

OLADELE T.O.



BOOK OF PROCEEDINGS

Series 7

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University of Ilorin,
Ilorin, Kwara State, Nigeria.

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ISTEAMS Research Nexus Conference

International Science, Technology,
Engineering, Arts, Management
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Multidisciplinary Conference

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4th ISTEAMS Research
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BOOK OF PROCEEDINGS

SERIES 7

Theme: Together Towards Tomorrow – Leveraging on Multidisciplinary Research for Human
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Ilorin, Kwara State, Nigeria

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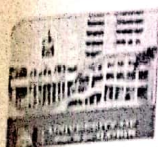
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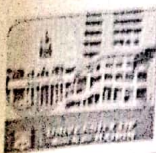


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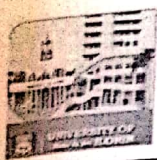
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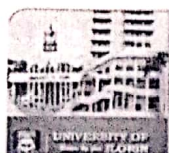
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Information and Communication Technology Approach to Antimalarial Drug Discovery

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ABSTRACT

Globally, malaria is a disease of public health importance. Currently, malaria is one of the three epidemic diseases that Global Fund is accelerating fight against. In 2014, there were 97 countries and territories that had ongoing malaria transmission. According to world Health Organization (WHO), 3.2 billion people were estimated to be at risk of malaria infection of which 1.2 billion were at high-risk areas in 2014. With regards to the high-risk areas, there was more than one malaria case per 1000 population. World-wide, there were estimated 484,000 malaria-related deaths in 2013, of which 90% occurred in Africa. Malaria killed an estimate of 1241 children under 5 years of age daily, or 52 children (under-fives) every hour in 2013. One of the four basic technical elements of WHO's Global Malarial Control Strategies is prompt treatment of the disease using antimalarial medicines. In Nigeria, artemisinin-based combination therapies (ACTs) are the first-line treatment of uncomplicated malaria. Despite ACTs are highly efficacious, Plasmodium falciparum resistance to artemisinin has been reported. Hence, there is urgent need to develop new and effective antimalarial drugs. Since the process of drug discovery and development are both time and capital intensive, it is essential to use simple cost-effective and rigorous screening methods to identify and validate just the very best new antimalarials at an early stage in the process. This is possible through the use of Information and Communication Technology techniques, hence the focus of this paper.

Keywords: Information and Communication Technology, Drug Discovery, Antimalarial Drugs
Malaria, Disease.

1. INTRODUCTION

Information and Communication Technology (ICT) has been in use in the field of medicine via medical care information systems in which electronic medical records are being manipulated. It has also been used in the diagnosis of various diseases including malaria. Currently it is being widely applied in drug discovery. The most widely applied techniques are Computational Chemistry and Molecular Modelling. Malaria, protozoal infection is caused by Plasmodium falciparum, Plasmodium malariae, Plasmodium knowlesi, Plasmodium ovale and Plasmodium vivax, (Williams et al., 2013, Medicines for Malaria Venture (MMV), 2013, Ninanet et al, 2012). It is a disease of public health importance. The reservoir of infection for the P. falciparum, P. vivax, P. malariae and P. ovale is man while for P. knowlesi is macaque (Williams et al., 2013, Figtree, et al, 2010). The vector is female anopheles mosquito (Figtree, et al, 2010, Luchavez, et al., 2008;). The transmission is through the bite of the anopheles mosquito (Williams et al., 2013, Collins, 2012).

Malaria has been endemic in our society since the dawn of history (Carter and Mendes, 2002). It is currently one of the major tropical communicable diseases adversely affecting the health of people and the economic development of many developing countries, particularly in the Sub-Saharan Africa (SSA). According to World Health Organization (WHO) 2014, 97 countries and territories had ongoing malaria transmission and 3.2 billion people were estimated to be at risk of malaria infection of which 1.2 billion were at high-risk areas in 2014. Also, there was more than one malaria case per 1000 population in these high-risk areas. Globally, an estimated 484,000 malaria-related deaths occurred in 2013, of which 90% was in Africa. Malaria killed an estimate of 1241 children under 5 years of age daily, or 52 children (under-fives) every hour in 2013. Moreover, 60% of the malarial-related deaths in 2010 were from Nigeria along with other 5 Sub-Saharan African countries (WHO, 2011).

Enormous efforts have been put in to fight malaria. It is one of the three epidemic diseases that Global Fund is accelerating fight against (The Global Fund, 2014). One of the four basic technical elements of WHO's Global Malarial Control Strategies is prompt treatment of the disease using antimalarial medicines (WHO 2012). According to MMV, 2013 antimalarial medicines such as chloroquine (CQ), quinine (QUI), sulphadoxine-pyremethamine (SP) and mefloquine (MQ) have been developed and used. However, treatment of malaria is very difficult due to emergence of resistant strains of *P. falciparum* to these cheap and widely available antimalarial medicines (Williams et al., 2013). Artemisinin-based combination therapies (ACTs), recommended in November 2004, and formally adopted nationwide in January 2005 as the first-line treatment of uncomplicated malaria (Federal Ministry of Health, Nigeria, 2005; WHO, 2010) are ACTs that are highly efficacious (Kamuhabwa and Silumbe, 2013).

Drug Discovery is a multi-step process involving target selection, lead identification and clinical candidate selection before clinical trials. With the rapid advances in Structural Biology and Computer Technology, the drug discovery process has been enriched by genomic and proteomic technologies. However, it must be understood that genomic technologies can be fully exploited provided the data acquisition process is highly efficient and highly automated, (Rastogi et al, 2008). In view of the foregoing, there is a necessity to provide a computerized system. That is, a knowledge-based system that will enhance the drug discovery process. Bioinformatics is an emerging field with the potential to significantly improve how drugs are found, brought to clinical trials and eventually released to the market. The Human Genome Project has provided a large number of potential target and therapeutic intervention for malaria and various diseases in recent years. Assessment of targets has become crucial to the success of the drug discovery process. The Pharmaceutical industry has so far relied on the traditional methods which are too slow and cumbersome. The industry has to adopt a new strategy of process biology which integrates genomics and bioinformatics tools to discover new drugs. Proteomics technologies have contributed immensely towards drug target identification, validation and lead selection. Drug target discovery is a decision-making process based on a huge amount of scientific data pertaining to the identification and validation of disease-associated targets. A major challenge lies in the compound selection process (Rastogi et al, 2008). However, various ICT techniques and infrastructures can be explored in order to facilitate the drug discovery process.

2. ICT AND FIGHT AGAINST MALARIA

In view of malaria disease burden and the malaria parasite resistance to currently used anti-malarials, there is an urgent need to develop new and effective antimalarial molecules. This goal can be achieved in two ways; either by focusing on validated targets in order to generate new drug candidates; or by identifying new potential targets for malaria chemotherapy. The advent of functional genomics and structure-based drug design has helped in the search for new targets. The genomic sequences of parasitic diseases are rapidly becoming available and recently, the full sequence of *Plasmodium falciparum* was published (Dyann, 2002). Much has been promised from this genomic revolution including the identification of new drug targets and novel chemotherapeutic treatments for the control of parasitic diseases. The recently concluded *Plasmodium* genome sequencing project has led to a dramatic increase in the amount of genome data available in public databases (Aguero et al, 2008). A major challenge confronting researchers on malaria is how to analyze and mine the data from this database. It has, therefore, become important to develop computational tools for data mining in novel genomes. The phenomenon of parasite resistance to drugs has also compounded the problem of malaria control. Chemotherapy is one of the major control strategies in the fight against the malaria parasite.



However, the development of drug resistance to many of the currently available drugs is causing a crisis in malaria endemic areas. The mechanism of drug resistance is still poorly understood, and if the problem is to be tackled successfully, new antimalarial drugs must be found to replace those that have been rendered ineffective in controlling malaria (Oladele et al., 2012). The challenge to use this information effectively will require functional genomics tools such as bioinformatics, micro arrays, proteomics and chemical genomics to identify potential drug targets, and to allow the development of optimized lead compounds. The information generated from these tools will provide a crucial link from genomic analysis to drug discovery. It is well understood that the development of new chemotherapeutics agents is a long and expensive process, and that many potential targets and lead compounds will fail at various steps in the process. The sequence of the different parasite genomes has already revealed a long list of potential drug targets. If promising candidates are to be identified, it will be essential to use simple cost-effective and rigorous screening ICT techniques to identify and validate just the very best new targets at an early stage in process (Oladele et al., 2012).

3. OVERVIEW OF DRUG DISCOVERY AND DEVELOPMENT

It is the mission of pharmaceutical research companies to take the path from understanding a disease to bringing a safe and effective new treatment to patients. Scientists work to piece together the basic causes of disease at the level of genes, proteins and cells. Out of this understanding emerge "targets," for potential new drugs. Researchers work to:

- validate these targets,
- discover the right molecule (potential drug) to interact with the target chosen,
- test the new compound in the lab and clinic for safety and efficacy and
- gain approval and get the new drug into the hands of doctors and patients.

This whole process takes an average of 10-15 years. For the first time in history, scientists are beginning to understand the inner workings of human disease at the molecular level. Recent advances in genomics, proteomics and computational power present new ways to understand illness. The task of discovering and developing safe and effective drugs is even more promising as our knowledge of disease increases. As scientists work to harness this knowledge, it is becoming an increasingly challenging undertaking. The average cost to research and develop each successful drug is estimated to be over \$800 million (DiMasi et al., 2003). Only one compound may ultimately receive marketing approval out of thousands of compounds that enter the research and development (R&D) pipeline (Cato et al., 2002). Furthermore only 30% of drugs that reach market place generate sufficient revenue to recover cost of the development (Grabowski et al., 2002). Success requires immense resources - the best scientific minds, highly sophisticated technology and complex project management, time, money and information.

3.1 Pre-discovery

Before any potential new medicine can be discovered, scientists work to understand the disease to be treated as well as possible, and to unravel the underlying cause of the condition. They try to understand how the genes are altered, how that affects the proteins they encode and how those proteins interact with each other in living cells, how those affected cells change the specific tissue they are in and finally how the disease affects the entire patient. This knowledge is the basis for treating the problem. Researchers from government, academia and industry all contribute to this knowledge base. However, even with new tools and insights, this research takes many years of work and, too often, leads to frustrating dead ends. And even if the research is successful, it will take many more years of work to turn this basic understanding of what causes a disease into a new treatment.

3.2 Drug Discovery

There are five key sequential stages in the Drug Discovery Process as shown in figure 1 (Piera):

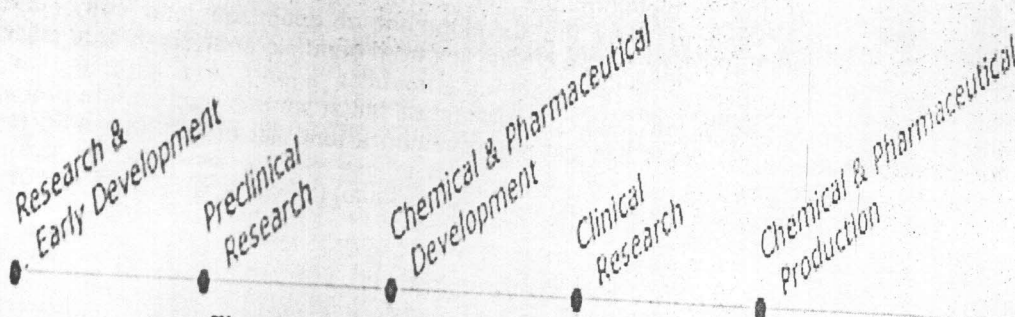


Figure 1: Sequential Stages of the Drug Discovery Process

1. Research & Early Development

This first phase of the drug development process is basic research. During this phase researchers try to understand the underlying mechanism or cause of a certain disease. Researchers look for new chemical or molecular entities that display promising activity against a particular biological target thought to be important for the disease. Other properties (including safety, toxicity, etc) and metabolic effects of the identified entities in humans are not focused on at this stage.

2. Preclinical Research

Preclinical research must be completed before clinical trials (testing in humans) can start. During this stage important feasibility, iterative testing and safety data is collected. The main goal of preclinical study is to determine a product's ultimate safety profile. Products may be new or iterated medical devices, drugs and gene therapy solutions. Each class of product may undergo different types of preclinical research. For instance, drugs may undergo pharmacodynamic, pharmacokinetic, ADME, and toxicity testing through animal testing. Typically, both in vitro and in vivo tests will be performed.

3. Chemical & pharmaceutical development

During the chemical and pharmaceutical development phase the aim is to design a quality product and its manufacturing process to consistently deliver the intended performance of the product. The information and knowledge gained from the studies and manufacturing experience provide scientific understanding to support the establishment of the design space, specifications, and manufacturing controls.

4. Clinical Research

In this phase clinical trials are conducted to collect safety and efficacy data for new drugs. These trials can only take place once there is adequate information about the quality of the product, its non-clinical safety and once health authority approval has been granted. As positive safety and efficacy data are gathered, the number of patients is typically increased. Clinical trials can vary in size from a single centre in one country to multi-centre trials in multiple countries. After conclusion of the clinical trials the drug will be submitted for regulatory approval, for example with the Food and Drug Administration in the US or with the European Medicines Agency.

5. Chemical & Pharmaceutical Production

Once a new drug has been approved by the regulatory agencies such as the Food and Drug Administration in the US a full scale manufacturing plant will be built based on the scientific understanding gathered during the chemical and pharmaceutical development phase.

3.3 Drug Development

Drug development refers to the processes involved in taking a candidate drug or Biological molecule through the stages necessary to obtain marketing approval. The end goal of drug development is to have a product that is approved by relevant regulatory authorities and can be prescribed to or otherwise made available to patients. As a general rule, the drug development process is lengthy and expensive. There is much debate to just how expensive the process is. The cost of development for a drug is being estimated to be around \$800 million dollars.

This high estimate reflects the fact that successful (or even unsuccessful) drug development, starting from the point at which an appropriate molecule/compound is identified, requires consideration and strategy on a wide range of factors including (Goulding and Marden, 2009):

- identification of the disease indication to be treated,
- potential for adverse events,
- intellectual property landscape,
- regulatory requirements and hurdles,
- the ability to conduct research and trials in a regulatory compliant manner,
- potential to manufacture and deliver the drug/compound,
- willingness to pay for the end product, and
- the potential market for the product.

4. INFORMATION AND COMMUNICATION TECHNOLOGY BASED DRUG DISCOVERY

ICT is used more and more for scientific research. Almost all scientific fields explore the use of ICT. The development of new technologies and new products is impossible nowadays without ICT. The main tasks in ICT include (Boyanov):

- Building high-speed network connectivity;
- Building and developing Grid technology platforms;
- Building and developing supercomputing platforms;
- Building virtual organizations, helping new ICT implementation;

The present trends for scientific activity organization involve basic e-infrastructure of network connectivity, above which new computer platforms such as Grid, Supercomputers, and Cloud are built, as well as storage device for keeping large databases.

ICT Network Infrastructures for Drug Discovery include:

(A) Grid Computing

Grid computing is currently developing into a major driving force for new approaches towards collaborative large scale science. Several national and international eScience programs have fostered collaboration between researchers from different scientific domains and the first large scale experiments on grids infrastructures such as EGEE are underway as reported in Wisdom (2015). Scientists are using grids high-speed computing networks as a large-scale and cheaper way to kick-start new drug development against malaria parasites.

In the biomedical community, grid computing has initiated several projects on large scale in silico drug screening approaches. The project WISDOM was amongst the first projects in the public domain that made use of grid enabled in silico docking to simulate the interaction of potential drugs with target proteins. In silico docking is the first step in the virtual screening process, which is one of the most promising approaches to speed-up and to reduce the costs of the development of new drugs (Wisdom, 2015). WISDOM was organised in the course of the first biomedical data challenge for drug discovery on the EGEE grid production service and was effectively run between 11 July 2005 and 31 August 2005. In the course of this first real large scale biomedical application on EGEE.



WISDOM

WISDOM (Wide In Silico Docking On Malaria) is an European initiative to enable the in silico drug discovery pipeline on a grid infrastructure. Initiated and implemented by Fraunhofer Institute for Algorithms and Scientific Computing (SCAI) scai.fraunhofer.de in Germany and the Corpuscular Physics Laboratory (CNRS/IN2P3) clrwww.in2p3.fr of Clermont-Ferrand in France. WISDOM has deployed a large scale docking experiment on the EGEE www.eu-egee.org infrastructure (Wisdom, 2015).

Three goals motivated this first experiment:

- The biological goal was to propose new inhibitors for a family of proteins produced by Plasmodium falciparum, a malaria parasite.
- The biomedical informatics goal was the deployment of in silico virtual docking on a grid infrastructure.
- The grid goal is the deployment of a CPU consuming application generating large data flows to test the grid operation and services.

(B) Cloud Computing

Cloud computing is a computing paradigm which makes computer facilities to be available in a remote location called cloud. This makes it accessible to computer users irrespective of location. This is significant in enhancing the drug discovery process.

(C) Supercomputing

The idea of supercomputing arises from the need to process data at very high speed, much faster than the conventional computer system. This has made it a useful infrastructure for drug discovery technology.

5. CONCLUSION

Discovery and development of new medicines is a long and complicated process. Every success is built on many prior failures. Advances in understanding human biology and disease are opening up exciting new possibilities for breakthrough medicines. At the same time, researchers face great challenges in understanding and applying these advances to the treatment of disease. These possibilities will grow as our scientific knowledge expands and becomes increasingly complex. Research-based pharmaceutical companies are committed to advancing science and bringing new medicines to patients. ICT technologies and infrastructures have been found to accelerate and enhance the drug discovery process thereby reducing the cost and time to discover new and efficient antimalarials.



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