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Artificial intelligence in drug-drug interaction checking

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Abstract

Artificial Intelligence (AI) has revolutionized modern medicine by providing computational solutions to manage complex clinical data and improve therapeutic outcomes. In pharmacology, AI particularly machine learning (ML) and deep learning (DL) models has demonstrated significant potential in predicting drug–drug interactions (DDIs), a major cause of adverse drug reactions (ADRs) and increased healthcare costs. This study focuses on the DANN-DDI (Deep Attention Neural Network for Drug–Drug Interaction) model, which integrates diverse pharmacological data to enhance the accuracy of DDI prediction. Drug features including chemical substructures, targets, enzymes, pathways, and existing interactions were extracted from the DrugBank (version 5.1.0) and KEGG databases. These features were used to construct five drug-feature networks, and structural deep network embedding (SDNE) was employed to learn drug representations. The DANN-DDI framework consists of three components: drug feature learning, drug-pair feature learning, and interaction prediction using a deep neural network optimized via the Adam algorithm and binary cross-entropy loss. Model performance was evaluated using 5-fold cross-validation and assessed through AUC, AUPR, accuracy, and F-measure metrics. The results indicated that optimal parameters (embedding dimension = 128, 7 hidden layers, 150 epochs, dropout rate = 0.4) yielded superior prediction outcomes. Compared with traditional computational methods such as similarity analysis and matrix factorization, the DANN-DDI model demonstrated improved capability to detect potential DDIs effectively. Overall, this study highlights the value of integrating AI-based approaches into pharmacovigilance systems to predict and prevent harmful drug interactions, ultimately enhancing patient safety and treatment efficacy.

Keywords: Artificial Intelligence; Drug-Drug Interaction; Deep Learning; Pharmacovigilance; Structural Deep Network Embedding

1. Introduction

Modern medicine has the challenge of acquiring, analysing, and using the enormous amount of knowledge needed to address complex clinical problems. Medical AI development has been closely associated with artificial intelligence algorithms that help physicians with diagnosis formulation, treatment decision-making, and outcome prediction. By supporting tasks that call for the manipulation of information and data, they are meant to assist healthcare professionals with their regular duties. Examples of such systems include evolutionary computation, fuzzy expert systems, artificial neural networks (ANNs), and hybrid intelligent systems. [1] Drugs are substances that can be used to treat, stop, or prevent disease; reduce its symptoms; or aid in the diagnosis of specific conditions. Drug developments have allowed physicians to save lives and treat a wide range of illnesses. [2] When an inpatient is released from the hospital, they are in the healing phase and are given prescriptions for different medications to address their illness. Because of comorbid

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diseases, frequent dose changes, and the critical nature of their illness, patients who are discharged from the medicine ward are more likely to experience polypharmacy, which increases the risk of pDDI. [3]

Adverse drug responses (ADRs) and higher healthcare expenses are frequently caused by them [4]. DDIs are rare, difficult to notice clinically, and only verifiable experimentally, which often limits our understanding of them. [5] According to one systematic review and metaanalysis of research from Australia, the US, and Europe, DDIs were thought to be responsible for 0.11% of hospital visits and an estimated median of 1.1% of hospital hospitalisations.[6]. Predicting protein–ligand binding affinities, finding new antiviral medications, and improving therapy for viral infections are just a few of the ways artificial intelligence (AI) has been applied to pharmacological effects [7]

One of the most useful applications of artificial intelligence is machine learning (ML), which is the development of software that can automatically learn from historical data to gather expertise and progressively enhance its learning behaviour to make predictions based on fresh data. Deep Convolutional Neural Networks (DL) are a longstanding family of machine learning models. These days, DL is highly famous because they are achieving amazing outcomes even at human performance levels. The positive results of identifying diabetic retinopathy and related eye conditions.[8]. Most of these difficulties have been attributed to the healthcare provider. The clinical acceptability of standalone diagnostic applications, for example, has been shown to be low unless they are linked into systems such as electronic medical records. [9]. One medication used to alleviate pain and fever from a variety of causes is acetylsalicylic acid, also referred to as aspirin. This drug prevents blood clots and myocardial infarction by inhibiting platelet aggregation and having anti-inflammatory and antipyretic properties. However, acetylsalicylic acid and 1-benzylimidazole together may enhance the risk or severity of hypertension (e.g., negative drug-drug interaction) [10].

Over the past half-century, AIM has experienced substantial transformation. Since the advent of ML and DL, applications of AIM have expanded, paving the way for personalised treatment as opposed to algorithm-only medicine. Predictive models could be used in the future for disease diagnosis, treatment response prediction, and preventative medicine.[11]. Employed five classifiers to construct the prediction models and incorporated a range of drug-drug similarities to characterise drug-drug combinations. Foukoue and associates.[12]. Developed a label propagation system that focused on high-order similarity and calculated the similarities between side effects, off-label adverse effects, and chemical structure. Park and others.[13]. Suggested a multimodal deep learning architecture to predict 65 types of DDI occurrences using different pharmacological characteristics. Integrating heterogeneous pharmacological characteristics is crucial for DDI prediction, according to recent research [14]. DDINMF was created using semi-nonnegative matrix factorisation, which enhances and degressively predicts DDI by breaking down the DDI adjacent matrix using regular nonnegative matrix factorisation (NMF). Methods based on similarity make the assumption that medications that are similar to one another may interact. Gottlieb and others.[15].

1.1. Drug- Drug Interaction

Drug interactions are described as interactions between a drug and another substance that can either improve or reduce the drug's effectiveness or cause the drug's side effects to worsen.[16]. There are several processes that might lead to drug interactions. These procedures could involve changes to the drug's pharmacokinetics, which include changes to the drug's absorption, distribution, metabolism, and excretion. Drug interactions can also be caused by the pharmacodynamic characteristics of the drug, such as when an agonist and a receptor antagonist are administered together for the same receptor.[17] A drug's anticipated effectiveness may be significantly altered when taken with another medication, certain foods, or when it interacts with gut microorganisms. Comprehending drug interactions, including drug-drug interactions (DDI) [18].

Predicting drug interactions (DDIs) can improve the process of medication development and post-marketing surveillance while lowering the likelihood of adverse responses. Clinical trials are costly, time-consuming, and impractical when dealing with the limits of experimental conditions and enormous amounts of data. In order to speed up the prediction process, the researchers implement numerous computational techniques. The current computational DDI prediction approaches fall into five general categories: methods based on deep learning, network analysis, similarity analysis, matrix factorisation, and literature extraction. Techniques based on literature extraction treat the extraction of DDIs as a multi-class classification task. Typically, they gather data from educational literary sentences, identify potential DDIs, and categorise them.[19]. Pharmacists utilise several forms of computerised medication-related clinical decision assistance, including drug-interaction alerting, to enhance patient safety.[20] To lessen the incidence of DDIs, computerised DDI alarm systems were developed since traditional manual data analysis methods are ineffective for making therapeutic choices.[21]

Systems based on AI and ML span many disciplines for the analysis and visualisation of heterogeneous healthcare data. Combining chemical, biological, behavioural, and network data to predict possible drug-drug interactions.[28].

2. Materials

2.1. Dataset Description

Chemical informatics and bioinformatics resources are combined in this database to provide comprehensive drug information, including targets, enzymes, pathways, drug chemical substructures, and drug-drug interactions. The DrugBank database, which was made available in April 2018 (version 5.1.0), provided the drug dataset with several drug attributes that we used in this work. Next, the target proteins of the medications are mapped into the KEGG drug database using the ID mapping service.

2.2. Overview of Methods

In this study, we provide the DANN-DDI deep attention neural network architecture for predicting possible interactions between drug pairs in different drug feature networks.[22]

Three components make up DANN-DDI, as shown in Figure 1: the drug feature learning component, the drug-drug pair feature learning component, and the drug-drug interaction prediction component. Using graph representation learning, the drug feature learning component first builds drug feature networks before learning the drug representations from these networks (Figure 1a). To obtain the comprehensive embeddings for drugs, the drug-drug pair feature learning component concatenates the five embeddings. It then creates an attention neural network to learn the representations of drug-drug pairings (Figure 1b). The drug-drug combination

A deep neural network, which takes as input the representations of drug-drug pairs, is used by the interaction prediction component to forecast possible drug-drug interactions (Figure 1c).

2.3. Drug Feature Learning

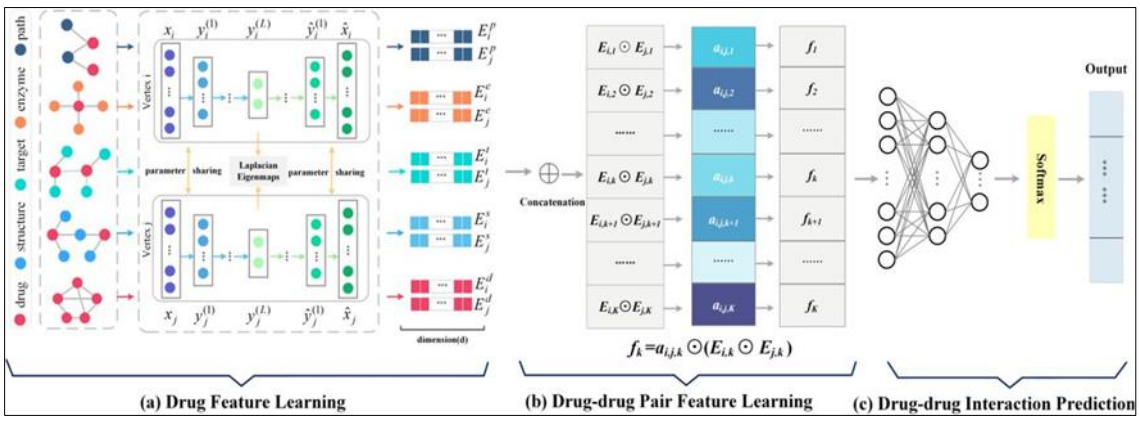

Figure 1 An overview of DANN-DDI. (a) Drug Feature Learning. (b) Drug-drug pair feature learning. (c) Drug-drug interaction prediction

The five drug properties that we have gathered in this work are chemical substructures, targets, enzymes, pathways, and drug-drug interactions. In Figure 1, the fundamental concept of pharmacological feature learning is explained.

2.3.1. Construction of Drug Feature

We take into consideration all of these drug features in order to construct five drug feature networks: drug-substructure, drug-target, drug-enzyme, drug-pathway, and drug-drug interaction. This is because different drug features have varying effects on the performance of DDI prediction. Drug nodes, feature nodes, and the links connecting them are all part of each drug feature network. Associations between medicines and traits are represented by the networks' linkages. For instance, a drug may have substructures, in which case its node is connected to some substructure nodes in the drug-substructure network.

2.3.2. Graph Representation Learning

Graph embedding, also known as representation learning, is becoming more and more popular in bioinformatics as a way to learn the feature vectors of nodes in networks. [23]. There have been numerous approaches to graph representation learning, and research has indicated that structural deep network embedding (SDNE) may be able to produce competitive results. For this reason, we use SDNE to learn drug node embeddings from drug feature networks.

The simultaneous preservation of first-order and second-order closeness is possible with SDNE. When two vertexes (i.e., vertex *i* and vertex *j*) have latent representations (i.e., *yi*^(*L)*and *yj*^(*L*)), their similarity is constrained by the first-order closeness. In order to reconstruct the second-order closeness, the reconstruction error of the input *x*i and the output *x̂*i is minimised. Additional information is available.[24] Five drug feature networks are used to extract drug node representations. Assume we have *n* medications; the five Drug embeddings from the aforementioned networks are represented as Drug embeddings from the aforementioned networks are represented as

2.4. Model Optimization

Model Enhancement There are three parts that make up DANN-DDI. The initial step is to train and optimise the pharmacological feature learning component. The drug-drug pair feature learning component is then trained and optimised in tandem with the end-to-end drug-drug interaction prediction component.

We choose the binary cross-entropy loss function and apply the Adam optimiser to optimise the DANN-DDI models.[25] to maximise the drug-drug interaction prediction component, using default values. Batch normalisation layers are used to speed up convergence between hidden layers, and dropout layers [26]

2.5. Problem Formulation

We approach the DDIs prediction challenge as a link prediction issue, similar to Shtar et al. [29], since DDIs comprise a complicated network in which nodes represent medications and links represent possible interactions. Given a directed DDI KG as G = (V, E), where every edge e = (u,v) ∈ E denotes a drug interaction between u and v.

Let N be the number of medicines. The DDIs matrix Y ∈ {0, 1} N x N can be defined as follows:

yu,v = { 1, if interaction exits between drugs u and v 0,}

If there is an interaction between medications u and v, yu,v = 1; otherwise, it is 0. (A) A value of 1 for yu,v in equation (1) denotes a current interaction between medicines u and v. A result of 0, however, does not imply that there is no interaction in the KG; rather, it may indicate that the interaction has not yet been identified [30]. We next move on to DDI extraction, which would be followed by KG construction.

2.6. DDIs extraction and KG construction

We first concentrate on the data and knowledge source selection since the two most crucial steps in our method are developing an integrated KG and extracting DDIs. The medications and drug-target related information from DrugBank, KEGG drug, and PharmGKB served as the foundation for our integrated knowledge graph. Conversely, OFFSIDES, TWOSIDES, and scientific literature from MEDLINE are used to identify DDI with sufficient proof.

2.6.1. Data Collection

There is currently no automatic technique or data source that can offer comprehensive DDI information. Additionally, the data that is now accessible comes from a variety of sources. As a result, we get information about drugs from a number of sources. The Drug Bank database is a bioinformatics and cheminformatics resource that integrates extensive drug target information with detailed drug-related data, such as chemical, pharmacological, and pharmaceutical data. There are 12,664 medication entries in the PharmGKB database1, including 2,588 approved small molecule pharmaceuticals, 1,287 approved biotech drugs, 130 neutraceuticals, and more than 6,305 investigational drugs.

3. Experiment

3.1. Evaluation Metrics

Prediction models were assessed using 5-fold cross validation in the earlier study.[27] 42In this work, we use 5-CV, or *K*-fold cross validation, to assess DDI prediction models. The known drug-drug interactions were divided into equal-

sized subsets at random. One subset and all unlabelled data are chosen for the testing set in each fold, and the remaining subsets and all unlabelled data are chosen for the training set. To train the prediction model and forecast unseen drug interactions, we use the known drug-drug interactions.

Here, the prediction model's performance is measured using a number of assessment metrics, including the accuracy (ACC), precision, recall, F-measure (F), area under the precision-recall curve (AUPR), and area under the ROC curve (AUC). Only a small percentage of drug-drug pairings in our research have known interactions. As a result, the main evaluation statistic we utilise is AUPR, which emphasises positive cases.

3.2. Parameter Discussion

The size of drug embeddings d, the number of DNN hidden layers α, the total number of DNN training epochs β, and the dropout rate ε for DNN hidden layers are the four essential parameters. Here, we go over how these parameters affect DANN-DDI's performance.

We examine the following parameter combinations: $\alpha \in \{4, 5, 6, 7, 8\}$, $\beta \in \{50, 100, 150, 200, 250\}$, $d \in \{32, 64, 128, 192, 256, 300\}$, and $\varepsilon \in \{0, 0.1, 0.2, 0.3, 0.4, 0.5\}$. DANN-DDI models are constructed using various parameter combinations, and 3-CV is used to assess the models. Prediction model performance is measured using the AUC and AUPR scores, which are the main metrics. DANN-DDI performs best among all parameter combinations when d = 128,

3.3. Analysis of DDIs predictions

The prediction task results based on various embedding techniques are compiled in Table 3. Generally speaking, the Conv-LSTM model fared better than all baseline models, with an AUPR of 0.93 in the best scenario. Additionally, the LR, NB, KNN, and SVM models did the lowest overall. Feature selectors based on these techniques may be discriminating drug-related features very strongly, forcing these classifiers to lose part of their intrinsic simplicity, low variance, and resistance to over-fitting. beneficial pharmacological characteristics that lead to reduced performance. With an F1-score of 0.91, the best of the ML baselines, RF outperforms the other tree-based classifiers. When compared to the best Conv-LSTM model in terms of F1 score, the model averaging ensemble of top-3 models (GBT, RF, and Conv-LSTM) improves performance by 1.5%. It's interesting to note that all classifiers' MCC scores demonstrate a strong correlation between the prediction and the ground truth (measured using a Pearson product-moment correlation coefficient we obtained 0.70). This is likely due to the embeddings produced by the embedding methods being learnable quality drug features. The Conv-LSTM network produced the highest AUC score, which is at least 3% higher than the RF classifier's second-best score, while the LR classifier did the worst. Figure 02 ROC curve displays constant AUC scores across the folds, indicating that the predictions are much superior to haphazard guesswork.

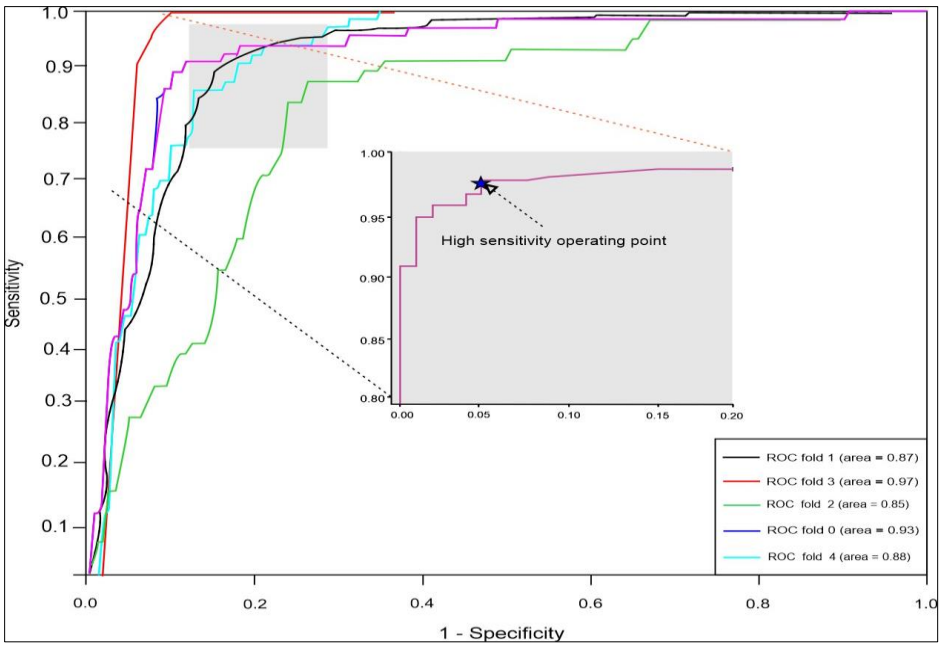

Figure 2 ROC curves of cross-validated Conv-LSTM model

3.4. Comparison of graph embedding methods

Table 3 shows that the classifiers perform better using drug characteristics produced by the KGloVe, SimpleIE, and ComplEx approaches. Specifically, the GBT, RF, and Conv-LSTM classifiers consistently get the highest F1, MCC, and AUPR scores on the embeddings produced by ComplEx. On the other hand, we encounter the lowest DDI prediction accuracy while utilising characteristics produced by the RDF2VEc technique. This differs from previous research.[31]. where RDF2Vec with a uniform weighting option produced the greatest results. In our instance, we believe that the classifiers did not gain much from additional training samples. In order to verify this, we calibrate the top-performing Conv-LSTM classifier against several embedding techniques for which the classifier's output probability can be directly understood as a confidence level in terms of "fraction of positives"; the outcome is shown in fig. 03 . As can be observed, the Conv-LSTM classifier provided a probability value ranging from 0.82 to 0.93, indicating that 93% of the predictions are true positive predictions produced by the PBG embeddings.

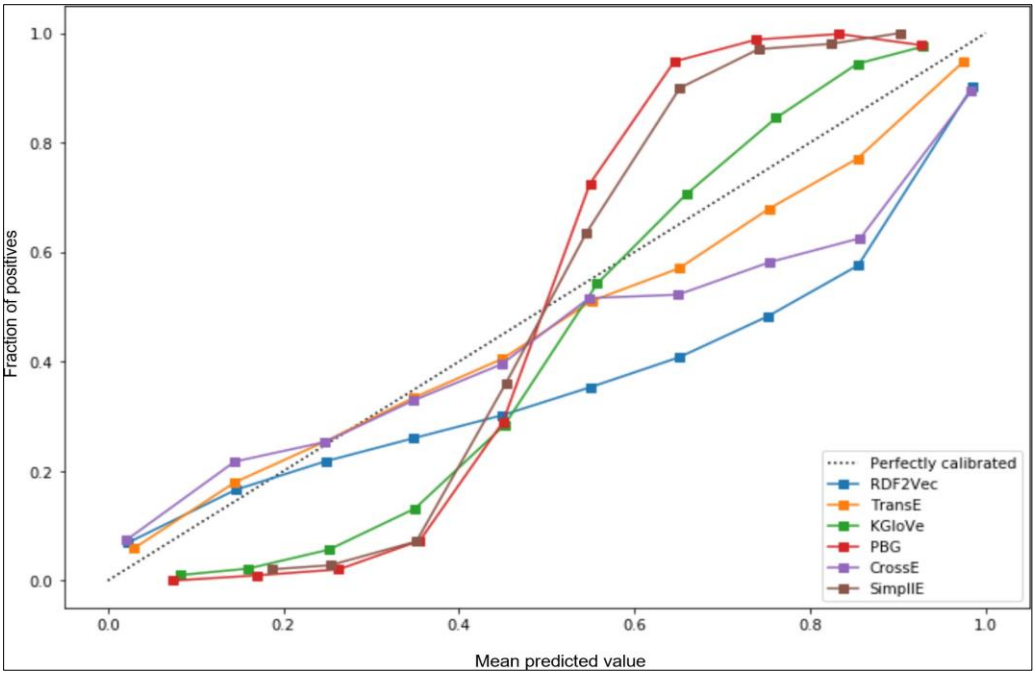

Figure 3 Calibrating Conv-LSTM with embedding methods

3.5. Effects of number of drug sample

We examined the learning curves of the top three classifiers (i.e., RF, GBT, and Conv-LSTM) and SVM (a linear model) for varied amounts of training data in order to comprehend the implications of having more training examples and to determine whether our classifiers suffer more from variance errors or bias errors. As the size of the training set increases, the validation and training scores for SVM converge to a low value, as illustrated in Figure 6. As a result, extra training data did not significantly improve SVM. Nevertheless, the Conv-LSTM network can learn more intricate ideas from the drug characteristics, while RF and GBT are tree-based ensemble techniques. Higher training scores indicate that there is less bias as a result of this. the validation scores for the greatest quantity of drug samples, demonstrating that increasing the amount of training samples does improve generalisation. [32].

3.6. Comparison with state-of-the-art

A one-to-one comparison was not feasible, particularly with Tiresias framework, because our methods for data collecting and preparation differ from others and we have more samples.[33].

4. Conclusion

Artificial Intelligence (AI) has transformed the landscape of pharmacology and clinical decision-making by providing advanced computational tools capable of processing complex biomedical data. The present study demonstrates the effectiveness of the Deep Attention Neural Network for Drug–Drug Interaction (DANN-DDI) model, which integrates heterogeneous pharmacological data to enhance the accuracy and reliability of DDI predictions. By incorporating drug features such as chemical substructures, targets, enzymes, pathways, and interaction networks from comprehensive

databases like DrugBank and KEGG, the model successfully learns intricate relationships among drugs using structural deep network embedding (SDNE).

The optimized model parameters—embedding dimension of 128, seven hidden layers, and a dropout rate of 0.4—yielded superior results across performance metrics such as AUC, AUPR, accuracy, and F-measure. Compared to traditional computational methods, DANN-DDI offers improved predictive power, demonstrating its ability to uncover potential DDIs that may otherwise go undetected in clinical settings. These findings emphasize the growing importance of AI-based systems in pharmacovigilance, drug discovery, and personalized medicine.

The integration of deep learning frameworks into DDI prediction enables researchers and clinicians to identify harmful drug interactions early, reducing adverse drug reactions (ADRs) and healthcare costs while improving therapeutic safety. Furthermore, the study highlights the significance of combining diverse data sources and graph representation learning to capture the multidimensional nature of pharmacological relationships.

In conclusion, DANN-DDI represents a significant advancement in computational pharmacology, showcasing how AI can be leveraged to strengthen drug safety and optimize clinical outcomes. Continued refinement of such models, supported by larger datasets and real-world validation, will further bridge the gap between data-driven prediction and precision healthcare, ultimately leading to safer and more effective treatment strategies.

Compliance with ethical standards

Disclosure of conflict of interest

No conflict of interest to be disclosed.

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