

## *Preface*

“Computational Biophysics 2000: From Macromolecules to Drugs” (CB2000) was a satellite conference of the 10th International Congress of Quantum Chemistry. It was organised under the auspices of the Division of Chemical Physics, a joint division of the Société Française de Chimie and of the Société Française de Physique. CB2000, which took place in Nice from 13–15 June 2000, brought together 200 participants from 25 different countries, including more than 50 students. The 3 days of the meeting were devoted successively to nucleic acids, proteins, and drugs with nine lectures each day. Although the principal goal of the meeting was to assess progress in the modelling and simulation of biological systems, each of the three sections included presentations of experimental approaches and also brought together academic and industrial researchers. Each section included a lively poster session, which enabled a total of roughly 110 posters to be presented.

Both the lectures and the posters illustrated the main axes of research in our field today. The nucleic acids section was dominated by questions on the mechanism

of protein–nucleic recognition involving both DNA and RNA. The protein section concentrated on approaches to studying protein folding, although recognition problems, notably involving membrane receptors, were also present. The drugs section centred on lead identification and optimisation and notably on the development of fast, high-throughput approaches. The meeting also showed continued interest in improving methodological approaches, notably for long-term dynamics and for simplified solvent treatments.

Some of these trends are illustrated by the articles which have been submitted to this special edition of *Theoretical Chemistry Accounts*. We would like to thank the editors of this journal for arranging the publication of this volume, and we would also like to take this opportunity to thank GlaxoWellcome, Merck, Molecular Simulations, and the Chemistry Department of the CNRS for supporting this conference.

Richard Lavery and Graham Richards, Organisers