"The contributed chapters in the book written by the faculties of science stream in the light of the recent thinking and developments in the field of science and education.- Science& Technology is now dominates almost every field of our activities.In summary, The faculties (Science stream) of GEMS Arts & Science college have made an excellent attempt to bring about this book Homo Scientia", covering almost all the important areas from biological sciences to artificial intelligence. Every article has its own merits in both academic and research fronts..I record my grateful appreciation and thanks to the contributors of this book for their untiring efforts."

**Dr. Balagopalan Unni**

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# HOMO SCIENTIA

Dr. Balagopalan Unni,
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Dr. K Gopalakrishnan,
Smitha Pramod V

GEMS

# HOMO SCIENTIA


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# Brief Biography

Dr. B.G.Unni, (Balagopalan Unni) Ph.D
(Allahabad central University)
FRES (London), FIANSc , FISAgBc, FICCE

Former Chief Scientist and Area Coordinator (Biotechnology & Biological Sciences) DADD and Fulbright Fellow retired from CSIR service in 2015 after 38 years of research career at CSIR North East Institute of Science & Technology Jorhat Assam. Appointed at Assam down town University as Director-Research in March 2015 and continued up to June 2019 and then re-designated as Adviser Research in August 2019). Back in Kerala, Dr.Unni is appointed as Director Academic & Research at GEMS College of Arts & Science affiliated to University of Calicut from August 2019. Both the positions are on honorary basis to strengthen the institutions in research areas. He did his BSc Biology (1972-74, Ewing Christian College, Alld University), MSc in Biochemistry(1974-76)(Second Rank) and Ph.D in Biochemistry from Allahabad University(1976-80) and PDF in Molecular Biology from Texas A&M University, USA(1988-91). Dr. Unni is specialized in Biochemistry, Molecular Biology, and Biotechnology and well established in his area of research and completed more than 40 years of research in both basic and applied fields of research. Dr.Unni got more than 130 research papers, 190 abstracts, 35 papers in proceedings, 7 patents,1 technology.18 chapters in books, edited 3 books and 29 students

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received PhD degrees under his guidance and supervision. Dr. Unni had completed more than 20 projects sponsored by Commonwealth Science Council, London, Ministry of Non conventional Energy Sources, Department of Non conventional Energy Sources Govt of India, North Eastern Council Govt of India, Department of Science &Technology, Department of Biotechnology, Central Silk Board,GB Pant Institute of Himalayan Environment and Development, CSIR and DRDO, Ministry of Defense, Govt of India during his scientific tenure at CSIR NEIST. Dr Unni received- Fulbright Travel Award/ Fellowship (USA) Dr. B.M. Das Memorial Science award, Hebrew University Award , H.R. Cama Memorial Travel Award,COSTED Travel Award,. DAAD- fellowship-Germany, Well Mark International Scholarship (USA) & Technology award in life sciences by CSIR,Govt of India . Best Fulbright Alumni Chapter Leader-South Asia Selected by the United States Education Foundation In India ( USIEF), New Delhi .Nominated to represent India at the International Fulbright Scholars meet at Marrakech, Morocco- Nominated by United States Education Foundation In India, New Delhi . Dr. Unni is in the editorial board of more than eight indexed journal in the country .Dr.Unni was nominated to various state and central committees such as High power committee for development of sericulture activities Muga, Eri,Tassar and Mulberry in Assam nominated by Governor of Assam, .Expert in the area of non mulberry sericulture, Ministry of Textiles, Advisory Board, Post graduate Biotechnology programme, Academic Council, Assam Agricultural University, Research Council, Central Silk Board, Ministry of Textiles , DBT's Nominee for Biosafety Committee ,Vice President SBC (India) Indian Institute of Science Bangalore, Vice President Indian Academy of Neuro-sciences, Member Fulbright Academy of Science & Technology, USA, Board of studies- Botany Nagaland University and Biotechnology Saugar University Madhya Pradesh., Fellow, Indian Academy of Neurosciences & Indian Society of Agricultural Biochemists, Fellow Royal Entomological Society, London UK and Scientific

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Advisor International Foundation of Science, Sweden, Member, Board of Studies Raiganj University ( 2017----), Member Research Review committee Tea Board of India (2016-2019), Member Advisory Committee Cancer Research Advisory Board, North East Cancer Hospital & Research Institute ( 2017--) President, Tea Improvement Consortium, Ltd, Tocklai Assam ( 2018-2020) .

Dr.Unni visited USA, Germany, Israel, Jordan, France, Morocco ,UK, Thailand ,Jordan, Singapore , China and UAE under various exchange program.

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# Preface

I am very happy to learn that, the GEMS Arts & Science College is bringing out a series of books written by the faculty in this academic year. The college is occupying a very important position among the colleges in Kerala, the same way the college is having unique standing in both academic and research fronts too. This is because of the excellent management, faculties and the best performances of the students.. I have full confident that in the course of time, and with the sincere commitment and dedication of the faculties , students and with management , the college will attain high level perfection and excellence and became a model college in the state of Kerala

This book entitled " Homo Scientia" had comprehensive research topics in various aspects in the topics of cyber security, biotechnology, microbiology and geology.A brief description about the cybersecurity, the protection of computer set up such as hardware, software data from several threats have been described in the chapter The best practices for deploying and managing IPS network security tools have been explored. The integration of intrusion prevention system (IPS) solutions, adherence to security policies, regular updates, monitoring and the implementation of incident response procedures are considered to be the essential components of a comprehensive network security framework. The risk management in cyber security, various cyber-attack kinds, malware, and some strategies to tackle these attacks are also explained by the authors. A comprehensive overview of the evolution of computer graphics, exploring the advancements in hardware, software, algorithms, and techniques that have propelled the field from its early pixel-based beginnings to the current state of realism etc also described. Optical character recognition has been extensively investigated in the past few years, and has been proven that high recognition rates can be achieved in specific

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application scenarios using some standard and well-studied methods such as neural network, support vector machine (SVM), etc. The possibility of learning an appropriate set of features for designing optical character recognition (OCR) has been investigated

Biotechnology is an interdisciplinary science using modern technologies to construct biological processes in research, agriculture, formulation of pharmaceutical products and other related fields. The better understanding of advances in plant genetic resources, genome modifications, omics technologies to generate new solutions for food security under changing environmental scenarios etc have been discussed in this chapter. The increasing demand for food had a great impact on the agriculture sector to address the various challenges associated with crop productivity. The tremendous advancement in plant research helps in understanding plant biology for sustainable food security, functional ecosystems, crop improvement and human health. One of the sustainable farming techniques is the use of fertilizer at nano level. Nanomaterials that enhance plant nutrition could be considered as an alternative to the conventional chemical fertilizers. one chapter covered the importance of nano fertilizer to enhance metabolic processes in plants and reviewed the concerns in developing nanotechnological methods in the future. Metabolomics has now emerged as a powerful tool for the comprehensive analysis of metabolites within biological systems. One of the chapters provides a review on metabolomics, encompassing its methodologies, applications, potential impact on personalized medicine ,and discusses further the need for advancements in analytical technologies. The antifungal activity of mangroves, particularly Rhizophora species are one of the main sources for fungicidal compounds due to the presence of high concentration of phenols. The antifungal activity of Rhizophora species has been elucidated, and could be further utilized as biocontrol agents for fungal disease in agricultural crops. One of the chapters discussed the species identification and its impact on economical and ecological level in the species like Nutmeg, one of the important medicinal plants that had a greater attention ,however, it was very difficult to differentiate the sexual identity

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in the seedling stages. But the protein content screening among the studied plantlets had differentiated the sexes in the species as explained by the author.

AI (Artificial Intelligence) or machine intelligence enables farmers to enhance the quality and ensure a quick go-to market strategy for crops, and adoption of these algorithms to improve food industries. Artificial intelligence (AI) has also the potential to revolutionize education, from personalized learning to assessment and grading. Additionally, AI-powered tools can provide greater accessibility to students with disabilities, while also enabling more engaging and interactive content. AI continues to develop and become more prevalent in education, towards responsible and equitable implementation. However the negative and positive part of the AI may also be looked into.

The chapters related to microbiological aspects have also been incorporated in this book . Carbapenem-resistant A. baumannii (CRAb), bacteria that cause multi-infections in humans and resistant to multiple drugs too. The study attempted to isolate and characterize the bacterial species from the clinical specimens using biochemical techniques. The enzyme, carbapenemase produced by the bacteria was isolated and determined by different assays. Another study identified the antibacterial, antioxidant and anticancer activities of Ganoderma lucidum by various chromatographic techniques. Anticancer activity was also assessed on HeLa cell lines using MTT assay and DPPH assay. In one of the chapters,the author discussed L-asparaginase, one of the widely exploited enzymes for the treatment of acute lymphoblastic leukemia (ALL). Also attempted to isolate and characterize the enzyme from soil samples collected from different locations at Kerala. The study indicated that soils can provide a rich source for L-asparaginase which has got ample application in pharmaceutical industries.

The studies on various geological aspects with respect to different geographical areas in Kerala soil has been included in the book. The vertical geochemical variation and elemental mobility of the lateritic terrain in the Makkaraparamba of Malappuram District, Kerala has been very well investigated. Under extremely oxidizing and leaching conditions, laterite


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soil transformed into a variety of rocks and further developed into stable secondary product in the existing humid tropical and subtropical environments. The hydrogeological conditions in Kumbala- Kaliyar river basin, Kasaragod district, Kerala was assessed by means of Vertical Electrical Sounding (VES). The digital spatial data output of the present study would be much helpful for planning and management of surface and sub-surface water resources of Kasaragod River basin in which the Kasaragod township is centrally located

The contributed chapters in the book written by the faculties of science stream in the light of the recent thinking and developments in the field of science and education.Science& Technology is now dominates almost every field of our activities. In summary , The faculties ( Science stream) of GEMS Arts & Science college have made a n excellent attempt to bring about this book Homo Scientia".covering almost all the important areas from biological sciences to artificial intelligence. Every article has its own merits in both academic and research fronts..I record my grateful appreciation and thanks to the contributors of this book for their untiring efforts.

**Dr.Balagopalan Unni**

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# METABOLOMICS: AN INTEGRATIVE APPROACH TO UNRAVELING BIOLOGICAL COMPLEXITY

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**ABSTRACT:**

Metabolomics has emerged as a powerful tool for the comprehensive analysis of small molecule metabolites within biological systems. It offers insights into the dynamic metabolic profiles and pathways that underlie various physiological and pathological processes. This review paper provides an extensive overview of the field of metabolomics, encompassing its methodologies, applications, and potential impact on personalized medicine. We discuss different analytical techniques, data acquisition and processing strategies, as well as computational tools for metabolite identification and data interpretation. Furthermore, we explore the diverse applications of metabolomics in areas such as disease biomarker discovery, drug development, nutritional sciences, and environmental research. Finally, we address the current challenges and future perspectives in the field of metabolomics, emphasizing the need for data integration, standardization, and further advancements in analytical technologies.

## INTRODUCTION

Metabolomics is a rapidly evolving field that focuses on the comprehensive analysis of small molecule metabolites within a biological system. It provides a snapshot of the metabolic state and offers insights into the biochemical pathways and networks

that underlie various physiological and pathological processes. By profiling the metabolome, which encompasses the entire repertoire of metabolites within a cell, tissue, or organism, metabolomics aims to unravel the complex interplay between genes, proteins, and environmental factors that shape cellular metabolism.

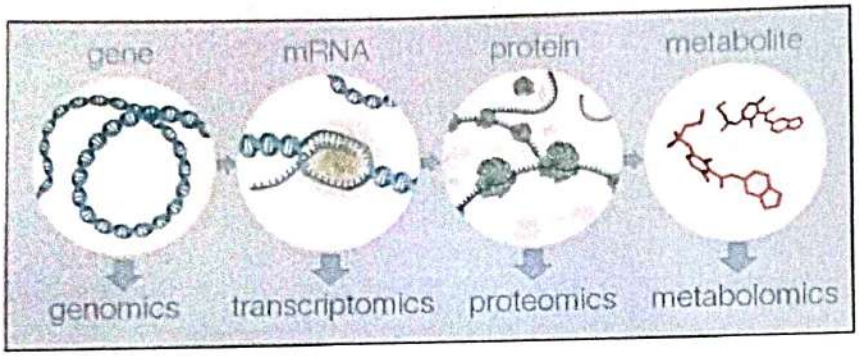


Fig. 1: Overview of the four major "omics" fields, from genomics to metabolomics (Courtesy: EMBL's European Bioinformatics Institute).

Metabolomics has gained significant attention in systems biology as it offers a holistic perspective on the functional status of a biological system. It complements genomics, transcriptomics, and proteomics by providing a direct measure of the end products of cellular processes. Through the analysis of metabolite patterns and signatures, metabolomics enables the identification of biomarkers for disease diagnosis, prognosis, and treatment response. Additionally, it facilitates the discovery of novel therapeutic targets and the evaluation of drug efficacy and toxicity.

**Analytical Techniques in Metabolomics**

A wide array of analytical techniques has been developed and employed, offering valuable insights into the metabolic pathways, dynamics, and interactions that underlie various physiological and pathological processes. Among the most prominent analytical platforms used in metabolomics are mass spectrometry and nuclear magnetic resonance spectroscopy.

Mass spectrometry is a versatile technique that enables sensitive and high-throughput analysis of metabolites. Gas chromatography-mass spectrometry is commonly used for volatile and semi-volatile metabolites. GC separates the metabolites based on their volatility, and the compounds are then ionized and fragmented in the MS. This technique provides information about the mass-to-charge ratio, fragmentation patterns, and relative abundance of the metabolites, facilitating their identification and quantification. Liquid chromatography-mass spectrometry is suitable for a broader range of metabolites, including polar and nonpolar compounds. LC separates the metabolites based on their physicochemical properties, and the eluted compounds are ionized and analyzed by the MS. MS-based techniques offer high sensitivity, selectivity, and accuracy, allowing for the detection and quantification of metabolites in complex biological samples.

Nuclear Magnetic Resonance spectroscopy, particularly proton NMR (^1H-NMR), is another powerful analytical technique in metabolomics. NMR provides detailed information about the chemical structure and dynamics of metabolites. It is non-destructive, reproducible, and does not require extensive sample preparation, making it advantageous for high-throughput analyses. NMR spectra provide signals corresponding to different functional groups present in the metabolites, enabling their identification and quantification. Moreover, NMR allows for the measurement of metabolite concentrations in a relative or absolute manner, providing valuable quantitative information.

The choice of analytical technique in metabolomics depends on several factors, including the research question, the metabolite classes of interest, and the available instrumentation. Each technique has its advantages and limitations. MS offers high sensitivity and versatility, allowing for the detection of a wide range of metabolites. It provides quantitative and qualitative information but may require complex data processing and metabolite identification strategies. NMR, on the other hand, is advantageous for its non-destructive nature, high reproducibility, and the ability to directly measure concentrations. However, NMR may have lower sensitivity

compared to MS and may require larger sample volumes.

To enhance metabolite separation and coverage, analytical techniques such as liquid chromatography or gas chromatography are often coupled with MS or NMR. LC-MS and GC-MS provide improved separation of metabolites prior to their detection, enabling the analysis of complex samples with higher resolution. Various separation modes, such as reversed-phase, normal-phase, and ion exchange chromatography, can be utilized to enhance metabolite separation based on their physicochemical properties. Additionally, advancements in data acquisition techniques, such as tandem MS (MS/MS), enable the elucidation of metabolite structures and the identification of metabolites with higher confidence.

**Other Emerging Techniques in Metabolomics**

Several emerging techniques are being explored and developed to further enhance the capabilities of metabolomics research. These techniques offer unique advantages in terms of sensitivity, spatial resolution, and coverage of the metabolome. Here, we discuss some of these emerging techniques in metabolomics.

**Direct Infusion Mass Spectrometry (DIMS):** Direct infusion mass spectrometry is a label-free technique that allows for the rapid analysis of intact metabolites without the need for prior separation. It enables high-throughput analysis, as it eliminates the time-consuming step of chromatographic separation. DIMS is particularly useful for targeted metabolomics approaches, where specific classes or groups of metabolites are of interest.

**Capillary Electrophoresis (CE):** Capillary electrophoresis is a separation technique that separates charged metabolites based on their electrophoretic mobility. CE coupled with MS offers high separation efficiency, sensitivity, and resolution for the analysis of polar metabolites. It complements other analytical techniques by expanding the coverage of the metabolome, particularly for small polar compounds.

**Imaging Mass Spectrometry (IMS):** Imaging mass spectrometry combines MS with spatial information, enabling the mapping of metabolite distributions within tissues or cells.

IMS allows for the visualization of metabolite localization, which is valuable for understanding metabolic heterogeneity and investigating disease processes. It has applications in fields such as cancer research, neuroscience, and drug metabolism studies.

**High-Resolution Mass Spectrometry (HRMS):** High-resolution mass spectrometry offers improved mass accuracy and resolution compared to conventional MS. HRMS enables precise determination of molecular formulas and structural elucidation of metabolites. It is particularly useful for the identification of unknown or unexpected metabolites, as well as the differentiation of isobaric species.

**Ion Mobility Spectrometry (IMS):** Ion mobility spectrometry is a separation technique that measures the mobility of ions in a gas-phase based on their size, shape, and charge. IMS coupled with MS provides an additional dimension of separation, enhancing metabolite identification and resolution. IMS is advantageous for the analysis of isomeric compounds and the characterization of complex mixtures.

**Ambient Mass Spectrometry:** Ambient mass spectrometry techniques allow for the direct analysis of samples in their native state, without prior sample preparation or extraction. Techniques such as desorption electrospray ionization , direct analysis in real-time , and laser ablation electrospray ionization enable rapid and non-destructive analysis of metabolites in tissues, bio fluids, and surfaces.

**Applications of Metabolomics:**

Metabolomics has found extensive applications in various fields, providing valuable insights into the metabolic alterations associated with health, disease, and environmental exposures. By comprehensively analyzing the metabolome, metabolomics offers unique opportunities for biomarker discovery, understanding disease mechanisms, advancing drug development, and optimizing nutritional interventions.

**Disease Biomarker Discovery and Clinical Applications:** Metabolomics has emerged as a powerful tool for the discovery and validation of biomarkers for various diseases, including cancer, cardiovascular diseases, diabetes, and neurodegenerative

disorders. By comparing metabolite profiles between diseased and healthy individuals, metabolomics can identify specific metabolites or metabolic patterns that serve as potential diagnostic, prognostic, or therapeutic response biomarkers. These biomarkers can aid in early disease detection, risk assessment, treatment monitoring, and personalized medicine approaches.

**Drug Discovery and Development:** Metabolomics plays a vital role in drug discovery and development by providing insights into drug metabolism, efficacy, and toxicity. Metabolomics studies help identify metabolic pathways affected by drug treatments and evaluate drug-induced changes in metabolite levels. This information can guide the selection and optimization of drug candidates, identify potential off-target effects, and improve our understanding of drug mechanisms of action.

**Nutritional Metabolomics and Food Sciences:** Metabolomics is valuable in understanding the impact of diet and nutrients on human health. It allows for the assessment of dietary intake, identification of metabolic signatures associated with specific diets or nutritional interventions, and evaluation of nutritional status. Metabolomics also contributes to food science and safety by characterizing metabolite profiles in food products, assessing food quality and authenticity, and detecting contaminants or adulterants.

**Environmental Metabolomics:** Environmental metabolomics investigates the effects of environmental exposures on living systems. It helps identify biomarkers of exposure, understand metabolic responses to environmental stressors, and assess the impact of environmental pollutants on human and ecological health. Environmental metabolomics is crucial for monitoring environmental contaminants, elucidating mechanisms of toxicity, and developing strategies for environmental risk assessment and management.

**Personalized Medicine:** Metabolomics has the potential to enable personalized medicine approaches by considering an individual's unique metabolic profile. Metabolomics data can guide treatment selection, predict drug response, and

identify subgroups of patients who may benefit from specific therapies. The integration of metabolomics with other omics technologies, clinical data, and machine learning approaches offers a comprehensive understanding of disease heterogeneity and the development of precision medicine strategies.

## CONCLUSION

As metabolomics continues to evolve, challenges remain. Standardization of protocols, data analysis workflows, and metabolite annotation are critical for reproducibility and data integration. Additionally, advancements in computational methods, data sharing, and collaboration among researchers are necessary to fully exploit the potential of metabolomics.

In conclusion, metabolomics is a powerful tool that provides a comprehensive understanding of the metabolic landscape within biological systems. Its applications in biomarker discovery, disease mechanisms, drug development, nutritional sciences, environmental research, and personalized medicine have the potential to transform healthcare, improve disease management, and optimize treatment strategies. With further advancements in technology, data analysis, and collaborative efforts, metabolomics will continue to unravel the complexities of the metabolome and contribute to our understanding of the intricate metabolic networks in health and disease.