Preface

"Biomolecules", including proteins, nucleic acids and saccharides, perform various biological activities in "water". Biomolecules and water molecules simply represent "chemical substances" when each of them exists alone. However, we find various biological processes expressed when these substances function together. This book "Water and Biomolecules – Physical Chemistry of Life Phenomena" covers the physical chemistry of such biological processes, and deals with "folding", "dynamics", and "function" of biomolecules as they are expressed in close relation to water molecules. Protein misfolding and amyloidogenesis are also included, because these are closely related to protein folding and functional expression, and hence responsible for a number of human diseases.

This book is also related to our recent Research Project "Water and Biomolecules", which was supported for five years by a Grant-in-Aid for the Scientific Research in Priority Areas from the Ministry of Education, Science, Culture, Sports and Technology (MEXT) of Japan, and concluded at the end of March of 2008. During the project period, we held an open workshop annually, at which we had several invited talks by expert researchers in our field, several oral activity reports from our project members, and poster presentations representing the activities of all the members of the project team. The last workshop was organized by Mikio Kataoka (Nara Institute of Science and Technology), and held in Nara, the oldest capital of Japan, on January 24 and 25, 2008. This book thus consists of 15 chapters, including seven chapters contributed by seven invited speakers (C.M. Dobson, H.J. Dyson, R.M. Levy, J.A. McCammon, C.A. Royer, C.M. Rao, and P.E.Wright) in the last workshop and eight chapters contributed by eight members (Y. Goto, F. Hirata, M. Kataoka, K. Kuwajima, Y. Okamoto, M. Sakurai, M. Terazima, and K. Yoshikawa) who were involved in our project.

The chapters are arranged thematically: Chaps. 1–5 describe experimental and simulation studies on the folding of biomolecules, Chaps. 6–12 are related to the dynamics and function of biomolecules, and Chaps. 13–15 deal with the amyloidogenesis of proteins.

In Chap. 1, Peter E. Wright and his colleagues describe recent advances in mapping transient long range interactions, which are directly implicated in kinetic folding pathways of apomyoglobin. They use NMR relaxation techniques to map out the apomyoglobin folding landscape. Chapter 3 by Takahiro Sakaue and Kenichi Yoshikawa gives an overview and recent developments in the higher-order structure transition between dispersed coil and condensed compact states in giant DNA molecules. The rich transition behaviors found in experiments are analyzed based on the statistical mechanical concept and are discussed in relation to biological significance. Chapters 4 and 5 deal with theoretical and computational studies of protein folding. Yuko Okamoto in Chap. 4 gives an excellent overview of generalized-ensemble algorithms for molecular simulations of protein folding, and Ron M. Levy and his colleagues in Chap. 5 describe studies using replica-exchange simulations to explore the complex binding and folding landscapes of proteins, particularly focusing on their recent work using simplified continuous and discrete representations of these landscapes. Kunihiro Kuwajima and colleagues in Chap. 2 also describe experimental and simulation studies of folding/unfolding of goat α-lactalbumin, and demonstrate the power of combination of experiments and simulations for studying the problems of protein folding.

In Chap. 6, H. Jane Dyson and her colleagues describe the structural properties and dynamics of sizable disordered proteins in solution characterized by spectroscopic methods such as NMR. The chapter thus deals with intrinsically disordered proteins, whose functional role in crucial areas such as transcriptional regulation, translation and cellular signal transduction has only recently been recognized. Chapter 7, by Mikio Kataoka and Hironari Kamikobo, describes studies on protein dynamics and the effect of hydration water on the dynamics using photoactive yellow protein as a model protein. Chapter 8 by Masahide Terazima describes studies on the biological reactions in several new techniques developed by his group. The techniques can monitor spectrally silent dynamics in time-domain, using the pulsed laser induced transient grating and transient lens methods. Catherine A. Royer and Roland Winter in Chap. 9 describe the pressure perturbation calorimetry, along with results from many previous densitmetric and high pressure studies to calculate quantitatively the specific volumes of a model protein, staphylococcal nuclease in both the folded and unfolded states as a function of temperature. Minoru Sakurai in Chap. 12 describes studies on the biological functions of a non-reducing disaccharide, α,α-trehalose as a substitute for water, and on their underlying mechanisms from viewpoints of thermodynamic, hydration and structural characteristics of this sugar. Chapters 10 and 11 deal with theoretical and computational studies of protein dynamics and functions. Fumio Hirata and his colleagues in Chap. 10 describe the application of the 3D-RISM theory, a statistical mechanics theory of molecular liquid, to characterization of proteins in aqueous solutions, particularly focusing on detection of water molecules and ions trapped in pores of proteins. J. Andrew McCammon in

Chap. 11 gives an excellent overview of how computer simulations can be used quantitatively to interpret the behavior of proteins, including their binding of ligands.

In Chap. 13, Chris M. Dobson gives an overview and the conceptual basis of the problems of protein folding and misfolding. The misfolding can often give rise to serious cellular malfunctions that frequently lead to disease. He also describes the results of experiments designed to link the principles of misfolding and aggregation to the effects of such processes in model organisms such as *Drosophila*. Chapter 14 by Abhay Kumar Thakur and Ch. Mohan Rao describes the recent studies of their group on the possibility of UV exposure as a structural perturbant using mouse prion protein and other amyloidogenic proteins as model systems. Finally, Chap. 15 by Yuji Goto and his colleagues describes the results of recent studies of their group on the direct observation of nucleation and growth of amyloid fibrils using total internal reflection fluorescence microscopy combined with thioflavin and atomic force microscopy.

We thank all the contributors to this book for their time and effort in preparing the manuscripts, and particularly Chris M. Dobson (Cambridge) and Ron M. Levy (Rutgers), who were international advisors to our project, for their interest in the project and a number of very useful suggestions regarding the project. Thanks are also due to Claus E. Ascheron, Balamurugan Elumalai and Adelheid Duhm of Springer Science for their help in publishing this book.

Okazaki
January 2009

Kunihiro Kuwajima
Yuji Goto
Fumio Hirata
Mikio Kataoka
Masahide Terazima

http://www.springer.com/978-3-540-88786-7

Water and Biomolecules
Physical Chemistry of Life Phenomena
Kuwajima, K.; Goto, Y.; Hirata, F.; Terazima, M.; Kataoka, M. (Eds.)
2009, XVII, 307 p., Hardcover
ISBN: 978-3-540-88786-7