

PHARMA DIGITALIZATION - TRANSFORMATION IN THE PHARMA SECTOR

Abstract

Digitalization plays a pivotal role in the advancement of various sectors. The growth of information technology has contributed a lot in the health care system. Digitalization in the pharma sector has paved a way for the less time consumption in the drug design and has refined the drug discovery process through various softwares. Digitalization can help in reduction of use of raw materials, human resources, time and it has also reduced the risk for low quality final products through automated systems in the pharma industries. In community and hospital pharmacy, the inclusion of computers has been a boon to fasten their business growth and to easily monitor the stocks of the purchased and the sold drugs. Digitalization has also opened the gate for the online pharmacies through which the customers can access and get their drugs delivered at their door steps. Moreover, digital clinical trial has led to the improvement of participant access, engagement and has also lowered the cost.

Keywords: Digitalization, Artificial intelligence, Computers, Online pharmacy, Digital clinical trials.

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I. INTRODUCTION

The healthcare sector is undergoing a profound change due to digitalization. As a crucial component of healthcare, the pharmaceutical sector is no exception to this. Since, there is a steady increase in the world's population, the demand for pharmaceutical product also increases¹. Better information on the effectiveness of medications and enhanced patient quality of life are required by healthcare payers and other clients of pharmaceutical companies. These requirements cannot be met only through conventional methods. It is achieved by digitalization². Digitalization is a process of utilizing digital technology to promote the revenue, production outcomes, innovation in process, new drug design, and consuming less time³. The digitalization process involves digital tools such as IoT, Cloud computing, AI, blockchain to enhance and improve the business process and outcomes⁴.

In this chapter, we will look towards digitalization in a) drug discovery and design, b) manufacturing companies, c) pharmaceutical supply chains, d) community and hospital pharmacy, e) clinical trials.

II. DIGITALIZATION IN DRUG DISCOVERY AND DEVELOPMENT

- 1. Role of AI in drug discovery:** AI (artificial intelligence) can identify the lead and hit compounds, as well as enhances drug target validation and optimise drug design^{5,6}. A computer model based on the QSAR can rapidly determine a large number of chemical compounds or basic physicochemical characteristics like log P or log D^{7,8}. But it is hard to find complex biological properties like ADR and potency. The virtual chemical space shows a geographical map of arrangements of molecules and characteristics that are used to search for bioactive compounds. Available chemical spaces include PubChem, ChemBank, DrugBank, and ChemDB. Hence, QSAR tools are used to determine the potent drug molecule⁹. These tools have developed into AI-based QSAR methods like LDA and SVMs.
- 2. Role of AI in drug screening:** Algorithms like Nearest-Neighbour classifiers, extreme learning machines, RFDNNs, and SVMs are used to identify feasibility and to analyse in vivo activity and toxicity¹⁰.
- 3. Study of physico-chemical properties:** The usage of computer softwares for drug design and drug discovery will fasten the process (Fig.1) and will pave way for proceeding with the discovery of newer drugs with some predictions instead of following a blindfold procedure. The list of some softwares used for drug design and drug discovery are listed as follows in the table no.1

Table 1: List of Software's used For Drug Design and Drug Discovery

Sl. No	Software	To Predict
1	ADMET predictor and ALGOPS program	Lipophilicity And Solubility
2	ANN-based models, graph kernels, and kernel ridge-based models	Acid Dissociation Constant
3	SVMs, ANNs, k-nearest neighbour algorithms, LDAs, probabilistic neural network algorithms, and partial least square (PLS)	Intestinal absorptivity, molecular surface area, molecular mass, total hydrogen count, molecular refractivity, molecular volume, log P, total polar surface area, the sum of E-states indices, solubility index (log S), and rotatable bonds

4. Evaluation of bioactivity: The affinity of drug molecules for the target protein or receptor determines the potency and therapeutic effect of a drug ¹¹.

- Applications like ChemMapper and the similarity ensemble approach (SEA) are used to identify drug–target interactions.
- KronRLS, SimBoost, DeepDTA, and PADME are used to predict drug target binding affinity.
- ML algorithms like MANTRA and PREDICT can be used to predict the therapeutic effectiveness of medications and target proteins of existing and undiscovered pharmaceuticals ¹¹.

5. Evaluation of toxicity: The cost of developing new drugs is increased by the frequent use of cell-based in vitro tests and animal trials to determine a compound's toxicity. Several web-based programmes are available to lower the cost, which include LimTox, pkCSM, admetSAR, and Toxtree. The ML algorithm DeepTox is used to predict the toxicity of a molecule accurately by locating static and dynamic information within the chemical properties of the molecules. The environment for repeatability of studies is improved by IoT-based data analysis of drug discovery systems, which also decreases human participation and human error in the process and testing. Through the use of defined procedures, the quality of the products can be greatly refined ¹².

6. Digital microscopy imaging: It is a digital and microscopic integrated technology to study quantitative microscopic images. Multinational microscopy imaging is very and is needed for biological research and drug discovery ¹². It has created technologies for sectioning microscopy and 3D image remaking. The cameras employed for this purpose are Nikon DXM 1200, Diagnostic SPORT, Pulnix TMC1000, Zeiss AxioCAM, Sony ST5. Integration of automated microscopic imaging with a controlled microscopic stage can yield high resolution image which can be used for studying the physiochemical property of the drugs.



Figure 1: Digitalization Fastening the Process of Drug Discovery

III. THE DIGITALIZATION IN MANUFACTURING COMPANIES

Pharmaceuticals Companies make use of new technology and information systems, which are used to monitor the processes by using multiple dedicated IT systems. It helps to monitor manufacturing activities from any remote location by using real-time monitoring and enhance them by minimising waste, increasing equipment utilization, and lowering production costs. Technology should be accessible so that it increases the productivity of employers who use computers and software.

1. Advantages of implementing digitalization in industry

- **Productivity:** Digitalization provides new and more ways to increase production by enhancing the manufacturing process and maintaining product quality.
- **Product quality:** By using technologies, it helps to decrease the risk of mistakes and promotes data collection. It helps to collect various data and standardise it. An alarm rings once the quality fails to fall under the range automatically.
- **Control:** digitalization aids in the control of the manufacturing process and the regularisation of high-quality products. Helps monitor the entire process.

2. Uses of internet in manufacturing plants

- **Preventive maintenance:** it can able to detect equipment problems and act rapidly in urgent circumstances by examining the data collected over time, algorithms may be created using the machine learning process. It makes decision on correct time.
- **Unified factory:** it helps to monitor and control the whole factory at any place as the whole factory connected through internet.
- **Connected mine:** personal safety equipments are all connected in mining operations and vehicle

- 3. Pharmaceutical supply chain:** The manufacturing, supply, distribution, and sales of necessary pharmaceutical goods are delivered to the end users at the proper location and time through the pharmaceutical supply chain, which is made up of a network of internal and external stakeholders and their connections. To optimise revenue and customer satisfaction, the pharmaceutical supply chain includes efficient management of financial, information, and material movement across network components.

There are many different digitalization methods, which include

- remote monitoring of production and distribution processes in real time,
- safeguarding production blueprints and utilising a secure supply chain channel,
- late-stage customization to reduce turnaround times based on market demand
- Using AI for more productive and cost-effective manufacturing, as well as blockchain to increase technology security.

Uses of digitalization in supply chains

- Information may be accessed anywhere in real-time by storing content and data in a controlled cloud repository in an electronic format.
- It helps in maintaining risk management, which includes four stages that are identification, prioritization, management, and monitoring of risk.
- It helps to maintain the cold temperature of delivery products.
- The good supply chain prevents the shortage of pharmaceutical products from reaching the market.

- 4. Digital supply chain:** The digital supply chain has been described as a smart, customer-focused, system-integrated, globally linked, and data-driven mechanism that makes use of new technology to produce useful products and more easily available and reasonably priced services¹³. The digital supply chain is a component of Industry 4.0 that assists enterprises in connecting environments within their functional areas. The digital supply chain provides new networked business systems that go beyond isolated, local, and single-company applications to supply chain-wide systematic and intelligent implementations. The main aim of the digital chain is to maintain the client's demand and supply with good quality .

There are three types of digital supply chain models:

- **First model:** It is based on the establishment of digitally integrated supply chain eco system. It provides transparency, flexibility, communication.
- **Second model:** It implements usage of virtual supply chain control tools, integrated supply chain, cloud computing and various digital tools like sensors, radio frequency, barcode, etc.
- **Third model:** It implements modern self-thinking software, AI reduces the cost and wastage, regulates the flow of product and supply by using digital supply chain.^{15,16}

- 5. Digital enablers:** Digital enablers are tools like IoT, AI, cloud computing and BDA which helps to promote the data and information collection from various sources and area. These tools are backbone of digital supply chain.

- **IoT:** The IoT (Internet of things) are smart devices which linked through sensors and internet. The IoT application, like cold chain monitoring, packaging, resources (man and machine), tracking and warehouse management helps to manage supply chains. The IoT integrates the data using radio frequency identification, mobile apps, wired wireless sensors, and machine to machine system that allow decision making in supply chain. By integrating sensors on tracking device with automatic start and stop mechanisms in warehouses, trucks which assist pharmaceutical producers in monitoring and maintaining cold chain conditions in real-time using smartphones and tablets. The data given by IoT models are vaccine carrier condition, location and temperature alert, etc.
- **AI:** AI play a vital role in digital supply chain in maintenance of factory as well as supply chain. It has the ability to solve issues independently using programs which includes deep learning, machine learning, computer vision and supervised learning ¹⁷.

The algorithms and database of AI provides:

- Obtaining 100 percent accurate prediction and forecasting of consumer demand,
- Optimising R&D by raising quality and lowering costs,
- Identifying proper customers
- Providing satisfaction to consumers.

- 6. Cloud-based supply chain (Cloud computing):** Cloud computing provides computing, storage and delivers at less cost with short lead time and less cost. The basis of business processes is Cloud SCM, which uses GPS installed in trucks to continually update predicted arrival and departure times as well as the actual time of departure. Correct forecasting of the raw material availability is possible, as is the updating of production information regarding planning, work-in-progress, completion, and shipment verification of the finished product to the partners ¹⁶.

IV. DIGITALIZATION IN COMMUNITY AND HOSPITAL PHARMACY USES OF COMPUTERS IN RETAIL PHARMACY

Community pharmacists use computers for a variety of tasks. A few accounting tasks are creating a medication label, generating a paper copy receipt for the patient copy the transaction history, billing the cost of a prescription, automatically ordering the cheap medications using electronic transitions, a large number of items annual withholding payroll preparation, making sales estimation, inventory control ¹⁸. There are multinational data banks used for information collection, which Drug bank, MEDLARS (Medical Literature Analysis and Retrieval System), includes World standard drug database and DIALOG.

- 1. Digital pharmacy:** Digital revolution has led to the rise of online pharmacies. Digital pharmacies provide increased access for the drugs with limited mobility to the consumers, reduced transaction and product costs, convenience and less time consuming ¹⁹. Most of the leading online pharmacies provide their consumers with extra discounts and medical alerts like personalized medicine purchase reminder (Fig.2). These online pharmacies also

provide complete information about the drugs along with their actions and side effects to their consumers which can help them to gain the required information of the products²⁰.

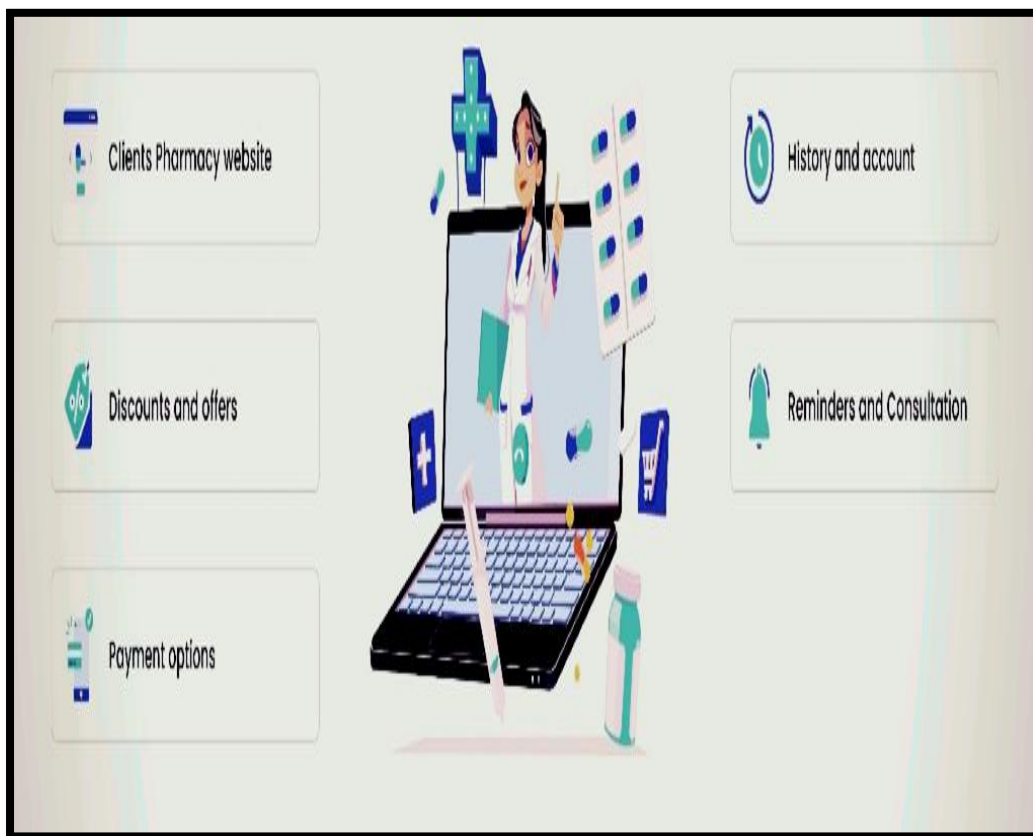


Figure 2: Features of Online pharmacy website

- 2. Clinical and hospital pharmacy:** Hospital pharmacy is a department of the hospital which regulates distribution of drugs, medicines, and professional supplies, stores them, and dispenses them to inpatients and outpatients. It may also have a manufacturing extension that produces pharmaceuticals and parenteral in large quantities. In hospitals, maintaining patient records is an important step, but with the use of computers, data can be simply preserved and regularly updated. Computers are used for inventory control²¹. Computers may be used by clinical pharmacists to monitor therapeutic drugs outcomes, especially narrow therapeutic index and high potency, such as anticonvulsants and cardiac glycosides. Drug-drug interaction can be identified by MEDIPHOR and PAD.
- 3. ADR management:** Analysis of adverse drug events can be aided by the creation of a computerised collection of post-marketing voluntary adverse drug event report. In order to ensure efficient data analysis and decision-making, the pharmaceutical industry and drug regulatory agencies have started building a computerised repository of premarketing and post-marketing clinical trial data^{22,23}. This effort eventually led to the implementation of new softwares for assessing and monitoring adverse drug events. A number of databases were created using computers, including spontaneous reporting systems and adverse event reporting systems for coding are programmed using COSTART, that include MeDRA.

V. DIGITALIZATION IN CLINICAL TRIAL

Pharmaceutical manufacturers, Contract Research Organizations use IoT for producing new drug molecule in quick period of time with less investment. The data collected are stored in cloud that provides better understanding in research. Clinical trial companies can remotely monitor patients thanks to the convergence of medical equipment and IoT networks. Various factors, including body temperature, hydration, sleep patterns, and Other everyday activities are passively and actively gathered from the subjects²⁴.

Clinical trial companies can remotely monitor patients thanks to the convergence of medical equipment and IoT networks. Various factors, including body temperature, hydration, sleep patterns, and Other everyday activities are passively and actively gathered from the subjects. This approach information conveyance is efficient. Oracle clinical V4i from Oracle Corporation., Trial master from Omni-comm system can be used for this purpose.

VI. CONCLUSION

Digitalization is always a challenging task in any health care system. Pharma sector being a crucial part in the health care system, is no exception to this. Like a coin has two sides, digitalization has its own challenges and drawbacks. The major challenges faced in the digitalization of pharmacy sector involve a very huge investment in bringing out the automated systems to operate in an effective way. Another major challenge in digitalization of pharma sector is the demand for uninterrupted functioning. Finally, not all the pharmacists/health care workers are willing to adopt these digital technologies and they prefer to traditional methods. These challenges should be taken into consideration and the importance of digitalization in pharma sector should be educated to the upcoming younger generation in-order to meet the increasing demand for medicine day by day.

LIST OF ABBREVIATIONS

AI	Artificial Intelligence
QSAR	Quantitative Structural Activity Relationship
ADR	Adverse Drug Reactions
LDA	Linear Discriminant Analysis
SVMs	Support Vector Machines
RFDNNs	Radio Frequency Deep Neural Networks
ADMET	Absorption, Distribution, Metabolism, Excretion and Toxicology
ANN	Artificial Neural Network
PLS	Partial Least Square
SEA	Similarity Ensemble Approach
IoT	Internet of things
BDA	Big Data Analytics
R&D	Research and Development
SCM	Software Change Management
GPS	Global Positioning System
MEDLARS	Medical Literature Analysis and Retrieval System

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