, and Robert Brown of the NIST Chemical Kinetics and Thermodynamics Division. This combination of a database retrieval system and estimation software is designed for both finding and estimating chemical property data. The

database contains thermochemical data for almost 4900 compounds or species from three NIST databases. These are the NIST Positive Ion Energetics Database, NIST Chemical Kinetics Database, and the NIST JANAF Thermochemical Tables Database.

The NIST S&P also contains a complete implementation of Benson's group additivity estimation method for gas-phase heats of formation, entropies, and heat capacities. There is