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ORİJİNAL ARAŞTIRMA / *Original Research*

Eczacılık, Eczacılık Bilimleri ve İlgili Alanlarda Yapay Zekâ Uygulamalarının Kullanımı

Usage of Artificial Intelligence Applications in Pharmacy, Pharmaceutical Science and its Related Fields

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Öz

Teknolojinin gelişmesi ile birlikte değişen meslek şartları, her meslek için yeni tanımlamalar gerektirmiştir. Eczacılık, birçok farklı alanı barındıran multidisipliner çalışmaların mümkün olduğu bir alandır. İlk defa 1960'ta tıptan ayrı bir meslek olarak tanımlanan eczacılık mesleği, 1960'tan sonraki her dönemde, çağın gerektirdiği değişikliklere uğramıştır. Majistral ilaçların hazırlandığı eczane laboratuvarları, müstahzar ilaç sayısının artması, ilaç takip sistemi ve Medula sisteminin eczanelere entegre edilmesi gibi örnekler, eczacılık hizmetinin bulunduğu çağa uymasının bir sonucu olarak yorumlanabilir. Günümüzde, teknolojinin getirdiği değişim zorunluluğu da göz önüne alınınca, hiçbir eczacılık hizmeti teknolojiden bağımsız düşünülememektedir. Eczacılığın neredeyse her alanında yapay zekâ algoritmaları kullanılabilir. Akılcı ilaç kullanımında, hastane eczanesinde, serbest eczanelerde, ilaç geliştirilmesinde ve üretilmesinde kullanılan yapay zekâ uygulamaları bilinmektedir. Bu çalışmanın amacı; güncel veriler ve literatür ışığında, eczacının sorumluluklarını ve eczacılık uygulamalarını genel olarak değerlendirmek; yapay zekâyı ve yapay zekânın özelliklerini açıklayarak eczacılık alanında kullanılan yapay zekâ uygulamalarına örnekler sunmaktır.

Anahtar Kelimeler: *Eczacılık, Akılcı ilaç kullanımı, İlaç üretimi, Yapay zekâ, Eczacı*

Abstract

The occupational conditions have been changing with the technology development in each of the profession. Pharmaceutical Science is a field which diverse perspectives are possible with multidisciplinary studies in many of the subjects. Pharmacy profession, which was defined as a separate profession from medicine since 1960 and has undergone changes required by the age in every period after 1960. Examples such as pharmacy laboratories where magistral medicines were prepared; from there an increase in the number of official drugs, arise of the drug tracking system and the integration of the Medula system into pharmacies can be interpreted as a result of the pharmacy service's adaptation to the era. Nowadays, considering the necessity of change brought by technology, no pharmaceutical service can be considered as an independent of technology. Artificial intelligence algorithms have been using in every field of pharmaceutical science. Artificial intelligence applications are used in rational drug use, hospital pharmacy, community pharmacy, drug development and production. The aim of this review is; To evaluate the pharmacist's responsibilities and pharmacy practices in general in the light of current data and literature to explain artificial intelligence and its properties whit current examples of artificial intelligence applications using in pharmaceutical science.

Key Words: *Pharmaceutical Science, Rational drug use, Pharmaceutical production, Artificial intelligence, Pharmacist*

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Introduction

Today, technology is very important in pharmaceutical science as in every profession and in every field of science. Technology is used in almost every field of pharmaceutical science. In some fields of pharmaceutical science, the importance of technology and the opportunities provided by technology are more from others:

- Rational drug use,
- Treatment, drug, and vaccine development studies,
- Pharmacy services,
- Hospital pharmacy,
- Patient data collection and storage (1-3).

In this review article, the concepts of pharmaceutical science and artificial intelligence are explained, and artificial intelligence applications used in pharmaceutical science have been reviewed. Among the duties and responsibilities of pharmacists, those related to technology were discussed. The advantages and disadvantages of using artificial intelligence applications in pharmaceutical science were discussed.

Duties and responsibilities of pharmacists

A pharmacist is a person who has successfully completed 4-8 years of education, which varies according to countries, knows the pathways art of drug preparation and presentation, and can train the patient for drug use (4). Generally, pharmacies are the last place patients stop by before using the drug, and therefore the pharmacists is the last person they consult before using the drug. Members of this critical profession, pharmacists, have duties and responsibilities towards medicine, patients and society. The duties and responsibilities of pharmacists are given in Table 1 (4-6). Some parts of this table can be improved and modified using technology. It is important to benefit from technology in issues that cause worldwide problems, deaths, and high costs, such as rational drug use.

Artificial intelligence (AI)

AI systems can be considered simply as a two-stage system: In the first stage, it understands the thinking and decisionmaking mechanism of the human mind; In the second stage, it repeats these mechanisms autonomously. The definition of the concept of artificial intelligence is defined as "Digital technology and/or applications that have the ability to imitate human beings, interact, learn, adapt and apply by expanding their experience" (7). The concept of AI was brought to the agenda for the first time by Turing in the 1950s and the possibility of a machine to think like a human is philosophically discussed (8).

AI algorithms have the ability to understand experiences, evaluate the results, and identifies the similarities between different situations (9). In the literature review, it was seen that different subcategories were used together with the concept of AI. AI can be examined under three subcategories; Rule-based AI (Expert Systems, Decision Support Systems, etc.), Decision-maker AI (Genetic Algorithm Code, Text Mining, etc.), and Learning AI (Artificial Neural Networks, Deep Learning, etc.) (10-12). The explanations and details of the sub categorization of AI are given in Table 2 (12-20).

Artificial intelligence applications in pharmaceutical science

1. Artificial intelligence in rational drug use

According to the definition of the World Health Organization (WHO), rational drug use is a set of rules that enable patients to take drugs in accordance with their clinical needs, in doses to meet their personal needs, in sufficient time, and at the lowest cost to themselves and to the society (6). This definition is put into practice in the form of the right medicine, the right dose, the right time, the right patient, the appropriate cost, the right follow-up, the right information, and the documentation (4).

Advice on rational drug use is generally obtained from healthcare professionals in Turkey. However, sometimes due to lack of time, sometimes due to excessive intensity, healthcare professional may not be able to make the necessary warnings. The use of AI algorithms can contribute to rational drug use by helping healthcare professionals at this point.

· **Artificial intelligence applications in detecting interactions:**

Drug-drug and drug-nutrient interactions are very risky and can be fatal. In a study, death due to drug-drug interaction was detected in 6.7% of hospitalized patients. The cost of deaths due to undesirable effects to the USA is 136 billion dollars annually (21). Systems created by using ES and ANN have begun to use to prevent interactions. Expert systems can provide the following features:

1- Comparing the compatibility of drugs,
2- Active ingredient control,
3- Medication possible side effects control,
4- Drug-nutrient interaction control,
5- Examination of drug prospectuses,
6- Side effects and disease symptoms control (9).

These data, which are evaluated by expert systems, are presented to the user as information. If the patient enters the drugs to be used in the system, patient sees information that the active substances and nutrient interactions are evaluated by databases (9).

Supplement X is a project in the production stage by Pharmaino established in Turkey. Supplement X is the pharmacy kiosk system that will analyze the drugs people have used and the diseases they have by artificial intelligence and then make suggestions. The purpose of SupplementX is to ensure the rational use of supple-ments (22).

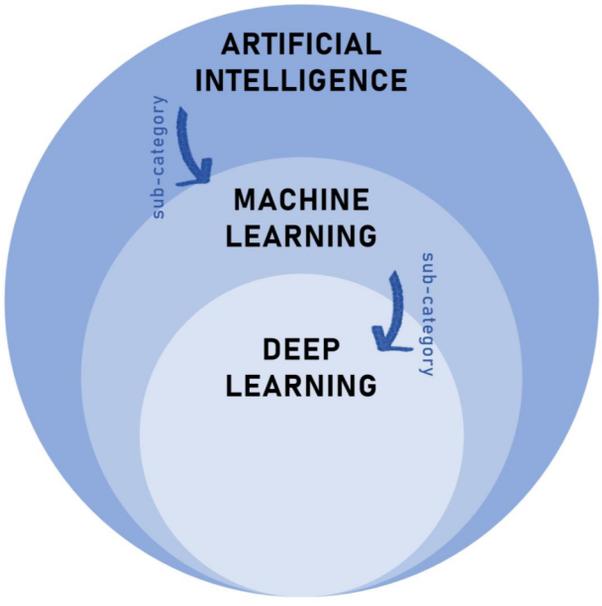

Figure 1. Artificial Intelligence, Machine Learning and Deep Learning Titles

· **Artificial intelligence applications in providing patient compliance:**

Patient compliance is to comply with what needs to be done for the treatment. Presence of compliance ensures maximum benefit from drug therapy. Communication between the doctor and pharmacists with the patient is very important. There is a direct relation between compliance and rational drug use (5).

Based in the United States of America (USA), the AiCure application works with an AI algorithm connected to the phone camera to check the accuracy of the medication used and the accuracy of the time used. The camera first recognizes the drug and then alerts the person by sending a notification when the time of use of the drug comes (23, 24). Thus, it helps the patient and the healthcare professional in the right time and the right medication titles. In another example, the interactions of drugs with other drugs are detected with the AI algorithm, helping healthcare professionals and preventing the patient from being harmed (9). Thus, the correct information is provided. In another example, through AI algorithms, the patient's information is processed, critical dose calculation is made, and healthcare professionals are supported to make more precise decisions on this issue (25). Thus, the correct dose will be provided.

SuperPharmacist is a mobile application in software stage designed by Pharmaino. It offers patients a personal treatment scheme with AI and enables patients to get the maximum efficiency from drugs (22).

· **Artificial intelligence applications in the rational use of antibiotics and antivirals:**

Unnecessary or incorrect use of antibiotics in Turkey as in other countries is a common problem. Misuse of antibiotics causes many health problems, especially resistance development (26). This problem has been recognized as a global risk by the WHO. AI was used for rational use of antibiotics and antivirals.

FluAI is a mobile application made by Yesil Science from Turkey. Users with symptoms such as throat ache and fever, after answering the questions, take a picture of their throat and upload it to the application. The photograph and the anamnesis given are evaluated by the artificial intelligence and tells the user that the infection is bacterial or viral over a percentage (27).

Researchers at Massachusetts Institute of Technology's (MIT) Computer Science and Artificial Intelligence Laboratory (CSAIL) announced that they developed a recommendation algorithm that predicts the likelihood that a patient's urinary tract infection will be treated with first or second-line antibiotics. It claims its models, trained with data from more than 10,000 patients, will allow clinicians to reduce second-line antibiotic use by 67 percent (28).

Using IDentif.AI, a team at the National University of Singapore identified combinations of antivirals that could be used in treatment of Covid-19 using AI algorithms. In the combinations, the combination of lopinavir/ritonavir was found to be relatively ineffective against Covid-19, while remdesivir alone was not found to be highly effective, it was found that taking lopinavir/ritonavir and remdesivir in combination inhibited the replication of the virus. Experiments have also supported these findings (29).

2. Treatment, drug, and vaccine development studies

Drug development and production is not an easy task. A pharmaceutical company can take as long as 12-14 years to develop a new drug, and it can cost up to $ 2.6 billion. One of the biggest advantages of AI is that it reduces the time required for drug development and in turn reduces the costs associated with drug develop-ment. A lot of research is being done to improve present AI technology to make the pharmacy profession more efficient (30).

Sanofi has signed an agreement to research the United Kingdom-based Exscientia's AI platform to research metabolic disease treatments, and Genentech is using an AI system created by GNS Healthcare in Cambridge, Massachusetts to help research cancer treatments. It appears that the largest biopharma companies go for similar collaborations (31).

According to a study, a library of small peptides with broad spectrum antibiotic activity was created and integrated with ANN. Thus, silico models representing antibiotic activity were created. When randomly generated samples

were examined, it was observed that the activity of peptides predicted by AI was very high. It has also been shown that the predicted peptides are highly effective against multiple superbugs which are multidrug resistant and have activities equal to or even better than the four of the most commonly used antibiotics. It was also observed to be effective against Staphylococcus aureus infections when tested in animal models (30).

Vaccine development is one of the most difficult parts of drug development. AI methods and systems biology approach have the potential to reduce failures while increasing efficiency and speeding up the development process (7). In 2020, humanity faced a pandemic that changed our lives and caused the death of many people. Governments and healthcare organizations are cons-tantly working to combat the disease. Many scientists benefit from AI, especially in the development of vaccines and antivirals. Artificial intelligence can help as an effective tool to study the virus and its capabilities, virulence, and genome. It can also help predict the protein structure of the virus and its interaction with other chemical compounds (32).

Manufactured by IBM with AI technology, the Watson computer is designed for oncologists to make better decisions in cancer treatment. It functions by analyzing a patient's medical information from a wide network of data and expertise, and then offering treatment options based on the evidence obtained (30). Watson is also used in researching oncology drugs, selecting the correct pharmacophore groups, and evaluating the three-dimensional structures of molecules (33).

University of California San Francisco (UCSF) Medical Center uses robotic technology integrated with AI for the preparation and follow-up of medicines to increase the safety of patients. It has been observed that the robot, which works with AI technology, prepares 3,5 millions drug doses without error (34).

The MEDi Pain Control Robot was developed as part of a project led by Tanya Beran, Professor of Community Health Sciences at the University of Calgary in Alberta. This robot first establishes a relationship with the children and then tells them what to expect during a medical procedure. Provides guidance on how to breathe and cope with their fears during the medical procedure. MEDi can speak 20 different languages by taking data of Google Translate (35).

BERG is a biotechnology-based pharmaceutical company that uses AI in drug discovery. The company uses artificial intelligence technology to find various biomarkers that cause disease, verify them, and then decide treatments based on the data obtained. The company's goal is to speed up the drug discovery process and achieve a cost reduction with the help of AI (30).

3. Artificial intelligence applications in pharmacy services

There are different machine learning algorithms created for prediction purpose. One of the biggest problems in the field of health is to evaluate all illnesses of the patient when a patient comes to the pharmacy. ML algorithms can be used to accurately predict diseases and the most appropriate medication for that disease. The pharmacist can provide the

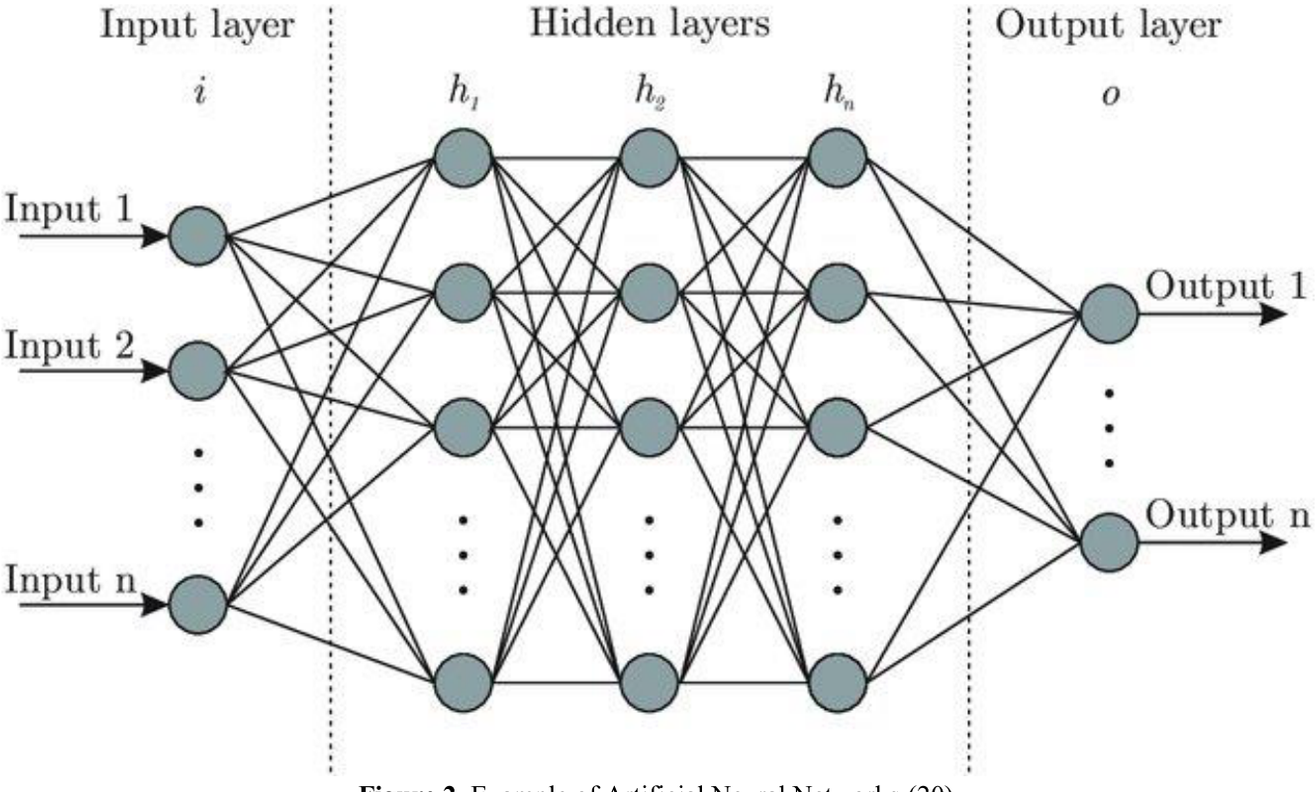

Figure 2. Example of Artificial Neural Networks (20)

effective medication to the patient with the help of machine learning prediction algorithms, instead of delivering the known drug. In addition, management can be achieved through ML algorithms in stock management (1).

Traditional pharmaceutical practices include categorizing medications manually, creating dosages, and tailoring medicines to patients' needs. Pharmacists spend a lot of time doing these tasks. The presence of robotic pharmacies in drug preparation is used to perform all these activities such as mixing, categorizing, and sealing drugs with minimal human intervention. There are automation systems in robotic pharmacies and systems such as ML, DL and Natural Language Processing (NLP) are used in this system according to the desired feature (36). The advantages of robotic and automation systems can be listed as follows (1):

- It is efficient. A pharmacy robot can fill and organize a large number of medications without any human intervention and without any mistakes. In addition to increasing the efficiency of operations, this also enables pharmacists to perform more value-added tasks.

- Creates an error-free environment for medical distribution. Human errors can be reduced with robots. "Once you program the robot to do the right thing, it always does the same thing over and over," says Rita Jew, UCSF Hospital Pharmacy Manager.

- It's safe. In a robotic pharmacy, medicines are securely stored in dispensing machines. With good security, the probability of drug theft or error is significantly reduced.

- There is a decrease in the waiting time of the patients. Robotic systems can meet thousands of prescriptions and fill desired drugs very quickly.

- It reduces risks in the sterile environment. Robotic pharmacies minimize microorganism contact in a sterile environment.

Robot Charlie, which is being used in some pharmacies in Germany, is involved in customer welcoming and sales. While hosting the customer, it communicates directly and directs it to the products on the shelves. It can give simple information and advice taught by its pharmacist. If the customer comes with a more complex problem or with a prescription, they can refer the person to the pharmacist or pharmacy staff. According to the feedback received from customers, the presence of Robot Charlie in the pharmacy makes customers and patients feel more comfortable (37). Robotic pharmacists can provide high efficiency in terms of workflow, reduce medication errors, provide drug delivery safety, minimize drug waste, and provide a sterile environment for the patient. On the other hand, it costs a lot and it can minimize human contact and needs to be updated frequently.

4. Artificial intelligence applications used in hospital pharmacy

· Data collection and processing

The digitalization of health and medicine, the increased availability of Electronic Health Records (EHRs) has encouraged healthcare professionals and clinical researchers to adopt the latest methodologies in the field of artificial intelligence to take advantage of the large medical databases available. More than 75% of hospital pharmacists in the USA use data mining functions to regularly document and collect patient-centered data. These include important information regarding drug safety, drug history, and therapeutic outcomes (2).

Patients' EHRs contain a large amount of valuable information, including drug history, adverse drug reactions, interactions, medication errors, and pharma-cokinetics. Results are achieved through a combination of NLP and machine learning techniques. The informa-tion processed by deep learning classification methods that are fed and learned from the large amount of data in the EHR is then structured by artificial neural networks. Thus, clinical pharmacists can easily use a large number of data for patients (2).

· Artificial intelligence in drug preparation and drug delivery methods in hospital pharmacies:

Robot pharmacists are used in the preparation of chemotherapy drugs in an oncology unit in a hospital in China. These robots can minimize pharmacists' exposure to cytotoxic drugs. It can prepare 10-15 bags of chemotherapy drug per hour (38).

United Arab Emirates (UAE) opened its first "robot pharmacy" at Rashid Hospital in Dubai. It is the first time a robot is being used in the UAE to dispense prescription drugs by clicking a button based on a barcode. This robot can store up to 35,000 drugs and can enter approxi-mately 12 prescriptions in less than a minute (38).

The University of Maryland Medical Center (UMMC) uses robotic technology to deliver medicines from pharmacies to patient care units. After the implemen-tation of the robotic delivery system, the time from fax to label, order preparation time and idle time of the drugs to be delivered decreased, while nurses' overall satisfac-tion with the pharmacy and the reliability of pharmacy delivery increased significantly (39).

Ethical Considerations

The advancement of technology in healthcare has many benefits, but there are some situations that need to be considered. Patient rights and ethics are a very important issue in the age of technology in health. Although the number of errors decreases, it is not possible to be zero. It should be determined who will be responsible in case of an error. When an error occurs, it should be investigated forensic. The responsible person should also be responsible for the

technology used in the errors accepted as malpractice. However, it is very difficult to detect technology-related problems. It is also debatable to what extent it would be possible or correct to take some strict measures in this regard (40). Another disadvantage is that patients do not adopt AI-based healthcare adequately. The patient should be able to choose the treatment from among the options. The decision should be made by the patient, even if there is guidance by the doctor about treatment. This situation will decrease as the usefulness of AI is proven.

Conclusion and discussion

It is estimated that the contribution of AI technolo-gies to the global economy between 2020 and 2030 will be 15 trillion US Dollars (41). Even if this estimate is approached, considerably high amounts will be invol-ved. Therefore, as Turkey, we should not fall behind, not depend on the outside, understand AI, and create our domestic and national AI algorithms.

Pharmaceutical science has developed considerably from past to present and continues to develop. It is possible to divide these periods as Pharmaceutics 1.0, Pharmaceutics 2.0 Pharmaceutics 3.0 and Pharmace-utics 4.0. Pharmaceutics 1.0 represents the use of herbal drugs for diseases, Pharmaceutics 2.0 represents the transition from the herbal period to the chemical production period, and Pharmaceutics 3.0 represents the use of an era-opening technology such as the internet in the field of pharmaceutics. Pharmaceutics 4.0 is a new concept, and it will develop the health technologies for future. As humanity know from the definition of Industry 4.0, disruptive technologies such as AI have begun to have a say in the industry. Today, machine-human cooperation in the industry can manage well. The concept of Pharmaceutics 4.0 has emerged with the use of destructive technologies in many stages from the production of drugs to their presentation to the patient. This concept continues today. Pharmacists who working in the period of Pharmaceutics 4.0 should have the competencies to fulfill the requirements of the age, that is, they should be closely interested in technology and use this technology to benefit their profession.

Using of different AI algorithms can contribute to different topics of the pharmaceutical science. However, pharmacists are essential for all topics at the same time.

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Table 1. Duties and Responsibilities of the Pharmacist

Title	**Explanation**
Providing Medication	Medications that must be available in the pharmacy must be kept in stock.
Reporting Drug Analysis	Analysis reports can be prepared in case of a problem regarding the content and/or formulation of drugs.
Pharmacovigilance Statements	The pharmacist is obliged to report when there are situations that need to be reported to Turkey Pharmacovigilance Center while monitoring the patient.
Medication Distribution	Medicines must be provided, stored, and presented under appropriate conditions.
Recommending Medication	Medication recommendations can be made if necessary ordered, in accordance with the needs and health status of the patient.
Patient Monitoring	It is necessary to follow up both the patient and the drug use in the long-term treatment of patients for the chronic diseases.
Cooperation with The Doctor	Communication is important to resolve prescription or patient-related problems.
Patient Care	Since the last person the patient speaks to before taking the drugs is usually a pharmacist, disease education, understanding of what the drugs are given and how they should be used are the most important factors that increase compliance in the treatment.
Patient Education	Pharmacists who gain the trust of patients on health-related issues should inform people periodically.
Reporting Drug Use Habits	Statistical analysis and evaluation of these data is the responsibility of the pharmacist. It is important for public health to keep regular records and to present them when requested by the relevant authorities.
Staff Education	The pharmacist carries out the task distribution of its staff and pharmacy faculty interns, supervises, and coordinates their work.

Table 2. Explanations and Details of the Subcategorization of AI

Rule Based AI	**Expert systems (ES)**	ES using AI algorithms on the basis of the decision mechanism are defined as "The information is ready to be processed or combined with the machine after it is processed" (13, 14). ES interpret the information obtained from experts using AI algorithms and output to non-experts. An ES includes four basic parts: database, exit mechanism, forward chaining mechanism and user interface (15).
Decision-maker AI	**Text Mining (TM)**	TM is defined as the discovery and extraction of new information from unstructured text (Kao & Poteet). Unlike computer-aided text analysis, which is widely used in this field, instead of extracting information based on word/term repetitions, TM usually makes use of other textual features such as grammar and uses natural language processing, computational linguistics, corpus linguistics, machine learning, and statistical techniques (16).
Learning AI	**Machine learning (ML)**	ML is an algorithm that provides self-learning and improvement with the results obtained from the presented data or based on previous solutions. It is based on mathematical and statistical results (12). It is aimed for machines to make inferences and make decisions by evaluating the data and experiences (17). There are multiple ways to teach a machine the desired information. These are: • *Supervised learning*: In this method, machines are trained using data containing targeted results. • *Unsupervised learning*: There is no need for an additional promotional tool in this method. The machine alone classifies by extracting meanings from the data. • *Reinforcement learning*: In this method, the concept of 'Agent' is available. The aim of the agent is to achieve the goal by experimenting with trial and error. With the gamification method, it learns by getting reward for correct moves and punishments for wrong moves.
	Deep learning (DL)	Deep learning is the sub-category of ML. The relationship between AI, ML, and DL concepts is shown in Figure 1. DL is a very useful method especially for the recognition and interpretation of images. It has a large number of data entries and automatically learns the distinguishing features (18). The biggest disadvantage of deep learning method is that all algorithms need big data.
	Artificial neural networks (ANN)	Artificial Neural Networks are systems that imitate biological neural networks (19). ANN performs the desired tasks by learning from the examples given. In ANN systems, input passes the information through the layer and interprets it as output. The structure of these systems is shown in Figure 2 (20).