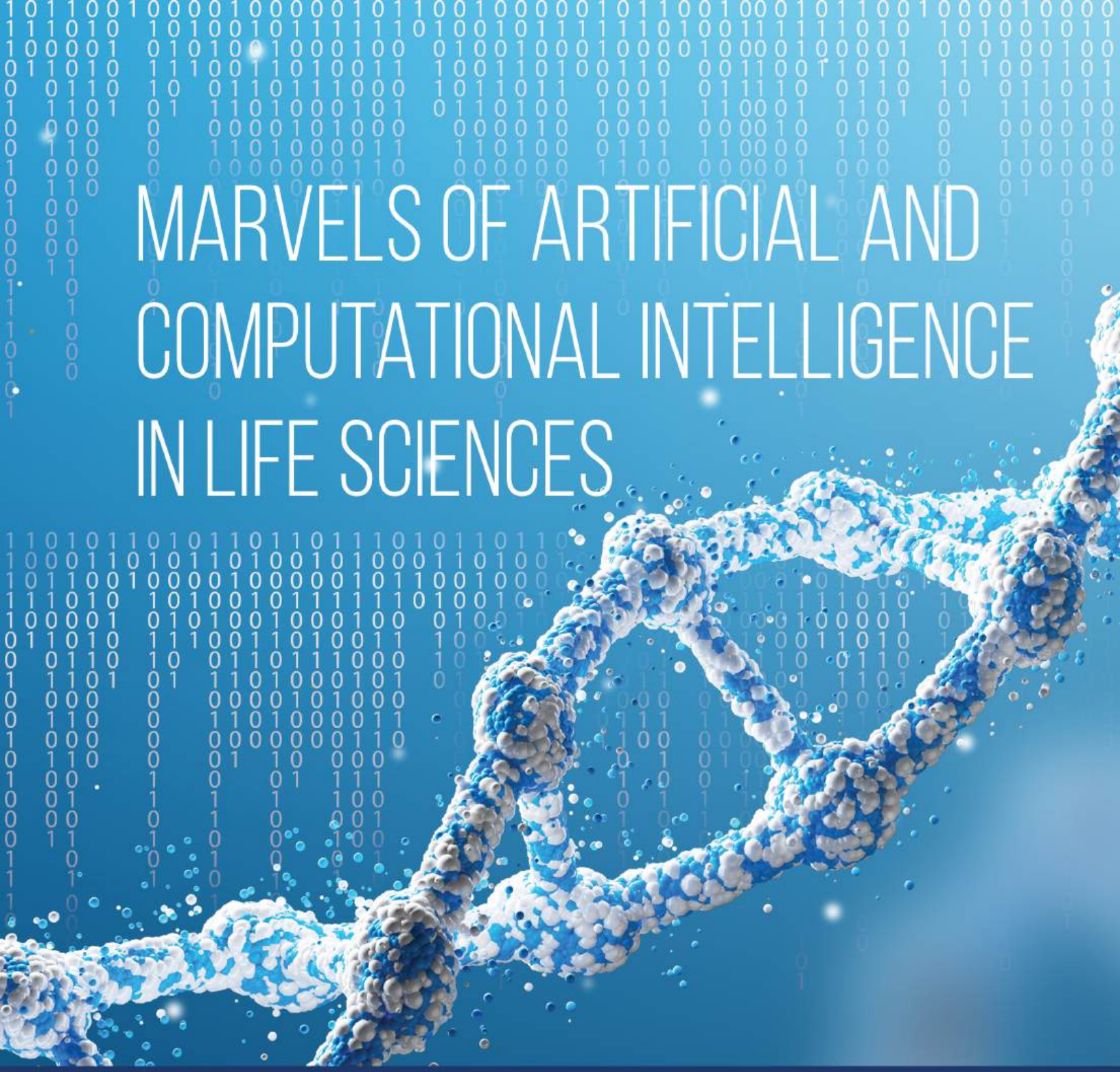
MARVELS OF ARTIFICIAL AND COMPUTATIONAL INTELLIGENCE IN LIFE SCIENCES



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Marvels of Artificial and Computational Intelligence in Life Sciences

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FOREWORD I

I am glad to learn that a book on "Marvels of Artificial and Computational Intelligence in Life Sciences", an undisputed lead technology that rules the world, is the combination of different computing technologies. AI & CA are not just about computers but the life, threat, and security of science, individuals, and humanity. AI & CA are composite fields involving computer science, mathematics, database, and network management. A common objective of AI is to enrich and enhance the experience of the users of different gadgets and information systems by ensuring their availability, integrity, authentication, confidentiality, and non-repudiation so that the right people can access accurate information at the right time. One should not forget that the use of the internet, social media, smartphones, and tablet computers are indispensable in daily life. In this context, this book focuses on the applications and futuristic trends in the perspective direction to address the dreams of the younger generations, who aspire to gain knowledge on applications that would provide imaginative thinking and forethought. The reader would gain new avenues of thought for applications of AI in IoT, and computational approaches for data analytics would be the expected lines of development in all fields of life. I hope that ideas and futuristic prospects underlined by the contributors will evolve into research hubs as the contributors have done extensive work to kindle the novel thoughts of research.

The young population has become increasingly dependent on computers and gadgets as information resources for communication, entertainment, financial transactions, education, socializing, and private and government services. Today, the infrastructure is information technology infrastructure rather than other physical structures. Many computer users think that their firewall and antivirus software provides them with all the protection they need to keep their computers secure. On the other hand, ever-evolving data science and data analytics of information systems also raise security concerns from many facets. However, AI and CA have become resourceful to users for the addition of more information to a growing number of databases. Meanwhile, the phenomenon coexists with increased expectations of exposure to hacking and attacks, misuse of information, and other security breaches. This book also describes informative systems that are vulnerable to illegal usage through internet connections.

I also envisage the editors and authors will continue to do the same work on different topics of interest in years to come. The efforts by the authors, editors, and publishers are commendable, and I wish the team to continue to serve the student community on a large scale in the coming days.

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FOREWORD II

I am happy to realize that the editors of the book "Marvels of Artificial and Computational Intelligence in Life Sciences" provide a valuable window on applications of AI & CA and cover the necessary components from various quarters of life, science and technological advancements of today. AI is becoming a critical technology that takes on life and productive scenarios of human beings and being human in ever-evolving situations of life. The book discusses the wide scope of research and deployed ability of AI & CA. All the chapters are highly impressive, well-researched, and authoritative in introducing all the facets of sciences and trending technologies, which integrate the highest volume of data. On the basis of available data, analytical research algorithms are being designed to address many questions/tasks in the present scenario. For instance, in restaurants, shops, or even on road walks, the data of individuals are being captured for analysis to decide on the needs of the individual, popularly known as 'proactive internet analytics'. Hence, artificial intelligence and computational approaches emerged as the indispensable technologies of the current decade and will continue to rule even for more decades. In this new age of global interconnectivity and interdependence, it is necessary for students to have awareness and knowledge about AI & CA and their supremacy. Hence, the initiative of these professional editors and authors is highly appreciated.

This book can help teachers develop a shared vision and understanding of interpretive discussion and its flexible uses across subjects and grade levels. The framework annotated examples and appendixes can structure and guide teachers' joint work as they prepare questions, co-lead discussions, observe and analyze classroom experiments, and discuss emergent questions and problems. As teachers gain confidence and skill through collaborative experimentation and development, they can also study the impact of participating in such discussions on students' confidence and academic skills. Tie-together, this book offers a curriculum for teacher learning at every career stage. Reading the book, you will find it hard to defend the view that good teachers are born, not made. I hope that this book will become a primer for teachers, teacher educators, and professional developers, helping teachers across the globe with applications of AI & CA to learn, teach, and practice the marvels of AI & CA.

I hope the book is a good resource for the students' community and teachers of contemporary technologies. I congratulate the editors and the authors for their efforts in bringing this book to the perspectives of researchers and as well teachers.

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PREFACE

At present, we are living in a technology-advanced world, which was not dreamt of by most of us when we were in our childhood. Similarly, how many of us are dreaming about the world that would be in the next century? In everyday life, we are using many non-living things that are functioning on par with human actions: alarm clocks, air-conditioners, refrigerators, washing machines, micro ovens, rice cookers, TV remotes, speed controllers for vehicles, smart watch/phone/TV and so on. In science, performing computational analysis before starting any research work is becoming mandatory to design and complete the tasks smartly. In general, Artificial Intelligence (AI) is dealing with simulations of human processes by a combination of mechanical, electrical, biological and computer engineering in particular. Computational approaches help to speed up calculation processes, which may be either simple mathematics or complex mathematics accounting for various physical forces acting on object(s). Thus, AI, a higher version of computational analysis, is becoming indispensable from sophisticated science and general lifestyle standpoints: For instance, robots in industries, in defense forces, and so on. Simply, it is the order of the day for humankind that a person cannot live without the influence of artificial intelligence and its applications.

With this background, we brought this book titled "Marvels of Artificial and Computational Intelligence in Life Sciences" for young aspiring candidates who have intellectual enthusiasm to pursue a career in the subject areas of artificial intelligence (AI) and computational approaches (CA). The book consists of 16 chapters (9 and 7 chapters are under the headings of AI & CA, respectively) describing the roles and applications of AI and CA in the different parts of our life systematically and lucidly. As you can refer, the contents are a good blend of topics in such a way the readers would clearly understand the multi-disciplinary nature of the emerging fields. The first 9 chapters of the book deal with the applications of AI in disease surveillance, disease diagnosis, drug discovery, drug design, home appliances, bio farms, power engineering & CAD modeling. The next 7 chapters of the book deal with the uniqueness of CA in identifying inhibitors to various druggable protein molecules, in health care systems, in numerical simulations, and data analysis of biophysical experiments. We trust that this book throws light on the things to come in the years to go. Let us all celebrate smartness and be in line with advanced technologies.

Taking this opportunity, the Editors would like to thank all authors of the book chapters for their sincere contributions, and anonymous reviewers for their constructive and perspective comments on the book chapters in their previous versions, which are the combined prime factors behind the present scientific merit of the book. The Editors express heartfelt thanks to the Editorial board and professional members of the Bentham Science Publishers for their intellectual encouragement, technical support, and entrepreneurship patronage for successfully bringing the book in all possible ways. The Editors also thank all the personnel, well-wishers, and almighty, who are behind this achievement.

Constructive suggestions on any parts of the book may be sent to the Editors and as well to the Publishers, and those suggestions will be addressed in future editions of the book.

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CHAPTER 1

Artificial Intelligence for Infectious Disease Surveillance

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Abstract: Artificial intelligence (AI) is a branch of science that mainly deals with computers. It can store massive data through built-in programs that can accumulate the required data and convert it into intellectual actions with a reason. In recent years, AI has played a vital role in various governmental and non-governmental sectors such as engineering, medicine and economics. The development of AI in the field of infectious diseases is colossal with a spectrum of applications including pathogen detection, public health surveillance, cellular pathways and biomolecules in host-pathogen interactions, drug discovery and vaccine development. Similarly, early detection is the key to controlling any disease outbreak. Systematic collection and analysis of data will yield vital data on the required tools for controlling the outbreak situation. The antibiotic stewardship program is being implemented in very few healthcare institutions due to its intense cost and work. AI is used for tackling the rise in antibiotic use and developing an algorithm that can effectively control the use of antibiotics along with diagnostic and treatment measures.

Keywords: Artificial intelligence, Algorithm, Antibiotics, COVID, Diseases outbreak.

INTRODUCTION

Artificial intelligence (AI) is a branch of science that deals with computers and built-in programs that can accumulate required data and convert it into intellectual actions with a reason. IBM defines AI as "that computers and machines mimic the problem-solving and decision-making capabilities of the human mind". AI heavily relies on reasoning, machine learning, and application development.

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AI includes systems that mimic human intelligence such as rational thinking and perform tasks with the available trained datasets. This helps to understand and solve problems efficiently and rapidly. The root relies on the inputs from trained and untrained datasets from various sources. The capability of the supercomputers in a specific format brings AI to act like humans and enhance the capabilities and contributions to human society.

The transformation from the "Human approach" in which systems think and act like humans to the "Perfect approach" in which systems think and act rationally is warranted to make problem-solving systems. The field of AI is a combination of computers and validated datasets. These are utilized including machine learning and deep learning algorithms. The developed systems make targeted predictions based on trained datasets. Machine learning utilizes algorithms with the previous data to predict the newer data. For this, different approaches to machine learning are implemented. Classical machine learning is implemented through supervised learning, unsupervised learning, semi-supervised learning and reinforcement learning. Depending on the data and the required output, any of the above approaches is chosen.

The application in medicine including dental sciences, optics and allied health sciences is widely spread recently. The convergence of AI and meta-optics has resulted in major developments in design, simulation and optical applications in terms of device testing and interpretation [1]. The development of AI in the field of infectious diseases is massive with a spectrum of applications including pathogen detection, public health surveillance, cellular pathways and biomolecules in host-pathogen interactions, drug discovery, and vaccine development.

The swift emergence of machine learning algorithms and computational resources in genomics and proteomics and other databases results in greater efficiency, precision, and dependability. These current techniques have provided growing prospects for their regular use in healthcare. Apart from medical sciences, AI has found its applications in different disciplines including engineering and economics as well.

The UK National Screening Committee assessed the use of AI systems that can screen, examine and classify mammograms and efficiently interpret and implement them into the UK Breast Screening Program. Improved programs to include specificity and detect a wide spectrum of diseases were taken into important consideration for obtaining maximum benefits. Retrospective and prospective studies could provide substantial evidence for the health professionals for women's well-being [2].

Several models have been built of which the “black box” model is one of the recently evolved models with high precision for healthcare systems. A model was built for cardiologists with different techniques for making predictions based on interpretable agnostic explanations and surrogate decision trees. A similar “black box” model has been reported to decide on pharmacovigilance.

The recent pandemic experiences of COVID-19 increased the search for new drugs and the repurposing of drugs for the control of the hyperinflammatory immune response. The anti-inflammatory drug baricitinib, a Janus Kinase (JAK) 1/2 inhibitor approved for rheumatoid arthritis has recently been strongly recommended by the WHO for use in COVID-19 patients. Assisted by AI, the drug’s antiviral and anti-inflammatory activities swiftly navigated to the clinical trials for use along with other immune modulators and JAK inhibitors. This indicates that drug discovery including drug repurposing that is assisted by AI can tremendously benefit therapy [3]. A smart contract-based solution has been developed for analysing the impact of contact tracing, and digital records for COVID-19 vaccinees with encrypted data chains and interplanetary file systems [4 - 7].

A model for the prediction of patients’ need for ICU admission and risk assessment on mortality was developed based on trained deep-learning model datasets of clinical features and chest radiographs. The AI tool and random forest analysis were used on the datasets to build the architecture and it was tested on prospectively recruited patients successfully [8]. The influence of AI on mobile users in the form of applications for monitoring and improving health has created now future perspectives on infectious disease control and therapeutic solutions.

Clinical diagnosis and appropriate therapeutic strategies are the areas that require immediate attention from AI. Antimicrobial resistance is the biggest challenge all over the globe, especially in intensive care unit settings. The extensive and unnecessary use of antibiotics has contributed to antimicrobial resistance that increases morbidity and mortality rate. The antibiotic stewardship program is being implemented in very few healthcare institutions due to its intense cost and work. The use of AI has been seen in tackling the rise in antibiotic use and developing an algorithm that effectively controls the use of antibiotics along with diagnostic and treatment applications. Suitable antibiotic therapy could be devised for specific infections or scenarios based on trained datasets of clinical data and suggest appropriate antibiotics for a better outcome. This could help establish antimicrobial stewardship more effectively to combat the nightmares of multi-drug-resistant pathogens [9].

CHAPTER 2

Recent Innovations in Artificial Intelligence (AI) Algorithms in Electrical and Electronic Engineering for Future Transformations

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Abstract: This chapter explores recent Artificial Intelligence (AI) innovations in core engineering domains, especially in Electrical and Electronics Engineering. The major grounds for these innovations arise due to the engineer's work toward the forefront innovative technologies, by contributing in research, design, development, testing, and manufacturing of next-generation equipment. The Electrical and Electronics Engineering expands its research and development methodology in applications with artificial intelligence subsets such as machine learning, deep learning, and data science algorithms. This as an upshot made an industrial revolution 4.0. In the evolution of new generation areas of research and development, which are discussed in this chapter, AI algorithms are implemented in the field of power systems, power electronics, smart grids, and renewable energy technologies. The experimental verification for these innovations has been executed using Matlab/Simulink design environment.

Keywords: Artificial intelligence, Deep learning, Machine learning, Power system, Power electronics, Renewable energy.

INTRODUCTION

Recently, Artificial intelligence (AI) is a fast-growing field and during the last few decades, it plays an important role in research areas [1, 2]. The goal of AI is to make machines (systems) simulate the intelligence of humans in it such as learning and reasoning. It has numerous advantages and has been effectively implemented in most industrial applications which include image classification,

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speech recognition, autonomous cars, *etc.* Because of its high potential value, power electronics and power systems also benefit from the evolution of AI, especially in the power module heatsink design optimization [3] and maximum power point tracking control for renewable energy sources such as wind and solar power plants [4, 5]. Autonomous power electronic components can be enabled by implementing/integrating AI with the system. This feature may improve the self-adaptability and self-awareness of the system. In addition, the power electronic component requires a variety of data throughout its life cycle, it can be fulfilled by the development of the internet of things (IoT), sensor technology, and big data analytics [6, 7].

AI is utilized to extract the data to revamp a product rival by design optimization, automation, system health monitoring, *etc.* Subsequently, the research in power electronics and power systems (electrical engineering) can be conducted from a data-driven perspective which is advantageous to challenging cases. AI (machine learning) is important in power systems and power electronics due to its nonlinear and complex characteristics such as tuning speed in control implementation, high sensitivity in condition monitoring for aging detection, *etc.* As a result, there is a demand for an overview of AI in electrical engineering to enhance the combined research in various applications. Based on the literature available in the sources, in this chapter, the applications of AI in electrical engineering are categorized as follows. *i.e.*, design, control, and maintenance.

Over the decades, applications of AI are almost ubiquitous and experienced spectacular dynamism. The continuously growing research area is the system control and correspondingly the number of publications has also increased over the past few years. Several existing pieces of literature related to AI in electrical engineering are presented here. Neural networks in industrial applications are discussed with the design of network structure, applications, and training methods [8]. The metaheuristic methods for stochastic optimization for power quality and waveform, circuit design, and control tuning are elaborated in a study [9]. By using AI techniques, such as fuzzy logic, metaheuristic methods are discussed [10], and highlighted with examples. A detailed discussion of metaheuristic methods for MPPT in a photovoltaic system is also presented [11]. Fault detection methods *via* AI technology in power electronics are discussed in most of the literature [12 - 15]. Nevertheless, it requires more details of the algorithm and a comparative analysis of machine learning methods. Subsequently, the complete review of AI algorithms and applications in electrical engineering is not discussed in detail. From the emerging perspective, this chapter aims to bridge this gap and consolidate the systematic needs of AI techniques in power electronics as well as power systems. Further, AI (fuzzy logic and machine learning technique) is impl-

emented and compared *via* MATLAB simulation for electrical engineering applications.

PROS AND CONS OF AI IN ENGINEERING

The advantages and disadvantages of emerging technology, *i.e*, Artificial Intelligence (AI) in electrical and electronics engineering are detailed in this section.

Pros of AI in engineering systems are as follows;

• Reduction in human error

• Saftey of human labor

• Speed of decision making

• Availability (continues working 24/7)

By looking at the various advantages of AI in the engineering field, we see the other side of the shortcomings of AI discussed below.

Cons of AI in engineering systems are as follows;

• Making Unemployment in human society

• Lack of emotional intelligence

• High cost and time required for an implementation

Now, the following pros and cons are understood from the above sections. From this, the integration of AI into electrical and electronics engineering applications can be addressed clearly in the upcoming sections [16].

ROLE OF AI IN POWER SYSTEMS

The most commonly implemented AI algorithms in power system engineering are Expert System Techniques, Artificial Neural Networks, and Fuzzy Logic Systems [16].

• Expert system is a computer system-based algorithm that incorporates the right decision-making as human experts. This system is used for calculating and determining the parameters and values in Power system generation, transmission and distribution.

CHAPTER 3

An Introduction to Diabetes Drug Discovery in Biomedical Industry through Artificial Intelligence, Using Lichens' Secondary Metabolites

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Abstract: Proven history in science shows that natural products play a vital role in drug discovery, specifically for immune deficiencies, infectious diseases, and other therapeutic areas, including cardiovascular diseases and multiple sclerosis. Monk Agastyar and Pandit Ayothidhas contributed more to the field of Siddha through mono- and polyherbal medicine and cured many diseases, including oxidative stress and diabetes. Using computational and analytical intelligence methods, this study aims to develop a natural phycobiont (lichens) edible source of metabolites for the chronic and metabolic disorder type II diabetes. The level of docking was ranked based on the iGEMDOCK grading function, with zero being the most accurate ligand. Ultimately, each complex from each fungus that ensured different binding pockets of the 6AK3 had been designated throughout the virtual screening process. Based on the uppermost energy value, the best compounds from each fungus showed accurate molecular docking. Out of the 22 compounds tested, the anthracene-9-one and acetamide found in *R. conduplicans* showed a high binding capacity. Meanwhile, the binding energy potential of M-Dioxan-4-ol, 2,6-dimethyl, obtained from *X. curta*, and 2-Chloroethyl Methyl Sulfoxide, obtained from M. fragilis, was enormous. *3, 4-13, 14-dodecahydr--18,18a-dihydroxy-2-methyl-, and 1,4-Bis (trimethylsilyl) benzene were all found in P. reticulatum.*

Keywords: Binding Energy, Docking, Metformin, Orsellinic Acid, Octasiloxane, Paraldehyde, Simulation, *Xylaria Curta*.

INTRODUCTION

Metabolic disorders from various humanised pathways are found in diseases as follows: Parkinson’s disease, inflammation, neurodegeneration, infection, cancer,

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diabetes, and obesity. These diseases have been reported since the beginning of scientific days and are not ignorable. By using the integrated drug discovery and product development programs, we were focusing on the following treatments: inflammation and its related proliferative diseases, various types of cancer, metabolic disorders including diabetes, neurodegenerative diseases, psoriasis, and infectious diseases. To prevent and secure against this, many natural and biologically proven scientific ailments were found. As a recent advancement in technology, epigenetic modulation was found in diabetic nephropathy through miRNA technology. Several decades after the identification and efficacy testing of natural products from higher and lower plants with GLP-1R agonist activities, other microbially-derived natural metabolites are recognised to have anti-diabetic potential. Along with this, the identified metabolites were artificially synthesised and treated for different types of diabetes. Many impressive studies have been reported in other developing countries such as one of the screening processes of Indian biodiversity and Indian systems of medicine in the search for newer compounds in the following domains: inflammation, arthritis, diabetes, cancer, and hepatoprotective activities [1]. Proven history in science shows that natural products play a vital role in drug discovery, specifically for immune deficiencies, infectious diseases, cardiovascular diseases and multiple sclerosis. Natural products offer unique markers resembling conventional synthetic molecules. Naturally, they have a higher molecular mass, an unbent number of sp3 carbon traces and oxygen particles but lesser nitrogen and halogen fractions, higher digits of H-bond acceptors and donors, and the lowest calculated octanol-water breakup coefficients and more significant molecular rigidity, which correspond with manufactured compound libraries. They denoted vast scaffold variations and structural complexities. Natural or synthetic drug molecules are often collected and identified in phenotypic, wet-lab experimental assays. Deconvolution of their molecular mechanisms of action can be a time-consuming methodology. But the artificial intelligence and computerised molecular evaluation and experimental analysis processes conserved time and were economical in terms of expenses with manpower support. The outcome of screening assays is likely, leveraging the prospect of rejuvenated cells and gene editing therapies, as well as approaches to determining the modes of activity of functional treatments. These treatment methodologies were being used by three premier operations. They are in first-generation analytical techniques, second-generation genome mining with an engineering approach, and cultivation systems, respectively. Similar to the image processing method that previously identified butterflies and lichens using artificial intelligence approaches, this search determined the pharmaceutical intelligence method for diabetes and various cancers. There is a standard concurrence that concentrated target validation is an essential part of exploring medication and has

more magnificence in the directive to boost the evolution of unexplored treatments..

Monk Agastyar and Pandit Ayothidhas contributed more to the field of Siddha through mono- and polyherbal medicine and cured many diseases, including oxidative stress and diabetes. It has been known since ancient times that humans use lichens for different types of daily needs. In this way, polypharmacy was taught through the diverse indigenous peoples of the world [2]. The pharmaceutical industry has dramatically increased its data digitization during the last few years. The difficulty of gathering, examining, and utilising that knowledge to resolve challenging healthcare problems comes with this digitalization, too. Because AI can handle massive amounts of data with improved automation, this encourages its use. Technology-based artificial intelligence (AI) systems can replicate human intelligence by using a variety of cutting-edge tools and networks. It does not, however, pose a danger if it totally displaces human physical presence. AI employs hardware and software that can analyse and learn from input data to make independent decisions in order to achieve predetermined goals. As this review describes, its uses in the pharmaceutical industry are constantly expanding. The McKinsey Global Institute predicts that the rapid advancements in AI-guided automation will fundamentally alter society's approach to work [3]. AI encompasses several fields of application, including machine learning as its core paradigm as well as intelligence, deep learning, and resolution search. In machine learning, algorithms are used to find patterns in a data collection that has been further classified. Deep learning is a branch of machine learning that uses artificial neural networks. These are a group of intricately connected computing components called “perceptons” that resemble biological human neurons in their ability to transmit electrical impulses. Each node in an ANN receives a distinct input, and the nodes combine their outputs into mono- or multi-linked outputs by utilising methods to solve issues. Convolutional neural networks, (RNNS) recurrent neural network, and multilayer perceptron networks are a few examples of ANNs that use either supervised learning or unsupervised learning and workout regimens [4]. CNNs are used in the processing of images and videos, in the modelling of biological systems, in the analysis of complicated brain operations, in pattern recognition, and in advanced signal processing. CNNs are a collection of complex behaviours with local connections that are distinguished by their topology. Kohonen networking, backpropagation neural broadcasters, LVQ communications, and ADALINE channels are some of the more complicated varieties [5]. Functional protein identification and their interactions have become crucial steps in the post-genomic age for comprehending the molecular machinery of the cell. The amount of information being produced by structural genomics and proteomics advances is enormous. Because the biological function of proteins is frequently closely

CHAPTER 4

Structural Bioinformatics and Artificial Intelligence Approaches in *De Novo* Drug Design

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Abstract: *De novo* drug design is a computational technique to develop novel chemical compounds from scratch without prior knowledge. Traditionally, structural bioinformatics approaches used either structure-based or ligand-based design; the former uses the active site information of the protein, and the latter uses known active binders. Modern methods based on artificial intelligence help design *de novo* drugs in less time by using pre-trained models. One of the major bottlenecks of the *de novo* drug design is the synthetic feasibility of the active compounds, which is addressed using AI-based methods that help reduce the time and cost of analysis of those compounds. Recent success stories from several companies show the strength of the AI-based *de novo* drug design programs, and many advances can be expected shortly.

Keywords: Artificial intelligence, Computer-aided drug design, Deep learning, Machine learning, Molecular docking, Scoring functions.

INTRODUCTION

Over the decades of drug discovery, several advancements happened in the field of drug discovery like database screening (finding a potential lead molecule for the target protein from the in-house database or public chemical compound database) or drug repurposing (using existing drugs for a novel protein target) using computational/experimental and its combination [1]. Designing or developing novel drug molecules with the desired biological activity for a potential protein target is crucial for pharmaceutical companies [2]. *De novo* design is the most preferred approach due to the higher possibility of developing novel molecules from the vast unexplored chemical space without any issue in claiming Intellectual Property Rights (IPR), as it never existed before.

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De novo denotes the designing compounds "starting from scratch" without prior knowledge (reference template). Though the rate at which protein structures were experimentally determined exponentially increased, the recent breakthroughs using the artificial intelligence method 'AlphaFold' predictions changed the entire scenario [3]. Artificial intelligence (AI) applications are predominantly increased in almost all fields, starting from the weather forecast, online shopping, several other predictions, and even drug discovery. In the field of drug discovery, it is widely used in the virtual screening of several millions of compounds in lesser time compared to the conventional methods, accessing the druggability of the target, predicting the pharmacokinetics properties (Adsorption, Distribution, Metabolism, Excretion –ADME) including the toxicity of the compounds, synthetic feasibility of the designed compounds, drug repurposing (studying the effect of existing drugs for the new targets) and *de novo* drug design (Fig. **1**). But the question is whether AI is a real hope or just a hype, though we can't get a straightforward answer; currently, we are getting promising results, but over time, we will come to know more about it [4].

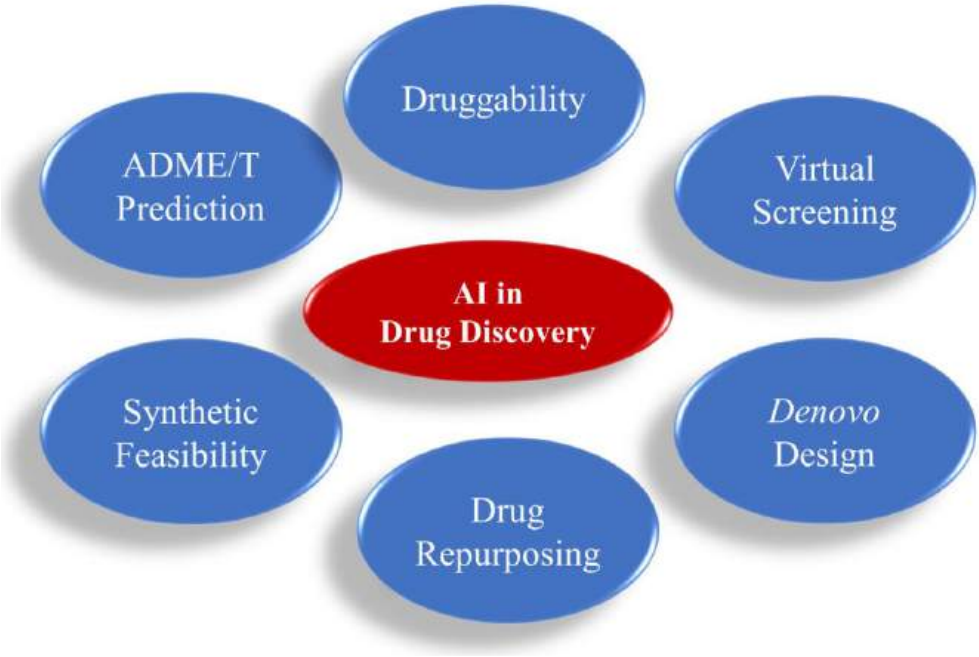

Fig. (1). Artificial Intelligence and its role in different fields of drug discovery.

Before the AI era, *de novo* small molecule designing methods could be classified into structure-based or ligand-based methods. In general, structure-based methods used active site information like size, shape, and physicochemical properties and

reported critical interactions of the protein [1]. Novel ligands can be grown from a bound scaffold/core structure in the active site region. To achieve the tight and effective binding, complementary properties of the ligand with the protein were considered in selecting the desired fragments (Fig. **2**). Alternatively, fragments interactions were studied (bound) in the active site region, and the desired fragments were linked to form a novel ligand. Since the molecule in both the cases was designed without considering the synthetic feasibility, there are high chances the molecules show effective computation and cannot even confirm the activity experimentally due to synthetic difficulties. Similarly, toxicity is also one of the crucial reasons for the failure of the *de novo*-designed compounds.

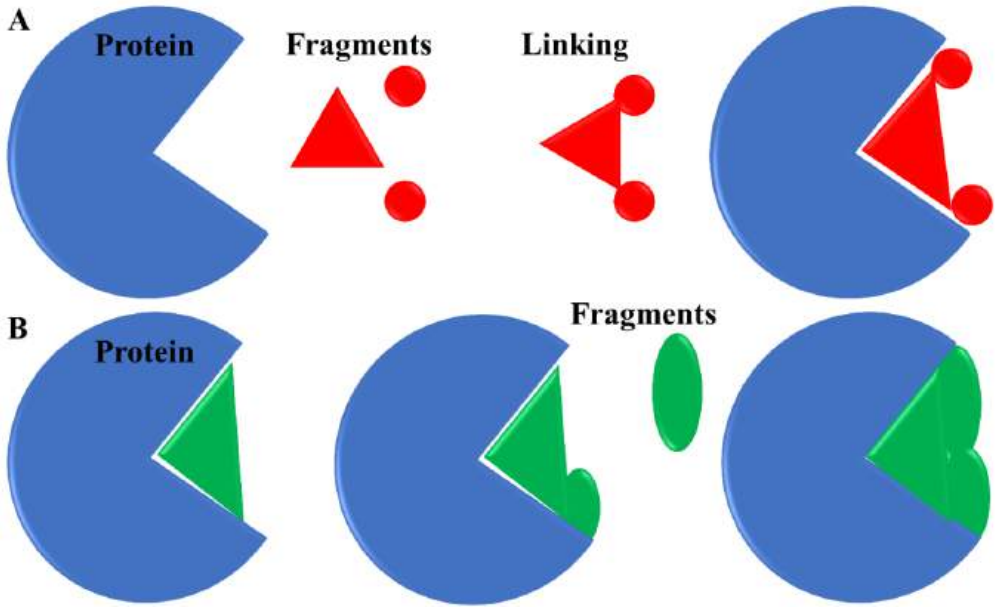

Fig. (2). Commonly used classical *de novo* design approaches. **A**) Link approach **B**) Grow approach.

Ligand-based *de novo* methods were used when the structural information of the protein was not available or not of good quality (say predicted model or poor resolution *etc.*) [2]. The reported compounds with known activity values were considered to build a pharmacophore/quantitative structure-activity relationship (QSAR) model to assess the vital features or properties essential for the binding. This active site structural information can be indirectly inferred from these active ligands.

CHAPTER 5

Artificial Intelligence (AI) Game Changer in Cancer Biology

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Abstract: Healthcare is one of many industries where the most modern technologies, such as artificial intelligence and machine learning, have shown a wide range of applications. Cancer, one of the most prevalent non-communicable diseases in modern times, accounts for a sizable portion of worldwide mortality. Investigations are continuously being conducted to find ways to reduce cancer mortality and morbidity. Artificial Intelligence (AI) is currently being used in cancer research, with promising results. Two main features play a vital role in improving cancer prognosis: early detection and proper diagnosis using imaging and molecular techniques. AI's use as a tool in these sectors has demonstrated its capacity to precisely detect and diagnose, which is one of AI's many applications in cancer research. The purpose of this chapter is to review the literature and find AI applications in a range of cancers that are commonly seen.

Keywords: AI, Cancer cases, Cancer therapy, Drug development, Hallmarks of cancer and targeted therapy, Types of cancer.

INTRODUCTION

In the medical profession, AI has been used in different tasks [1]. The application of AI technology in fundamental biology, pharmacology, and medicine has resulted in several technological advances, with outcomes equivalent to those of human professionals [2]. According to a study, there is indeed a possibility that AI will surpass humans in all tasks in four decades. This prediction indicates that AI will have a big impact on a variety of activities in areas including technology and healthcare [3].

Traditional expert systems based on symbols and information dominated early AI technology. Machine learning is ushering in a new era in AI. Machine learning is

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a typical AI technique that provides a variety of algorithms that can increase the accuracy of prediction using large amounts of data [4].

Neural network models are used in deep learning, a branch of AI, to solve problems that classical machine learning cannot. Since its initial application in 2012 [5] for image recognition, deep learning has been the de facto approach for researching computer vision, and its accuracy in image recognition has significantly increased [1].

The architecture, layer type, updating of linking weights, feedback method, and other elements of deep learning techniques are categorized [5]. The most popular deep learning models are recurrent neural networks or feedback neural networks, deep structural learning, and convolutional neural networks or shift-invariant [6 - 8]. In terms of data collection and processing, Stephens *et al.* (2015) [9] predicted that within ten years, the usage of AI in genomic information would be on par with or surpass that of social media, online video, and other information-related industries. Automated algorithms that extract relevant patterns can give useful information and influence therapy development, patient categorization, and illness research [10].

While processing data, AI may give access to private information such as genomic sequences, which raises privacy concerns. Before collaborating with AI researchers and incorporating deep learning into their projects, medical practitioners and biological scientists should have a fundamental understanding of deep learning, including its uses and potential drawbacks [10]. This is because the use of deep learning technology requires large datasets with appropriate data annotation. Cancer is the most significant cause of mortality in industrialized nations, and its prevalence is expected to rise as the population ages (Fig. **1**) [11 - 13].

Each year, about 1 million people in Japan are diagnosed with cancer, and around 400,000 people die from it [10]. Thus, during the next ten years, cancer research will continue to be a significant focus in order to save lives. The use of AI in cancer biology is the main topic of this section (Figs. **2** and **3**). This study examined current developments in AI in cancer biology, including its application to various types of cancer, cancer therapy, and drug discovery. This section searches numerous publications and internet sources for interpretation using search criteria such as “AI,” “chemotherapy,” and “drug discovery.” To strengthen the conclusions, we simultaneously analyze different literature.

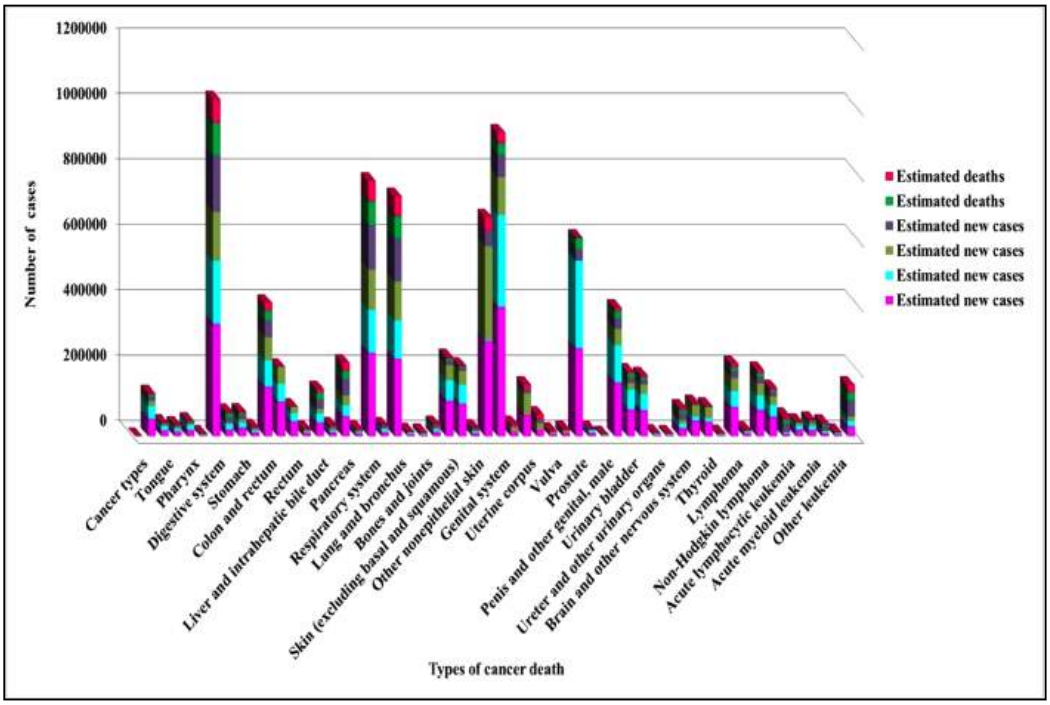

Fig. (1). Number of new cancer cases and fatalities in the United States by gender in 2022.

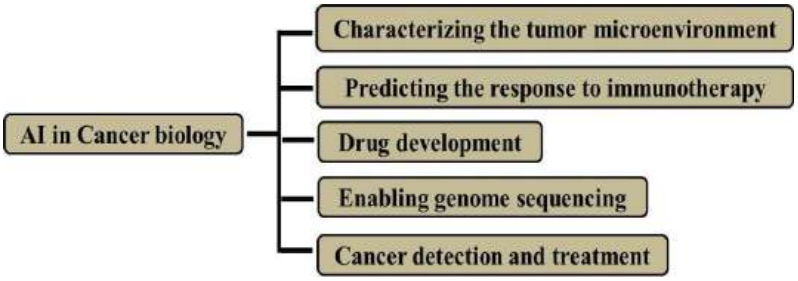

Fig. (2). Application of AI in CB.

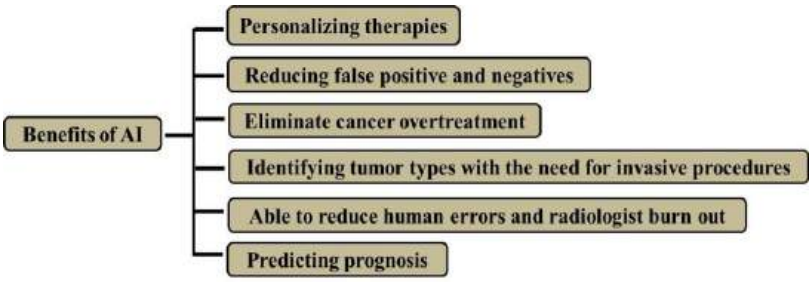

Fig. (3). Benefits of AI in CB.

CHAPTER 6

AI-Based Energy Management for Domestic Appliances

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Abstract: Energy conservation is the need of the hour for various reasons, including the depletion of fossil fuels. The domestic sector is the major consumer of generated electricity across the globe. Artificial Intelligence is a powerful decision-making tool. Building AI-based techniques will be effective in conserving energy for domestic appliances. The general framework of AI-based lighting, room comfort, refrigerator and other load systems have been addressed in this chapter. The AI-based systems can effectively manage the operation of these loads, thereby reducing energy consumption.

Keywords: Artificial intelligence, Air-conditioner, Dish-washer, Energy management, Lighting system, Room comfort system, Refrigerator system, Washing machine.

INTRODUCTION

Electricity Generation and Consumption

India is the world's third-largest power generator. As of December 31, 2021, India's national electric grid has a total installed capacity of 393.389 GW. The Central Electricity Authority of India (CEA) estimated India's energy surplus and peak surplus for the 2020–21 financial year at 2.7% and 9.1%, respectively, in its 2020 Load Generation Balance report [1].

At 1,284.44 trillion kilowatt-hours, the utility energy supply fell 6.5 billion kilowatt-hours short of demand in the 2019-20 fiscal year (-0.5 percent). There

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were 1,229 MW (-0.6 percent) less peak demand met than required, which was 182,533 MW (peak load). A limited amount of power would be made available through regional transmission networks to those states that were predicted to be in low supply. Electricity generation in India has been less of an issue than power distribution since 2015 [2].

According to the Ministry of Environment and Energy Statistics, out of the energy generated, 41% is consumed by the industrial sector, followed by the domestic segment with 26%. The agriculture division utilizes 18%, commercial 8%, other consumers 6%, and railways and traction systems use 1% of the total electricity generated. Conferring to the Energy Conservation Act of 2001, industrial consumers with more than 120 kVA demand must conduct an energy audit and submit the report to the state-designated agencies once in three years. In this way, the industrial sector is used to conserve electricity. The next significant segment that consumes more power is the domestic sector. Researchers evidenced that following appropriate practices and properly utilizing domestic appliances would result in higher energy conservation in household appliances.

Artificial Intelligence

Digital computers can execute activities often associated with intelligent entities because of Artificial Intelligence (AI). Human-like reasoning, meaning, generalization, and the capacity to learn from prior experience all fall under the umbrella of cognitive science [3]. We attribute intelligence to all but the most superficial human behaviours, yet even complex insect behaviours are not considered to be the evidence of intelligence. Human intelligence, according to psychologists, is not best described by a single characteristic but rather by a composite of many distinct talents. Intelligence studies have concentrated on the following areas: learning, reasoning, problem-solving and perception. AI systems can learn in a variety of ways. The simplest one is through trial and error. In AI-based systems, the software may store the situation and its response. It recalls it when the computer encounters the same situation. AI-based systems get trained with these situations and results and make appropriate decisions with reasoning. The reasoning assists in making reasonable conclusions. AI aims to solve problems that may be general or specific. General problems may have a broad range of issues, whereas specific problems may need tailor-made solutions depending on the circumstances and situations. At the outset, AI-based systems give better decisions or solutions for problems encountered through holistic learning and problem-solving methods.

AI's effective decision-making and problem-solving skills can be effectively utilized to conserve energy. The depletion of fossil fuels and the capital cost of

renewable energy sources lead to AI's usage in energy management. The systems developed through AI for energy conservation and management are called Smart Energy Management Systems. These systems create awareness and alarms and insist the consumers on the energy conservation approaches when applied in any energy conservation sector. These systems can be applied for industrial, domestic, agricultural, commercial and traction systems [4 - 7]. In this chapter, an AI-based energy management system has been attempted for domestic appliances. The aimed system effectively manages energy consumption and contributes to an individual's environmental and economic growth and, thereby, the nation.

HOME ENERGY MANAGEMENT SYSTEM

An intelligent network control system constructed on top of a smart grid, bright house, and smart meter technologies is referred to as a home energy management system (HEMS). It integrates each of these components into a unified management and command structure. The characteristics include the generation of power, the use of electricity, and the use of technologies that store energy. Customers that use HEMS have a better chance of lowering the cost of their monthly power bills and improving the performance of their renewable home energy sources. The conventional power market does not incorporate customers randomly; it simply provides a single-price model for energy [8 - 10]. As a direct result of this, there is an insufficient amount of accessible power during peak hours, and electricity is wasted during off-peak hours [9, 11]. After this, the system of charging different prices during peak and off-peak hours is implemented. This method contributes to the overall goal of assisting customers in shifting the time of day during which they utilize electricity. On the other hand, it is less flexible and cannot fully depict the relationship between the demand for electricity and its supply. In addition to this, HEMS can fully interact with the power grid to obtain an accurate real-time price, cooperate with generation and load forecasting, perform an intelligent allocation of household energy, optimize the allocation of household load in the time dimension, achieve demand response on the customer side, relieve the pressure that is placed on the grid during peak hours, and improve the stability of the grid [12 - 15].

A smart grid is a new generation of information technologies such as the Internet of Things, cloud computing, mobile Internet, and big data that are combined with the household as a carrier to achieve a low-carbon, healthy, intelligent, comfortable, and safe family lifestyle. Smart grids are designed to help families live more comfortable, intelligent, and safe lives. The HEMS serves as the fundamental component of the smart grid. The Internet of Things, cloud computing, mobile Internet, and big data are all examples of the next generation of information technologies that make up the smart grid [16 - 18]. It accomplishes

CHAPTER 7

AI-Based Domestic Load Scheduling and Power Management for Renewable Energy Exporters

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Abstract: Residential Photovoltaic systems (RPV) are flattering and widespread among customers due to government policies. The power sources available in RPV include a grid, a PV system and a battery. The principal cost of residential photovoltaic systems is a bit high. When more power is exported, the customer who has installed it will export more power for their benefit. It can be achieved by efficiently scheduling the three sources and managing the power export. Artificial Intelligence-based systems can effectively take care of it because they provide effective decision-making solutions.

Keywords: Artificial intelligence, Citical loads, Optimal scheduling, Power management, Residential photovoltaic systems.

INTRODUCTION

Population expansion, technological innovation, and growing living standards have contributed to increased global energy use during the previous two decades. The energy we consume now is 25 times more than it was 25 years ago. Increased fossil fuel use has resulted in environmental problems, *viz.* Climate change worldwide due to the increased NOx, CO_2, and CO in the air, and decreased air quality [1]. For long-term growth that is both sustainable and low in emissions of greenhouse gases, the only option is to shift from conventional to clean energy generation [2].

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The 2015 Paris Agreement demands a positive action from the world to climate change. By 2050, the goal is to reduce greenhouse gas emissions significantly.

Over the last decade, renewable energy sources, like solar, wind, hydropower, *etc.*, have grown from 1% to 27% of the world's total power production. The increase is primarily due to wind and solar electricity [3 - 5]. The EU and countries like the United States, China, India, Japan, and Australia have all implemented ambitious climate policies, which have resulted in reducing solar and wind energy prices.

The energy from the sun is limitless, and no one can monopolise it. The simple and secure road to a sustainable future is solar electricity. Popularity has grown due to technological breakthroughs and lower production costs. At the moment, renewable energy is responsible for producing 35 percent of the electricity used in the United States, 27 percent in the European Union, and 21 percent in China. One of the countries with the most rapid economic expansion is India, which has a population of 1.4 billion people and has 18 percent of the generation of renewable energy. Clean, renewable energy for cooking and power for every home has come a long way. Industries are encouraged to construct wind and solar power projects directly from the energy reforms. The government also encourages household consumers to install renewable energy systems to meet rising energy needs. Rooftop solar plants are becoming increasingly common owing to government incentives. India obtains 4 - 7 kWh of energy per day and can generate 5,000 trillion kWh annually [6 - 8]. Many utilities and customers have chosen solar power generation. The installed capacity of Solar PhotoVoltaic (SPV) plants reached 34.831GW towards the end of 2019. After two disastrous floods in two years, Kerala is currently renovating and focusing on sustainable growth. Due to the high population density, large solar parks are impracticable. Thus the Kerala State Electricity Board (KSEB) is on a quest to create 500MW of electricity using rooftop solar plants. This is in addition to numerous residential structures having standalone solar plants and floating panel solar farms [9, 10].

TYPES OF ROOFTOP SOLAR PV SYSTEM

There are three distinct types of solar photovoltaic systems for rooftops. Off-grid, grid-tied, and grid-tied with backup are the three options. The following describes the essential topology of each type:

Grid-tied System

The solar power generated by grid-connected systems is reversed and sent back into the distribution network. There is no storage component in a system connected to the grid. Installing solar panels on residential rooftops connected to

the power grid qualifies homeowners for financial incentives from the government. The topology of a grid-linked system is shown in Fig. (**1**). Because there is no need for storage, this technology has a lower overall cost. The goal of constructing a system connected to the grid is to make customers eligible for more incentive benefits while simultaneously lowering their overall energy costs. Inverters that were linked to the grid immediately became inactive. This technology is incapable of handling power outages or other urgent situations. This technique is also incapable of controlling use during peak hours. Calculating monthly energy costs requires comparing the amount of energy generated by photovoltaic panels (PV) to the amount used when the customer's load need is lower than the energy production of the PV system, the customer benefits.

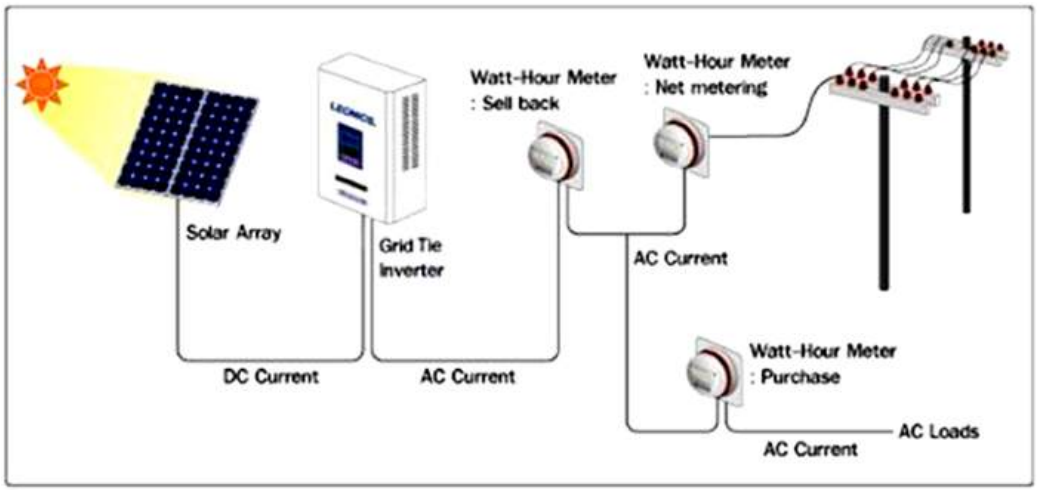

Fig. (1). Grid Tied System.

Grid-tied System with a Backup

A utility grid, a solar photovoltaic (PV) system, and batteries comprise a hybrid system, *i.e.* the grid-tied system with backup. This approach works particularly well in areas that often experience power outages. The customer's requirements for backup and autonomy determine the battery's capacity. To bring down the overall cost of the system, the backup battery could only be utilised for critical loads in an emergency. It is more costly than a system that is connected to the grid. A system that is connected to the grid and has a battery backup is shown in Fig. (**2**).

CHAPTER 8

Artificial Intelligence in Physical Science

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Abstract: The study of matter and energy, as well as their relationships with one another, is the focus of the scientific field known as physics. It is possible to describe physics as the study of nature or as that has been belonging to natural things. This branch of science is concerned with the laws and characteristics of matter, in addition to the forces that act upon it. Physics is often recognized as one of the most challenging scientific disciplines-because, it draws concepts and ideas from other academic subfields, such as biology and chemistry. At the beginning of physics, mathematical models had to be meticulously compiled and then evaluated manually. Scientists are now capable of simulating and solving difficult physics problems with notably more speed, precision, and creativity than ever before because of breakthroughs in artificial intelligence and machine learning. Frameworks powered by artificial intelligence are speeding up the research in a wide variety of fields of physics such as nuclear technology, windmill energy production, thermal power plant, space research and energy management. The application of artificial intelligence for the development of new models and solutions for challenging physics problems has the potential to significantly accelerate the rate of progress of scientific advancement across the most basic field of physics.

Keywords: Artificial intelligence, Energy management, Nuclear physics, Physical science.

INTRODUCTION

Physical science is one of the scientific disciplines that underpin the physical world and is actively integrated into peoples' daily lives [1]. The benefits of physics in daily life may be as simple as converting electrical energy into heat to make coffee every morning or as complicated as planning a space shuttle voyage

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from Earth into an orbit [2]. Given the immense relevance of physics in research, even if certain ideas are first difficult to understand, the return in terms of pleasure and knowledge may make all the work worthwhile. The emergence of cutting-edge technology demonstrates the significance of understanding physics. Technological advances are often centered on physics' inventions and innovations based on a contemporary comprehension of emerging physics understanding and illustrating the relevance of physical science. Wilhelm Rontgen discovered X-rays more than a century ago and X-ray machines are today a part of medical devices taken for granted, created and refined by scientists and researchers working off the original study. Enrico Fermi examined current information on nuclear fission and explored it until he created the first nuclear chain explosion in the first part of the twentieth century. The benefits of physics in daily life can now be seen in the functioning of nuclear energy plants, which generate electricity to power homes and manufacturers all around the globe.

However, studying physics may be personally satisfying when individuals come to grasp daily objects and events in terms of the physics ideas that underpin them, such as automobile acceleration, gravity causing an apple to fall from a branch, or electricity powering gadgets. We have been witnesses to a transformation in artificial intelligence [3] over the journey of the last 10 years (Fig. **1**). Two primary factors have indeed been vital in driving this transformation ahead. First, the widespread availability of computers and processors has resulted in large amounts of computation capability that is quite low-cost and easily accessible. With today's graphics processing units, it is now possible to do millions of operations at once, although it is still sluggish. Second, there has been a significant drop in the price of data storage, which has led to the widespread availability of terabyte computers in people's residences [4].

Fig. (1). Artificial Intelligence and deep learning (Credit: metamorworks/Shutterstock.com).

Furthermore, the internet has made it possible to acquire and retain data in an analytically competent way. The use of this technology may be found almost everywhere. Voice recognition in the smartphone, automated types of vehicles and the opportunity of promoting advertisements are already anchored through Al technologies [5], and an increasing number of businesses are pooling together to market with these AI technologies. As a first step, this chapter discusses the concept of artificial intelligence and demonstrates how it could be used in science and engineering to develop novel artificial intelligence products.

The objective of this chapter is to highlight the potential of artificial intelligence in solving scientific challenges (Fig. **2**) that have historically remained unanswered. The fields of statistical physics and mathematics have made significant strides in our comprehension of artificial intelligence technologies. There seem to be certain concepts that may be a computer can and cannot understand, as said by mathematics. It has also been mathematically demonstrated that there are some specific methods of the program that should be designed to understand a particular task successfully [6]. To discover the dog in the whole picture, you have to use a programme that performs the same function for all regions of the image, such as if one wants a computer to identify it in a pet shop.

Fig. (2). Applications of AI in science, Engineering and Technology.

The paradigms of physics and mathematics, when combined with the engineering aspect of artificial intelligence, have delivered several genuinely astonishing findings [7]. It has been hypothesized that physics challenges can be solved *via* machine learning. Artificial intelligent technologies were employed to eliminate noise from the observations when LIGO discovered its first gravitational wave in 2017 [8]. A ground-breaking article that was published in Science demonstrated that a machine can understand how a spring functions by just viewing repeating recordings of an item being moved back and forth across the spring. Deep learning is trying to infiltrate many different domains of physics, and it's already bearing valuable harvest in those fields. However, there have been no comprehensive answers available [9].

CHAPTER 9

Artificial Intelligence Based Global Solar Radiation Prediction

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Abstract: Solar energy is one of the cleanest renewable energy sources and has no environmental impact. Solar radiation data is important to solar engineers, designers and architects which is also fundamental for efficiently determining irrigation water needs and potential yield of crops, among others. Solar energy is mainly used to meet the growing electricity demand and decline the amount of CO_2 emission thus preserving fossil fuels and natural resources. The temperature and sunshine duration are measured by most of the meteorological services all over the world but global solar radiation measurements are limited due to the restricted number of solar radiation measuring stations and some of the data are missing. In order to estimate the solar radiation in the other areas where the meteorological stations are not established, the theoretical solar radiation estimation models proposed by various researchers have proved handy. One of the main important assignments is to recognize the site with high solar energy potential for renewable power generation. This assists in accomplishing the target of the Indian solar mission project by the year 2022. The present work aims at the prediction of solar radiation using artificial neural network models which are applied to four different locations across India. As validation, measured and estimated solar radiation data were analyzed in terms of the square of the correlation coefficient and RMSE. The outcomes of this study will play a vital role in the estimation of global solar radiation with less percentage of error.

Keywords: Artificial intelligence, ANN, Global solar radiation, Prediction, Solar energy.

INTRODUCTION

Knowledge of solar radiation data is very essential for solar energy based applications including sizing solar systems, performance monitoring, site selection, architectural designs, and design of irrigation systems and many other uses. However, for many countries, solar radiation measurements are not available

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in all locations due to the cost, maintenance, and calibration requirements of measuring equipments, thus causing the need to develop artificial intelligence-based models for the prediction of solar radiation based on meteorological data. The available solar radiation at any particular location is essential for planning as well as the successful implementation of solar-based systems in practical applications. This study is of great importance, as the results can be applied to estimate the available solar radiation at any place in India before implementing solar-based systems. Various approaches are available in the literature to predict the solar radiation data and weather parameters namely the mathematical model [1, 2], artificial intelligence-based models [3 - 5], machine learning [6 - 8] deep learning [9 - 15] and hybrid models [16 - 19]. Artificial Neural Network (ANN) models have been utilized for a wide range of applications such as pattern recognition, prediction, forecasting, optimization, and simulation [20 - 23]. Researchers have predicted solar radiation using artificial intelligence based models based on the relevant meteorological parameters as input variables.

This paper has been organized into 4 sections. Section 1 covers an introduction to solar radiation estimation and its need in the current context. Section 2 includes the prediction of solar radiation using the ANN model. Section 3 contains the result and discussion and finally, section 4 covers the conclusion of the study.

ARTIFICIAL NEURAL NETWORK METHODOLOGY

ANN models have been widely used for a wide range of applications such as pattern recognition, speech recognition, prediction, and forecasting of renewable energy. In this study, the input parameters that ANN models generally use include the month of the year (MOY), and geographical parameters namely the latitude (Lat), longitude(Long), altitude(Alt), declination(δ), extraterrestrial radiation(H_0), bright sunshine hour(BS), Day length(S_0), maximum temperature(T_{max}) and minimum temperature(T_{min}).

Artificial neural networks imitate biological neural networks. Fig. (**1**) shows the simple model of an artificial neuron. The basic small individual element of ANN is the neuron. The ANN model consists of three layers namely input, output and hidden layers. X_1, X_2,. X_n are the inputs to the artificial neuron and w_1 w_2…w_n are the weights attached to the input links. The input details are captured and are processed by the sum function and the new signal generated by the neuron is set by the transfer function. The output of the ANN model is given by the following equation (1):

$$y = f[\sum_{i=1}^{N} I_i w_i] \quad \textbf{(1)}$$

Where Ii is the i[th] input of the network, wi= weight and f is the transfer function.

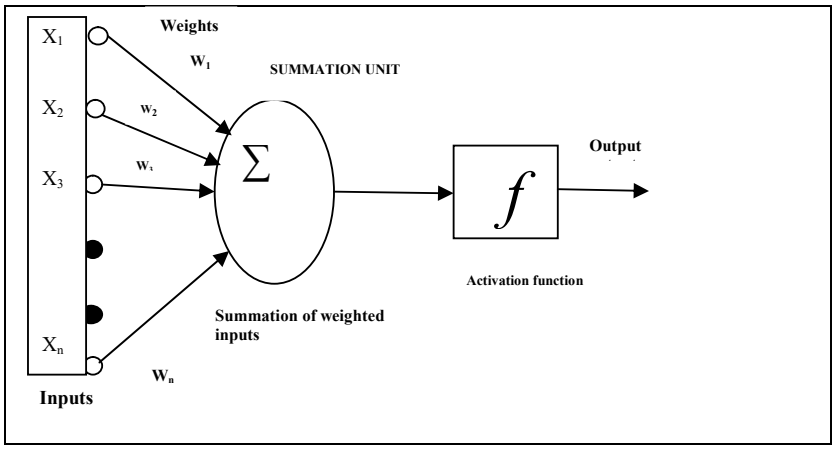

Fig. (1). Model of an artificial neuron.

The multi-input single-output ANN is given by the following equation:

$$y = f_1\left[\sum_{i=1}^{nh} w_{i1f_i} \sum_{k=1}^{ni} I_{ki} w_k\right] \quad \textbf{(2)}$$

In the above equation (2), *nh* is the neuron numbers available in the hidden layer, *ni* is the number of inputs*; fi* is the transfer function of the hidden layer and f_1 is the activation function of the output layer. In this work, tansig activation function is used in the neurons of the hidden layer and linear function in the neuron of the output layer.

RESULTS AND DISCUSSION

The predicted global solar radiation data using the ANN model for the selected four Indian locations namely Bhubaneswar, Hyderabad, Nagpur and Trivandrum is available in Table **1**.

Table 1. Predicted GSR data for the selected Indian locations using the ANN model.

Month Number	Monthly Average Solar Radiation MJ/m2 /Day			
	Bhubaneswar	**Hyderabad**	**Nagpur**	**Trivandrum**
1	16.30	18.60	15.82	17.64
2	18.45	21.31	18.90	19.20
3	19.85	22.84	22.20	18.99
4	21.77	23.72	23.59	18.76

CHAPTER 10

In silico Approaches to Tyrosine Kinase Inhibitors' Development

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Abstract: Many cellular communications and cellular activities are regulated by a class of enzyme tyrosine kinases. Mutations or increased expression of these enzymes lead to many proliferative cancers as well as other non-proliferative diseases such as psoriasis, atherosclerosis and some inflammatory diseases. Hence, they are considered vital and prospective therapeutic targets. Over the past decade, considerable research work has been carried out to develop potential inhibitors against these tyrosine kinases. So far, a number of compounds have been identified successfully as tyrosine kinase inhibitors and many compounds were developed as drugs to treat tyrosine kinase-induced diseases. Behind the successful development of these inhibitors, many Computer Aided Drug Design (CADD) (*in silico*) approaches include molecular modelling, high throughput virtual screening against various chemical databases, and docking (both rigid and flexible method of docking). Further many studies identified the possible features which are responsible for tyrosine kinase inhibition activities for a number of series of compounds through the quantitative structure-activity/property relationship (QSAR/QSPR) process. In this review article, the structural characteristics, mechanism of action, and mode of inhibition of tyrosine kinases are discussed followed by the successful applications of a variety of *in silico* approaches in tyrosine kinase inhibitors development.

Keywords: Artificial intelligence, Computer-aided drug design, Computational intelligence, Docking, EGFR, *In silico* approaches, Ligand based drug design, Machine learning, Pharmacophore, Protein tyrosine kinases, QSAR, Structure based drug design, Tyrsoine kinase inhibitors (TKI), Virtual screening, VEGFR.

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INTRODUCTION

Protein Tyrosine Kinases (Ptks)

One of the largest gene families in the human genome is the protein kinase family consisting of 560 genes which corresponds to about 1.7% of the total genome [1]. This gene family plays a vital role in many cellular regulation processes such as apoptosis, proliferation and progression of the cell cycle, developmental processes, immunological response, cell differentiation, and nervous system function [2]. Among the many types of post-translational modification processes, phosphorylation is one of the most widespread classes and is mainly used in signal transduction. Protein kinases phosphorylate the serine/ threonine, tyrosine and histidine amino acids by transferring a phosphate group from ATP and attaching covalently to the free hydroxyl group of these amino acids. Based on the type of amino acid residues phosphorylated, the protein kinases are classified as serine/threonine kinases consisting of 385 members and tyrosine kinase consisting of 90 members and tyrosine-like kinases which include 43 members.

Historically, the protein tyrosine kinases (PTKs) were used to define the typical class of oncogenes causing many forms of malignancies in human beings [3]. These were also involved in diabetes and different types of heredity syndromes [4]. These play vital roles in many signal transduction pathways and cellular regulation processes. Structural and functional alterations of many PTKs result in a number of diseases including cancer [5, 6].

Many PTKs involved in the oncogenesis lead to various types of tumours [7]. Over the past several years, intensive research has been carried out on targeting these oncogenic PTKs by small molecule inhibitors. In this review, the structural, and functional aspects of PTKs are briefly discussed along with their role in diseases. This is followed by a brief view of how the different types of computational (*in silico*) approaches help in identifying or developing small molecule inhibitors for a variety of PTKs thus facilitating the development of some novel small molecule inhibitors against PTKs.

CLASSIFICATION OF PROTEIN TYROSINE KINASE FAMILY

The 90 unique genes which encode tyrosine kinases have been broadly classified into receptor tyrosine kinases (58 members) and non-receptor tyrosine kinases (32 members). Based on the nature of the domain sequence, the tyrosine kinases have been divided into different subfamilies. There are 20 approximately different subfamilies of kinases *viz.*, ALK, AXL, DDR, EGFR, EPH, FGFR, INSR, MET, MUSK, PDGFR, PTK7, RET, ROR, ROS, RYK, TIE, TRK, VEGFR and AATYK in the receptor tyrosine kinases and 10 different subfamilies *viz.*, ABL,

ACK, CSK, FAK, FES, FRK, JAK, SRC, TEC & SYK in non-receptor tyrosine kinases [3].

Architecture and Regulation of Receptor Protein Tyrosine Kinases (RPTKs)

The overall architecture of RTKs consists of three different portions, namely polypeptide ligand binding extracellular portion, helical transmembrane portion and tyrosine kinase catalytic cytoplasmic domain [8]. The extracellular region consists of diverse numbers of distinct globular domains: immunoglobulin-like domain, cysteine-rich domain, EGF-like domain and fibronectin type III-like domain; the cytoplasmic domain consists of the juxtamembrane region, tyrosine kinase catalytic region, and a carboxy-terminal region. Various lengths of juxtamembrane and carboxy-terminal regions are seen among the RTKs. In the binding of a ligand molecule, tyrosine residues present in these regions were autophosphorylated [9] which regulate the catalytic function as well as serve as docking sites for SH2 domain-containing proteins [10]. Except in insulin receptors (includes their family members) and MET subfamily of kinases, the majority of RTKs consist of a single polypeptide chain and exists as monomer in the absence of a ligand molecule. Considering the polypeptide RTKs ligands, except the ligand of the Eph receptor family (ephrins), most of the ligands are soluble [11, 12]. As a result of ligand-mediated oligomerization, tyrosine residues are autophosphorylated thus helping to increase the intrinsic catalytic activity and forming binding sites for downstream signaling proteins. Hence, the RTKs are activated. Autophosphorylation of tyrosine residues in the activation loop and cytoplasmic domain results in kinase activity stimulation in a number of RTKs [13] such as insulin receptor [14], EGF receptor [15], PDGF receptor [16], MET receptor [17], VEGF receptor [18], and TrkA [19] and the generation of docking sites for phosphotyrosine thus recognizing modular domains *viz.* SH2 domains and phosphotyrosine binding domain (PTB) [20]. Further, the autophosphorylation of tyrosine residues in the activation loop occurs in the receptor (otherwise called trans – autophosphorylation). A change in the conformation of the receptor takes place upon ligand-induced dimerization whereas in other regions like juxtamembrane or carboxy-terminal regions, it occurs within a receptor (otherwise called cis - autophosphorylation) without having any conformational change of receptors upon dimerization [21, 22]. The processes namely proteolysis mediated by ubiquitin [23], and receptor-mediated endocytosis [24] and phosphotyrosine phosphatases [25] regulate the RTKs.

CHAPTER 11

Computer-Aided Drug Discovery Studies in Ethiopian Plant Species

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Abstract: Since ancient times, plants with therapeutic properties play a major role and are used as medicine by several groups of people all over the world. Ethiopia can be considered a hub of medicinal plants due to their diverse species and traditional usage by the local people. Medicinal plants in Ethiopia hold high therapeutic value and hence, most of them are preserved and saved from extinction. Also, most of the plants are yet to be studied due to a lack of documentation and experimental validation. Secondary metabolites from these plants possess numerous pharmacologically active compounds. Computer-aided drug discovery using Artificial Intelligence and high throughput technologies saves time and is more cost-efficient than traditional clinical studies. In this chapter, we discuss the computational studies done on ten important Ethiopian medicinal plants that have antioxidant, antimicrobial, anticancer and antidiabetic properties using phytochemical analysis and *In-silico* approach for plant-based drug development, which could serve as a potential pharmacological lead against different disease targets.

Keywords: Artificial intelligence, Antioxidant, Anticancer, Antimicrobial, Drug discovery, Ethiopia medicinal plants, *In-silico*, Molecular docking.

INTRODUCTION

Ethiopia, entitled the Horn of Africa is located in Eastern Africa (9.4969° N, 36.8961° E). It has a high plateau varying from 1,290 to 3,000 m (4,232 to 9,843 ft) above the sea level with a central mountain range comprising the highest of 4,533 m (14,872 ft) divided by the Great Rift Valley that splits the plateau diagonally. The plateau has a number of small and large rivers like the Blue Nile Crossing on them. The climate is mostly temperate on the plateau and hot on the lowlands. Though the country lies within the tropics, it's nearness to the equator

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counterbalances the elevation of the land. They experience three seasons, winter or cold season (October to February) followed by a dry season (hot) and a Rainy season (June to October, October is occasionally a wet month). The valleys and lowlands have dense vegetation but the plateaus usually appear thin with trees and bushes scattered on them. In the northern region, the hillside is densely wooded. Vegetation in the southern region, on the uplands, is very rich.

The country is diverse in its Flora with varied agroecological zones due to its agroclimatic conditions. It is estimated that Ethiopia consists of 6500-7000 plant species which include medicinal plants as well. Nearly 19 percent of the medicinal plants are native to the country. 80 percent of the Ethiopian population and 90 percent of their livestock depend on traditional medicine and these medicinal plants are very effective in treatment. The data on recognizing and managing the therapeutic plants with their classification, parts, and uses are mostly related either to local or elder people, who transmitted their knowledge verbally. In Ethiopia, traditional therapists use herbal resources existing in nature for treating numerous diseases. Secondary metabolites, small molecules and other natural compounds harvested from different parts of the plants (roots, stem, leaves, fruits and seeds) revealed admirable medicinal properties. They provide therapeutic effects for many skin diseases, and bacterial, viral, parasitic and infectious diseases. Also, conditions such as cancer, diabetes and arthritis are cured using these medicinal plants. This chapter focuses on the following Ethiopian medicinal plant species, *Brucea antidysentrica, Clausena anisate, Ocimum cufodontii, Cucumis prophetarum, Cadia purpurea, Zanthoxylum chalybam, Uvaria schefflera, Clematis burgensis, Euphorbia schimperiana,* and *Rhynchosia ferruginea*, whose medicinal values are not yet studied thoroughly and are of research interest [1 - 7].

Computer-aided drug discovery and development (CADDD) is a fast-growing field as this technology keeps evolving [1, 8 - 11]. It is important to conduct computational studies in the process involving biological and chemical space to modernize drug design, development, discovery and optimization. Computer-aided or *in silico* design is used to ease and enable hit identification, selection, absorption, distribution, metabolism, excretion and toxicity properties (ADMET) for safety criteria. Computational approaches usually include protein modelling for unknown structures (Adinitio, threading, homology-based on the sequence identity), ligand-based drug design (pharmacophore modelling, a 3D spatial arrangement of chemical features essential for biological activity), structure-based drug design (drug-target docking), and quantitative structure-activity and quantitative structure-property relationships (Density Functional Theory analysis). In modern drug design, *in silico* methods are largely used to understand drug-receptor interactions and quantum chemical properties. The computational tools

and software developed for this purpose are aimed to improve the effectiveness and efficiency of the drug discovered and its development process by reducing the time invested for animal studies, in fact decrease their usage, and also for better prediction purposes.

BRUCEA ANTIDYSENTRICA

Brucea antidysentrica is a perennial tree that grows up to 7-9m tall in regions having tropical climate. The local Ethiopian name of the plant is Aballo. Every part of the plant holds a therapeutic value and substances prepared from them are used to treat conditions such as dysentery, diarrhea, leprosy, cancer, eye disease, rabies and fever. Reports from the past have revealed the abundance of quassinoids in the genus. It has a broad range of biological activities like antiviral, antitumor, herbicidal, anti-parasitic and antioxidant. Isolation, spectroscopic identification, antibacterial, antioxidant evaluation, and molecular docking analysis of the roots of *B. antidysentrica* have been reported in the article [1, 9, 12]

For ages, traditional medicines are chosen as an alternate tactic on treatment for several diseases. Phytochemical analysis of the roots of *B. antidysentrica* showed the presence of alkaloids, tannins, flavonoids, steroids and saponins, terpenoids, and phytosterols. Silica gel column chromatographic separation of the crude extracts directed to the separation of three indole alkaloids, compound 1 – [derivative flazin methyl ether], compound 2 – [canthin-6-one] and compound 3 – [1,11-dimethoxycanthin-6-one], all of which were identified for the first time from the species. It is mentioned that compound 1 was isolated for the first time from the genus. The antibacterial test results have revealed that the twelve isolated compounds show promising antibacterial activity against *S. aureus, E. coli, S. Typhimurium, and B. subtilis.* Compounds **1** and **2** exhibited medium (12.66±0.60 and 12.5±0.87 mm zone of inhibition) antibacterial activity against *E. coli* and *S. typhimurium* compared to that of ciprofloxacin (27.3±2.52 and 29±1.00 mm zone of inhibition). Compound 2 had strong DPPH free radical scavenging activity (87.5% at 100 µg/mL) when compared to ascorbic acid. Molecular docking analysis showed good scoring pose of the lowest energy with values -5.8 Kcal/mole, -5.7 Kcal/mol and -5.7 Kcal/mol for alkaloids 1-3, respectively. These findings of pharmacologically important secondary metabolites, the biological activity observed by molecular docking analysis and the free radical activity support the traditional usage of the plant to treat various infectious diseases.

CLAUSENA ANISATE

Clausena anisate belongs to the family Rutaceae. It is an evergreen small tree or shrub that grows up to 10 m tall in tropical regions of Africa. Their leaves are

CHAPTER 12

Artificial Intelligence-genomic Studies in The Advancement of Agriculture

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Abstract: Artificial Intelligence in agriculture biology plays a vital role in the improvisation of crop production and enhances resistance against plant pathogens. Artificial intelligence brings about changes in crop production by predicting the gene data, showing the ability of plants to resist plant pathogens and environmental conditions. Machine learning methods, namely artificial, neural, and Deep Neural networks. Computational approaches were used to determine Plant Genomics. The main aim of this review study was to understand plant genomics data, predict plant genomes based on machine learning and reduce the cost of fertilizers and side effects. The seven important factors include soil moisture, the electric conductivity of soil solution, evapotranspiration, humidity, soil aeriation, and soil pH and air temperature. The red, green, and infrared channels of sensors in three layers of ANN were used for the determination of genomic data. Chemical fertilizers are used to kill pests damaging crops and affecting the ecosystem. Farmers and agricultural scientists are looking forward to implementing advanced machine learning techniques such as sensors mounted on vegetable and fruit orchards. The traps were manufactured and installed by using sensors to detect parasites infecting crops of agricultural importance. This review study was focused on computational data on plant genomics and promoting less usage of fertilizers to prevent carcinogenic and genomic diseases. The researchers performed an experiment and stated that eight master transcription factors are the most vital to enhance the ability to fix nitrogen from the atmosphere. Farmers are future artificial intelligence Engineers. Based on the review of the literature, it was evident that artificial intelligence enhances crop improvement for better productivity.

Keywords: Artificial intelligence, ANN, CI, CNN, DNN, Gene editing, Machine learning, ML Algorithms, Plant Genomics, Sensors.

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INTRODUCTION

Artificial intelligence plays a vital role in the determination of patterns in data that represent genes of importance leading to the prediction of specific characteristics in plants. Computational approaches were used to enhance the basics of plant genomic research. Computational artificial intelligence research in the field of agriculture is promising and challenging for researchers to develop novel methods for the determination of data regarding unique traits in plants. The genomic data enhances the capability of plants to respond to physical factors like extremes of temperature, pH, humidity, toxins, and pathogens. The Phenotypic-Genotypic methods were found to be excellent genetic tools in the determination of multidimensional data at an affordable cost and were characterized by means of high throughput techniques. This review explained the preparation of the model by the transfer of genomic DNA sequences to molecular phenotypes and the prediction of functional variants. Machine Learning is the science of Programming computers and the Programme could be divided into models which aim at target variables and prediction of DNA sequences. Artificial neural networks are efficient methods to rectify machine learning-associated problems. The ANN is made up of input and output layers. The deep neural network is a kind of ANN. The DNN could be differentiated from ANN as it consists of various layers. The network namely the co-evolutionary neural network reduces the number of weights [1].

For thousands of years, human life has been sustained and improved through agriculture for food, fiber, and fuel. Agriculture needs to be optimized because of the changing environment, growing population, and rising nutritional demands. Utilizing genetic breakthroughs in agriculture will allow for more efficient and sustainable approaches to these problems. The development of crops and livestock with desirable agronomic features is accelerated by developments in genomic selection (GS) and, gene editing [2]. The foundation of GS is based on the idea that data from numerous markers dispersed throughout the genome can be utilized to determine an individual's breeding value and capture population diversity. It was initially described in 2001 and depends on creating a breeding equation using a training population with certain features while breeders have relied on a small number of molecular markers for many years, and improvements in genome-wide technology have resulted in a substantial expansion of the genetic resources accessible for agriculture. Breeders now have strong tools to develop agriculture thanks to advancements in genetics, bioinformatics, and biotechnology. To link genotypes to phenotypes, sequence data and well-studied marker sets can be used, and the maintenance of databases holding genomic data is crucial to comprehending genetic variation within and between populations and settings. The ability to define novel species, conduct meta-analyses, explain complicated

features, and ultimately enable genomic selection and gene editing for the improvement of agriculture are all made possible by this data. The study of agrigenomics has revolutionized the breeding and management of plants, animals, and crops thanks to genetic technologies. Since the sequencing and assembly of the rice genome in 2005, breakthroughs in sequencing technologies and bioinformatics tools have enabled rapid development. However, plant genome assembly and the process of creating a genome sequence from fragmented sequencing are still constrained by frequent long repetitive areas, huge genome sizes, and frequent polyploidy. Rice's genome was still sequenced using bacterial artificial chromosomes (BAC) and Sanger sequencing, whereas the grape genome was the first to use a combination of the less expensive 454 sequencings and Sanger sequencing. Two years later, the cucumber genome was assembled using Illumina short reads and Sanger sequencing, which launched the fast adoption of next-generation sequencing (NGS) 40 of the 55 plant genomes that have been sequenced by 2013, belonged to crops. Crop genome sequencing now has access to a new tool thanks to the development of third-generation sequencing technology that can produce lengthy reads longer than 10 kb. The majority of the major crops are among the over 260 nuclear genomes of land plants that are currently freely accessible in GenBank. In order to produce superior genotypes through genetic recombination, crop breeding has traditionally depended on cycles of phenotypic selection and crossing [3].

The bread wheat genome has been annotated with the aid of the RNA-seq mapping program me Portcullis, which uses ML to distinguish between genuine and fake splicing junctions. A promising area for discovering hitherto undiscovered prospects for crop improvement is the inference of the links between regulatory elements and genes. An *in silico* regulatory network built only on gene co-expression levels has limitations since the relationship of genes may not accurately reflect common gene regulation. As a result, an ML-based technique that can combine diverse types of regulatory signals from different data sources has gained popularity for interactive inference of gene regulatory networks. DNN has many applications namely moderate usage of energy in orchards, achievement of effective scalability by application-oriented computational abilities, and employing low data radio procedures [4].

All genes and genetic variants influencing agronomics traits can be discovered once genome sequences are available, and modifications performed during breeding processes can be evaluated at the genotype level. In many facets of crop breeding, including genome-wide association studies (GWAS) and quantitative trait loci (QTL) mapping, where genomic sequencing of crop populations can enable gene-level resolution of agronomic variation, genomics plays an increasingly significant role. This is due to the ready availability of genomic data

CHAPTER 13

Computational EPR and Optical Spectral Investigation of VO(II) Ion Doped in Aqualithiumaquabis (Malonato) Zincate Lattice

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Abstract: Electron Paramagnetic Resonance studies are carried out at room temperature on single crystals of aqualithiumaquabis (malonato) zincate doped with VO(II) using X-band frequencies. Rotations in three mutually orthogonal planes indicate three chemically inequivalent sites, with intensities ratios of 1:2:9. However, only one site, with the highest intensity, could be followed during crystal rotations. The calculated spin Hamiltonian parameters are: g_{xx}=1.976; g_{yy}=1.973; g_{zz}=1.933; A_{xx}= 7.01 mT; A_{yy}= 6.77 mT; A_{zz}= 18.01 mT. The impurity has entered the lattice in an interstitial position. The analysis of the powder spectrum also reveals the presence of only one site. Admixture coefficients, Fermi contact and dipolar interaction terms have also been evaluated. IR, UV-Visible and powder XRD data of the doped complex confirm the structure and symmetry of the host lattice.

Keywords: Electron paramagnetic resonance, Inorganic compound, Location, Vanadyl, Vrystal growth.

INTRODUCTION

Electron Paramagnetic Resonance (EPR) studies on diamagnetic host lattices by incorporating paramagnetic transition metal ions provide information about the strength of the ligand field around the central metal atom. In these cases, the resonances are sharp due to the absence of dipole-dipole interaction.

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Vanadyl ion, *i.e.*, VO(II), being one of the most stable molecular paramagnetic transition metal ion, is widely used as an EPR probe to understand phase transitions, distortion, strength and magnitude of crystal fields, relaxation times, *etc.* Vanadium exists as bivalent, trivalent and tetravalent. Out of these, the ion commonly exists as VO(II), with a single unpaired 3d electron bound to an oxygen atom by the strong bond in its tetravalent state. The orientation of the V=O bond in complexes depends on the nature of the ligands and hence shows very interesting results [1 - 4]. Most of the EPR results reported for this ion can be classified into two types, one in which the vanadyl ion freely rotates at normal temperatures and the second category in which the ion is preferentially oriented. For example, if the ligands are water or sulfate ions, the vanadyl ion has a fixed orientation, while in others, it has a random orientation. In addition, the analysis of the EPR spectra of VO(II) ion in various host lattices indicates that the paramagnetic impurity was found to enter the host lattice, predominantly substitutionally [5 - 8]. However, interstitial position or both is also known [9, 10]. Malonato ligand has importance in treating malignant tumors when coordinated with platinum (United States Patent 4140707). Coordination polymer compounds containing malonic acid as a ligand have been recently intensively studied due to their potential application as materials in molecular electronics, catalysts, biologically active compounds, molecular-based magnetic materials, microporosity, electrical conductivity, non-linear optical activity, *etc* [11, 12]. Malonic acid acts as a ligand with various dentate abilities. Additionally, the carboxylate group provides an efficient pathway that couples the magnetic centres either ferro- or antiferromagnetically [13 - 19]. In view of the importance of the ligand, the present single crystal EPR study of VO(II) in aqualithiumaquabis(malonato)zincate has been undertaken to identify the presence and nature of impurity in the host lattice.

EXPERIMENTAL

Material and Method

Preparation of Single Crystal of VO(II)-doped $[Li(H_2O)]_2[Zn(mal)_2(H_2O)]$

Malonic acid, zinc(II) basic carbonate, and lithium hydroxide were purchased from commercial sources and used as received. $[Li(H_2O)]_2$ $[Zn(mal)_2(H_2O)]$ is synthesized by adding solid zinc(II) basic carbonate to an aqueous solution of malonic acid under continuous stirring. The suspension is heated at 40-50° C, until a colorless solution is obtained. This solution is filtered and mixed with an aqueous solution of lithium hydroxide. To this solution, five different concentrations of vanadyl sulfate (1.0, 1.5, 2.0, 2.5, and 5.0%) are added as paramagnetic impurity. All the crystals are transparent and light blue in color,

well-shaped and separated out on concentrating the solution at room temperature. Aqualithiumaquabis (malonato) zincate is abbreviated here as ALMZ.

EPR Measurements

EPR spectra are recorded at 300 K on a JEOL JES-TE100 ESR spectrometer operating at X-band frequencies, having a 100 kHz field modulation to obtain the first-derivative EPR spectrum. 1,1-Diphenyl-2-picrylhydrazyl (DPPH) with a g-value of 2.0036 is used as a reference for g-factor calculations.

UV-Visible, FT-IR, Powder XRD Measurements

The optical spectrum has been recorded at room temperature using a Varian Cary 5000 ultraviolet-visible (UV-Vis) near-infrared spectrophotometer in the range of 200-1300 nm. FT-IR spectra are recorded for doped and undoped materials on a Shimadzu FT-IR-8300/8700 spectrometer, in the frequency range of 4000-400 cm^{-1}. The measurements are made using almost transparent KBr pellets containing fine-powdered samples at room temperature. Powder XRD studies are carried out for doped and undoped materials on a PANalytical X'pert PRO diffractometer with Cu Kα radiation of wavelength λ = 0.15406 nm, 2θ values between 5-75°, at room temperature.

CRYSTAL STRUCTURE

$[Li(H_2O)]_2[Zn(mal)_2(H_2O)]$ is isostructural with $[Li(H_2O)]_2[Cu(mal)_2(H_2O)]$ [20]. It belongs to the triclinic crystal system with space group *P*1, having unit cell parameters a = 0.6851 nm, b = 0.8852 nm, c = 1.0529 nm, α = 80.65°, β = 75.04°, γ = 70.36° and Z = 2. The copper atom is coordinated with a distorted square pyramidal environment. Four carboxylate-oxygen atoms from two crystallographically independent malonate groups build the equatorial plane around the copper atom. A water molecule occupies the apical position.

RESULTS AND DISCUSSION

Single Crystal EPR Studies

For a vanadyl impurity, along a crystallographic axis, an eight-line pattern is observed since the electron spin is 1/2 and ^{51}V nuclear spin is 7/2. In order to obtain spin Hamiltonian parameters at room temperature, single crystal rotations were performed along the three mutually orthogonal axes a*, b and c*, where axis b is the crystallographic axis b, axis a* is orthogonal to axis b in ab plane and axis c* is mutually perpendicular to both the axes b and a*. Crystals with 1 and 1.5% concentrations of dopant ion gave resonances that are relatively weak and hence

CHAPTER 14

Morphological and Structural Characterizations of Strontium in Strontium Sulphate as a Perceptive Factor in the Computational Method for the Forensic Analysis of Tool Paint by Non-destructive Analytical Studies

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Abstract: The morphological and structural characterization of strontium in strontium sulphate in forensic analysis is highlighted in this chapter. Strontium sulphate is a polymeric compound with structural similarities to barium sulphate. The best tool for forensic applications is the SEM's non-destructive microscopic inquiry, which has been utilized as a reference technique to support the study. This study further demonstrated that the main screening of samples using the XRD does not require any special sample preparation. Crystallite size and miller plane for specific peak values are computed using computational data and statistical techniques to obtain accuracy in the forensic investigation. In comparison to previous descriptions of X-rays as tool paintings in forensic analysis, this paper is the one that receives the most citations. A thorough study of these tool coatings might effectively connect an optimistic presumption to particular crime scene locations.

Keywords: Computational data, Crime scene, Forensic analysis, Paint analysis, SEM, XRD.

INTRODUCTION

Paint analysis is one of the forms of trace evidence that are most frequently studied in forensic science labs. Other instances of tool paint analysis include artistic, architectural, and automotive paints [1]. Raman spectroscopy has recently

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been employed by forensic investigators to clarify the conformation of paints, vehicle lenses, and everyday archaeological artefacts. In addition, efficient adopted methods and user-friendly equipment are used with the sophisticated introduction to paint analysis. These methods are frequently applied in forensic environments. Paint shards are a frequent sort of trace evidence discovered in burglaries, vandalism, and traffic accidents [2]. These tool paints can be thoroughly examined to relate a strong suspicion to particular crime scene locations.

The primary components that are used to distinguish between different paints consist of pigments and resins. Infrared technology, which is non-destructive and rapid has been demonstrated to be a viable and accurate method for tool paint testing since the 1970s [3]. The examination of pigments and the study of inks both employed the molecule-vibrating data of resins supplied by Raman spectroscopy successfully [4]. By using spectroscopy and chemometrics in forensic investigation, none of the research studies on differentiating tool paint samples have been published [5 - 7]. The word forensic refers to using science to administer justice, often known as forensic science. With the increase in crimes, forensic science has developed to be more exact and quicker to respond to new issues. In accordance with the environment, an extensive range of crimes were perpetrated every day. As a result, forensic professionals handle a variety of evidence [8, 9]. With one instance, a bed sheet is covered with blood; in another, a single hair. Forensic science employs a plenty of techniques to gather evidence at the scene of a crime. Raman spectroscopy, which has been employed up to now in forensic laboratories, is of interest to forensic researchers [10]. Due to its non-destructive nature, limited sample preparation requirements, and convenience for the forensic expert, Raman spectroscopy is the widely used technology for the study of forensic samples. When the paint layers are divided using the scraping technique, the ATR-FTIR spectroscopy makes sure that spectra are drawn from the first few microns of the transparent paint coat. Then transmission IR spectroscopy is used to characterize it; caution must be exercised while analyzing such spectra [11, 12]. In the meanwhile, IR chemical imaging has served as a replacement since it allows for the simultaneous acquisition of chemical and spatial information. One of the technologies employed in the past is pyrolysis gas chromatography/mass spectrometry (Py-GC/MS) [13 - 16]. It is regarded as a beneficial analytical approach because of its enormous discrimination capacity, especially when chemical differences exist between tiny size samples and the harmful technique procedure is the main drawback [17]. In some cases, specifically SEM/ EDS provides a more in-depth report of the inorganic fillers and pigments included in the tool paint analysis, carried out by the tool paint expertise, in order to improve the analytical technique for this sort of material testing. Also it determines whether an expanded use of this methodology would

allow the differentiation of various instruments that are indistinguishable or not sufficiently distinguished by the current analytical strategy [18, 19]. Strontium sulphate is a polymeric compound with structural similarities to barium sulphate. It is noteworthy to note that strontium sulphate was discovered naturally in more valuable strontium compounds. Based on this filler in the data provided in this work, X-ray mapping and local X ray analysis reveal detailed variation [20].

METHODS AND MATERIALS

Metal salts were ordered and received from Merck (Darmstadt, Germany). All the solvents were purified by standard techniques employed for spectroscopic and electrochemical studies. All samples were characterized by Fourier-transform infrared (FT-IR), Raman micro spectroscopy and ultraviolet-visible spectroscopy (UV–Vis). Some additional characterizations were made to gather the chemical frequency information and the discrimination power of these techniques.

XRD Analysis

The XRD of the samples presented in this work was produced in two Philips X-ray diffractometers: D8 Advance ECO XRCD Systems with SSD160 1 D Detector (Bruker) by using Cu K(λ = 1.54056 A) radiation which is the most popularly used X-ray radiation for the analysis of both powdery and poly crystalline materials. Many samples of each pigment from different manufacturers were selected and the best findings are provided here, which were used as a standard for commercial pigments for comparing results from unknown sources or samples. The pigments were kept under flexible conditions during the grinding procedure without any sample preparation to ensure that the polymorphic pigments do not undergo any state change or any reaction [21]. The pigment sections were separated from the paints using dilution and centrifuging methods, washed and dried. Then, it became easy to find the pigment from the paint samples.

UV–VIS Microspectroscopy

Each sample was put in glycerol on a quartz microscope slide that was about 5 μm thick, and the slide was then covered with a quartz cover slip. It was a 35-model PERIN ELMER LAMBDA. Glycerol is not itself fluorescent. Both clear and color top coats were examined using UV–Vis micro spectroscopy. Within a single tool paint sample, heterogeneity or variability could occur. Therefore, more than ten spectra from different locations of the same sample, for each clear and color coat, were gathered to get a precise representation of the paint. To use the CRAIC data software, statistical analyses were conducted for every layer of each sample. Every 10 spectrums from each layer (*e.g.*, clear or color coat) of each sample were

CHAPTER 15

Functional Prediction of Anti-methanogenic Targets from *Methanobrevibacter Ruminantium* M1 Operome

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Abstract: *Methanobrevibacter ruminantium* M1 is one of the abundant methanogenic archaea found in ruminants, which is influential in livestock production by enteric methane emission. Several methane mitigation strategies have been employed to curtail enteric methane emissions, most of which have not been successful to date. Hence, it is imperative to discover new targets for the development of organism-specific vaccines and inhibitors of methanogenesis. In this study, we predicted the functions and characterized chemogenomic and vaccine proteins from their operomes using a combined bioinformatics approach. A precise function of 257 hypothetical proteins was assigned based on their sequence-structure-function relationships, as evidenced by the literature. We identified 12 virulence genes and 18 vaccinogenic proteins as reliable antigenic determinants. The predicted virulence proteins were found to promote the survival of this organism in the intestine of ruminant animals. The toll-like receptor, nudix hydrolase, pseudo murein-binding repeat protein, and phosphonoacetate hydrolase identified in this organism have shown more immunogenic and vaccinogenic characteristics. Therefore, the new virulence factors and vaccine candidates identified in this study would provide a quest for new anti-methanogenic drugs to mitigate the methane emitted in ruminant animals.

Keywords: Hypothetical proteins, Immunoinformatics, *Methanobrevibacter*, Methanogenesis, Protein function, Vaccine.

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INTRODUCTION

Methane is a potent greenhouse gas produced by rumen methanogens *via* enteric fermentation in the gastrointestinal tract of livestock. Enteric methane emissions represent a loss of approximately 5–7% of dietary energy in ruminants [1]. It is predicted that reducing methane emissions from ruminants will also increase the energy available to animals for meat and milk production, leading to meeting the demand for ruminant-based agriculture by 2050 [2, 3].

Methane mitigation interventions have been developed to inhibit the methanogenic activity of ruminants. Most interventions have failed or met with only limited success owing to the lack of organism-specific targets studied in rumen methanogens [4 - 8]. To address this issue, several genome-wide analyses have been used to investigate new chemogenomic and vaccine proteins from rumen methanogens [9 - 11].

Methanobrevibacter and *Methanobacterium* are the dominant rumen methanogenic archaea in ruminant livestock. *Methanobrevibacter ruminantium* M1 (MRU)is experimentally investigated to be a dominant rumen methanogen and accounted for 27.3% on average, accounting for 61.6% of rumen archaea [12]. MRU is a hydrogenotrophic rumen methanogen that uses H_2 to reduce carbon dioxide (CO_2) for methane biosynthesis. Formate is also used as a carbon source for growth and energy metabolism. This organism has a circular chromosome (2.93 Mbp) with 2,278 coding genes and 144 metabolic pathways with 722 reactions, 557 enzymes, and 751 metabolites [13]. However, 756 coding genes (73%) were annotated as hypothetical proteins (HPs) from this genome, suggesting that the entire proteome function remains to be elucidated.

Automated genome sequence analysis provides a function of only 50-70% of the coding genes of the most completely sequenced bacterial genomes [14]. The operome characterizes proteins with unknown biological functions [15]. Conserved hypothetical proteins (HPs) and uncharacterized proteins have known and unknown gene homologs, respectively [16, 17]. Although several computational efforts have been made to assign the function of prokaryotic operomes, only a few investigators have attempted a combined bioinformatics approach [10, 11, 18, 19]. Summative information derived from the sequence, structure, and literature of related homologs supports precise functional annotation of prokaryotic operomes [20].

A combined bioinformatics approach is of great concern to realize our fragmentary knowledge of potential drug targets [9 - 11, 16, 19]. In this study, it was used to assist in the precise molecular function of the MRU operome based on the sequence-structure-function link. Currently available antibiotics, inhibitors,

and vaccines have shown narrow-spectrum activity against rumen methanogens [6 - 8]. The new virulence and vaccine proteins identified in the operome can resolve the current demand for veterinary therapeutics.

The predicted vaccine candidates that would work in the laboratory as well as in clinics is a challenging problem. Hence, vaccine development strategies such as molecular modeling and dynamic simulation, vaccigenic target (antigens) discovery and the selection and simulation of B and T cell epitopes and simulations should be assisted by Artificial Intelligence (AI) and Machine Learning (ML). ML models have been used to investigate immunogenic components to be exploited as vaccine candidates. AI models have been used to reach the right targets and design vaccines by combining several hundred parameters. Various bioinformatics software and tools used in the vaccine target discovery process are consolidated in this chapter. However, AI and ML offer promising solutions that could accelerate the optimization of new viable vaccines.

MATERIALS AND METHODS

Sequence-based Functional Annotation

A total of 756 HPs were identified from the MRU genome using keyword search ("hypothetical proteins, unknown, uncharacterized, and putative") against the Kyoto Encyclopedia of Genes and Genomes (KEGG) [21]. Conserved motifs were detected from the identified HPs using the KEGG-Motif search tool (http://www.genome.jp/tools/motif/). A protein that showed a cutoff value below 10-5 and harbored a domain with an unknown function was excluded from the dataset. Conserved domains and architectures were identified using the NCBI-CDD v3.16 search tool [22] and SMART V7 [23], respectively. Functional site-associated patterns in the sequences were analyzed using ScanProsite [24].

Structure-based Functional Annotation

The functions of protein families and related Gene ontology terms were deduced from the evolutionary relationships of HPs using the SIFTER server [25]. The primary (instability index, aliphatic index, grand average of hydropathicity, *etc.*) and secondary (helix, sheets, extended coil, loops, *etc.*) structural characteristics of HPs were predicted using Expasy's ProtParam server (http://web.expasy.org/protparam/) and SOPMA [26], respectively. The 3D structural characteristics of HPs were predicted from their respective homology models generated using the Swiss Model [27]. The functions of the HPs were classified using the CATH database based on the conserved domain, protein fold, family, and biological function [28].

CHAPTER 16

Comparative Prediction of Electrical Interplay Systems in *Methanothermobacter thermautotrophicus* ΔH and Metal-loving Bacteria

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Abstract: Bioelectrochemical technology has been developed to elucidate the mechanisms of electrical interplay systems for electromethanogenesis in microbial electrolysis cells (MEC). In the present study, we evaluated the electrical interplay systems for electromethanogenesis in *Methanothermobacter thermautotrophicus* ΔH (MTH). The modular structure of its protein-protein interaction (PPI) network was compared with the electrical interplay systems of metal-loving eubacteria (*Geobacter metallireducens* and *G. sulfurreducens*). The structure-function-metabolism link of each protein pair was evaluated to mine experimental PPI information from the literature. The results of our study indicate that the topological properties of the PPI networks are robust and consistent for sharing homologous protein interactions across metal-loving eubacteria. A large fraction of genes and associated PPI networks were established in the MTH for direct interspecies electron transfer systems, which were divergent from metal-loving eubacteria. MTH is predicted to generate CH_4 by reducing CO_2 with hydrogen in the geothermal environment through growth-associated electromethanogenesis. Thus, the present computational study will facilitate an understanding of the proteomic contexts and mechanisms of interspecies electron transfer between thermophilic autotrophic methanogenic archaea and metal-loving Eubacteria for electromethanogenesis.

Keywords: Electrical interplay system, Electromethanogenesis, Geobacter, *Methanothermobacter*, Nanowire, Protein networks, Systems biology.

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INTRODUCTION

Methanothermobacter thermautotrophicus ΔH (MTH), an obligate thermophilic methanogen, is used to reduce CO_2 with H_2 into CH_4 gas in an anoxic environment. The growth and energy metabolism of this organism depends on the concentrations of H_2, formate, and many trace metals under syntrophic conditions [1]. Comparative proteomic analysis revealed its physiological adaptation and interspecies H_2 transfer under pure culture and syntrophic conditions [2 - 14]. H_2 and formate act as the primary shuttle compounds to transfer electrons from donors to acceptors within the methanogenic consortia. Regarding diffusivity, H_2 diffuses 30 times faster than formate; therefore, formate is more soluble than H_2, with approximately 1000-fold higher solubility. The presence of hydrogenases or formate dehydrogenases is essential for chain biochemical reactions through extracellular electron transfer in syntrophic methanogenic consortia [15, 16].

Over 50% of CH_4 production could be ascribed to direct interspecies electron transfer (DIET) between *Geobacter* and *Methanosaeta* in an electric-anaerobic sludge digester [17]. DIET is more energy-conserving than interspecies H_2 or formate transfer; however, the relationship between them has not yet been elucidated [15]. *G. sulfurreducens* PCA (GSU) [18], *G. metallireducens* GS-15 (GME) [17, 19], and *Shewanella oneidensis* [20, 21] are exoelectrogenic metal-loving eubacteria. These microorganisms can form extracellular nanowires that transfer electrons to minerals and between cells. Recent studies demonstrated that the oxidation of ethanol by GME GS-15 is electrically coupled to the reduction of fumarate by GSU PCA [22] and to the reduction of CO_2 to produce CH_4 biofuel by *M. harundinacea* and *Methanosarcina barkeri* through nanowires [19, 23] and conductive carbon materials [24, 25]. However, direct evidence is required to support the role of nanowires and multiheme c-cytochrome in transferring electrons from methanogenic archaea to metal-loving bacteria.

The extracellular electrical interplay between microorganisms and minerals links the redox transformation of metal ions to the oxidation of organic carbon compounds and fixation of CO_2 to CH_4 through hydrogenotrophic methanogenesis [26]. According to the electron diversion hypothesis, electrons from H_2 could have diverted to Cr_6^+despite CO_2 to produce CH_4, suggesting cooperative and competitive microbial metal reduction and methanogenesis [27 - 31]. MTH was reported to reduce Fe_3^+ in smectite minerals [27], V_5^+ under both growth and non-growth conditions [28], and toxic Cr_6^+ to less toxic Cr_3^+ at 65°C *via* ferredoxin-dependent reactions in the electron transport chain [29]. Hence, a metallic-like electron transfer mechanism supports a conduction process in which electrons are delocalized and can move freely without thermal activation, as in metals and conductive polymers [26].

Genome sequencing of MTH was completed, and its genomic context was characterized to understand the complexity of the proteome in biological functions [32]. To address this metabolic complexity, there is no genome-scale metabolic network for this organism. Genome-scale metabolic reconstructions have been developed for GME iAF987 with 987 genes and 1285 reactions with 1109 metabolites [33, 34] and GSU with 588 genes and 523 reactions with 541 metabolites [35]. These genomes contain approximately 50% of the proteome with unknown functions and no high-throughput experimental data in the databases [13]. A genome-scale study of the cellular metabolism of these microorganisms highlights the importance of protein-protein interaction (PPI) networks. Therefore, we evaluated the modular structure of the PPI network of the MTH from a gene set consisting of pilin, archaellin, archaella assembly proteins, and electron carrier proteins. The reconstructed network model was compared with the GME and GSU to better understand the electrical interplay systems for electromethanogenesis. This will provide a clue for exploiting MTH for the production of CH_4 from CO_2 with hydrogen in microbial electrolysis cells (bioelectrochemical reactors).

Computational Intelligent approaches have become an obvious need in proteomics research. These techniques have been used to investigate protein function predictions, PPI networks and differential gene expression by mining proteomic information from large-scale datasets. However, more studies are needed to complete our knowledge of the PPI network, which represents a challenging research problem in computational biology. Artificial intelligence (AI) provides massive openings to accelerate bioinformatics applications through a deeper and more reliable way of interrogating proteomics data. Intelligent search algorithms that combine deep learning and Machine learning (ML) have become central to extracting new proteome information from PPI data and inferring properties. Recently, integrating deep learning algorithms and ensemble classifiers and integration of multiple heterogeneous data are useful for protein function prediction and PPI network interpretations. Hence, Al and ML models are more effective for future proteomics research work than the existing bioinformatics tools.

MATERIALS AND METHODS

Identification and Functional Characterization of Pilin and Archaellin

A text-mining approach was used to identify proteins involved in the electrical interplay of MTH. The conserved domains and architecture of the identified proteins were detected by the NCBI conserved domain search [36] and the SMART server [37], respectively. Common conserved motifs found in the

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