ABSTRACT: There is no science without communication. The enormous amount and the quick growth of scientific literature means it can be treated, organized, stored and retrieved only in digital form. Learning to master the use of new information and communication technology (ICT), and getting to know how to collect and select appropriate scientific information is imperative during university education. The essential requirements, both information sources and technical equipment, have been established for the Hungarian academic community within the framework of a national government project EISZ (Ministry of Education, 2001). In the Department of Chemistry at the University of Szeged the old course “Chemical Literature” has been re-formed into “Chemical Information Retrieval”. A short survey of the literature related to the subject, a brief description of the project EISZ and the course content, methods and assignments are presented here. [Chem. Educ. Res. Pract.: 2003, 4, 373-385]

KEY WORDS: chemical information; information retrieval; ICT; university education

INTRODUCTION:

“Communication is the essence of science” (Francis Crick)

At the very beginning scientists communicated their results by gathering together for talks or by private letters. These informal methods have been developed into formalized regular meetings and scientific papers during the 17th century (Williams & Bowden, 1999). The first chemical journal was established in the 18th century (Chemisches Journal established by Lorenz von Crell in 1778). Progression of the last 225 years can be summarized in 5 periods, which are getting shorter and shorter:

- 1778-1940s, birth of primary journals and compilations, indexes, abstract journals, reviews stored and retrieved manually;
- 1940s-1960s, although the chemical literature is stored using mechanical or electromechanical sorters, retrieval still relies generally on printed sources;
- 1960s-1970s, the chemical literature is stored and retrieved using electronic computers, the first completely computer indexed Science Citation Index started in 1964;

Francis Crick is one of the Nobel Prize Winners in Medicine, in 1962, who were given the award "for their discoveries concerning the molecular structure of nucleic acids and its significance for information transfer in living material" (Press Release, Nobel Foundation) http://www.nobel.se/medicine/laureates/1962/
1980s, the chemical information is supplied on-line, the trial running of CAS On-line started in 1976 and the on-line equivalent of Chemical Abstracts in 1983;

1990s-nowadays, scientific communication takes place via the Internet.

One of the most dedicated information scientists is Eugene Garfield (Garfield, 2002), who was originally a chemist. Current Contents, the Index Medicus, the Science Citation Index are all related to him. He is the founder of the ISI (Institute for Scientific Information) and the bi-weekly journal for research professionals, The Scientist.

THE LITERATURE OF TEACHING CHEMICAL INFORMATION RETRIEVAL

The literature of teaching chemical information is enormous. This paper does not make an attempt to give a complete bibliography on this subject. Instead it refers to Carol Carr’s annotated bibliography (Carr, 2000) of the time period of 1993-1998 and lists articles which have been published since then (Ricker & Thompson, 1999; Wilk & Wiger, 2000; Murov, 2001; Ridley, 2001a; Ridley, 2001b; Zass, Braendle, & Bizzizzero, 2001; O’Reilly, Wilson, & Howes, 2002; Christensen, Franzyk, Frolund, Jaroszewski, Staerk, & Vedso, 2002; Gallagher & Adams, 2002; Landolt, 2002; Jackson, 2002; Porter, Lee, & Wiggins, 2002).

A brief overview of the literature of teaching chemical information retrieval can be centered around four questions. Why teach? What to teach? How to teach? Who should teach?

Why teach? It is beyond dispute that chemical information retrieval must be included in the chemistry curriculum. But it may be useful and perhaps necessary to list considerations for the faculty as well as for the students. One of the most important things in becoming an independent scientist, not merely a technician, is having information skills. The expanding scientific information, the diversity of the sources and the new information technology have transformed our libraries into library and information centers, and the scientific literature into scientific information. Students should learn the basic techniques: to handle computers, to select the most appropriate source, to build up and run a searching process, and to evaluate sources/information. It is too much, and too complicated, for self-learning. This perception led to the creation in 1991 of The Chemical Information Instructor, the special column in the Journal of Chemical Education for discussing methodology of this subject.

Some further considerations are as follows: (i) good information skills save time and money for the scientist and his employer; (ii) to be involved in a scientific community

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The compilation is based on a three step literature searching procedure:

1) Subject search in three databases (the Web of Science/ISI, the SciFinder Scholar and the Elsevier’s Science Direct) using the following search strategy:

- chemical information retrieval AND education AND 1999-2003
- chemical literature AND education AND 1999-2003
- information retrieval AND chemistry curriculum AND 1999-2003

2) Author search in the same timespan in WoSc using the “author” search field, and the “address” field when required, to focus on some of the most acknowledged specialists of the subject: Carr C, Murov S, Rzepa HS, Somerville AN, Whitaker BJ, Wiggins G and Winter M. In this step related- and cited records as well as the citing articles have been checked.

3) Browsing the Journal of Chemical Education issues of the same period as the special source of the subject.
nowadays is impossible without information skills; (iii) information skills help to make a successful career.

What to teach? The content of courses has been changed in the last three decades, which can be indicated with three words: literature, information, Internet. Undergraduate and graduate courses can be categorized into four main types: general courses in information retrieval, courses in specific subject area (e.g., organic chemistry), courses in specific information sources (e.g., Beilstein or Chemical Abstracts), and courses in specific types of source (e.g., Internet).

How to teach? Independently or integrated within chemistry courses? Separate traditional and online techniques? Problem- or source-driven approach? Each solution has advantages and drawbacks and the right choice basically depends on the possibilities in the department.

Who should teach? Co-operation of librarian and chemist is a suitable solution but it is more and more desirable to have an instructor educated both in chemistry and library science as well. Reflecting this new demand there are special university programs e.g., Chemical Information Specialization and Master of Library Science at Indiana University (Indiana University, 2002).

EISZ (Elektronikus InformációSZolgáltatás)
THE HUNGARIAN ELECTRONIC INFORMATION SERVICE

Electronic information service or electronic library or digital library is a completely new organization resulting from the new information and communication technology. The definition of the digital library according to the Digital Library Federation (2000) is as follows:

“Digital libraries are organizations that provide the resources, including specialized staff, to select, structure, offer intellectual access to, interpret, distribute, preserve the integrity of, and ensure the persistence over time of collections of digital works so that they are readily and economically available for use by a defined community or set of communities.”

In the mid 1990’s several initiatives aimed to maintain separate collections of digitized information. (Vikor, Gamound, & Heath, 1997, Ober 1999, Swartz 2000). Digital libraries can be hosted by academic institutions, government agencies or international organizations (Witten, 2003). They can group complex content or focus on a specific subject, e.g., medical sciences (Papadakis, Chrissikopoulos, & Polemi, 2001).

The exponential growth of information production makes it almost impossible to store information in printed form. Increased subscription fees, the costs of mailing, copying and interlibrary loans can be lowered by sharing information sources in an electronic format. Digital technology has much greater power regarding content organization and retrieval too. Moreover, Hungarian library collections were very poor regarding foreign scientific journals before 1989 because of political reasons. These facts have forced the government to build and maintain a digital library. To take the preliminary steps, already existing national electronic information services of other countries have been studied. The Finnish model has been taken into consideration predominantly (Szántó, 2000).

EISZ is the name of the Hungarian national project, which provides electronic information resources for the higher education and academic institutions. It was launched in 2001. The following sources are now available:
• **ISI Web of Science** (Science Citation Index Expanded, Social Science Citation Index and Arts & Humanities Citation Index back to 1973)
• **ScienceDirect (Elsevier Science)** (more than 1200 full-text journals back to 1998 and the abstract database: MEDLINE back to 1967)
• **Lecture Notes in Computer Science (Springer)** (timespan: back to 1982)
• **Hungarian journals online (Akadémiai Kiadó)** (34 international and 9 Hungarian)
• **Dictionaries (Akadémiai Kiadó)**
• **ARCANUM (Arcanum Adatbázis Kft.)** (10 databases on Hungarian language and literature, history, culture)
• **Tesztre készen! (prepared for test)** (interactive English and German exercises).

Highly respected specialists in library and information sciences are in charge of the acquisition of EISZ and developmental activities.

**TEACHING CHEMICAL INFORMATION AT THE UNIVERSITY OF SZEGED**

During the last few decades the one-hour class course *Chemical Literature* was included in the chemistry curriculum. The course introduced chemistry major students to the organization and use of the department’s chemistry library. Beside general library information, the printed Chemical Abstracts was the main field of study. Handling review publications and handbooks of specific subject areas were integrated in chemistry courses e.g., printed version of Beilstein in the advanced organic chemistry lab.

Making full use of our very limited possibilities, we have organized elective courses on portions of the title subject over the last ten years. Our tools were the non-commercial sites of chemical organizations and universities, the catalogues of chemicals and the MEDLINE, the free of charge bibliographic database of National Library of Medicine. As we had no access to any of the main commercial chemical information sources, we tried to give an insight by hunting for free trials. These courses were restricted regarding the number of students as well because our department did not have its own computer laboratory. Anyway, these first steps have resulted in an independent and comprehensive chemical information retrieval course.

Reform of the chemistry curriculum connected with the introduction of the credit system and the set up of the department’s computer laboratory (financed by a special fund of the government) have made possible the establishment of a new course. *Chemical Information Retrieval* is a compulsory two-credit hours course for chemistry major students from this year. It is a general introductory course, which does not focus on a specific subject area or information source and does not segregate traditional and digital technologies. We handle the chemical literature as a consistent unit. The fundamentals of library and information science, the use of the science library, the classification of sources, the basic concepts of starting and building up a searching process are handled regardless of the technology. But the electronic format is the main focus as it is very new for us and for our students. The teaching aims can be summarized briefly as follows:

- to make students realize that there is no single source having all the information we are looking for;
- to teach how to start information retrieval, what the starting points can be;
- to demonstrate that various types of information source exist and to show when to use each type;
- to give fundamental criteria for evaluating sources in order to choose the right one;
to train students in the basic steps of a searching process, to show how to develop an organized plan for gathering information on a particular topic;

- to become familiar with the major chemical reference tools and the full text sources available at our university;

- to show that the Internet is a great place for looking up information but critical evaluation of sources is essential.

**COURSE ORGANIZATION**

*Prerequisites:* The course is open for students who have completed 4 credits in informatics. It is strongly recommended to enroll on the course in the 4th semester or later after completing some basic chemistry courses.

*Participation:* Attendance is compulsory as all subjects are demonstrated and exercised. We meet students every week for one and a half hours in the department’s computer laboratory. The upper limit of the class size is 20 students.

*Teaching resources:* We do not use a textbook. There is no Hungarian textbook and no English one is available at the department or in the university libraries. Electronic “handouts” prepared by tutor are available during the semester on the tutor’s homepage.

*Expectations:* Homework assignments based on the previous week’s experience must be submitted in electronic format as attached files. Final grades are based on these simple library exercises, a compilation of data and information about a chosen topic and a structured bookmark file for personal use in chemical research.

*Teaching methods:* All possible methods that serve the use of new information technology are applied. Lectures are held in the computer laboratory of the department. Topics are discussed using a power point presentation and are illustrated mostly with the help of on-line sources. Students accomplish simple tasks in every class working on their own with a computer. During the semester we are in communication with students by e-mail; they get back their homework with comments, and they can ask help for making or improving assignments. The “handouts” as .ppt and .html files are available on the teacher’s homepage. These contain the outline of the course and links to the most important chemical sources. In addition students are referred to Internet based reference materials (Howe, 1993) and tutorials of database producers (ISI 2002, CAS 2003).

**COURSE CONTENT**

**Week 1**

*Information. Document types. Basic tools of new IT*

Terms like information, information society, information gap, information industry, are discussed briefly and some features of information are given (e.g., synergism, dependency on environment). Classification of documents are presented in detail:

- primary or secondary or tertiary
- based on information content (bibliography, catalog, full text document, facts or data collection)
 physical form (printed or electronic)

with further categorization of electronic sources with regard to access method, file format and method of payment.

There is a ‘brushing-up’ of basic information technology skills and tools at the beginning of the Chemical Information Retrieval course (e.g. creating and processing electronic files of different formats; Internet, www, e-mail, attaching file).

**Exercise 1:** Choose a topic in chemistry for practicing chemical information retrieval during this course. Define some general and specific terms, or a compound name related to your subject. Depending on the source/tool sometimes you will need general or specific terms or a single compound name.

**Exercise 2:** Send me an e-mail message (find my address) with the following content: your name, how often and for what purpose you use computers, your chosen topic.

**Scientific communication, tools for gathering information**

Scientific communication tools can be divided into informal and formal categories. The informal channels (conferences, lectures, discussions, correspondences) differ from the formal ones (patents, papers, books, research reports) regarding their content, aim and audience. As the formal tools are stored, indexed and processed (in libraries or databases) they can be retrieved, thus they communicate science across distance and time.

There is no single way to become well-informed. The following tools are available to gain information: libraries; conferences, seminars and workshops; publishers, journals and experts in special fields; personal scientific connections; and the Internet. The new information technology has not only improved the efficacy of the traditional channels greatly, but also produced new forms of them (e.g. electronic library, mailing list, e-mail, preprint servers).

**Exercise 3:** Connect to the university library web site (http://www.bibl.u-szeged.hu/), find OPAC (Online Public Access Catalogue) of our university and Oxford University. Run the same search. Indicate from the first ten items in the result lists the primary and secondary literature sources.

**Exercise 4:** Go to the catalogue (http://www.bibl.u-szeged.hu/bibl/online/ejou.html) of online periodicals and find two full-text primary and two full-text secondary sources with different publishers.

**Week 2**

*Search tools of the Internet: search engine, subject directory, meta-search engine, subject-gateway* (Online Information Review, 2000), *portal*

An appreciation of the advantages (e.g. more up-to-date material; easy handling and processing of information) and the problems (redundancy and overlap; the lack of quality control; constantly changing or disappearing sources; scattered, not integrated information) of the Internet, and a comparative understanding of the basic navigating tools, are essential for their effective use.

Search engines, web directories and subject gateways are prepared differently and therefore their way they are used, the size and quality control of their content, and their target audience are distinct. Further considerations within this topic are: the hybrid nature of many of the resource discovery tools, to the advisability of applying different tools to find adequate
information, and the availability of computer tools for discovering non-Internet sources via the Internet (bibliographic databases, online library catalogues).

Internet subject gateways are especially important in scientific information retrieval. According to T. Koch (2000) the key characteristics of the quality-controlled subject gateways are:

- editors, information and subject specialists are involved in the creation, development and management of the resource collection
- published selection criteria
- resource description (metadata, annotation/summary/abstract)
- deeper levels of classification (keywords/subject heading systems, thesauri)
- regular updates through record and link checking.

Several gateways have developed into portals providing other services (access to databases, personalization, news, conferences, and job vacancies). C. Glander-Höbel (2002) gives an overview of chemical subject services of the Internet. In the class some subject gateways of scholarly or academic Internet resources e.g. INFOMINE (University of California, 1994), BUBL (2003) and special chemical search engines/portals as ChemFinder (CambridgeSoft Corporation, 2003), MetaXChem (Chemie.DE Information Service GmbH, 2003), ChemIndustry (ChemIndustry.com Inc. 2003) are visited and discussed:

**Exercise 5:** Connect to http://www.infopeople.org/search/chart.html, select one search engine, one meta-search engine, one general directory and one scholarly directory. Compare their database size and ranking method. Run a search using Boolean operators. How many items have you found?

**Exercise 6:** Connect to http://www.chemweb.com/, join by registration and answer: Is it a gateway or a portal? Is it quality-controlled according to Koch?

**Week 3**

*The invisible web* (Price, 2002a)

In January 2003 Google was the number one Web search engine regarding the size of the database (Leita, 2003) (indexed pages were about three billions: $3 \times 10^9$!). In addition to this huge number there is a tremendous number of web pages, which are not found by the general search tools. The indexed part of the web is estimated from 20 up to 50 % (Clyde, 2002). The other 50-80 % of the web is called the invisible web (or hidden or deep web). As a chemical search is very different from any other search method, in that compounds can be characterised by their name, molecular formula, Chemical Abstract Services (CAS) Registry number, or structure, common search engines are almost useless in the field of chemical compounds. Therefore, chemical search engines/portals can be classified as the tools of the invisible web as well. Focusing on science, the following tools make possible to find information on the invisible web:

- building of our own collection (bookmark)
- invisible web directories (Sherman & Price, 2001; Price, 2002)
- the Librarian Index to the Internet (Berkeley Digital Library SunSITE, 2003), which is a hybrid tool (search engine and subject directory) maintained by library and information specialists
- Scirus, the special search engine from Elsevier Science (2003).
Scirus is a science-specific search engine. Beside digging far deeper than most search engine crawlers, it focuses on websites containing scientific content, and indexes important scientific journal sources (e.g. Medline, ScienceDirect, Beilstein Abstracts, or Chemistry Preprint Server).

**Exercise 7:** Visit the website http://www.scirus.com/, access About us and find answers to the following questions: Why use Scirus ahead of other search engines? How does Scirus rank results? What content is covered by Scirus? What is the Chemistry Preprint Server?

**Exercise 8:** You finish your MSc studies this year and you want to study for a PhD somewhere abroad. Using Scirus find a position in your selected field. Submit the data (name, address, phone, fax, e-mail) of the institution, a short description of the program, and a completed application form (or the url of the page providing admission information).

**Evaluating Internet resources**

There are several reasons (no reviewers and editors, no cost of publication, everybody can put information on the net, etc.) why an incredible amount of junk can be found on the Internet.

“The term grey literature refers to a wide range of types of informational material, which is made available to the general public by public and private sector organisations whose function is not primarily publishing.” (Quinion, 2003)

On the other hand there are very often so many advertisements built into a website that it is difficult to distinguish them from authentic information. A bibliography (Auer, 2003) of this subject can be found on the website of Virginia Tech University Libraries.

The most important criteria by which to judge the worth of an Internet source are its coverage, content, authority, accuracy, currency, currency, graphic and multimedia design, and ease of use. Students do one of the free interactive tutorials (Social Science Information Gateway, 2003, Henderson, 2003, The Ohio State University Library, 2003) teaching the critical evaluative skills through quizzes and practical exercises.

**Exercise 9:** Find the homepage of the Hungarian Chemical Society and review it in every respect. What is your final conclusion? Rate it on a five-point scale.

**Week 4**

**Description of databases**

The term database can be defined (The American Heritage Dictionary of English Language, 2000) as “a collection of data arranged for ease and speed of search and retrieval”. In library and information science we use it in a narrower sense. It refers to regularly updated file of digitized information related to a specific subject or field (Reitz, 2002). As chemistry produces an especially enormous output of data, databases have great importance. To be effective in information retrieval it is necessary to know all about different databases. The following description helps students to make themselves familiar with any scientific database:

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3 The CAS Registry Number is assigned to a substance when it enters the CAS REGISTRY database. On Tuesday 7 October 2003, the CAS Registry had reached number 600115-98-8, counting 22,243,508 organic and inorganic substances. Approximately 4,000 new substances are added each day: http://www.cas.org/substance.html
Exercise 10: Characterize the National Periodical Database http://www.iif.hu/db/npac/, which is the union catalogue of foreign periodicals held by the Hungarian libraries.

Searching databases

Though databases are different from the whole span of the Internet, any general electronic research process consists of the following steps:

- determine goals (to define topic in the form of a question)
- choose database (by checking coverage, type and cost of available databases)
- identify search terms (to collect broader and more specific terms and synonyms, to consult controlled lists and indexes of the database, to gather specific authors and specific journals/sources related to the subject)
- build search (to combine terms with operators, to choose search fields and limit fields, to adjust settings, to determine how results are displayed
- run search
- analyze results and modify search strategy
  - results not on target (check spelling, find more exact terms, check that the appropriate database has been chosen)
  - too many results (use narrower terms, use limit fields, use more AND, use less OR)
  - too few results (check spelling, use more general terms, use more OR, use less AND, find additional search terms from within papers you have already found: co-authors, paper’s keywords, cited, citing and related articles)
- re-run search
- save, print, export or e-mail the list of records retrieved (and selected)
- document the search process (date, database, exact search strategy, number of retrieved and selected records).

Exercise 11: Spectra Online http://spectra.galactic.com/SpectraOnline/Default_ie.htm is a web-based free spectral database. Describe it according to the characteristics discussed earlier. Supply the names, formula, structure, physical data, mass spectrum, FT-IR spectrum and NMR spectra of the compound CAS Reg.#: 121-33-5. Search an organic molecule involved in your chosen topic and collect the same data in one file.

Weeks 5-8

The EISZ: Web of Science and Science Direct

This is the core source of the course as it provides two major commercially available databases for the academic community. Web of Science and Science Direct are characterized in detail regarding coverage, type, search tools, search rules, elaboration of results and special services. Three points are especially emphasized:
Beside traditional subject-author searching the ISI Web of Science has a unique tool, cited reference searching. Thus, information seeking both forward and backward in time can be done.

The coverage of a database created by the producer can be different from the coverage of the database to which we have access depending on our subscription. This should be made clear.

Services and tools depend on the version of the database as vendors are improving their products continuously. It is recommended sometimes to check the version number and consult notices for new features.

Subsequent to the overview, students test all available functions of the two databases during the lessons.

**Exercise 12:** Run a search according to the given process in a three-step search strategy.

**Week 9**

*Chemical Abstracts and SciFinder Scholar*

The different sections of Chemical Abstracts (CA) in printed form are available in different libraries of Szeged. The electronic version is not included in EISZ; our university has one access at a time as a member of a consortium. As a consequence the main aspect of teaching this topic is to demonstrate the differences between the two forms, such as coverage (content and timespan), effectiveness, currency of information, search tools (the chemical structure search option). The library terms index, abstract, author abstract, abstracting service are also discussed here.

Beside on-line demonstration of the SciFinder Scholar the downloadable interactive guided tutorial (CAS, 2003) helps training. This provides key facts about the databases and guides the student’s ‘hands-on’ experience in operating this database.

**Exercise 11** Starting with the index guide formulate a question and make a literature search in the printed CA on your chosen topic.

**Week 10**

*Beilstein: Beilstein Handbook of Organic Chemistry, Beilstein CrossFire, Beilstein Abstract*

Students get an introductory overview of the printed Beilstein including coverage, content, a detailed summary of the Beilstein System, its indexes and the general procedure for determining the Beilstein volume relevant for a particular organic compound. Detailed instructions, examples and exercises are given during the organic chemistry laboratory course.

A general survey is given about Beilstein CrossFire too. It is explained, that in addition to factual data, the abstracts of papers published since 1980 are available. Furthermore, the program AutoNom, which can translate chemical structures into systematic IUPAC names, is integrated. Due to our limited access to CrossFire, only one on-line presentation is possible, so students cannot practice during the class. It is highlighted that regardless of the publication technology (printed or electronic) Beilstein is the oldest secondary source with references to the chemical literature back to 1771 and the largest and most comprehensive factual data collection of organic chemistry. It publishes only critically reviewed data and literature references are given for all data. It is also noted that the printed version of Beilstein is no longer published.
Week 11

**How to find chemical information?**

At the end of the course students get a practical overview of chemical resources and tools. The pieces of the subject discussed during the semester are assembled into a very simple manual: “How to find chemical information”. This manual consists of a strategy and a list of references. While the former is a general approach the latter is a time-specific and institution-specific part of a comprehensive one. The strategy of information retrieval can be summarized in the following items (Hill & Culp, 2000):

- choose the appropriate source/tool,
  - introductory or overview information - books, reviews, encyclopedic works
  - individual pieces of data - handbooks, tables
  - original research - journal/patent indexes
- start with the easiest tools (accessibility and handling),
- find the keys which will unlock other tools (CAS registry number, review articles)
- use reference sources at the start of a research project (to get an overview, to clear up the jargon, to find the most important works associated with the topic)
- use pearl growing or the iterative approach (build on good results by searching its keywords and checking its cited/citing/related articles).

The list of electronic documents (free and commercial databases) available at the University of Szeged is structured according to the type of the required information:

- chemistry related information (e.g. societies, institutions, publishers, suppliers, conferences, jobs)
- fundamental constants, units, quantities
- chemicals (property data, CAS registry number, synonyms, structure, safety and hazardous data, spectral data, preparation)
- chemical reactions
- terms and concepts (dictionaries, encyclopedias, glossaries)
- research topic
  - locate primary sources on the topic (bibliographic databases)
  - obtain the journal articles/dissertations/patents.

**Exercise 13** Make a compilation on your topic containing the following items:

- bibliography of the last ten/five years research, sorted by date
- accessibility of the three most important articles in Hungarian libraries
- any Nobel prize (laureates, date, press release) connected with the topic, or a part of it, or a technique associated with it
- a compilation of data and information about a compound (involved in your topic), CAS Registry Number, 2D structure, property data, spectra, MSDS, any biological/medical importance.

**Exercise 14** Save your favorites in an organized bookmark file so, that either Internet Explorer or Netscape Navigator can import it. Beside the URLs visited during the course add new web pages interesting for a chemical researcher.
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