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A REVIEW ON SCOPE OF ARTIFICIAL INTELLIGENCE IN PHARMA

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ABSTRACT: Artificial Intelligence (AI) focuses on producing intelligent modelling, which helps in imagining knowledge, cracking problems and decision-making. Recently, AI played an important role in various fields of pharmacy like drug discovery, drug delivery formulation development, poly-pharmacology, hospital pharmacy, *etc*. In drug discovery and drug delivery formulation development, various Artificial Neural Networks (ANNs) like Deep Neural Networks (DNNs) or Recurrent Neural Networks (RNNs) are being employed. Several implementations of drug discovery have currently been analysed and supported the power of the technology in quantitative structure-property relationship (QSPR) or quantitative structure-activity relationship (QSAR). In addition, de novo design promotes the invention of significantly newer drug molecules with regard to desired/optimal qualities. In the current review article, the uses of AI in pharmacy, especially in drug discovery, drug delivery formulation development, poly-pharmacology and hospital pharmacy are discussed.

INTRODUCTION: •Artificial Intelligent machine learning, particularly intelligent computer learning, is a field of study known as Artificial Intelligence (AI). Programs that deliver outcomes in the comparable to how human attention is processed [1]. Typically, this process entails gathering data, creating effective mechanisms for using that data, and demonstrating clear orarough conclusion and oneself corrections/ adjustments [2]. The practical uses of AI technology in various technical and business fields have recently made it a highly fundamental part of industry fields of study [3, 4]. Predicting *in-vivo* reactions, pharmacokinetics, and other outcomes is also made possible by the application of AI models. Parameters of the treatments, appropriate *etc.*, Suitable dosage [2, 5].

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According to the importance of pharmacokinetic prediction of drugs, the uses of *in-silico* models facilitate their Effectiveness and in expensiveness in the drug research [6]. Person who finally coined the term artificial intelligence and is regarded as father of AI is John Mc Carthy. Artificial intelligence in Pharma refers to the use of automated algorithms to perform tasks which traditionally rely on human intelligence.

Over the last five years, the use of artificial intelligence in the pharma and biotech industry has redefined how scientists develop new drugs, tackle disease, and more [7]. The main objective of this artificial intelligence to identify useful information processing problems and give an abstract account.

History OFAI: After playing a significant role in defining the area devoted to the creation of intelligent machines, John Mc Carthy, an American computer scientist pioneer and inventor, was called the "Father of Artificial Intelligence [9]."

FIG. 1: JOHN MC CARTHY [8]

Maturation of AI (1943-1952):

Year 1943: The first work which is now recognized as AI was done by Warren McCulloch and Walter pits in 1943. They proposed model of artificial neurons.

Year 1949: Donald Hebb demonstrate and updating rule for modifying the connection strength between neurons. His rule is now called Hebbian learning.

Year 1950: The Alan Turing who was an English mathematician and pioneered machine learning in 1950. Alan Turing publishes "Computing machinery and intelligence" In which he proposed at a test. The test can check the machine ability to exhibit intelligent behavior equivalent to human intelligence, called a Turing test.

The Birth of AI (1952-1956):

Year 1955: An Allen Newell and Herbert A. Simon created the first artificial intelligence program which was named as "Logic theorist". This program had proved 38 of 52 mathematics theorems, and find new and more elegant proofs for some theorems.

Year 1956: The word AI first adopted by American computer scientist John McCarthy at Dartmouth conference. For the first time, AI coined as an academic field [10, 11].

The Golden years-early Enthusiasm (1956-1974):

Year 1966: The researchers emphasized developing algorithms which can solve mathematical problems. Joseph Weizenbaum created the first Chabot in1966, which was named as ELIZA.

Year 1972: The first intelligent humanoid robot was built in Japan which was named as WABOT-1.

The First AI Winer (1974-1980): The duration between years 1974 to 1980 was the first AI winer duration. AI winer refers to the time period where computer scientist dealt with a severe shortage of funding from government for AI research. During AI winer, an interest of publicity on AI was decreased [12].

A Boom of AI (1980-1987):

Year 1980: After AI winter duration, AI came back with "Expert system." Expert system was programed that emulate the decision-making ability of human expert. In the year 1980, the first national conference of the American association of AI was held at Stanford University.

The Second AI Winer (1987-1993): The duration between the years 1987 to 1993 was the second AI winer duration.

Again, investors and government stopped funding for AI research as due to high cost but not efficient result. The expert system such as **XCON** was very cost-effective.

The Emergence of Intelligent agents (1993-2011):

Year 1997: In this year, IBM deep blue beats world chess champion, Gary Kasparov, and became the first computer to beat a world chess champion.

Year 2002: For the first time, AI entered the home in the form of Roomba, a vacuum cleaner.

Year 2006: AI came in the Business world till the year 2006. Companies like Facebook, Twitter, and Netflix also started using AI [13, 14].

Deep Learning, Bigdata and Artificial General Intelligence (2011-present):

Year 2011: In the year 2011, IBM's Watson won jeopardy, a quiz show, where it had to solve the complex questions as well as riddles. Watson had proved that it could understand natural language and can solve tricky questions quickly.

Year 2012: Google has launched an Android app feature "Google now ", which was able to provide information to the user as a prediction.

Year 2014: In the year 2014, Chabot "Eugene Goostman" won a competition in the infamous "Turing test".

Year 2018: The "Project Debater" from IBM debated on complex topics with two master debaters and also performed extremely well.

Google has demonstrated an AI program "Duplex" which a virtual assistant was and which has hairdresser appointment on call and lady on other side didn't notice that she was talking with the machine [15].

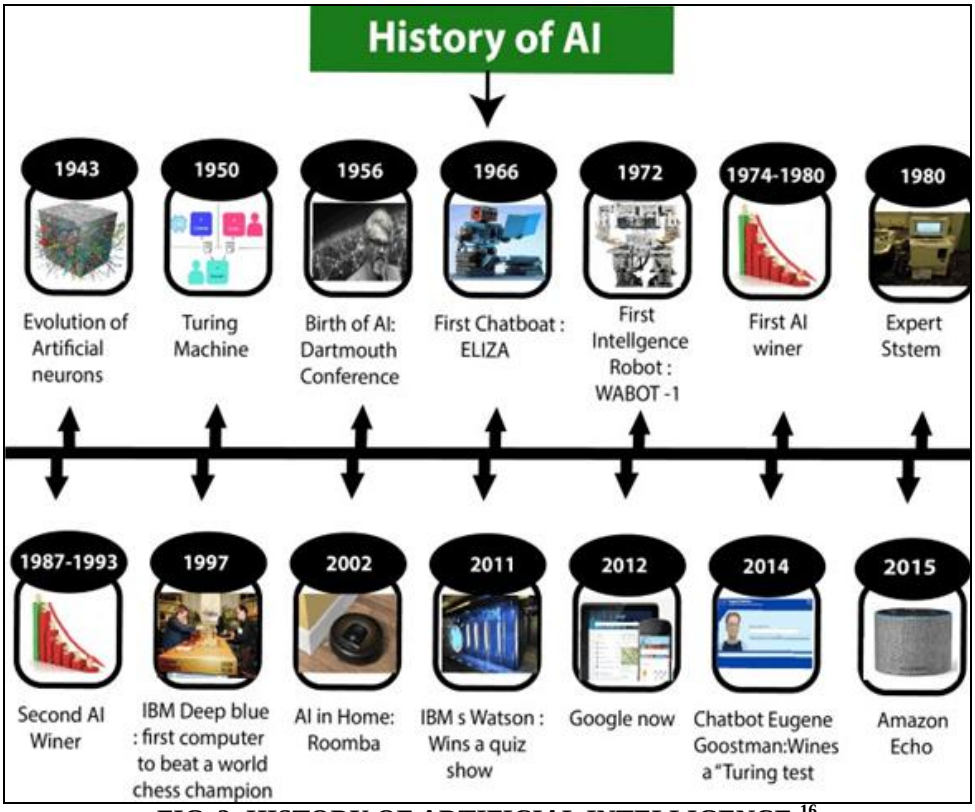

FIG. 2: HISTORY OF ARTIFICIAL INTELLIGENCE [16]

AI Classification: AI can be classified in two different ways [17, 18].

- ❖ According to caliber
- ❖ According to the presence

Based on the caliber	Weak intelligence Artificial narrow intelligence Artificial general intelligence Artificial super intelligence
Based on presence	Type1 reactive machine Type 2 limited memory system Type 3 is based on the theory of mind Type 4 self-awareness

Classification Based on Caliber [19, 20]:

Weak Intelligence or Artificial Narrow Intelligence (ANI): It is also known as Artificial Narrow Intelligence. This system is designed and trained to perform a narrow task, such as facial recognition, driving a car, playing chess, and traffic signaling.

E.g.: Apple SIRI virtual personal assistance, tagging in social media.

Artificial General Intelligence (AGI) or Strong AI: It is also called Human-Level AI. It can simplify human intellectual abilities. Due to this, when it is exposed to an unfamiliar task, it can find the solution. AGI can perform all the things as humans.

Artificial Super Intelligence (ASI): It is brainpower, which is more active than smart humans in drawing, mathematics, space, etc. in every field from science to art. It ranges from the computer just little than the human to a trillion times smarter than humans.

Classification Based on Presence: Arend Hintze [21], an AI scientist classified the AI technology based on its presence and not yet present. They are as follows:

Type 1: This type of AI system is known as **"Reactive Machine".** e.g., Deep Blue, the IBM chess program which hit the chess champion, Garry Kasparov, in the 1990s. It can identify checkers on the chessboard and can make predictions; it does not have the memory to use past experiences. It was designed for narrow purposes use and is not useful in other situations. Another example is Google's Alpha Go.

Type 2: This type of AI system is known as "Limited Memory System". This system can use past experiences for present and future problems. In autonomous vehicles, some of the decision-making functions are designed by this method only. The recorded observations are used to record the actions happening in the future, such as changing the lanes by car. The observations are not in the memory permanently.

Type 3: This type of AI system is known as "Theory of Mind". That means that all humans have their thinking, intentions, and desires which impact the decisions they make. This is a non-exist AI.

Type 4: This type of AI system is known **as "Self-awareness."** The AI systems have a sense of self and consciousness. If the machine has self-awareness, it understands the condition and uses the ideas present in other's brains. This is a non-existing AI.

Devices Worked On Artificial Intelligence [22]:

1. Social media feeds (FB, TWITTER, INSTA)
2. Music and media streaming services
3. Video games
4. Online adds network
5. Navigation and travel
6. Banking finance
7. Alexa
8. Tesla etc.

AI in Pharmacy: Each phase of the medication design process uses AI technology, which significantly lowers the cost and lowers the health risks associated with preclinical trials. Based on the vast amount of pharmaceutical data and machine learning process, AI is a useful tool for data mining [23].

In the pharmaceutical industry, AI is mostly utilized for:

1. Drug discovery
2. Clinical research
3. Disease diagnosis
4. Novel medication
5. Prediction

Drug Discovery [63, 65, 66, 68]: Klopman introduced a new program to study the structure activity relationship (SAR) of organic molecules [4].

Drug discovery often takes a long time to test compounds against samples of diseased cells. Finding compounds that are biologically active and are worth investigating further requires even more analysis. To speed up this screening process, Novartis research teams use images from machine learning algorithms to predict which untested compounds might be worth exploring in more details. As computers are far quicker compared to traditional human analysis and laboratory experiments in uncovering new data sets, new and effective drugs can be made available sooner, while also reducing the operational costs associated with the manual investigation of each compound [7].

The current AI initiative by the top biopharmaceutical companies includes:

Mobile Platform to Improve Health Outcomes: The ability to recommend patients by means of real time data collection and thus improve patient outcomes. Drug discovery Pharma companies in conjunction with software companies are trying to implement the most cutting edge technologies in the costly and extensive process of drug discovery [25].

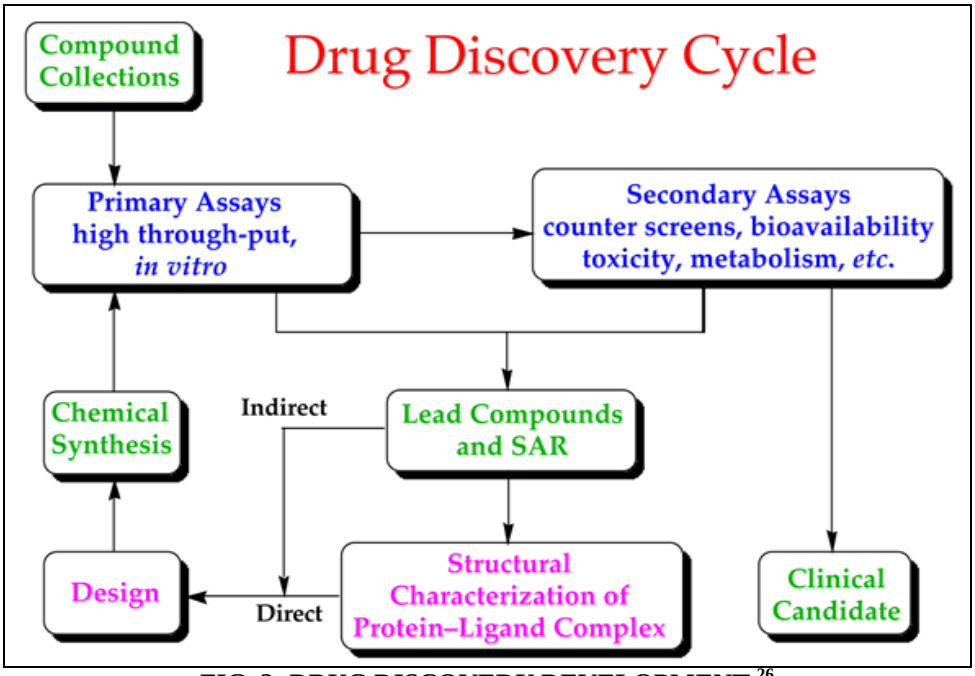

FIG. 3: DRUG DISCOVERY DEVELOPMENT [26]

Clinical Research: Big data and AI technologies are complimentary as AI can help to synthesize and analyses ever-expanding data [54, 55, 56].

Uses: AI can identify suitable cohorts for clinical trials by analyzing medical records and social media content. Trial recruitment can be sped up by using AI technologies to alert medical staff and patients about trial opportunities, as well as simplifying entry criteria to be more accessible for potential participants [27].

FIG. 4: CLINICAL RESEARCH [28]

Disease Diagnosis: The AI techniques are also most efficient in identifying the diagnosis of different types of diseases. The presence of computerized reasoning (AI) as a method for improved medical services offers unprecedented occasions to recuperate patient and clinical group results, decrease costs, *etc* [29, 51, 58].

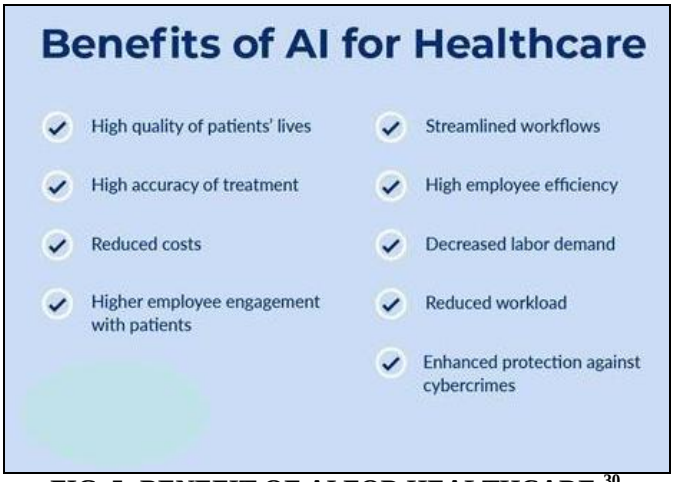

FIG. 5: BENEFIT OF AI FOR HEALTHCARE [30]

Novel Medication: Artificially intelligent computer systems are used extensively in medical sciences. Common applications include diagnosing patients, end-to-end drug discovery and development, improving communication between physician and patient, transcribing medical documents, such as prescriptions, and remotely treating patients [60, 62].

In the 1970s, AI applications were first used to help with biomedical problems. From there, AI-powered applications have expanded and adapted to transform the healthcare industry by reducing spend, improving patient outcomes, and increasing efficiencies overall.

Data Analysis: Artificial Intelligence and Data Analytics is the power to analyze and learn about large amounts of data from multiple sources and detect patterns to make future trend predictions. Business and industry benefits from predictive analytics to make decisions about production, marketing and development [52].

AI in Data Analysis: Artificial intelligence (AI) is the basis for mimicking human intelligence processes through the creation and application of algorithms built into a dynamic computing environment. Stated simply, AI is trying to make computers think and act like humans.

AI Applied in Top Companies in the Word: The application of AI in the pharmaceutical and biotech industries has completely changed how researchers approach disease; develop new drugs, and more over the last five years [31, 32, 60].

Pfizer: Immune Oncology.

Roche: Diabetic Macular edema.

Novartis: Decode Cancer Pathology Images.

Johnson Johnson: Stroke Related Death, Skin Scanner Merck & Co MSD: Emphasis On Diabetic at Cancer Prevention.

Sanofi: Drug repurposing identifies new uses of some of its Clinical strength molecule for genetic Disease.

Glaxo Smith Kline: Drug Discovery has Artificial Intelligence unit, *in-silico* drug discovery unit.

Amgen: Precision medicine in GNS health care medical research.

Gilead Sciences: Drug Discovery in April 2019.

Application of AI in Pharmacy:

1. Research development
2. Drug development
3. Diagnosis
4. Disease prevention
5. Epidemic prediction
6. Remote monitoring
7. Manufacturing
8. Marketing
9. Rare diseases and personalized medicine
10. Processing biomedical and clinical data
11. Identifying clinical trial candidates

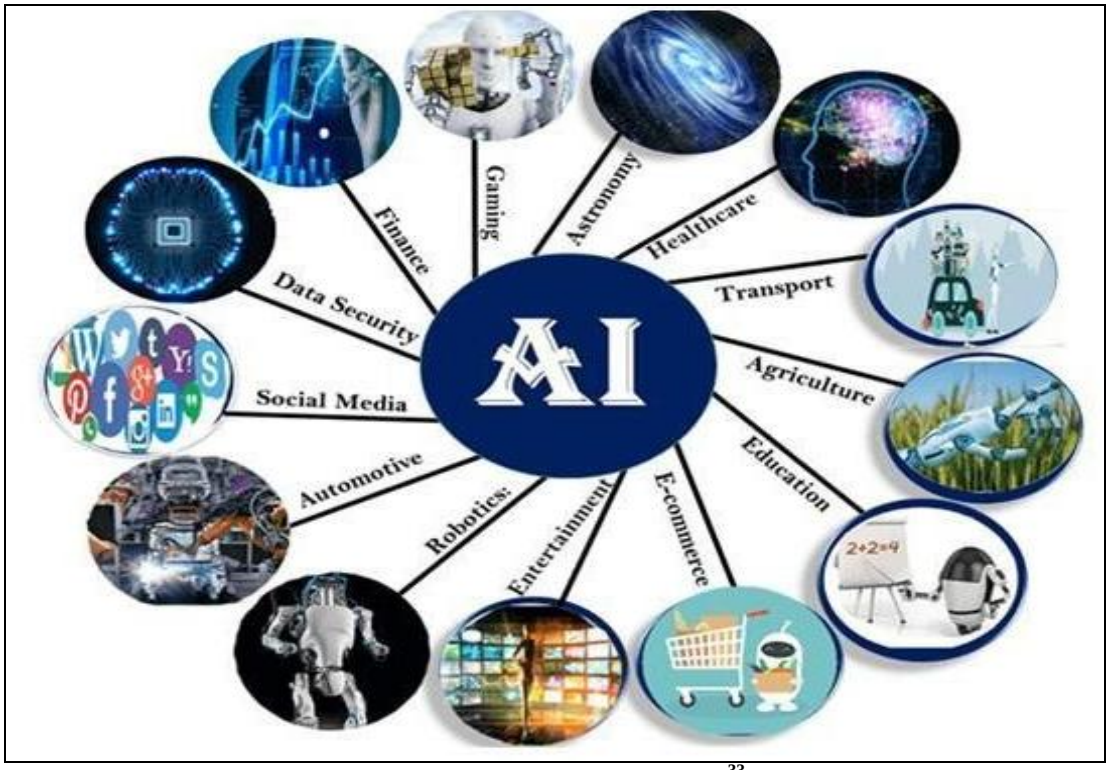

FIG. 6: APPLICATION OF AI [33]

Research and Development: Pharma companies all over the world are using cutting-edge ML Algorithms and AI- powered tools to speed up the drug discovery process. These intelligence technologies can be utilized to address issues related to complex biological networks because they are made to find nuanced patterns in vast datasets [34].

Drug Development: The application of AI has the potential to advance R&D. AI is capable of anything, from creating and finding new compounds to target-based medication validation and discoveries [35].

Diagnosis: Large volumes of patient healthcare data may be collected, processed, and analyzed by doctors using cutting-edge machine learning systems. Sensitive patient data is being safely stored in the cloud or other centralized storage systems by healthcare providers all over the world utilizing ML technology. Electronic medical records, or EMRs, are what this is [36, 59, 62, 52].

Disease Prevention: Pharma Companies can use AI to develop cures for both known diseases like Alzheimer's and Parkinson's and rare diseases. Generally, pharmaceutical companies do not spend their time and resources on finding treatments for rare diseases since the ROI is very low compared to the time and cost it takes to develop drugs for treating rare diseases [37].

Epidemic Prediction: AI and ML are already used by many pharma companies and healthcare providers to monitor and forecast epidemic outbreaks across the globe.

These technologies feed on the data gathered from disparate sources in the web, study the connection of various geological, environmental and biological factors on the health of the population of different geographical locations, and try to connect the dots between these factors and previous epidemic outbreaks. Such AI/ML models become especially useful for underdeveloped economies that lack the medical infrastructure and financial framework to deal with an epidemic outbreak [38, 61].

Remote Monitoring: It is a breakthrough in the pharma and healthcare sectors. Many pharma companies have already developed variables powered by AI algorithms that remotely monitor patients suffering from life-threatening diseases.

Manufacturing: Pharma companies can implement AI in manufacturing process for higher productivity, improved efficiency, and faster production of lifesaving drugs.

AI can be used to manage and improve all aspects of the manufacturing process, including:

- Quality control
- Predictive maintenance
- Waste reduction
- Design optimization
- Process automation

Marketing: Given that the industry is a purchases industry, artificial intelligence (AI) can be a useful tool in pharma marketing. Pharma businesses use AI to research and create distinctive marketing tactics that promise great sales and brand recognition.

Future Scope of Artificial Intelligence:

- ❖ AI in science and research
- ❖ AI in cyber security
- ❖ AI in data analysis
- ❖ AI in transport
- ❖ AI in home
- ❖ AI in health care *etc*

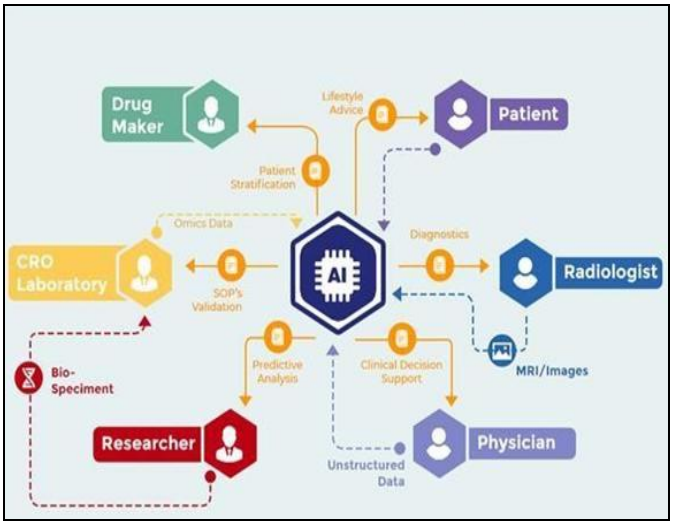

FIG. 7: FUTURE SCOPE OF AI 39

AI in Science and Research: AI is making lots of progress in the scientific sector. Artificial intelligence can handle large quantities of data and processes it quicker than human minds. This makes it prefect for research where the sources contain high data volumes. AI is already making breakthroughs in this field [40, 53, 54, 67].

AI in Cyber Security: Cyber security is another field that's benefitting from AI. As organizations are transferring their data to IT networks and cloud, the threat of hackers is becoming more significant.

AI in Data Analysis: Data analysis can benefit largely from AI and ML. AI algorithms are capable of improving with iteration, and this way, their accuracy, and precision increase accordingly. AI can help data analysts with handling and processing large datasets.

AI in Transport: The transport sector has been using AI for decades. Airplanes have been using autopilot to steer them in the air since 1912. An autopilot system controls the trajectory of a plane, but it isn't restricted to aircraft alone. Ships and spacecraft also use autopilot to help them maintain the correct course.

AI in Home: AI has found a special place in people's homes in the form of Smart Home Assistants. Amazon Echo and Google Home are popular smart home devices that let you perform various tasks with just voice commands.

AI in Healthcare: The medical sector is also using this technology for its advantages. AI is helping medical researchers and professionals in numerous ways [41, 64].

Advantages of AI [42, 43, 44]: The potential advantages of AI technology are as follows [42, 43, 44]:

Error Minimization: AI assists to decrease the errors and increase the accuracy with more precision. Intelligent robots are made of resistant metal bodies and capable of tolerating the aggressive atmospheric space, therefore, they are sent to explore space.

Difficult Exploration: AI exhibits its usefulness in the mining sector. It is also used in the fuel exploration sector. AI systems are capable of investigating the ocean by defeating the errors caused by humans.

Daily Application: AI is very useful for our daily acts and deeds. For examples, GPS system is broadly used in long drives. Installation of AI in Androids helps to predict what an individual is going to type. It also helps in correction of spelling mistakes.

Digital Assistants: Now-a-days, the advanced organizations are using AI systems like 'avatar' (models of digital assistants) for the reduction of human needs. The 'avatar' can follow the right logical decisions as these are totally emotionless. Human emotions and moods disturb the efficiency of judgement and this problem can be overcome by the uses of machine intelligence.

In general, human beings can perform single task at a time. In contrast to the human beings, machines are capable of performing multi-tasking jobs and can analyze more rapidly in comparison to the human beings. Various machine parameters, i.e., speed and time can be adjusted according to their requirements.

Medical uses: In general, the physicians can assess the condition of patients and analyze the adverse effects and other health risks associated with the medication with the help of AI program. Trainee surgeons can gather knowledge by the applications of AI programs like various artificial surgery simulators for examples, gastrointestinal simulation, heart simulation, brain simulation, *etc*.,

No Breaks: Unlike human beings who have the capacity of working for 8 h/day with breaks, the machines are programmed in such a way that these are capable of performing the work in a continuous manner for long hours devoid of any kinds of confusions and boredom.

Increase Technological Growth Rate: AI technology is widely used in most of the advanced technological innovations worldwide. It is capable of producing different computational modelling programs and aims for the invention of the newer molecules. AI technology is also being used in the development of drug delivery formulations.

No Risk: In case of working at the risky zone like fire stations, there are huge chances of causing harm to the personnel engaged. For the machine learning programs, if some mishap happens then broken parts can be repairable.

Acts as Aids: AI technology has played a different function by serving children as well as elders on a 24x7 basis. It can perform as teaching and learning sources for all.

Limitless Functions: Machines are not restricted to any boundaries. The emotionless machines can do everything more efficiently and, also produce more accurately than the human beings.

Disadvantages of AI [42, 43, 44]: The important disadvantages of AI technology are as follows [42, 43, 44].

Expensive: The launch of AI causes huge money consumption. Complex designing of machine, maintenance and repairing are highly cost effective. For the designing of one AI machine, a long period of time is required by the R & D division.

AI machine needs updating the software programmers, regularly. The reinstallations as well as recovery of the machine consume longer time and huge money.

No Replicating Humans: Robots with the AI technology are associated with the power of thinking like human and being emotionless as these add some advantages to perform the given task more accurately without any judgement. If unfamiliar problems arise, robots cannot take the decision and provide false report.

No Improvement with Experience: Human resource can be improved with experiences. In contrast, machines with AI technology cannot be enhanced with experience. They are unable to identify which individual is hard working and which one is nonworking [45].

No Original Creativity: Machines with AI technology have neither sensitivity nor the emotional intelligence. Humans have the ability to hear, see, feel and think. They can use their creativity as well as thoughts. These features are not achievable by the uses of machines.

Unemployment: The widespread uses of AI technology in all the sectors may cause large scale unemployment. As because of the undesirable Un-employment, human workers may lose their working habits and creativity [46, 47].

Risks [48]:

- Automation-spurred job loss
- Privacy violations
- Weapons automatization
- Deep fakes
- Market volatility
- Algorithmic bias caused by bad data
- Socioeconomic inequality

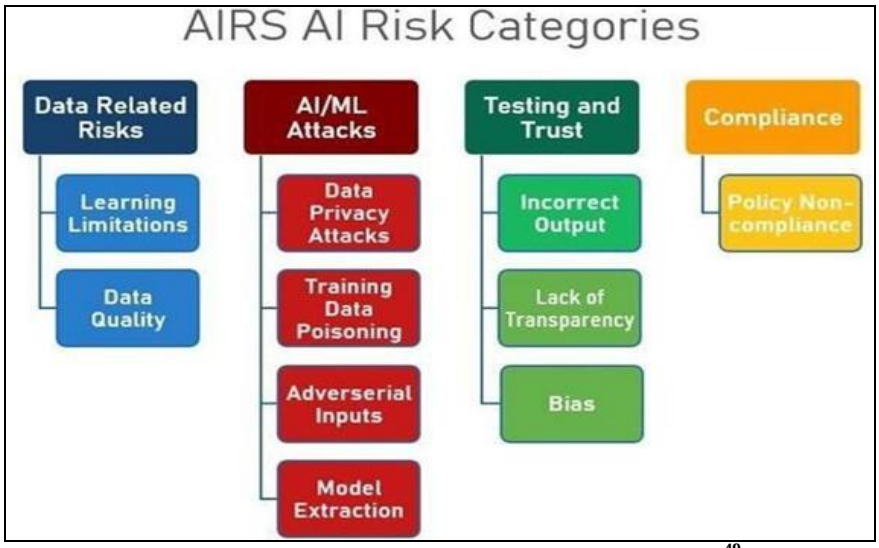

FIG. 8: RISK OF ARTIFICIAL INTELLIGENCE [49]

CONCLUSION: During past few years, a considerable amount of increasing interest towards the uses of AI technology has been identified for analyzing as well as interpreting some important fields of pharmacy like drug discovery, dosage form designing, polypharmacology, hospital pharmacy, etc., as the AI technological approaches believe like human beings imagining knowledge, cracking problems and decision making. The uses of automated workflows and databases for the effective analyses employing AI approaches have been proved useful. As a result of the uses of AI approaches, the designing of the new hypotheses, strategies, prediction and analyses of various associated factors can easily be done with the facility of less time consumption and inexpensiveness.

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CONFLICTS OF INTEREST: Nil

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