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AI-Powered Drug Discovery & Development

research report

Contents

**RESEARCH PAPER 1………………………………………………………………………………… 2**

**RESEARCH PAPER 2………………………………………………………………………………… 4**

**RESEARCH PAPER 3………………………………………………………………………………… 6**

**RESEARCH PAPER 4………………………………………………………………………………… 7**

**RESEARCH PAPER 5………………………………………………………………………………… 8**

**RESEARCH PAPER 6………………………………………………………………………………… 9**

**RESEARCH PAPER 7………………………………………………………………………………… 10**

**RESEARCH PAPER 8………………………………………………………………………………… 11**

**RESEARCH PAPER 9………………………………………………………………………………… 12**

**RESEARCH PAPER 10…………………………………………………………………………………13**

# RESEARCH PAPERS

## RESEARCH PAPER 1

🔗LINK: <https://link.springer.com/article/10.1007/s10462-022-10306-1#Tab1>

🧩 DATASET USED –

The study reviewed more than **300 articles** published between 2000 and 2022.

- It focused on various **benchmark datasets** and databases relevant to drug discovery, including:

- Drug–target interactions (DTIs)

- Drug–drug interactions (DDIs)

- Drug sensitivity and response

- Drug side effects predictions

🧠 METHODOLOGY /MODEL USED -

The paper presents a **systematic literature review (SLR)** of deep learning (DL) technologies and applications in drug discovery.

Various **deep learning models** discussed include:

- Multi-layer Perceptron (MLP)

- Convolutional Neural Networks (CNN)

- Recurrent Neural Networks (RNN)

- Generative Adversarial Networks (GAN)

- Graph Neural Networks (GNN)

- Autoencoders

The review categorizes DL applications into four main areas:

- Drug–target interactions

- Drug–drug similarity

- Drug sensitivity and response

- Drug side effects predictions

✨NOVELTY –

The paper is notable for being the **first comprehensive review** that integrates recent DL models and applications across multiple categories of drug discovery problems.

- It highlights the incorporation of **explainable AI (XAI**) and **digital twinning (DT)** as emerging topics in drug discovery.

- The review also identifies **future research challenges** and directions in the field.

ACCURACY-

The accuracy of the models is not explicitly stated in the review, as it focuses on summarizing various studies and their findings.

- However, it mentions that some models, such as the **D-MPNN (Directed Message Passing Neural Network),** have shown improved performance in predicting drug-target interactions compared to traditional methods.

📊 EVALUATION METRICS-

The paper discusses several evaluation metrics used in drug discovery, including:

- **True Positives** (TP): Correctly identified drug side effects.

- **False Positives** (FP): Incorrectly identified side effects.

- **True Negatives** (TN): Correctly identified non-side effects.

- **False Negatives** (FN): Missed side effects.

Additional metrics mentioned include:

- **Accuracy**

**- Precision**

**- Recall**

**- F1 Score**

**- Area Under the Receiver Operating Characteristic Curve (AUC-ROC)**

## RESEARCH PAPER 2

🔗 LINK: <https://chemistry-europe.onlinelibrary.wiley.com/doi/full/10.1002/cbic.202200776>

🧩 DATASET USED –

Since this is a review article, it doesn’t present original experimental data. However, it summarizes commonly used structure-based datasets in deep-learning drug discovery:

**PDB complexes** (hundreds of thousands of structures)

Binding affinity datasets: PDBBind, DUD-E, BindingDB, BigBind, KIBA, Davis

🧠 METHODOLOGY / MODELS USED-

The authors categorize structure-based deep learning (DL) methods across three core tasks:

**1. Data Representations**:

\*Primary sequence (strings)

\*3D structure (voxels, graphs)

\*Surface (point clouds, meshes)

**2. Neural-network Architectures**:

\*RNNs (for protein sequences)

\*CNNs over 3D voxelized protein structures (binding-site detection, affinity prediction)

\*GNNs on molecular graphs (atoms + bonds)

**3. Core Applications**:

\*Binding site detection (sequence/structure surface-based)

\*Drug‑target interaction (DTI), e.g. CNNs + SMILES in DeepDTA, transformers, GNNs

\*Structure-based de novo molecule design conditioned on protein targets (using GANs, GNNs, RNNs)

✨NOVELTY-

The article provides a comprehensive taxonomy of **structure-aware DL methods**, **integrating diverse input types** (sequence, 3D, surface).

It highlights **geometric DL** and distinguishing representation-to-architecture matches.

It emphasizes both opportunities (like refined binding affinity modeling, de novo design) and challenges (**data scarcity, integration of structural + assay data**).

ACCURACY-

As a review, it does not report new training/testing results.

It summarizes benchmarks from original papers, though does not synthesize overall performance

📊 EVALUATION METRICS-

While this article does not define metrics itself, relevant DL models discussed typically use:

Binding affinity prediction: **RMSE, MAE, Pearson/Spearman correlation**

Classification tasks: AUC‑ROC, precision, recall, **F1-score**

De novo molecule design: chemical validity, novelty, docking scores, synthetic accessibility

## RESEARCH PAPER 3

🔗 LINK: https://link.springer.com/article/10.1007/s44163-025-00266-0

🧩 DATASET USED-

None – the study is a conceptual review/perspective and did not generate or analyze any datasets.

🧠 METHODOLOGY / MODELS USED-

The paper dives into ethical and technical analysis of **Distributed Machine Learning (DML) frameworks** used for sensitive medical data, particularly:

**1. Split Learning** – parts of the model are trained locally and on a central server.

**2. Federated Learning** – clients train locally; only model updates (weights) are shared, preserving data privacy.

**3. Swarm Learning** – peer-to-peer model training using a decentralized ledger (e.g., blockchain) without a central server.

The methodology is largely analytical and philosophical, comparing technical mechanisms–like edge computing, parameter aggregation, and privacy techniques–with ethical frameworks (the “5 P’s,” informed consent, fairness, responsibility, etc.).

✨ NOVELTY-

A comprehensive ethical analysis of DML methods specifically **in healthcare,** framing them under five major ethical principles:

**1. Informed Consent**

**2. Safety & Transparency**

**3. Algorithmic Fairness**

**4. Data Privacy**

**5. Ethical Implementability.**

📊 EVALUATION METRICS AND ACCURACY-

Since this is not an empirical study, it does not present accuracy figures, performance metrics, or quantitative evaluation. Rather, it qualitatively examines ethical trade-offs, limitations (e.g., bias, privacy threat, resource constraints), and conceptual benefits.

## RESEARCH PAPER 4

🔗LINK: <https://www.sciencedirect.com/science/article/pii/S1359644617303598>

🧩 DATASET-

The paper is a comprehensive review, not an empirical study, and thus does not introduce a specific dataset itself. However, it discusses benchmark datasets frequently used in deep learning for drug discovery:

**Molecule Net**: a collection of diverse public datasets encompassing over 700,000 compounds with various bioactivity, **ADMET** (absorption, distribution, metabolism, excretion, toxicity), and physicochemical properties.

🧠 METHODOLOGY/ MODELS USED-

This review summarizes various deep learning architectures and reinforcement learning used in molecular modeling, including:

Feed-forward networks for **QSAR** (quantitative structure–activity relationship) predictions.

**Graph neural networks**, capturing molecular structures.

**Sequence models** (e.g., RNNs, LSTMs) and Reinforcement Learning (RL) for de novo molecule generation and optimization.

Use of **deep generative models** to design novel compounds.

✨ NOVELTY-

The article highlights:

Pioneering applications of deep learning in drug discovery beyond activity prediction, such as **de novo molecular generation.**

Case studies demonstrating deep reinforcement learning to **generate molecules with specific desired properties**.

A review of **successes, obstacles, and the future integration of AI in pharmaceutical R&D**.

📊 EVALUATION METRICS-

Again, as a review, the paper doesn’t present original experimental metrics. However, it references how performance is measured in the domain:

**AUC‑ROC & AUC‑PRC** for classification/bioactivity models.

Regression metrics: **RMSE and MAE** for continuous properties.

## RESEARCH PAPER 5

🔗LINK: <https://www.mdpi.com/1422-0067/24/3/2026>

🧩 DATASET USED-

This paper is a review and doesn’t present new experimental datasets. Instead, it synthesizes AI/ML methods applied in drug development workflows—covering use cases ranging from target identification to clinical trials.

🧠 METHODOLOGY / MODELS USED-

As a literature survey, it collates various AI-driven methods used in modern drug discovery, such as:

**Supervised Learning**: Random forests, SVMs, neural networks for QSAR and ADMET prediction.

**Deep Learning**: CNNs, GNNs, and transformer architectures for molecular property prediction and generation.

**Reinforcement Learning** (RL): Policy-gradient or actor-critic agents for de novo molecule generation.

**Unsupervised Learning:** Dimensionality reduction and clustering for compound library design.

✨ NOVELTY-

Offers a panoramic overview of how AI/ML methods have revolutionized each stage of drug discovery—from hit identification to **lead optimization and safety profiling**.

Highlights case studies showing significant **reductions in time and cost**, including the successful application of **deep reinforcement learning to design novel compounds**.

Presents a framework for **AI integration in pharma R&D**, emphasizing cross-talk between computational outputs and experimental pipelines.

📊 EVALUATION METRICS AND ACCURACY-

As a review, original metrics are not reported, but the paper discusses standard performance measures used in each domain:

**Classification Models**: AUC‑ROC, AUC‑PRC

**Regression Models**: RMSE, MAE

**Generative Models**: Validity, novelty, uniqueness of generated molecules

## RESEARCH PAPER 6

🔗 LINK: <https://arxiv.org/abs/2401.14665?utm_source=chatgpt.com>

🧩 DATASET USED-

**Peptide–protein interaction (PepPI)** datasets curated by authors, likely from databases like PDB or specialized peptide assays.

🧠 METHODOLOGY / MODELS USED-

**Graph Neural Network framework** with:

Fine-grained perturbation module

Dual-view objective using contrastive learning and peptide pre-training

Extended version **diPepGB** handles heavily imbalanced data with directed edges

✨ NOVELTY-

Introduces a **domain-specific peptide GNN** with contrastive pre-training and directed-edge handling for imbalance.

**Performance: Outperforms baseline PepPI models**—exact metrics not in abstract, but described as “greatly outperforms.”

📊 EVALUATION METRICS AND ACCURACY-

Likely **ROC-AUC, Precision, Recall**—though the abstract omits specifics, these models typically report **AUC, accuracy, F1**.

## RESEARCH PAPER 7

🔗 LINK: <https://arxiv.org/abs/2206.07015>

🧩 DATASET USED-

**PDBbind v2016 core set for drug–target binding affinity**

🧠 METHODOLOGY / MODELS USED-

A compact (~0.6 M parameters) GNN that:

**Builds an undirected graph** based on distance thresholds

**Ignores covalent bonds to reduce complexity**

**Uses GNN‑MLP** with independent atom/edge feature extraction

Pools learned features to **predict affinity**

✨ NOVELTY-

Achieves **state-of-the-art performance** with efficient**, non-geometric GNN**, **reducing compute overhead.**

Performance: Pearson correlation , a 5.2% improvement over other GNN-based methods.

📊 EVALUATION METRICS AND ACCURACY-

**Pearson’s correlation coefficient**; underlying regression **uses MSE.**

## RESEARCH PAPER 8

🔗 LINK: <https://www.sciencedirect.com/science/article/pii/S1046202324001282>

🧩 DATASET USED-

DrugBank**: 1,706 drugs, 191,808 positive samples, 86 interaction types**

TWOSIDES dataset

🧠 METHODOLOGY / MODELS USED-

Multiscale **GNN (MGNN**) to capture local/global structure

Substructure interaction learning with attention between drug pairs

✨ NOVELTY-

**Combines multiscale molecular representations with pairwise attention to better predict adverse interactions.**

Performance: Demonstrates state-of-the-art predictive performance on DrugBank and TWOSIDES.

📊 EVALUATION METRICS AND ACCURACY-

**Likely uses AUC, AUPR, accuracy, F1.**

## RESEARCH PAPER 9

🔗 LINK: <https://www.sciencedirect.com/science/article/pii/S0957417423030002>

🧩 DATASET USED-

**Multiple virtual screening benchmarks with protein pockets and ligand libraries**

🧠 METHODOLOGY / MODELS USED-

**Unsupervised graph-autoencoder** for protein pocket representation

**Graph-CNNs** for 2D ligand and pocket graphs

Binding classification without explicit complex structures

✨ NOVELTY-

Learns latent representations for both **proteins and ligands, enabling complex-free binding prediction.**

Performance: Comparable or superior to 3D‑CNNs, docking (AutoDock Vina), RF-Score, and NNScore.

📊 EVALUATION METRICS AND ACCURACY-

**ROC‑AUC, likely Precision/Recall, binding classification accuracy**

## RESEARCH PAPER 10

🔗LINK: <https://arxiv.org/abs/2107.06773>

🧩 DATASET USED-

**Drug molecules with BBB permeability annotations**, plus drug–protein interaction networks; uses Mordred descriptors

🧠 METHODOLOGY / MODELS USED-

**Relational Graph Convolutional Network (RGCN)** combining drug–protein interactions and molecular descriptors

Enhancements using drug similarity graphs to improve generalization

✨ NOVELTY-

**Integrates relational graph learning to explicitly model drug–protein relationships affecting BBB penetration.**

ACCURACY-

**Accurac**y = 0.872

AUROC = 0.919

AUPRC = 0.838

With similarity, improved to accuracy = 0.876, AUROC = 0.926, AUPRC = 0.865

📊 EVALUATION METRICS AND ACCURACY-

**Accuracy, AUROC, AUPRC**

### THE END