Global Journal of Basic Science ISSN : XXXX-XXXX

Review

Role of artificial intelligence in cancer diagnosis and treatment: current trends and future directions

Haisam Khurshid [1,*]

[1] Department of Mechanical Engineering, Zakir Husain College of Engineering and Technology, Aligarh Muslim University, Aligarh, 202202, U.P., India; khurshidhaisam@gmail.com.

* Correspondence: khurshidhaisam@gmail.com (H.K.)

Citation: Khurshid H. Role of artificial intelligence in cancer diagnosis and treatment: current trends and future directions. *Jour. Bas. Sci.* 2024, 1(1). 1-13.

Received: September 07, 2024
Revised: October 11, 2024
Accepted: October 19, 2024
Published: November 01, 2024

doi: 10.63454/jbs20000001

ISSN: XXXX-XXXX

Abstract: Artificial Intelligence (AI) in healthcare is essential in the fight against several deadly illnesses, including lung, breast, and skin cancer. AI is a sophisticated system that recognizes difficult healthcare unit challenges by using mathematically based algorithmic concepts that are similar to those of the human mind. Many aetiologies, including a large number of genetic and epigenetic abnormalities, contribute to the deadly disease known as cancer. It is challenging to diagnose cancer early on since it is a complex disease. Thus, using AI and machine learning (ML), genetic variants and other important elements could be found in due time. AI is a synergistic way to mining large amounts of raw data for pharmacological targets, mechanisms of action, and interactions with organisms. Although there are a number of data mining issues with this synergistic method, computational techniques from various scientific groups for multi-target drug discovery are particularly beneficial in overcoming the AI bottlenecks for drug-target discovery. In the near future, AI and ML may serve as the central hub for the diagnosis, management, and assessment of nearly any illness in the medical field. In this thorough analysis, we examine the enormous potential of artificial intelligence (AI) and machine learning (ML) in conjunction with the biological sciences, particularly with regard to cancer research. Here, we explored the recent updates related to AI and ML applications in cancer diagnosis and therapeutics.

Keywords: Artificial Intelligence (AI); cancer diagnosis; cancer treatment; machine learning; digital pathology

1. Introduction

In cancer research, diagnosis, and treatment, artificial intelligence (AI) is becoming a game-changer, providing previously unheard-of chances to tackle the intricacies of this difficult area. Computational systems that can efficiently handle and analyse large volumes of data related to cancer are necessary for the integration of complex research findings with this data. AI offers strong tools for addressing the complex issues related to biological anomalies like cancer by applying sophisticated algorithms created to mimic human cognitive processes[1-11].

AI's potential, especially when paired with machine learning (ML), is becoming more widely acknowledged as being essential to contemporary healthcare. Large, diverse datasets can be processed with the help of these technologies to find patterns and insights that are hard, if not impossible, to find with conventional techniques. Researchers and medical professionals can improve the accuracy and effectiveness of cancer detection and therapy by applying these cutting-edge computational tools. Furthermore, new diagnostic tools that may detect diseases at incredibly early stages have been developed as a result of recent developments in AI and ML[12-15]. Tools for diagnosing autonomic neuropathy, which is frequently linked to a number of systemic disorders, serve as an example of how these technologies might be used in more general medical settings (Figure 1). These developments in oncology have great potential for early cancer detection, which would enable prompt treatments and better patient outcomes.

It is anticipated that as AI and ML develop further, their incorporation into healthcare systems will transform the field of illness management and make them essential for promoting precision medicine and individualised treatment.

A branch of machine learning called deep learning (DL) uses artificial neural networks to automatically extract valuable features from data. In contrast to conventional techniques, deep learning enables the creation of end-to-end prediction models by combining feature extraction and model training into a single procedure. More thorough and precise predictions are made possible by this method, which lessens the constraints and biases brought about by manually created characteristics[6, 16-24].

The capacity of deep learning to examine large and complicated datasets, revealing complex patterns and drawing insightful conclusions that could be impossible for humans to decipher, is one of its main advantages. Deep learning has changed the game in the field of medical imaging. These algorithms can help medical personnel locate lesions, identify abnormalities, and provide diagnostic support by automating the interpretation of medical pictures. In addition to reducing medical professionals' burden, this improves diagnostic precision and reduces mistakes.

Numerous medical imaging tasks, including as image classification, segmentation, lesion identification, and registration, have found use for deep learning approaches.They have been effectively used to analyse a variety of imaging modalities, including CT scans, MRIs, and X-rays. Lung, rectal, pancreatic, stomach, prostate, brain, and breast cancers are among the many tumors that these technologies have shown excellent promise in identifying[25-31].

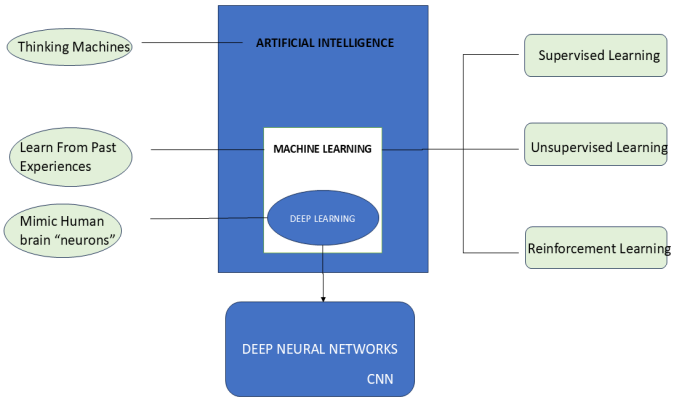

Figure 1. AI applications and the layout.

Researchers from all across the world are paying close attention to deep learning's enormous promise in cancer diagnoses. It is anticipated that the technology's use in medical picture analysis will grow as it develops further. This article offers a thorough summary of deep learning's contributions to cancer diagnosis through medical imaging, acknowledging the significance of these developments. It seeks to provide the most up-to-date information and techniques to seasoned researchers who want to improve their work, as well as a thorough resource for novices in the subject.

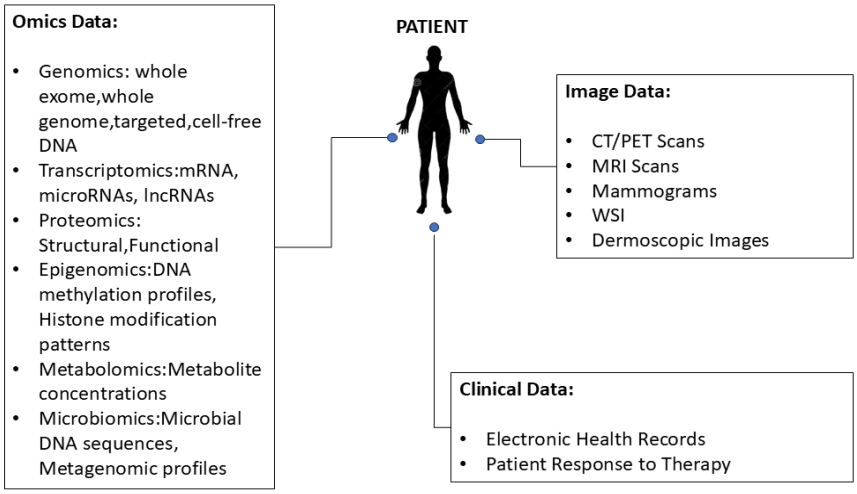

Figure 2. Data integration for patient diagnosis and the potential need to use AI/ML.

2. Application of Deep Learning in Cancer Diagnoses

2.1. Medical Image Analysis in Cancer Diagnosis Using Deep Learning: One of the most important uses of deep learning (DL) in cancer diagnosis is now medical image analysis. DL has revolutionised the way academics and physicians analyse medical pictures by processing vast amounts of imaging data and revealing complex patterns. Cancer detection, diagnosis, and monitoring have advanced significantly as a result of this use, frequently with greater accuracy and efficiency than with conventional techniques[26, 27, 32-36].

2.1.1. Image Classification: Medical image classification into predetermined classes, such as differentiating between normal and diseased tissues, is a strength of deep learning algorithms. For example, medical image classification is a common application of convolutional neural networks (CNNs), a family of deep learning models (Figure 3). In order to find patterns suggestive of malignancy, these models examine characteristics like texture, shape, and intensity. By categorising mammograms, chest CT scans, and MRI pictures, respectively, this has been especially helpful in the diagnosis of cancers such as breast, lung, and brain tumors[6, 7, 33, 37-39].

2.1.2. Tumor Segmentation: In medical imaging, segmentation is an essential step for separating malignant tissues from nearby healthy structures. Tumor boundaries in imaging modalities including CT, MRI, and PET scans can be accurately delineated by DL-based segmentation algorithms like U-Net and its variations. These models help with treatment planning, including identifying targets for radiation therapy, by precisely determining the area of a tumor. For instance, segmentation aids in the visualisation of tumor areas and their infiltration into nearby brain tissues during the diagnosis of glioblastoma[33, 40-44].

2.1.3. Lesion Detection: Finding lesions in medical imaging can be difficult, especially when the cancer is still in its early stages and the abnormalities are typically minor and undetectable. DL models that have been trained on large datasets are remarkably sensitive in detecting suspicious regions. For example, algorithms for the diagnosis of lung cancer can

examine CT scans of the chest to find small nodules that might be signs of cancer. Similar to this, DL models help detect masses and microcalcifications in mammograms that are suggestive of early-stage breast cancer[45-50].

2.1.4. Image registration: Aligning images acquired from several modalities or time points for comparative analysis is known as image registration. By automating the alignment of datasets, DL techniques simplify this procedure and make it simpler to track the course of a disease or the effectiveness of treatment. In the diagnosis of prostate cancer, for instance, the alignment of MRI and PET scans aids in the integration of functional and anatomical data, offering a more thorough comprehension of the condition[34, 51-53].

2.1.5. Radiomics and feature extraction: The extraction of radiomic features—quantitative aspects of medical imaging that reveal underlying tumor biology—is aided by deep learning. Tumor aggressiveness, responsiveness to treatment, and patient outcomes can all be predicted with the use of these characteristics, which include texture, shape, and intensity distributions. By automating this extraction procedure, DL models can reveal hidden traits that human observers would miss[18, 34, 54-60].

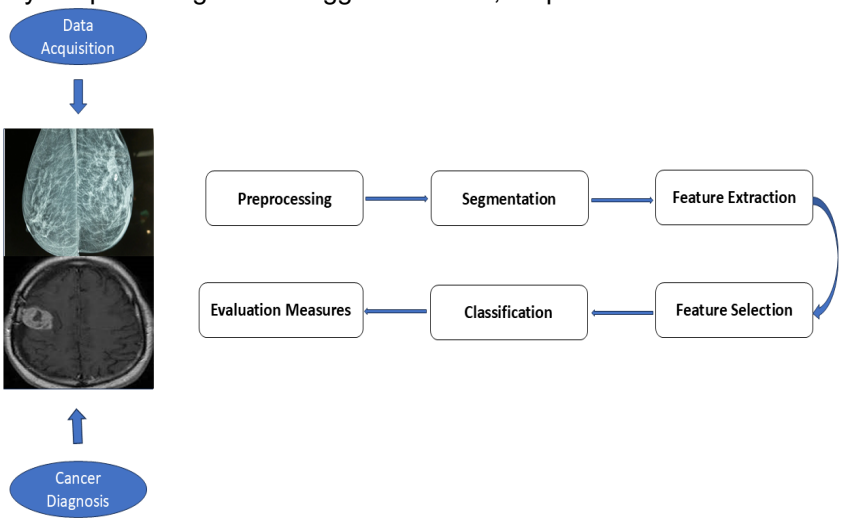

Figure 3. Digital pathology and AI/ML application.

2.1.6. Enhanced accuracy and workflow efficiency: By lowering false positives and negatives, deep learning has greatly improved diagnostic accuracy. Additionally, by automating repeated procedures, it increases workflow efficiency in medical environments. AI systems, for example, pre-screen mammograms in breast cancer screening programs, freeing up clinicians to concentrate on the most urgent cases and maximising their workload[51, 61-65].

2.1.7. Multimodal Analysis: DL makes it possible to analyse several imaging modalities at once. For instance, a more thorough understanding of lung cancer can be obtained by integrating pathology images and CT scans. This multimodal method helps guide individualised treatment strategies by facilitating a more thorough and accurate assessment of cancer[27].

3. Histopathology and cytology in cancer diagnosis using deep learning

Two fundamental methods for diagnosing cancer are histopathology and cytology, which use microscopic analysis of tissue and cell samples to find cancers. Nevertheless, these techniques are frequently time-consuming, labor-intensive, and dependent on pathologists' knowledge, which may result in inconsistent diagnostic precision. In this field, deep learning (DL) has become a game-changing technique that makes it possible to analyze histopathological and cytological data automatically, consistently, and with extreme accuracy[66-71] (Figures 3 and 4).

3.1.1. Automated tissue classification: Convolutional neural networks (CNNs), a type of deep learning algorithm, have demonstrated remarkable success in dividing tissue samples into benign, precancerous, and malignant groups. These models are highly accurate in identifying cancer by examining the morphological and structural characteristics of tissues. The time needed for manual evaluation has been greatly decreased by using DL models, for instance, to differentiate between normal and malignant areas in whole-slide images (WSIs) of breast, lung, and prostate tissue[38].

3.1.2. Subtype classification and grading: In addition to identifying the existence of cancer, DL models are able to categorize it into distinct subtypes and assign a severity rating. For example, DL has been used to distinguish between invasive ductal carcinoma (IDC) and ductal carcinoma in situ (DCIS) in breast cancer, allowing for more individualized treatment planning. Similar to this, algorithms evaluate Gleason patterns in prostate cancer to provide precise grades that inform prognostic and treatment choices[6, 33, 37-39, 72].

3.1.3. Nucleus detection and segmentation: When diagnosing cancer, the morphological features of the cell nucleus are crucial. In histopathology slides, DL methods like U-Net and Mask R-CNN are excellent at detecting and segmenting nuclei. These algorithms provide information on tumor heterogeneity and progression by identifying differences in nuclear structure, size, and density linked to malignancies. Additionally, automated nucleus segmentation makes quantitative analysis easier, including the computation of mitotic indices—a critical component of tumor grading[33, 34, 39, 73].

3,1,4. Cytological analysis: Developments in DL are particularly advantageous for cytology, which is concerned with individual cells rather than tissue architecture. Pap smears and other cytological images can be used to train algorithms

that can detect anomalies suggestive of cervical cancer. By detecting early-stage lesions with high sensitivity and specificity, these systems help screening programs by lowering the number of false positives and negatives[33].

3.1.5. Biomarker detection and prediction: Patterns found in histopathological images are linked to genetic biomarkers, such as IDH mutations in gliomas or HER2 status in breast cancer. To avoid the necessity for extra molecular testing, DL models are being created to predict these indicators straight from histopathological slides. This reduces expenses and turnaround times while also streamlining the diagnostic workflow[10, 11, 70, 74-97].

3.1.6. Tumor microenvironment analysis: By examining the interactions between cancer cells and the stromal or immune cells that surround them, deep learning is also improving our understanding of the tumor microenvironment. DL offers information on immune response, tumor growth, and possible treatment targets by measuring these interactions. Tumor-infiltrating lymphocyte (TIL) spatial analysis employing DL, for example, has been connected to immunotherapy response in a number of malignancies[1, 98-108].

3.1.7. Enhancing pathologist efficiency: By identifying regions of interest and pre-analyzing slides, DL systems assist pathologists in making decisions. Pathologists are able to concentrate on challenging cases, reduce workload, and minimize diagnostic errors as a result. Algorithms included into digital pathology systems, for instance, can rank instances that need urgent care, increasing the overall effectiveness of cancer diagnosis.

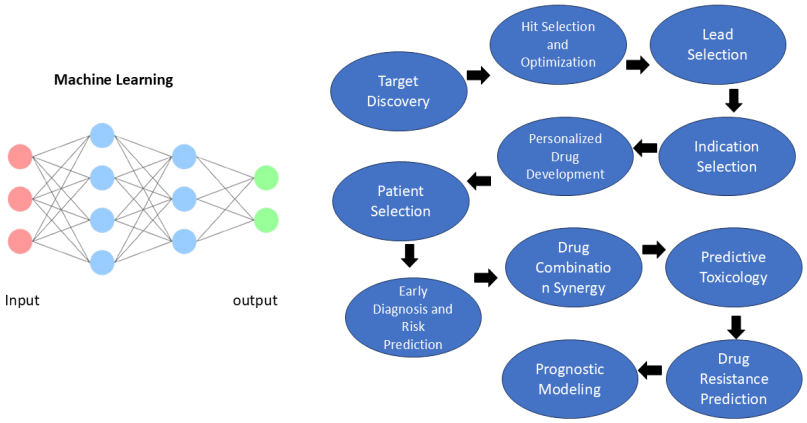

Figure 4. Machine learning application and processing layout.

4. Genomic and molecular data analysis

In order to facilitate precision oncology and comprehend the complex mechanisms behind the advancement of cancer, it is essential to analyse genetic and molecular data. A potent technique for handling the enormous and intricate datasets produced by genomic and molecular profiling methods is deep learning (DL). By using these methods, scientists and medical professionals can find useful biomarkers, create individualised treatment plans, and gain important insights into the biology of cancer.

Because it provides previously unheard-of insights into the biological causes of the disease, the analysis of genomic and molecular data has emerged as a key component of contemporary cancer research and clinical practice. Researchers can learn vital details about the processes behind cancer growth, progression, and treatment resistance by examining the genetic and molecular makeup of tumors. These analyses change the way cancer is identified, treated, and managed by facilitating a greater knowledge of the disease at the systems biology level. The advancement of precision medicine is among the most important contributions made by genomic and molecular data analysis. Clinicians can customise treatment plans to the particulars of each patient's cancer by detecting molecular markers, aberrant gene expression patterns, and particular genetic abnormalities. For example, the development of targeted treatments that increase treatment success while reducing adverse effects has been directed by genetic markers like EGFR mutations in lung cancer or HER2 overexpression in breast cancer. In addition to improving patient outcomes, this individualised strategy lessens needless treatment burdens[79, 84, 109-125].

Another crucial component of the importance of genomic and molecular data is its capacity for prediction. By assisting in the stratification of patients according to their risk profiles and anticipated course of disease, biomarkers obtained from such analysis can offer useful prognostic information. This makes it possible for medical professionals to decide on follow-up care and the severity of treatment with knowledge. Predictive biomarkers can also indicate how a patient will react to particular treatments, like immunotherapy or chemotherapy, which helps to improve treatment plans and steer clear of ineffective ones. Analysis of genetic and molecular data is crucial for speeding up the development of cancer drugs, in addition to its influence on clinical practice. Researchers can find possible treatment targets and create medications that specifically block these pathways by determining the molecular causes of cancer. Additionally, a thorough grasp of tumor biology is provided by the integration of multi-omics data, such as proteomics, metabolomics, and genomes, which promotes the identification of new targets and combination treatments.

Analysing genomic and molecular data is crucial for comprehending tumor heterogeneity, which is a defining feature of cancer. Different cell subpopulations with unique genetic and molecular features frequently make up tumors. By clarifying the mechanisms underlying treatment resistance and disease recurrence, an analysis of these variances aids in the development of solutions. Furthermore, the knowledge gathered from these studies helps to design clinical trials, which increases the chances of trial success by allowing the selection of suitable patient groups.

To sum up, the analysis of genetic and molecular data is a game-changing tool in the fight against cancer, propelling advancements in drug development, precision medicine, biomarker discovery, and tumor biology knowledge. In the years to come, it has the potential to transform cancer care and improve patient outcomes through its ongoing integration into clinical and research workflows.

4.1.1. Application of deep learning in genomic data analysis: In the analysis of genetic data, deep learning models have proven very effective, providing new avenues for cancer research and diagnosis:

I. Mutation detection and classification: Single nucleotide variations (SNVs) and structural variants, two genetic changes that are major causes of cancer, can be found using DL algorithms. For example, transformer-based models and recurrent neural networks (RNNs) have been used to examine DNA sequences and find oncogenesis-related mutations like TP53 or KRAS mutations.

II. Biomarker discovery: DL models make it easier to find biomarkers that can be used as indicators of the occurrence, course, or response to treatment of diseases by utilising extensive genetic information. For instance, BRCA1/2 mutations and other clinically significant markers have been found using DL, allowing for early detection and focused treatments for ovarian and breast malignancies.

III. Gene expression analysis: Differential gene expression patterns across cancer subtypes can be revealed by applying DL to RNA sequencing data. These studies help identify possible therapy targets, classify tumors, and predict prognoses.

4.1.2. Application of deep learning in molecular data analysis: To provide a more thorough understanding of cancer biology, DL has been effectively used to molecular-level data in addition to genomes, including proteomics, metabolomics, and epigenomics:

I. Protein structure prediction: Protein function and its role in carcinogenesis may now be understood with unparalleled accuracy thanks to DL models like AlphaFold, which have completely changed the prediction of protein structures[25, 126-130].

II. Pathway modeling and analysis: Rebuilding and examining the metabolic networks and signalling pathways linked to cancer is made possible by DL methods. This aids in clarifying the molecular processes behind the development and spread of tumors.

III. Drug target identification: Finding new therapeutic targets is made possible by deep learning algorithms that examine interactions between proteins and between drugs. This is especially important for creating customised medication regimens or inhibitors for undruggable targets.

5. Application of AI/ML in therapeutic target discovery and drug development

The combination of artificial intelligence (AI) and machine learning (ML) technologies is causing a radical change in the drug research and development process, which has historically been linked to high prices and lengthy delays. AI is playing a significant role in expediting and simplifying the identification of therapeutic targets and the development of new medications, particularly with the introduction of reasonably priced next-generation sequencing (NGS) technology and the growing accessibility of extensive cancer-related datasets. Clinical, genomic, proteomic, and imaging data are just a few of the numerous and varied data sets that AI models can now combine to improve every step of the drug discovery process.

5.1. Therapeutic target discovery: The way that researchers find promising drug targets is changing as a result of AI-driven therapeutic target discovery techniques. Target identification has always depended on an understanding of biological processes and recognised disease mechanisms, which is laborious and prone to error. Large datasets, including gene expression profiles, protein-protein interaction networks, and clinical data, are now analysed using AI and ML approaches to more accurately and efficiently discover possible therapeutic targets.

Tong et al., for example, used a one-class support vector machine approach to suggest potential therapeutic targets in liver cancer research by integrating clinical data, gene expression patterns, and protein interaction networks. With an area under the curve (AUC) of 0.88, this method produced a strong model that demonstrated AI's ability to identify promising treatment targets from intricate biological data sets. Similarly, to anticipate proteins important in breast cancer pathogenesis, López-Cortés et al. used deep learning-based categorisation approaches and integrated multiple cancer-related databases, including TCGA, PharmGKB, and Cancer Genome Interpreter. A number of intriguing medication development prospects were found using this integrative technique. Additionally, programs like the DepMap Consortium have made useful resources available, including as loss-of-function screen datasets, which have made it possible to use AI in more ways to find therapeutic targets that are particular to cancer. Applying AI to datasets like the DepMap is assisting in identifying the most pertinent experimental data types that should be given priority for therapy discovery, in addition to possible targets.

5.2. Drug design and molecule generation: AI may be used for more than only finding targets; it can also be used to create therapeutic compounds. AI has the potential to simplify the labour-intensive, iterative trial-and-error processes that are the foundation of traditional drug design methodologies. AI-assisted in silico drug design makes it possible to

quickly generate and optimise new drug candidates with desired physicochemical characteristics and particular target binding affinities.

Molecular generation has benefited greatly from reinforcement learning, a branch of artificial intelligence. With this method, a reward system provides feedback to an AI model, directing it to produce molecules that satisfy predetermined standards. For instance, Olivecrona et al. showed how a recurrent neural network (RNN) model could produce Celecoxib analogues and molecules devoid of sulphur when it was optimised using policy-based reinforcement learning. This approach has a lot of potential for effectively producing new therapeutic compounds. Similar to this, You et al. created new compounds using a graph convolutional network (GCN), a model that is especially well-suited for creating chemical molecules. Compared to conventional 2D representations, GCNs have the benefit of being able to model molecules in three dimensions, which enables a more realistic depiction of chemical interactions.

Additionally, drug design is using Generative Adversarial Networks (GANs), which are made up of two competing networks (a discriminator and a generator). GANs have shown promise in generating compounds with desired pharmacological characteristics, such as drug-likeness, solubility, and synthesizability. One such method is the MolGAN approach. The identification and optimisation of new drug candidates has been completely transformed by these AI-based methods, which has resulted in quicker and more focused drug development.

5.3. Drug Repurposing: An economical and successful substitute for conventional drug discovery techniques is drug repurposing, which entails discovering novel therapeutic applications for already-approved medications. By discovering possible new uses for medications based on gene expression patterns, chemical structural similarities, and clinical data, artificial intelligence (AI) models—in particular, deep neural networks, or DNNs—have sped up the repurposing process. AI may use the comprehensive transcriptional datasets from the Library of Integrated Network-Based Cellular Signatures (LINCS), including gene perturbation profiles, to find potential candidates for drug repurposing. For instance, AI models can find medications that reverse cancer-specific markers and recommend their repurposing in oncology by comparing the gene expression profiles of cancer cells with those of normal cells. Repurposing candidates can be ranked according to their structural resemblance to recognised cancer treatments, and DNNs trained on these data sets have demonstrated promise in predicting therapeutic categories for medications (such as vasodilators and antineoplastics).

Based on each patient's unique genetic alterations, AI also uses publicly accessible datasets, such as those from cell viability tests like GDSC, PRISM, and NCI-60, to forecast which medications will work best for cancer patients. Using these datasets, the CDRScan tool—an ensemble of five convolutional neural network (CNN) models—offers a customised approach to drug repurposing by recommending the best medication for each patient. Furthermore, by combining known clinical annotations and drug chemical structures, AI models such as DeepDR and PREDICT are being used to find new drug-disease connections, perhaps leading to new therapeutic indications for already-approved medications.

6. Current challenges and future perspectives in AI applications for cancer

AI has the ability to completely change the way that cancer is treated by providing revolutionary opportunities in prevention, diagnosis, therapy, and research. Even while AI applications in the lab have shown impressive results, there are still many obstacles to overcome before these developments can be applied in clinical settings. In order to fully utilise AI to improve cancer outcomes, several issues must be resolved.

6.1. Challenges in data diversity and representation: For AI algorithms to produce precise predictions, large and complete datasets are necessary. However, varied communities are frequently under-represented in contemporary datasets. Although the differences in cancer incidence and progression by socioeconomic status, race, and gender are well established, training datasets often contain data from certain populations, such as people with European ancestry. Furthermore, a lot of datasets only include primary tumors, ignoring metastatic occurrences, which restricts their usefulness for comprehending advanced cancer stages.

Due to problems like genetic drift, cell lines—which are commonly employed in preclinical research—also fall short in reproducing the intricacies of patient-specific profiles. Although patient-derived organoids have emerged as a more precise and reliable substitute, their incorporation into conventional research is still developing. To create AI models that are inclusive and generalisable across populations, these gaps must be filled.

6.2. Data sharing and accessibility: The restricted availability of important datasets because of corporate limitations and privacy concerns is another major obstacle. Although there are now more public data platforms available, private or controlled-access datasets are still not being used to their full potential. A crucial first step in encouraging cooperation and improving the repeatability of AI models is making sure that data repositories are open-access, standardised, and harmonised.

In a similar vein, code sharing is crucial to reproducibility and transparency in AI-driven cancer research. Many studies lack well-documented and annotated code, even with the advent of platforms like GitHub and Docker for sharing version-controlled settings. Code sharing is becoming more and more required by journals, which encourages open science and cooperative developments in AI-driven cancer treatment.

6.3. Underutilization of electronic health records (EHR): Though their potential is yet mostly unrealised, electronic health records are a treasure trove of patient data that capture comprehensive clinical histories. Actionable insights are difficult to draw from EHR data because of its unstructured and inconsistent nature. These problems are starting to be addressed by recent initiatives including standardising patient data using common data models and developing approachable frameworks for longitudinal data visualisation. Effective use of EHR will greatly expand AI's application in predictive analytics and personalised treatment.

6.4. Building trust among clinicians: Gaining physician trust is crucial to the complete integration of AI into clinical practice. Quantifying and resolving uncertainty in AI predictions is one crucial issue. Prediction variability can be caused by a variety of factors, including model bias, artefacts, and data accuracy. Creating methodical techniques to evaluate and mitigate uncertainty will boost trust in AI-assisted decision-making.

The "black-box" aspect of deep learning models, which frequently obscures their decision-making procedures, is another issue. To increase AI models' adoption in clinical settings, efforts must be made to improve model interpretability by comprehending how these models process data and discovering the biological insights they disclose.

7. Future directions: prevention and personalization

In the future, prevention rather than therapy may be where AI has the biggest influence on cancer care. Thanks to wearable technologies, electronic health records, and genetic testing, it is now possible to gather enormous volumes of data about individual patients. AI systems can combine these data sources to provide individualised, real-time insights into cancer risk, assisting people in implementing preventative measures.

AI may, for example, evaluate cancer risk with previously unheard-of accuracy by combining genetic predispositions with environmental and lifestyle data. The creation of customised preventative strategies, early intervention, and even remote patient monitoring that notifies doctors of possible problems could all be made possible by this connection.

By improving efficiency, accuracy, and personalisation in these areas, artificial intelligence is revolutionising the fields of patient care, cancer therapy, and drug development. It has already proven that it can quickly identify therapeutic targets, create new medications, and repurpose current therapies. Nevertheless, there are certain difficulties in incorporating AI into clinical practice. The need for more inclusive and standardised methods is highlighted by dataset biases, restricted access to high-quality data, and the underutilisation of electronic health records.

Furthermore, efforts must be made to increase interpretability and foster clinician trust due to the opaque nature of AI models and the "black-box" nature of deep learning. The clinical application of AI will depend on addressing these problems through open data sharing, reproducibility of AI models, and uncertainty quantification.

In the future, AI may be crucial in identifying cancer risk and customising preventative care, demonstrating that its promise goes beyond therapy. AI has the ability to deliver real-time, patient-specific suggestions by combining genetic, clinical, and environmental data, thereby completely changing the way that cancer is treated.

In conclusion, even though there are still obstacles to overcome, artificial intelligence (AI) offers enormous and revolutionary potential in the fields of oncology and drug development. AI will become a pillar of contemporary medicine through cooperative efforts to overcome present constraints, leading to innovations that benefit patients everywhere.

Author Contributions: Conceptualization, H.K.; methodology, H.K.; software, H.K.; validation, H.K.; formal analysis, H.K.; investigation, H.K.; resources, H.K.; data curation, H.K.; writing—original draft preparation, H.K.; writing—review and editing, H.K.; visualization, H.K.; supervision, H.K.; project administration, H.K.; funding acquisition, H.K. The author has read and agreed to the published version of the manuscript.; funding acquisition, H.K. The author has read and agreed to the published version of the manuscript.

Funding: This research received no external funding.

Acknowledgments: I am thankful to Department of Mechanical Engineering, Zakir Husain College of Engineering and Technology, Aligarh Muslim University, Aligarh, 202202, U.P., India for providing us the resources and the facility to carry out the work.

Conflicts of Interest: The authors declare no conflict of interest. The funders had no role in the design of the study; in the collection, analyses, or interpretation of data; in the writing of the manuscript, or in the decision to publish the results.

Institutional Review Board Statement: Not applicable.

Informed Consent Statement: Not applicable.

Data Availability Statement: Not applicable.

References

1. Allam, M., S. Cai, and A.F. Coskun, *Multiplex bioimaging of single-cell spatial profiles for precision cancer diagnostics and therapeutics.* npj Precision Oncology, 2020. **4**(1): p. 11.
2. Attolini, C.S.O., P.F. Stadler, and C. Flamm, *CelloS: A multi-level approach to evolutionary dynamics.* Advances in Artifical Life, Proceedings, 2005. **3630**: p. 500-509.
3. Banerji, C.R.S., et al., *Clinical AI tools must convey predictive uncertainty for each individual patient.* Nature Medicine, 2023. **29**(12): p. 2996-2998.

4. Bang, D., et al., *Biomedical knowledge graph learning for drug repurposing by extending guilt-by-association to multiple layers.* Nat Commun, 2023. **14**(1): p. 3570.
5. Bernett, J., et al., *Guiding questions to avoid data leakage in biological machine learning applications.* Nat Methods, 2024. **21**(8): p. 1444-1453.
6. Eftekharian, M., A. Nodehi, and R. Enayatifar, *ML-DSTnet: A Novel Hybrid Model for Breast Cancer Diagnosis Improvement Based on Image Processing Using Machine Learning and Dempster-Shafer Theory.* Comput Intell Neurosci, 2023. **2023**: p. 7510419.
7. Esteva, A., et al., *Dermatologist-level classification of skin cancer with deep neural networks.* Nature, 2017. **542**(7639): p. 115-118.
8. Gupta, A., et al., *Artificial intelligence guided conformational mining of intrinsically disordered proteins.* Communications Biology, 2022. **5**(1): p. 610.
9. Hager, P., et al., *Evaluation and mitigation of the limitations of large language models in clinical decision-making.* Nat Med, 2024.
10. Khan, B., et al., *Deciphering molecular landscape of breast cancer progression and insights from functional genomics and therapeutic explorations followed by in vitro validation.* Scientific Reports, 2024. **14**(1).
11. Qahwaji, R., et al., *Pharmacogenomics: A Genetic Approach to Drug Development and Therapy.* Pharmaceuticals, 2024. **17**(7).
12. Akl, M.A., et al., *Design, spectral, molecular modeling, antimitotic, analytical and mechanism studies of phenyl isothiocyanate Girard's T derived metal complexes.* BMC Chem, 2023. **17**(1): p. 153.
13. Audagnotto, M., et al., *Machine learning/molecular dynamic protein structure prediction approach to investigate the protein conformational ensemble.* Scientific Reports, 2022. **12**(1): p. 10018.
14. Berger, B., J. Peng, and M. Singh, *Computational solutions for omics data.* Nature Reviews Genetics, 2013. **14**(5): p. 333-346.
15. Boudin, M., et al., *The OREGANO knowledge graph for computational drug repurposing.* Sci Data, 2023. **10**(1): p. 871.
16. Cichonska, A., et al., *Computational-experimental approach to drug-target interaction mapping: A case study on kinase inhibitors.* PLoS Comput Biol, 2017. **13**(8): p. e1005678.
17. Dietterich, T.G., *Machine Learning.* Annual Review of Computer Science, 1990. **4**(1): p. 255-306.
18. Harrison, P.J., et al., *Deep-learning models for lipid nanoparticle-based drug delivery.* Nanomedicine, 2021. **16**(13): p. 1097-1110.
19. Herman, S., et al., *Disease phenotype prediction in multiple sclerosis.* iScience, 2023. **26**(6): p. 106906.
20. Hu, Y., et al., *A machine learning approach for the identification of key markers involved in brain development from single-cell transcriptomic data.* BMC Genomics, 2016. **17**(Suppl 13): p. 1025.
21. LeCun, Y., Y. Bengio, and G. Hinton, *Deep learning.* Nature, 2015. **521**(7553): p. 436-44.
22. Libbrecht, M.W. and W.S. Noble, *Machine learning applications in genetics and genomics.* Nature Reviews Genetics, 2015. **16**(6): p. 321-332.
23. Menden, M.P., et al., *Machine Learning Prediction of Cancer Cell Sensitivity to Drugs Based on Genomic and Chemical Properties.* PLoS ONE, 2013. **8**(4): p. e61318.
24. Ruff, K.M., T.S. Harmon, and R.V. Pappu, *CAMELOT: A machine learning approach for coarse-grained simulations of aggregation of block-copolymeric protein sequences.* The Journal of Chemical Physics, 2015. **143**(24): p. 243123.
25. Ahdritz, G., et al., *OpenFold: retraining AlphaFold2 yields new insights into its learning mechanisms and capacity for generalization.* Nat Methods, 2024. **21**(8): p. 1514-1524.
26. Fass, L., *Imaging and cancer: A review.* Molecular Oncology, 2008. **2**(2): p. 115-152.

27. Gutman, D.A., et al., *Cancer Digital Slide Archive: an informatics resource to support integrated in silico analysis of TCGA pathology data.* Journal of the American Medical Informatics Association, 2013. **20**(6): p. 1091-1098.
28. Nielsen, R.V., et al., *Personalized Intervention Based on Early Detection of Atherosclerosis: JACC State-of-the-Art Review.* J Am Coll Cardiol, 2024. **83**(21): p. 2112-2127.
29. Quaranta, V., et al., *Mathematical modeling of cancer: The future of prognosis and treatment.* Clinica Chimica Acta, 2005. **357**(2): p. 173-179.
30. Vartholomeos, P., et al., *MRI-Guided Nanorobotic Systems for Therapeutic and Diagnostic Applications.* Annual Review of Biomedical Engineering, 2011. **13**(1): p. 157-184.
31. Weber, W.P., et al., *ASO Visual Abstract: Impact of Imaging-Guided Localization on Performance of Tailored Axillary Surgery in Patients with Clinically Node-Positive Breast Cancer: Prospective Cohort Study Within TAXIS (OPBC-03, SAKK 23/16, IBCSG 57-18, ABCSG-53, GBG 101).* Ann Surg Oncol, 2023.
32. Binzer-Panchal, A., et al., *Integrated Molecular Analysis of Undifferentiated Uterine Sarcomas Reveals Clinically Relevant Molecular Subtypes.* Clin Cancer Res, 2019. **25**(7): p. 2155-2165.
33. Filipczuk, P., et al., *Computer-Aided Breast Cancer Diagnosis Based on the Analysis of Cytological Images of Fine Needle Biopsies.* IEEE Transactions on Medical Imaging, 2013. **32**(12): p. 2169-2178.
34. Giger, M.L., N. Karssemeijer, and J.A. Schnabel, *Breast Image Analysis for Risk Assessment, Detection, Diagnosis, and Treatment of Cancer.* Annual Review of Biomedical Engineering, 2013. **15**(1): p. 327-357.
35. Powell, B.M. and J.H. Davis, *Learning structural heterogeneity from cryo-electron sub-tomograms with tomoDRGN.* Nat Methods, 2024. **21**(8): p. 1525-1536.
36. Zysk, A.M. and S.A. Boppart, *Computational methods for analysis of human breast tumor tissue in optical coherence tomography images.* Journal of Biomedical Optics, 2006. **11**(5): p. 054015-054015-7.
37. Candia, J., et al., *From Cellular Characteristics to Disease Diagnosis: Uncovering Phenotypes with Supercells.* PLoS Computational Biology, 2013. **9**(9): p. e1003215.
38. Jackson, H.W., et al., *The single-cell pathology landscape of breast cancer.* Nature, 2020. **578**(7796): p. 615-620.
39. Rietdijk, J., et al., *A phenomics approach for antiviral drug discovery.* BMC Biology, 2021. **19**(1): p. 156.
40. Balluff, B., et al., *De novo discovery of phenotypic intratumour heterogeneity using imaging mass spectrometry.* J Pathol, 2015. **235**(1): p. 3-13.
41. Chen, X., et al., *CONSERTING: integrating copy-number analysis with structural-variation detection.* Nature Methods, 2015. **12**(6): p. 527-530.
42. Koboldt, D.C., et al., *VarScan 2: Somatic mutation and copy number alteration discovery in cancer by exome sequencing.* Genome Research, 2012. **22**(3): p. 568-576.
43. Zakov, S., M. Kinsella, and V. Bafna, *An algorithmic approach for breakage-fusion-bridge detection in tumor genomes.* Proceedings of the National Academy of Sciences, 2013. **110**(14): p. 5546-5551.
44. Zhang, Q., et al., *CMDS: a population-based method for identifying recurrent DNA copy number aberrations in cancer from high-resolution data.* Bioinformatics, 2010. **26**(4): p. 464-469.
45. Morris, D.S., et al., *Integrating Biomedical Knowledge to Model Pathways of Prostate Cancer Progression.* Cell Cycle, 2007. **6**(10): p. 1177-1187.
46. Schreer, I., *Early Detection and Diagnosis of Breast Cancer.* Breast Care, 2006. **1**(4): p. 227-228.
47. Shyamala, M., et al., *Detection of Mutations in EGFR in Circulating Lung-Cancer Cells.* New England Journal of Medicine, 2008. **359**(4): p. 366-377.
48. Stangis, M.M., et al., *The Hallmarks of Precancer.* Cancer Discov, 2024. **14**(4): p. 683-689.
49. Visvader, J.E., *Cells of origin in cancer.* Nature, 2011. **469**(7330): p. 314-322.

50. Wu, C.-L., et al., *Metabolomic Imaging for Human Prostate Cancer Detection.* Science Translational Medicine, 2010. **2**(16): p. 16ra8.
51. Ekvall, M., et al., *Spatial landmark detection and tissue registration with deep learning.* Nat Methods, 2024. **21**(4): p. 673-679.
52. Mishra, A., J. Nair, and A.M. Sharan, *Coping in Post-Mastectomy Breast Cancer Survivors and Need for Intervention: Systematic Review.* Breast Cancer (Auckl), 2023. **17**: p. 11782234231209126.
53. Pantazis, P. and W. Supatto, *Advances in whole-embryo imaging: a quantitative transition is underway.* Nature Reviews Molecular Cell Biology, 2014. **15**(5): p. 327-339.
54. Arinkin, V., et al., *Phenotyping date palm varieties via leaflet cross-sectional imaging and artificial neural network application.* BMC Bioinformatics, 2014. **15**(1): p. 55.
55. Berg, B.A.v.d., et al., *SPiCE: a web-based tool for sequence-based protein classification and exploration.* BMC Bioinformatics, 2014. **15**(1): p. 93.
56. Berry, M.W., et al., *Algorithms and applications for approximate nonnegative matrix factorization.* Computational Statistics & Data Analysis, 2007. **52**(1): p. 155-173.
57. Bray, M.-A., et al., *Cell Painting, a high-content image-based assay for morphological profiling using multiplexed fluorescent dyes.* Nature Protocols, 2016. **11**(9): p. 1757-1774.
58. Capobianco, E., *Model validation for gene selection and regulation maps.* Functional & Integrative Genomics, 2008. **8**(2): p. 87-99.
59. Hazes, B., *CDSbank: taxonomy-aware extraction, selection, renaming and formatting of protein-coding DNA or amino acid sequences.* BMC Bioinformatics, 2014. **15**(1): p. 61.
60. Li, C., et al., *BioModels Database: An enhanced, curated and annotated resource for published quantitative kinetic models.* BMC Systems Biology, 2010. **4**(1): p. 92.
61. Buggenthin, F., et al., *An automatic method for robust and fast cell detection in bright field images from high-throughput microscopy.* BMC Bioinformatics, 2013. **14**(1): p. 297.
62. Lång, K., et al., *Artificial intelligence-supported screen reading versus standard double reading in the Mammography Screening with Artificial Intelligence trial (MASAI): a clinical safety analysis of a randomised, controlled, non-inferiority, single-blinded, screening accuracy study.* The Lancet Oncology, 2023. **24**(8): p. 936-944.
63. Meijering, E., et al., *Imagining the future of bioimage analysis.* Nature Biotechnology, 2016. **34**(12): p. 1250-1255.
64. Olsson, H., et al., *Estimating diagnostic uncertainty in artificial intelligence assisted pathology using conformal prediction.* Nature Communications, 2022. **13**(1): p. 7761.
65. Shi, Y., et al., *Predicting early breast cancer recurrence from histopathological images in the Carolina Breast Cancer Study.* NPJ Breast Cancer, 2023. **9**(1): p. 92.
66. Elston, C.W. and I.O. Ellis, *Pathological prognostic factors in breast cancer. I. The value of histological grade in breast cancer: experience from a large study with long-term follow-up.* Histopathology, 1991. **19**(5): p. 403-10.
67. Hoffmann, L., et al., *Ganglioglioma with adverse clinical outcome and atypical histopathological features were defined by alterations in PTPN11/KRAS/NF1 and other RAS-/MAP-Kinase pathway genes.* Acta Neuropathol, 2023. **145**(6): p. 815-827.
68. Toivanen, R., et al., *A Preclinical Xenograft Model Identifies Castration-Tolerant Cancer-Repopulating Cells in Localized Prostate Tumors.* Science Translational Medicine, 2013. **5**(187): p. 187ra71.
69. Tsagozis, P., et al., *Sarcoma Tumor Microenvironment.* Adv Exp Med Biol, 2020. **1296**: p. 319-348.
70. Vorontsov, E., et al., *A foundation model for clinical-grade computational pathology and rare cancers detection.* Nat Med, 2024.

71. Yao, L., et al., *Human umbilical cord-derived mesenchymal stromal cells alleviate liver cirrhosis through the Hippo/YAP/Id1 pathway and macrophage-dependent mechanism.* Int Immunopharmacol, 2023. **123**: p. 110456.
72. Gordonov, S., et al., *Time series modeling of live-cell shape dynamics for image-based phenotypic profiling.* Integrative Biology, 2015. **8**(1): p. 73-90.
73. Li, F., et al., *Chapter 17: Bioimage Informatics for Systems Pharmacology.* PLoS Computational Biology, 2013. **9**(4): p. e1003043.
74. Prensner, J.R., et al., *Beyond PSA: The Next Generation of Prostate Cancer Biomarkers.* Science Translational Medicine, 2012. **4**(127): p. 127rv3.
75. Zhang, L., et al., *Salivary Transcriptomic Biomarkers for Detection of Resectable Pancreatic Cancer.* Gastroenterology, 2010. **138**(3): p. 949-957.e7.
76. Ahmed, S., et al., *A Network-Guided Approach to Discover Phytochemical-Based Anticancer Therapy: Targeting MARK4 for Hepatocellular Carcinoma.* Front Oncol, 2022. **12**: p. 914032.
77. Almowallad, S., R. Jeet, and M. Mobashir, *Systems-level understanding of toxicology and cardiovascular system.* Jour. Bas. Sci., 2024. **5**(1): p. 1-16.
78. Anwer, S.T., et al., *Synthesis of Silver Nano Particles Using Myricetin and the In-Vitro Assessment of Anti-Colorectal Cancer Activity: In-Silico Integration.* Int J Mol Sci, 2022. **23**(19).
79. Bajrai, L.H., et al., *Gene Expression Profiling of Early Acute Febrile Stage of Dengue Infection and Its Comparative Analysis With Streptococcus pneumoniae Infection.* Front Cell Infect Microbiol, 2021. **11**: p. 707905.
80. Bajrai, L.H., et al., *Understanding the role of potential pathways and its components including hypoxia and immune system in case of oral cancer.* Sci Rep, 2021. **11**(1): p. 19576.
81. Balling, R. and P.J. Stover, *Nutrition in the Age of Precision and Systems Biology.* Annual Review of Nutrition, 2023. **43**(1): p. v-vi.
82. Baylin, S.B. and P.A. Jones, *A decade of exploring the cancer epigenome — biological and translational implications.* Nature Reviews Cancer, 2011. **11**(10): p. 726-734.
83. Choudhry, H., et al., *Study of APOBEC3B focused breast cancer pathways and the clinical relevance.* Jour. Bas. Sci., 2024. **2**(1): p. 1-12.
84. El-Kafrawy, S.A., et al., *Genomic profiling and network-level understanding uncover the potential genes and the pathways in hepatocellular carcinoma.* Front Genet, 2022. **13**: p. 880440.
85. Eldakhakhny, B.M., et al., *In-Silico Study of Immune System Associated Genes in Case of Type-2 Diabetes With Insulin Action and Resistance, and/or Obesity.* Front Endocrinol (Lausanne), 2021. **12**: p. 641888.
86. Helmi, N., D. Alammari, and M. Mobashir, *Role of Potential COVID-19 Immune System Associated Genes and the Potential Pathways Linkage with Type-2 Diabetes.* Comb Chem High Throughput Screen, 2022. **25**(14): p. 2452-2462.
87. Huwait, E. and M. Mobashir, *Potential and Therapeutic Roles of Diosmin in Human Diseases.* Biomedicines, 2022. **10**(5).
88. Khan, B., et al., *Nivolumab and Ipilimumab Acting as Tormentors of Advanced Tumors by Unleashing Immune Cells and Associated Collateral Damage.* Pharmaceutics, 2024. **16**(6).
89. Khouja, H.I., et al., *Multi-staged gene expression profiling reveals potential genes and the critical pathways in kidney cancer.* Sci Rep, 2022. **12**(1): p. 7240.
90. Krishnamoorthy, P.K.P., et al., *In-silico study reveals immunological signaling pathways, their genes, and potential herbal drug targets in ovarian cancer.* Informatics in Medicine Unlocked, 2020. **20**: p. 100422.
91. Mobashir, M., et al., *An Approach for Systems-Level Understanding of Prostate Cancer from High-Throughput Data Integration to Pathway Modeling and Simulation.* Cells, 2022. **11**(24).
92. Mullard, A., *When can AI deliver the drug discovery hits?* Nature Reviews Drug Discovery, 2024. **23**(3): p. 159-161.

93. Mustafa, S. and M. Mobashir, *LC-MS and docking profiling reveals potential difference between the pure and crude fucoidan metabolites.* Int J Biol Macromol, 2020. **143**: p. 11-29.
94. Saddeek, S., R. Almassabi, and M. Mobashir, *Role of ZNF143 and Its Association with Gene Expression Patterns, Noncoding Mutations, and the Immune System in Human Breast Cancer.* Life (Basel), 2022. **13**(1).
95. Alammari, D., *Cytokine Signaling Pathways are involved in Lung Cancer and COVID-19.* Jour. Bas. Sci., 2024. **3**(1): p. 1-12.
96. Huwait, E.A., *Therapeutic agents for the management of atherosclerosis from herbal sources: A computational approach.* Jour. Bas. Sci., 2024. **4**(1): p. 1-24.
97. Almowallad, S., R. Jeet, and M. Mobashir, *A systems pharmacology approach for targeted study of potential inflammatory pathways and their genes in atherosclerosis.* Jour. Bas. Sci., 2024. **6**(1): p. 1-12.
98. Alexander, S. and P. Friedl, *Cancer invasion and resistance: interconnected processes of disease progression and therapy failure.* Trends in Molecular Medicine, 2012. **18**(1): p. 13-26.
99. Alkasalias, T., et al., *Fibroblasts in the Tumor Microenvironment: Shield or Spear?* Int J Mol Sci, 2018. **19**(5).
100. Allavena, P., et al., *Pathways connecting inflammation and cancer.* Current Opinion in Genetics & Development, 2008. **18**(1): p. 3-10.
101. Anderson, A.R.A., et al., *Microenvironmental Independence Associated with Tumor Progression.* Cancer Research, 2009. **69**(22): p. 8797-8806.
102. Balandrán, J.C., A. Lasry, and I. Aifantis, *The Role of Inflammation in the Initiation and Progression of Myeloid Neoplasms.* Blood Cancer Discovery, 2023. **4**(4): p. OF1-OF13.
103. Besse, B., et al., *Biomarker-directed targeted therapy plus durvalumab in advanced non-small-cell lung cancer: a phase 2 umbrella trial.* Nature Medicine, 2024: p. 1-14.
104. Cairns, R.A., I.S. Harris, and T.W. Mak, *Regulation of cancer cell metabolism.* Nature Reviews Cancer, 2011. **11**(2): p. 85-95.
105. Chan, N., M. Milosevic, and R.G. Bristow, *Tumor hypoxia, DNA repair and prostate cancer progression: new targets and new therapies.* Future Oncology, 2007. **3**(3): p. 329-341.
106. Chen, K.-W. and K.J. Pienta, *Modeling invasion of metastasizing cancer cells to bone marrow utilizing ecological principles.* Theoretical Biology and Medical Modelling, 2011. **8**(1): p. 36.
107. Diaz-Cano, S.J., *Tumor Heterogeneity: Mechanisms and Bases for a Reliable Application of Molecular Marker Design.* International Journal of Molecular Sciences, 2012. **13**(2): p. 1951-2011.
108. Friedl, P. and S. Alexander, *Cancer Invasion and the Microenvironment: Plasticity and Reciprocity.* Cell, 2011. **147**(5): p. 992-1009.
109. Ala, U., et al., *Prediction of Human Disease Genes by Human-Mouse Conserved Coexpression Analysis.* PLoS Computational Biology, 2008. **4**(3): p. e1000043.
110. Ali, H.R., et al., *Genome-driven integrated classification of breast cancer validated in over 7,500 samples.* Genome Biology, 2014. **15**(8): p. 431.
111. Barrett, T., et al., *NCBI GEO: archive for functional genomics data sets--update.* Nucleic Acids Res, 2013. **41**(Database issue): p. D991-5.
112. Best, C.J.M., et al., *Molecular Alterations in Primary Prostate Cancer after Androgen Ablation Therapy.* Clinical Cancer Research, 2005. **11**(19): p. 6823-6834.
113. Bild, A.H., et al., *An integration of complementary strategies for gene-expression analysis to reveal novel therapeutic opportunities for breast cancer.* Breast Cancer Research, 2009. **11**(4): p. R55.

114. Boutros, P.C., et al., *Spatial genomic heterogeneity within localized, multifocal prostate cancer.* Nature Genetics, 2015. **47**(7): p. 736-745.
115. Brockmoller, J. and M.V. Tzvetkov, *Pharmacogenetics: data, concepts and tools to improve drug discovery and drug treatment.* Eur J Clin Pharmacol, 2008. **64**(2): p. 133-57.
116. Durand, A., et al., *Identification of Novel Genetic Risk Factors for Focal Segmental Glomerulosclerosis in Children: Results From the Chronic Kidney Disease in Children (CKiD) Cohort.* Am J Kidney Dis, 2023. **81**(6): p. 635-646 e1.
117. Iorio, F., et al., *A Landscape of Pharmacogenomic Interactions in Cancer.* Cell, 2016. **166**(3): p. 740-754.
118. Jaiswal, A., et al., *Multi-modal meta-analysis of cancer cell line omics profiles identifies ECHDC1 as a novel breast tumor suppressor.* Mol Syst Biol, 2021. **17**(3): p. e9526.
119. Loscalzo, J. and A.L. Barabasi, *Systems biology and the future of medicine.* Wiley Interdisciplinary Reviews: Systems Biology and Medicine, 2011. **3**(6): p. 619-627.
120. Muzny, D.M., et al., *Comprehensive molecular characterization of human colon and rectal cancer.* Nature, 2012. **487**(7407): p. 330-337.
121. Parikshak, N.N., M.J. Gandal, and D.H. Geschwind, *Systems biology and gene networks in neurodevelopmental and neurodegenerative disorders.* Nature Reviews Genetics, 2015. **16**(8): p. 441-458.
122. Peidli, S., et al., *scPerturb: harmonized single-cell perturbation data.* Nature Methods, 2024: p. 1-10.
123. Scharfe, C.P.I., et al., *Genetic variation in human drug-related genes.* Genome Med, 2017. **9**(1): p. 117.
124. Yang, Z. and B. Rannala, *Molecular phylogenetics: principles and practice.* Nature Reviews Genetics, 2012. **13**(5): p. 303-314.
125. Zhao, S. and R. Iyengar, *Systems pharmacology: network analysis to identify multiscale mechanisms of drug action.* Annu Rev Pharmacol Toxicol, 2012. **52**: p. 505-21.
126. Bryant, P. and F. Noe, *Structure prediction of alternative protein conformations.* Nat Commun, 2024. **15**(1): p. 7328.
127. Bryant, P., G. Pozzati, and A. Elofsson, *Improved prediction of protein-protein interactions using AlphaFold2.* Nat Commun, 2022. **13**(1): p. 1265.
128. Fang, X., et al., *A method for multiple-sequence-alignment-free protein structure prediction using a protein language model.* Nature Machine Intelligence, 2023. **5**(10): p. 1087-1096.
129. Jumper, J., et al., *Highly accurate protein structure prediction with AlphaFold.* Nature, 2021. **596**(7873): p. 583-589.
130. Wayment-Steele, H.K., et al., *Predicting multiple conformations via sequence clustering and AlphaFold2.* Nature, 2024. **625**(7996): p. 832-839.