

Review of Personal Computer Literature Abstract Sources for Mass Spectrometry

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People who work in mass spectrometry have a larger volume of literature available than ever before. With the ever-increasing power of the microcomputer, it has become easier to have these data at hand for reference and to keep current in the field. Electronic abstract programs for use to search and maintain a knowledge of current activities in mass spectrometry from four different sources are compared (see Table 1). Although the reviewed programs and databases cover different periods, all have data through their last distribution for 1994. Comparisons were done on this basis. All four sources have different degrees of specificity. The databases, in order of their specificity, follow:

Current Contents[®] on CD-ROM
Physical, Chemical & Earth Sciences
Institute for Scientific Information[®]
FREE Demo Available

Analytical Abstracts on CD-ROM
The Royal Society of Chemistry
FREE 30-Day Trial Subscription

CASurveyor
Mass Spectrometry and Applications
Chemical Abstract Services (American Chemical Society)
FREE Demo Available

LC/MS Update
GC/MS Update Part A: Environmental
GC/MS Update Part B: Biomedical, Clinical, Drugs
(includes forensics) HD Science
FREE Demo Available

The availability of large volumes of data on a computer is a very good way to do literature searches. There is some question as to its value for keeping current in the field. Many people like to review information on a regular basis in a printed format. If this is restricted to a specific, relatively narrow field like environmental gas chromatography/mass spectrometry (GC/MS), it is not too difficult a task. Even the broader field of mass spectrometry is easy to review when the data come once a week. Looking at these small volumes of data allows an opportunity to see things in an adjacent abstract that can spark an idea. This type of free association is not as available in

digital searches of databases. Large databases probably have the greatest benefit when used for subject searches. However, all of the reviewed products do have software features that allow the user either to look at the most recently distributed information or to perform specific search strategies on it. This capability prevents the need to review the entire database when new issues are distributed.

All four programs were evaluated on a 60-MHz Pentium microcomputer with 32-MB RAM. A 4X CD-ROM drive was used for the databases that required CD-ROM capabilities, and the database that used only a hard drive was loaded onto a 500-MB IDE drive with a 10- μ s access time. All displays were on a 17-in. monitor that operated at a resolution of 1024 \times 768 with 256 colors via a 2-MB RAM video accelerator card. Both Microsoft[®] Windows[™] for Work Group 3.11 and Windows 95[™] were used with all programs. DOS versions of these search programs are available from HD Science, the Institute for Scientific Information, and the Royal Society of Chemistry. Macintosh[®] versions are available from the Royal Society of Chemistry and Chemical Abstract Services. None of the DOS or Macintosh versions was evaluated.

Current Contents on CD-ROM. Physical, Chemical & Earth Sciences

Current Contents Physical, Chemical & Earth Sciences is the most nonspecific of the four databases with respect to mass spectrometry. This database is distributed every week on CD-ROM at a 1995 annual subscription price of \$1995 plus \$50 shipping and applicable taxes. The weekly CD-ROM contains information for the prior 52 weeks. The last issue of the year is an annual archive. The 1995 subscription price includes the 1994 Annual Archive. Annual archives for 1993 and 1994 also are available separately at \$397.50 each. The price for the 1995 Annual Archive will be \$795 if it is purchased as a separate item. The 1996 subscription price is \$80 higher and also will include the prior year's annual archive. According to Barbara Gladney, Market Manager for *Current Contents* products, "*CC on CD-ROM* is intended to be used for both current awareness and for retrospective." In addition to the reviewed product, the Institute for Scientific Information (ISI) offers six other multidisciplinary products. Special pricing is available for group purchases of these products with the *Physical, Chemical & Earth Sciences* edition. A printed version of this database is offered for \$468 per year. However, the printed version does not contain the author abstracts found in the

Table 1. Program comparison

Features	<i>Current Contents</i>	<i>Analytical Abstracts</i>	<i>CASurveyor</i>	HD Science Updates
Degree of specificity	Phys., chem. & earth sci.	Analytical chemistry	Mass spectrometry	Specific areas of mass spectrometry
Available program types	Windows and DOS	Windows, DOS, and Macintosh	Windows and Macintosh	Windows and DOS
Availability and type of demo	CD-ROM with full prog.; limited data FREE	30-Day FREE subscription	CD-ROM with full prog.; limited data FREE	Diskette with limited prog. & data \$10
Distribution media	CD-ROM	CD-ROM	CD-ROM	Diskette
Frequency of distribution	Weekly	Quarterly	Monthly ^a	6 Times/year
Period covered by each distribution	Rolling 52 weeks	January 1980 until present	Rolling 36 months	Since last distribution
Prior issues available	1993, 1994, 1995 annual archives	Not applicable	No	1991-1994 as yearly files
Type of searching	Hypertext	Hybrid hypertext and Boolean logic	Boolean logic	Hypertext
Ability to create and annotate personal database	No ^b	No ^b	No ^b	Yes
Ease of installation	Poor	Good	Good	Fair
Ease of updating	Poor	Unnecessary ^c	Unnecessary ^c	Good
Ease of use	Excellent	Excellent	Fair	Good
Mass spectrometer and conditions identified	Very rare	Seldom	Seldom	Almost always
Ability to search latest data only	Yes	Yes	Yes	Yes
Number of journals covered	900 +	250 +	Up to 3000	250 +
Includes table of contents from cited journals	Yes	No	No	No
Networking	3 Simultaneous users/\$9975	2-4/\$2243; 5-8/\$2990; 9-12/\$4111; site \$5980	2-8 Users/ \$1895	2-5 Users/ price on request
Annual subscription ^d	\$2075 ^e			\$295/series
Price	\$398/'93 & '94	\$1495	\$995	\$695/series
Prior issues/periods	\$795/'95			1991-1994

^a Prior to October 1995, this was distributed quarterly.

^b Records can be exported as text to files in other database management programs.

^c These programs are distributed with all available data.

^d All pricing is single user price.

^e The yearly subscription includes the prior year's annual archive.

CD-ROM version. ISI also has a weekly diskette version that is available with or without author abstracts. The annual subscription rate for the version that contains the author abstracts is \$845. A local area network (LAN) version also is available. The price for a three-simultaneous user annual subscription to the 1995 volume is \$9975; this includes the 1994 Annual Archive.

CC on CD-ROM uses search software from Ovid Technologies, Inc. (New York, NY). This search engine is very good and intuitive. The provided documentation includes a Quick Reference Guide published by ISI and other documentation from Ovid. The Quick Reference Guide, along with a very good interactive help system, is all that is needed. The data provided

are broken into a few clearly labeled fields in an easy-to-read format. This was the only database whose entire 1994 volume contained references to two test articles that appeared in the November 1, 1994 issue of *Analytical Chemistry* and in the October 1994 issue of the *Journal of the American Society for Mass Spectrometry*. The abstracts are the author abstracts provided in the original journals; ISI does no abstracting. If an article does not have an author abstract, there will be no abstract included with the *Current Contents* citation. The citations contained in this database are from over 900 journals. There are 46 journals listed for analytical chemistry. It is very easy to obtain copies of the cited articles. One of the selections on the menu bar's file

menu is "Order Document," which allows you to directly print or FAX an order (provided you have a FAX modem that can be used as a printer output). The full text of the article will then be sent to you through the ISI document delivery service, "The Genuine Article[®]," by either 30-min FAX, 24-h FAX, Federal Express, or U.S. Mail. Many of the articles sent by mail or Federal Express are tear sheets, which provide for better quality charts and graphics. The price for this service, based on establishing a \$300 deposit/monthly bill account, is \$9 for the first 10 pages and \$2.75 for each additional 10 pages. There are varying delivery charges plus the publisher's royalty fees, which vary by journal. None of the other programs tested had this feature. You can still take advantage of this service at slightly different rates without having a deposit/monthly bill account.

The Ovid search engine was, by far, the most difficult to install. It was originally installed when Windows for Work Group 3.11 was loaded on the test computer. It has to be installed from DOS and requires a very large amount of memory below 640 KB. Each database (annual archive) must be installed individually because of the copy protection algorithm used. This is done from an installation program on the CD-ROM. No real difficulty was encountered in the installation of the 1994 Annual Archive. The installation instruction sheet was very poor and, in the hands of someone not really familiar with computers, can cause a lot of problems. Installation of the 1993 Annual Archive was possible only after calling technical support, which was the best I have ever encountered on any computer product. To install the 1993 Annual Archive, it was necessary to edit the CONFIG.SYS file temporarily to free more memory below 640 K. When the demo was installed, memory was corrupted to the point that the computer had to be rebooted prior to running Windows. Ms. Gladney said an October 1995 new release of the software would address these installation issues. The search engine requires about 8 MB of hard drive space; another 75-85 KB is required for each annual archive.

Each annual archive is on a separate CD, which means that the CDs have to be changed as each year is searched. The availability of only a single year of data at one time is not as convenient as access to multiple years, but the ability to maintain search strategies from one database to another helps to limit this inconvenience. When a search is carried out, the criteria are displayed followed by the fields in which they appear in the various selected citations. This step is then followed by the number of citations in a separate column. To display search results, the user may choose a full record view that includes the abstract, an author-title view, or a number of other display options. It also is possible to view the table of contents of the journal in which the selected citation appears.

The inclusion of the tables of contents in the ISI products also enables users to scan the contents as an

alternative to key-word searching. Journals can be selected by discipline and by date, which includes "most recent week." Author abstracts and author and publisher addresses can be accessed from the contents page display. This access allows for a higher degree of free association than usually is found in electronic databases.

The two primary advantages of the ISI *Current Contents Physical, Chemical & Earth Sciences* database are its degree of current data and its weekly distribution. The display characteristics and options of the search engine are superior to some of the other programs reviewed. This product and *CASurveyor* have, by far, the best demo distributions. The ISI demo is a CD-ROM that contains three months of data from four of the multidisciplinary editions, which include *Physical, Chemical & Earth Sciences*. The demo is a fully functioning program that allows the user to see how the search engine works.

Analytical Abstracts

The Royal Society of Chemistry offers the *Analytical Abstracts on CD-ROM*. It is distributed as quarterly updates and is more specific with respect to mass spectrometry than *Current Contents on CD-ROM*. The CD has data from 1980 through the quarter of issue. There are over 180,000 records on each. Over 1200 citations are generated each month from a core list of over 250 journals, selected because of their importance to analytical chemistry. The entire database contains citations from over 3000 journals. Each CD-ROM issue will contain 3600 + new citations. The database contains abstracts of all the citations since 1984; those prior to 1984 are not abstracted. Like the American Chemical Society, the Royal Society of Chemistry prepares its own abstracts. According to the brochure, "The specially written English abstracts highlight the analytical method..." Information seldom is provided as to the mass spectrometer or its operating conditions other than those for the gas chromatograph in references to GC/MS.

The search software installs very easily by using the Windows program manager file/run command and the SETUP.EXE program that is on one of the two program diskettes. The resulting program group has two icons: one for the program and one to configure the program. The search software requires a little more than 2.6 MB of hard disk space.

This database uses a fairly straightforward search engine developed by SilverPlatter International, N.V. (Norwood, MA). Search results and strategies can be saved from session to session. Individual records can be selected and a record of this selection can be saved. The display of the search result was well organized and offered several options. The default installation configuration did have some limitations: it would allow saving only to a floppy diskette in drive A and it would allow only 20 records at a time to be printed.

This limitation was remedied quickly by using the program called from the reconfiguration icon. The records are saved in a text format only. They could be imported into some other database manager, but the user would have to develop the appropriate data links to the imported text field labels. The searches were fast on the test computer and accumulated from search to search, which allows return to an earlier search without repetition. When key words are entered, several searches can be generated. As an example, a search on "mass spectrometry" yielded search results for "mass," "spectrometry," and "mass spectrometry." The data associated with each abstract are arranged in up to 26 separately labeled fields, dependent on the available information. The CD-ROM labeled January 1980 through December 1994 was missing citations to the two test articles that appeared in *Analytical Chemistry* and the *Journal of the American Society for Mass Spectrometry* in the last quarter of 1994. According to Judith Barnsby, Marketing Officer for *Analytical Abstracts* at the Royal Society of Chemistry, the lag time between the publication of an article and its appearance in *Analytical Abstracts* is three to nine months, whereas that of the printed format is three to six months due to its monthly publication. It should be remembered that this database is a general analytical database. Of the 180,000 + records on the examined CD-ROM, only 8868 records were found when a search was done for "mass spectrometry."

In addition to the *Analytical Abstracts* (AA on CD-ROM), the Royal Society of Chemistry also offers other CD-ROM products: *Environmental Chemistry, Health & Safety* (ECH & S on CD-ROM) updated quarterly, *Chemical Business News Base* (CBNB on CD-ROM) updated every two months, and *Chemical Engineering and Biotechnology Abstracts* (CEABA on CD-ROM) updated quarterly. These other database products use DIALOG OnDisc[®], from DIALOG Information Services, Inc. (Palo Alto, CA), as the search engine.

AA on CD-ROM has several advantages, two of which are the period of prior data covered and the specificity of the abstracts to the analytical method. Another unique feature is the inclusion of separately labeled fields for the analyte, matrix, and general analytical techniques. According to Ms. Barnsby, "[Like *Current Contents*,] the wider coverage of *Analytical Abstracts* means that it is most useful to people who are working with several techniques, not just mass spectrometry or departments with several analytical specialties."

The price for AA on CD-ROM is \$1495 annually. The Royal Society of Chemistry also publishes *Mass Spectrometry Bulletin*, which is a monthly current awareness service for mass spectrometry, that is available in printed and diskette formats. The price is \$995 if you subscribe to the hardcopy form of *Analytical Abstracts* (\$970 for a one-year subscription published monthly). Several local area networking options are

available: 2-4 users, \$2243; 5-8 users, \$2990; 9-12 users, \$4111; site license, \$5980.

CASurveyor. Mass Spectrometry and Applications

CASurveyor is produced by the Chemical Abstracts Service organization, a division of the American Chemical Society. *CASurveyor*, now published monthly, is specific to the overall field of mass spectrometry. Prior to October of 1995, *CASurveyor* was published quarterly. Each CD-ROM contained citations for the prior two years plus the current cumulative year to date. This was a rolling three years of information. The volume tested contained abstracts for the years 1992 through the end of 1994. Now that *CASurveyor* is published monthly, it will contain a rolling 36-months of data. Expired versions are not available. The annual subscription for the 12 issues is \$995. There was no price increase with the increased number of issues when the distribution went from quarterly to monthly. The material contained on the CD-ROM is broader than that which appears in *CA Selects for Mass Spectrometry*. According to Charles Hatfield, Product Manager for *CASurveyor*, the inclusion definition was broadened from that used for *CA Selects*. The price for the 26-issue annual subscription to *CA Selects* is \$210, and there is no bundled pricing for the hardcopy and CD-ROM. A 2-8 simultaneous user local area network license is available at a yearly subscription rate of \$1895.

The contents come from a core of 1300 journals reviewed in their entirety by Chemical Abstracts Service. Another approximately 7000 journals are surveyed and partially abstracted. CAS implemented *CA Plus*, a service that has been available on-line, that includes author abstracts rather than CAS-generated abstracts. These eventually are replaced by the CAS abstracts. *CA Plus* allows for an earlier reference to articles. The *CA Plus* citations for mass spectrometry articles will be included in the monthly issues of *CASurveyor*. The records will be noted when they are author abstracts. Citations to the two test articles were not found in the database through the end of 1994. This was explainable because, according to Mr. Hatfield, without the inclusion of the *CA Plus* contents, it could take as long as six months until a citation appears in *CASurveyor*, dependent on the time when an article appeared and the degree of complexity to abstract it. With the inclusion of *CA Plus* and the monthly distribution, the maximum time for a citation to appear in *CASurveyor* should be no more than a month.

The search software easily installs from SETUP.EXE located on the CD-ROM. Less than 1 MB of hard disk space is required. Searches were quick. The software was not as intuitive as the other three programs but, once understood, was somewhat easy to use. This program came with a single User Guide for both the Macintosh and Microsoft Windows versions, which

created some difficulties. You have to be careful you are not in a Macintosh section when you are using the Windows version and trying to figure out how something works. The User Guide is provided with its own support stand and is spiral bound at the top of the pages, which allows it to be used as a hands-free standup reference while working with the program. This proved to be very convenient when first learning the program. On the Windows menu of the menu bar were "Tile" and "Close All" selections. These were nice features to view and deal with the program's multiple windows. Each time an abstract is displayed, a new window is opened. This program, unlike the other three reviewed, uses mostly Boolean logic searches rather than hypertext or a hybrid of hypertext and Boolean logic. The exception is the use of hypertext for CAS Registry number and similarity word searches. Each search criterion (word, author, journal name, MOL formula, etc.) must be correct in its totality or followed by an appropriate wild card symbol (* or ?). A good example of this had to do with an "author" search. If a "word" search was done by using only the last name of an author, hits that matched the author's name would be found along with the names of organizations and so forth. If an "author" search was done by using only the last name of the author, no hits would be found. The last name of the author had to be followed by the string wild card (*). This produced hits for all authors with that last name. Each time the program starts, you are prompted to select a database by using a standard Windows file selection dialog box: the default drive and directory contain the search program. This annoyance can be eliminated by specification of the location and name of the desired database as an argument to the command line. Unfortunately, this information is not included in any of the reviewed documentation. Mr. Hatfield said this information was contained in the help screens for version 2 of the search engine. Version 2 was received just as this evaluation was being completed and currently is being shipped to subscribers. It addresses a number of issues that have been raised by users. Unfortunately, if you want to look at older versions of the data (1991-1993 CD-ROMs), you must maintain the previous version of the software. This really is not a concern because of the small amount of disk space required by both versions. Version 2 actually requires about 200-KB less disk space than version 1.

The search results are displayed as a list of document titles preceded by the number of times your search criteria appear in the citation. Version 2 has wordwrap added to this display, which is a great improvement over the single line that extends off the right edge of the screen. Once a citation is displayed, it is easy to jump to another by using the "Next Doc" or "Prev Doc" buttons located at the top of the window. The fields are not labeled as in the other three pro-

grams tested, and the author field is very specific. This database contains CAS Registry numbers, which are absent in the other reviewed databases, for all named compounds in an article. You can place the cursor on a CAS Registry number and select the "Goto RN" button on the program's button bar or double click the CAS Registry number to display the substance record. This record may include the substance's CA Index name, IUPCA name, other related common and trade names, molecular formula, and chemical structure.

The primary advantages of *CASurveyor* are its price, timeliness (both in terms of delivery and data contained), amount of literature reviewed, specificity to mass spectrometry, and inclusion of the CAS Registry data.

LC/MS Update, GC/MS Update Part A: Environmental, and GC/MS Update Part B: Biomedical, Clinical, Drugs (includes forensics)

The three separate *Update* series offered by HD Science are, by far, the least expensive and most specific of the four products tested. The annual subscription price is \$295 each plus \$40 for shipping and handling. Because the HD Science *Updates* are distributed for specific restricted disciplines, the price for a specific interest area is relatively very low. The prior four years of any of the three can be purchased for \$695. This is the only non-CD-ROM distribution tested. Each *Update* series is distributed in six issues yearly on diskette. Each issue is a separate file, but a cumulative file for the year is included. The volumes for previous years are distributed as single files for each year. Hardcopy versions of the three series are also available at the same price. There is no bundled pricing. HD Science also offers a *Mass Spectrometry Analytes 1991-1993* series. There are four titles in this series: *Pesticides, PCDDs/PCDFs/PCBs, Water and Sediments, and Drugs and Drug Metabolites*. They are abstracts selected from the *Update* series. Supplemental editions of the *Analytes* series will be available.

The *Update* series use *Info Select* (Micro Logic Corp., Hackensack, NJ), a personal information manager, as its search engine. This is distributed through HD Science for \$145 and is required to use the data in the *Update* and *Analytes* series. This program installs very easily from a single diskette by using a Windows SETUP.EXE program run from the file selection on the program manager's menu bar. All the data are stored on the hard disk in the same directory as the program. The amount of space required depends on how you arrange the files. Each annual *Update* in the series requires between 750 KB and 1.9 MB. Cumulative files for each are now between 4 and 6 MB (this is 1991 through the first issue of 1995). The limiting factor for this program is the amount of extended memory available on your computer. All data are loaded into RAM

and you must have sufficient memory for the file you load.

Use of the program is very straightforward. Setup and maintenance are a little more difficult. If you want to combine the annual volumes or if you want a specific database to be loaded automatically when *Info Select* starts, a number of steps must be taken. These steps require some knowledge of computer software and some time to get an understanding of *Info Select*. Some users may find this tedious. The data in an individual issue can be reviewed easily without interference from prior data because each issue is distributed as an individual file. Each issue for each of the *Update* series has around 200 abstracts. The abstracts are taken from a review of over 250 journals. Book reviews and proceedings of some meetings are included.

In addition to its low price, the *Update* series has several other features that make it unique. It is the only one of the four reviewed products that allows for creation of separate databases that can be used in exactly the same way and by the same program as the distributed data. The individual abstracts can be annotated by the user. They can become a part of the distributed data or they can be used with a personal database. The personal annotations can be saved as underlined and/or bold text.

The search engine is very easy to use. Any string, no matter where it occurs in the abstract, is searched by typing the text in the find field of the search dialog box. As you type, the database is searched. If you get to a point where there are no hits for an entered string, then the letters to the last string found are erased automatically. Once a search is complete, you can select the search dialog box's OK button and the first found abstract will be displayed. It is very easy to move from abstract to abstract. The location of the abstract in the database is shown graphically on a vertical scroll bar on the right side of the display. Another unique feature of the HD Science abstracts is their meaningful identification numbers, whereas the other three products use esoteric identification numbers. The number in each abstract has a specific meaning, which is intuitive. As an example, the first abstract in issue 1 of the 1995 volume of *GC/MS Update Part B: Biomedical, Clinical, Drugs* is B95:1:1.

The most unique feature of the *Update* series is the abstracts themselves. They emphasize the sample preparation and instrumental technique. An abstract of an article in one of the other three reviewed products on the identification of a protein, where mass spectrometry was used, will emphasize the structure of the protein and its significance. The HD Science *Update* series abstract will, in many cases, provide sufficient information to begin to explore the analytical technique prior to obtaining a copy of the complete article. The specific instrument used, operating conditions, sample introduction mechanism, and sample prepara-

tion details nearly always are included. The abstracts in the *Update* series emphasize the mass spectrometry technique; however, there is still information included as to the significance of the work.

The dates on the three CD-ROM products not only are supposed to reflect the period covered but also the actual date of issue. The HD Science *Update* series usually will have more than one of a year's issues sent to subscribers well into the next year. There is a two to five simultaneous user LAN option for *Info Select* and the HD Science abstracts. Pricing is available on request from HD Science.

According to Steve Down, Publisher at HD Science, the biggest single advantage of the *Update* series is inclusion of information that pertains to the instrumental technique, which allows an investigator to do early experimentation prior to receipt of the complete article. This, along with the ability to easily create a personal annotated database, makes for a very good product for persons responsible to extract data from a mass spectrometer. It also is very useful in the overall study of mass spectrometry.

The helpfulness and knowledge of all marketing, sales, and support people contacted with regard to these four products was very refreshing, especially when compared to other personal computer products.

Addresses and telephone numbers for the four organizations that provide the reviewed products follow:

Institute for Scientific Information, Inc.
3501 Market Street
Philadelphia, PA 19104, USA
Tel: 215-386-0100 Fax: 215-386-2911
Toll-free: 1-800-336-4474 and press 2 for an ISI Sales Representative
email: isioder@isinet.com
or

Institute for Scientific Information, Inc.
Brunel Science Park
Brunel University
Uxbridge UBS 3PQ, UK
Tel: +44-1895-270016 Fax: +44-1895-256710
email: uksales@isinet.com

The Royal Society of Chemistry
Thomas Graham House
Science Park, Milton Road
Cambridge, CB4 4WF, UK
Tel: +44-1223-420066 Fax: +44-1223-423429
Toll-free: 1-800-473-9234 (US only)
e-mail: marketing@rsc.org
or

SilverPlatter Information, Inc.
100 River Ridge Drive
Norwood, MA 02062-5026, USA
Tel: 617-769-2599 Fax: 617-769-8763
Toll-free: 1-800-343-0064

Chemical Abstract Services (American Chemical Society)

CASurveyor, Department 84M
2504 Olentangy River Road
P.O. Box 3012
Columbus, OH 43210-0012, USA
Tel: 614-447-3776 Fax: 614-447-3671
Toll-free: 1-800-848-6538

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