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# Internet – Where Is Chemistry Going?

## EDITORIAL

The Internet, and especially the World-Wide Web (WWW), continues to be a buzzword no professional can escape from. Initial hesitation whether this medium really would be suitable for professional information processing for chemists and other scientists or engineers did certainly exist. These voices are becoming less and less audible. This is of course also due to the fact that major players in the chemical information and software business have now launched ambitious development projects to provide building blocks or complete program suites that are Internet-savvy, and are reshaping many data sources which previously required individual client programs for access to Inter- and Intranet Web interfaces.

So when the Internet is supposed to change the way we deal with professional information, where is chemistry going? How do today's bleeding-edge applications look like, and how do they work internally? How did they evolve, and what will the foreseeable future bring?

In this CHIMIA issue, I have tried to assemble a group of renowned authors from a broad range of backgrounds, which could answer some of these questions. They are working on quite different aspects related to the adoption of established chemical information processing methodology to this medium. The typical chemist and reader of this nonspecialist journal is naturally mostly interested in how he or she can profit from using Internet technology at the workplace or in education, now or in the near future. For the benefit of this class of readers, the major focal point of this collection of articles are prototypical end-user applications. This kind of Internet-based information or computational services is becoming increasingly common. They begin to be delivered in company environments for routine tasks such as standard database access, compound purchase or simple spectra interpretation, and are often integrated into university courses.

The series of articles begins with a paper by *Henry Rzepa* from the Imperial College, London. He recalls the few intensive years of development and standards shaping which led to the current state of the art and provides us with a historical perspective. *Henry Rzepa* was among the first chemists to recognize the potential of a then very young medium, the WWW, for chemical information distribution. His name is inseparably linked to many of the underlaying official and informal standards such as *Chemical MIME* which make transparent transport and proper handling of non-textual information, such as chemical structure files and spectra, a reality today.

The next contribution by *Jonathan Brecher* deals with the problem of making the immense body of chemical data available from hundreds of open sources on the Internet accessible for the chemist. For various reasons, text-based queries on the standard WWW search engines are mostly useless when trying to obtain structure-oriented chemical information. The CambridgeSoft

ChemFinder has become the premier source for locating this kind of data. His paper details the concepts and behind-the-scene workings of this public service.

Publishing specialist journals as Web editions is an idea which looks straightforward, is immediately appealing and has been implemented very early in the history of the WWW. The *Journal of Molecular Modeling* was the first fully electronic chemistry journal and now is able to look back onto a four-year history. *Tim Clark* and *Henryette Roth* review the impact this journal has had, and whether the expectations linked to its launch were met.

After covering the aspect of delivering existing information, from the uncontrolled realms of the open WWW or peer-reviewed journals, we move on to the problems related to the implementation of computational services in a WWW environment. These need to respond to variable user submissions and are supposed to become a part of the workplace for most chemists. *Anatoli Krassavine*, associated with *Cherwell Scientific* and the chief developer of one of the most advanced Java packages for handling structure information, presents a tour through the design of his system which will also satisfy the more technically inclined reader.

We close this CHIMIA edition with two sample applications which both use client-server computing and Java applets for the implementation of computational services. *Peter Ertl* of *Novartis* illustrates his in-house structure-oriented QSAR analysis tools, while *Paul Selzer* from the University of Erlangen-Nürnberg established a public IR-spectra simulation service. These are two prototypical applications for chemical data processing which demonstrate the type of computational services which I believe will become a model for the next generation of computational software packages.

Finally, I would like to add a few comments regarding some major underlying trends in Internet-based chemical information processing. These are not directly visible at the user level, but will probably determine the general course of future development in a crucial way. Currently, we see many building blocks which are yet isolated, but I expect the tendency to increase interoperability to continue. The traditional model of huge packages, *e.g.*, in the modeling sector, may be outdated quite soon. However, interoperability can be defined in various ways, not just as programs exchanging data, but also as computers and browsers of different manufacturers being able to access the same information sources and processing services. The ideal of many developers is to achieve both platform and browser independence at least on the client side (the computer of the chemist).

This is definitely possible, but can sometimes be difficult and time-consuming to implement. The problems begin with Web browsers which are not completely compatible, and unfortunately they tend to diverge in their functionality precisely in those areas which are needed for sophisticated active Web-based applications which go beyond the simple display of text, images, and standard forms. In addition, companies such as *Microsoft* offer enticing proprietary features which make development easy and attractive, but are bound to a single platform, and in a complementary strike do their best to sabotage platform-independent technologies such as Java. Chemical software is only a microscopic part of the whole software business and can hardly influence the ongoing battle of giants which provide the underlying technological basis. For me it is still an open question which development

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trend will prevail. Portable Java is still gaining momentum, but typical plug-ins and add-ons which are traditionally compiled program parts are now generally only published for MS Windows and MacOS.

In the area of information exchange and encoding, interesting developments are happening. It is generally being recognized that both HTML for text presentation and the traditional structure exchange formats such as MDL Molfiles possess serious shortcomings. A big convergence is taking place right now: HTML, the coding format of the pages on the WWW, will eventually be replaced by a more powerful successor, XML. The most exciting aspect of XML is that it allows for structuring conventions to encode any kind of data, including the content of structure exchange files. An XML-based standard for chemical data, CML, is currently being defined and has the potential to become the next model for storage of annotated chemical information. Unfortunately, we were not able to include an article about CML in this issue. You will, however, encounter various references to this emerging standard in several contributions. If you desire to learn more about the background of CML, please visit the relevant Web sites.

I hope you will enjoy this issue.

W.-D. Ihlenfeldt

*Glossary*: Bleeding edge: Ironical computer slang term for applications at the very edge (or slightly beyond) of current technology. Implies experimental, novel, and enterprising character.

It's a great pleasure for the Editorial Board of CHMIA to thank the coordinating guest editor Dr. *Wolf-Dietrich Ihlenfeldt* (Computer Chemistry Center, University of Erlangen-Nürnberg, Germany) for his most successful getting together of a group of renowned authors to the hot topic of the present issue: 'Internet – Where is Chemistry Going?'.

# 3rd Lausanne Conference on Bioorganic Chemistry

**Thursday, March 4, 1999, 13.30**
**to Friday, March 5, 1999, 17.00**

The meeting offers a forum especially for young scientists to discuss various aspects of this rapidly expanding interdisciplinary field. Beside the plenary lectures, a poster session will be organized.

**Invited Speakers:**

- **Bernard Cuenoud, Novartis, Basel, Switzerland**
  Targeting Double-Stranded DNA with Modified Oligonucleotides
- **Alois Fürstner, MPI für Kohlenforschung, Mühlheim/Ruhr, Germany**
  Studies on Bio-Active Pyrrole Alkaloids
- **Claude Hélène, Muséum National d'Histoire Naturelle, Paris, France**
  Molecular Recognition of DNA and Control of Gene Expression by Oligonucleotide Derivatives
- **Donald Hilvert, ETH-Zürich, Switzerland**
  Directed Evolution of Protein Catalysts
- **Jean-Marie Lehn, Université Louis Pasteur, Strasbourg, France**
  Bioorganic Topics in Supramolecular Chemistry
- **Jean-Louis Reymond, University of Bern, Switzerland**
  Discovering Catalytic Antibodies using Fluorescence Assays
- **Daniel H. Rich, University of Wisconsin-Madison, USA**
  Merging Rational Drug Design with Combinatorial Chemistry: Reasonable and Unreasonable Expectations
- **John A. Robinson, University of Zürich, Switzerland**
  Molecular Recognition of Peptides and Proteins
- **Bernard Roques, Université René Descartes, Paris, France**
  Structural Data for New Chemical Approaches in Regulation of Exo and Endo Signal Transmission
- **Herbert Waldmann, University of Karlsruhe, Germany**
  Peptide Conjugates – Tools for the Study of Biological Signal Transduction

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