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SOLVED AND UNSOLVED PROBLEMS OF CHEMOINFORMATICS

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From early beginnings in the 1960s Chemoinformatics has developed into a scientific field of its own. Without the many tools provided by chemoinformatics modern scientific research and development in chemistry and related fields would simply not be possible.[1,2]

Mature as the field has now become there are nevertheless many problems that still wait to be satisfactorily solved: The efficient search for the bioactive conformation, the representation of polymers, the prediction of the course of chemical reactions, the analysis of biochemical reaction networks, the design of organic syntheses, automatic structure elucidation to name just a few. In addition, dramatic changes are occurring in the way we get access to data and information, the role of publishing houses is being challenged by information becoming freely available on the internet.

Furthermore, it must be realized that chemoinformatics has not yet found its proper place in the chemical community, the power of chemoinformatics has not yet been utilized in every corner of chemistry. As of now, most efforts have been directed to drug design but chemoinformatics methods could increase our understanding of chemistry across all fields, from analytical chemistry through organic chemistry to physical chemistry.

Thus, there is still a lot of work to be done to prove the importance of chemoinformatics, from producing excellent chemoinformatics applications in all areas of chemistry, through training chemoinformatics specialists to incorporating chemoinformatics topics into regular chemistry curricula.

1. Handbook of Chemoinformatics - From Data to Knowledge, 4 volumes, J. Gasteiger, Editor, Wiley-VCH, Weinheim, 2003. ISBN: 3-527-30681-1

2. Chemoinformatics - A Textbook, J. Gasteiger, T. Engel (Editors), Wiley-VCH, Weinheim, 2003. ISBN: 3-527-30680-3