

Contents

1	Introduction	1
	Michael Levitt	
2	Modeling RNA Molecules	5
	Neocles Leontis and Eric Westhof	
3	Methods for Predicting RNA Secondary Structure	19
	Kornelia Aigner, Fabian Dreßen, and Gerhard Steger	
4	Why Can't We Predict RNA Structure At Atomic Resolution? . . .	43
	Parin Sripakdeevong, Kyle Beauchamp, and Rhiju Das	
5	Template-Based and Template-Free Modeling of RNA 3D Structure: Inspirations from Protein Structure Modeling	67
	Kristian Rother, Magdalena Rother, Michał Boniecki, Tomasz Puton, Konrad Tomala, Paweł Łukasz, and Janusz M. Bujnicki	
6	The RNA Folding Problems: Different Levels of sRNA Structure Prediction	91
	Fredrick Sijenyi, Pirro Saro, Zheng Ouyang, Kelly Damm-Ganamet, Marcus Wood, Jun Jiang, and John SantaLucia Jr.	
7	Computational Prediction and Modeling Aid in the Discovery of a Conformational Switch Controlling Replication and Translation in a Plus-Strand RNA Virus	119
	Wojciech K. Kasprzak and Bruce A. Shapiro	
8	Methods for Building and Refining 3D Models of RNA	143
	Samuel C. Flores, Magdalena Jonikas, Christopher Bruns, Joy P. Ku, Jeanette Schmidt, and Russ B. Altman	
9	Multiscale Modeling of RNA Structure and Dynamics	167
	Feng Ding and Nikolay V. Dokholyan	

10	Statistical Mechanical Modeling of RNA Folding: From Free Energy Landscape to Tertiary Structural Prediction	185
	Song Cao and Shi-Jie Chen	
11	Simulating Dynamics in RNA–Protein Complexes	213
	John Eargle and Zaida Luthey-Schulten	
12	Quantum Chemical Studies of Recurrent Interactions in RNA 3D Motifs	239
	Jiří Šponer, Judit E. Šponer, and Neocles B. Leontis	
13	Nonredundant 3D Structure Datasets for RNA Knowledge Extraction and Benchmarking	281
	Neocles B. Leontis and Craig L. Zirbel	
14	Ions in Molecular Dynamics Simulations of RNA Systems	299
	Pascal Auffinger	
15	Modeling RNA Folding Pathways and Intermediates Using Time-Resolved Hydroxyl Radical Footprinting Data	319
	Joshua S. Martin, Paul Mitiguy, and Alain Laederach	
16	A Top-Down Approach to Determining Global RNA Structures in Solution Using NMR and Small-Angle X-ray Scattering Measurements	335
	Yun-Xing Wang, Jinbu Wang, and Xiaobing Zuo	
17	RNA Structure Determination by Structural Probing and Mass Spectrometry: MS3D	361
	A.E. Hawkins and D. Fabris	
	Appendix	391
	Index	395

RNA 3D Structure Analysis and Prediction

Leontis, N.; Westhof, E. (Eds.)

2012, X, 402 p., Hardcover

ISBN: 978-3-642-25739-1