INVESTIGATING DRUG INNOVATIONS USING ARTIFICIAL INTELLIGENCE: A NEW PIPELINE

Dr. Mahmood Khan Yousufi[1]

Professor and Head, Department of Microbiology, Jawaharlal Nehru College, Bhopal, Madhya Pradesh, India[1]

Abstract: Drug innovations have entered the battle of the host-pathogen evolutionary arms race by focusing on invading species. In the recent studies it has been observed that majority of the assorted drugs utilized in medications are being challenged from the pathogens. This is leading to the blooming of antimicrobial resistance or AMR. The emergence of drug-resistant microbes coupled with a lengthy and expensive pipeline for drug or antibiotic research, has sparked a critical interest in computational techniques that could hasten candidate discovery. Advances in AI have promoted its use in a variety of computer-aided drug design contexts, with an expanding utility in drug discovery. Along with the crucial prediction of antimicrobial activity, *de novo* molecular design, determination of drug-likeness features, and antimicrobial compound representation are also being fetched by employing AI. This review describes developments in the innovations of drugs, antibiotics and antimicrobial peptides, which have been made possible by AI. Further this investigation also examines the adoption of open scientific best practices in AI-driven drug innovations in the current urgency of the antimicrobial resistance challenges and makes the case for openness and reproducibility as a way to quicken preclinical research. It was observed in this study that numerous new corporate start-ups are eagerly approaching to AI based drug innovations. The conclusion of this investigation opined that artificial intelligence advancements in the drug innovation arena offer numerous prospects for future applications.

Keywords: Drugs, Innovation, discovery, Artificial Intelligence, Machine Learning, Antibiotics, Antimicrobial resistance, Pipeline.

I. INTRODUCTION

It is a very hard job to discover a secondary metabolite that has cidal or static properties. Although various secondary biochemicals often show inhibition or killing effects on microbes, on the contrary they cannot be utilized in individuals due to their hazardous side effects. Antibiotic drugs are secondary biochemicals that are created by natural living organisms in order to survive in natural state [1]. In recent times it has been experienced in the world arena that pathogenic microbes have developed resistance against several antibiotic drugs used in treating human illnesses [2].

According to the world health organization antimicrobial resistance is one of the top threats the world is facing concerning public health [3]. It has been depicted by WHO that exponential use of antibiotics have led to the development of drug resistant pathogenic microbes [3]. Artificial intelligence is a branch of computer science that deals with constructing intelligent machines that can perform required tasks through human intelligence [4]. The recent trends in the healthcare sector exhibit that AI can be quite supportive in diagnosis of maladies and securing it through decent treatment prototypes [5]. AI is a new approach to combat antimicrobial resistance that is peaking enormously [6]. In the present investigation AI is being explored concerning its proficiency in overcoming antimicrobial resistance and new drug innovations.

II. LITERATURE REVIEW

In the year 2021, Lau et al., studied the efficiency of AI in battling antimicrobial resistant bacteria [7]. Melo and his associates in their study explored how artificial intelligence can accelerate antibiotic discovery [8]. In the year 2020, Fanelli and his coworkers investigated the role of AI in opposing antimicrobial resistance in children [9]. AI equipped molecular diagnostics was used for detecting antimicrobial resistance in *Pseudomonas aeruginosa* by Khaledi et al [10]. David et al., in the year 2021 investigated the possibilities of AI in discovery of antibiotics [11]. In the year 2018, Veltri, Kamath and Shehu in their study determined that deep learning enhances antimicrobial peptide identification [12].The antimicrobial peptide design using QSAR modeling and computers was examined by Jenssen et al., in the year 2008 [13]. Determination of new antibacterial peptides by AI and chemoinformatics was carried out by Fjell and his coworkers in

the year 2009 [14]. Fields et al., in the year 2019 used machine learning and biophysical selecting of minimum bacteriocin domain for a new antimicrobial peptide innovation [15]. A white-box approach based on machine learning was used for identifying mechanisms of antibiotic action by Yang et al in the year 2019 [16]. Jukic and Bren in the year 2022, in their investigation studied numerous AI based approaches useful in innovation of antibacterial agents and different molecular targets [17]. Patel and his coworkers in the year 2020 examined various machine learning based protocols used for drug discovery [18]. Lee et al., in the year 2022 determined the methods for computer linked drug designing through big data and artificial intelligence [19]. Ivanenkov et al in the year 2019 in their investigation explored novel antibacterials using machine learning methods [20]. Drug delivery through AI and machine learning for efficiently treating infections in humans was studied by He et al., in the year 2021 [21]. Ekins and his associates studied the exploitation of AI for end to end drug innovation and its development in the year 2019 [22]. Zhang et al., in the year 2021 in their study explored deep learning based drug discovery for tackling Coronavirus 2 [23].

III. DRUG INNOVATIONS

A large volume of finance is drained during the drug development procedures. The global corporations are eagerly looking for novel methods for innovating drugs especially for antibiotic resistant microbes. The hunt for novel drugs is getting quicker and effective by the use of machine learning and artificial intelligence. The investment in artificial based drug discovery has raised to 2.4 billion US dollars in the year 2020 to 5.2 US dollars by the end of 2021[24]. The process of drug discovery involves significant steps viz. target discovery and validation, hit discovery and validation, assay development, defining a hit series and hit to lead phase, and lead optimization phase [25].The merging of AI in drug discovery is newly born and shall improve with the latest advancements in this field. It takes around 15 years to raise a single novel drug to reach the patient for treatment [26]. A German biotech corporation, Evotec has declared clinical trials of a novel anticancer drug molecule that has been developed through AI [27]. The researchers at Massachusetts Institute of Technology in Cambridge have innovated a premiere antibiotic, halicin through artificial intelligence [28].

IV. BENEFITS OF INCORPORATING AI IN DRUG INNOVATIONS

The modern medications can be revolutionized by utilizing AI in drug discovery. It has been exhibited that use of machine learning in drug innovations shall lead to a monetary benefit of about 70 billion dollars till 2028 [29].Several benefits have been devised upon fusion of AI with drug discovery. It is observed that artificial intelligence does not depend on set targets [30]. Through AI a large volume of data can be isolated from a data reservoir [31]. AI is a reliable tool that can predict a useful and accurate drug molecule [32].The drug innovation and manufacturing process can be boosted by artificial intelligence [33]. The utilization of AI in drug processing offers elimination of animal models that play a vital role in clinical trial procedures [34]. AI also has the capability to design human-like tissues, thus excluding dependability on animals for drug testing [35]. Several patents on drugs created through AI have been filed recently. The patent KR2018022537A exhibits the utilization of AI in predicting combination of drugs [36]. The patent KR20200145835A describes the combination of thioridazine for treating metabolic liver disorders [37]. The patent WO2021080295A1 describes how AI is capable of designing a molecular structure of a novel drug [38]. The patent No. US11,076,824 B1 describes the detection of COVID-19 using artificial intelligence [39].

V. AI BASED STARTUPS ON DRUG INNOVATIONS

Recently various startups have been established that are performing miraculously in the field of drug innovations through artificial intelligence [40]. Exscientia corporation has created an AI integrated designing domain alluded to as Centaur Chemist that can identify novel drug targets plus manoeuvre to create drugs and use them for clinical trials [41]. This corporation is set to bag seven patents with respect to AI [42]. A US based startup data2discovery was founded in the year 2012 [43]. It is employing a healthcare data analytical percept to obtain conclusions from a huge volume of complicated heterogeneous data [42]. A South Korean based artificial intelligence coupled startup Standigm was raised in the year 2015 [44]. It utilized AI to create avant garde chemical constituents with requisite traits [44]. Using AI based workflow technique Standigm is running twenty two in house drug pipelines [44]. Unlearn AI, is a startup that works on synthetic, patient data, created by using AI so as to provide life saving therapies to patients as early as possible [45]. It is the only corporation employing artificial intelligence to create digital twins that are useful in creating the clinical trials rapidly along with accurate results [46]. An American based startup Genesis Therapeutics was created in the year 2019 [47]. It has united AI with biotechnology to promote innovation of new meds [47]. Genesis Therapeutics has a protein structure forecast technology called Dynamic PotentialNet technology [48].

VI. CONCLUSION

From this investigation it is inferenced that use of drugs in human wellness is playing a notable role. The integration of AI with the drug development protocols has reasonably advanced the drug manufacturing process. Artificial intelligence is not only reducing the cost of drug manufacturing but also saving the precious time being consumed during clinical trials. It is being concluded in this investigation that more research is adequately required for perfectly utilizing AI in the drug innovation procedures.

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