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## **A review on digitalization on pharmacological experiment**

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### **Abstract**

Pharmacology is primarily concerned with clinical pharmacokinetics and pharmacodynamics, yet as pharmacological mechanisms. Ostwald Schmiedeberg, the "Father of Pharmacology" within the 19th century. The pharmaceutical industry must embrace variety of technologies, like 3D printing, precision medicine, or patient design, silico trials, animal testing, and side impacts on human and animal participants. Three differing kinds of exploration patterns are proposed: hypothetical, methodical, and even-minded. Growing the archive concept, reengineering abstracting, and planning interdisciplinary models are hypothetical requirements. Digital transformation has shifted projects during a type of industries. Encourage pharmaceutical companies to seem for a brand new strategy to deal with computerised benefits that are currently available. Projects in a very range of industries are changed because of digital transformation. Encourage pharmaceutical businesses to develop a replacement strategy for managing currently accessible computerised benefits. Increased usage of robots, automation solutions, and computerization are all a part of the digitalization process, which allows for cost savings, increased efficiency and production, and greater adaptability to vary. The healthcare industry is being transformed by digitalisation. The pharmaceutical sector, being an important component of healthcare, isn't any exception. Pharma businesses are already using new technology and innovations to enhance pharmaceutical development and patient care. More data on pharmaceutical efficacy and improved quality of life for patients is being demanded by healthcare payers and other pharma consumers. For building and operating large-scale system-level pharmacology models utilised within the drug development process, a spread of software tools are available. Scientists is also obliged to use many modelling tools, looking on the challenge, which could raise model project duration, IT costs, etc. As a result, having one platform that permits for the setup and execution of large-scale simulations for models created using various modelling tools is very important.

**Keywords:** pharmacy, pharmacology, P kinetics, P dynamics, digitalization, softwares, pharma industry, GMP, FDA, 3D printing

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### **Introduction**

Pharmaceutical Science is a discipline of science that includes a variety of scientific areas that deal with different elements of pharmaceutical ingredients used in the production of therapeutic products. Pharmaceutical Science is thus the scientific foundation for understanding the physical, chemical, biological, and biomedical aspects of drug characteristics and activities.

The digital shift has already begun. Technology is being used by businesses across all industries to change and improve how they operate and serve their customers. Pharmacy is no exception. As businesses discover different ways to operate in the wake of the pandemic, technology has risen to the fore. There was a pressing need to stay officially open, but from afar. The move was far easier for individuals who already had a digital presence than for all those who have to start from zero. The term "digitalisation" can refer to a number of different topics. It could be a shift in how you manage client records, how you supply products and services, or how you actually contribute to your end users. It can assist you in being more efficient and identifying new opportunities to generate more revenue for your location.

### **Literature Review**

#### **Digitalization In Pharma**

Digitalization has evolved into an integral part of everyday life. Every segment has been adapting to the digital time frame at a faster rate. Apart from the website, the pharmaceutical industry hasn't exactly been able to embrace modern advertising. More pharmaceutical companies are using internet-based living destinations or web-based business locales as a computerised advertising platform these days. This allows customers to purchase products online. A few organisations are attempting to appreciate the true worth of advanced, while others are incorporating it into a larger advertising system. However, none of the organisations can sell their products online because they manufacture physician-recommended pharmaceuticals that cannot be marketed online. There are a few companies that are quite innovative when it comes to computerised development, but the lack of excellent contextual assessments of digitalization in the pharmaceutical industry limits its use. The Pharmaceutical industry isn't particularly well-versed in web promoting. While marketers in financing, proficient

administrations, assembling, and business administrations have raced ahead online, the medicines division has been held back by the part's apprehensive conduct, which is coupled with doubtful direction. However, online specialist and patient groups have emerged to accommodate patients' increased use of mobile, web-based living, and online data.

However, the pharmaceutical industry (PI) has been resistive to digitization, thanks to a scarcity of experience and also the complexity of the event and manufacturing procedures involved. Despite this, there's a particular must digitalize PI, as demand for both traditional and novel pharmaceuticals continues to rise. CDMOs (Contract Development Manufacturing Organizations) have a singular digitalization problem. The first features of excellent Manufacturing Practice (GMP) should be closely linked to PI digitalization, and CDMO specifically, and success in PI digitalization necessitates an even target GMP. Basic concepts of fine Manufacturing Practice (GMP) in Pharmaceutical Industries also are covered and discussed, as GMP may be a critical component of business digitalization deployment. Another key thing to think about during CDMO digitalization is close communication with continually changing stakeholders. This text provides an outline of the key components of CDMO digitization and covers both the advantages and downsides of the method, with a spotlight on practical solutions for further digital implementation.

Life sciences firms that embrace the shape of digital transformation can improve patient care while also offering care at a lower cost. Digitalization will have far-reaching consequences, destroying traditional value chains and dismantling existing organisations. In consequence, the industry are going to be shifting faraway from a revenue model supported generating blockbuster pharmaceuticals and toward one supported a technology ecosystem.

### **Benefits of Digitization in Pharmacy**

Focusing on digitizing pharmacy can create a variety of advantages, including :

- The opportunity to provide more customised service to clients online, in real time, and outside of regular store hours
- Creating extra sources for your location (online sales, selling new product lines, online exclusive items and services)
- Positioning your pharmacy to compete with big box retailers, pharmacy chains, and local grocers
- Providing your clientele with better overall value

### **Examples of Digitization in Pharmacy**

There is a long list of innovative ways you can digitize your pharmacy:

- Customer portals so they can manage their personal information
- Online prescription renewal
- Selling products online
- Online chat and wellness advice
- Informational blogs and email newsletters to inform your customer base about health tips and current news in the medical field.
- Mobile apps
- Online appointment booking for wellness checks
- Home delivery and curbside pickup coordination
- Patient design
- Silico Experiments
- New Technologies Pharmaceuticals
- New Business Strategies

### **Silico experiments**

The combination of current computing technologies with mathematical or theoretical characterizations of cancer cell biology, known as "in silico experimentation," is an unique approach to guiding the beginning stages of hypothesis development and experimental design that has the possibilities to save time and money in the lab. This computational approach is helpful because it allows for the implementation of large numbers of experiments that may be seen at any degree of detail and repeated and manipulated at will.

It's tough to dispute that preclinical cancer biology research is costly. Such studies incorporating in vitro and in vivo animal tests entail hypothesis creation and testing to find out whether additional trials are necessary, and they are exceedingly time and money consuming for researchers. Laboratory setup, equipment, and space, as well as the time, equipment, and materials costs needed in continuous, hands-on experimental work, all contribute to the expenditure of laboratory-based experimental research. In silico experiments can be used to guide the creation of more defined hypotheses and experimental research as a precursor to, or in conjunction with, preclinical experimental studies. Basic data such as toxicity, pharmacokinetics, and efficacy can be determined via in silico and mathematical modelling, which can subsequently be used to drive preclinical and clinical investigations.

To develop biological models, in silico experimentation combines biological data and expert opinion with numerical and software representations. These models can then be used to conduct computer-based studies instead of or in addition to laboratory research. It is possible to build what are basically "computational patients" to experiment on by using parameter distributions based on current expert opinion ("fuzzy" inputs) or biological

data (random variables) as inputs into in silico models. Smaller-scale and even multiscale investigations on the molecular, cellular, and tissue/organ levels are also possibilities. Appropriate application of in silico models entails creating assumptions based on experimental data and specialized knowledge, allowing the models to be utilised to effectively advise clinical trials with the goal of lowering costs and boosting efficiency.

### Patient design or digital medical

- Academic researchers and clinical trial sponsors, both of whom require the facilitation of internal team conversations (e.g., data science teams working with protocol designers in the translational medicine teams).
- Clinicians, who will be introduced to digital medication in their practise on a more regular basis.
- Patients, who, as medicine becomes more individualised and consumer-oriented, we expect will be more in charge of their own care.

Projects like an open-source DIY artificial pancreas, discussion boards, and cloud-based solutions like Tidepool have sprung up as a result of this trend, making diabetic research more accessible and actionable. In response to patient demand, the FDA approved the first artificial pancreas two years after the DIY artificial pancreas was made widely available. In order to better incorporate patient input, the FDA formed its own patient engagement advisory council. The FDA must be followed by pharmaceutical businesses. As seen by the rise of DIY medicine initiatives, people want their voices heard when it comes to making medicine more accessible and inexpensive.

### New digital technologies in pharma

Let's look at how digital transformation can reorganize the pharmaceutical sector in marketing strategy after we've gone through the meaning of the term. Anything from direct-to-consumer advertising (DTCA) to larger medical marketing could benefit from a digital transformation. However, it must fulfil unique, specified aims in addition to be significant, as stated previously. The recent changes in the digital marketing landscape require creativity in this regard. Take a look at the following instances from among them: According to studies, consumers favour brands that support social concerns.

### Future Ecosystem in Digitalization in Pharmacy

Following are trends of digitalization in pharma sciences:



Fig 1

#### Drug dose adjustment

Doses will be tailored to each patient's needs based on their stage of disease and personal characteristics.

#### Drug impact monitoring

The medication is monitored in real time to provide ad hoc feedback.

#### Healthcare tree

A lifetime health report that includes all treatments. Its representation will incorporate the origin as the background and reasons of illness and disease, allowing therapy and prevention to be more personalised.

**Smart pharma hub**

A smart medication production hub that uses robotics and 3D printing to create tailored pharmaceuticals.

**Individualized drug printing**

Ad hoc printing of each patient's modified medicine dose.

**Medical prescription agent**

Prescription and drug dose are handled by a smart, technological agent.

**Bioprinting**

Bioprinting, like 3D printing, is an additive manufacturing technology that employs a digital version as a blueprint to print a layer - by - layer. Bioprinters, unlike 3D printers, use cells and biomaterials to create organ-like structures that allow living cells to reproduce. Human livers, kidneys, and hearts are being bioprinted at laboratories and research institutes.

**Health data clearance**

All of a patient's data will be contained in private medical health records, so data security in decentralised blockchain ecosystems is paramount.

**Preventive therapy**

Therapy will be possible even before medicine is required, thanks to the identification of health history and personal health consultancy support.

**Experimental Pharmacology**

Experimental pharmacology is the first phase in developing novel drugs. It is the process of investigating the pharmacological activities of previously created drugs using both preclinical and clinical study methodologies in a stepwise manner. At get to a chemical that is both safe and effective, as well as display the intended pharmacological quality or behaviour, it is necessary to go through a number of important steps in the drug discovery and development process. However, in the 1st phase of experimental pharmacology, investigations are frequently completed with an assumption hypothesis that has not been adequately validated by scientific evidence. It is usually carried out in a biomedical laboratory setting, where in vitro and in vivo study approaches are possible.

An in vitro experimental research is a test that takes place outside of a living creature in a test tube, culture plate, or other container to examine the biological properties of test material. In vitro investigations are significant because they enable for faster discovery of new treatments because numerous medications can be tested at once (and in a large number of cell samples), with only those that look to be effective moving forward to human trials. One of the major limitations of in vitro investigations is the lack of biokinetics (how the body distributes and metabolises medications and toxins). This, along with a number of other considerations, can make extrapolating the results of in vitro experiments to what might be assumed when the medicine is taken in vivo extremely challenging.

An in vivo experimental study differs from an in vitro study in that it is conducted within a living creature to evaluate the pharmacological properties of test material. In vivo tests are frequently performed before in vitro tests to identify the toxicity of test material, and both studies are critical in the drug development process. In vivo investigations are critical for drug development because they allow researchers to assess a drug's properties, including physiological and biochemical processes like side effects and drug-drug interactions, which are difficult to see in vitro.

In experimental pharmacology, many kinds of laboratory animals are employed to study the dose–biological response connection and the pharmacokinetics of various test compounds. Mice, rats, Guinea pigs, and rabbits are the most commonly employed laboratory animals.

**Pharmacological animal experiments involve**

Pure Research = Behavioural, Developmental, Functional

Applied Research = Specific Activity

Xenotransplantation = Transplant of tissue or organ from one species to other

Toxicological studies = Safety studies

**Softwares in pharmacological Expt**

The development and deployment of mechanistic, systems-level models to aid decision making has increased in recent years in pharmaceutical R&D. These models perform better than more traditional and empirical pharmacokinetic/pharmacodynamics (PK/PD) models at describing disease biology and therapeutic pharmacology. They're sometimes referred to as quantitative systems pharmacology (QSP) models to separate them from other systems biology models that don't include medication pharmacology or pharmacokinetics, and don't always account for disease biology and progression. QSP models have a substantially higher no. of

equations and parameters than typical PK/PD models due to their extensive description of physiology and pharmacology.

### **Following are Some of the Softwares**

#### **Ex-Pharm pro**

This is a computer-assisted learning (CAL) tool that includes several modules that imitate animal trials in pharmacology. These applications can also be used to show how medications affect various animal systems..

These software carries experimental studies such as:

- Various devices are used to investigate analgesic activity.
- Activity that relaxes the muscles.
- Research on drugs that affect the central nervous system.
- Anticonvulsant properties.
- Tests on thyroid and antithyroid medications
- Research into pupil control stimulation.
- Drug effects on the ileum of guinea pigs.
- Experiment with your blood sugar levels.
- A metabolic cage was used to investigate diuretic action.

#### **ViPS**

##### **Details about ViSP, as well as its use to the MDSP model.**

The MDSP mathematical model was created to mechanistically characterise the fundamental physiological and pathological mechanisms involved in T2DM. It depicts key systems and pathways that regulate glucose and lipid metabolism, as well as pathophysiological alterations associated with T2DM and the PKPD effects of several antidiabetic medications. The model's core mimics nutrient intake and digestion, as well as their distribution and usage by various human tissues and organs. The nutrients are delivered in the form of meals (up to three per day) with a specified percentage of carbohydrates, lipids, and proteins, as well as a specific calorie intake. The nutrients are absorbed into the blood via the gastrointestinal tract, and the model follows glucose and lipid metabolism in the brain, liver, muscle, and adipose tissue.

The Explorer is the first of several key user-interface components in the ViSP programme. It arranges the models and data of users in a tree-like hierarchical structure, with projects at the top. A ViSP project normally contains all information about simulation tasks that are relevant to the research issue. Each project can include one or more models, such as distinct versions developed during the model development process. Every time a new model is developed, it is characterized by an executable file that is posted into the ViSP databases.. A text file containing a list of model input data and their baseline values is included with the programme. Every model can be linked to one or more user interfaces (UIs) that are tailored to specific project requirements or user preferences. The next level of the hierarchy contains groupings of parameters that are subgroups of input parameters as defined in the Methods. Each group may also have various value sets, which could represent settings for different treatment regimens, for example. The model, data, and results are all kept in a database, which makes handling the model, data, and results much easier.

#### **Lt**

The Lt's Pharmacology Collection includes professionally produced lectures and labs that investigate ligand-receptor binding and dose-response connections in a variety of tissue preparations. Use a variety of medication and tissue preparations to engage your students in hands-on experiments examining dose-response relationships and ideas in ligand-receptor binding.

These programmes aid in the study, comprehension, or acquisition of additional knowledge about the mammalian heart, uterus, cervix, airway resistance, and other topics.

#### **Pharmavirtua**

Information and communication technologies are now key teaching aids for both descriptive and nondescriptive sciences like anatomy and histology. In the biological and health sciences, software has been utilised to aid in the learning of certain ideas at the molecular and cellular levels. Although instructional software, virtual environments, and e-learning are not new, their applications have grown to include more sophisticated fields of science and higher degrees of education. Despite the abundance of pharmacological software available on the internet, few of these applications have been pedagogically reviewed. Developing educational software differs significantly from non-educational programs, such as business applications. Educational software must be built to make learning easier for users who may not be familiar with the material being studied. In this regard, our group created "PHARMAVIRTUA," a Creative Commons-licensed software suite aimed at assisting pharmacology teachers by encouraging active and engaged student learning.

The PHARMAVIRTUA academic software programme was evaluated for its utility in teaching and learning fundamental pharmacology in this study. PHARMAVIRTUA was founded in the discipline of pharmacology with an emphasis on pharmacokinetics and pharmacodynamics, where they thought to be key ideas in the field.

### **CAL**

Previous research has suggested that some students chose traditional laboratory-based experiments to CAL simulations and vice - versa, so an experiment was conducted to see whether any factors influenced students' perspectives. The unpredictability in tissue response is a well-known concern when doing tissue-based research. The speed at which the preparation is developed in the organ is at least partially responsible for tissue variability. Langedroff Heart, Neuromuscular Pharmacology, Autonomic and Respiratory Pharmacology, and other topics are studied here.

### **Abbreviations**

**CDMO** = Contract Development Manufacture Organizations

**GMP** = Good Manufacturing Practices

**PI** = Pharmaceutical industry

**PK** = Pharmacokinetic

**PD** = Pharmacodynamic

**QSP** = Quantitative System Pharmacology

**CAL** = Computer Assisted Learning

**CNS** = Central Nervous System

**ViSP** = Virtual Systems Pharmacology

**MDSP** = Metabolic Diseases Systems Pharmacology

**T2DM** = Type 2 Diabetes Mellitus

**UI** = User Interfaces

**DTCA** = Direct-to-Consumer Advertising

**FDA** = Food and Drug Administration

### **Conclusion**

The pharmaceutical industry must embrace a number of technologies, such as 3D printing, precision medicine, or patient design, silico trials, animal testing, and side effects on human and animal participants. In August 2015, the FDA authorised a 3D-printed medicine product, signalling the start of a new era in pharmaceutical production. Three patterns of exploration are proposed: hypothetical, methodical, and even-minded. Digital transformation has shifted strategies in a variety of industries. Encourage pharmaceutical companies to look for a new strategy to deal with computerised benefits that are currently available. Any manufacturing industry's digitalization is an important phase in the production process. Higher usage of robots, automation solutions, and computerization are all part of the digitalization process, which allows for cost savings, increased efficiency and production, and greater adaptability to change. The healthcare industry is being transformed by digitalisation. Pharma businesses are already using new technology and innovations to improve pharmaceutical development and patient care. More data on pharmaceutical efficacy and enhanced quality of life for patients is being demanded by health insurers and other pharma clients. For building and operating large-scale system-level pharmacology models utilised in the drug development process, a variety of software tools are available. Following that, other data including such patient longitudinally, medical claims, electronic health record, social data, and patient services will be incorporated. As a result, having a single platform that enables for the setup and execution of large-scale simulations for models created using various modelling tools is important. Pharmaceutical businesses can no longer rely solely on personal interactions with healthcare professionals and clinics to earn revenue. Rather, they have to use digital measures to get in touch with healthcare professionals.

### **References**

1. Abou-El-Enein M, Römhild A, Kaiser D, Beier C, Bauer G, Volk HD, *et al.* Good Manufacturing Practices (GMP.) manufacturing of advanced therapy medicinal products: a novel tailored model for optimizing performance and estimating costs *Cytotherapy*,2013;15(3):362-383
2. Alagarsamy S, Kandasamy R, Subbiah L, Palanisamy S. Applications of Internet of Things in Pharmaceutical Industry, 2019. Available at SSRN 3441099s3)
3. Awad A, Trenfield SJ, Gaisford S, Basit AW. 3D printed medicines: a new branch of digital healthcare *Int. J. Pharm.*,2018;548(1):586-596
4. Awad A, Trenfield SJ, Goyanes A, Gaisford S, Basit AW Reshaping drug development using 3D printing *Drug Discov. Today*,2018;23(8):1547-1555
5. DeFronzo RA. Pharmacologic therapy for type 2 diabetes mellitus. *Ann. Intern. Med.*,1999;131:281-303. 10.7326/0003-4819-131-4-199908170-00008
6. www. <https://www.adinstruments.com/lt/pharmacology>
7. www. <https://norecopa.no/norina/expharm-pro>
8. www. <https://journals.physiology.org/doi/full/10.1152/advan.00033.2014>
9. www. <https://www.ncbi.nlm.nih.gov/pmc/articles/PMC4205926/>