Weekly Report - Patent Review

Week No : 30.07.2025 - 19.08.2025

Reg. No : Class: IV B.E CSE

Name of the student:

1) **Domain** : AI & ML in Healthcare

2) **Problem statement**:

Drug–Drug Interactions (DDIs) have become a serious safety concern in modern healthcare, especially with the rise in multi-drug treatments for chronic and complex diseases. When two or more drugs are taken together, they can interact in ways that reduce the effectiveness of treatment or cause harmful side effects, which may sometimes be life-threatening. Identifying these interactions early is essential to avoid adverse drug reactions and ensure patient safety. However, manually detecting DDIs through clinical trials or expert analysis is time-consuming, expensive, and not always feasible for every drug combination. As the number of available drugs continues to grow, there is a pressing need for accurate, scalable, and efficient systems that can predict potential interactions automatically. Addressing this challenge can greatly improve treatment planning and reduce risks in healthcare.

3) **No. of patent papers reviewed** : 5

Patent 1

Field	Details
Patent Title	Predicting Drug-Drug Interactions Based on Clinical Side Effects
Patent Number	US 10,803,144 B2
Inventor(s)	Jianying Hu,Robert K. Sorrentino,Fei Wang,Ping Zhang
Filing Date / Grant Date	Filed : 2014-05-06 Granted : 2020-10-13
Assignee / Organization	International Business Machines Corp
Patent Office / Country	USPTO / United States

Abstract	Proposes a processor-implemented method, system, and computer program to predict adverse DDIs using clinical side-effect data. It builds a training dataset (pharmaceutical/PK/PD DDIs) from multiple sources, constructs per-drug side-effect features, trains a DDI classifier, and evaluates which side effects differentiate positive vs. negative predicted DDIs via 2×2 contingency tables and Fisher's exact test. Includes a label-propagation approach over a drug similarity graph to capture higher-order relationships.
Keywords / Domain	Drug–Drug Interaction (DDI); Clinical Side Effects; Label Propagation; Similarity Graph; Fisher's Exact Test; Phenotype-driven ML; Pharmacodynamic DDIs; Machine Learning
Problem Addressed	Phase IV surveillance and PK/pharmaceutical methods miss many PD interactions; existing structure-based predictions have limited clinical translation and explanation. Need early, clinically grounded, explainable DDI prediction.
Proposed Innovation	Use side-effect profiles to construct a drug similarity network and propagate labels to predict DDIs; statistically test which side effects distinguish risky pairs. Multitask label propagation yields DDI profiles simultaneously for multiple drugs.
Key Claims	• Building a DDI training dataset from multiple sources (DrugBank/labels/FAERS/text mining). • Constructing per-drug side-effect feature vectors. • Training a DDI classifier to predict adverse interactions for drug pairs. • For each side effect, forming 2×2 tables and applying Fisher's exact test to detect differential occurrence between predicted positive and negative DDI pairs.
Drawings / Diagrams	FIG. 1: Processing system FIG. 2: System architecture for DDI prediction FIG. 3: Method workflow FIG. 4: Label propagation method FIG. 5–7: Similarity graph before/after propagation rounds
Comparison with Project Idea / Literature	• Uses ensemble/knowledge-based approaches. • Project extends by using GCN+DNN hybrid on DrugBank + SIDER. • Adds XAI + NLP interpretability, absent in this work.
Identified Gap / Scope for Improvement	• Limited generalization to novel drug structures. • Lacks molecular graph learning and ADE integration. • No explainability mechanisms.
Similarity Check / Plagiarism Possibility	• Conceptual overlap in DDI prediction. • Low risk if hybrid deep model and XAI contributions are emphasized.

Patent 2

Field	Details
Patent Title	Multimodal Cell Complex Neural Networks for Prediction of Multiple Drug Side Effects Severity and Frequency
Patent Number	US20230086217A1
Inventor(s)	Mustafa Hajij; Ghada Alzamzmi; Nina Miolane
Filing Date / Grant Date	Filed: 2022-09-22 Granted: 2024-07-30
Assignee / Organization	Santa Clara University; University of South Florida; University of California, Berkeley; University of California, San Diego
Patent Office / Country	USPTO / United States
Abstract	The invention presents a novel method using Multimodal Cell Complex Neural Networks (MCXNs) to predict the side effects (both severity and frequency) of multiple drugs taken concurrently (polypharmacy). Unlike graph neural networks which only capture pairwise drug-drug interactions, MCXNs model k-wise higher-order relations (where $k \geq 2$) between drugs and proteins. The system outputs probabilities of side effects, their severity classes, and frequency categories, and ranks drug combinations from best to worst. It can also monitor dynamic changes in side effects over time based on patient health records or lifestyle changes.
Keywords / Domain	Polypharmacy; Side Effect Prediction; MCXN; Higher-Order Neural Networks; Frequency & Severity Estimation; Personalized Medicine; Drug Safety
Problem Addressed	Traditional graph- and matrix-based models fail to capture higher-order drug interactions (more than two drugs concurrently). They also separately address either severity or frequency of side effects but not both together. Current methods are static and cannot account for dynamic patient health changes or new drugs added during treatment.
Proposed Innovation	• Introduces MCXNs that model higher-order relations among drugs, proteins, and side effects. • Predicts both severity and frequency of side effects simultaneously. • Monitors temporal changes in side effects during treatment (dynamic modeling). • Provides drug ranking and alternative recommendations to optimize safety. • Allows prediction for new drugs without retraining the model by inferring new drug-protein interactions.

Key Claims	• Training a multimodal cell complex neural network (MCXN) on drug–protein–side effect data. • Modeling pairwise and k-wise interactions ($k \geq 2$). • Predicting probabilities, severity, and frequency of polypharmacy side effects. • Ranking drug combinations based on severity & frequency. • Incorporating patient health/lifestyle vectors to personalize side effect prediction.
Drawings / Diagrams	FIG. 1: High-level deployment illustration FIG. 2: Cell complex showing drug-protein-drug interactions FIG. 3: Adjacency matrices of simplicial/cell complex FIG. 4: Training and deployment pipeline diagrams
Comparison with Project Idea / Literature	• Focuses on ADR detection via signal/semantic data. • Project differs by chemistry-first graph learning with ADE mapping. • Real-time explainable outputs not included in this paper.
Identified Gap / Scope for Improvement	• Strong bias towards reported/co-occurrence data. • No structure-based predictive modeling. • No integration of DrugBank + SIDER datasets.
Similarity Check / Plagiarism Possibility	• Overlap in ADR focus. • Low risk if approach remains graph/deep learning-driven.

Patent 3

Field	Details
Patent Title	Prediction and Generation of Hypotheses on Relevant Drug Targets and Mechanisms for Adverse Drug Reactions
Patent Number	US20190050538A1
Inventor(s)	Heng Luo; Ping Zhang; Achille B. Fokoue-Nkoutche; Jianying Hu
Filing Date / Grant Date	Filed: 2017-11-21 Published: 2019-02-14
Assignee / Organization	International Business Machines Corporation (IBM)
Patent Office / Country	USPTO / United States
Abstract	This invention introduces a machine learning–based system for predicting adverse drug reactions (ADRs) using molecular docking features. The framework generates 3D structural representations of drugs, computes their binding interactions with unique human proteins, and applies machine learning classifiers to predict ADRs.

	Beyond prediction, the system highlights relevant protein targets that may explain ADR mechanisms, thereby bridging prediction and interpretability. This approach enables both ADR detection for marketed drugs and early risk assessment in drug development.
Keywords / Domain	Adverse Drug Reactions; Molecular Docking; Machine Learning; Drug Safety; Drug-Target Interaction; Hypothesis Generation; Precision Medicine
Problem Addressed	Existing ADR prediction models achieve accuracy but lack biological interpretability. They focus on performance metrics without providing hypotheses about underlying mechanisms, making it difficult to guide wet-lab validation or precision medicine decisions.
Proposed Innovation	• Uses 3D drug structures and molecular docking features as model input. • Predicts ADRs through logistic regression classifiers trained on drug–protein binding scores. • Identifies relevant protein targets linked to ADRs, enabling hypothesis generation for mechanisms. • Incorporates data from DrugBank, PDBBind, and SIDER databases. • Supports early-stage drug development and post-marketing safety analysis.
Key Claims	• Method for predicting ADRs using molecular docking–based drug–protein interaction features. • Generation of drug-target interaction matrices and ADR label matrices. • Logistic regression classifiers developed for ADR prediction (one per ADR). • Integration with docking tools (e.g., AutoDock Vina) to compute binding scores.
Drawings / Diagrams	FIG. 1–4: Framework for predicting ADRs using molecular docking + ML FIG. 5–10: Case study results (e.g., Mometasone, ADR prediction, protein binding) FIG. 11–12: Example computing system for ADR prediction framework
Comparison with Project Idea / Literature	• Employs network propagation and interaction profiles. • Project provides direct molecular graph encoding with GCN. • Multi-task prediction (DDI + ADE) is missing in this paper.
Identified Gap / Scope for Improvement	• Struggles with sparse/new drug entities. • Lacks explainability of predictions. • No multi-dataset (DrugBank + SIDER) fusion.
Similarity Check / Plagiarism Possibility	• Moderate conceptual overlap. • Low–Moderate risk, mitigated by hybrid GCN+DNN and XAI novelty.

Patent 4

Field	Details
Patent Title	Method and System for Predicting Drug-Drug Interactions
Patent Number	US20250111905A1
Inventor(s)	Guy Shtar, Adir Solomon, Eyal Mazuz, Lior Rokach, Bracha Shapira
Filing Date / Grant Date	Filed:2023-02-02 Granted: 2025-04-03
Assignee / Organization	BG Negev Technologies and Applications Ltd.
Patent Office / Country	USPTO / United States
Abstract	The invention proposes a machine learning–based system for preclinical drug–drug interaction (DDI) prediction using only chemical structure information. A DDI data structure of known interactions is combined with line-notation chemical descriptors (e.g., SMILES) of drugs and new substances of interest. Structural similarity metrics (Tanimoto, Edit Distance, LCS, NLCS, TF, etc.) are applied to compare new drugs with baseline drugs. A lookup adjacency matrix factorization with propagation (LAMFP) algorithm is used to infer DDIs, even for unseen drugs, by leveraging known DDIs of structurally similar molecules. This enables accurate in-silico prediction of DDIs before clinical data is available.
Keywords / Domain	Drug–Drug Interaction (DDI), Preclinical Safety, Machine Learning, Matrix Factorization, SMILES, Similarity Metrics, Cold-Start Problem, In-Silico Drug Testing
Problem Addressed	• Laboratory DDI testing is expensive, slow, and resource-intensive. • Existing ML methods for DDI prediction depend on clinical trial or post-marketing data, making them unusable in preclinical stages. • Conventional molecular structure encodings produce large, complex representations, leading to overfitting and poor generalization. • Current recommender-based approaches fail to handle unseen (new) drugs due to the cold-start problem.
Proposed Innovation	• Introduces simplified chemical structure representations (SMILES + similarity metrics) to avoid overfitting. • Novel Lookup Adjacency Matrix Factorization with Propagation (LAMFP) algorithm, enabling prediction for new/unseen drugs. • Uses ensemble similarity scoring (Tanimoto, Edit Distance, LCS, NLCS, TF) for robustness. • Integrates GRU + Char2Vec embeddings to capture hidden sequence-level patterns in SMILES.

Key Claims	• A method for predicting DDIs using: (i) DDI data structure, (ii) chemical structure descriptors of baseline drugs, (iii) SMILES-based descriptors for new drugs. Calculation of similarity metrics (Tanimoto, Edit Distance, LCS, NLCS, TF). • Prediction of DDIs between (a) new drugs and baseline drugs, or (b) pairs of new drugs. • Use of Adjacency Matrix Factorization with Propagation (AMFP), extended with Lookup mechanism (LAMFP) for unseen drugs.
Drawings / Diagrams	FIG. 1: Pseudo-code of LAMFP algorithm FIG. 2: Block diagram of computing device for DDI prediction FIG. 3A–3B: Applications of system for DDI prediction FIG. 4: System modules for predicting DDI FIG. 5: Flow diagram of method
Comparison with Project Idea / Literature	• Clinical decision support focus using EHR data. • Project focuses on molecular structure + ADE prediction. • Adds patient-agnostic NLP explanations not seen here.
Identified Gap / Scope for Improvement	• Opaque risk scores without interpretability. • Dependent on data-source quality. • No structure-to-side-effect modeling.
Similarity Check / Plagiarism Possibility	• Minimal overlap due to data/method differences. • Low plagiarism risk.

Patent 5

Field	Details
Patent Title	Prediction of Drug-Drug Interactions and Specific Adverse Drug Reactions
Patent Number	US10223500B2
Inventor(s)	Jianying Hu, Yashu Liu, Ping Zhang
Filing Date / Grant Date	Filed:2015-12-21 Granted: 2019-03-05
Assignee / Organization	International Business Machines Corporation (IBM)
Patent Office / Country	USPTO / United States
Abstract	This invention provides methods, systems, and devices for analyzing drug-drug interactions (DDIs) and predicting specific adverse drug events (ADEs). Chemical structures for one or more drug pairs are obtained from a user or database, and chemical fingerprints are generated for each drug. Using a bi-linear logistic regression model, the probability of a DDI is predicted. If an interaction is predicted, a

	multi-task bi-linear regression model is applied to predict specific adverse events (e.g., bleeding, nausea, arrhythmia). The invention increases drug regimen safety by providing DDI and ADE predictions in real time.
Keywords / Domain	Drug–Drug Interaction (DDI), Adverse Drug Reactions (ADR), Chemical Fingerprint, Bi-linear Model, Multi-task Learning, Machine Learning, Medication Safety, Healthcare Informatics
Problem Addressed	• Adverse drug-drug interactions cause severe morbidity and mortality (74,000 ER visits & 195,000 hospitalizations annually in the US). • Existing methods (e.g., Phase IV trials, post-marketing surveillance) are slow, incomplete, and unable to predict ADEs before drug release. • Current computational models fail to predict specific adverse events associated with DDIs.
Proposed Innovation	• Uses chemical fingerprints (vectorized molecular structures) for pairwise drug comparisons. • Introduces a two-level prediction system: Level 1: DDI probability prediction via bi-linear logistic regression. Level 2: Multi-task bi-linear regression to predict specific adverse events. • Incorporates sparse group LASSO for feature selection of chemical substructures most relevant to ADEs. • Cloud-based system supports integration with wearables, mobile devices, and clinical software.
Key Claims	• A method for obtaining chemical structures, generating chemical fingerprints, and predicting DDIs using bi-linear logistic regression. • An extended multi-task regression model to predict specific ADEs per DDI. • A system comprising processors + memory modules executing these prediction tasks. • Identification of specific chemical fingerprints responsible for DDIs/ADEs. • A computer program product for implementing DDI and ADE predictions across devices and cloud environments.
Drawings / Diagrams	FIG. 1: Workflow for DDI & ADE prediction methodology FIG. 2: System architecture for DDI/ADE prediction FIG. 3: Process flow for DDI prediction via bi-linear regression FIG. 4: Process flow for ADE prediction via multi-task regression FIG. 5–6: Training data matrices and models for DDI and ADE tasks FIG. 7–8: Cloud computing infrastructure for deployment
Comparison with Project Idea / Literature	• Uses chemical fingerprints + bi-linear logistic regression. • Project improves with end-to-end GCN+DNN hybrid. • Introduces XAI (substructure attribution) + NLP for interpretability.

Identified Gap / Scope for Improvement	• Restricted to fixed descriptors and linear models. • No integration of DrugBank + SIDER datasets. • No user-facing explanation components.
Similarity Check / Plagiarism Possibility	• Moderate thematic overlap (DDI + ADE). • Novelty secured by deep graph learning, hybrid modeling, and XAI+NLP modules

Patent Review Summary

S.No	Patent Title	Patent Number	Country	Year	Key Claim(s)	Relation to Mini Project	Similarity Detected
1	Predicting drug-drug interactions based on clinical side effects	US10803144B2	US	2015 (file.), 2020 (grant)	DDI prediction using side-effect features, similarity graph label propagation, Fisher's test to identify discriminative side effects; system/CPP embodiments	Core prior art for clinically explainable DDI prediction; informs side-effect feature design and graph reasoning	• Conceptual overlap in DDI prediction. • Low risk if hybrid deep model and XAI contributions are emphasized.
2	Multimodal Cell Complex Neural Networks for Prediction of Multiple Drug Side Effects Severity and Frequency	US20230086217A1	US	2023 (file.), 2024 (grant)	Predict side effect severity & frequency using MCXNs, model k-wise drug-protein relations, dynamic monitoring, ranking & alternative recommendations	Core to our topic—side effect forecasting for multiple drugs; informs higher-order modeling	• Overlap in ADR focus. • Low risk if approach remains graph/deep learning-driven.
3	Prediction and Generation of Hypotheses on Relevant Drug Targets and Mechanisms for Adverse Drug Reactions	US20190050538A1	US	2017 (file.), 2019 (grant)	ADR prediction using drug–protein docking features + logistic regression; identifies mechanistic protein targets	Strong relevance to ADR forecasting; supports hypothesis-driven interpretation	• Moderate conceptual overlap. • Low–Moderate risk, mitigated by hybrid GCN+DNN and XAI novelty.

4	Method and System for Predicting Drug-Drug Interactions	US20250111905A1	US	2023 (file.), 2025 (grant)	ML-based preclinical DDI prediction using SMILES, similarity metrics, and LAMFP algorithm	Strong alignment with DDI prediction; complements with structural similarity approach	• Minimal overlap due to data/method differences. • Low plagiarism risk.
5	Prediction of Drug-Drug Interactions and Specific Adverse Drug Reactions	US10223500B2	US	2015 (file.), 2019 (grant)	Bi-linear regression for DDI, multi-task model for ADE prediction, fingerprint-based feature vectors	Directly relevant (predicts both DDI & ADR)	• Moderate thematic overlap (DDI + ADE). • Novelty secured by deep graph learning, hybrid modeling, and XAI+NLP modules

Signature of the Student **Course Instructor**