

Computational and Experimental Studies in Alzheimer's Disease



Edited by
Kunal Bhattacharya
and **Atanu Bhattacharjee**



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Computational and Experimental Studies in Alzheimer's Disease

This reference book compiles the recent advances in computational and experimental modelling to screen and manage Alzheimer's disease. It covers basic etiopathology and various in vitro and in vivo strategies of disease intervention. The book discusses how computer-aided drug design approaches reduce costs and increase biological test efficiency. It reviews the screening for anti-Alzheimer drugs and biomarker analysis of disease inhibitors. The book also explores mechanistic aspects of neurodegeneration and the use of natural products as therapeutics for Alzheimer's disease.

Key features:

- Elaborates on the computational modelling of protein target inhibitors as anti-Alzheimer's agents
- Explains the role of phytomolecules and natural products in Alzheimer's therapy
- Reviews preclinical ways to assess drugs focusing on Alzheimer's disease
- Covers biomarker analysis for Alzheimer's disease
- Discusses the onset and progression of Alzheimer's disease

The book is meant for professionals, researchers, and students of neuroscience, psychology, and computational neurosciences.



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Foreword



I am highly delighted to put my views and endorse the forthcoming publication of the book titled *Computational and Experimental Studies in Alzheimer's Disease*. This comprehensive reference book represents a compilation of scholarly articles in the field of neuroscience, as it focuses on latest advances in computational and experimental modeling for screening and managing Alzheimer's disease. Authored by distinguished experts, this book is an invaluable source of knowledge for professionals, researchers, and students in neuroscience, psychology, and computational neurosciences etc.

I appreciate the timeliness efforts of the authors and significance of this compilation. The book not only delves into the basic etiopathology of Alzheimer's disease but also explores various in vitro and in vivo strategies for disease intervention.

It provides valuable insights into the use of computational modeling in identifying protein target inhibitors as potential anti-Alzheimer agents. Furthermore, it discusses the crucial role of phytomolecules and natural products in Alzheimer's therapy, an area that holds great promise for effective treatments. One of the key strengths of this reference book is its coverage of biomarker analysis for Alzheimer's disease. Identifying reliable biomarkers is pivotal in early diagnosis and monitoring, and the insights offered in this book can potentially impact clinical practice and future research efforts significantly. The insight in this field is essential for developing targeted interventions and improving our understanding of the disease process.

In conclusion, it is worth mentioning that the book offers a comprehensive and up-to-date resource for those deeply committed to addressing the challenges of Alzheimer's disease. I wholeheartedly recommend this book to professionals, researchers, and students in neuroscience, psychology, and computational neurosciences, as well as anyone interested in making a meaningful contribution to the fight against Alzheimer's disease.

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Preface

Alzheimer's disease (AD) has become a major issue in global health in recent decades, impacting millions of people all over the world. Memory loss, confusion, and other cognitive difficulties, as well as severe impairment in everyday functioning, are hallmarks of this progressive neurodegenerative condition. The prevalence of AD has increased rapidly with the aging population and rising life expectancy, inflicting a significant burden on health care systems, families, and society at large.

The goal of the book "Computational and Experimental Studies in Alzheimer's Disease" is to further advance our understanding of this disease by combining computational and experimental methods. To provide a thorough review of the present status of study in this difficult domain, this book compiles a wide variety of themes, approaches, and views.

In the first chapter, we set the stage by discussing the neuropathology, neurochemistry, and epidemiology of Alzheimer's disease. It explores the nuances and gaps in our knowledge of the disease, covering topics like risk factors and the influence of age, genetics, lifestyle, and comorbidities. Alterations in neurochemistry and the emergence of neuropathological markers like β -amyloid plaques and neurofibrillary tangles are also discussed in this chapter.

Preclinical procedures for assessing anti-AD medications are discussed in Chapter 2, which mainly covers *in vivo* and *in vitro* testing. It delves into using *ex vivo* models and cell-based tests in addition to transgenic and nontransgenic animal models. This chapter emphasizes the value of preclinical research in determining if a therapy intervention is safe and effective before proceeding with clinical trials.

In Chapter 3, we look at how computational methods can be used to investigate the feasibility of AD treatments derived from plants. Methods for identifying natural chemicals that interact with important targets implicated in AD pathogenesis are discussed, including the use of molecular docking, virtual screening, and molecular dynamics simulations. The potential of computational approaches to promoting efficient treatments for AD is highlighted in this chapter.

The fourth chapter examines recent advances in the application of computer-aided drug design (CADD) to AD. It emphasizes the use of high-performance computing and advanced algorithms to identify and modulate key protein targets implicated in the pathology of Alzheimer's disease. The combination of computational models, virtual screening, and experimental methods opens up new avenues for the discovery of effective Alzheimer's disease (AD) treatments.

Analysis of biomarkers for Alzheimer's disease is the subject of Chapter 5. The possibility of different biomarkers for use in early diagnosis, prognosis, and therapy of AD is discussed. The chapter highlights the potential of biomarkers in generating new treatments and facilitating drug development for AD, and emphasizes their usefulness in clinical practice and research.

In Chapter 6, we delve into the role of phytochemicals and the underlying mechanisms of neurodegeneration in AD. It explores the therapeutic potential of plant-based substances like curcumin and resveratrol in slowing the progression of Alzheimer's disease. In this chapter, we learn more about the potential benefits of phytochemicals and how they can be used to attack AD at several points in the disease's development.

As anti-AD agents, Chapter 7 concentrates on computational modelling of BACE-1, AChE, and phosphodiesterase inhibitors. It presents the results of molecular dynamics simulations and binding free energy calculations and discusses the identification of potent antagonists using *in silico* techniques. This chapter provides insightful information regarding potential lead molecules and their interactions with key targets in Alzheimer's disease.

Therapeutic applications of natural products for AD utilizing computational approaches are explored in Chapter 8. It emphasizes natural compounds' potential as a source of structurally varied molecules with extensive biological activity. This chapter delves into how computational methods

can be used to discover new natural chemicals and their underlying mechanisms of action, paving the path for novel AD treatments.

Potential AD inhibitors are analysed in Chapter 9 using computational modelling of several target proteins. The article talks about how virtual screening, molecular docking, and molecular dynamics simulations can be used to find new lead compounds. This chapter provides information about how to create new treatments for Alzheimer's disease.

In summary, "Computational and Experimental Studies in Alzheimer's Disease" integrates computational approaches and experimental investigations to present an interdisciplinary approach to understanding AD. This book aims to contribute to the growing body of knowledge and inspire further research toward developing effective treatments for this life-threatening condition by exploring various aspects of AD pathology, preclinical evaluation, computational modelling, and therapeutic applications.

**Editors Kunal Bhattacharya
Atanu Bhattacharjee**

About the Editors

Kunal Bhattacharya is currently working as an assistant professor at the Pratiksha Institute of Pharmaceutical Sciences, Assam, India. His area of specialization includes computer-aided drug design, bioinformatics, and analytical chemistry. Kunal Bhattacharya obtained his M.Pharm in pharmaceutical chemistry from Nitte University, Mangalore, India. He is currently pursuing his Ph.D. in pharmaceutical sciences in neurodegenerative diseases from The Assam Royal Global University, Assam, India. He has worked extensively on multiepitope vaccine designing and developing various essential drug molecules. He has reviewed various research articles and book chapters from reputed publishers. He has published various Research and Review articles in various reputed journals of academic importance. He has also contributed chapters to numerous books in the fields of mental health and pharmaceutical science. He has received prestigious summer research fellowships in India: CSIR in 2020 and IASc-INSA-NASI in 2021.

Atanu Bhattacharjee is currently working as a professor in the School of Pharmacy, The Assam Royal Global University, Assam, India. He is considered a pioneer in the fields of pharmacognosy and phytochemistry. Dr Bhattacharjee achieved his Ph.D. in Pharmaceutical Sciences in the areas of phytochemistry and neuro-pharmacology from Nitte University, Mangalore, India. He worked extensively on various in silico, in vitro and in vivo experiments to encounter neuro-degenerative disorders such as Alzheimer's disease with folklore medicine from the Indian diaspora and to determine safety profiles and standardize medicinal plants. Many research and review articles published in internationally acclaimed journals are under his credentials. In 2021, he received the prestigious "Young Scientist Award" from the VDGGOOD Professional Association in India for his significant contribution to scientific research. His extensive work on natural products to encounter SARS COV-2 has been recognized globally as he received a patent from South Africa in 2022 on "Bioinformatics platform for identification of quercetin derivatives as immunity booster molecules against SARS COV-2". He was the Honorable Academic Editor of the *Asian Journal of Medicine and Health*, SCIENCEDOMAIN International, India till 2021. He is also an editorial board member and reviewer of many internationally reputed journals. Dr Bhattacharjee is also a member of the Alzheimer's Association.



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