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SMART PHARMACEUTICAL DRUG REPURPOSING USING AI TECHNIQUES

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ABSTRACT

PHARMA: AI-Driven Drug Repurposing Platform is an innovative system designed to accelerate the discovery of new therapeutic uses for existing drugs by leveraging artificial intelligence and machine learning techniques. Traditional drug development is a time-consuming and costly process; therefore, drug repurposing offers a faster and more cost-effective alternative by identifying new applications for approved or investigational drugs. The proposed platform integrates diverse biomedical data sources such as gene expression profiles, protein–protein interaction networks, clinical trial data, and scientific literature. Advanced AI models, including deep learning and natural language processing (NLP), are utilized to analyze complex biological relationships and predict potential drug-disease associations. The system also employs data mining and network-based approaches to uncover hidden patterns and generate actionable insights. By providing a user-friendly interface and real-time predictions, the platform supports researchers, healthcare professionals, and pharmaceutical companies in making informed decisions. Overall, the proposed system enhances drug discovery efficiency, reduces development costs, and contributes to precision medicine by identifying effective treatments for various diseases.

KEYWORDS:

Drug Repurposing, Artificial Intelligence, Machine Learning, Deep Learning, Natural Language Processing, Biomedical Data, Drug Discovery, Precision Medicine, Bioinformatics, Healthcare Analytics

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I. INTRODUCTION

The process of drug discovery and development is traditionally long, expensive, and complex, often taking more than a decade and requiring substantial financial investment before a drug reaches the market. This challenge has driven the need for alternative approaches that can accelerate therapeutic development while reducing costs and risks. One such promising approach is **drug repurposing**, which involves identifying new therapeutic uses for existing or previously approved drugs. By leveraging already available safety and pharmacological data, drug repurposing significantly shortens the development timeline and improves success rates compared to traditional methods.

With the rapid growth of biomedical data, including genomic information, clinical records, and scientific literature, there is an increasing opportunity to apply **Artificial Intelligence (AI)** and machine learning techniques to transform the drug discovery process. AI-driven systems can analyze large-scale, complex datasets to uncover hidden patterns, predict drug-disease relationships, and generate valuable insights that are difficult to obtain through conventional approaches. Techniques such as deep learning, network analysis, and natural language processing (NLP) enable automated extraction of knowledge from diverse data sources, improving the efficiency and accuracy of predictions.

The proposed **PHARMA: AI-Driven Drug Repurposing Platform** aims to utilize these advanced technologies to build an intelligent system capable of identifying potential drug repurposing opportunities. The platform integrates multiple data sources, including gene expression data, protein interactions, and clinical trial information, and applies AI models to predict novel drug-target and drug-disease associations. This approach not only accelerates the discovery of effective treatments but also supports precision medicine by tailoring therapies to specific diseases and patient profiles.

Overall, the integration of AI in drug repurposing represents a significant advancement in healthcare and pharmaceutical research, offering a scalable, data-driven solution to address global medical challenges and improve patient outcomes.

II. LITERATURE REVIEW

Recent research in drug repurposing has increasingly focused on leveraging artificial intelligence and data-driven approaches to identify new therapeutic uses for existing drugs. Early studies primarily relied on traditional computational methods such as molecular docking, similarity-based approaches, and statistical analysis to predict

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drug–target interactions. These methods provided useful insights but were limited in handling large-scale and heterogeneous biomedical data [1][2].

With the growth of biomedical databases and omics data, researchers began adopting machine learning techniques to improve prediction accuracy. Algorithms such as support vector machines (SVM), random forests, and logistic regression were used to analyze gene expression data and drug features, enabling better identification of potential drug-disease associations [3]. These approaches demonstrated improved performance compared to conventional methods but still required significant feature engineering.

The advancement of deep learning has further transformed drug repurposing research. Models such as convolutional neural networks (CNNs), recurrent neural networks (RNNs), and graph neural networks (GNNs) have been applied to automatically extract complex patterns from biomedical data. These models are particularly effective in analyzing molecular structures, protein interactions, and biological networks, leading to more accurate and scalable predictions [4][5].

Natural language processing (NLP) techniques have also been widely used to extract valuable information from scientific literature, clinical trial reports, and electronic health records. By analyzing large volumes of unstructured text, NLP-based systems can identify hidden relationships between drugs, diseases, and genes, significantly enhancing drug repurposing capabilities [6].

Several studies have explored network-based approaches, where biological entities such as drugs, proteins, and diseases are represented as interconnected graphs. These methods use graph analysis and link prediction techniques to discover new associations, providing a holistic view of biological systems and improving the effectiveness of repurposing strategies [7].

Recent works have also focused on integrating multi-modal data sources, including genomic data, proteomics, chemical structures, and clinical information, to develop more comprehensive drug repurposing models. These hybrid approaches improve prediction accuracy and robustness by combining diverse data types and analytical techniques [8].

Despite these advancements, challenges such as data heterogeneity, model interpretability, and validation of predicted drug candidates remain significant. Additionally, ensuring data privacy and handling incomplete or noisy datasets continue to be important research areas, indicating the need for more robust and explainable AI-driven drug repurposing systems [9].

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III. EXISTING SYSTEM

Existing drug repurposing systems primarily rely on traditional computational and experimental approaches to identify new uses for existing drugs. One common method is **similarity-based analysis**, where drugs are compared based on chemical structure, target proteins, or biological pathways. If two drugs share similar properties, they are assumed to have similar therapeutic effects. While this approach is simple and interpretable, it often fails to capture complex biological relationships.

Another widely used approach is **molecular docking**, which predicts how a drug molecule interacts with a target protein at the molecular level. This technique helps identify potential drug-target bindings but requires significant computational resources and is often limited to small datasets and specific targets.

Network-based methods are also used in existing systems, where drugs, diseases, and proteins are represented as interconnected nodes in a biological network. These systems apply graph-based algorithms to identify potential relationships. Although effective in capturing interactions, they are limited by incomplete or noisy biological data and often lack scalability.

Traditional systems also make use of **machine learning models** such as support vector machines (SVM), decision trees, and regression techniques. These models analyze features derived from biomedical data to predict drug-disease associations. However, they require extensive manual feature engineering and may not perform well with highly complex or high-dimensional datasets.

Furthermore, many existing systems rely heavily on **structured data** and do not fully utilize unstructured data sources such as scientific literature, clinical notes, and research articles. As a result, valuable information remains underutilized, reducing the overall effectiveness of the repurposing process.

In addition, these systems often face challenges such as high computational cost, limited accuracy, lack of real-time analysis, and difficulty in handling large-scale heterogeneous data. They also provide limited interpretability and may not adapt well to rapidly evolving biomedical knowledge.

IV. PROPOSED SYSTEM

The proposed system, **PHARMA: AI-Driven Drug Repurposing Platform**, is designed to overcome the limitations of traditional drug discovery and repurposing approaches by integrating advanced artificial intelligence techniques with large-scale biomedical data. The system aims to identify potential new uses for existing drugs by analyzing complex relationships between drugs, diseases, genes,

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and proteins in an efficient and scalable manner.

In this system, data is collected from multiple heterogeneous sources, including gene expression datasets, protein–protein interaction networks, drug chemical structures, clinical trial databases, and scientific literature. The collected data undergoes preprocessing steps such as cleaning, normalization, and transformation to ensure consistency and quality for further analysis.

The core component of the proposed platform is an AI-based prediction engine that utilizes machine learning and deep learning models. Techniques such as graph neural networks (GNNs), convolutional neural networks (CNNs), and natural language processing (NLP) models are employed to extract meaningful features from structured and unstructured data. These models analyze biological networks and textual information to identify hidden patterns and predict potential drug-disease associations.

The system also incorporates a network-based analysis module where drugs, targets, and diseases are represented as nodes in a graph. Link prediction algorithms are applied to discover new relationships and suggest possible repurposing opportunities. Additionally, NLP techniques are used to extract relevant insights from biomedical literature, enhancing the knowledge base of the system.

A hybrid approach is adopted by combining multiple models and data sources to improve prediction accuracy and robustness. The system continuously learns from new data, allowing it to adapt to evolving biomedical knowledge and provide updated recommendations.

The platform includes a user-friendly interface that enables researchers and healthcare professionals to input queries, visualize results, and explore potential drug repurposing candidates. It supports real-time analysis and provides explainable outputs to assist in decision-making.

Overall, the proposed system offers a comprehensive, scalable, and intelligent solution for drug repurposing by leveraging AI and big data technologies, significantly reducing time, cost, and effort in identifying effective treatments.

V. METHODOLOGY

The methodology of the proposed **PHARMA: AI-Driven Drug Repurposing Platform** follows a systematic pipeline that integrates data collection, preprocessing, feature extraction, model training, and prediction to identify potential drug repurposing opportunities effectively.

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Initially, data is collected from multiple heterogeneous biomedical sources such as gene expression datasets, drug databases, protein–protein interaction (PPI) networks, clinical trial records, and scientific literature. This includes both structured data (drug properties, target proteins, clinical outcomes) and unstructured data (research articles and medical reports). The collected data is then preprocessed to remove inconsistencies, handle missing values, normalize formats, and ensure high-quality input for analysis.

Next, feature extraction is performed to transform raw data into meaningful representations. For structured data, features such as molecular descriptors, gene expression patterns, and interaction networks are extracted. For unstructured textual data, Natural Language Processing (NLP) techniques such as tokenization, stemming, and embedding methods are used to convert text into machine-readable formats.

Following feature extraction, multiple AI models are applied. Machine learning algorithms such as support vector machines (SVM), random forests, and logistic regression are used for baseline predictions, while deep learning models such as convolutional neural networks (CNNs), recurrent neural networks (RNNs), and graph neural networks (GNNs) are employed to capture complex biological relationships. Network-based models are used to analyze interactions between drugs, genes, and diseases, enabling link prediction and discovery of hidden associations.

The system adopts a hybrid modeling approach where outputs from different models are combined to improve prediction accuracy and robustness. Ensemble techniques or weighted scoring methods are used to integrate results from various components. The system is trained and validated using known drug-disease associations to ensure reliability.

After training, the model predicts potential new uses for existing drugs by identifying strong associations between drugs and diseases. The results are ranked based on prediction confidence and relevance. Visualization tools are used to present the findings in an understandable format, aiding researchers in decision-making.

Finally, the system is evaluated using performance metrics such as accuracy, precision, recall, F1-score, and ROC-AUC. Continuous learning mechanisms are incorporated to update the model with new biomedical data, ensuring adaptability and improved performance over time. This methodology ensures a scalable, efficient, and intelligent approach to drug repurposing.

VI. SYSTEM MODEL

System Architecture

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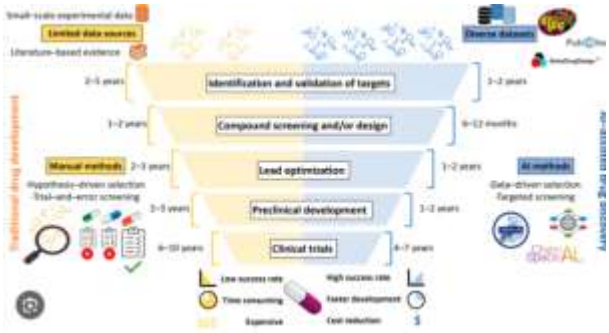
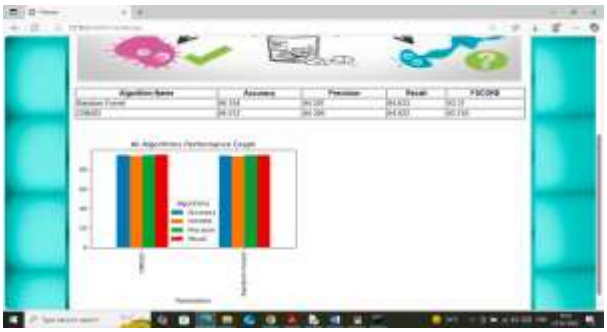


VII. RESULTS AND DISCUSSIONS

In above screen user is entering sign up details and then press button to save user data to Blockchain and then will get below page

In above screen user sign up process completed and then in red colour text I am displaying all log details obtained from Blockchain after user data storage. This log contains details like Transaction no, hash code, Block no and many other details. Now click on 'User Login' link to get below page

In above screen user is login and after login will get below page



In above screen in table format can performance of each algorithm in form of accuracy, precision, recall and FSCORE. In graph also we are comparing both algorithm performance where x-axis represents algorithm names and y-axis represents accuracy and other metrics in different colour bars. In both algorithms CNN got high accuracy. Now click on 'Predict Alternate Uses' link to get below page

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In above screen selecting and uploading 'testData.csv' file and then click on 'Open and submit' button to get below page

VIII. CONCLUSION

The **PHARMA: AI-Driven Drug Repurposing Platform** presents an advanced and efficient approach to modern drug discovery by leveraging artificial intelligence and data-driven techniques. By integrating diverse biomedical data sources such as gene expression profiles, protein interactions, and clinical information, the system is capable of identifying meaningful drug–disease relationships that are difficult to detect using traditional methods.

The use of machine learning and deep learning models enables the platform to analyze complex biological patterns, improve prediction accuracy, and reduce the dependency on manual analysis. Additionally, the incorporation of natural language processing allows the system to utilize valuable insights from unstructured data such as research articles and clinical reports. This comprehensive approach significantly enhances the effectiveness of drug repurposing.

The proposed system addresses key challenges in conventional drug discovery, including high cost, long development time, and limited scalability. By focusing on repurposing existing drugs, the platform accelerates the identification of potential treatments while minimizing risks associated with new drug development.

Overall, the system contributes to the advancement of precision medicine and healthcare by providing a scalable, intelligent, and reliable solution for identifying new therapeutic opportunities. With further improvements and real-world validation, the platform has the potential to play a crucial role in transforming pharmaceutical research and improving patient outcomes.

IX. FUTURE WORK:

The **PHARMA: AI-Driven Drug Repurposing Platform** can be further enhanced in several directions to improve its accuracy, scalability, and real-world applicability. Future work can focus on integrating advanced deep learning architectures such as transformer-based models (e.g., BERT and BioBERT) to improve the understanding of complex

biomedical text and enhance the extraction of drug–disease relationships from scientific literature.

Another important extension is the incorporation of **multi-omics data**, including genomics, proteomics, metabolomics, and epigenomics, to provide a more comprehensive understanding of biological systems. This will enable the system to generate more precise and personalized drug repurposing predictions aligned with the principles of precision medicine.

The platform can also be improved by implementing **explainable AI (XAI)** techniques, allowing researchers and healthcare professionals to understand the reasoning behind model predictions. This will increase trust, transparency, and adoption in clinical and pharmaceutical settings.

Future enhancements may include **real-time data integration** and **continuous learning mechanisms**, enabling the system to update its knowledge base dynamically as new biomedical data and research findings become available. This will ensure that the platform remains up-to-date and responsive to emerging healthcare challenges.

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