Minireview Article

Pharmacoinformatics: Development Through History and its Role in Pharmaceutical Industry

Abstract: Medicine has displayed miraculous developments during the past century or so. Credit goes to the emergence of scientific research methods. Research on the disease, its causes, effects, precaution, and especially cure has revolutionized the world. Man has been liberated from epidemics and other deadly diseases. All this would not have been possible, had there not been research and development in medication simultaneously. The pharmaceutical industry is an integral part of the medical field. A real boost was given to all kinds of research with the invention of the computer. Data saving, processing, and analysis were never easier. This paper aims at highlighting the great role and importance of Pharmacoinformatics in drug discovery. It also elucidates how drug discovery is done. A portion of it also targets how this science has evolved over time. The particular purpose is to trace the transformations that came with the introduction of Information Technology in this field.

Keywords: Pharmacoinformatics; pharmacy informatics; information technology, health informatics; drug discovery.

Introduction

Pharmacoinformatics is almost the same science as medical informatics (Hammond & Cimino, 2001). It can be defined as the field of science related to the analysis, use, and propagation of medical data through the application of information technology to different aspects of healthcare and medicine (Gautam, Bhambu, Rai, & Sahu, 2013). The Healthcare Information and Management Systems Society defines Pharmacoinformatics as "the scientific field that focuses on medication-related data and knowledge within the continuum of healthcare systems – including its acquisition, storage, analysis, use, and dissemination." It can also be defined as the combination of drug information and pharmacy information systems (Venkateswarlu, 2018). This science is also involved in the scope of medical informatics and drug discovery which relate to drug properties and its management (López-López, Naveja, & Medina-Franco, 2019; Bisht & Singh, 2018). In medicine, informatics has been successfully applied to the following fields apart from Pharmacoinformatics:

a) Toxico-informatics
b) Neuro-informatics
c) Immuno-informatics
d) Cancer informatics
e) Chemo-informatics
f) Bioinformatics
g) Metabolomics
h) Genome informatics
i) Proteome informatics
j) Biomedical informatics

Pharmacoinformatics has two broad categories relating to the research and discovery process:

a) Scientific Aspect
b) Service Aspect

The scientific aspect involves the management of drug discovery and drug development activities, while the service aspect includes patient-centered activities (Olğaç, Türe, Olğaç, & Möller, 2019).

Method of Developing New Drug

"I like to think about drug discovery as solving a very complex jigsaw puzzle with many thousands of pieces," says Mark Noe, Vice President of Discovery Sciences in Pfizer's Groton, CT Research and Development site.

Development of new medicines is a complex procedure involving the combination of various scientific and technological disciplines which include chemistry, biology, pharmacology, pharmaceutical technology- all in coordination with information technology. Researchers have to make observations and record them continuously. This data is then used while research. Informatics has revolutionized the way this is done. There are the following stages of the drug discovery procedure:

1. Choose a Target

To start the procedure, the first step is to comprehend what changes that particular disease has on biological processes in the body. The typical protein involved in the disease process is isolated. The target of a drug can also be DNA or RNA.

2. The Search

This part of the mission is about finding a compound to interact with the target. It is not as simple because millions of compounds have to be tried, and the search narrows down step by step (Sehgal et al., 2018). One or more narrowed compounds called "lead" compounds will continue to be optimized through safety and efficacy testing. At last the scientists reach a compound to test it in the next stages. The methods include:

a) Pharmacology
b) Rational Drug Design
c) High throughput Screening

3. Candidate is Chosen

It takes months or even years to locate a compound that works! After hundreds to thousands of tests, there is something that can relieve the suffering of millions of people.

4. Toxicity Testing

At this stage, the scientists starting testing what other effects other than the target effect will that compound cause on biological processes.

5. Phase 1 Clinical Trials

The main goal of a Phase I trial is to test the safety of a medicine in healthy volunteers at the predicted active dose (Urquhart, 1995). The safety of the medicine is tested on a healthy body at this stage. Volunteers are required for this stage, typically a control group consisting of 20 to 100 people.

6. Formulation, Bottling, and Packaging

After successfully isolating the active ingredient, it is turned into a medicine that can be tested at the next stages. The amount and form to be administered have to be decided at this stage.

7. Phase 2 Clinical Trials

The drug is now tested on real patients of the target disease. The effectiveness and possible side effects come to light in a real-life situation.

8. Phase 3 Clinical Trials

At this stage, the drug is tried on a control group of patients ranging from 300 to 3,000 volunteers. It is also compared with other available rivals if present.

9. Final Registration

Congratulations world! Science has created another miracle for you.

The newly discovered medicine is now presented to regulatory agencies like the U.S. Food and Drug Administration (FDA). They have their own procedure to adopt for every new drug before giving it approval.

Role and Advantages of Information Technology

The cure for a disease is not expensive at all. The actual expense is caused by research on the diagnosis and discovery of drugs. It requires a huge investment in the collection of data, testing, and experimenting, repeat processes, errors, delays in care, etc. By introducing information technology all this can be saved (Shaikh & Khoja, 2011a). Let us see how technology and informatics have served the world.

1. Startling Savings

As described above, the discovery and development of new medicines is a long and patient work involving huge investments. Information Technology has come to the rescue by saving huge amounts of testing and experimenting costs.

2. Shared Knowledge

Healthcare is called 'practice' as people related to it keep on learning and refining their skills and knowledge (Ming & Khan, 2018). Information technology has brought great convenience in sharing each-others' knowledge and experience (Shaikh & Khoja, 2011b). There are huge databases about drugs and patients' data to benefit from.

3. Patient Participation

Information Technology has made it a lot easier to get feedback on a larger scale (Shaikh & Khoja, 2012). This has greatly helped to refine the effectiveness of drugs. Patients are a lot better educated and informed about their condition and add to the crucial database regarding their particular condition.

4. Impersonal Care

The healthcare providers don't have to remember each and every patient as the record of the patients is saved digitally. Even a great part of the diagnosis process is done algorithmically by optimized technology.

5. Time-Saving

By improving coordination and by facilitating different processes, information technology saves a great deal of time (Shaikh & Khoja, 2013). The discovery and development of new medicines now take a lot less time than a few decades ago.

6. Better Results

The biggest advantage that information technology has brought to the field of pharmaceuticals is the improved results (Shaikh & Khoja, 2014a). Digital record-keeping of medical data has improved diagnosis and dropped the ratio of errors. It has helped not only the discovery process but also the hospitals, clinics, providers, patients, insurance companies, and governments, too by saving time and money.

Development through History

The article which is considered to be the pioneer in pharmacy informatics was published in Fortune Magazine on October 5, 1981, under the title “Next Industrial Revolution: Designing Drugs by Computer at Merck” (Van Drie, 2007). This article is said to have caused great enthusiasm for computer-aided drug design (CADD). Interest in CADD remained on high throughout, but High-Throughput Screening (HTS) became the chief method of discovery for new treatments (Bisht & Singh, 2018). This is a very aggressive approach basing on the screening of a huge number of molecules to find one that has desired results on the disease. Since HTS is almost a hit and trial method, the success rate is often extremely low. Greater faith, therefore, remains on CADD as it narrows the number of candidate-compounds and saves a lot of time and effort as a result. The experimenting through HTS requires extensive effort and time for the development and validation of drug. On the other hand, CADD asks for less time and can be used in parallel with the processes of HTS. The better way has been found to combine both. India claims to have set up the first dedicated department for Pharmacoinformatics at the National Institute of Pharmaceutical Education And Research, S.A.S. Nagar, India in 2003 (Venkateswarlu & Kiran, 2018). The other countries followed it and now it is taught as a fully commissioned discipline. Informatics pharmacists are among the highest-paid professionals (Jelliffe & Tahani, 1993).

The remarkable comparison between CADD and HTS came in 2003 and established CADD as definitely a better method in every respect. The case was to transform growth factor-β1 receptor kinase inhibitors. The researchers at Eli Lilly adopted the traditional HTS method to find a lead compound that would be improved later on by examination of structure-activity relationship using in vitro assays (Hammond & Cimino, 2001). On the other hand, a team of researchers at Biogen Idec took to CADD and by adopting virtual HTS based on structural interactions between a weak inhibitor a factor-β1 receptor kinase (Hanson, Levin, & Scott, 2012). The Biogen Idec team identified 87 hits by virtual screening of compounds, and the best hit was identical in structure to that discovered by Eli Lilly’s team through a rigorous HTS approach. (Hickey & Smyth, 2010). This case proved that computer-based research could produce the same results as the years-long full-scale HTS procedure. (Hammond, Jaffe, Cimino, & Huff, 2014).

Incredible Present

During the past 10 years, there has been a visible increase in the number of pharmacy institutions and departments in the US which offer pharmacy informatics courses up to the PharmD level. The number of pharmacy institutions has also increased at the same rate. However, this increase has not been consistent on a percent per year basis. There have been fact-finding studies by agencies like Flynn, Fox, and colleagues by analysis of websites and surveys to analyze the syllabi of pharmacy schools. Although incomplete information came up in these studies, however, the findings were consistent in a way that there is a dearth of informatics educational offerings and there is a lack of progress over the study time (Nouri, Hassali, & Hashmi, 2019). The original Flynn analysis 2005 showed an increase of 33%, while the recent study shows it to have reached 36%. However, it is attributed to the increase in the number of schools offering pharmacy informatics courses. Considering that the accreditation procedure has gone remarkable changes during the past 10 years (making it harder to get), the trend towards an increase in pharmacy schools and informatics courses is encouraging.

Future Prospects

There is a huge scope for advancement in Pharmacoinformatics, like any other field of science (Allen, Ruan, King, & Ruan, 2019). The technologies like Artificial Intelligence (AI), Blockchain, Telepharmacy, and Digiceuticals have great promise for this science.

7. Artificial Intelligence (AI)

Machine algorithms are already in practice, but AI is a service to bring sweeping improvements in how to manage data with analytics and how to run operations (Toma, Dinu, & Diguta, 2019). The greater the involvement of AI, the more extensive will be the results.

8. Blockchain

Sharing of experience was a big challenge when pharmacies worked independently. Uploading patient health information onto the block-chains, assigning personalized keys to patients for transference and access and applying regulations for privacy, safety and availability concerns will greatly help in the development of drugs.

9. Telepharmacy

This too is, in no way, a new idea. But the issues of internet bandwidth bring limitations in serving remote patients who are most in need of this service (Yap, 2016). The introduction of 5G technology and infrastructure improvements will help resolve the issues and to expand this service.

10. Digiceuticals

Now, this surely is something quite new. It comprises digital health technologies that can be applied to cure certain conditions or to assist medication therapies. This is the future of healthcare and is bound to develop and expand further.

Conclusion

Information Technology has, without a hint of doubt, refashioned almost every aspect of life (Shaikh & Khoja, 2014b). But its advantages in the field of medicine are unmatched, solely because it is directly related to life, physical well-being, and healthcare. Pharmacoinformatics is certainly the top field benefitting from information technology. The job of developing new drugs has been expedited and facilitated by informatics. The research that took years is now completed a lot quicker as every step is assisted by technology. The future of this field, and as a result, of the whole healthcare industry is promising. It is hard to abandon the traditional practice and to adopt an innovative approach, but the delay caused in this delay directly results in prolonging suffering (Ikram, Ghani, & Abdullah, 2015). Caution is certainly required in decision making, but once something proves its worth, there should be no reluctance.

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