Chapter 1
Role of Molecular Docking in Computer Aided Drug Design and Development
Subhabrata Sen, Department of Chemistry, Shiv Nadar University, India
Rahul Agarwal, Department of Life Sciences, Shiv Nadar University, India
Ashutosh Singh, Department of Life Sciences, Shiv Nadar University, India

Chapter 2
Application of docking methodologies in QSAR-based studies
Omar Deeb, Al-Quds university, Palestine
Heidy Martínez-Pachecho, División de Estudios de Posgrado, Universidad del Papaloapan, Mexico
Guillermo Ramírez-Galicia, Universidad del Papaloapan, Mexico
Ramón Garduño-Juárez, Universidad Nacional Autónoma de México, Mexico

Chapter 3
Molecular Docking Challenges and Limitations
Jahan B. Ghasemi, University of Tehran, Iran
Azizeh Abdolmaleki, Islamic Azad University of Touyserkan, Iran

Chapter 4
Application of molecular docking in studies on the binding mechanism of three enzymes with natural products
Huajin Zeng, Zhengzhou University, China
Ran Yang, Zhengzhou University, China
Ling-bo Qu, Zhengzhou University, China

Chapter 5
Molecular Docking of Biologically Active Substances to Double Helical Nucleic Acids: Problems and Solutions
Kateryna V. Miroshnichenko, O. Ya Usikov Institute for Radiophysics and Electronics of NAS of Ukraine, Ukraine
Anna V. Shestopalova, O. Ya Usikov Institute for Radiophysics and Electronics of NAS of Ukraine, Ukraine

Chapter 6
Molecular Docking-Based Drug Design and Discovery: Rational drug design for the subtype selective GPCR ligands
Soo-Kyung Kim, California Institute of Technology, United States
William A Goddard III, California Institute of Technology, United States

Chapter 7
Molecular Modelling, Dynamics and Docking of Membrane Proteins – Still a Challenge
Nanda Kumar Yellapu, Vector Control Research Centre, India
Chapter 8
In silico Perspective into Interactions and Mutations in Human TLR4 and Ebola Glycoprotein: An In silico Insight to Defend Ebola Virus Entry

Sujay Ray, Department of Biochemistry and Biophysics, Kalyani University, India
Arundhati Banerjee, Department of Biotechnology, NIT, India

Chapter 9
Molecular docking based antiallergic drug design

Anamika Basu, Gurudas College, India
Piyali Basak, School of Bioscience & Engineering, Jadavpur University, India
Anasua Sarkar, Government College of Engineering and Leather Technology, India

Chapter 10
Protein-Protein Interactions (PPIs) As An Alternative To Targeting The ATP Binding Site Of Kinase: In Silico Approach To Identify PPI Inhibitors

Sailu Sarvagalla, Centre for Bioinformatics, Pondicherry University, India
Mohane Selvaraj Coumar, Centre for Bioinformatics, Pondicherry University, India

Chapter 11
Applications of Molecular Docking- Its impact and importance outside the purview of Drug Discovery: Industrial Applications of Molecular Docking

Josephine Anthony, ESSO-National Institute of Ocean Technology, India
Vijaya Raghavan Rangamaran, ESSO-National Institute of Ocean Technology, India
Kumar T Sivashankarasubbiah, ESSO-National Institute of Ocean Technology, India
Dharani Gopal, ESSO-National Institute of Ocean Technology, India
Kirubagaran Ramalingam, ESSO-National Institute of Ocean Technology, India