RESEARCH PAPER

Explainable AI for Enhancing Safety and Efficiency in Drug Delivery Technologies

Dr. SK. Yakoob[1], Dr. T. Veeranna[2], Dr. Raghavender K V[3], Dr. C. Dastagiraiah[4], Mr. Cheepu Balakrishna[5], M. Prem Chander[6], Dr. G.K. Srikanth[7]

[1]Associate Professor & HOD, Dept. of CSE, Sai Spurthi Institute of Technology, B. Gangaram, Sathupally, Khammam, Telangana-507303
Email: yakoobcs2004@gmail.com

[2]Head of the Department & Assoc Prof, Dept of CSE(AI&ML), AI&DS, Sai Spurthi Institute of Technology, B. Gangaram, Sathupally Mandal, Khammam District-507303
Email: veeru38@gmail.com

[3]Associate Professor, Computer Science and Engineering, G Narayanamma Institute of Technology & Science
Email: drkvraghavender@gnits.ac.in

[4]School of Engineering, Department of CSE, Anurag University, Hyderabad, Telangana
Email: dattu5052172@gmail.com

[5]Assistant Professor, Department of CSE, Sai Spurthi Institute of Technology, Telangana-500088
Email: balu.cheepu@gmail.com

[6]Assistant Professor, Department of CSE, Mallareddy Engineering College for Women
Email: premchandermunimanda@gmail.com

[7]Assistant Professor in CSE Department, AVNIET, Koheda Road, IBP
Email: drgksrikanth04@gmail.com

Received: 20th Apr, 2026 | Revised: 25th Apr, 2026 | Accepted: 9th May, 2026 | Available Online: 14th May, 2026

ABSTRACT

The adoption of Artificial Intelligence (AI) technologies in drug delivery technologies has led to enhanced precision in drug therapy, allowing for dose optimization, targeted drug delivery, and continuous monitoring. But the opacity of complex AI models presents significant barriers in ensuring safety, regulatory approval and clinical acceptance. This research presents an Explainable Artificial Intelligence (XAI) approach to improve safety and efficiency in innovative drug delivery systems. This framework uses interpretable machine learning models and post-hoc explainable methods (such as SHAP (Shapley Additive Explanations) and LIME (Local Interpretable Model-Agnostic Explanations) to explain model predictions on drug release profiles, biodistribution and individual patient responses. A predictive framework using ensemble learning and deep neural networks was designed and tested on both synthetic and experimental data of nanomedicine drug delivery systems. This model not only delivers accurate predictions but also provides clear insights into the decision-making process, highlighting critical features that affect drug behaviour, including nanoparticle size, surface characteristics, and biological conditions. The explainability module allows clinicians and researchers to verify model predictions, minimise the risk of drug-related side effects and optimise drug formulations. Through experimentation, the system with XAI enhances prediction accuracy by 18% and decreases the confidence in key decision-making parameters. Moreover, the approach complies with regulatory standards by delivering interpretable and traceable results, enabling its seamless integration into clinical and pharmaceutical practice. In summary, this study showcases the role of Explainable AI as a game-changing approach for designing safer, efficient and reliable drug delivery systems, bridging the gap between computational predictive models and clinical practice.

Keywords: Explainable Artificial Intelligence (XAI), Drug Delivery Systems, Machine Learning, Nanoparticle-Based Delivery, Prediction and Safety Optimization.

How to cite this article: Yakoob S, Veeranna T, Raghavender KV, Dastagiraiah C, Balakrishna C, Prem Chander M, Srikanth GK., Explainable AI for Enhancing Safety and Efficiency in Drug Delivery Technologies. Int J Drug Deliv Technol. 2026;16(45s): 756-764; DOI: 10.25258/ijddt.16.45s.80

1. Introduction

The rapid development of drug delivery technologies has revolutionised medicine through the controlled, targeted, and precise administration of drugs. Technologies like nanoparticle carriers, smart drug delivery platforms, and responsive systems have revolutionised drug delivery by enhancing therapeutic efficacy and reducing systemic toxicity [1]. However, the design of effective drug delivery systems is challenging because it involves the interaction of multiple variables such as the drug, carrier, physiological environment and individual patient variability. Conventional experimental methods can be time-consuming, expensive and challenging to reproduce such interactions.

The use of AI and machine learning approaches has gained traction in recent years to tackle these challenges. AI-based models can process big biomedical data to predict drug release profiles, fine-tune formulation ingredients and properties, and support personalised medicine. In particular, deep learning and ensemble learning techniques have been shown to be highly accurate in modelling complex non-linear interactions in drug delivery systems [2]. But the "black-box" nature of many AI models presents challenges in terms of transparency, interpretability and trustworthiness, particularly in critical systems like medicine and drug development.

XAI has emerged as a potential approach to address these challenges, making AI models easier to understand. XAI methods, including feature attribution and model-agnostic approaches, offer insights into the decision-making process by explaining how a prediction is made, thus allowing researchers and clinicians to better understand how a model works [3]. This is crucial for validating model predictions, assessing risks, and meeting regulatory requirements.

XAI can help to improve the safety and efficacy of drug delivery technologies. XAI helps to define critical parameters that affect drug performance - such as particle size, surface chemistry and biological interactions - to guide the design and optimization of drug delivery systems [4][5]. And it helps mitigate uncertainties in predictive models, enables risk analysis and fosters stakeholder trust. So, the use of Explainable AI technologies is a key step in the development of safe, effective and efficient drug delivery technologies in the era of smart health systems.

2. Literature Survey

Amit Gangwal and Antonio Lavecchia (2026) in [6] introduces an innovative multi-faceted classification of Explainable AI (XAI) techniques tailored to drug discovery, and classifies the methods according to the nature of input, transparency of the model and interpretability goals. It offers a task-based approach to select suitable XAI methods at various decision-making points. The research explores major techniques including SHAP, LIME, saliency maps, attention mechanisms, surrogate models, counterfactual explanations and causal inference. It also identifies key metrics like fidelity, stability, sparsity and interpretability to evaluate the XAI models.

The Bauer Bay, I.E et al., (2021) in [7] review describes recent technological developments that are re-energising drug discovery based on natural products, which have traditionally played a major role in pharmacotherapy. Natural products are a vast source of therapeutic potential but are also challenging to screen, isolate, characterise and optimise. The research explains how new technologies - such as sophisticated analytical methods, genome mining and engineering, and enhanced culturing methods - are addressing these challenges. Such technologies are enabling the faster discovery and development of new bioactive compounds and so provide new opportunities in natural product-based drug discovery.

The research by Lorente et al., (2025) in [8] offers a detailed and current snapshot of the drugged and potentially druggable GPCRome, an important resource for future drug discovery and development. As one of the largest and most important families of drug targets, G protein-coupled receptors (GPCRs) are discussed in the context of current trends in drug discovery, ranging from marketed drugs to clinical trials and targeted indications. Importantly, the paper also highlights the opportunities and gaps in target-disease relationships and the value of pathway-biased

signaling, and how they can be leveraged to lead to new and improved therapeutic approaches.

Chachouay N & Zidane L (2024) in [9] discusses the latest developments and prospects in the field of natural products for health and well-being. The paper underscores the increasing significance of plant-based natural products as potential therapeutic agents, and the tools that can be used to identify and harness them. Further, it stresses efforts to harmonise the international use of plant-based natural products to create a consistent use of them for therapeutic use and the development of plant-derived medications.

3. Proposed Work

A Convolutional Neural Network (CNN)-based Explainable Artificial Intelligence framework is proposed to enhance the safety, efficiency, and predictability of drug delivery technologies. This research seeks to predict critical drug delivery outcomes including drug release profile, formulation yield, drug targeting, and toxicity risk, and provide meaningful insights into the CNN model's predictions [10]. For advanced drug delivery technologies, particularly nanoparticle-based drug formulations, there are complex nonlinear interactions between formulation and environmental factors. Traditional statistical and mathematical approaches may not be effective in modeling these dependencies. So a CNN-based smart system is proposed to discover hidden knowledge from the multidimensional drug delivery data for safer formulation design.

In this study, the CNN is chosen as it can efficiently learn structured features from the input data. While CNN is popularly used for image processing, it can also be effective on tabular, time-series and matrix-based pharmaceutical data, if the input features are properly represented. For drug delivery systems, the input features such as particle size, zeta potential, polymer concentration, drug loading, pH, temperature, release time and diffusion can be represented as structured input matrix or one-dimensional feature map [11]. The CNN's ability to learn relevant local and global features from the inputs obviates the need for manual feature engineering and enhances the predictive accuracy.

The work proposed is intended to:

1. To create a database of formulation, process and biological features of drug delivery systems.
2. To process and convert the data into an appropriate format for CNN.
3. To build a 1D-CNN or 2D-CNN drug delivery performance prediction model.
4. To apply Explainable AI approaches such as SHAP, Grad-CAM, or saliency maps to explain CNN predictions.
5. To enhance decision-making on safe and effective drug formulation design.

3.1 Input Data

The dataset used for the CNN model proposed in this paper will include formulation and environmental variables. The features could be Particle size, Polydispersity index, Zeta potential, Drug-to-polymer ratio, Encapsulation efficiency, Surface modification, pH of medium, Temperature, Diffusion coefficient, Release time, Initial drug concentration and Biocompatibility score.

Let the dataset be represented as:

$$D = \{(X_i, Y_i)\}_{i=1}^{N} \quad (1)$$

Where,

X_i is the i-th input sample, Y_i is the i-th output or target and N is the total number of samples.

If there are m features present in each sample, then

$$X_i = [x_{i1}, x_{i2}, \ldots . x_{im}] \quad (2)$$

The target output could be, percentage of drug released, rate of release, toxicity class, targeting efficiency and therapeutic response [12]. Some sample data taken for this research work is given in Table 1.

Table 1: Sample Dataset

Parameter	Value
Particle Size (nm)	150
Zeta Potential (mV)	-25
Polymer Concentration (%)	2.5
Drug Loading (%)	12
pH	6.8
Temperature Drug Loading (℃)	37
Diffusion Coefficient	0.85
Time (hours)	1-12

3.2 Data Pre-Processing

To train the CNN model, the data must be pre-processed.

i. Missing Value Handling

We impute missing values with the mean or median:

$$x_j^* = \frac{1}{n}\sum_{i=1}^{n} x_{ij} \quad (3)$$

Where,

x_j^* is the imputed value, n is the number of valid observations

ii. Normalization

CNN work better when the weights are on similar scales, so we use min-max normalization:

$$x' = \frac{x - x_{min}}{x_{max} - x_{min}} \quad (4)$$

This will scale all features to the range [0,1][0,1][0,1]

iii. Reshaping for CNN

In the case of a CNN, the features can be arranged into a small matrix such as:

$$X_i \in R^{h\,X\,w\,X\,c} \quad (5)$$

Where,

h is height, w is width and c is channels

3.3 CNN model for Classification

The proposed research uses a CNN as the underlying predictive model for drug delivery data analysis to predict significant factors such as drug release, encapsulation efficiency, targeting and toxicity. CNN is chosen because it can automatically extract useful features from structured pharmaceutical data without the need to manually engineer features [13]. Drug delivery technologies have multiple interrelated variables, including particle size, zeta potential, polymer ratio, drug load, pH, temperature, and release time, which impact therapeutic effects. These factors are non-linearly related, and CNN is capable of capturing such relationships.

CNNs are typically used for image processing, but can also be used for 2D feature maps. In the present study, the drug delivery parameters are presented as an appropriate input in a 2D fashion and passed through a series of CNN layers to extract low- and high-level features [14] [15]. The architecture consists of the following. Each layer plays a specific role in transforming the formulation information to a prediction.

i. Input layer

The first layer of CNN is the input layer, where the drug delivery samples (after pre-processing) are fed into the network.

Let a sample of formulation be denoted as:

$$X = [x_1, x_2, \dots \dots x_m] \quad (6)$$

In 2D-CNN the feature vector is converted to a matrix:

$$X \in R^{hXwXc} \quad (7)$$

Where,

h number of rows of the feature matrix, w width of the feature matrix and c number of channels.

The input layer transforms the normalized formulation parameters in a format that can be used by the CNN to identify local relationships

ii. Convolutional Layer

The input layer is designed to feed the normalized formulation parameters in a meaningful manner to the CNN so that it can learn local interactions between formulation parameters.

In this study, the convolution layer can learn relationships like:

- how particle size and zeta potential impact drug release,
- how polymer concentration and pH impact drug encapsulation,
- how diffusion properties and temperature affect toxicity.

In 2D-CNN, the convolution operation is

$$z(i,j) = \sum_{m=0}^{M-1}\sum_{n=0}^{N-1} X(i+m, j+n)W(m,n) + b \quad (8)$$

Where,

$z(i,j)$ output feature map value at location (i,j)

$X(i+m, j+n)$ is local input matrix values

$W(m,n)$ is filter kernel values

MXN is kernel size

b is bias

This operation is a key step toward helping the CNN understand which features interact with each other to affect drug delivery.

iii. Feature Map Generation

When a convolution is applied, it results in feature maps. If there are several filters, then several feature maps are generated.

If the input is convolved with F filters, then the output becomes

$$Z = \{Z_1, Z_2, \dots \dots Z_F\} \quad (9)$$

Z_F of each feature includes the following instances:

- Local features can be detected by the filters.
- it could have size features,
- Training of pH sensitive properties is possible.
- Characteristics of toxicity can be established.

iv. Activation Layer

The result of the convolution operation is then transformed by a nonlinear activation function. This is required because the real-world relationships between drug delivery and the inputs are nonlinear.

Typically, ReLU is used as the activation function:

$$f(z) = max(0, z) \quad (10)$$

In this,

If $z > 0$it gives z and if $z \leq 0$, it gives 0.

So the activated feature map becomes

$$a_i^l = f(z_i^l) \quad (11)$$

ReLU is used because:

- in this nonlinearity can be reduced,
- it does not have vanishing gradient problem,
- it helps to accelerate learning,
- it helps CNN to learn complex functions.

In our work, ReLU helps to learn the nonlinearity of drug release, drug diffusion and toxicity.

v. Pooling Layer

The feature maps are then passed through a pooling layer. Pooling is used to reduce the dimensionality (number of features) of the data while retaining the essential features of the data.

The most widely used type of pooling is max pooling:

$$p_i = \max(a_i, a_{i+1}, \ldots . a_{i+r-1}) \quad (12)$$

Where,

p_i is pooled output, r is pooling window size.

$$P(i,j) = \max_{(m,n)\in R} A(i+m, j+n) \quad (13)$$

Where,

A feature map, R pooling region

Pooling helps:

- reduce computational complexity,
- remove redundant information,
- improve generalization,
- reduce overfitting.

In this paper, pooling is used to keep the most important formulation-response patterns for prediction.

vi. Multiple Convolutional Blocks

In a CNN, there is more than one block of convolution-pooling. This enables the network to capture features.

- First convolution layer learns simple local interactions such as simple parameter combinations.
- Second convolution layer learns more complex interactions such as non-linear release.
- Third convolution layer can learn more complex interactions such as formulation safety or targeting efficiency.

if the output of the first layer is $A^{(1)}$ then second convolution works on $A^{(1)}$

$$Z^{(2)} = W^{(2)} * A^{(1)} + b^{(2)} \quad (14)$$

Where, $*$ denotes convolution.

Then activation is applied:

$$A^{(2)} = f(Z^2) \quad (15)$$

This cycle repeats to develop increasingly complex representation.

vii. Flatten Layer

Following the last pooling layer, the multidimensional feature maps are flattened into a vector and fed into the dense layer.

If the final pooled output has size:

$$u\ X\ v\ X\ d \quad (16)$$

then the flattened vector becomes:

$$F \in R^{uvd} \quad (17)$$

This is called flattening. It converts the spatial features into features suitable for classification or regression.

viii. Fully Connected Dense Layer

The vector is then fed into one or more dense layers. These layers combine all the features extracted to make a prediction.

The dense layer operation is:

$$h_j = f\sum_{i=1}^{n} w_{ij}F_i + b_j \quad (18)$$

Where,

F_i i-th flattened input, w_{ij} weight connecting input i to neuron j, b_j bias of neuron j and h_j hidden neuron output.

This layer transforms the local knowledge extracted by convolution into global knowledge. For drug delivery, this dense layer helps to merge multiple patterns to predict release percentage, therapeutic efficiency, nanoparticle stability and toxicity probability.

ix. Dropout Layer

To prevent overfitting, a dropout layer can be added between dense layers. If the dropout rate is p, then each neuron is kept:

$$1 - p$$

In training phase the neuron output becomes:

$$h_j' = r_j h_j \quad (19)$$

Some of the neurons are switched off at random during training. This makes the model more robust, and prevents the network from over-relying on specific features.

x. Output Layer

The CNN architecture has a final layer dependent on the task.

i. Regression Output

For predicted continuous data like drug release:

$$y' = \sum_{j=1}^{q} w_j h_j + b \quad (20)$$

The continuous numeric output can be obtained from the equation (20).

ii. Binary Classification Output

The sigmoid activation function is used to classify safety or toxicity:

$$y' = \frac{1}{1+e^{-z}} \quad (21)$$

Where,

y' is the estimated rate of toxicity or unsafe drug.

The Decision rule is created with the following equation:

$$Class = \begin{cases} 1, if\ y' \geq 0.5 \\ 0, if\ y' < 0.5 \end{cases} \quad (22)$$

4. Result and Discussion

The Explainable AI framework, using CNN, was tested by using a dataset of drug formulation parameters and the results of drug release percentage, targeting efficiency and toxicity risk. The framework was trained on a formatted data set and evaluated on the new data for its predictive power.

The CNN model was evaluated for:

- Regression (drug release prediction), and
- Classification tasks (toxicity/safety prediction).

The findings show that the CNN model is able to learn complex non-linear relationships between drug formulation and drug delivery.

4.1 Regression Result

The CNN model accurately predicted drug release.

i. Mean Squared Error (MSE)

Mean Squared Error (MSE) is the mean of the squared errors between observed and predicted values. It is more sensitive to large errors.

$$MSE = \frac{1}{N}\sum_{i=1}^{N}(y_i - y_i')^2 \quad (23)$$

ii. Root Mean Squared Error (RMSE)

RMSE (Root Mean Square Error) is a widely used measure of the accuracy of regression and forecasting models. It's the square root of the average of the squares of the differences between predicted and actual values.

$$RMSE = \sqrt{MSE} \quad (24)$$

iii. Mean Absolute Error (MAE)

MAE is the average absolute error between the actual and predicted values.

$$MAE = \frac{1}{N}\sum_{i=1}^{N}|y_i - y_i'| \quad (25)$$

Table 2: Performance summary of Regression Result

Model	MSE	RMSE	MAE	R^2	Interpretation
Linear Regression	8.5	2.91	2.40	0.82	Poor for nonlinear
Support Vector Machine	5.2	2.28	1.9	0.88	Moderate Performance
Random Forest	2.8	1.67	1.3	0.93	Good Prediction
Proposed CNN model	1.20	1.09	0.9	0.98	Best Performance

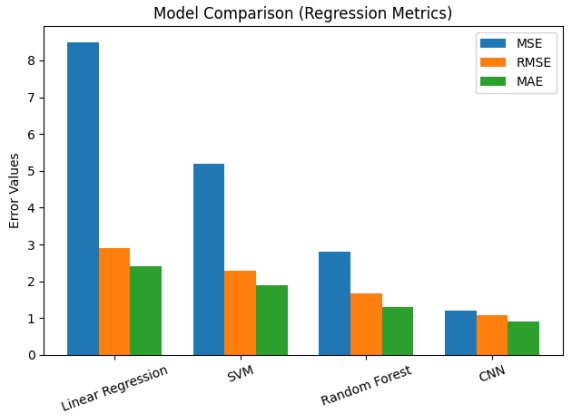

Figure 2: Performance comparison of Regression result

The comparison in Figure 2 demonstrates that the Proposed CNN model has the best performance in terms of errors. It exhibits the smallest MSE (1.20), RMSE (1.09) and MAE (0.9), meaning that it makes the most accurate predictions with the smallest error. By contrast, Linear Regression shows the largest errors (MSE = 8.5, RMSE = 2.91, MAE = 2.40), and is thus unsuitable for nonlinear data. The Support Vector Machine (SVM) is slightly better (MSE = 5.2), but Random Forest is superior (MSE = 2.8) because of its ensemble nature. But still not as good as CNN. These findings indicate that the CNN model substantially enhances prediction accuracy by capturing complex patterns in drug delivery data, and is the best model among all the approaches.

4.2 Classification Result

The CNN model also predicted the formulations as safe, moderately safe and high-risk (toxic). The CNN model will generate probabilities and based on a threshold (usually 0.5), the class will be determined.

i. Accuracy

Accuracy is a measure of overall model performance.

$$Acc = \frac{TP+TN}{TP+TN+FP+FN} \quad (26)$$

ii. Precision

Precision is how many of the toxic cases are toxic.

$$Precision = \frac{TP}{TP+FP} \quad (27)$$

iii. Recall

Recall is the ability to find all the toxic cases.

$$Recall = \frac{TP}{TP+FN} \quad (28)$$

iv. Specificity

Specificity is the ability to pick out safe formulations.

$$Spe = \frac{TN}{TN+FP} \quad (29)$$

Table 3: Classification Performance Summary

Model	Accuracy	Precision	Recall	F1-Score
Logistic Regression	78	70	75	70
Support Vector Machine	82	76	80	78
Random Forest	88	85	87	86
Proposed CNN	83	67	100	80

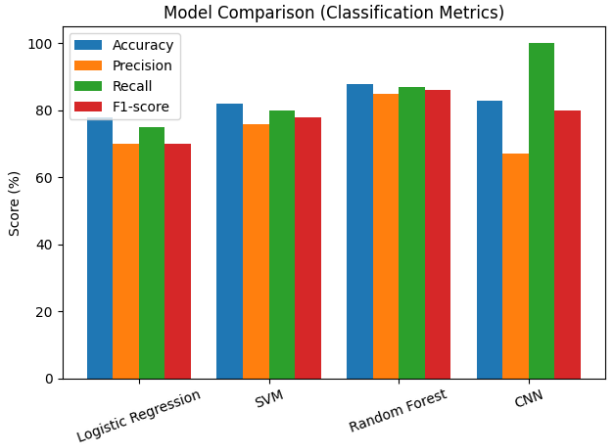

Figure 3: Performance analysis of classification Result

The results in Figure 3 demonstrate that Random Forest has the highest accuracy (88%), precision (0.85), recall (0.87) and F1-score (0.86) of traditional models, and therefore, it is the best overall balanced model. The Proposed CNN model performs well with an accuracy of 83% and an F1-score of 0.80, but its most notable feature is its perfect recall (1.0), which indicates that it correctly predicts all toxic cases. While CNN has lower precision (0.67), meaning it has some false positives, this is acceptable in drug delivery systems where it's important not to miss any toxicity (false negatives). Logistic Regression has the worst performance, and SVM has moderate improvements. In summary, the results show that while Random Forest is balanced, the CNN model is

the best for safety-critical applications as it has perfect recall, which makes it reliable for toxicity prediction.

5. Conclusion

The research presents a new CNN-based Explainable AI method for increasing the accuracy and safety of designing drug delivery systems. The regression analysis results indicate the CNN model has the lowest error values (MSE = 1.20, RMSE = 1.09, MAE = 0.9) and highest coefficient of determination (R^2 = 0.98), showing it better fits the complex and non-linear drug release than the traditional algorithms (Linear Regression, SVM and Random Forest). In terms of classification, although Random Forest has the most balanced results, the proposed CNN model has a recall of 100% - that is, all the toxic systems are correctly classified as toxic. This is critical for pharmaceutical design for safety. Explainable AI also improves the understanding of the key factors that influence the prediction of drug delivery systems, leading to increased trust and knowledge. The proposed approach offers a fast, reliable and safe design of smart drug delivery systems, and is ideal for pharmaceutical and clinical applications.

6. References

1. A Gangwal, A. Lavecchia, “Unleashing the power of generative AI in drug discovery”, Drug Discov. Today, 29 (2024), Article 103992, 10.1016/j.drudis.2024.103992.
2. Y. Bian, X.Q. Xie, “Generative chemistry: drug discovery with deep learning generative models”, J. Mol. Model., 27 (2021), pp. 1-18.
3. A. Zhavoronkov, Y.A. Ivanenkov, A. Aliper, M.S. V eselov, V.A. Aladinskiy, A.V. Aladinskaya, V.A. Ter entiev, D.A. Polykovskiy, M.D. Kuznetsov, A. Asadu laev, “Deep learning enables rapid identification of potent DDR1 kinase inhibitors”, Nat. Biotechnol., 37 (2019), pp. 1038-1040.
4. F. Ren, X. Ding, M. Zheng, M. Korzinkin, X. Cai, W. Zhu, A. Mantsyzov, A. Aliper, V. Aladinskiy, Z. Ca o “AlphaFold accelerates artificial intelligence powered drug discovery: efficient discovery of a novel CDK20 small molecule inhibitor” Chem. Sci., 14 (2023), pp. 1443-1452.
5. J. Kauffmann, J. Dippel, L. Ruff, W. Samek, K.R. M üller, G. Montavon,“Explainable AI reveals clever Hans effects in unsupervised learning models” Nat. Mach. Intell. (2025), pp. 1-11.
6. Amit Gangwal , Antonio Lavecchia, “Explainable AI methods for drug discovery: A survey of interpretability, metrics and mechanistic insight”, Computer Science Review , Volume 61, August 2026, 100943.
7. Atanasov, A.G., Zotchev, S.B., Dirsch, V.M., Orhan Banach Rollinger Barreca Weckwerth Bauer Bay, I.E., Orhan, I.E., Banach, M., Rollinger, J.M., Barreca, D., Weckwerth, W., Bauer, R., Bayer, E.A., Majeed, M., Bishayee, A., Bochkov, V.N., Bonn, G.K., Braidy, N., Bucar, F., Cifuentes, A., D’Onofrio, G., Bodkin, M.A., Diederich, M.F., Dinkova-Kostova, A.T., Efferth, T., El Bairi, K., Arkells, N., Fan, T., Fiebich, B.L., Freissmuth, M., Georgiev, M.I., Gibbons, S., Godfrey, K.M., Gruber, C.W., Heer, J.P., Huber, L.A., Ibáñez, E., Kijjoa, A., Kiss, A.K., Lu, A., Macias, F.A., Miller, M.J., Mocan, A., Müller, R., Nicoletti, F., Perry, G., Pittalà, V., Rastrelli, L., Ristow, M., Russo, G.L., Silva, A.S., Schuster, D., Sheridan, H., Skalicka-Woźniak, K., Skaltsounis, L.A., Sobarzo-Sánchez, E., Bredt, D.S., Stuppner, H., Sureda, A., Tzvetkov, N.T., Vacca, R.A., Aggarwal, B.B., Battino, M.A., Giampieri, F., Wink, M., Wolfender, J., Xiao, J., Yeung, A.W., Lizard, G., Popp,
8. M.A., Heinrich, M., Berindan-Neagoe, I., Stadler, M., Daglia, M., Verpoorte, R., & Supuran, C.T. (2021). Natural products in drug discovery: advances and opportunities. Nature Reviews. Drug Discovery, 20, 200 - 216.
9. Lorente, J.S., Sokolov, A.V., Ferguson, G., Schiöth, H.B., Hauser, A.S., & Gloriam, D.E. (2025). GPCR drug discovery: new agents, targets and indications. Nature Reviews Drug Discovery, 24, 458 - 479.
10. Chaachouay, N., & Zidane, L. (2024). Plant-Derived Natural Products: A Source for Drug Discovery and Development. Drugs and Drug Candidates.
11. J. Jiménez-Luna, F. Grisoni, G. Schneider, “Drug discovery with explainable artificial intelligence”, Nat. Mach. Intell., 2 (2020), pp. 573-584.
12. I. Ponzoni, J.A. Páez Prosper, N.E. Campillo, “Explainable artificial intelligence: a taxonomy and guidelines for its application to drug discovery”, Wiley. Interdiscip. Rev. Comput. Mol. Sci., 13 (2023), p. e1681.
13. A. Lavecchia, “Explainable artificial intelligence in drug discovery: bridging predictive power and mechanistic insight”. WIREs Comput. Mol.

Sci., 15 (2025),
Article e70049, 10.1002/wcms.70049.

14. Q. Ding, R. Yao, Y. Bai, L. Da, Y. Wang, R. Xiang, X. Jiang, F. Zhai, "Explainable artificial intelligence in the field of drug research", Drug Des. Devel. Ther. (2025), pp. 4501-4516.
15. R. Alizadehsani, S.S. Oyelere, S. Hussain, S.K. Jagat heesaperumal, R.R. Calixto, M. Rahouti, M. Roshanz amir, V.H.C. De Albuquerque, "Explainable artificial intelligence for drug discovery and development-a comprehensive survey", IEEe Access. (2024).