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A Path to 2030

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Chukwuabuka Egbuna
Shashank Kumar
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Shahira M. Ezzat
Sargunan Kaliyaperumal

Phytochemicals as Lead Compounds for New Drug Discovery

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Chukwuabuka Egbuna

Department of Biochemistry, Faculty of Natural Sciences, Chukwuabuka Obasogie Okeke University, Uyo, Nigeria

Shashank Kumar

Center for Biochemical and Molecular Sciences, Qadiri University of Health, Bafra, India

Jonathan C. Iremaja

Department of Biochemistry, Faculty of Natural Sciences, Chukwuabuka Obasogie Okeke University, Uyo, Nigeria

Shahira M. Ezzat

Department of Pharmacology, Faculty of Pharmacy, Suez Canal University, Egypt

Department of Pharmacology, Faculty of Pharmacy, Suez Canal University for Medical Sciences and Arts, Egypt

Sargunan Kaliyaperumal

Department of Zoology, Vellore Veterinary College, Tamil Nadu, India

Phytochemicals as Lead Compounds for New Drug Discovery provides complete coverage of the recent advances in the discovery of phytochemicals from medicinal plants as models to the development of new drugs and chemical entities. Functional bioactive compounds of plant origin have been an invaluable source for many natural therapeutic drugs and have played a major role in the treatment of diseases around the world. These compounds possess structural, molecular, and chemical diversity and have led to many important discoveries. The book presents fundamental theories and factors affecting the choice for plant-based products, as well as various advanced computational drug discovery and ADME-Tox complexity compliance criteria. It also details the natural bioactive lead compounds and molecular targets for a range of life-threatening diseases including cancer, diabetes, and neurodegenerative diseases.

Written by a global team of experts, *Phytochemicals as Lead Compounds for New Drug Discovery* is an ideal resource for drug developers, pharmacists, post-graduate, and academic researchers, practitioners and specialists, chemical engineers, biochemists, analytical chemists, and other researchers in these fields. It will also be very valuable to professors, students, and researchers in the domain.

Key Features

- Presents fundamental concepts and factors affecting choice for plant-based products
- Details the FDA drug complexity acceptance criteria, including substructure and way forward
- Highlights recent advances in computational-based drug discovery
- Focuses on the discovery of new drugs and potential therapeutic targets for the treatment of chronic diseases of world importance



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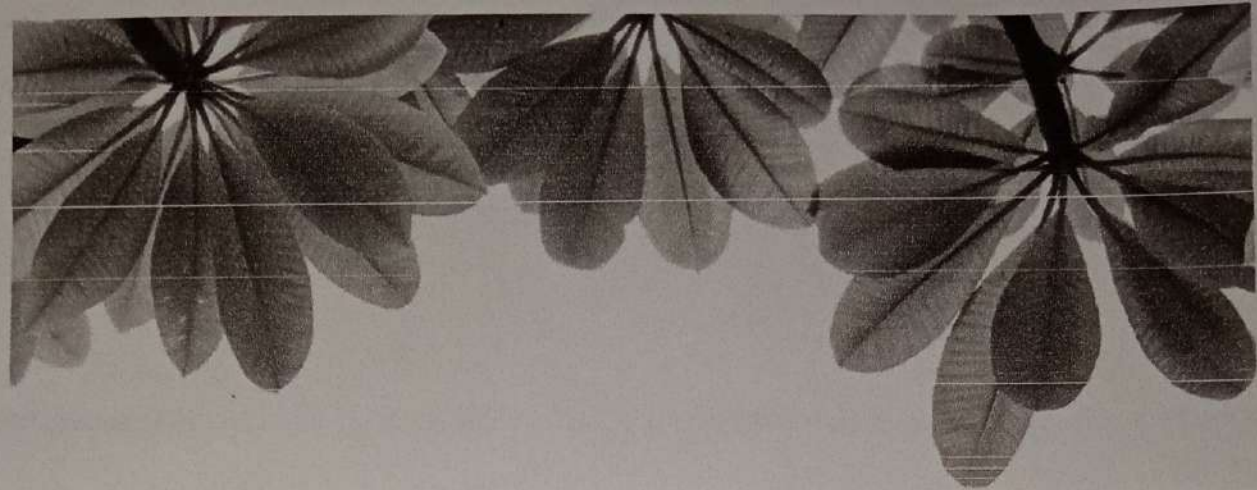
A MANUAL FOR STUDY OF MAJOR INVERTEBRATES

Dr. K. SARAVANAN

Dr. G. REVATHI

**DEPARTMENT OF ZOOLOGY
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Volume 1

Fundamentals, Modern Techniques,
and Applications



Editors

Chukwuebuka Egbuna • Jonathan Chinenye Ifemeje
Stanley Chidi Udedi • Shashank Kumar

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GAS CHROMATOGRAPHY–MASS SPECTROMETRY ANALYSIS AND IN VITRO ANTICANCER ACTIVITY OF *TECTONA GRANDIS* BARK EXTRACT AGAINST HUMAN BREAST CANCER CELL LINE (MCF-7)

ARUL PRIYA R.¹, K. SARAVANAN^{1,*}, and UMARANI B.¹

¹PG and Research Department of Zoology, Nehru Memorial College (Autonomous), Puthanampatti, Tiruchirappalli 621007, India

*Corresponding author. E-mail: kaliyaperumalsaravanan72@gmail.com
ORCID: *<https://orcid.org/0000-0003-4082-3143>

ABSTRACT

This chapter presents an investigation of the presence of secondary metabolites in the ethyl acetate extract of *Tectona grandis* bark extract and the cytotoxic effect against MCF-7 cell lines. Phytochemical compounds were determined by gas chromatography–mass spectrometry (GC-MS) analysis. The cytotoxic activity, morphological assessment of cell death, potential of mitochondrial membrane potential and deoxyribonucleic acid (DNA) damage pattern were evaluated by MTT assay, acridine orange/ethidium bromide (AO/EB) staining technique, JC-1 staining method and comet assay, respectively. GC-MS chromatogram showed the presence of five major phytochemical compounds in ethyl acetate extract of *T. grandis* bark which includes flavonoids, phenols, and tannins. The inhibition concentration (IC_{50}) of ethyl acetate extract of *T. grandis* bark was calculated as 1.57 mg/mL for MCF-7 cell line and induced significant DNA damage. Thus, the present study concludes that the ethyl-acetate extract of *T. grandis* bark possesses potent antibreast cancer activity.

Antiviral phytochemicals for drug development: a data mining studies

Saravanan Kaliyaperumal¹, Karuppannan Periyasamy², Umarani Balakrishnan³, Premalatha Palanivel¹ and Chukwuebuka Egbuna³

¹PG & Research Department of Zoology, Nehru Memorial College (Autonomous), Tiruchirappalli, Tamilnadu, India; ²PG & Research Department of Zoology, Holy Cross College (Autonomous), Tiruchirappalli, Tamilnadu, India; ³Department of Biochemistry, Faculty of Natural Sciences, Chukwuemeka Odumegwu Ojukwu University, Anambra State, Nigeria

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15.1 Introduction

A huge number of pathogens, especially the viruses have the capacity to adjust themselves according to the new trends of human society. The population explosion, globalization, and sex revolution have collectively caused an increase in the incidence and prevalence of viral diseases. By the year 2020, it is projected that viral diseases will become the deadliest of all the pandemics in human history. Therefore, virus poses a continuous threat to human health and the global economy. Viruses have efficient means to survive and broadcast in a number of varieties of hosts such as birds, insects, fish, humans, and other mammals and various cell types with respect to their host distribution, genomic organization, and clinical presentations. Virus may possess DNA or RNA as genome and may follow diverse routes for replication, transcription, and translation processes. Clinically, they may present themselves as self-resolving, localized infections or may attain several forms to affect the whole body. Although belonging to various classes, viruses follow similar general pathway for causing pathogenesis in the host. Repetitive replication of viruses results in the appearance of clinical features. Although there has been an increase in the number of approved antiviral agents, yet these drugs cover a very narrow range of viruses. Moreover, an increased incidence of resistance to these antivirals further decreases their therapeutic potential [1,2].

Plants form a fundamental part of many medicinal systems under practice today. Around 50% of prescribed drugs are either produced from plants or are derivatives of plant products [3]. Plants represent a large, untapped, potential source of antiviral agents. Although there has been relatively few studies seeking antiviral agents from plants, those studies have revealed an unexpectedly frequent occurrence of antiviral activity in plants. A large number of compounds of varied chemical structures isolated from medicinal plants have been shown to possess antiviral activity. Thus, this chapter made an attempt to explore various antiviral compounds from plants for the development of antiviral drugs.

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Chukwuebuka Egbuna

Shashank Kumar, PhD

Jonathan Chinenye Ifemeje, PhD

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TOXIC PLANTS AND PHYTOCHEMICALS

CHUKWUEBUKA EGBUNA^{1,*}, ALAN THOMAS S.²,
ONYEKA KINGSLEY NWOSU³, OLUMAYOWA VINCENT ORIYOMI⁴,
TOSKA L. KRYEZIU⁵, SARAVANAN KALIYAPERUMAL⁶, and
JONATHAN C. IFEMEJE¹

¹*Department of Biochemistry, Chukwuemeka Odumegwu Ojukwu University, Anambra State, Nigeria, Tel.: +2347039618485*

²*National Institute of Plant Science Technology, Mahatma Gandhi University, Kottayam, Kerala 686560, India*

³*National Biosafety Management Agency, Abuja, Nigeria*

⁴*Institute of Ecology and Environmental Studies, Obafemi Awolowo University, Ile-Ife, Osun State, Nigeria*

⁵*Department of Clinical Pharmacy, University of Pristina, Kosovo*

⁶*PG and Research Department of Zoology, Nehru Memorial College (Autonomous), Puthanampatti-621007, Tiruchirappalli, India*

**Corresponding author. E-mail: egbuna.cg@coou.edu.ng;
egbunachukwuebuka@gmail.com*

**ORCID: <https://orcid.org/0000-0001-8382-0693>*

ABSTRACT

Poisonous plants produce toxic compounds when in contact with living organisms such as plants, animal, and microorganism are capable of eliciting undesirable aftermath effects even death. These compounds include anticholinergic, severe gastrointestinal (GI) irritants, cardiac glycosides, central nervous system stimulants/hallucinogens, and cyanogens. Some of

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