Contents

Preface v
Contributors xi

PART I EXPERIMENTAL APPROACH

1 Molecular Design of Performance Proteins With Repetitive Sequences: *Recombinant Flagelliform Spider Silk as Basis for Biomaterials* 3
Charlotte Vendrely, Christian Ackerschott, Lin Römer, and Thomas Scheibel

2 Creation of Hybrid Nanorods From Sequences of Natural Trimeric Fibrous Proteins Using the Fibritin Trimerization Motif 15
Katerina Papanikolopoulou, Mark J. van Raaij, and Anna Mitraki

3 The Leucine Zipper as a Building Block for Self-Assembled Protein Fibers 35
Maxim G. Ryadnov, David Papapostolou, and Derek N. Woolfson

4 Biomimetic Synthesis of Bimorphic Nanostructures 53
Joseph M. Slocik and Rajesh R. Naik

5 Synthesis and Primary Characterization of Self-Assembled Peptide-Based Hydrogels 61
Radhika P. Nagarkar and Joel P. Schneider

6 Periodic Assembly of Nanospecies on Repetitive DNA Sequences Generated on Gold Nanoparticles by Rolling Circle Amplification 79
Weian Zhao, Michael A. Brook, and Yingfu Li

PART II COMPUTATIONAL APPROACH

7 Protocols for the *In Silico* Design of RNA Nanostructures 93
Bruce A. Shapiro, Eckart Bindewald, Wojciech Kasprzak, and Yaroslava Yingling

8 Self-Assembly of Fused Homo-Oligomers to Create Nanotubes 117
Idit Buch, Chung-Jung Tsai, Haim J. Wolfson, and Ruth Nussinov

9 Computational Methods in Nanostructure Design: *Replica Exchange Simulations of Self-Assembling Peptides* 133
Giovanni Bellesia, Sotiria Lampoudi, and Joan-Emma Shea

10 Modeling Amyloid Fibril Formation: *A Free-Energy Approach* 153
Maarten G. Wolf, Jeroen van Gestel, and Simon W. de Leeuw

11 Computer Modeling in Biotechnology: *A Partner in Development* 181
Aleksei Aksimentiev, Robert Brunner, Jordi Cohen, Jeffrey Comer, Eduardo Cruz-Chu, David Hardy, Aruna Rajan, Amy Shih, Grigori Sigalov, Ying Yin, and Klaus Schulten

12 What Can We Learn From Highly Connected β-Rich Structures for Structural Interface Design? 235
Ugur Emekli, K. Gunasekaran, Ruth Nussinov, and Turkan Haliloglu

Index 255