World Journal of Pharmaceutical Science and Research
www.wjpsronline.com
Review Article
ISSN: 2583-6579
SJIF Impact Factor: 5.111
Year - 2025
Volume: 4; Issue: 1
Page: 123-140

A REVIEW ON ARTIFICIAL INTELLIGENCE IN ANTICANCER DRUG DEVELOPMENT

Pasam Jyothirmayi*[1], A. Anusha[2], Dr. N. Srinivasarao[3], Ch. Nagadeepthi[4], M. Sreelasya[5] and P. Nagakusuma[6]

[1,2,3]Faculty of Pharmacy, Vikas College of Pharmacy, Vissannapeta, Krishna District, Andhra Pradesh.

[4,5,6]Department of Pharmaceutics, Vikas College of Pharmacy, Vissannapeta, Krishna District, Andhra Pradesh.

Article Received: 14 December 2024 || Article Revised: 05 January 2025 || Article Accepted: 27 January 2025

***Corresponding Author: Pasam Jyothirmayi**
Faculty of Pharmacy, Vikas College of Pharmacy, Vissannapeta, Krishna District, Andhra Pradesh.
DOI: https://doi.org/10.5281/zenodo.14783830

How to cite this Article: Pasam Jyothirmayi, A. Anusha, Dr. N. Srinivasarao, Ch. Nagadeepthi, M. Sreelasya, and P. Nagakusuma (2025). A REVIEW ON ARTIFICIAL INTELLIGENCE IN ANTICANCER DRUG DEVELOPMENT. World Journal of Pharmaceutical Science and Research, 4(1), 123-140. https://doi.org/10.5281/zenodo.14783830

ABSTRACT

Artificial intelligence is progressively spreading through the world of health, particularly in the field of oncology. AI offers new, exciting perspectives in drug development as toxicity and efficacy can be predicted from computer-designed active molecular structures. Their wider use is eagerly awaited as they should markedly reduce durations and costs. Health authorities cannot neglect this new paradigm in drug development and should take the requisite measures to include AI as a new pillar in conducting clinical research in oncology. Artificial intelligence (AI) has strong logical reasoning ability and independent learning ability, which can simulate the thinking process of the human brain. AI technologies such as machine learning can profoundly optimize the existing mode of anticancer drug research. But at present AI also has its relative limitation. Artificial intelligence based on big data can extract the hidden patterns, important information, and corresponding knowledge behind the enormous amount of data. Anti-cancer drug design has been acknowledged as a complicated, expensive, time-consuming, and challenging task. How to reduce the research costs and speed up the development process of anti-cancer drug designs has become a challenging. Computer-aided drug design methods have played a major role in the development of cancer treatments for over three decades. Recently, artificial intelligence has emerged as a powerful and promising technology for faster, cheaper, and more effective anti-cancer drug designs.

KEYWORDS: Artificial intelligence, Computer-aided drug design, Cancer.

1. INTRODUCTION

Artificial intelligence (AI) is a set of technologies that enable computers to perform a variety of advanced functions, including the ability to see, understand and translate spoken and written language, analyze data, make recommendations, and more.

AI is the backbone of innovation in modern computing, unlocking value for individuals and businesses. For example, optical character recognition (OCR) uses AI to extract text and data from images and documents, turns unstructured content into business-ready structured data, and unlocks valuable insights. While the specifics vary across different AI techniques, the core principle revolves around data. AI systems learn and improve through exposure to vast amounts of data, identifying patterns and relationships that humans may miss.

In recent years, many companies have ramped up their R&D (research and development) efforts for anti-cancer drugs.[1] There is a growing number of large and long-term clinical trials providing a possible therapeutic opportunity for more cancer patients.[2] Recently, the American Cancer Society announced that the three-year survival rate for lung cancer from 2014 to 2021 was raised from 21% to almost 31%.[3] The efficacy of targeted therapies and immunotherapeutics has been investigated in a variety of solid tumors.[4] Artificial intelligence (AI) refers to the intelligence shown by machines made by humans. It is a comprehensive science including computer science, cybernetics, neurophysiology, psychology, and linguistics. AI is believed to have been born at the Dartmouth conference in 1956. After decades of vigorous development, the meaning of AI continues to expand, and it has become the general name of artificial neural networks, machine learning, deep learning and other technologies.[5] Deep learning, an important branch of AI.[6] As one of the cutting-edge cancer treatments, targeted drug therapy has the advantages of high efficiency, few side effects, and low drug resistance for patients.[7] However, there are several drawbacks to the existing targeted therapies, such as a few druggable targets[8] ineffective Coverage of the patient population, and the lack of alternative responses to drug resistance in patients.[7]

Therefore, identifying novel therapeutic targets and evaluating their druggability.[9,10] The current cancer research focus of targeted drug therapy. Since we have difficulty in comprehensively understanding the pathogenesis of cancer due to the complexity of the disease.[11] As a result, these therapies could have undesired impacts on normal tissues and even provoke serious side effects for patients.[12,13] Over the past few decades, we have sa fast development of artificial intelligence biology analysis algorithms. To make this study easy to understand, we not only divide these artificial intelligence algorithms into network-based biology analysis algorithm and machine learning-based (ML-based) biology analysis algorithm according to the data of biological network structure, but also employ Fig. 1 to describe the historical milestone for these artificial intelligence biology analysis algorithms.

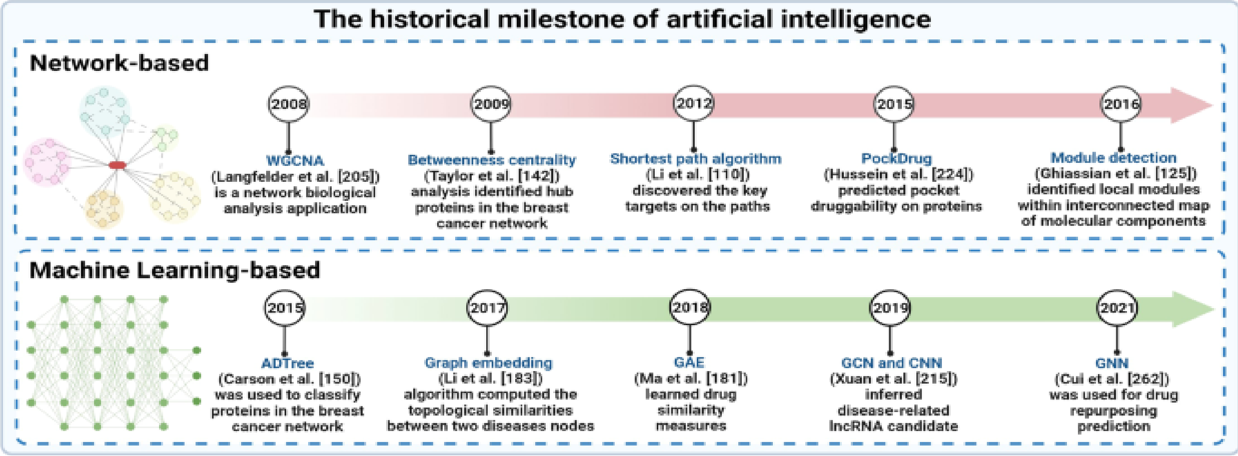

Fig. 1: The historical milestones of network-based and ML-based biology analysis.

On the onehand, network-based biology analysis algorithms provide a variety of alternative network approaches to identify cancer targets. More importantly, various network-based biology analysis algorithms can investigate network data from different perspectives, therefore they can compensate each other to provide accurate biological explanations.[14] On the other hand, ML-based biology analysis[15,16,17] not only can efficienly handle high throughput, heterogeneous, and complex molecular data, but also can mine the feature or relationship in the biological networks. Thus, we should develop more ML-based biology analysis algorithms to provide such advanced biology analyses that can allow precise target identification and drug discovery for cancer. Cancer is a generic term for a broad category of disease that occurs due to the transformation of normal cells into tumor cells comprising of multi-stage progress from cancerous lesions to malignancy. Over a million cancer incidences are reported yearly, leading to high mortality rates.[18]

Conventional cancer treatment involves surgical procedures for cancer in a localized stage, followed by radiation therapy and chemotherapy for advanced stages of cancer.[19] Nanotechnology plays a vital role in developing modern drug delivery systems as natural compounds are now being investigated for treating cancer and several other microbial and inflammatory diseases.[20,21] Employing nanotechnology enables the application of nanostructures and other curative agents developed at a nanoscale level for nanomedicine. The field of biomedicine encompasses nanobiotechnology, drug delivery, biosensors, and tissue engineering, which are significantly influenced by the use of NPs.[22] In the past decade, several advances have been witnessed in nanotechnology, and possible fabrication, characterization, and modifications of NPs functional properties are now implemented for medical diagnosis and biomedical applications.[23] NPs comprise materials designed at an atomic and molecular level, resulting in smaller nanospheres. Hence, nanoscale-sized particles can navigate freely in the human body compared to more extensive materials.[24] Cancer treatment is challenging as there are various cancer biomarkers, and each patient has a distinct molecular profile. This diversity is apparent in different cancer types as patients have unique molecular signatures and distinct driver mutations leading to tumor heterogeneity which is a critical challenge in cancer treatment.[25,26]

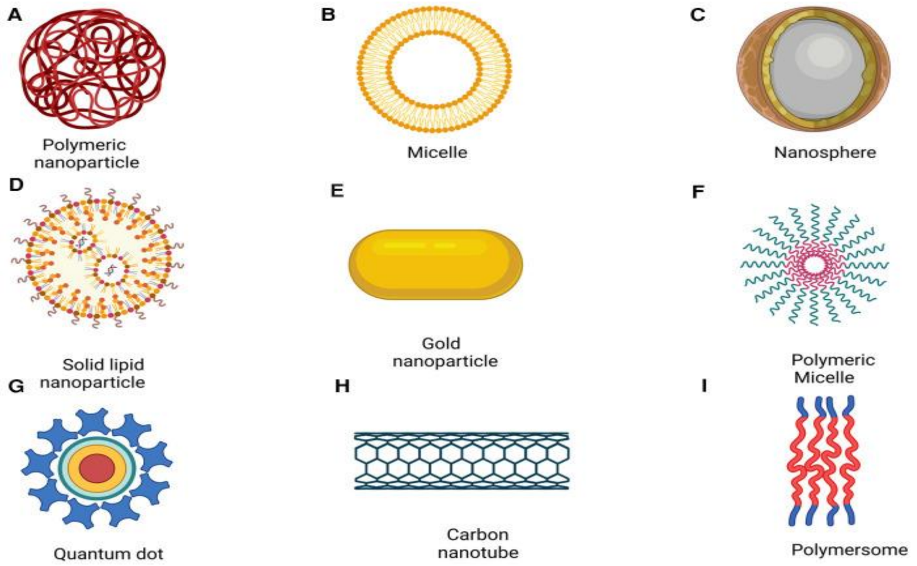

Figure 2: Nanoparticles for drug delivery. (Reprinted from "Nanoparticle-Mediated Targeted Drug Delivery to Cancer Stem Cells by Bio Render", June 2020.

The advances in AI and its potential contribution to bionanotechnology present a unique opportunity to realize its full potential in precision medicine for cancer diagnosis and treatment. This is because AI has immense capabilities for automation and faster patient analysis of complex disease information by faster processing of complex medical data and delivering accurate results, thereby improving treatment outcomes.

The complete approach for drug design and discovery comprises target recognition, hit exploration, hit-to-lead development, lead optimization, preclinical drug candidate identification, and preclinical and clinical research. Conferring to statistics, the mean research and development (R&D) period generally take 10–17 years for developing a new form of drugs prescribed.[27] Artificial intelligence in drug discovery and development.Drug Discov. Today (2021) In addition to substantial time and cost factors concerning the development of modern minute molecular pharmaceuticals, the ratio of success for developing these drugs are below 10%.[27] Computerized drug molecule design approaches provide wise supervision for drug design and discovery accompanied by decreased costs with improved productivity. Subsequently, the present context of higher costs, large threat, and long periods that is depicted by drug industries will be reformed.[28] The continuous progression in innovative computing technologies could transform design and discovery of drugs with remarkable success rates.

According to FDA's illustrations[29] the discovery and development of drug have five phases: (i) drug discovery and development: new drug is tested from the perception of disease mechanisms and its effects on molecular compounds; (ii) preclinical research: new drug is tested in various test centers, and experiments are done with animals to acknowledge the reliability and challenges; (iii) clinical research: various phases of clinical experiments are done to check the new drug on people for analyzing its reliability and success rates; (iv) FDA review: FDA organizations analyze the details of new drug and make a result to sanction or not; and (v) post-marketing research: pharmacosurveillance and performance comparison research is done to monitor the safety of drugs. In modern era, artificial intelligence (AI) is one of the innovative technologies for drug design and discovery. AI is the simulation of digital computers or machines to perform decision-making and problem-solving tasks that are usually associated with a human mind. It has various methods for processing the data which enables devices and computers to train human intellectual skills through experiences in handling complex data challenges. Conventional computational techniques process data operations manually and are further utilized for optimizing tasks that are complex for human insight (e.g., performing testing on all drug-dose combinations). Later, the tasks which are non-trivial to identify are incorporated with AI through small-scale commands, such as identification and classification of cancer.Cancer is a severe threat to human health with a high mortality and a rising incidence rate.[30] Several types of cancer can be cured if they are diagnosed and treated early.

However, the treatment of cancer is not ideal at present. Cancer mortality rates remain high and continue to rise, including for prostate, colorectal, and cervical cancer.[31] These tumors lack effectivescreening and treatment methods, resulting in patients not getting timely and effective treatment. Secondly, the heterogeneity of tumors is high, which can create great challenges in their treatment.[32] Therefore, new diagnostic and treatment methods that are tailored to individual patients are needed. Precision medicine (PM) is a promising approach that takes individual genetics, environment and lifestyle into account and concentrates on clarifying, diagnosing and treating diseases to create a customized treatment plan for patients through obtaining multi-omics or multi-mode information from individuals.[33] Tumors are generally caught sight of in the following two situations: one is the screening of high-risk groups.[34] Based on these results, tumors will be accurately diagnosed, staged, and classified to help the patients benefit from precision treatment. AI can play a part in tumor prevention, screening, diagnosis, treatment, and prognosis predication.[35-38] In addition; a framework diagram (Figure 3) is added to this article, which shows a series of processes from the discovery of tumor patients to the end of their diagnosis, treatment, and the changes that AI can bring.

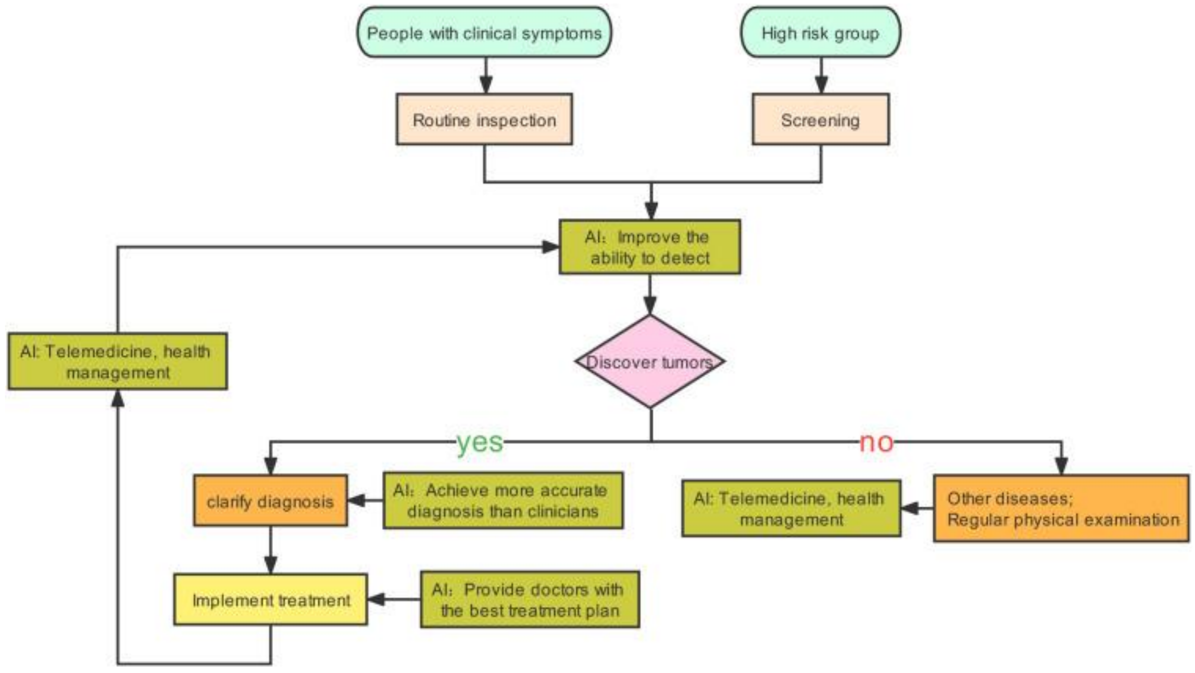

Figure 3: Possible changes caused by AI injection into clinical practice.

With the development of next-generation sequencing (NGS) technology, omics data, such as genomics, proteomics and transcriptomics, have been accumulated.[39] In the present review, we first introduced the application of AI in omics, and then in pathology and medical imaging, and expanded on how these applications assist PM. Finally, we described the challenges and future directions of AI assisted PM for tumors.

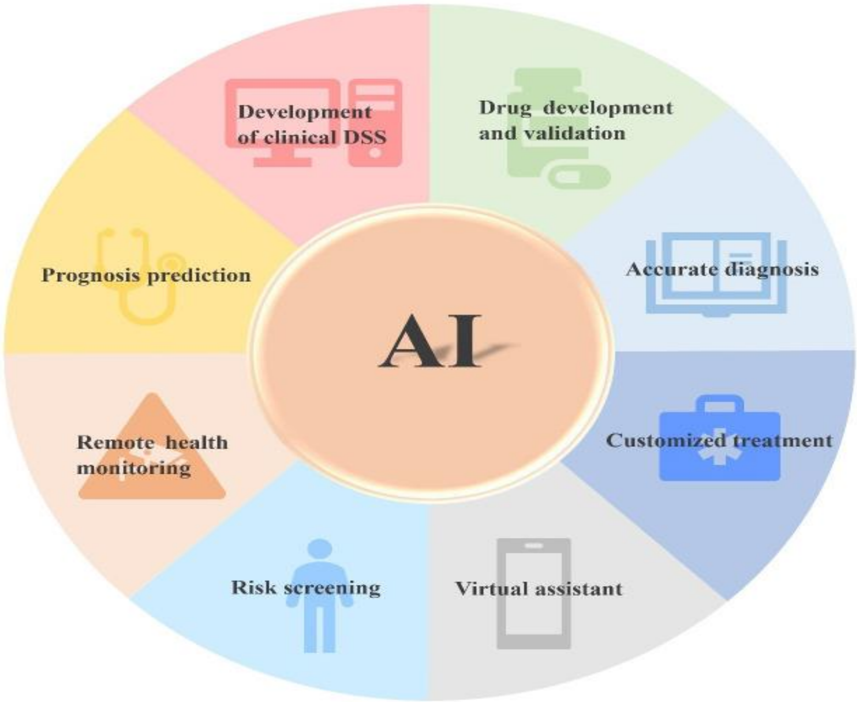

Figure 4: Application prospect of AI in tumor.

Artificial intelligence (AI) is concretely reshaping our lives and it is time to understand its evolution and achievements to model future development strategies. This is true also for oncology and related fields, where AI is now opening new important opportunities for improving the management of cancer patients, as will be highlighted in this perspective paper.

In 1950, Alan Turing was the first that conceives the idea of using computers to mimic intelligent behaviour and critical thinking.[40] The human body comprises trillions of cells, and the chance of occurrence of cancer in any part of it is fairly significant. Non-communicable diseases (NCDs) are now a major cause of global deaths, and cancer is expected to top the ranked list of leading causes of deaths in every country.[42] Cancer incidences and mortality are rapidly growing worldwide.[43] As per the report of the World Health Organization (WHO) in 2015, cancer is one of the topmost ranking causes of death before the age group of 70-75 years in 91 countries out of 172 and holds the third or possibly fourth position in 22 other countries. One of the major factors that play a vital role in tackling cancer is its early detection and prompts diagnosis. There are different imaging techniques available for cancer screening and diagnosis among which the investigative methods that top the list are mammography, ultrasound, and thermography. Mammography is one of the most important early diagnostic methods for breast cancer but it is not very successful for dense breasts. For this reason, ultrasound or diagnostic sonographic techniques are recommended.[44] In recent years, technological advancement in medical imaging as well as the discovery of minimally invasive biomarkers have shown possibilities of curbing such challenges across a wide spectrum including detection of cancer, therapeutics and monitoring techniques. However, one of the major challenges lies in the interpretation of the large volume of data being generated by such advancements.

2. Artificial Intelligence in Anti-Cancer Drug Target Identification

The identification of drug–target interactions (DTIs) is the initial step in anti-cancer drug design. The strength of drug–target binding is often described by binding affinity constants, including indicators such as a dissociation constant (Kd), an inhibition constant (Ki), and a half-maximal inhibitory concentration (IC50).[45] Since the experimental determination of DTIs is a time-consuming and expensive process, its computational prediction is of great interest. Accurate and effective DTI predictions can greatly aid drug development and accelerate comp92-94 discovery.

2.1. Artificial Intelligence Efficiently Elevates the Prediction Accuracy of DTI

Traditionally, the computational methods for DTI predictions have included molecular docking simulation and machine learning-based methods. However, these studies would be expensive, time-consuming, and difficult to conduct without knowing the 3D structures of the drug targets. Peng et al. developed a novel end-to-end learning framework based on heterogeneous graph convolutional networks (EEG)-DTI for DTI predictions. A graph convolutional network-based model was used to learn the low-dimensional feature representations of drugs and targets and predict the DTI based on the learned features. It achieved a promising DTI prediction performance even when the 3D structures of the drug targets were not used.[46] Meanwhile, to address the explanation problem of deep learning, Yang et al. proposed a drug–target interaction prediction method based on mutual learning mechanisms without 3D structural information and with explanation.[47]

2.2. Artificial Intelligence Could Integrate Data from Multiple Sources to Help with Anti-Drug Target Identification

Drug target identification is a key step in drug development. However, most previous studies were confined to a single data type and did not integrate multiple data types. Thus, they were vulnerable to data-specific noise and needed to be improved in terms of practicality and accuracy.[48] Recently, there has been a growing number of methods within similarity-based or data-driven frameworks that attempt to use artificial intelligence to improve the predictive power by integrating multiple different data types. Madhukar et al. developed a Bayesian-based machine learning method (BANDIT), which achieved approximately 90% target prediction accuracy on more than 2000 small molecules by integrating six types of data, including growth inhibition data, gene expression data, adverse reaction data, chemical structure data, and drug data.[49] Proposed a method named DDR to investigate how to predict drug–target interactions more efficiently by using data from different sources, which included eight drug similarity networks and eight target similarity networks. The drug similarity networks included the following: gene expression similarity, disease-based similarity, drug side effect-based similarity, chemical structure fingerprint-based similarity, etc. The target similarity networks included the following: gene ontology-based similarity, protein sequence-based similarity, etc.[50] The above studies illustrated that integrating data from multiple sources through artificial intelligence could increase the biological explanation of drug target prediction and prediction accuracy.

2.3. Artificial Intelligence Could Help Predict the Druggability of Anti-Cancer Drug Targets

The selection of drug targets is also a very critical step in the cancer drug design process, and it has a great impact on the success rate of later clinical trials. Therefore, many related methods were developed. Raies et al. proposed a prediction model called Drugnome AI to address the problem of targeted drug synthesis. The stochastic semi-supervised machine learning framework was used to develop Drugnome AI for predicting the druggability of drug targets in the human exome. It also demonstrated how the application of Drugnome AI can predict the druggability of drug targets in oncology diseases.[51]

3. AI and anticancer drug development

AI can be used to predict anti-cancer drug activity or assist in anti-cancer drug development. Different cancers and the same drugs may have different reaction modes, and data from high-through put screening procedures often reveal the relationship between genomic variability of cancer cells and drugactivity Lindetal.[52] Developed a drug sensitivity prediction model based on a machine learning model called elastic net regression. Machine Learning Models Were Proved To Successfully predict the drug sensitivity of patients with ovary an cancer.[53] These patients predicted by the model to be resistant include ovary an cancer patients treated with tamoxifen, gastric cancer patients treated with 5FU and endometrial cancer patients treated paclitaxel. All of these patients were proved to have poor prognosis. This study shows that artificial intelligence has great potential in predicting the sensitivity of anticancer drugs. AI also plays a prominent role in addressing drug resistance in cancer.[54] AI can quickly understand how cancer cells become resistant to cancer drugs by learning and analyzing data on large drug-resistant cancer, which can help improve drug development and adjust drug use. Figure (5)

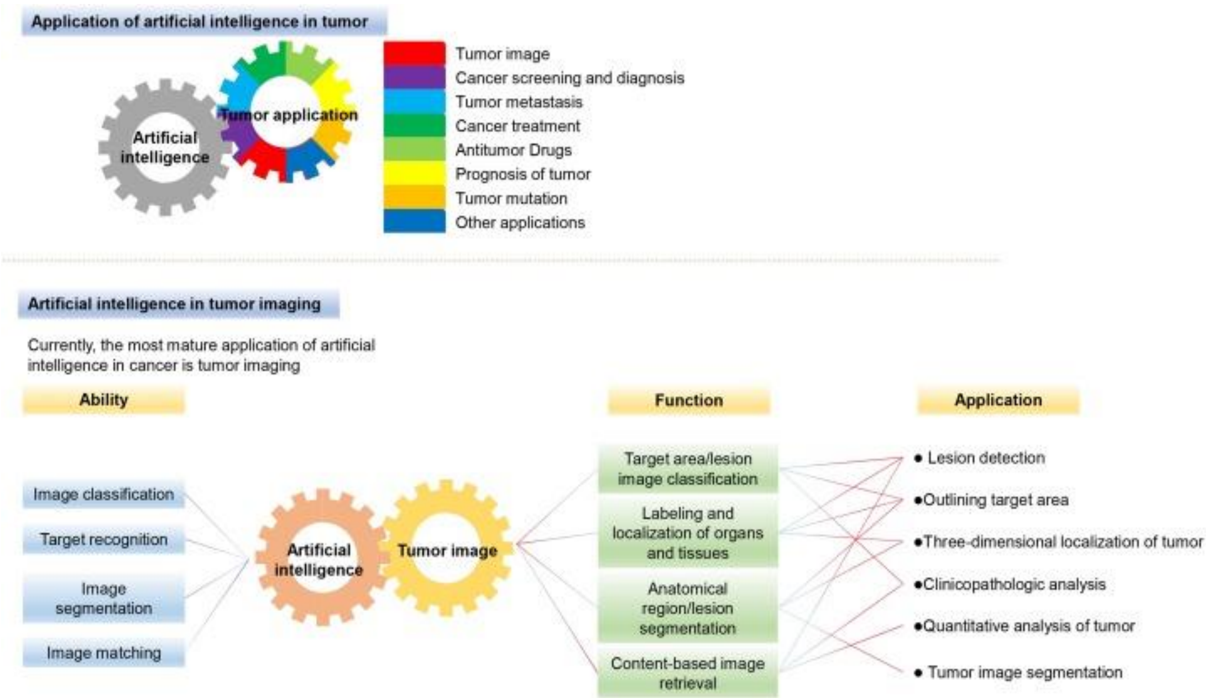

Fig. 5: The applications of AI in tumors.

The AI could improve cancer imaging, cancer screening and diagnosis, cancer treatment and cancer drugs and other fields. AI can promote cancer research and clinical practice.

At present, the most mature application of AI in the field of cancer should be cancer imaging. Some excellent performances of AI fittheneeds of medical imaging, and the combination of the two can promote the progress of cancer research.

3.1. AI and chemotherapy

In the field of cancer chemotherapy, AI focuses more on the response between drugs and patients. The main application achievements of AI include management of chemotherapy drug use, prediction of chemotherapy drug tolerance and optimization of chemotherapy program.[55] AI can perfect and accelerate the optimization process of combined chemotherapy. In one study, the researchers successfully determined the optimal dose ofzen-3694and enzalutamide by using "CURATE. AI" (anartificial intelligence platform created by National University of Singapore using deep learning and other technologies), thus improving the efficacy and tolerance of the combined treatment (56) developed a machine learning algorithm that can predict the tolerance of breast cancer to chemotherapy. The study, which explored the relationship between chemotherapy drugs and patients' genes, was able to distinguish between the effects of two chemotherapy drugs, taxolor gemcitabine. In addition, studies have shown that deep learning method is significantly better than the Epstein-Barr Virus-DNA-based model in risk stratification and guidance of induction chemotherapy for naso-pharyngeal carcinoma.[57] It means that the guiding role of deep learning method can be used as a potential indicator to predict single induction chemotherapy for advanced nasopharyngeal carcinoma.[58]

3.2. AI and radiotherapy

In the course of cancer radiotherapy, the application of AI technology more specific AI can help radiologists map out target or automatically plan radiation regimens for treatment[59] used the three-dimensional convolutional neural network (3DCNN) to achieve automatic delineation of nasopharyngeal carcinoma, with an accuracy of 79%, which is comparable to that of radio therapy specialists. Cha et al.[60] combined deep learning technology with radiomics (a method of extracting image features from radiographic images) to build a predictive model that can evaluate the response to treatment of bladder cancer. Babier et al.[61].developed automations based on deep earning technology that reduced the time it took to plan radiation therapy to just a few hours. The treatment plan generated by he AI software is comparable to patients' conventional treatment plan and the time is greatly reduced (Fig.6).

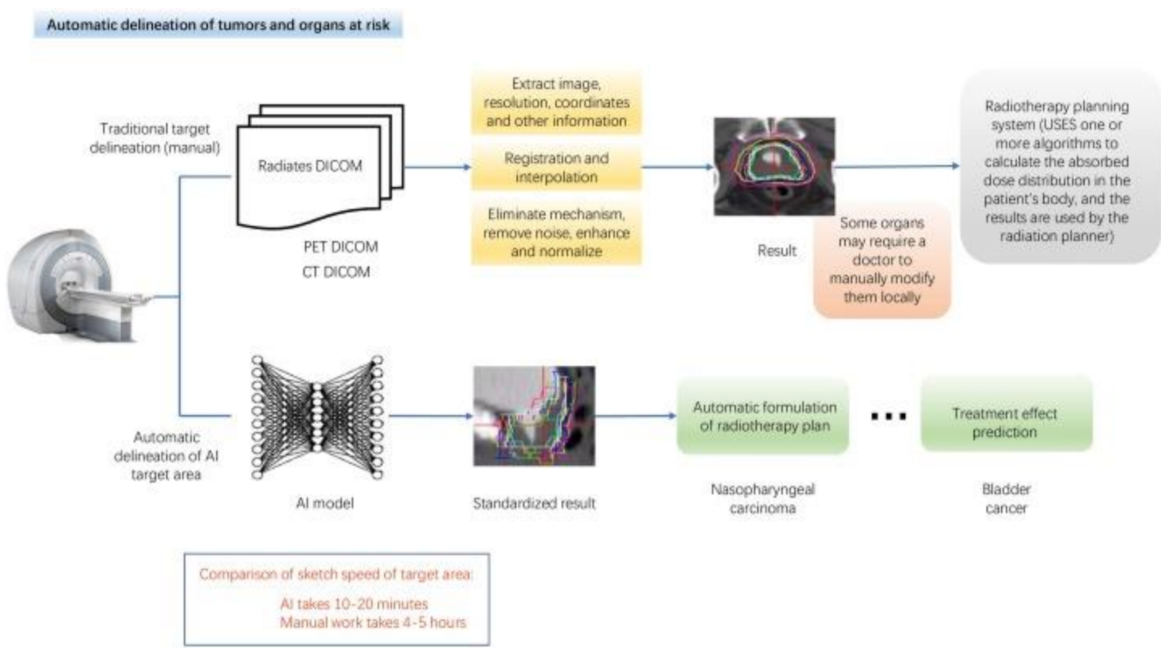

Fig. 6: Automatic delineation of tumors and organs at risk.

The application of AI in cancer radiotherapy mainly includes cancer target area, the delineation of organs at risk, and the automatic formulation of radiotherapy plans. The AI system can automatically realize the intelligent delineation of radiative images without manual registration, interpolation, and other operations. In addition, AI can directly predict three-dimensional dose distributions based on mapped organs and target areas, automating more personalized treatments.

3.3 AI and immunotherapy

In the application of cancer immunotherapy, AI mainly focuses on evaluating the treatment effect and helping physicians adjust the treatment plan.[62] Developed an AI platform based on machine learning to accurately predict the therapeutic effect of programmed cell death protein 1 (PD-1) inhibitors. This platform can effectively evaluate the effect of immunotherapy in patients with advanced solid tumors who are sensitive to PD-1 inhibitors. Bulik-Sullivanetall.[63] Developed a machine learning method based on a human leukocyte antigen (HLA) mass spectrometry database, which can improve the identification of cancer neoantigens and improve the efficacy of cancer immunotherapy.

4. Targeted drug delivery methods for cancer treatment

Over the past decades, there have been several advances and successes in cancer treatments. Due to an improved understanding of carcinogenesis processes, cell biology, and tumor microenvironment.[64] However, cancer is a complex disease; therefore, many types of cancer still have a high fatality rate. Targeted drug delivery in this context is highly critical for improving the survival rates of cancer patients with information that can ensure the accurate delivery of anticancer drugs.[65] In addition, drug targeting helps to define the selective release of cancer drugs at the specific tumor site with a higher pharmacological impact. Two targeting methods can be achieved using NPs: active Machine development.[66].In passive targeting, localization of NPs is best achieved for the organ of interest within the tumor microenvironment, whereas active targeting allows for identifying the uptake levels of NPs by the tumor cells.[67] (see Figure 7).

Through the revolutionization of artificial intelligence(AI) technologies in clinical research, significant improvement is observed in diagnosis of cancer. Utilization of these AI technologies, such as machine and deep learning, is imperative for the discovery of novel anticancer drugs and improves existing. However, building a model for complicated cancers and their types remains a challenge due to the lack of effective therapeutics that hinders the establishment of effective computational tools.

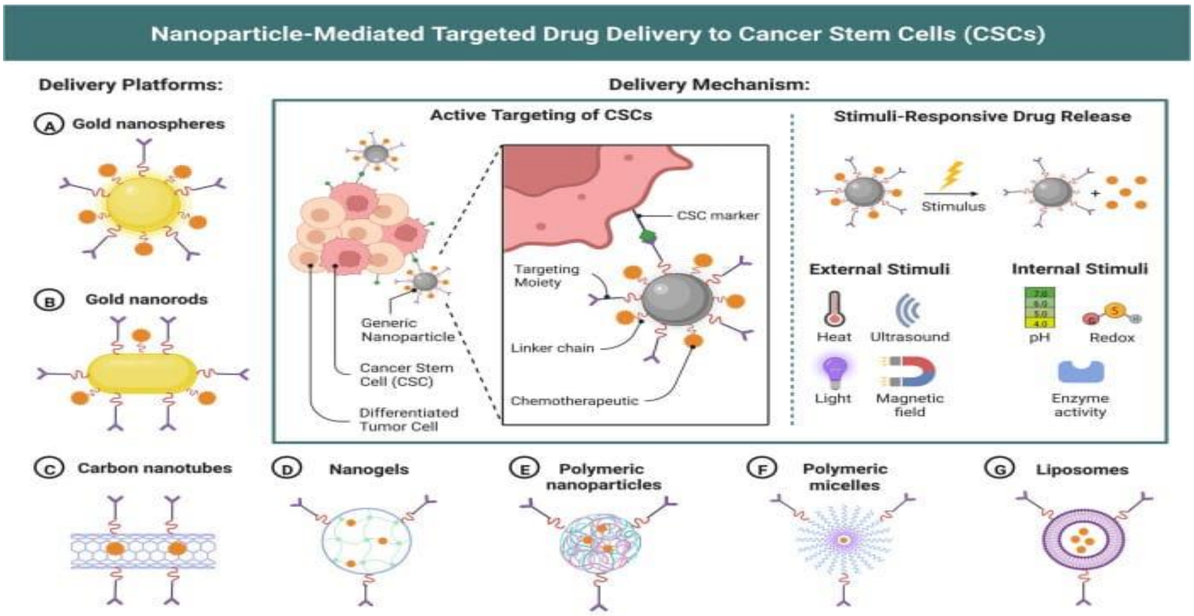

Fig 7: Nanoparticles mediated targeted drug delivery for cancer treatment.

4.1 .AI methods for cancer imaging

Recent empowerment and analysis in cancer imaging help to visualize tumor dissemination, screening of compound effects, multiple biological features of a cell, staging, and cancer treatment decision. Which are utilized for revolutionizing drug discovery. Radiomics and AI is an ideal platform for breast image analysis since it deals with various applications including breast cancer risk prognosis, lesion spotting and classifying, radiogenomics, and predicting medical results.

4.2 Anticancer drug design and discovery using AI

AI and its technologies have made a huge impact in multiple facets of cancer research. The complexity of drug synergy research relies on estimating broad range of drug combinations with broad range of drugs taken for estimations, which is rapidly evolving through the broad range of cancer types and dosages of drugs. A potential drug combination was discovered based on clinical research, which usually consumes more time and cost, and when the solution is not feasible, treatments may cause side.

4.3. Artificial Intelligence in pathology assists the accurate diagnosis of tumors

Pathological analysis is considered the gold standard of the clinical diagnosis of tumor.[68] However, the current shortage of clinical pathologists and their reliance on subjective consciousness for diagnosis leads to low repeatability and unequal diagnostic levels of clinical pathologists, which is not helpful for clinicians' decision-making with regards to treatment.[69] Computational pathology has seen significant developments from the use of improved AI algorithms and computing power.

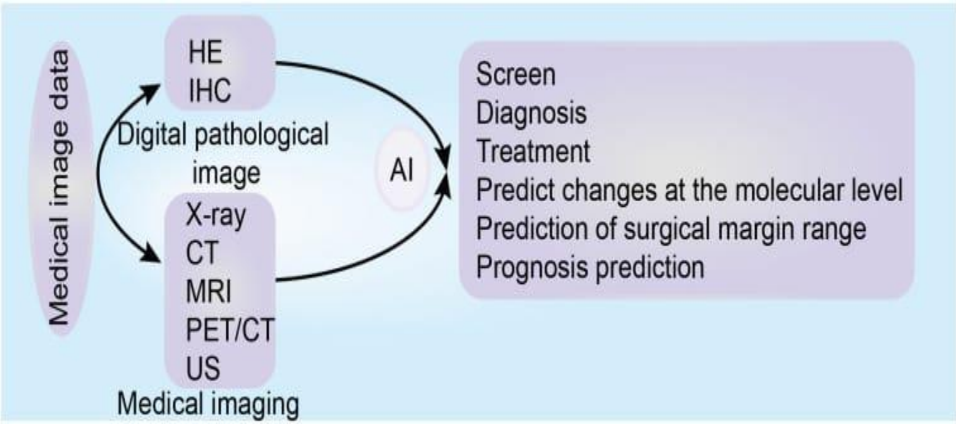

Figure 8: The role of AI in the digital pathological.

4.4. AI assists radiologists in accurately diagnosing tumors

AI has three main tasks in tumor imaging: Detecting, characterizing and monitoring tumors.[70] Detection refers to the location of the region of interest in the image. Characterization includes tumor diagnosis, and staging. Monitoring refers to the monitoring of the changes in tumors with time.[71] The process of ML-assisted tumor detection and diagnosis is as follows: Image data acquisition, image preprocessing, segmentation of regions of interest, feature selection, establishing the model and carrying out training, verification and testing.[72]

5. Future perspectives

A comprehensive overview on current applications of AI in oncology-related areas is provided, specifically describing the AI-based devices that have already obtained the official approval to enter into clinical practice. Starting from its birth, AI demonstrated its cross-cutting importance in all scientific branches, showing an impressive growth potential for the future. As highlighted in this study, this growth has interested also oncology and related specialties.

6. Applications of AI in Cancer

AI in Lung Cancer: Biomedical imaging and ML provided a new dimension to research. The initial stage of lung cancer detection is always important. ML added new features and possibilities to enhance lung cancer diagnosis and tracking treatment response. Various models are being designed to propagate the initial stage of detection and enable AI to meaningfully categorize lung nodules into two classes namely benign or malignant.[73]

AI in Breast Cancer: A statistical report says, among the various cancers, breast cancer is the most frequently diagnosed cancer.[74]

AI in CNS Tumor: CNS tumors occurrence present itself with a large spectrum in the field of pathology and are possibly more diverse with respect to any other tumors in the human body. This wide range of diagnoses demands a very unique and accurate estimation of imaging modalities. One of the most important biomarkers that aid in determining the prognosis in CNS tumors is Isocitrate Dehydrogenase (IDH). The changes in the presence of IDH mutation can be effectively recognized using machine learning methods including deep CNNs trained on conventional MR images.[75-76]

7. Limitations and Future prospects of AI in cancer

AI is continuing to prove its potential and efficacy in various stages of disease confronting such as early detection, treatment planning and prediction of future outcomes. Despite the increased advancements being made in AI and its applications in oncology, there are numerous limitations and setbacks that needs to be addressed. Few of them include issues with data access, generalizability, developing real-world applications, interpretation issues, ‘black box’ problem, and challenges pertaining to education and expertise in the field. Although various literature evidences have proved AI to be efficient in diagnosing and outcome prediction of various cancers, the generalizability of the said AI application needs to be validated, as most studies would be confined to a particular disease type in a specific population, with data being obtained from a particular institution/repository. Efforts needs to be made in terms of promoting medical data sharing among institutes and carrying out multiple external validations. Numerous attempts are being carried out in developing real world applications, however, AI training is a data-hungry method requiring a multi-faceted approach from all the institutions worldwide. One of the other major challenges that’s being currently faced while using AI in medical domain, is trying to interpret as to how AI model came up with the solution. This limitation in the ability to precisely understand the logic behind these algorithms is termed as the “black box” problem.

Artificial Intelligence used in anticancer drug development

Artificial intelligence (AI) is used in many ways to improve the development and use of anticancer drugs, including:

Predicting patient response

AI tools can predict how a patient's cancer will respond to a specific drug by analyzing data from individual cells within tumors.

Understanding drug resistance

AI can help identify how cancer cells become resistant to drugs, which can help improve drug development and use.

Identifying tumor neoantigens

AI can help identify tumor neoantigens, which can improve the efficacy of tumor immunotherapy.

Managing chemotherapy

AI can help manage the use of chemotherapy drugs, including predicting how well a patient will tolerate them.

Designing drug combinations

AI can help design combinations of drugs with different targets and pathways.

Predicting patient survival

AI tools like chief can predict patient survival and the risk of death.

In silico clinical trials

AI-based in silico clinical trials are still in the early stages, but they could significantly reduce the cost and duration of clinical trials

Artificial Intelligence works on anticancer drug development

Artificial intelligence (AI) is helping to improve anticancer drug development in several ways, including

Identifying drug targets: AI can analyze large amounts of data to identify novel targets for anticancer drugs.

Predicting drug efficacy and toxicity: AI can predict the efficacy and toxicity of drugs from their computer-designed molecular structures.

Improving drug combinations: AI can help design drug combinations that target different pathways.

Understanding drug resistance: AI can help identify how cancer cells become resistant to drugs, which can help improve drug development.

Predicting patient survival: AI tools can predict patient survival and the risk of death.

Improving chemotherapy regimens: AI can help manage chemotherapy drugs and predict how well patients will tolerate them.

Planning radiation treatment: AI can help radiologists map target areas and plan radiation treatment programs.

Artificial intelligence (AI) can be used in many ways in the pharmaceutical industry

Drug discovery: AI can help predict a drug's bioactivity by analyzing data on known compounds. AI can also help speed up the process of discovering new drugs, reducing the time it takes from 5-6 years to just one year.

Quality control: AI can monitor dosage, temperature, and ingredient types to help maintain product integrity throughout the supply chain.

Manufacturing: AI can help streamline biopharma manufacturing.

Clinical trials: AI can help improve the flow of clinical trial data.

Supply chain: AI can help enable self-healing supply chain applications.

Patient education: AI can help patients learn how and when to take their medication, and how to adhere to their treatment plan.

Healthcare collaboration: AI can help improve collaboration between different healthcare services for a single patient.

Precision medicine: AI can help cluster patients based on predictive factors to improve patient selection for clinical development.

CONCLUSION

AI has shown promising results in certain fields of oncology, including tumor screening, detection, diagnosis, treatment, and prognosis prediction. With the progress of AI, the improvement of computer performance, and the explosive growth of various data, new learning methods, such as the hybrid learning method, will continue to emerge, further improving the overall performance of the model, such as efficient data analysis and accurate prediction. The recent model generated by the ML and DL that can analyze various data sets will also improve the prospects of PM. In conclusion, AI-assisted PM can help detect, diagnose and treat cancer early, as well as assist in the selection of the best treatment scheme, consequently improving the prognosis of patients and improving their treatment results.

REFERENCES

1. Moreau, P.; Garfall, A.L.; van de Donk, N.W.C.J.; Nahi, H.; San-Miguel, J.F.; Oriol, A.; Nooka, A.K.; Martin, T.; Rosinol, L.; Chari, A.; et al. Teclistamab in Relapsed or Refractory Multiple Myeloma. N. Engl. J. Med. 2022; 387: 495–505.
2. Avery, R.K.; Alain, S.; Alexander, B.D.; Blumberg, E.A.; Chemaly, R.F.; Cordonnier, C.; Duarte, R.F.; Florescu, D.F.; Kamar, N.; Kumar, D.; et al. Maribavir for Refractory Cytomegalovirus Infections With or Without Resistance Post-Transplant: Results From a Phase 3 Randomized Clinical Trial. Clin. Infect. Dis., 2022; 75: 690–701.
3. Siegel, R.L.; Miller, K.D.; Fuchs, H.E.; Jemal, A. Cancer statistics, 2022. CA Cancer J. Clin. 2022; 72: 7–33.
4. Li, N.; Spetz, M.R.; Li, D.; Ho, M. Advances in immunotherapeutic targets for childhood cancers: A focus on glypican-2 and B7-H3. Pharmacol. Ther. 2021; 223: 107892.
5. C.M. Lo, U. Iqbal, Y.J. Li Cancer quantification from data mining to artificial intelligenceComput. Methods Programs Biomed., 2017; 145: A1
6. W.L. Bi, A. Hosny, M.B. Schabath, M.L. Giger, N.J. Birkbak, A. Mehrtash, T. Allison, O. Arnaout, C. Abbosh, I.F. Dunn, R.H. Mak, R.M. Tamimi, C.M. Tempany, C. Swanton, U. Hoffmann, L.H. Schwartz, R.J. Gillies, R.Y. Huang, H. AertsArtificial intelligence in cancer imaging: clinical challenges and applicationsCA Cancer J. Clin., 2019; 69(2): 127-157 .
7. Shabani, M. & Hojjat-Farsangi, M. Targeting receptor tyrosine kinases using monoclonal antibodies: the most specific tools for targeted-based cancer therapy. Curr. Drug Targets, 2016; 17: 1687–1703.
8. Paananen, J. & Fortino, V. An omics perspective on drug target discovery platforms. Brief. Bioinform, 2019; 21: 1937–1953.
9. Hopkins, A. L. & Groom, C. R. Opinion: The druggable genome. Nat. Rev. Drug Discov, 2002; 1: 727–730.

10. Bushweller, J. H. Targeting transcription factors in cancer—from undruggable to reality. Nat. Rev. Cancer, 2019; 19: 611–624.
11. Colaprico, A. et al. Interpreting pathways to discover cancer driver genes with Moonlight. Nat. Commun, 2020; 11(69).
12. Manzari, M. T. et al. Targeted drug delivery strategies for precision medicines. Nat. Rev. Mater, 2021; 6: 351–370.
13. Rosenblum, D., Joshi, N., Tao, W., Karp, J. M. & Peer, D. Progress and challenges towards targeted delivery of cancer therapeutics. Nat. Commun, 2018; 9: 1410.
14. Chen, L. & Wu, J. Bio-network medicine. J. Mol. Cell Biol., 2015; 7: 185–186.
15. Ghanat Bari, M., Ung, C. Y., Zhang, C., Zhu, S. & Li, H. Machine learning-assisted network inference approach to identify a new class of genes that coordinate the functionality of cancer networks. Sci. Rep., 2017; 7: 6993.
16. Muzio, G., O'Bray, L. & Borgwardt, K. Biological network analysis with deep learning. Brief. Bioinform, 2021; 22: 1515–1530.
17. Camacho, D. M., Collins, K. M., Powers, R. K., Costello, J. C. & Collins, J. J. Next-generation machine learning for biological networks. Cell, 2018; 173: 1581–1592.
18. World Health Organization. Cancer. (2022). Available at: https://www.who.int/news-room/fact-sheets/detail/cancer (cited August 29, 2022).
19. Olusanya TOB, Haj Ahmad RR, Ibegbu DM, Smith JR, Elkordy AA. Liposomal drug delivery systems and anticancer drugs. Molecules, 2018; 23(4): 907. 10.3390/molecules23040907
20. Kumar A, Sharipov M, Turaev A, Azizov S, Azizov I, Makhado E, et al. Polymer-Based hybrid nanoarchitectures for cancer therapy applications. Polymers (Basel), 2022; 14(15): 3027. 10.3390/polym14153027.
21. Qindeel M, Sargazi S, Hosseinikhah SM, Rahdar A, Barani M, Thakur VK, et al. Porphyrin-based nanostructures for cancer theranostics: chemistry: fundamentals and recent advances. Chemistry Select, 2021; 6(48): 14082–99. 10.1002/slct.202103418.
22. Patra JK, Das G, Fraceto LF, Campos EVR, Rodriguez-Torres MDP, Acosta-Torres LS, et al. Nano based drug delivery systems: recent developments and future prospects. J Nanobiotechnol, 2018; 16(1): 71. 10.1186/s12951-018-0392-8.
23. Gupta AK, Gupta M. Synthesis and surface engineering of iron oxide nanoparticles for biomedicalapplications. Biomaterials, 2005; 26(18): 3995–4021. 10.1016/j.biomaterials.2004.10.012.
24. Rudramurthy GR, Swamy MK, Sinniah UR, Ghasemzadeh A. Nanoparticles: alternatives against drug resistant pathogenic microbes. Molecules, 2016; 21(7): 836.10.3390/molecules21070836.
25. McGranahan N, Swanton C. Clonal heterogeneity and tumor evolution: past, present, and the future. Cell, 2017; 168(4): 613–28. 10.1016/j.cell.2017.01.018.
26. Longo DL. Tumor heterogeneity and personalized medicine. N Engl J Med, 2012; 366(10): 956–7. 10.1056/NEJMe1200656.
27. L. Wang et al.Artificial intelligence facilitates drug design in the big data era Chemometr. Intell. Lab. Syst, 2019.
28. P. Moingeon et al. Artificial intelligence-enhanced drug design and development: toward a computational precision medicine Drug Discov, Today 2022.
29. S.R. Khan et al.Integration of AI and traditional medicine in drug discovery Drug Discov. Today, 2021.
30. Bray F, Ren JS, Masuyer E, Ferlay J. Global estimates of cancer prevalence for 27 sites in the adult population in 2008. Int J Cancer, 2013; 132(5): 1133–45. doi: 10.1002/ijc.27711.

31. Torre LA, Siegel RL, Ward EM, Jemal A. Global cancer incidence and mortality rates and trends–an update. Cancer Epidemiol Biomarkers Prev, 2016; 25(1): 16–27. doi: 10.1158/1055-9965.EPI-15-0578 .
32. Consortium, I.T.P.-C.A.o.W.G . Pan-cancer analysis of whole genomes. Nature, 2020; 578(7793): 82–93.
33. MacEachern SJ, Forkert ND. Machine learning for precision medicine. Genome, 2021; 64(4): 416–25. doi: 10.1139/gen-2020-0131 .
34. Zhou J, Sun H, Wang Z, Cong W, Wang J, Zeng M, et al.. Guidelines for the diagnosis and treatment of hepatocellular carcinoma (2019 edition). Liver Cancer, 2020; 9(6): 682–720. doi: 10.1159/000509424 .
35. Le Berre C, Sandborn WJ, Aridhi S, Devignes M-D, Fournier L, Smail-Tabbone M, et al.. Application of artificial intelligence to gastroenterology and hepatology. Gastroenterology, 2020; 158(1): 76–+. doi: 10.1053/j.gastro.2019.08.058.
36. Senan EM, Jadhav ME, Rassem TH, Aljaloud AS, Mohammed BA, Al-Mekhlafi ZG. Early diagnosis of brain tumour MRI images using hybrid techniques between deep and machine learning. Comput Math Methods Med, 2022; 2022. doi: 10.1155/2022/8330833.
37. Rajput G, Agrawal S, Biyani K, Vishvakarma SK. Early breast cancer diagnosis using cogent activation function-based deep learning implementation on screened mammograms. Int J Imaging Syst Technol, 2022; 32(4): 1101–18. doi: 10.1002/ima.22701.
38. Qiu H, Ding S, Liu J, Wang L, Wang X. Applications of artificial intelligence in screening, diagnosis, treatment, and prognosis of colorectal cancer. Curr Oncol, 2022; 29(3): 1773–95. doi: 10.3390/curroncol29030146.
39. Kaczmarek E, Pyman B, Nanayakkara J, Tuschl T, Tyryshkin K, Renwick N, et al.. Discriminating neoplastic from nonneoplastic tissues using an miRNA-based deep cancer classifier. Am J Pathol, 2022; 192(2): 344–52. doi: 10.1016/j.ajpath.2021.10.012.
40. Kaul V, Enslin S, Gross SA. History of artificial intelligence in medicine. Gastrointest Endosc, 2020; 92: 807–12.
41. Hamamoto R, Suvarna K, Yamada M, Kobayashi K, Shinkai N, Miyake M, et al. Application of artificial intelligence technology in oncology: towards the establishment of precision medicine. Cancers, 2020; 12: 3532.
42. World health statistics 2018: monitoring health for the SDGs, sustainable development goals OMS, 2018.
43. Global Cancer Incidence and Mortality Rates and Trends--An Update Torre L. A., Siegel R. L., Ward E. M., Jemal A.. Cancer Epidemiology Biomarkers & Prevention, 2015; 25.
44. Hou Ming-Feng, Chuang Hung-Yi, Ou-Yang Fu, Wang Chen-Ya, Huang Chyi-Lie, Fan Hui-Mei, Chuang Chieh-Han, Wang Jaw-Yuan, Hsieh Jan-Singh, Liu Gin-Chung, Huang Tsung-Jen. Ultrasound in Medicine & Biology, 2002; 28.
45. Ghimire, A.; Tayara, H.; Xuan, Z.; Chong, K.T. CSatDTA:Int. J. Mol. Sci., 2022; 23: 8453.
46. Peng, J.; Wang, Y.; Guan, J.; Li, J.; Han, R.; Hao, J.; Wei, Z.; Shang, X. An end-to-end heterogeneous graph representation learning-based framework for drug-target interaction prediction. Brief. Bioinform, 2021; 22: bbaa430.
47. Yang, Z.; Zhong, W.; Zhao, L.; Chen, C.Y.-C. ML-DTI: Mutual Learning Mechanism for Interpretable Drug-Target Interaction Prediction. J. Phys. Chem. Lett., 2021; 12: 4247–4261.
48. Dara, S.; Dhamercherla, S.; Jadav, S.S.; Babu, C.M.; Ahsan, M.J. Machine Learning in Drug Discovery: A Review. Artif. Intell. Rev., 2022; 55: 1947–1999.

49. Madhukar, N.S.; Khade, P.K.; Huang, L.; Gayvert, K.; Galletti, G.; Stogniew, M.; Allen, J.E.; Giannakakou, P.; Elemento, O. A Bayesian machine learning approach for drug target identification using diverse data types. Nat. Commun, 2019; 10: 5221.
50. Olayan, R.S.; Ashoor, H.; Bajic, V.B. DDR: Efficient computational method to predict drug-target interactions using graph mining and machine learning approaches. Bioinformatics, 2018; 34: 1164–1173.
51. Raies, A.; Tulodziecka, E.; Stainer, J.; Middleton, L.; Dhindsa, R.S.; Hill, P.; Engkvist, O.; Harper, A.R.; Petrovski, S.; Vitsios, D. DrugnomeAI is an ensemble machine-learning framework for predicting druggability of candidate drug targets. Commun. Biol., 2022; 5: 1291.
52. A.P. Lind, P.C. Anderson Predicting drug activity against cancer cells by random forest models based on minimal genomic information and chemical properties PLoS One, 2019; 147): Article e0219774.
53. J.F. McDonald Back to the future - the integration of big data with machine learning is re-establishing the importance of predictive correlations in ovarian cancer diagnostics and therapeutics Gynecol. Oncol., 2018; 149(2): 230-231.
54. J.T. Beck, M. Rammage, G.P. Jackson, A.M. Preininger, I. Dankwa-Mullan, M.C. Roebuck, A. Torres, H. Holtzen, S.E. Coverdill, M.P. Williamson, Q. Chau, K. Rhee, M. Vinegra Artificial intelligence tool for optimizing eligibility screening for clinical trials in a large community Cancer center JCO Clin. Cancer Inform., 2020; 4: 50-59.
55. M. Smail-Tabbone, B. Rance, I.Y.S.O.B. Section Editors for the I. Translational Contributions from the 2018 literature on bioinformatics and translational informatics Yearb. Med. Inform., 2019; 28(1): 190-193.
56. A.J. Pantuck, D.-K. Lee, T. Kee, P. Wang, S. Lakhotia, M.H. Silverman, C. Mathis, A. Drakaki, A.S. Belldegrun, C.-M. Ho, D. Ho Modulating BET bromodomain inhibitor ZEN-3694 and enzalutamide combination dosing in a metastatic prostate Cancer patient using CURATE.AI, an artificial intelligence platform Adv. Ther., 2018; 1(6): Article 1800104.
57. X. Tang, Y. Huang, J. Lei, H. Luo, X. Zhu The single-cell sequencing: new developments and medical applications Cell Biosci., 2019; 9: 53.
58. H. Peng, D. Dong, M.-J. Fang, L. Li, L.-L. Tang, L. Chen, W.-F. Li, Y.-P. Mao, W. Fan, L.-Z. Liu, L. Tian, A.-H. Lin, Y. Sun, J. Tian, J. Ma Prognostic value of deep learning PET/CT-Based radiomics: potential role for future individual induction chemotherapy in advanced nasopharyngeal carcinoma Clin. Cancer Res., 2019; 25; 4271-4279.
59. P. Meyer, V. Noblet, C. Mazzara, A. Lallement Survey on deep learning for radiotherapy Comput. Biol. Med., 2018; 98; 126-146.
60. K.H. Cha, L. Hadjiiski, H.P. Chan, A.Z. Weizer, A. Alva, R.H. Cohan, E.M. Caoili, C. Paramagul, R.K. Samala Bladder Cancer treatment response assessment in CT using radiomics with deep-learning Sci. Rep., 2017; 7(1): 8738.
61. A. Babier, J.J. Boutilier, A.L. McNiven, T.C.Y. Chan Knowledge-based automated planning for oropharyngeal cancer Med. Phys., 2018; 45(7): 2875-2883.
62. S. Trebeschi, S.G. Drago, N.J. Birkbak, I. Kurilova, A.M. Calin, A. Delli Pizzi, F. Lalezari, D.M.J. Lambregts, M.W. Rohaan, C. Parmar, E.A. Rozeman, K.J. Hartemink, C. Swanton, J. Haanen, C.U. Blank, E.F. Smit, R.G.H. Beets-Tan, H. Aerts Predicting response to cancer immunotherapy using noninvasive radiomic biomarkers.Ann. Oncol., 2019; 30(6): 998-1004.

63. B. Bulik-Sullivan, J. Busby, C.D. Palmer, M.J. Davis, T. Murphy, A. Clark, M. Busby, F. Duke, A. Yang, L. Young, N.C. Ojo, K. Caldwell, J. Abhyankar, T. Boucher, M.G. Hart, V. Makarov, V.T. Montpreville, O. Mercier, T.A. Chan, G. Scagliotti, P. Bironzo, S. Novello, N. Karachaliou, R. Rosell, I. Anderson, N. Gabrail, J. Hrom, C. Limvarapuss, K. Choquette, A. Spira, R. Rousseau, C. Voong, N.A. Rizvi, E. Fadel, M. Frattini, K. Jooss, M. Skoberne, J. Francis, R. YelenskyDeep learning using tumor HLA peptide mass spectrometry datasets improves neoantigen identification Nat. Biotechnol, 2018; 10.1038/nbt.4313.
64. Sonnenschein C, Soto AM. Over a century of cancer research: inconvenient truths and promising leads. PLoS Biol, 2020; 18(4): e3000670. 10.1371/journal.pbio.3000670.
65. Veselov VV, Nosyrev AE, Jicsinszky L, Alyautdin RN, Cravotto G. Targeted delivery methods for anticancer drugs. Cancers (Basel), 2022; 14(3): 622. 10.3390/cancers14030622.
66. Singh R, Lillard JW. Nanoparticle-based targeted drug delivery. Exp Mol Pathol, 2009; 86(3): 215–23. 10.1016/j.yexmp.2008.12.004.
67. Bazak R, Houri M, El Achy S, Kamel S, Refaat T. Cancer active targeting by nanoparticles: a comprehensive review of literature. J Cancer Res Clin Oncol, 2015; 141(5): 769–84. 10.1007/s00432-014-1767-3.
68. Wu Y, Cheng M, Huang S, Pei Z, Zuo Y, Liu J, et al.. Recent advances of deep learning for computational histopathology: Principles and applications. Cancers, 2022; 14(5): 1199. doi: 10.3390/cancers14051199.
69. Robertson S, Azizpour H, Smith K, Hartman J. Digital image analysis in breast pathology–from image processing techniques to artificial intelligence. Trans Res, 2018; 194: 19–35. doi: 10.1016/j.trsl.2017.10.010.
70. Bi WL, Hosny A, Schabath MB, Giger ML, Birkbak NJ, Mehrtash A, et al.. Artificial intelligence in cancer imaging: Clinical challenges and applications. CA Cancer J Clin, 2019; 69(2): 127–57. doi: 10.3322/caac.21552.
71. Dhahri H, Al Maghayreh E, Mahmood A, Elkilani W, Faisal Nagi M. Automated breast cancer diagnosis based on machine learning algorithms. J Healthcare Eng, 2019; 2019: 4253641. doi: 10.1155/2019/4253641.
72. Hawkins Samuel, Wang Hua, Liu Ying, Garcia Alberto, Stringfield Olya, Krewer Henry, Li Qian, Cherezov Dmitry, Gatenby Robert A., Balagurunathan Yoganand, Goldgof Dmitry, Schabath Matthew B., Hall Lawrence, Gillies Robert J.. Journal of Thoracic Oncology, 2016; 11(12).
73. Liu Ying, Balagurunathan Yoganand, Atwater Thomas, Antic Sanja, Li Qian, Walker Ronald C., Smith Gary T., Massion Pierre P., Schabath Matthew B., Gillies Robert J.. Clinical Cancer Research, 2016; 23(6).
74. Ciompi Francesco, Chung Kaman, van Riel Sarah J., Setio Arnaud Arindra Adiyoso, Gerke Paul K., Jacobs Colin, Scholten Ernst Th., Schaefer-Prokop Cornelia, Wille Mathilde M. W., Marchianò Alfonso, Pastorino Ugo, Prokop Mathias, van Ginneken Bram. Scientific Reports, 2017; 7(1).
75. Global cancer statistics 2018: GLOBOCAN estimates of incidence and mortality worldwide for 36 cancers in 185 countries Bray Freddie, Ferlay Jacques, Soerjomataram Isabelle, Siegel Rebecca L., Torre Lindsey A., Jemal Ahmedin. CA: A Cancer Journal for Clinicians, 2018; 68(6).
76. Chang Ken, Bai Harrison X., Zhou Hao, Su Chang, Bi Wenya Linda, Agbodza Ena, Kavouridis Vasileios K., Senders Joeky T., Boaro Alessandro, Beers Andrew, Zhang Biqi, Capellini Alexandra, Liao Weihua, Shen Qin, Li Xuejun, Xiao Bo, Cryan Jane, Ramkissoon Shakti, Ramkissoon Lori, Ligon Keith, Wen Patrick Y., Bindra Ranjit S., Woo John, Arnaout Omar, Gerstner Elizabeth R., Zhang Paul J., Rosen Bruce R., Yang Li, Huang Raymond Y., Kalpathy-Cramer Jayashree. Clinical Cancer Research, 2017; 24(5).