International Spring School on the Digital Library and E-publishing for Science and Technology
CERN, Geneva, Switzerland, 3 – 8 March 2002

Digital Library and E-Publishing Developments in Chemistry

Engelbert Zass
Chemical Information Specialist, ETH (Swiss Federal Institute of Technology) Zürich, Chemistry Biology Information Center, Switzerland

ABSTRACT

Based on the author's experience with chemical information retrieval in an academic special library, trends in scientific information and their consequences for libraries are outlined. The ETHZ Chemistry Biology Information Center is used in this context as an example for an ongoing transformation from a traditional special library to a digital library and information services center.

INTRODUCTION

A significant amount of scientific information is now available in electronic form, secondary information like abstracting & indexing services already since the early seventies, primary publications like journals or patents since the mid-nineties. There can be no doubt that this availability has a dramatic influence on the operation of science libraries. This influence extends far beyond the rather simple effect of replacing the medium paper by electronic storage and presentation forms like e-journals, databases on servers, handbooks on CD-ROM, etc.

Let us take a look at some important traditional library functions in order to analyse the recent and future changes:

- major source of information access for users;
- archiving information;
- Collection development: procuring (selecting) and organizing information (cataloguing).

Information **access** is certainly affected most: scientists in the first half of the 20th century had most of the needed information sources available to them by personally subscribing to journals, abstracting services, and (in chemistry) to handbooks like *Beilstein* or *Gmelin*. In the second half of the last century, however, they became very much dependent on the holdings of their library as the increasing number of scientific journals and the increasing cost for journals and reference works eroded and later eliminated the feasibility of covering major information needs with personal subscriptions. Nowadays, with databases marketed as "end-user systems" (cf. below), electronic journals, and the entire Web as informal medium, a significant part of scientific information is again available at the office/workbench of the individual scientists. The amount of information thus available is growing fast. This implies that users need to go to the library much less than before, and that traditional library holdings are reduced in their importance.

A similar development is being observed regarding **archiving** of information, one of the central functions of large regional and national libraries. With more and more information in electronic form, archived under the current system by the producers, not the libraries, this function is at least significantly diminished, with future roles quite uncertain at present. Likewise, even the "freedom" of selectively licensing electronic information is partly taken over by large library consortia, and further reduced by producer-defined information "packages" (e.g., e-journals) that may only be licensed in their entirety, or not at all. For cost reasons, a lot of local **cataloguing** is replaced by buying standard catalogue records from catalog consortia in the US, or in Europe by "Bibliotheksverbünde" [1] that share catalog data via a common OPAC system.

Consequently, libraries are converted all over the world to "digital libraries", "electronic libraries", "hybrid libraries", "virtual libraries" to react to these changes – somewhat unfortunately, these changes were mostly forced on libraries by technological developments, publishers, and user demands, and not influenced, let alone determined by them to an extent that represents their traditional importance in the scientific information chain.

Before we discuss our experiences and ideas about such an ongoing transformation in the ETHZ Chemistry Biology Information Center [2], it is necessary to mention some aspects particular to chemical information [3] that influence this process.

CHEMICAL INFORMATION

Chemical information is distinguished from information in other scientific fields by the aggregation of the following factors:

- The **chemical structure** [4] as the visually and conceptually "outstanding" quality in chemical information: structures are a very precise means for communicating chemical information even across language barriers which cannot be matched by any other method of description like indexing. The "price to pay" for this was additional complexity and expense already in the print age. This is aggravated in the electronic form by the need not just to display structures as graphics besides (much simpler to handle) text, but also to make them searchable in a chemical sense as a whole or in part. This is still a demanding process, both for algorithms trying to cope with the complexity of chemical structures (which are not as straightforward as the graph-theoretical concepts borrowed from mathematics used to handle them), and for the computer systems to search very large structure collections.

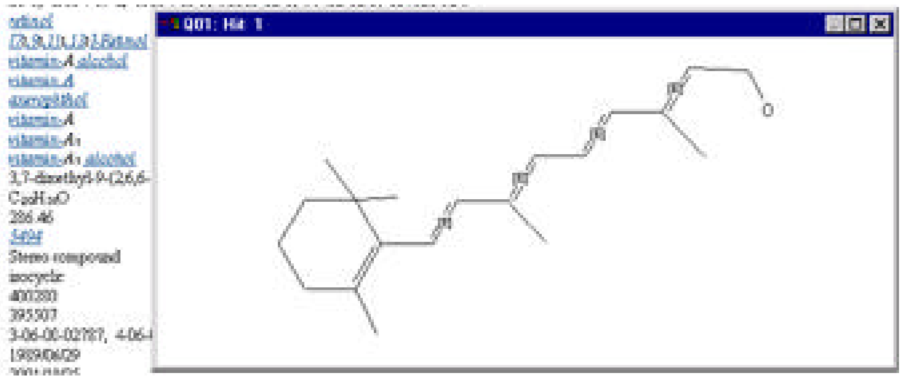

Figure 1. Structure of Vitamin A from the *CrossFire Beilstein* database (screen dump, © Beilstein Institut zur Förderung der Chemischen Wissenschaften)

- The **quantity** of chemical information: almost 40 million chemical compounds are reported in databases, growing by no less than about 130'000 new compounds per week [5]! Further, there are more than 20 million corresponding publications, and in excess of 10 million chemical reactions; these involve also chemical structures, but need their own special databases and search facilities because of additional features particular to chemical reactions. In the order of 50 million (the exact number is not known) property data are reported and searchable for chemical compounds. Not surprisingly, chemistry databases are surpassed in size and number of records only by patent databases (which contain to large extent chemical information!).

- The remarkable **tradition** for chemical information sources: journals devoted to chemistry (*Crells Chemische Annalen*, 1778) followed a century after the first scientific journal ever, the *Philosophical Transactions of the Royal Society of London* in 1665. In order to make the already at that time large volume of primary publications accessible, secondary publications started in 1830 with the *Pharmaceutisches* (later *Chemisches*) *Central-Blatt*. The most typical chemical secondary sources, the appropriately structured/indexed Handbooks about chemical compounds and their properties partly antedated this: *Gmelin Handbuch der theoretischen Chemie* 1817, *Beilstein Handbuch der organischen Chemie* 1881, etc.

Figure 2. Printed Gmelin Handbuch der Anorganischen Chemie (part of 8th edition)

- A very large commercial **market** for chemical information sources due to the chemical industry: This is one of the major reasons why chemistry was among the first areas of science for which databases were produced, and probably has one of the most varied offerings in electronic information sources.

TOWARDS DIGITAL LIBRARIES

INFORMATION RESOURCES

Journals, reference works (abstracting & indexing publications, handbooks), and books (monographs) have all been moved to electronic media. There are, however, distinct differences at present regarding the extent of that "conversion", the acceptance of the electronic form with users, and the role they play in providing the necessary information for scientists. Some of these differences existed already for the print versions, but others are new due to the medium.

Historically, abstracting & indexing publications were the first to be available in electronic form. They preceded e-journals by almost a quarter of a century. Most scientists refer to such electronic collections of secondary information like *Chemical Abstracts* [6], *Science Citation Index* [7], etc. when they use the term "database" The introduction of this first category of electronic sources was rather gradual over time, and most libraries easily adjusted to this by offering guided searches in these databases for their customers; these first-generation databases were too expensive and too complex for end-users. Thus, scientists in this phase were actually even more dependent on the library for their information: they not only had to go to the library for the then dominating printed sources, but needed personal assistance there for database searching while they had used their printed predecessors on their own. At the ETHZ Chemistry Department, we already tried then to get electronic information to the workplace by training and supporting a "database specialist" in each research group. This measure in the eighties was successful within its supposed limits, but with the cost and effort involved certainly not the desired general solution to improve information supply for individual chemists.

This changed completely when improved graphic interfaces became available for chemistry databases. This development began already around 1985; at ETHZ, we started in 1985 to offer the reaction databases REACCS, ORAC, and SYNLIB via the network directly to chemists [8]. Effects on the way chemists searched for information were relatively minor at first with these specialized databases. Only about 10 years later, "usage-friendly" interfaces like *CrossFire* [9] and *SciFinder (Scholar)* [10] became available for the all-important large chemistry databases *Beilstein*, *Gmelin*, and *Chemical Abstracts*. Then, however, changes were fast and dramatic: users do no longer come to the library for searches, the printed secondary literature corresponding to these databases is no longer used at all, and consequently, subscriptions were terminated, or the production of the print equivalent was even discontinued as for the Handbooks *Beilstein* and *Gmelin*.

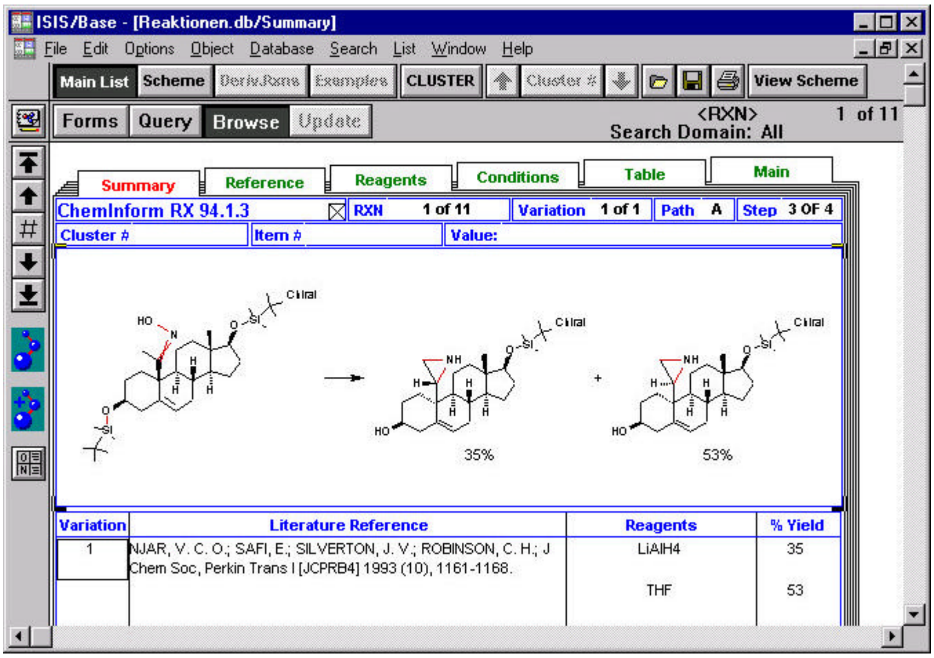

Figure 3. Modern GUI for chemical reaction database
(screen dump from MDL Reaction Browser, © MDL Information Systems)

Changes did not only occur in user behavior: while the public databases have been offered by hosts taking care of operating, accounting, and other necessary technical-administrative measures, end-user client-server database systems in chemistry were (and in their majority still are) only available as "in-house" systems. This implied that licensing institutions had to operate their own servers. In the case of the abovementioned reaction databases at ETHZ, the server was operated by our computer center. When we licensed *CrossFire Beilstein* in 1994, we were faced with the necessity to operate our own server as the computer center no longer offered such facilities. With other, smaller Swiss universities having the same problems, this led to the development of a *de facto* chemistry consortium to share hardware and operating expenses among Swiss universities in 1995 [11]. Similar developments happened in most other countries. In this way, libraries really started "going digital" by operating information servers not only for their OPACs and library Web sites, but also for databases. Cooperation among academic institutions, first to reduce operating overhead, then to license databases as a consortium, has become another important task for libraries.

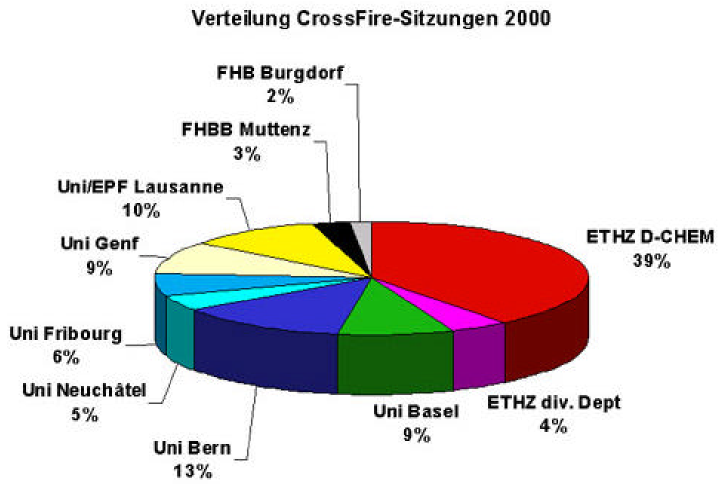

Figure 4. Swiss chemistry database cooperation: usage statistics for ETHZ chemistry server (distribution of searches in *CrossFire Beilstein* and *Gmelin* in the year 2000)

Electronic versions of journals became available on a broad front only in the second half of the nineties; their relatively fast introduction based on accepted standards (formats html/pdf, browser access), the popularity and success of the Web, and the parallel developments in the secondary literature mentioned above made them the fastest adopted electronic resource. Given the numbers and importance of journals in a science library, this had far-reaching effects on the role of libraries and the behaviour of users.

For libraries, electronic journals mean even more added cost to ever-mounting prices for scientific serials ("serials crisis"), and an additional workload that had usually to be covered without increase of staff. Printed issues have to be kept in parallel to electronic editions in most cases, to satisfy license requirement of some publishers, or to fulfill traditional archiving obligations. Printed issues are also often needed to provide copies for article delivery, as many publishers prohibit the production of such copies from the electronic versions. Despite the excellent acceptance of electronic journals by many scientists, they still want the printed issues for browsing and serendipity, and they want it near their working place, i.e., in their special library. With many multiple journal subscriptions already eliminated for cost reasons even before the advent of e-journals, this raises the issue of where to store the only remaining print copy: in the special library, where users strongly want it, or in the central library for archiving and article delivery? When discussing acceptance and use of e-journals, we have to keep in mind that they are usually not read on the screen, but printed out in the majority of cases. While copies from printed journals were usually only taken for the scientist's personal literature collection, or for thorough reading with marking pens, articles from e-journals are often printed out even for cursory reading and browsing. Offering printed journals for browsing may thus reduce waste of paper.

Even though they may no longer be physically available in the library, we found that electronic journals must be catalogued as individual issues like their printed counterparts; simply providing a link to the journal home page of the publisher is definitely not the kind of service a digital library can be content with. With the publishers unfortunately changing the links to the electronic issues on their servers from time to time, and with many such links not regular enough for automatic processing, keeping links to individual issues working requires a major effort.

Figure 5. Printed journals ready for browsing in the ETHZ Chemistry Biology Information Center

But being a digital library implies to treat all information units alike that are needed by users, regardless of their medium – their should be no principal difference between a printed book, a print or electronic journal issue, a video, a CD-ROM, or an important URL! We are well aware of the fact that this implies a break with several library cataloguing traditions, and lots of manual and intellectual labour for information entry and the even more important upkeep. When OPACs shall have a useful role in the future, they must incorporate all these features, and they must be enhanced with user-configurable portal functions instead of being only simple electronic lists of physical holdings in the library. The OPAC of a digital library must, for example, offer customisable tools to handle new journal issues, like the *Organiser* tool we realized as part of our Web OPAC CLICAPS [12].

Electronic journals are at present mostly used for current awareness, and the retrieval of more recent references. Scientists have to cope with a plethora of electronic sources for current awareness – Web pages, search engines, e-journal issues, alerting services by publishers, host database alert profiles (once called “SDI”: selective dissemination of information), and special TOC (table of content) databases like *ISI Current Content* [13]. Digital libraries should advise users on these information tools and how they differ in function.

For retrospective searching that usually starts in secondary literature databases, direct links from the literature references therein to the primary sources are strongly demanded by users, and essential to integrate the electronic secondary and primary literature. Despite the “back file conversion” projects of print to electronic journals already in progress by major commercial publishers and scientific societies [14], a large amount of primary information will only be available in print for some time to come. Unless these printed holdings are linked together with electronic journals to databases, we run the danger that users will try to circumvent the older, non-electronic sources because they are less easily accessed. This must be avoided by all means. We think that a combination of links to the printed sources as well as e-journals in the OPAC of the nearest library [15], augmented by an e-mail article delivery service from a large central library [16]., is a useful solution to this problem.

Not surprisingly, many initiatives and solutions for linking journal citations to full articles came up in the last few years, both from references in secondary sources (which I propose to call “vertical links”) as well as from a citation in a journal or patent to another primary source (“horizontal linking”): there are, for example, gateways like *ChemPort* [17], facilities like “hop out” in the *CrossFire* client software *Commander* to link *Beilstein* and *Gmelin* references to journals (both printed holdings and electronic full text [15]) and patents, more powerful, user-configurable software like *LitLink* [18] for the same purpose, and the *CrossRef* [19] initiative of important publishers.

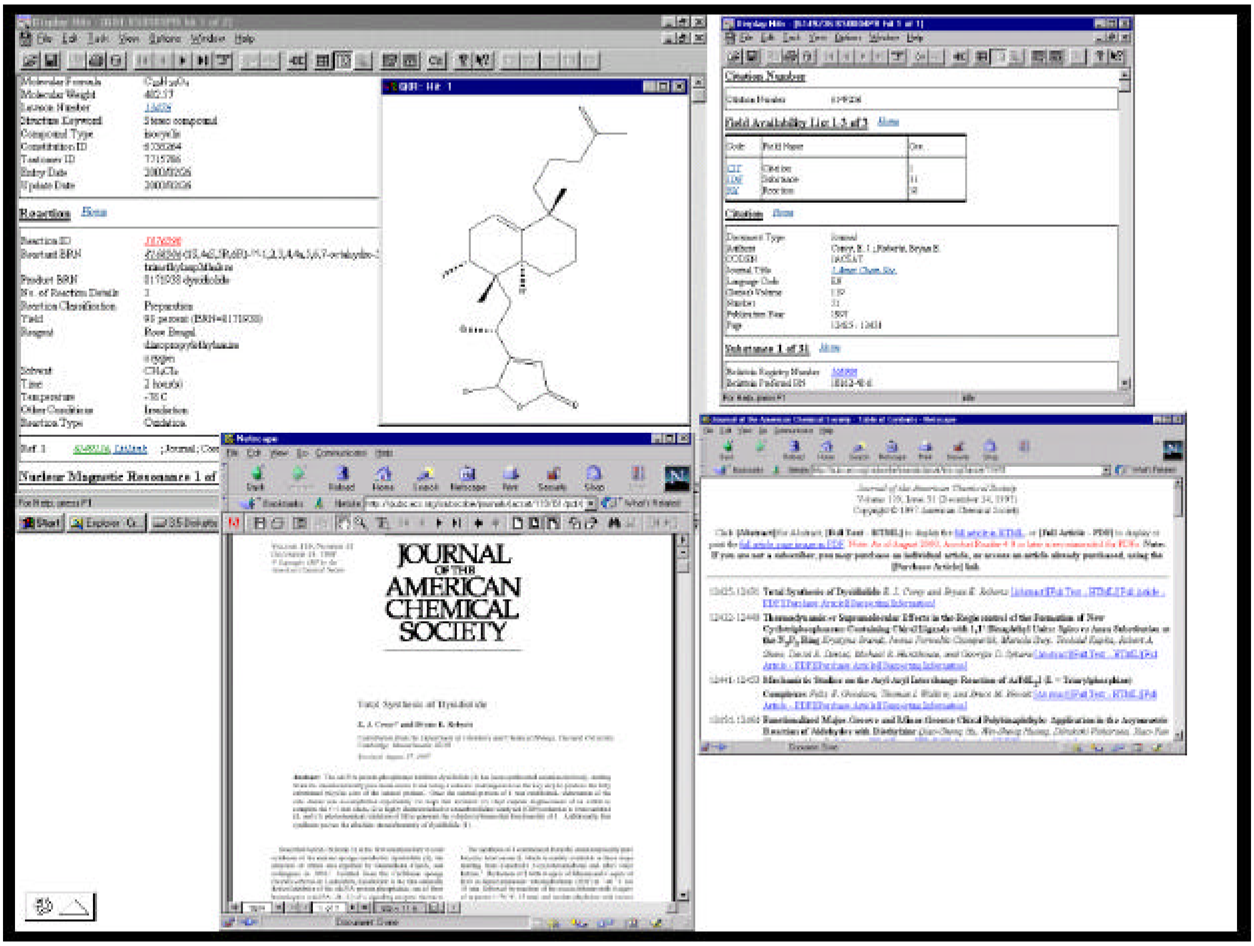

Figure 6. Linking databases to e-journals (collage of screen dumps from Beilstein CrossFire database to e-journal: clockwise from top left)

Electronic books are relative latecomers, they are so far the electronic sources least accepted by users, and are not yet widespread. It can be assumed that libraries will continue to play an important role in this information segment for the foreseeable future, provided they integrate the new e-books with their massive holdings of printed books.

STAFF AND FACILITIES

Many people working in scientific libraries have some formal scientific education in addition to their formal qualifications as librarians, but with the latter often dominating. For modern digital libraries with value-added services to users, the emphasis on staff qualification will change: the majority of staff at least in science areas will be fully trained scientists, and a certain number of IT specialists, both preferably with an additional qualification as librarians/documentation specialists.

Moving from the information offerings to the physical premises of a digital library (which cannot be entirely digital and virtual if it is to fulfil its task as we see it!), it is of course mandatory that every working place offers power supply and network connection. At the ETHZ, implementation of a laptop university has recently started in the context of the *ETH World* project concept [20]. In the ETHZ Chemistry Biology Information Center, we are ready for that by offering a wireless LAN for our users. Walk-in users, or those that did not want to carry their laptop around to the library, still need to work on library computers that we have to provide and maintain (Fig. 7). We found that users contact us often with their computer problems, both those directly related to information retrieval, as well as those of a more general nature. Consequently, a digital library needs a lot more IT expertise and appropriately qualified staff not only to cope with the internal IT demands (network, library servers, staff and user workstations), this experience and competence should also be made available to users.

This raises the wider context of integrating computer centers, network/communication IT staff, and libraries to a common information infrastructure for commercial and academic institutions. Particularly in the latter institutions, this means a significant reorganization, the breaking of many political barriers, and overcoming many cultural differences. Assuming that this will not be an easy and fast process, digital libraries are well advised to play that support role for users until a more encompassing solution will be available.

Figure 7. One of 32 user stations in the ETHZ Chemistry Biology Information Center

E-PUBLISHING

The "serials crisis" which has dominated discussions in library circles for years is now also a topic among scientists themselves. Many scientists have suggested that they or their institutions publish their papers directly, bypassing commercial publishers which many consider to be highly profitable at the expense of the taxpayer's money that finances to a large extent both the production of publishable scientific information (i.e., basic research) as well as the public (academic) libraries that have to buy the expensive publications on demand of the scientists. Many people involved agree that the present publication system may not be continued very much longer in the same way as before for economic reasons. The long-established scientific information chain author – primary publisher – abstracting & indexing service (database producer) – provider (library, host) – reader has shown changes recently for libraries and hosts. The latter lost database revenues due to sales of database systems like *Web of Science* [21], *CrossFire* [9] or *SciFinder* [10] directly from producer to customer. Primary publishers, however, were obviously much less negatively affected by the move to electronic sources. Both electronic-only journals, or journals published directly without commercial or society publishers are very few, and without significance yet [22]. Chemists and other scientists are obviously very conservative with regard to changes in a publication system that is very closely tied to peer recognition and rewards like tenure or promotion.

More engagement in the publication process by libraries is in my opinion desirable, but I doubt that they will play a significant role in e-publishing in the near future. This assumption is corroborated by several observations. With the majority of chemists taking a Ph.D., theses and research reports do contain a wealth of information not published elsewhere, but they are hard to find, and even harder to come by. Despite the fact that academic libraries have been in a very favourable position possessing these sources, projects for electronic theses are relative recent and not well known among users [23]. Recent additions to the "information scene" in medicine and science, "Web communities" like *BioMednet* [24] or *ChemWeb* [25] were not created by libraries, but by individuals or commercial publishers. It is probably realistic to assume that libraries will mostly stay at the "receiving end" in the publications chain, and thus only be able to react instead of acting and influencing developments in scientific communication.

For the far majority of scientific journals, e-publishing means just publishing an electronic version besides the print that looks (at least in the pdf format preferred by many users) just like the print. Added features like ASAP (full text "as soon as publishable" before completion of an issue), links from references to other publications, full-text search engines have not really changed the established paradigm. Features to overcome that paradigm, like including dynamic multimedia elements (animations, video sequences), or e-only-journals that significantly deviate from the time-honored journal structure, are still very few, and with very limited impact [22]. We have to face that fact that most scientists are "paper-minded" in the sense that the advantages of the electronic medium for retrieving information are well accepted, but that the working medium (and by consequence, also the publishing medium) is still paper.

The "serials crisis", the problem of journal pricing, cannot be solved by libraries by belatedly mimicking concentration processes on the publisher side with licensing consortia that are now so popular, but only by principal changes in the entire publication chain, involving authors, readers, publishers and libraries.

SERVICES: SUPPORT, TRAINING, EDUCATION

We have indeed come quite some way from the complex, yet feature-limited command-driven search interfaces of the first-generation databases to modern GUIs in client-server systems, with Web browsers the best-known and heaviest used example for this information retrieval architecture. But even one of the most advanced interfaces for searching chemical information, *SciFinder (Scholar)* [10], has its pitfalls, as the following examples try to illustrate.

A search [26] for literature on the important chemical compound Vitamin A (cf. Fig. 1) may be executed in two obvious ways with *SciFinder Scholar*. A first approach ("Explore by Chemical Compounds", Fig. 8) used the name of the compound to retrieve it in the compound database, and then retrieved 14'166 literature references for this compound. In a second approach, we used the name "Vitamin A" as a keyword ("Explore by Topic", Fig. 8) which gave 33'844 references. The difference is easily explained by the fact that although the database banner announces the availability of the literature back to 1907, the first (compound) approach misses most of the pre-1967 references (only 13 were retrieved) while the second (keyword) in contrast retrieved 12'323 references before 1967. The user is not properly notified about this handicap. Despite the obviously much larger result in the second approach, this misses quite a number of references found in the first; an approach combining both features retrieved 34'606 references. Users not appropriately trained will not only be unable to formulate the third, most comprehensive query used here, they will most probably incorrectly assume that any of the first two approaches gives the complete literature present in the database!

The situation becomes even more complex when one searches not for "straightforward" organic compounds like Vitamin A, but for inorganic compounds or materials: a search for Titanium Nitrides, important as ceramic materials, retrieved with an obvious, simple query ("molecular formula TiN") in SciFinder only 6 compounds; a slightly modified query "Ti.N" (using knowledge about CAS compound indexing that is unfortunately not really commonplace among chemists, as we keep noting) got 256 compounds in SciFinder Scholar, while a search using the command-driven STN Messenger interface [27] to exactly the same structure database retrieved no less than 307 compounds!

This demonstrates that the usage-friendly interfaces like *CrossFire* [9] or *SciFinder (Scholar)* [10] now at long last available in chemistry, do make the **handling** of searches much easier, but do not solve the majority of the problems originating in the underlying large and very complex databases. Another important aspect must be mentioned in this context: the developments discussed before have increased the number of different information sources, and made them available electronically at the "point of need" at the scientist's workplace.

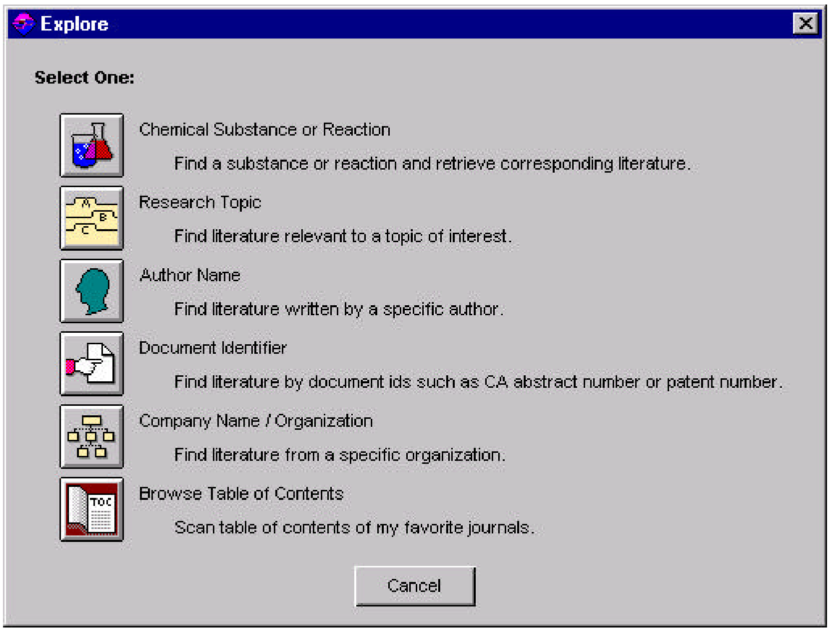

Figure 8. Search mode ("Explore") selection menu from SciFinder Scholar (screen dump, © American Chemical Society)

A lot of the potential for improved information supply inherent in these new and powerfully searchable sources, however, cannot be realized by users who do not have the proper "meta information" about content, coverage, strengthens and weaknesses of the many electronic sources. Producers are not providing appropriate "boiler plates" for their databases, although they are able and should be required to do so. They are, for obvious reason, in no position to critically compare their sources to those of competitors. Consequently, libraries have to come to the aid of users in both respect, and they are quite capable of doing that.

Another problem related to the increasing number of electronic sources is the increasing number of "electronic variants" of the basically same source. The single most important chemical information source is an example in point: while there existed only one print version of *Chemical Abstracts* (with indexes for keywords, compounds, etc.), there are now no less than five different media/interfaces for the corresponding database suite offered by *Chemical Abstracts Services* [6]: print, *CA on CD*, *CA Student Edition*, *SciFinder*, *SciFinder Scholar*. This number does not even include the different implementations of the *Chemical Abstracts* literature and structure databases offered by several hosts; the most important of them regarding chemistry, *STN International* [27], alone offers with the native command language *STN Messenger*, the front end *STN Express*, *STN on the Web*, and *STN Easy* four interfaces to these databases that not only differ significantly in the ease of use, but even more so in the search facilities offered. This variety for just a single source – I could have also used the well-known *Science Citation Index* [7] as an example to make the same point – is bewildering even for information specialists and potentially dangerous for the end-user, the scientist.

Nevertheless, the far majority of information searches are done now by scientists themselves at their workplace, and no longer by information specialists at a library/information center. One of the most common misconceptions in this context is the assumption that the availability of present electronic information sources with the so-called "user-friendly" interfaces like *SciFinder (Scholar)*, *CrossFire*, *Web of Science* and others will *per se* greatly improve information supply, and enable an average chemist to solve most of the questions her/himself. This notion is for obvious reasons propagated by the producers of such systems; however, it is not only invalid to the extent used, it is also dangerous concerning he quality of information supply. A certain degree of information literacy is indispensable to utilize the present systems, and this can be achieved with a reasonable efficiency only by appropriate education, training, and support for users. Experienced, qualified scientific staff in special libraries is predestined to provide this literacy in close contact with the science educators in academia.

With regard to this problem, we have since the early days of database use at our department (1979) offered training courses and support, both tailored to the specific needs of our customers. This was augmented in 1984 by a formal chemical information course to educate chemistry students [28]. Since 1998, most courses are taught with the assistance of a Web-based course system. The aforementioned collaboration among Swiss academic chemistry departments for the operation and licensing of chemistry databases has been extended in 1999 to a cooperation in teaching chemical information courses involving all eight Swiss university chemistry departments [29].

As a further means of local support, we pooled in 1994 the user stations for accessing electronic sources (at that time, mostly databases on CD-ROM) in an "Electronic Library" where a chemist as support person is on duty during opening hours to assist users. Since 1995, we use our Web pages not only as a means to inform users about our information offerings (Web OPAC, list of available databases etc.) and services (training courses etc.), but also as a platform for supporting the use of databases by providing installation instructions, troubleshooting information, meta information about databases, search examples, and tips and tricks.

The means described so far – courses, Web pages, personal support – are not yet considered sufficient to reach the majority of users. We therefore have recently started to develop multimedia training and teaching modules for chemical information. These modules are intended to augment and support our courses as well as for individual self-study [30].

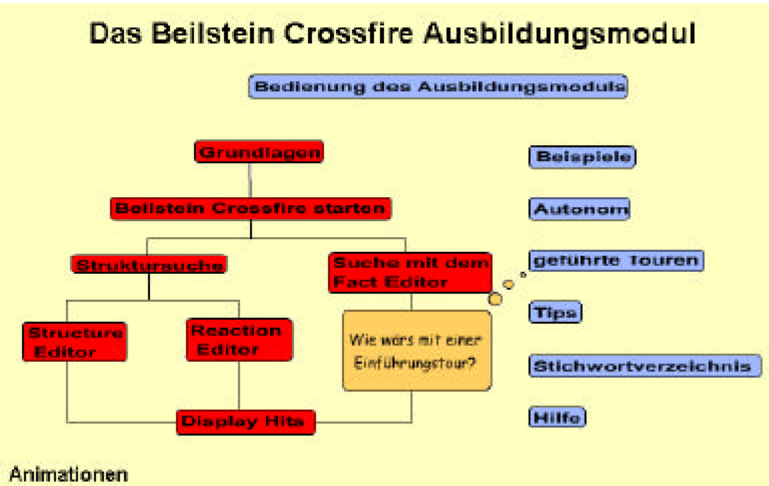

Figure 9. Start Screen of *CrossFire Beilstein* training module [30]

We are convinced that besides the services outlined here, libraries in research institutions will in the future delegate staff part-time to assist scientists with research project that are particularly information intensive research projects. This of course will only be possible if the libraries will be provided with enough qualifies staff, a major problem unresolved at present in many libraries.

We consider support services of the kind discussed here an important and indispensable part of digital libraries, augmented at least in academic libraries by educational services. As it is true that users no longer need to come to the digital library for a lot of the information they need, we should induce them also in our own interest to personally come to the library premises for services and support. Modern libraries will be much more dependent on their success to satisfy actual users needs, and before they can do this, they must find out these needs.

OUTLOOK

What we have to keep foremost in mind is that libraries have lost their long-time stronghold as information providers – people can and do get information in most other places independent of the library as a physical place, and (albeit to a lesser extent) also independent of the library as an institution. Consequently, if we want to stay in business and justify our existence (and the public money spent for many of us), we have to offer much more than just information access, and this tailored to real user needs to a larger degree than ever before. Information supply in general is still a “provider market”, particularly with regard to publishers/producers, but no longer so for libraries. For them, it dramatically changed to a “buyers market”. Consequences need to be taken from that, just “going digital” is not enough.

Good libraries have of course been much more than just nicely maintained collections on shelves, they always provided a variety of reference and other support services to help users get the information they need. Such services, however, were often regarded as subsidiary to holdings and catalogs. Nowadays, libraries can no longer just wait for the users to come and use their (once indispensable) sources, they must outreach to their customers and actively solicit problems they can help to solve. The key concept for digital libraries must thus involve more than a change of the medium, it must involve a change from a predominantly holdings orientation to a predominantly service orientation. According to our long-time experience, at least in a complex scientific area like chemical information, there are not yet user-friendly databases around, but there must be user-friendly librarians available right now.

Regarding the fact that some of the developments in digital information clearly need (and thus favour) large organizations like central libraries and consortia, one can specifically question the future of smaller, special libraries. Our answer is that with the necessary service and user-orientation, appropriately staffed special libraries in close physical and intellectual contact with users are more important than ever, as their roles in direct support, tailored training, and education cannot be adequately fulfilled by large central libraries or consortia alone.

ACKNOWLEDGMENT

I thank all my colleagues from the team of the ETHZ Chemistry Biology Information Center for their cooperation, and in particular Dr. Martin Brändle for helpful discussions while preparing this manuscript.

NOTES, LINKS, AND REFERENCES

Abbreviations:

GUI:	graphic user interface
IT:	information technology
LAN:	local area network

[1] For example, the Swiss German NEBIS consortium http://www.nebis.ch/, or Südwestdeutscher Bibliotheksverbund (SWB) the http://www.bsz-bw.de/verbundsys/.
[2] ETHZ Chemistry Biology Information Center: http://www.infochembio.ethz.ch/.
[3] W.A. Warr, C. Suhr: Chemical Information Management. VCH, Weinheim 1992.
[4] J. Ash, W.A. Warr, P. Willett (eds.): Chemical Structure Systems. E.Horwood, Chichester (UK) 1991.
[5] Average growth per week of the CAS Registry structure database in 2001.
[6] Chemical Abstracts Service: http://www.cas.org/.
[7] Science Citation Index: http://www.isinet.com/isi/products/citation/scie/index.html.
[8] E. Zass, S. Müller: *Chimia* **40**, 38 (1986). Neue Möglichkeiten zur Recherche von organisch-chemischen Reaktionen: Ein Vergleich der "in-house" Datenbanksysteme REACCS, SYNLIB und ORAC.
[9] CrossFire: http://www.beilstein.com/products/xfire; see also literature in http://www.infochembio.ethz.ch/Xfire_dokumentation.html.
[10] SciFinder: http://www.cas.org/SCIFINDER/scicover2.html; academic version SciFinder Scholar: http://www.cas.org/SCIFINDER/SCHOLAR/index.html; see also literature in http://www.infochembio.ethz.ch/SFS_dokumentation.html.
[11] E. Zass: Online Inf.Proc. 22, 39-46 (1998). Large chemical databases in-house: serving CrossFire and ISIS to an academic user community. For usage statistics of databases, see http://www.infochembio.ethz.ch/Xfire_statistics.html. Licensing is now handled by the "official" Swiss consortium established in 2000: http://lib.consortium.ch/.
[12] CLICAPS Web OPAC: http://www.clicaps.ethz.ch/CLICAPS.html; *Organiser*: Option "Persönliche Zs-Liste" on this page.
[13] ISI Current Contents: http://www.isinet.com/isi/products/cc/ccconnect/cccsitewide/index.html.
[14] See, for example, http://pubs.acs.org/liblink/PR_Journal_Archives.pdf, or http://www.diglib.org/preserve/ejp.htm.
[15] For our implementation of this feature to link to the primary literature, see http://www.infochembio.ethz.ch/datenbankvernetzung.html.
[16] For the delivery of articles scanned from print-only journals as pdf files by the ETH Library, see http://www.ethlife.ethz.ch/news/show/0,1046,0-5-1083,00.html.
[17] ChemPort: http://141.66.18.180/html/english/about.html.
[18] MDL LitLink: http://www.mdli.com/cgi/dynamic/product.html?uid=&key=&id=31.
[19] CrossRef: http://www.crossref.org/.

[20] ETH World: http://www.ethworld.ethz.ch/; laptop project: http://www.ethlife.ethz.ch/tages/show/0,1046,0-8-1102,00.html and http://www.neptun.ethz.ch/.

[21] ISI Web of Science: http://www.isinet.com/isi/products/citation/wos/index.html.

[22] Springer's originally "electronic only" *Journal of Molecular Modeling* founded in 1995 (http://link.springer.de/link/service/journals/00894/), for example, had to provide archival versions in both electronic (CD-ROM) and print from on request by users and libraries. Both the *Internet Journal of Chemistry* (http://www.ijc.com/), and *Molecules* (http://www.mdpi.org/molecules/) are examples for e-journals of a new type that are tailored to the facilities of the medium.

[23] For example, http://www.theses.org/ (US), http://www2.chemie.uni-erlangen.de/services/dissonline/ (one of several German projects), http://e-collection.ethbib.ethz.ch:80/diss/ (ETHZ Library), http://www.arcs.ac.at/DissDB/welcome;internal&action=_setlanguage.action?LANGUAGE=ge (Austrian National Theses Database).

[24] http://www.bmn.com/.

[25] http://www.chemweb.com/.

[26] Searches on Jan 21st 2001 in SciFinder Scholar, literaure restricted to *CA plus* database (i.e., *Medline* excluded).

[27] STN International: http://www.stn-international.de/.

[28] E. Zass: Chemical Information Education, in H.R. Collier (Ed.), "Proc. Montreux 1989 Int. Chem.Inf. Conf.", Springer, Berlin 1989, p. 55.

[29] http://www.infochembio.ethz.ch/troisiemecycle.html.

[30] The first example was a *CrossFire Beilstein* training module (Diplomarbeit S. Zwimpfer: Entwicklung eines multimedialen Ausbildungsmoduls für Beilstein CrossFire. Fachhochschule beider Basel 2000/2001). The majority of the present work is done in the context of the German "Leitprojekt "Vernetztes Studium – Chemie" (see http://www.vs-c.de/).

