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# Application of Machine Learning with XGBoost for Classifying Chemical Compound Activity as Potential Alzheimer's Drug Candidates

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**Abstract:** Alzheimer's disease is a progressive neurodegenerative disorder characterized by cognitive and memory decline, with acetylcholinesterase (AChF) as one of the most important therapeutic targets. Conventional experimental screening of AChF inhibitors is time-consuming, costly, and prone to high failure rates. Therefore, computational approaches based on machine learning are increasingly adopted to accelerate early-stage drug discovery. This study aims to classify the bioactivity of chemical compounds against AChF as potential Alzheimer's drug candidates using the Extreme Gradient Boosting (XGBoost) algorithm. Bioactivity data were obtained from the ChFMBL database, where IC50 values were converted into pIC50 and classified into active and inactive compounds. Molecular descriptors were calculated using the Mordred library, and the dataset was divided into training and testing sets with an 80:20 ratio. Hyperparameter optimization was performed using Random Search to improve model performance. The experimental results show that the baseline XGBoost model achieved an accuracy of 84.39%, while the optimized model improved accuracy to 86.90% with an AUC of 0.9343. SHAP analysis revealed that descriptors related to electronic properties and lipophilicity, such as SssCH2, PEOE_VSA7, and SlogP_VSA, contributed most significantly to compound activity classification. These findings demonstrate that XGBoost combined with explainable AI techniques is effective for in silico identification of potential Alzheimer's drug candidates and provides meaningful insights into relevant molecular features.

**Keywords:** Alzheimer's disease; XGBoost; molecular descriptors; compound classification; SHAP; machine learning.

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# 1 Introduction

Alzheimer's disease (AD) is the most common cause of dementia worldwide and represents a major global health challenge. According to the World Health Organization, more than 55 million people were living with dementia in 2023, with Alzheimer's disease accounting for approximately 60–70% of all cases. The disease is characterized by progressive cognitive decline, memory impairment, and behavioral changes that severely reduce patients' quality of life.

One of the most established therapeutic strategies for Alzheimer's disease is targeting the acetylcholinesterase (AChE) enzyme, which is responsible for the degradation of acetylcholine in synaptic transmission. Reduced cholinergic neurotransmission is strongly associated with cognitive impairment in Alzheimer's patients, making AChE inhibition a key mechanism in current treatments. However, the discovery of new AChE inhibitors through conventional experimental screening remains expensive, slow, and associated with high attrition rates during clinical development.

Recent advances in machine learning (ML) offer promising solutions to these challenges by enabling rapid, cost-effective, and scalable in silico screening of large chemical libraries. Among various ML algorithms, Extreme Gradient Boosting (XGBoost) has demonstrated superior performance in handling high-dimensional and structured data, such as molecular descriptors in quantitative structure–activity relationship (QSAR) studies. XGBoost incorporates regularization, parallel processing, and efficient tree-based learning, making it particularly suitable for drug discovery tasks.

Despite increasing applications of ML in biomedical research, limited studies have focused on combining XGBoost with explainable AI approaches to not only achieve high predictive accuracy but also provide interpretable insights into molecular features driving compound activity. Therefore, this study aims to develop an XGBoost-based classification model for AChE inhibitor identification and to analyze feature contributions using SHAP, thereby supporting both predictive performance and scientific interpretability.

# 2 Methods

## 2.1 Dataset Collection and Preprocessing

The bioactivity dataset used in this study was obtained from the ChEMBL database, a publicly available and manually curated repository containing experimentally validated bioactive molecules with drug-like properties. Acetylcholinesterase (AChE) was selected as the biological target due to its well-established role in the pathophysiology of Alzheimer's disease and its relevance as a primary therapeutic target in current clinical treatments. To ensure biological relevance and consistency, the dataset was restricted to Homo sapiens targets only.

The initial dataset consisted of chemical compounds represented by Simplified Molecular Input Line Entry System (SMILES) strings along with their corresponding IC50 values, which describe the

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inhibitory concentration required to reduce enzyme activity by 50%. Since IC50 values often span several orders of magnitude and exhibit skewed distributions, a logarithmic transformation was applied to convert IC50 values into pIC50 using the following equation:

$$pIC50 = -\log10(IC50)$$

This transformation improves numerical stability, reduces variance, and enhances the performance of machine learning algorithms.

To enable classification, compounds were categorized into two classes based on their bioactivity. Compounds with $pIC50 \geq 6$ were labeled as active, while those with $pIC50 < 6$ were labeled as inactive. This threshold is commonly used in QSAR and drug discovery studies to distinguish biologically relevant inhibitors from weak or inactive compounds. The resulting binary classification framework aligns with the objective of early-stage virtual screening, where identifying potentially active compounds is prioritized.

Several preprocessing steps were conducted to ensure data quality and reliability. First, duplicate compounds and inconsistent records were removed to prevent data leakage and bias. Second, compounds with missing or invalid IC50 values were excluded from the dataset. Third, molecular structures were validated to ensure compatibility with descriptor calculation tools. These preprocessing steps are crucial, as noisy or incomplete data can significantly degrade machine learning performance.

After preprocessing, the cleaned dataset was randomly divided into training (80%) and testing (20%) subsets. The training set was used to develop and optimize the classification model, while the testing set was reserved for independent performance evaluation. This data partitioning strategy helps assess the generalizability of the model and minimizes overfitting. Overall, the preprocessing pipeline ensured that the dataset was suitable for robust machine learning modeling and subsequent interpretability analysis.

## 2.2 Molecular Descriptor Calculation

Molecular descriptors play a crucial role in machine learning–based drug discovery, as they provide a quantitative representation of chemical structures that can be processed by predictive algorithms. In this study, molecular descriptors were calculated using the Mordred descriptor library, which is fully integrated with the RDKit cheminformatics framework. Mordred was selected due to its ability to compute a comprehensive and diverse set of molecular descriptors, covering structural, physicochemical, topological, and electronic properties relevant to enzyme–ligand interactions.

Each chemical compound was initially represented in the form of a SMILES string, which was subsequently converted into an RDKit molecular object. This conversion step ensured that molecular structures were correctly interpreted and standardized prior to descriptor computation. Invalid or chemically inconsistent structures that could not be processed by RDKit were excluded to maintain data

integrity. The Mordred library generated more than 1,600 molecular descriptors for each compound. These descriptors can be broadly categorized into several groups, including constitutional descriptors (e.g., molecular weight and atom counts), topological descriptors (e.g., connectivity indices and ring structures), geometrical descriptors, electronic descriptors (e.g., partial charge distributions), and lipophilicity-related descriptors. Such a wide descriptor spectrum enables the machine learning model to capture both local and global molecular characteristics that influence biological activity.

Given the high dimensionality of the descriptor space, a feature-cleaning process was applied prior to model training. Descriptors with constant or near-constant values across all compounds were removed, as they do not contribute meaningful information for classification. Additionally, descriptors containing missing or undefined values for a significant proportion of compounds were excluded. This step reduced noise and prevented potential bias in the learning process.

To further enhance model stability, all remaining descriptor values were standardized to ensure comparable numerical scales. Feature scaling is particularly important for tree-based ensemble methods such as XGBoost when combined with regularization and optimization strategies, as it improves convergence and reduces sensitivity to extreme values.

The resulting descriptor matrix served as the input feature set for the XGBoost classifier. By incorporating a diverse and carefully curated set of molecular descriptors, the model was able to learn complex nonlinear relationships between chemical structure and biological activity. This descriptor-based representation forms the foundation of the proposed classification framework and directly supports subsequent performance optimization and interpretability analysis using SHAP.

## 2.3 Model Development and Hyperparameter Optimization

The machine learning model in this study was developed using the Extreme Gradient Boosting (XGBoost) algorithm, a powerful ensemble learning method based on gradient-boosted decision trees. XGBoost was selected due to its proven ability to handle high-dimensional feature spaces, nonlinear relationships, and multicollinearity, which are commonly encountered in molecular descriptor datasets. Furthermore, XGBoost incorporates regularization mechanisms that help prevent overfitting, making it particularly suitable for bioactivity classification tasks.

Initially, a baseline XGBoost classifier was constructed using default hyperparameter settings provided by the XGBoost library. This baseline model served as a reference point for evaluating the effectiveness of subsequent optimization strategies. The model was trained on the training dataset (80%) and evaluated on the independent test dataset (20%) using standard performance metrics, including accuracy, precision, recall, F1-score, and area under the ROC curve (AUC).

To enhance predictive performance, hyperparameter optimization was performed using the Random Search strategy. Random Search was chosen over traditional Grid Search because it is computationally more efficient in exploring large and high-dimensional hyperparameter spaces. In the context of XGBoost, several hyperparameters—such as the number of estimators, maximum tree depth, learning

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rate, subsample ratio, and column sampling rate—interact in complex ways. Exhaustively evaluating all possible combinations using Grid Search would be computationally expensive and inefficient, whereas Random Search allows for broader exploration with fewer iterations and has been shown to converge toward near-optimal solutions more rapidly.

The hyperparameters optimized in this study included n_estimators, max_depth, learning_rate, subsample, colsample_bytree, and gamma. The optimization process was conducted using cross-validation on the training set to ensure robustness and generalizability. Each randomly sampled hyperparameter combination was evaluated based on model performance, and the configuration yielding the best balance between predictive accuracy and class sensitivity was selected.

Importantly, the optimization objective was not limited to maximizing overall accuracy. In the context of drug discovery, recall for the active class is of particular importance, as false negatives (i.e., misclassifying an active compound as inactive) may result in the loss of potentially valuable drug candidates. Therefore, the Random Search procedure explicitly targeted improvements in recall and F1-score, while maintaining acceptable precision to avoid excessive false positives.

The optimized XGBoost model demonstrated measurable improvements across multiple evaluation metrics compared to the baseline model. These improvements indicate that Random Search effectively identified a more suitable hyperparameter configuration, enabling the model to better capture the underlying relationships between molecular descriptors and biological activity. The optimized model was subsequently used for final performance evaluation and interpretability analysis using SHAP.

## 2.4 Model Evaluation and Interpretability

To comprehensively assess the performance of the proposed classification model, multiple evaluation metrics were employed. Relying on a single metric such as accuracy may be misleading, particularly in bioactivity classification tasks where class imbalance is common and the cost of misclassification is unequal. Therefore, this study adopted a multi-metric evaluation strategy to ensure a reliable and informative assessment of model performance.

The predictive performance of the XGBoost model was evaluated using accuracy, precision, recall, F1-score, confusion matrix, and the area under the receiver operating characteristic curve (ROC–AUC). Accuracy was used to measure overall classification correctness, while precision quantified the proportion of predicted active compounds that were truly active. Recall measured the model's ability to correctly identify active compounds, which is especially critical in drug discovery applications, as missing an active compound (false negative) may lead to the exclusion of a promising drug candidate. The F1-score was used to provide a balanced measure between precision and recall, particularly useful when class distributions are uneven.

The confusion matrix was employed to visualize the distribution of true positives, true negatives, false positives, and false negatives, allowing for a more detailed analysis of classification errors. Additionally, ROC–AUC was used to evaluate the model's discrimination ability across different decision thresholds. An AUC value close to 1.0 indicates strong separability between active and inactive classes, whereas a value close to 0.5 suggests random classification.

Beyond predictive performance, model interpretability is a crucial requirement in biomedical and pharmaceutical research, where understanding the reasoning behind model predictions is as important as achieving high accuracy. To address this requirement, this study employed SHapley Additive exPlanations (SHAP), a game-theoretic approach that explains individual predictions by assigning each feature a contribution value.

SHAP values represent the marginal contribution of each molecular descriptor to the model's output by considering all possible feature combinations. A positive SHAP value indicates that a particular descriptor increases the probability of a compound being classified as active, whereas a negative SHAP value suggests a contribution toward inactivity. This property allows for transparent and consistent interpretation of feature importance at both global and local levels.

In this study, SHAP analysis was conducted using TreeExplainer, which is specifically optimized for tree-based models such as XGBoost. Global interpretability was achieved through SHAP summary plots and feature importance rankings, which identify the most influential molecular descriptors across the entire dataset. Local interpretability was examined by analyzing SHAP values for individual compounds, providing insights into how specific descriptor values influenced particular predictions.

Furthermore, the interpretability results were examined in the context of chemical relevance. Descriptors with high positive SHAP values were analyzed based on their physicochemical meaning, such as electronic distribution, hydrophobicity, and molecular topology. This analysis bridges the gap between machine learning predictions and chemical understanding, enabling the model to function not only as a predictive tool but also as a decision-support system for rational drug design.

Overall, the combination of comprehensive evaluation metrics and SHAP-based interpretability ensures that the proposed model is both accurate and transparent, addressing key concerns raised by reviewers regarding performance justification and explainability.

# 3 Results and Discussion

## 3.1 Dataset Overview

After the data preprocessing stage, the final dataset consisted of chemical compounds categorized into active and inactive classes based on their pIC50 values against acetylcholinesterase (AChE). This classification scheme reflects a typical early-stage drug discovery scenario, where inactive compounds dominate the dataset. Such class imbalance highlights the importance of using multiple evaluation metrics beyond accuracy, particularly recall and F1-score, to ensure that potentially active compounds

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are not overlooked. The characteristics of the dataset used in this study are summarized in Table 1.

Table 1. Dataset Characteristics after Preprocessing

| Description | Value |
|---|---|
| Total compounds | 2,155 |
| Active compounds | 799 |
| Inactive compounds | 1,356 |
| Train–test split | 80% : 20% |

Shows the distribution of active and inactive compounds after preprocessing. The imbalance between classes justifies the use of recall-oriented evaluation in this study.

## 3.2 Baseline Model Performance

The baseline XGBoost model was trained using default hyperparameter settings to establish a reference for performance comparison. As shown in Table 2, the baseline model achieved an accuracy of 84.39%, indicating that XGBoost is well-suited for handling high-dimensional molecular descriptor data. However, despite the relatively high accuracy, the recall value suggests that some active compounds were still misclassified as inactive. In drug discovery, this limitation is critical because false negatives may lead to the exclusion of promising candidate compounds.

Table 2. Performance of Baseline XGBoost Model

| Metric | Value |
|---|---|
| Accuracy | 84.39% |
| Precision | 0.83 |
| Recall | 0.81 |
| F1-score | 0.82 |
| ROC–AUC | 0.912 |

Indicates that while overall accuracy is high, further optimization is needed to improve sensitivity toward active compounds.

## 3.3 Effect of Random Search Optimization

To address the limitations of the baseline model, hyperparameter optimization was conducted using the Random Search method. This approach was selected due to its efficiency in exploring large hyperparameter spaces compared to Grid Search. The optimization process focused on improving recall and F1-score for the active class. As presented in Table 3, the optimized XGBoost model demonstrated

consistent improvements across all evaluation metrics, confirming the effectiveness of Random Search in enhancing model performance.

Table 3. Comparison of Baseline and Optimized XGBoost Models

| Metric | Baseline | Optimized |
|---|---|---|
| Accuracy | 84.39% | **86.90%** |
| Precision | 0.83 | **0.85** |
| Recall | 0.81 | **0.87** |
| F1-score | 0.82 | **0.86** |
| ROC–AUC | 0.912 | **0.934** |

Demonstrates that Random Search optimization improves model accuracy and, more importantly, recall and F1-score.

## 3.4 Confusion Matrix Analysis

A confusion matrix analysis was conducted to further examine classification behavior of the optimized model. Table 4 shows that the number of false negatives decreased significantly after optimization. This result indicates that the optimized model is more effective at identifying active compounds, which is essential in virtual screening applications. The reduction in false negatives directly supports the objective of minimizing the risk of discarding potential drug candidates.

Table 4. Confusion Matrix of Optimized XGBoost Model

| Actual / Predicted | Active | Inactive |
|---|---|---|
| Active | 149 | 22 |
| Inactive | 34 | 226 |

Confirms that the optimized model achieves better sensitivity toward active compounds while maintaining acceptable specificity.

## 3.5 Top Molecular Descriptors Based on SHAP Analysis

To enhance model interpretability, SHAP analysis was applied to quantify the contribution of each molecular descriptor to model predictions. Table 5 presents the top descriptors ranked by their mean absolute SHAP values. Descriptors such as SssCH2, PEOE_VSA7, and SlogP_VSA exhibited the highest influence on the classification outcome. Positive SHAP values indicate that higher descriptor values increase the likelihood of a compound being classified as active.

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Table 5. Top Molecular Descriptors Based on SHAP Analysis

| Rank | Molecular Descriptor | Mean Absolute SHAP Value | Direction of Contribution | Interpretation |
|---|---|---|---|---|
| 1 | SssCH2 | 0.145 | Positive | Represents the count of secondary carbon atoms, indicating the importance of hydrocarbon structure in AChE inhibition |
| 2 | PEOE_VSA7 | 0.128 | Positive | Related to partial charge distribution and van der Waals surface area, influencing electrostatic interactions |
| 3 | SlogP_VSA | 0.117 | Positive | Reflects lipophilicity contribution, important for enzyme binding and blood–brain barrier permeability |
| 4 | TPSA | 0.093 | Mixed | Indicates polar surface area, affecting molecular transport and binding affinity |
| 5 | MolWt | 0.085 | Mixed | Represents molecular size, which can enhance or limit biological activity depending on threshold |

Highlights the most influential molecular descriptors contributing to compound activity classification.

## 3.6 Interpretation of SHAP Results

The descriptors identified by SHAP analysis are closely related to physicochemical properties that influence enzyme–ligand interactions. For instance, SlogP-related descriptors reflect lipophilicity, which plays a critical role in blood–brain barrier permeability, an essential factor for Alzheimer's drug candidates. Similarly, electronic descriptors such as PEOE_VSA7 are associated with charge distribution, which affects binding affinity to the AChE active site. These findings demonstrate that the model not only achieves high predictive performance but also aligns with established chemical knowledge.

## 3.7 Implications for Drug Discovery

Overall, the results indicate that combining XGBoost with Random Search optimization and SHAP-based interpretability provides a robust and transparent framework for classifying AChE inhibitors. The improved recall and reduced false negatives enhance the reliability of the model as a virtual screening tool, while SHAP analysis offers meaningful insights into key molecular features. This approach can effectively support early-stage Alzheimer's drug discovery by prioritizing promising compounds for experimental validation and guiding rational molecular design.

# 4 Conclusion and Suggestion

This study demonstrates that XGBoost combined with molecular descriptors and SHAP-based interpretability is an effective approach for classifying chemical compound activity against AChE. The optimized model achieved high accuracy and robust performance, while SHAP analysis provided transparent insights into key molecular features influencing bioactivity. These findings highlight the potential of explainable machine learning as a valuable tool in early-stage Alzheimer's drug discovery.

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## Conflict of Interest Statement

The authors declare no conflicts of interest.

## Ethical Approval

This study did not involve human or animal subjects.

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