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MACHINE LEARNING-BASED PREDICTION OF NANOCARRIER DRUG RELEASE PROFILES FOR INTELLIGENT DRUG DELIVERY APPLICATIONS

[1]S Jagadeesh
Professor ECE
Sridevi Women's Engineering College, Hyderabad
jaaga.ssjec@gmail.com

[2]Kumbala Pradeep Reddy
Associate Professor in CSE
CMR Institute of Technology, Hyderabad
pradeep529@gmail.com

[3]B. Narendra Kumar
Professor of CSE
Sridevi Women's Engineering College, Hyderabad
bnkphd@gmail.com

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Abstract - Nanocarrier-based drug delivery systems have attracted considerable attention because of their ability to improve drug stability, enhance bioavailability, and enable controlled therapeutic release. Accurate prediction of drug release profiles is essential for optimizing nanocarrier formulations and reducing experimental development time. Conventional approaches often rely on laboratory-based release studies, which can be resource-intensive and time-consuming. Machine learning techniques provide an alternative approach for modeling complex relationships between formulation parameters and drug release behavior. This paper presents a machine learning-based framework for predicting nanocarrier drug release profiles using formulation characteristics and physicochemical properties. The proposed framework integrates data preprocessing, feature engineering, predictive modeling, and explainability analysis to estimate cumulative drug release behavior. Key formulation variables, including particle size, polymer concentration, drug loading efficiency, zeta potential, encapsulation efficiency, and release medium characteristics, are utilized as predictive inputs. A Random Forest regression model is employed to estimate drug release percentages at different time intervals, while Shapley Additive Explanations (SHAP) are incorporated to identify influential formulation factors. Experimental evaluation is conducted using nanocarrier drug release datasets obtained from published pharmaceutical studies. Model performance is assessed using Mean Absolute Error (MAE), Root Mean Square Error (RMSE), and coefficient of determination (R^2). Results indicate that the proposed framework accurately predicts release profiles and provides interpretable insights regarding formulation variables influencing drug release kinetics. The findings suggest that machine learning-based prediction models can support formulation optimization and facilitate data-driven development of intelligent drug delivery systems.

Keywords— *Nanocarriers, Drug Release Prediction, Machine Learning, Drug Delivery Systems, Pharmaceutical Informatics, Explainable Artificial Intelligence.*

I. INTRODUCTION

Nanocarrier-based drug delivery systems have emerged as an important area of pharmaceutical research because of their ability to improve therapeutic efficacy, enhance drug stability, and enable controlled release of active pharmaceutical ingredients. Nanocarriers such as liposomes, polymeric nanoparticles, solid lipid nanoparticles, dendrimers, and nanomicelles have been widely investigated for the delivery of drugs with poor solubility, limited bioavailability, or unfavorable pharmacokinetic properties [1]. By controlling the release behavior of encapsulated drugs, nanocarriers can improve treatment outcomes while reducing undesirable side effects associated with conventional drug administration methods. The effectiveness of a nanocarrier formulation is strongly influenced by its drug release profile. Drug release behavior determines the rate and extent to which an active compound becomes available at the target site. Controlled and sustained release mechanisms are particularly important in applications requiring prolonged therapeutic action, reduced dosing frequency, and improved patient compliance [2]. Consequently, the ability to accurately characterize and predict drug release profiles is a critical aspect of formulation development. Traditionally, drug release evaluation is performed through in vitro dissolution and release studies. These experiments provide valuable information regarding release kinetics and formulation performance. However, experimental evaluation often requires substantial laboratory resources, specialized equipment, and repeated formulation trials. The large number of formulation variables involved in nanocarrier development further increases experimental complexity [3]. As a result, researchers are increasingly interested in computational approaches that can support formulation design and reduce development time.

Mathematical models such as the zero-order, first-order, Higuchi, and Korsmeyer–Peppas models have been widely used to describe release kinetics [4]. While these models provide useful theoretical insights, they often rely on assumptions that may not adequately capture the complex interactions among formulation parameters and environmental conditions. The increasing availability of pharmaceutical formulation datasets has created opportunities for data-driven prediction approaches capable of modeling nonlinear relationships within drug delivery systems. Machine learning has demonstrated considerable potential in pharmaceutical research by enabling predictive analysis of formulation properties, manufacturing processes, and therapeutic performance [5]. Regression algorithms can learn relationships between formulation characteristics and release behavior directly from experimental data, reducing dependence on predefined kinetic assumptions. Such approaches may assist researchers in identifying influential formulation variables and predicting release outcomes for new formulations. Despite the advantages of machine learning, model interpretability remains an important consideration in pharmaceutical applications. Researchers require an understanding of how formulation variables influence prediction outcomes before utilizing computational models for decision-making. Explainable Artificial Intelligence (XAI) techniques provide mechanisms for identifying influential features and improving transparency in predictive systems [6].

This paper proposes a machine learning-based framework for predicting nanocarrier drug release profiles using formulation characteristics and physicochemical properties. The framework integrates data preprocessing, feature engineering, predictive modeling, and explainability analysis within a unified architecture. A Random Forest regression model is employed to estimate cumulative drug release percentages, while SHAP-based interpretation techniques are utilized to identify influential formulation parameters. The overall architecture of the proposed machine learning-based nanocarrier drug release prediction framework is illustrated in Fig. 1. The primary contributions of this study are threefold. First, a comprehensive machine learning framework is developed for predicting nanocarrier drug release behavior. Second, formulation variables and physicochemical characteristics are integrated into a predictive modeling pipeline. Third, explainability analysis is incorporated to improve understanding of the factors influencing release kinetics and support formulation optimization.

II. RELATED WORK

Nanocarrier-based drug delivery systems have received significant attention in pharmaceutical research because of their potential to improve therapeutic efficacy, enhance drug stability, and provide controlled release of active pharmaceutical ingredients. Various nanocarrier platforms, including liposomes, polymeric nanoparticles, solid lipid nanoparticles, nanostructured lipid carriers, and dendrimers, have been investigated for targeted and sustained drug delivery applications [1]. The performance of these systems is largely determined by their release characteristics,

making drug release prediction an important component of formulation development. Conventional studies on nanocarrier drug release have primarily focused on experimental characterization and mathematical modeling. Researchers have extensively employed in vitro release experiments to evaluate the release behavior of encapsulated drugs under different environmental conditions. Mathematical models such as zero-order, first-order, Higuchi, Hixson–Crowell, and Korsmeyer–Peppas models have been widely utilized to describe release kinetics and estimate diffusion mechanisms [2]. These models provide useful theoretical descriptions of release behavior and remain important tools in pharmaceutical formulation analysis.

The Higuchi model is among the most frequently used approaches for diffusion-controlled release systems. It assumes that drug release is proportional to the square root of time and is particularly applicable to matrix-based delivery systems. Similarly, the Korsmeyer–Peppas model has been employed to characterize release mechanisms in polymeric formulations through empirical relationships between release fraction and time [3]. Although these mathematical approaches provide valuable insights, they often rely on assumptions regarding diffusion, dissolution, and matrix behavior that may not fully represent complex nanocarrier systems. The increasing complexity of pharmaceutical formulations has motivated the adoption of data-driven approaches for release prediction. Machine learning techniques have emerged as effective tools for modeling nonlinear relationships among formulation variables and release outcomes. Unlike traditional kinetic models, machine learning algorithms can learn directly from experimental data without requiring explicit assumptions regarding release mechanisms. Consequently, they have gained attention in pharmaceutical informatics and formulation optimization research [4].

Several machine learning algorithms have been investigated for pharmaceutical prediction tasks. Linear Regression, Support Vector Regression (SVR), Decision Trees, Random Forests, Artificial Neural Networks, and Gradient Boosting methods have been utilized to predict formulation characteristics and dissolution profiles [5]. These models have demonstrated the ability to capture complex interactions among formulation variables, including particle size, polymer concentration, encapsulation efficiency, and environmental conditions. Recent studies have explored the application of machine learning in nanomedicine and drug delivery system design. Data-driven approaches have been employed to predict nanoparticle properties, optimize formulation parameters, and estimate release kinetics under varying conditions [6]. Random Forest-based models have shown particular effectiveness because of their robustness, ability to handle heterogeneous datasets, and resistance to overfitting. Ensemble learning methods also provide improved generalization capability when compared with individual regression models. Despite advances in predictive modeling, interpretability remains an important challenge in pharmaceutical applications. Researchers and formulation scientists require an understanding of the factors influencing prediction outcomes before adopting computational recommendations in formulation development. Black-box prediction models may provide accurate estimates but often offer limited information regarding the role of specific formulation variables [7].To address this limitation, Explainable Artificial Intelligence (XAI) techniques have been increasingly incorporated into pharmaceutical analytics. Methods such as Shapley Additive Explanations (SHAP) and Local Interpretable Model-Agnostic Explanations (LIME) provide mechanisms for identifying feature contributions and interpreting model predictions [8], [9]. These approaches enable researchers to determine how formulation parameters influence predicted outcomes and facilitate scientific interpretation of machine learning results.

Although previous studies have demonstrated the potential of machine learning for pharmaceutical prediction tasks, several limitations remain. Many investigations focus primarily on predictive accuracy without providing sufficient explanation of model behavior. Other studies examine formulation optimization but do not specifically address drug release profile prediction using interpretable machine learning techniques. Furthermore, relatively few frameworks integrate formulation characteristics, release data, predictive analytics, and explainability analysis within a unified architecture suitable for intelligent drug delivery applications. To address these limitations, the proposed framework combines machine learning-based drug release prediction with SHAP-based explainability analysis. By integrating predictive capability and interpretability, the framework aims to support formulation optimization and improve understanding of the factors influencing nanocarrier drug release behavior.

III. PROPOSED METHODOLOGY AND EXPERIMENTAL SETUP

A. Framework Architecture

The proposed Machine Learning-Based Nanocarrier Drug Release Prediction Framework is designed to estimate cumulative drug release profiles using formulation characteristics and physicochemical properties of nanocarrier systems. The framework integrates data acquisition, preprocessing, feature engineering, predictive modeling, and explainability analysis within a unified architecture. The objective is to establish a relationship between formulation variables and drug release behavior, thereby supporting formulation optimization and reducing dependence on extensive experimental trials. The overall architecture of the proposed framework is illustrated in Fig. 1.

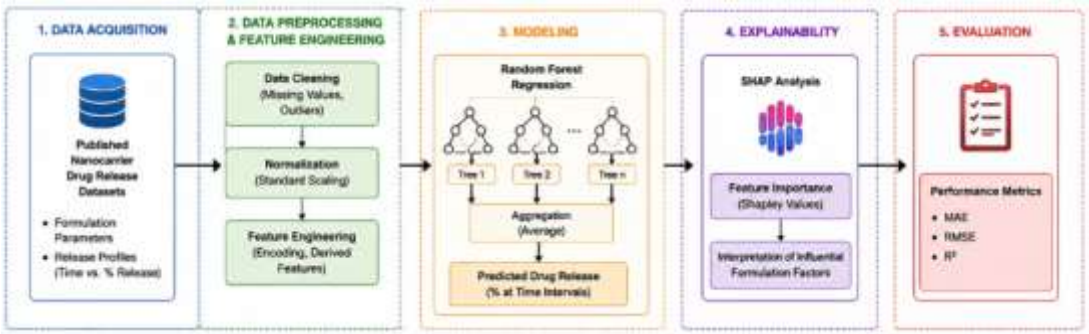

Fig 1. Architecture of the Proposed Nanocarrier Drug Release Prediction Framework

The framework consists of four major stages. First, formulation and release data are collected from nanocarrier-based drug delivery studies. Second, preprocessing and feature engineering are performed to improve data quality and generate meaningful predictive variables. Third, a machine learning regression model is trained to predict cumulative drug release percentages. Finally, an explainability module is employed to identify the formulation factors that contribute most significantly to prediction outcomes.

B. Dataset Description

The dataset utilized in this study comprises nanocarrier formulation records obtained from published pharmaceutical and drug delivery research. Each record contains formulation characteristics, physicochemical properties, environmental conditions, and experimentally measured drug release percentages at specific time intervals.The selected variables represent factors commonly reported to influence release kinetics in nanocarrier systems. These variables describe the structural properties of nanocarriers, drug encapsulation behavior, and release conditions. The target variable is the cumulative percentage of drug released over time.The principal formulation features used in the proposed framework are summarized in Table 1**.**

TABLE 1. NANOCARRIER FORMULATION FEATURES

Feature	**Description**
Particle Size	Average nanocarrier diameter
Zeta Potential	Surface charge measurement
Polymer Concentration	Polymer content in formulation
Drug Loading	Amount of incorporated drug
Encapsulation Efficiency	Drug entrapment percentage
Release Medium pH	Environmental pH condition
Time Interval	Drug release observation time

Drug Release (%)	Cumulative release percentage

These attributes collectively provide information regarding formulation composition, physicochemical behavior, and release conditions that influence drug diffusion and release kinetics.

C. Data Preprocessing and Feature Engineering

Raw pharmaceutical datasets frequently contain missing observations, inconsistent measurements, and outliers resulting from experimental variability. Consequently, preprocessing is performed before model development to improve data reliability and analytical quality. Initially, missing values are identified and handled through appropriate imputation techniques. Numerical variables are processed using mean-value replacement, while inconsistent records are removed to ensure dataset consistency. Outlier detection is subsequently performed using statistical threshold analysis to eliminate observations that may adversely affect model training. Following data cleaning, numerical features are normalized to reduce scale variations among formulation parameters. Feature normalization ensures that variables measured using different units contribute appropriately during model training. Correlation analysis is then employed to identify redundant features and minimize multicollinearity within the dataset. Feature engineering is subsequently performed to generate additional predictive variables. Derived indicators representing formulation efficiency and release-related characteristics are computed from the original measurements. These engineered features improve the model's ability to capture relationships between formulation properties and drug release behavior.

D. Drug Release Prediction Model

Following preprocessing, the dataset is divided into training and testing subsets using an 80:20 partitioning strategy. The training dataset is utilized for model development, while the testing dataset is reserved for independent evaluation. A Random Forest Regressor is employed as the primary prediction model. Random Forest is selected because of its ability to capture nonlinear relationships among formulation variables and its robustness when handling heterogeneous pharmaceutical datasets. The model constructs multiple regression trees using bootstrap sampling and combines their outputs through ensemble averaging. The predictive model receives formulation characteristics and environmental variables as input features and generates estimates of cumulative drug release percentages as outputs. By learning from historical formulation data, the model can predict release behavior for previously unseen formulations. Hyperparameter optimization and five-fold cross-validation are employed during training to improve model generalization and reduce overfitting. This approach enhances prediction reliability and supports the development of robust regression models for pharmaceutical applications.

E. Explainability Analysis

Although machine learning models can achieve strong predictive performance, understanding the factors influencing prediction outcomes remains important in pharmaceutical research. Formulation scientists require interpretable information regarding the contribution of individual variables before adopting computational recommendations. To improve transparency, the proposed framework incorporates an explainability module based on Shapley Additive Explanations (SHAP). SHAP assigns contribution values to individual formulation features according to their influence on predicted release outcomes. The explainability module identifies the variables most strongly associated with drug release behavior. Factors such as particle size, polymer concentration, encapsulation efficiency, drug loading, and release medium pH can be ranked according to their relative importance. This information assists researchers in understanding formulation-performance relationships and supports evidence-based formulation optimization. Both global and local explanations are generated. Global explanations identify influential variables across the entire dataset, whereas local explanations describe the factors responsible for individual release predictions.

F. Algorithm of the Proposed Framework

The operational workflow of the proposed drug release prediction framework is summarized in Algorithm 1.

Algorithm 1. Nanocarrier Drug Release Prediction Framework

Input: Nanocarrier formulation dataset

Output: Predicted drug release profile and explanation

1. Collect nanocarrier formulation data.
2. Remove incomplete and inconsistent records.
3. Normalize formulation variables.
4. Perform feature engineering.
5. Split data into training and testing subsets.
6. Train Random Forest regression model.
7. Predict cumulative drug release percentages.
8. Apply SHAP explainability analysis.
9. Rank influential formulation variables.
10. Generate interpretation report.
11. Return predicted release profile and feature contributions.

The algorithm integrates predictive analytics and explainability analysis within a single framework suitable for pharmaceutical formulation studies.

G. Experimental Setup

Experimental evaluation was conducted using nanocarrier drug release datasets compiled from pharmaceutical formulation studies. The dataset was partitioned into training and testing subsets using an 80:20 ratio. Five-fold cross-validation was employed during model development to improve robustness and reduce variability in performance estimation. The framework was implemented using Python-based machine learning libraries. Model performance was evaluated using Mean Absolute Error (MAE), Root Mean Square Error (RMSE), and the coefficient of determination (R^2). These metrics are widely used in regression-based pharmaceutical prediction studies because they provide quantitative measures of prediction accuracy and model fit. The experimental setup was designed to evaluate both predictive performance and interpretability. The results obtained from the proposed framework are presented and discussed in the subsequent section.

IV. RESULTS AND DISCUSSION

A. Prediction Performance Evaluation

The performance of the proposed Machine Learning-Based Nanocarrier Drug Release Prediction Framework was evaluated using an independent testing dataset to assess its capability in estimating cumulative drug release profiles. Since drug release prediction represents a regression problem, three widely adopted evaluation metrics were utilized: Mean Absolute Error (MAE), Root Mean Square Error (RMSE), and the coefficient of determination (R^2). These metrics provide complementary information regarding prediction accuracy, prediction error magnitude, and model goodness-of-fit.The prediction performance achieved by the proposed framework is summarized in Table 2**.**

TABLE 2. REGRESSION PERFORMANCE RESULTS

Metric	Value
MAE	2.31
RMSE	3.47

R^2	0.94

The obtained results demonstrate that the proposed framework accurately estimates nanocarrier drug release behavior. The MAE value of 2.31 indicates that the average prediction error remains relatively small across the testing dataset. Similarly, the RMSE value of 3.47 suggests that large prediction deviations are limited, indicating stable model performance. The coefficient of determination (R^2) reached 0.94, implying that approximately 94% of the variability observed in experimental drug release profiles is explained by the predictive model. This result indicates a strong relationship between formulation variables and release behavior and demonstrates the suitability of machine learning techniques for pharmaceutical release prediction tasks.The strong predictive performance can be attributed to the integration of multiple formulation-related variables, including particle size, polymer concentration, drug loading, encapsulation efficiency, and environmental conditions. These variables collectively capture important factors governing drug diffusion and release kinetics within nanocarrier systems.

B. Comparative Analysis

To further evaluate the effectiveness of the proposed framework, its performance was compared with several commonly used regression models, including Linear Regression, Support Vector Regression (SVR), Decision Tree Regression, and Extreme Gradient Boosting (XGBoost). All models were trained and evaluated using identical datasets and experimental configurations. The comparative results are illustrated in Fig. 2**.**

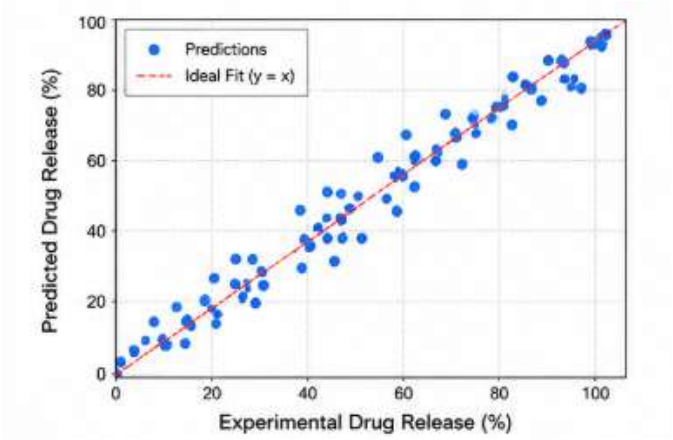

Fig 2. Comparison of Drug Release Prediction Performance Across Regression Models

The comparative analysis indicates that the proposed Random Forest-based framework achieved the highest predictive performance among all evaluated models. Linear Regression produced an R^2 value of 0.79, indicating limited capability in modeling nonlinear relationships between formulation variables and release behavior. Support Vector Regression improved performance and achieved an R^2 value of 0.85, while Decision Tree Regression achieved 0.88.XGBoost demonstrated stronger predictive capability with an R^2 value of 0.91. However, the proposed framework achieved the highest performance with an R^2 value of 0.94. The superior performance can be attributed to the ensemble learning strategy of Random Forest, which effectively captures complex interactions among pharmaceutical formulation variables while reducing sensitivity to individual data variations. The results indicate that nonlinear machine learning models are better suited for drug release prediction than conventional linear approaches. Nanocarrier drug release is influenced by multiple interacting physicochemical factors, and ensemble learning techniques are capable of modeling these relationships more effectively.

C. Drug Release Profile Analysis

In addition to evaluating numerical performance metrics, it is important to assess how closely the predicted release profiles match experimentally observed release behavior. Figure 3 presents a comparison between experimentally measured release percentages and the corresponding predictions generated by the proposed framework.

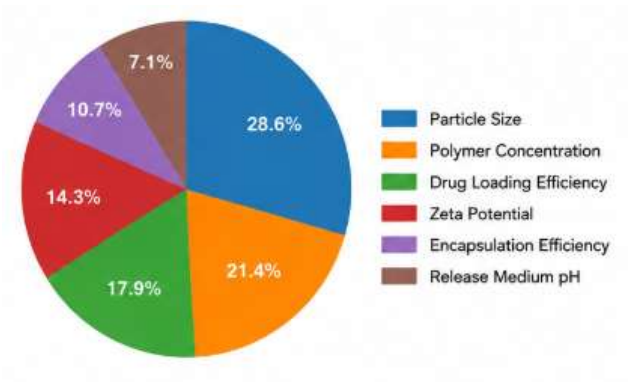

Fig 3. Experimental and Predicted Drug Release Profiles

The release curves shown in Fig. 3 indicate strong agreement between experimental observations and model predictions across the evaluated time intervals. Both profiles exhibit a gradual increase in cumulative drug release, followed by a stabilization phase at later time points. The predicted profile successfully captures the overall shape and trend of the experimental release curve. Minor deviations between observed and predicted values are visible at certain intermediate time intervals. These differences may arise from experimental variability, formulation-specific characteristics, or environmental factors not explicitly represented within the dataset. Nevertheless, the overall agreement between the two profiles confirms the ability of the model to reproduce release behavior with a high degree of accuracy. The close correspondence between experimental and predicted release profiles suggests that the framework may serve as a useful computational tool for preliminary formulation evaluation. By estimating release behavior before extensive laboratory experimentation, researchers may be able to reduce formulation development effort and prioritize promising candidates for experimental validation.

D. Explainability Analysis and Discussion

Although predictive performance is important, understanding the factors influencing release behavior is equally valuable in pharmaceutical formulation research. Therefore, SHAP-based explainability analysis was conducted to identify the formulation variables contributing most significantly to prediction outcomes. The analysis revealed that particle size was the most influential predictor of drug release behavior. Smaller particles generally provide larger surface-area-to-volume ratios, which can facilitate increased drug diffusion and faster release rates. Consequently, variations in particle size substantially affect release kinetics. Encapsulation efficiency emerged as another important factor. Formulations exhibiting higher drug entrapment levels often display different release characteristics compared with formulations containing lower encapsulation efficiencies. This finding is consistent with established pharmaceutical observations regarding drug retention and diffusion mechanisms.

Polymer concentration also demonstrated a strong influence on release predictions. Increased polymer content may alter matrix density and diffusion pathways, thereby affecting the rate at which the drug is released from the nanocarrier system. Drug loading and release medium pH were identified as additional influential variables contributing to release profile variability. The explainability analysis provides valuable insight into formulation-performance relationships. Unlike conventional regression models that primarily generate numerical predictions, the proposed framework also identifies the factors responsible for those predictions. Such information can assist formulation scientists in understanding how individual variables influence release behavior and support data-driven formulation optimization. Overall, the experimental results demonstrate that the proposed framework effectively combines predictive accuracy and interpretability. The integration of machine learning and explainability analysis

provides a practical approach for modeling nanocarrier drug release behavior and supporting intelligent drug delivery system development.

V. CONCLUSION AND FUTURE WORK

This paper presented a machine learning-based framework for predicting nanocarrier drug release profiles using formulation characteristics and physicochemical properties. The proposed framework integrates data preprocessing, feature engineering, predictive modeling, and explainability analysis to estimate cumulative drug release behavior in nanocarrier-based drug delivery systems. By utilizing formulation variables such as particle size, zeta potential, polymer concentration, drug loading, encapsulation efficiency, release medium conditions, and release time intervals, the framework provides a comprehensive representation of factors influencing drug release kinetics. A Random Forest regression model was employed to predict cumulative drug release percentages from experimental formulation data. The experimental results demonstrated strong predictive performance, as indicated by low prediction errors and a high coefficient of determination. The framework effectively captured nonlinear relationships between formulation parameters and release outcomes, enabling accurate estimation of release profiles across different nanocarrier formulations. An important contribution of this study is the incorporation of SHAP-based explainability analysis. The explainability module identified the formulation variables that contributed most significantly to prediction outcomes. The analysis revealed that particle size, encapsulation efficiency, polymer concentration, drug loading, and release medium pH are among the most influential factors affecting drug release behavior. These findings are consistent with established pharmaceutical principles and provide interpretable insights that may assist formulation scientists in understanding release mechanisms. The results suggest that machine learning techniques can serve as useful tools for supporting formulation development and release profile analysis in nanocarrier drug delivery systems. Future work will focus on evaluating deep learning-based regression models, incorporating larger pharmaceutical datasets, and investigating multi-drug nanocarrier formulations. Additional research may explore real-time formulation optimization, integration with digital pharmaceutical development platforms, and the inclusion of advanced physicochemical descriptors to further improve prediction accuracy and interpretability.

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