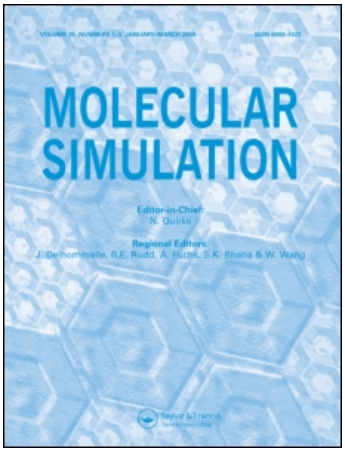

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Editorial

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EDITORIAL

When considering the development of science, three transition periods may be distinguished. About six centuries B.C. the old Greeks, like Thales and Pythagoras, brought about the concept of a theory to describe observed phenomena. About 2000 years later the Renaissance saw the emergence of a systematic use of experiments to validate theory, a famous example being Galileo's falling stones experiment. Nowadays, we benefit from the transition to the systematic use of computers to validate theory. It has been made possible by the rapid and sustained increase of computing power over the last decades: a factor of ten per 5 years at constant costs. This implies that when the years pass by, ever more complex chemical and physical phenomena can be tackled by computational means. One of the areas of rapid development is the simulation of chemical or physical processes on a computer. For example, the computer has almost completely replaced the wind tunnel in aircraft design, and the flow tank in ship design. Will it also replace chemical experiments? Fortunately not. The basic laws governing the behaviour of atoms and molecules are known, but so difficult to simulate with the required accuracy, that a replacement of chemical experiments is completely out of reach. The goal of molecular simulation is rather to provide insight in cause/effect relationships at the atomic level by performing controlled computer experiments. The challenge to the computational chemist is thereby not to wait for ever faster computers, but to propose more clever algorithms, based on simpler yet reliable approximations of the basic laws of atomic and molecular physics, in order to improve his model description of physical or chemical phenomena.

Over the past decade computer simulation of proteins and other biochemically relevant molecules has emerged as a rapidly growing area of research. The method of molecular dynamics is used to probe equilibrium properties, e.g. binding constants of biomolecular complexes, to predict the conformation and stability of parts of proteins or protein mutants. The Special Issue on *molecular simulation in biochemistry and pharmacology* is meant to give a picture, or snapshot (to use simulation terminology), of the use of computer simulation techniques in biochemistry and pharmacology. A variety of topics is treated. The availability of accurate, yet simple force fields for biomolecular systems is of crucial importance. This is the subject of the first three papers: those of Grootenhuis and Haasnoot, of Stouten et al, and of Schiffer *et al.* Given a force field, protein structure prediction can be attempted, either from scratch or using experimental data or the structure of a homologenous protein. This problem is treated in the papers of Bruccoleri and Havel. The understanding of the interaction between molecules forming a molecular complex is a determining factor in drug design, as is discussed by Gubernator *et al.* Methodology to compute free energy differences and its application to proteins is the subject of the papers of Mezei, Edholm and Ghosh, and Elofsson and Nilsson. The diffusion of a superoxide ion into the active site channel of the

enzyme superoxide dismutase is simulated by Wong *et al.* Schlitter *et al.* use molecular dynamics to simulate a conformational transition process in insulin, and Mehler *et al.* address differential calcium binding to the protein Calbindin. The larger time scale motions of a phosphatidylcholine bilayer are probed in nanosecond simulations performed by Stouch. The last two papers of the Special Issue consider the use of neutron and X-ray diffraction data when studying the structure and dynamics of biomolecules. Taken together, the 15 papers of this Special Issue illustrate the type of problems and applications that are currently investigated in the area of computational molecular biochemistry and pharmacology.

It is a pleasure to thank all authors for their efforts to bring about this Special Issue.

W.F. van Gunsteren