

Preface

Almost two decades ago we jointly edited a book (*Computational Approaches to Biochemical Reactivity*) with Arie Warshel. The volume summarized results in the rapidly developing computational aspects of biochemical reactivity, which were new at that time. Since then interested specialists faced a really spectacular development in the field, which was honoured by awarding the 2013 Nobel Prize in Chemistry to three scientists, among them Arie. Hundreds of first-class publications and dozens of successes in computer-aided drug design provide evidence for the high-level application of models and methods to practical problems related to the structure and function of proteins. Maybe the most important lesson we could learn from the history of *Protein Modelling* is that there is no single and omnipotent method available for the treatment of various problems, rather different levels of approximations should be applied. More than in case of quantum mechanical modelling of small and medium-sized molecules, the concept of the chemical bond provides a sound basis for computational methods, which can be extended and refined by the use of quantum mechanics. Therefore, *Protein Modelling* is now well established and used to facilitate the thorough understanding and rational design of biochemical processes.

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