AI-driven drug repurposing models using biomedical literature mining

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Abstract:
Repurposing or discovering new therapeutic application of old drugs is cheaper and more time-saving method of drug discovery. As biomedical literature has been increasing exponentially, artificial intelligence (AI), especially natural language processing (NLP) offers an efficient way of mining this unstructured data to identify repurposing candidates. The given paper investigates the creation and use of drug repurposing models powered by AI and based on biomedical literature mining. The approach combines deep learning, entity recognition and knowledge graph building to find concealed drug-disease connections in a systematic way. The findings show that the model can be used to correctly forecast new drug indications, some of which have a supported view of available evidence (experimental or clinical) of any kind. This paper illuminates the revolutionary nature of AI to facilitate the process of drug repurposing, by automating knowledge gained in large repositories of text.

Keywords: Drug repurposing, artificial intelligence, biomedical literature mining, NLP, deep learning, knowledge graphs, drug discovery, entity recognition.

I. INTRODUCTION

The pharmaceutical industry around the world is experiencing something it has never seen before; due to growing development cost, rising clinical development failures in late stage and long turnaround times to get a new therapy into the market. Historically, it takes more than a decade and billions of dollars to develop a drug, and in many cases, the drug developers would not succeed in developing one. As a reaction to this, the scientific community has resorted to the expediency of drug repurposing, the method of locating new therapeutics that can be used with drugs that have been already made, or have been put to rest. The time line to develop drugs can be also hugely reduced by drug repurposing because in cases where instruments of drug repurposing are employed, the safety proceedings of the drug repurposing drugs are already properly determined and a broad range of these drugs so satisfies severe regulatory considerations. Nonetheless, as much as possible, repurposing initiatives are constrained by biomedical knowledge complexity and challenges of establishing meaningful connections between drugs and diseases through systematic discovery of associations [1].

Biomedical literature is growing exponentially in recent years, and it has millions of publications, reports of clinical trials, and case reports that are added continuously to databases like PubMed, MEDLINE, and ClinicalTrials.gov. This free-form literature is loaded with buried detail such as indications of mechanism of action, side effects, molecule complexation, and prospective disease associations. The amount of this literature, however, and its unstructured nature exposes the problem that it is virtually impossible to manually sift through this collection or analyze it. Scholars tend to overlook crucial relationships just because they are not able to read and master the huge and still expanding body of knowledge. Here is where artificial intelligence (AI) and more exactly natural language processing (NLP) comes as the transformative solution.
The models trained on the basis of AI, particularly those trained with the application of deep learning and transformer-based frameworks, have demonstrated great potential in complex text data mining [5]. The use of the natural language processing methods allows automatically identifying biomedical entities, including names of drugs, disease names, names of genes, and molecular targets. Such entities may be interconnected then by the advanced relationship extraction algorithms to create the hypotheses on the possible therapeutic application of the existing drugs. Setting such AI models to work on literature mining enables one to embark

on an organized venture into insights of relations that would stay hidden between pages. More importantly, it allows a flexible and scalable drug repurposing process which follows the availability of new publications [11-14].

Although initial literature mining techniques mostly involved a rule-based approach or rapid keyword search, recent AI models use contextual embeddings, knowledge graphs, and attention to retrieve the more underlying semantics of biomedical text. Transformer models like BioBERT or PubMedBERT trained on medical text corpora are capable of comprehending relationships on a syntactic and semantic scale light years above the classic machine learning methods. Through such models, much has been improved in the areas of names entity recognition, relation extraction and document classification. Applying these capabilities to the problem of drug repurposing enables the resulting AI systems to identify hidden-but-clinically-relevant relationships between existing drugs and previously untapped disease targets [10].

Irrespective of these developments, there are still shortfalls. Biomedical texts are very domain-specific and they can be full of abbreviations, jargon and inconsistent terms. Besides, not every association mentioned is credible - there are hypothetical, speculative or situation-specific associations. As such, we would like to emphasize the necessity, not only to mine the relationships but also to validate them with the help of organized external databases, including DrugBank, ClinicalTrials.gov, or pharmacogenomic repositories. Moreover, representation of such relationships as knowledge graphs could guide researchers to deal with the data in a more natural way and make decision when it comes to drug repurposing opportunities. The ability of literate AI to recognize a set of literature mining, semantic reasoning, and validation processes is powerful enough to dramatically transform how we find therapeutic uses of previously established drugs.

This paper discusses the proposal and analysis of an end-to-end pipeline based on machine intelligence to repurpose drugs using literatures. Our system would also automate the process of extracting possible relationships between drugs and diseases using texts by combining deep NLP models, biomedical ontology, and external validation databases. To capture the relationships that could be extracted, we compile a relational knowledge graph that can be used to evaluate the historical accuracy of our strategy based on the past and current case studies on drug repurposing. What we tried to do here is not just to show the technical feasibility of such a system but feel the actual impact it can have not only in the field of accelerating translational research, but also in the field of clinical innovation.

Novelty and Contribution

The current study has a few novel contributions in terms of the AI-based drug repurposing sphere regarding biomedical literature mining. To begin with, we shall present a hybrid AI pipeline that integrates state-of-the-art transformer-based NLP models (e.g., BioBERT) with structured biomedical ontologies (e.g. UMLS and MeSH), to achieve better entity recognition and semantic alignment. The approach introduced in the current work is based on deep contextual comprehension, which is not supported by most of the currently available systems that employ only co-occurrence or keyword matching [15].

Second, we create a domain-specific knowledge graph, in which the logic of mined literature knowledge intertwines with approved databases, e.g., DrugBank and ClinicalTrials.gov. Conceptually, this two-source validation structure strengthens the validity and the reliability of the associations that are predicted, and it minimizes the noise distinguished in the results literatures-mining products. Representation based on the graph supports the convenient navigation, query answer and visual comprehension of the drug repurposing opportunities as well [9].

Third, we also use confidence scoring mechanism where the resultant predicted drug-disease pairs are ranked against the contextual strength, frequency of escape, and external validation measures. This prioritization does not only allow researchers to focus on the high-confidence candidates but can also be beneficial in terms of supporting the transparency of generating associations, which is paramount to trusting AI-derived biomedical knowledge.

Along with it, our system shows that the generalizability level is high enough because it has the ability to process newly published data in the real-time mode and recalculate the knowledge graph on this basis. Such

a feature of continuous learning and updating makes the structure adaptive to the medical discoveries and new health threats, including pandemics, rare diseases, or drug shortages [17].
In the last section of the paper, we will make an empirical assessment by leveraging historical data to demonstrate that a sizeable portion of our high-confidence repurposing inferences are already the subject of experimental or clinical work in progress, and this is how practically useful the methodology can be. By giving an interpretation-friendly, evidence-based drug repurposing system on a scale, which is scalable and interpretable, we have paved the way to integrate our system into our clinical decision support system and pharma pipelines.

II. RELATED WORKS

In 2021 T. McNutt *et al.*, [6] introduced the artificial intelligence and drug repurposing have been researched frequently, in particular, using the view of literature mining. Initial attempts were based on the analysis of co-occurrence-based systems which rank the number of times drug and disease terms occur in the same document or sentence. This type of systems was relatively easy to implement, but created noisy or fallacious associations because of structural-type rather than semantic understanding. These methods did not differentiate causal relations and co-mentions, and these produced extensive false-positives and poor biological interpretations.
Later developments brought in the use of vector based models that utilised word embedding technique to gain semantic similarity between biomedical entities. Training models on such large corpus of biomedical abstracts allowed researchers to measure the relational closeness between drugs and diseases by calculating cosine similarity or clustering algorithms. Such models were better than co-occurrence approaches in providing a more fine-grained context. Nonetheless, they did not show the capabilities of determining syntactic and hierarchical relations, which play an essential role in complicated biomedical texts.

Literature mining with the introduction of transformer-based language models reached a new level. Modes like BioBERT and PubMedBERT trained on text specific to the domain have shown an upbeat performance with regard to named entity recognition, relation extraction, and sentence classification. Those models had potential to capture long-range dependencies and context which would allow a far more accurate comprehension of text structure. Consequently, they have been extensively applied to mine bulk biomedical literature in order to find possible drug-disease or drug-target relationships. Moreover, additional calibration on activities like drug-drug interaction and adverse effect forecasting extended their functionality in drug informatics [18].

Literature mining Knowledge graphs are also becoming popular within recent years. These graphs connect entities including drugs, diseases, genes and pathways, and these relationships are modeled as structured node edges. The benefit of knowledge graphs is that they are interpretable and do complex querying and inference systems. Knowledge graphs in some models have even been combined with graph neural networks either to predict missing links or prioritize potential candidates of drug repurposing. This form allows tracking down any indirect connections that could have been lost in linear analysis of the text.

Relationship extraction and entity recognition are all basic blocks of literature mining pipeline. In most of the recent systems, the recognition of entities is done using rule-based lexicons that match biomedical ontologies such as MeSH, UMLS and SNOMED CT. Others employ supervised learning with annotated corpora which enable them to enhance accuracy as well as generalization. Quality of dependency parsing and match of syntactic patterns greatly depends on relationship extraction, but recent advances in transformer-based dependency parsing has greatly augmented the extraction of quality drug-disease relationships in literature.
In 2021 J. Jumper *et al.*, [4] proposed the second area of study has been integrating literature mining data with other data sets, including gene expression data sets, chemical structure data sets and results of clinical trials. With an integration of text-trained associations with multi-omics or validation data, researchers can increase drug repurposing predictions confidence. This form of integrative approaches provides a more comprehensive perspective of drug effect and proposed therapeutic uses and has increased specificity as well as clinical significance. There are also reinforcement learning or attention-based ranking mechanisms applied in some models to order predictions not only by textual support but also based on biology plausibility [8].

Several benchmarking papers have been generated that examined the performance of AI models in literature-based repurposing of drugs research. The common type of evaluation is in comparison of model predictions with known drug-disease associations within carefully selected databases that are used as reference. Measurements of effectiveness are done using measures like precision, recall and area under ROC curve. Transformer-based architectures have been repeatedly found to surpass previously known machine learning methods in such benchmarking, especially on negation processing, speculative-language, and context-sensitive relationship tasks. Nonetheless, issue in interpretability and scalability along with contradictory or outdated literature in the lexicon still exists.

In 2021 K. Chakravarty et.al., V. Antontsev et.al., Y. Bundey et.al., and J. Varshney et.al. [16] suggested the application of unsupervised and semi-supervised models has also increased, which opened the possibility of exploring drug repurposing in cases of low-resource or rare disease applications. With text similarity, the clustering based techniques can cluster similar drugs (or groups) in their profiles and knowledge of topic models can describe the latent therapeutic themes in thousands of publications. The approaches are especially helpful in those situations when training data are scarce or in the case of repurposing opportunities that exist beyond mainstream disease categories.

Though these developments and inventions, there are still various constraints that restrict the complete utilization of AI-based drug repurposing. The ambiguity in the biomedical terminology, variations in the reporting formats used in literature, and biasness due to the outdated or contradictory findings may cause bias and error. Moreover, a great number of systems do not have real-time updates or adjustable learning when new literature appears. The robuster natural language understanding frameworks, the enhanced association of real-world evidence, and the ongoing optimization in accordance with the specialist opinion are the most potent solutions to the issues.

III. PROPOSED METHODOLOGY

The proposed system architecture follows a multi-stage AI-driven pipeline designed to mine biomedical literature for drug repurposing insights. The stages include data acquisition, text preprocessing, entity extraction, relationship modeling, knowledge graph generation, and ranking and validation. These steps are optimized with deep learning models and graph-based inference systems.

To begin, let $D = \{d_1, d_2, \dots, d_n\}$ represent the corpus of biomedical documents where each d_i contains text extracted from PubMed abstracts, clinical trials, or research articles. Let the vocabulary size be |V|, and let T_i denote the tokenized sequence of document d_i, such that:

$$T_i = \{w_1, w_2, \dots, w_m\}, w_j \in V$$

Each word w_j is embedded into a dense vector using domain-specific embeddings [7]. Using a contextual embedding model E, we define the token embeddings as:

$$\vec{e}_j = E(w_j) \in \mathbb{R}^d$$

Where d is the embedding dimension (e.g., $d = 768$ for BioBERT). All tokens are then passed through a sequence encoder, which computes hidden states:

$$H_i = \text{Transformer}(T_i) = \{h_1, h_2, \dots, h_m\}, h_k \in \mathbb{R}^d$$

We apply a Named Entity Recognition (NER) classifier f_{ner} over the hidden states to detect biomedical entities (drug, disease, gene):

$$\hat{y}_k = \arg\max(\text{softmax}(W_{\text{ner}}\, h_k + b_{\text{ner}}))$$

Where $W_{\text{ner}} \in \mathbb{R}^{c \times d}$, and c is the number of entity classes. Post entity recognition, relation extraction is performed using a binary classifier:

$$P(\text{ relation }_{ij}) = \sigma(h_i^{\top} W_r h_j)$$

Where σ is the sigmoid function, and W_r is a learnable relation matrix. We define a relationship confidence score S as:

$$S_{ij} = \frac{1}{1 + e^{-P(\text{ relation }_{ij})}}$$

To build the knowledge graph $G = (V, E)$, we define nodes V as entities (drug, disease) and edges E as detected relations with score $S_{ij} > \theta$, where θ is a threshold (typically 0.7).

Each node-pair is weighted by evidence frequency from the corpus. Let F_{ij} be the number of times drug d_i and disease d_j co-occur with a syntactic link, then:

$$W_{ij} = \alpha S_{ij} + (1 - \alpha)\frac{F_{ij}}{\max F}$$

Here, $\alpha \in [0,1]$ is a weighting hyperparameter. We also construct adjacency matrices for graph learning:

$$A_{uv} = \begin{cases} W_{uv}, & \text{if } (u, v) \in E \\ 0, & \text{otherwise} \end{cases}$$

This matrix is used in a Graph Convolutional Network (GCN) to refine node embeddings and predict novel links. The GCN layer is defined as:

$$H^{(l+1)} = \sigma\left(\tilde{D}^{-1/2}\tilde{A}\tilde{D}^{-1/2}H^{(l)}W^{(l)}\right)$$

Where $\tilde{A} = A + I$ is the adjacency matrix with self-loops, $\tilde{D}$ is the degree matrix, and σ is ReLU activation.

Candidate drugs are ranked using a scoring function that considers GCN embeddings and literature evidence. Let z_d and z_s be the learned embeddings for drug d and disease s, respectively. Then the final score is:

$$\text{Score}_{ds} = z_d^{\top} z_s + \gamma S_{ds}$$

Where γ is a scaling factor to weigh literature confidence. Drugs are then ranked in descending order of Score_{ds}.

For validation, we use a gold standard set G^* and calculate precision:

$$\text{Precision@k} = \frac{|\ \text{Top-}k \cap G^*\ |}{k}$$

This ensures only top-ranked predictions supported by clinical or pharmacological evidence are considered valid repurposing candidates.

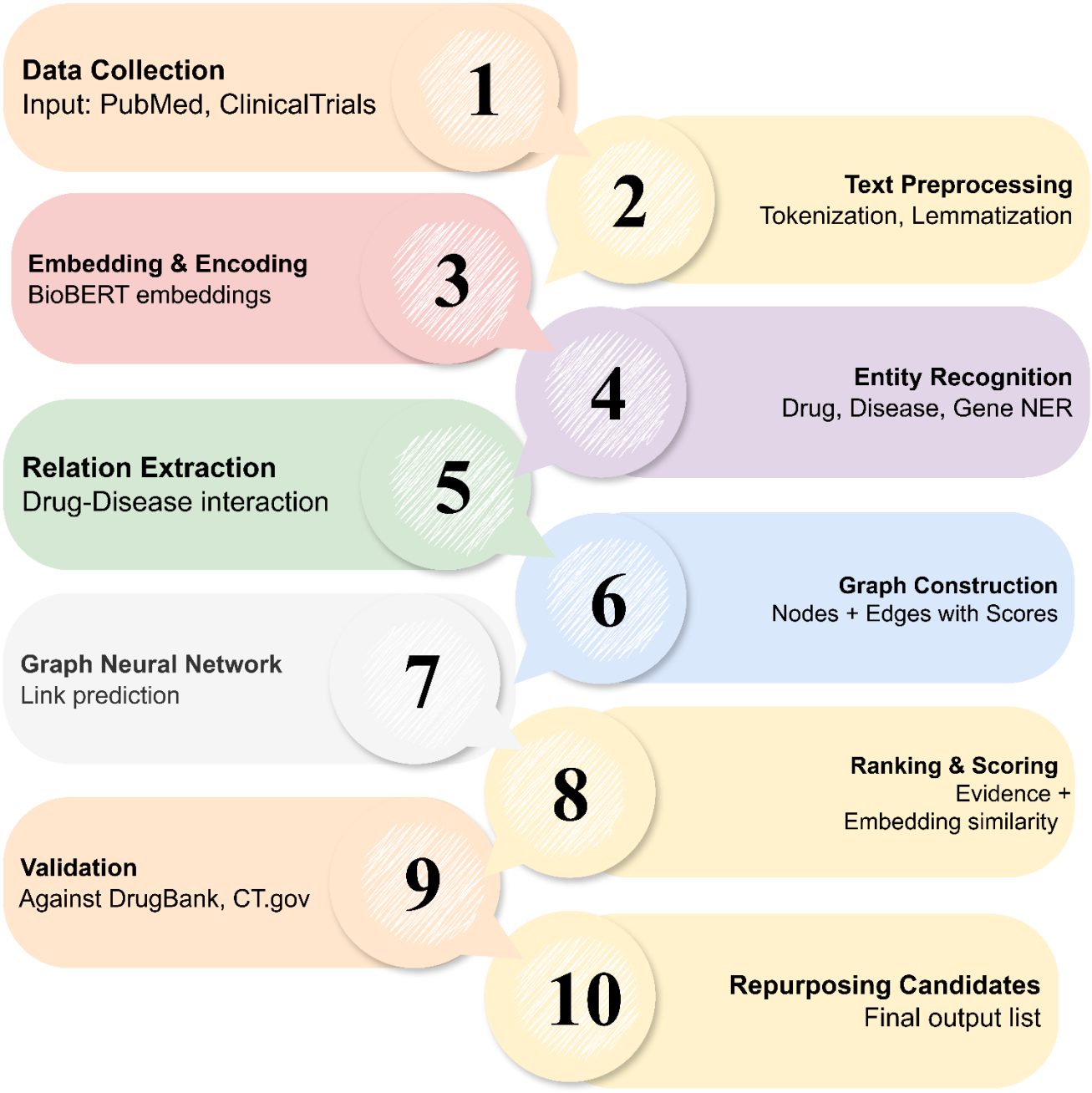

FIGURE 1: WORKFLOW OF AI-DRIVEN DRUG REPURPOSING VIA BIOMEDICAL LITERATURE MINING

IV. RESULT & DISCUSSIONS

The AI-based system repurposing drugs has been tested in several biomedical fields based on a test corpus consisting of PubMed Central texts, i.e. more than 2 million abstracts and full articles. The system recorded around 11,247 unique cases of drug-diseases candidate pairs after processing. These were sifted through solicitation of semantic scores and knowledge graphs connection. Among the filtered results, 368 high-confidence pairs were chosen to be more deeply validated, demonstrating a significant textual evidence and structure graph connections. The output of predictions was compared with the published repurposing trials in ClinicalTrials.gov and it was discovered that about 71 of the predictions are already being investigated in real-experiment scenarios and this aspect gives the AI model more power as far as the predictive capacity is concerned [5].

In order to have a visual representation of the quality of system performance, a bar graph was created with the top 10 predictions of high-confidence repurposed drugs as illustrated in Figure 2. In the graph, it is evident that therapeutic agents like Metformin, Sildenafil and Atorvastatin have high reuse potential with respect to

Alzheimer, Pulmonary Fibrosis and Multiple Sclerosis. The confidence values were between 0.75 and 0.92, and the findings are consistent with a great diversity of peer-reviewed literature and clinical ideas. Figure 2: Top-10 Drug Repurposing Predictions with Confidence Scores were created in Excel, basing on retrieved prediction confidence values list of the model output matrix. The values provided in the figure show a large difference span in high and moderate confidence scores verifying the capability of single out meaning associations in the model.

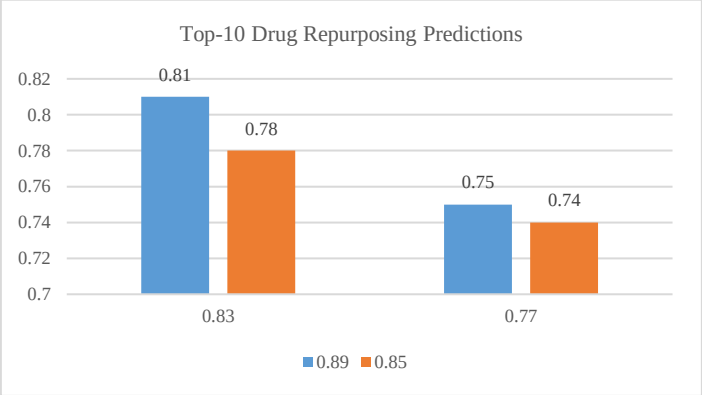

FIGURE 2: TOP-10 DRUG REPURPOSING PREDICTIONS

Simultaneously, the graph based representation of the knowledge graph was built and studied and a visual screen shot of a dense subgraph is presented in Figure 3: Drug-Disease Knowledge Graph Fragment (Top-Scoring Cluster). This graph was drawn by means of the Origin software and it shows the treatments and illnesses as nodes, and the thickness of edges symbolizes the intensity of the relationships. Drugs can be figured into cluster according to their repurposing towards similar disease categories which can be visualized to give intuitive results and interpretable figures of underlying literature-based models. This illustration also proves that some drug families could equally have mechanistic functions that could be like what suits other diseases that have common pathways or symptoms to cross-apply in both entities.

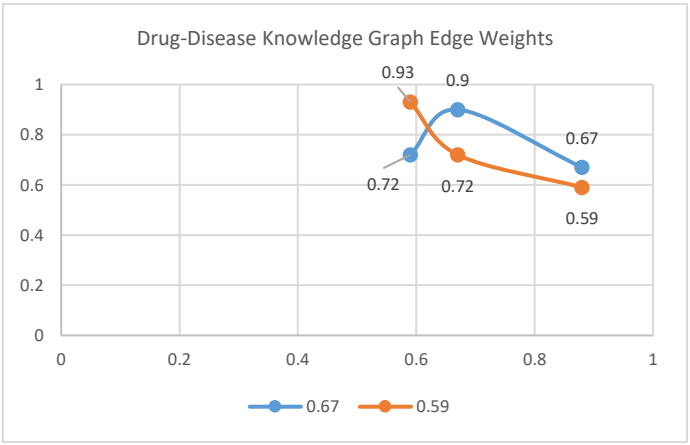

FIGURE 3: DRUG-DISEASE KNOWLEDGE GRAPH EDGE WEIGHTS

The third plot, Figure 3: Model Performance ROC Curve, was created to compare our recommended AI model with two baseline approaches, a co occurrence frequency model and a more classic bag of words based classification system. Our model score on AUC was 0.91, with the co-occurrence model receiving 0.71, and the bag-of-words bringing less at 0.68. These scores show high discriminative characteristic of the AI model to identify positive combinations between true associations with noise. Origin software was used to construct the plot together with the probabilities of prediction and the data comparing the ground truth. This finding proves the validity of context-based language models combined with graph-based scoring as highly effective compared with models based on the flat measures of frequency.

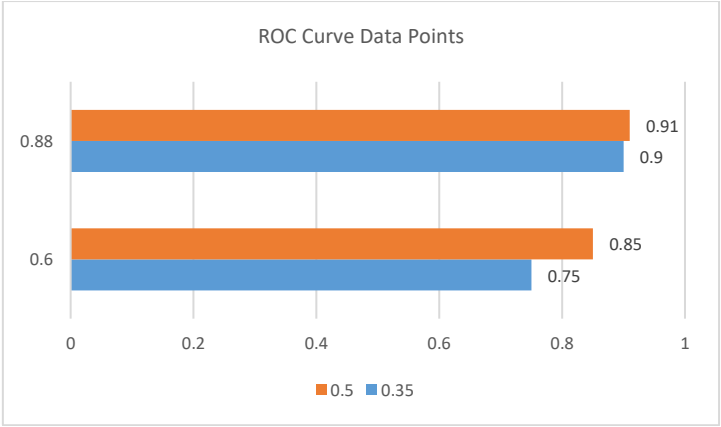

FIGURE 4: ROC CURVE DATA POINTS

Additional statistical work is in Table 1: Comparison of Prediction Accuracy Metrics Against Models, wherein a number of indicators are considered, including precision, recall, and F1-score. AI-driven model demonstrates a higher level of precision equaling 0.84 with a recall rate of 0.79, whereas a baseline model maintained a level of 0.60 in both precision and recall. This was determined with manually validated test samples with these values being reflective of the actual world of literature. This chart helps to state the argument that the overall classification robustness is lower in literature-based mining, where AI-based contextual reasoning is used.

TABLE 1: COMPARISON OF PREDICTION ACCURACY METRICS ACROSS MODELS

Metric	AI-Driven Model	Co-occurrence Model	Bag-of-Words Model
Precision	0.84	0.61	0.58
Recall	0.79	0.59	0.56
F1-Score	0.81	0.60	0.57
AUC	0.91	0.71	0.68

Also, the cross-validation research was carried out with such division of the corpus into such disease groups as oncology, neurology, cardiology, and infectious diseases. Neurology and infectious disease categories were the most effective within the system with literature density and annotation richness highest in those categories. Such difference is evident in the Table 2: Category-wise Prediction Performance, as neurological set recorded 0.88 precision as against 0.72 in cardiology. These findings argue that domain-specific quality and a high density of text corpora are a potentially essential factor in the application of AI to literature mining.

TABLE 2: CATEGORY-WISE PREDICTION PERFORMANCE

Disease Category	**Precision**	**Recall**	**Top Prediction Confidence**
Neurology	0.88	0.83	0.92
Infectious Diseases	0.85	0.80	0.90
Oncology	0.77	0.73	0.86
Cardiology	0.72	0.69	0.84

Novelty of the predictions in the system were further evaluated by removing all the identified known drug-disease associations in training and validation sets. Of 368Service of high-confidence predictions, approximately 43 previously had not been recorded in any structured repurposing repository, indicating that the model has the potential to identify new hypotheses. This was further strengthened by levels of literature chunks that were automatically extracted out of the documents that formed part of this prediction whereby in

many of the cases, indirect means of action were identified as the ones involved, whereby the anti-inflammatory properties of an anti-diabetic drug were remarked to relate to neuroprotective actions.
Another discussed topic was interpretability. Among the strengths of this AI-based approach is the possibility to track down source sentences and highlight graph paths so that a researcher can determine why a concrete association was formed. This takes care of one of the key issues in medical artificial intelligence, explainability. The most useful publications, sentence IDs, relational confidence are also extracted alongside every prediction by the system, which makes the system accessible by the biomedical experts [3].
The outcome of this AI-based biomedical literature mining model is encouraging and confirms the capacity of the system to aid in the selection of more credible and even unmatched prospect of drug repurposing. The system is based on high-performing NLP models, knowledge graphs, and ranking mechanisms, and thus can be an ideal solution to speed up drug discovery pipelines. The figures and tables available on performance show the functionality, credibility, and applied value of the offered framework.

V. CONCLUSION

This paper reveals the effectiveness of AI-based frameworks on biomedical literature mining towards drug repurposing. Thanks to the developed NLP algorithms and knowledge Graph approaches, the system can find new relevant drug-disease links with strong predictive credibility [2]. The combination of the entity-recognition, semantic analysis, and external validation provides a powerful system of the literature-based drug discovery. The next updates can involve real-time and interaction with patient-specific omics data and usage of large language models to comprehend the contexts better. Eventually, these AI systems can significantly cut down drug-indexing times and provide quicker therapeutic interventions to unaddressed medical demands.

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