25 Years Molecular Modeling Workshop:

Old Questions - New Answers?

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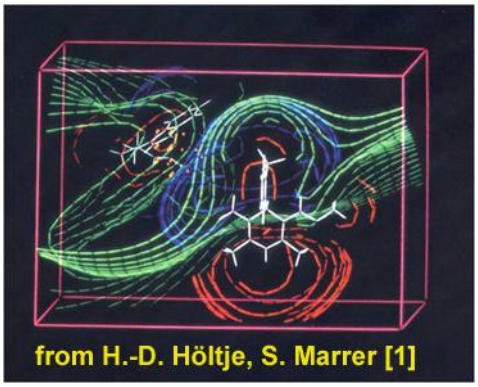
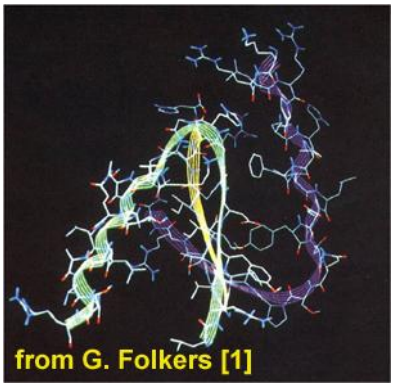
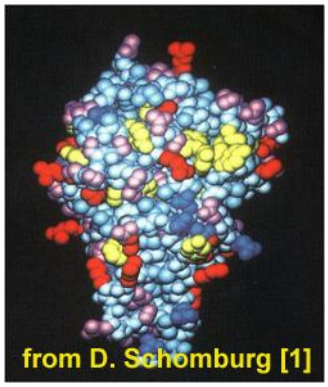
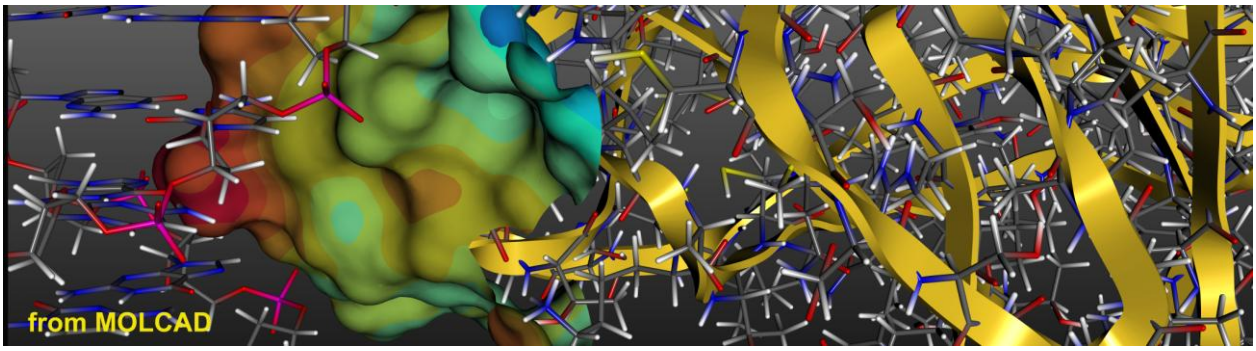
The first molecular modeling workshop took place in Darmstadt in 1987. The workshop was initiated and supported by the German Ministry of Science and Technology with the aim to bring together researcher from academia and industry from the field of computer aided molecular design. The background was a program of the German government directed towards the reduction of animal experiments in pharmaceutical research by alternative methods. Many scientist, well known in the field, contributed to this event. [1]







The basic questions have been the same as today: Industrial researcher mainly asked "How can computer aided methods be used in order to reduce the effort in the development process for new drugs?" while the questions from academia have been related to the understanding and the quantification of the molecular recognition process. The basic model scenario was crude and its visualisation and numerical treatment could only be handled with "super computers" with a capacity which is smaller than that of today´s laptops. The answers have been vague. The situation is much different today. According to Moore´s rule (computer capacity doubles roughly every two years) one may estimate a factor of about 10^4 to 10^5 in capacity. Moreover, there was a big step forward on the software side. Instead of crude models, we can use today sophisticated ones including quantum mechanical treatments and simulation techniques. Modern computer graphics techniques allows an effective real time man machine communication in the modeling and simulation business. Nevertheless, we are still far away from adequate answers to the old questions. Tim Clark formulated the situation of the modeling community as "Soothsayers or Scientists" [2]. The recent problems and some ideas for the future developments will be discussed in this contribution.



[1] BMBF, *Molecular Modelling - Informations and Trends*, **1988**
[2] T. Clark, *lab&more*, **2010**, *No. 2*, 17-19.