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Preface

Computational chemistry and the living world: from sequence to function

The articles which constitute this special issue of *Theoretical Chemistry Accounts* represent a cross-section of the work presented during an International Symposium held in France in April 1998 and entitled "Computational Chemistry and the Living World: From Sequence to Function". This meeting, which gathered together researchers and research students from around the world, was jointly organised, by the British, French, German and Italian physical chemistry divisions or societies along with the French Biophysical Society. The aim of the meeting was to see how computational chemistry can face the challenge posed by the many genome sequencing projects which have already led to an explosive growth in sequence data and are creating a revolution in the way in which we can understand the functioning of biological organisms, from simple bacteria through to human beings.

Computational chemistry can contribute to such understanding in many ways, by helping to identify protein families from their sequence alone, by explaining and simulating protein folding, by identifying the factors responsible for recognition processes between ligands, proteins and nucleic acids, by analysing enzyme catalysis and, most generally, by forming physically reasoned links between sequences, structures and biological functions. The articles in this special issue, which illustrate all of these applications, have been grouped into five broad themes:

1. From protein sequence to structure
2. Membrane and membrane-associated proteins
3. Nucleic acid structure and dynamics
4. Recognition processes
5. Electrostatics and solvation
6. Physical chemistry and biochemical reactions

Taken together, these articles show that progress has been made in many areas. Force fields and simulation algorithms are improving. Increasing computer power, and notably parallel processing, is allowing longer simulations on larger systems, more extensive conformational searches and is enabling hybrid quantum-classical methods to be applied. Nevertheless, the complexity of biological systems and the subtlety of the interactions which govern their behaviour leave us with many problems to occupy the young scientists now entering this very lively field of research.

Richard Lavery and Jacopo Tomasi, Guest-Editors

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