The Obernai Declaration

Preamble

The Workshop

Chemoinformatics in Europe: Research and Teaching

assembled on May 29-31, 2006 in Obernai, France 100 scientists from 18 European countries as well as from USA and Canada.
These scientists were members of a wide range of Chemical Societies of European countries such as SCF, RSC, GDCh, SCI as well as of organizations such as the QSAR and Modelling Society, Molecular Graphics and Modelling Society, and the Chemical Structure Association. The following declaration was unanimously accepted by the participants of this workshop.

Chemoinformatics Research

Chemoinformatics is a scientific discipline that has evolved in the last 40 years at the interface between chemistry and computer science. It has been realized that in many areas of chemistry, the huge amount of data and information produced by chemical research can only be processed and analyzed by computer methods. Furthermore, many of the problems faced in chemistry are so complex that novel approaches utilising solutions that are based on informatics methods are needed. Thus, methods were developed for building databases on chemical compounds and reactions, for the prediction of physical, chemical and biological properties of compounds and materials, for drug design, for structure elucidation, for the prediction of chemical reactions and for the design of organic syntheses.

Research and development in chemoinformatics is essential

- for increasing our understanding of chemical phenomena
- for industry to remain competitive in a global economy

Chemoinformatics methods can be applied in any field of chemistry, from analytical chemistry to organic chemistry. It is of particular importance in drug design and development. European scientists have made major contributions to chemoinformatics mostly funded by national programs of various sorts. Chemoinformatics is now obtaining major attention in the USA, Japan, China and India. As a case in point, the National Institutes of Health (NIH) in the U.S. are dedicating large amounts of funds for the further development of chemoinformatics in the framework of the NIH Roadmap Initiative:

Therefore, to keep European chemical science and industry competitive, an increase in funding of chemoinformatics is needed in Europe, both at the national and the European Union level.

Chemoinformatics: Teaching

The further development of chemistry in general and chemoinformatics in particular needs an increase in teaching of chemoinformatics. This is necessary

- to provide chemoinformatics specialists for academia and industry
- to train chemists in the use of chemoinformatics methods in all areas of chemistry

In order to achieve these goals

- chemoinformatics curricula have to be implemented in universities teaching chemistry in Europe
- essential topics of chemoinformatics have to be integrated into other scientific disciplines including biology and materials science.
- summer schools for training students and industrial chemists have to be initiated.

A general framework of a curriculum in chemoinformatics is contained at
http://infochim.u-strasbg.fr/chemoinformatics/

A list of the major topics of chemoinformatics considered to be essential for the training of all chemistry students is given at the same web site.

Cooperation Academia – Industry

The chemical and pharmaceutical industries produce massive amounts of data that needs to be understood for the more efficient planning of experiments. Academia develops methods for converting these data into information and knowledge. For the development of accurate predictive systems with a broad scope, an increase in the collaboration of academia and industry is considered essential. This is particularly true for the development of toxicity prediction systems as urgently needed in the framework of the REACH (Registration, Evaluation and Authorization of CHemicals) initiative of OECD.

To this endeavour

- bi- and multilateral collaboration of industry and academia are encouraged
- the release of non-confidential data from industry is recommended
- the methods developed in academia have to be carefully validated
- joint projects to develop the chemoinformatics infrastructure necessary for global competitiveness in research and development need to be initiated.