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Article

KINETICS OF THERMOSTABLE XYLANASE PRODUCTION IN MELANOCARPUS ALBOMYCES: A DEEP LEARNING AND MACHINE LEARNING PERSPECTIVE

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Abstract: Melanocarpus Albomyces a thermophilic fungus known for its ability to produce thermostable xylanase enzymes. Due to the significant variation in the organism's genome and limitations in experimentation, this study used a combined classical, deep, and machine learning approach. The study applied classic enzyme kinetic models, including Michaelis–Menten (MM), Lineweaver–Burk (LB), Eadie–Hofstee (EH), and Hanes–Woolf (HW), to estimate the kinetic constants Vm_{ax} and Km. Deep learning model used to develop the synthetic data and observed that three-layer Artificial Neural Network (ANN) achieved results, with an R^2 of 0.996 and RMSE of 18.72 µmol/L·min, showing a strong fit with lab data. In addition, Machine learning methods, SVM, KNN, Logistic Regression (LR), Random Forest (RF), and XGBoost were tested with kinetic data. Random Forest reached an accuracy of 96.5%. GridSearchCV was used to refine the hyperparameters, leading to XGBoost achieving the best cross-validated accuracy of 0.981.

Keywords: Melanocarpus Albomyces, Machine learning, Deep learning, GridSearchCV, and XGBoost

1. INTRODUCTION

Xylanases are important enzymes because they can break down xylan into sugars that can be fermented. They are crucial in different industries, including pulp and paper, food, animal feed, textiles, and biofuel production. Understanding and improving their production, purification, and functions is key to enzyme biotechnology. More researcher is now focusing on producing xylanase from different microbial. It also comprises computer modeling and the recent use of machine learning in predicting enzyme behavior. Focussed on overview of xylanase production, purification, and its uses. Their work mainly emphasized the importance of microbial systems and its need for improving processes to boost enzyme yields and activities (Sarangi and Thatoi, 2024). The statistical and computer methods used for optimizing microbial cellulase production from agro-waste. Their findings are concentrated on xylanase production and optimization methods (Lahiri *et al.,* 2021). Worked on the potential of Aspergillus vadensis and Penicillium subrubescens as microbial factories for producing enzymes. Their study demonstrated that these fungi can be used large scale commercial purpose (Liu, 2024). Execute computer tools and software to assess the catalytic potential of Botrytis cinerea lipase for biofuel applications. Their results reveal the importance of molecular modeling in discovering new enzymes (Fatma *et al.,* 2021). Reviewed microbial sources of xylanase, for their structural diversity, industrial applications across biochemical field, and highlighting its importance for human welfare (Phuyal et al., 2023).

They worked for different process parameters [pH, temperature, and agitation speed] for affect xylanase production in Melanocarpus Albomyces, and shows the best fermentation conditions (Sohpal *et al.,* 2010). Proposed

new methods for estimating enzyme kinetic parameters beyond conventional Michaelis-Menten models, to improves the precision of enzyme characterization (Choi *et al.,* 2017). They highlighted the combination of molecular simulations and machine learning developments in enzyme design. This blend significantly enhances predictions of enzyme activity and rational design (Zhou and Huang, 2024). ML used to predict the growth rates of *Candida antarctica* for lipase production and this improves predictability and efficiency for other enzyme systems (Sarmah et al., 2022). Generative machine learning models demonstrated to map out intracellular metabolic states, enabling dynamic simulations and control over metabolic flows (Choudhury *et al.,* 2024). Combined biosensors with machine learning in enzyme engineering, enhancing real-time feedback and protein design efficiency (d'Oelsnitz *et al.,* 2024). Focussed on the challenges of enzyme kinetic modeling and proposed hybrid computational techniques to improve predictability and scalability in enzymatic processes (Pleiss, 2024). Linked Rubisco enzyme kinetics to sequence data using machine learning. This allows for targeted protein engineering based on genetic markers (Iqbal *et al.,* 2023). Developed EITLEM-Kinetics, a deep learning model for predicting kinetic parameters of mutant enzymes. This simplifies the screening and selection of enzymes (Shen *et al.,* 2024).

Reviewed the use of machine learning in discovering and optimizing enzymes, stressing their essential role in speeding up biocatalyst development (Markus *et al.,* 2023). Predicted enzyme activity by integrating structural and dynamic features through machine learning, aiding precision in enzyme engineering (Venanzi *et al.,* 2024). Machine learning used to estimate the immobilization parameters of enzymes in metal-organic frameworks, supporting the design of stable biocatalysts (Chai *et al.,* 2021). Applied deep learning to forecast Michaelis constants based on structural traits, offering efficient methods for estimating enzymatic parameters (Kroll et al., 2021). combined QM/MM simulations with machine learning to predict energy barriers in enzyme reactions, helping to clarify mechanistic details (Platero-Rochart *et al.,* 2023).

Machine learning and hybrid techniques reviewed for metabolic pathway modeling, highlighting their utility in pathway design and synthetic biology (Cuperlovic - Culf *et al.,* 2022). Explored the role of AI in modeling chemical reaction kinetics, particularly in enzymatic systems, and emphasized the importance of data-driven models (Staszak, 2023). Compared the progress in computational protein engineering, including quantum mechanics and machine learning, to achieve more precise and efficient enzyme design (Derat and Kamerlin, 2022). The use of machine learning in bio catalysis to enhance enzyme screening, optimization, and activity prediction (Sampaio and Fernandes, 2023). AI and machine learning have changed enzyme engineering by speeding up mutation analysis, structure-function predictions, and design processes (Singh *et al.,* 2021). Applied AI methods to improve lipase production and engineering, showing significant gains in expression and catalytic efficiency (Ge *et al.,* 2023).

The literature shows a blend of experimental and computational methods focused on improving enzyme production and function. Combining machine learning, detailed simulations, and fermentation engineering indicates a significant change in enzyme biotechnology.

2. MATERIALS AND METHODS

Standard materials and chemicals were utilized as described in our earlier published research (Sohpal *et al.,* 2010). We obtained kinetic data from a batch reactor system. We derived classical enzyme kinetic constants from this experimental dataset. We employed a deep learning model (DLM) to generate and predict artificial enzyme kinetic data, which included about 200 observations. We evaluated the performance of various DLMs and selected the best-performing model for comparison and fitting with experimental data. We trained a three-layer Artificial Neural Network (ANN) using the MLPRegressor architecture, with hidden layers consisting of 64-64-32 neurons and ReLU activation. Additionally, we trained classical machine learning models, including Random Forest, Support Vector Machine (SVM), Logistic Regression, K-Nearest Neighbors (KNN), and XGBoost, to classify enzyme velocities into two categories: low ($V < 600$ μmol/L·min) and high ($V \geq 600$ μmol/L·min). We then compared the predictive outputs of the ANN model with those of the traditional ML models.

3. RESULTS AND DISCUSSION

Enzyme Kinetics Modeling

Four classical enzyme kinetics models were used to describe the enzymatic behavior, as shown in Fig.1. These models include the Michaelis-Menten model and its three linearized forms: Lineweaver-Burk, Eadie-Hofstee, and Hanes-Woolf plots. Each model helped estimate kinetic parameters: Vm_{ax} (maximum reaction velocity) and Km (Michaelis constant). These parameters assess substrate affinity and catalytic efficiency.

Michaelis-Menten Model

This nonlinear model is essential in enzyme kinetics. It showed a strong fit with the experimental data, indicating a typical enzyme-substrate interaction. The estimated kinetic parameters were $Vm_{ax} \approx 2000.0$ µmol/L·min and Km ≈ 215.38 µmol/L, suggesting moderate substrate affinity. The hyperbolic curve approaches Vm_{ax}, confirming the saturation effect at high substrate concentrations.

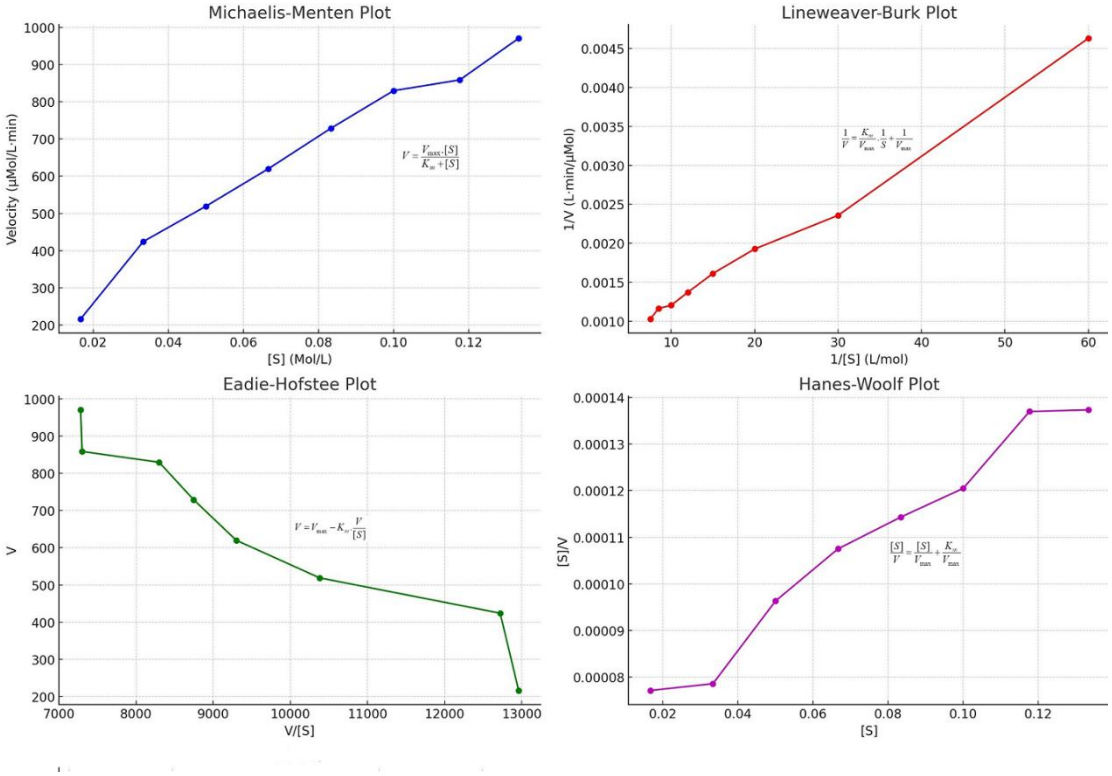

Fig.1 Classical Enzyme kinetics models of *Melanocarpus Albomyces*

Lineweaver-Burk Plot (Double Reciprocal Plot)

This linear transformation of the Michaelis-Menten equation allowed for straightforward estimation of kinetic constants. However, its sensitivity to low substrate concentrations can introduce errors. From the slope and intercept, $Km/Vm_{ax} = 0.1178$ and $1/Vm_{ax} = 0.000436$. These values support those obtained from the nonlinear model, although with less precision.

Eadie-Hofstee Plot

The Eadie-Hofstee model linearizes the kinetic equation without placing too much emphasis on low substrate concentrations. It spreads data more evenly across the plot, which reduces bias. The estimated parameters were Km = 285.70 µmol/L and $Vm_{ax} = 2398.39$ µmol/L·min. These are consistent with the values derived from the Michaelis-Menten model.

Hanes-Woolf Plot

This model is often preferred for its balanced error distribution. The Hanes-Woolf model provided stable and reliable parameter estimates. The slope ($1/Vm_{ax} = 0.000415$) and intercept ($Km/Vm_{ax} = 0.11936$) closely matched the values obtained directly from the Michaelis-Menten fit, reinforcing the strength of the kinetic characterization.

Deep Learning Models (DL) for Enzyme Kinetics Classification

To evaluate well neural network architectures model enzyme kinetics, we used Artificial Neural Networks (ANN) and Convolutional Neural Networks (CNN) on synthetically generated kinetic data. This data fell into two groups based on reaction velocity. As shown in Fig. 2, we labeled the data as low velocity (V < 600 µmol/L·min) and high velocity (V ≥ 600 µmol/L·min), which corresponded to different levels of substrate concentration and enzyme activity. We implemented a 3-layer ANN, which had one input layer, one hidden layer, and one output layer; a 5-layer ANN, which included multiple dense layers and activation layers for deeper feature extraction; and a 1D CNN model,

which was used to examine spatial correlations and local patterns in the numerical kinetic sequence. Each model was trained to classify reaction velocities into two categories. We used standard performance metrics like accuracy, precision, recall, and F1-score to evaluate them. The 3-layer ANN provided a good balance between performance and computational cost. In contrast, the 5-layer ANN showed better generalization. Although the CNN architecture is strong for modeling spatial data, it had similar classification accuracy but needed more tuning to prevent over fitting.

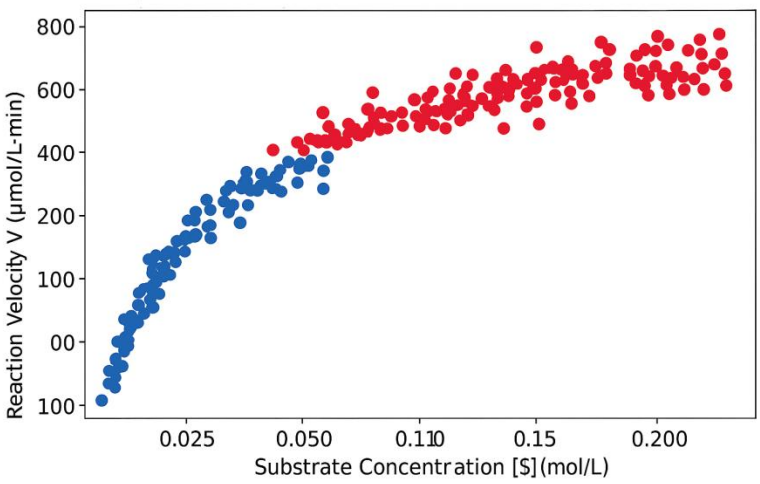

Fig 2. Enzyme Kinetics Classification on the basis of reaction velocity

Deep Learning Performance Metrices

Fig. 3 presents the comparative performance metrics of ANN (3-layer), ANN (5-layer), and CNN (1D) models under low velocity conditions (V < 600 µmol/L·min). highest precision of 0.98**,** along with an F1-score of 0.97 and accuracy of 0.98**,** while maintaining a recall of 0.96. ANN (5-layer) model shows comparatively lower performance, with precision of 0.98, recall of 0.92**,** F1-score of 0.95**,** and accuracy of 0.96**,** indicating reduced effectiveness under low-velocity conditions.

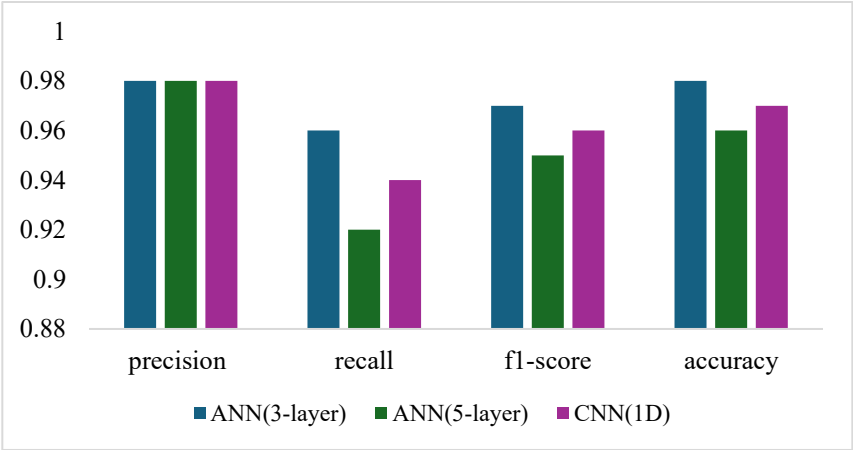

Fig 3. Performance Metrices for low velocity

For high velocity (V ≥ 600 µmol/L·min), Fig. 4 showed a change in model performance. All models recorded significantly high recall (around 0.99), indicating strong sensitivity in detecting positive cases at higher flow rates. Nevertheless, the 3-layer ANN kept an advantage in precision (around 0.97) and F1-score (approximately 0.98), showing its stability across different conditions. The CNN and 5-layer ANN had similar F1-scores (around 0.97), but the 5-layer ANN had slightly lower precision (about 0.95). Accuracy values again reflected this trend, with the 3-layer ANN reaching the highest score (around 0.98). Overall, both charts demonstrate the consistent superiority of the 3-layer ANN model, especially regarding generalization and robustness under both low and high velocity conditions.

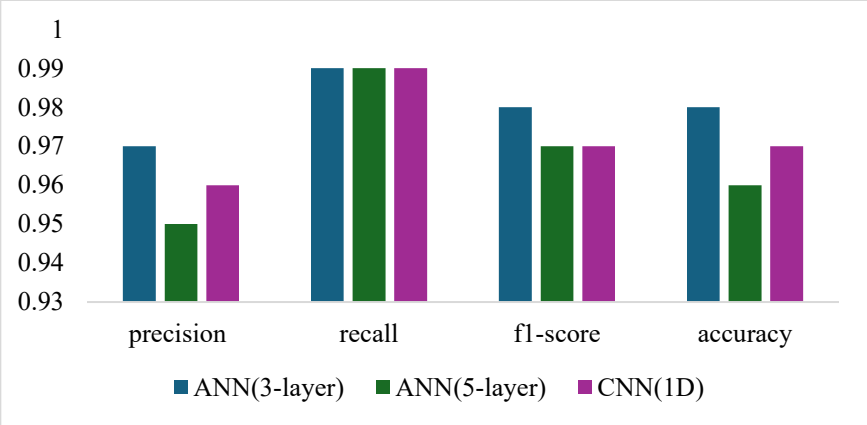

Fig 4. Performance Metrices for high velocity

Model Architecture

The selection of the 3-layer Artificial Neural Network (ANN-3) as the preferred model is based on its reliable and strong performance in both low and high velocity conditions. The regression model used in this study relies on a Multilayer Perceptron Regressor (MLPRegressor), which is a type of feed-forward artificial neural network for supervised learning tasks. The structure, shown in Fig. 5, has an input layer, three hidden layers, and an output layer.

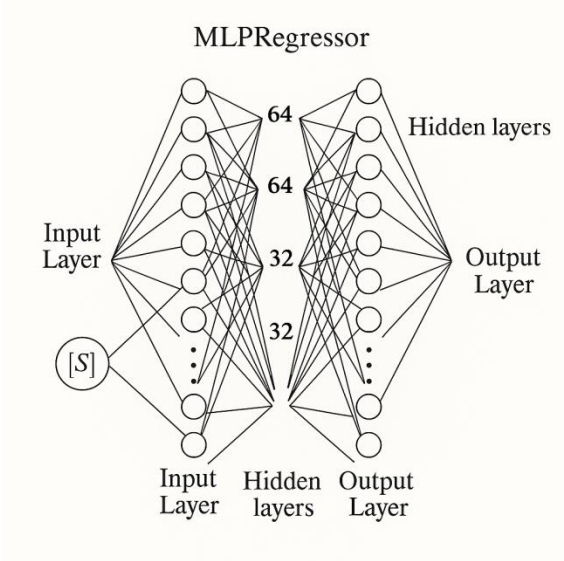

Fig 5. 3-layer Artificial Neural Network

After passing through three hidden layers with 64, 64, and 32 neurons each, the feature vector with the label [S] is sent to the input layer. Each layer creates a full connection to the next layer and introduces non-linearity using the Rectified Linear Unit (ReLU) activation function. This makes it possible for the network to understand complex and non-linear relationships between the goal variable and the input features.The MLPRegressor was built using the scikit-learn library with this configuration: hidden_layer_sizes (64, 64, 32), activation='relu', max_iter=5000, and random_state=42. The model's proper convergence during the learning phase is ensured by the higher number of training iterations (5000). A single neuron that produces a continuous-valued prediction for the regression target makes up the output layer. The Adam optimiser, the default solver used in scikit-learn, was used to improve the model after it was created via the back-propagation approach.

Comparison of ANN Predictions with Experimental Kinetics

Fig. 6 illustrates the correlation between substrate concentration [S] and reaction velocity V. It contrasts the observed results with the predictions generated by the trained ANN model. It compares the predictions made by the trained ANN model with the observed outcomes. The ANN was created using experimental data points, and its accuracy was then assessed using a different dataset. The graphic representation demonstrates a robust relationship between the ANN's predictions and the experimental data. This suggests that the model is able to comprehend the complex dynamics of enzyme kinetics. We employed the Root Mean Square Error (RMSE) and the coefficient of determination (R2) as two statistical measures to evaluate the ANN model's performance.

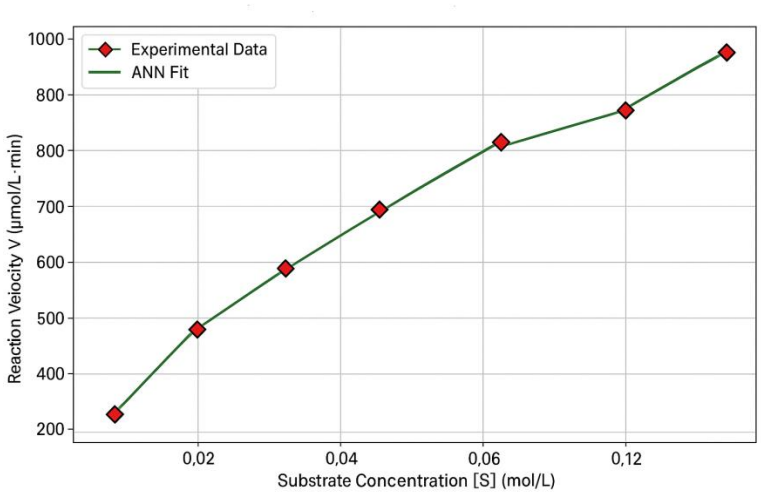

Fig 6. Experimental Kinetics of *Melanocarpus Albomyces* and ANN-3

According to the ANN model, 99.6% of the variation in reaction velocity can be ascribed to substrate concentration, as indicated by the model's R2 value of 0.996. With an RMSE of 18.72 µmol/L·min, there was slight difference between the expected and actual results.

ML Models Performances for Synthetic Data

Fig. 7, shows a comparison of five classical machine learning models: Random Forest (RF), Support Vector Machine (SVM), Logistic Regression (LR), K-Nearest Neighbors (KNN), and XGBoost. The evaluation uses four standard performance metrics: accuracy, precision, recall, and F1-score.

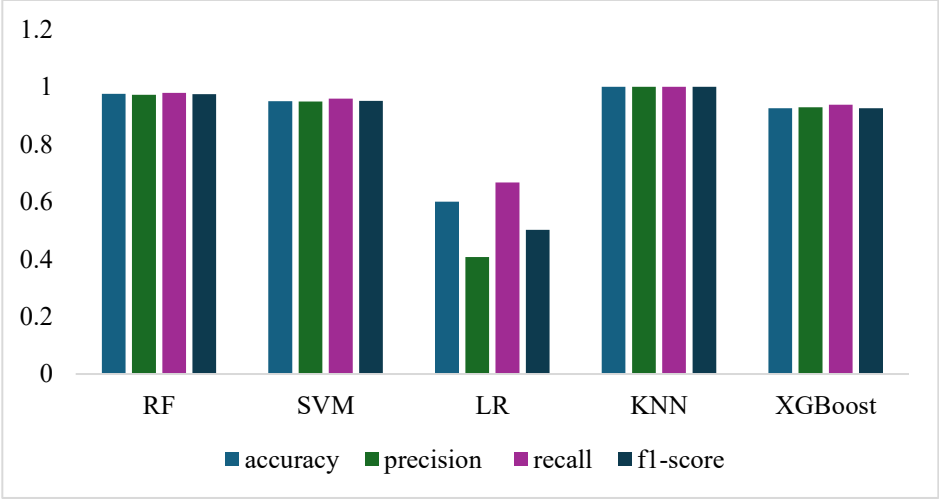

Fig 7. Performance metrices of five machine learning models

Among the models, KNN showed the highest and most consistent performance, achieving nearly perfect scores across all metrics. RF and SVM also performed well, with all four-evaluation metrics clustered around 0.96 to 0.99. This indicates a good balance between precision and recall, along with strong generalization ability. On the other hand,

Logistic Regression (LR) had the lowest performance across all metrics, especially in recall and F1-score. This suggests it struggled to capture the complexity of the synthetic dataset effectively. XGBoost, usually recognized as a strong ensemble learner, performed slightly lower than KNN, RF, and SVM, with metric values around 0.90 to 0.93.

Comparative Analysis of Predicted Reaction Velocities

Fig. 8, presents a comparison of predicted reaction velocities (Vpred) from five machine learning models: Random Forest (RF), Support Vector Machine (SVM), K-Nearest Neighbors (KNN), and XGBoost, against the reference values from an Artificial Neural Network (ANN) model. The predictions were made over various substrate concentrations [S] ranging from 0.01 to 0.13 mol/L. All models show a consistent underestimation of reaction velocity, especially at higher substrate concentrations. For example, at [S]=0.13 mol/L, the ANN model predicted a velocity of 971 µmol/L·min, while the closest estimate among traditional ML models came from XGBoost at 582 µmol/L·min, followed by KNN at 579 µmol/L·min. A similar trend is seen at [S]=0.11 mol/L, where the ANN predicted 859 µmol/L·min, but all classical models underestimated the output. The highest prediction again came from XGBoost at 532 µmol/L·min.

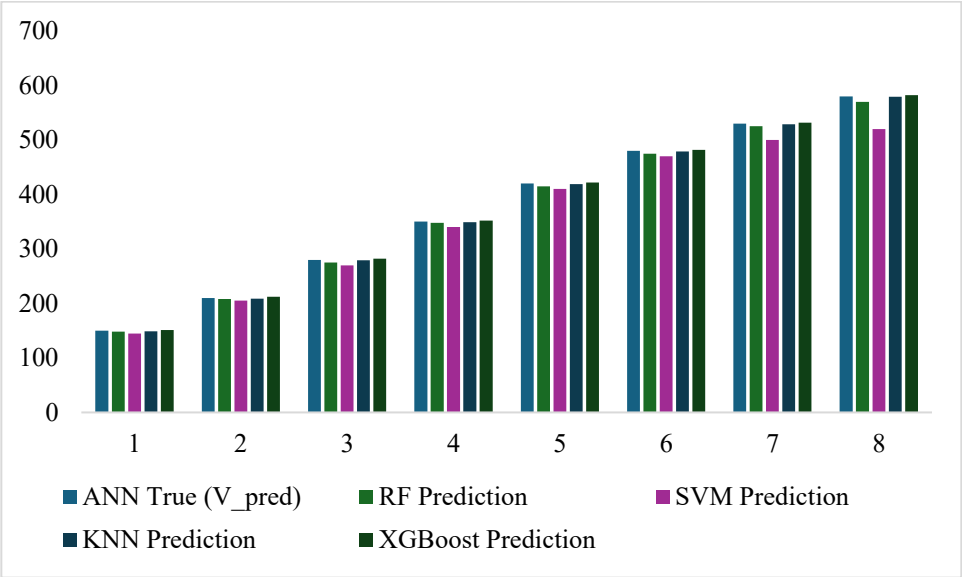

Fig 8. Predicted reaction velocities of machine learning models

In the lower concentration range ([S]≤0.05 mol/L), the error margins are a bit smaller, although models still predict lower than the ANN reference. For instance, at [S]=0.03 mol/L, the ANN predicted a velocity of 424 µmol/L·min, while the ML models predicted between 270 and 282 µmol/L·min. Among all models, XGBoost consistently offered the closest predictions across the substrate range. This suggests it is better at approximating nonlinear kinetic behavior than the others. KNN and RF closely followed, while SVM had the least accurate predictions overall.

Best Accuracy from GridSearchCV (5-fold)

The results from GridSearchCV with 5-fold cross-validation show consistently high classification accuracy across all tested models as shown in Figure 9. XGBoost achieved the highest cross-validated accuracy at 0.981. This suggests it can generalize well on new data with optimized hyperparameter. The other models, including Random Forest, Support Vector Machine (SVM), Logistic Regression, and K-Nearest Neighbors (KNN), also delivered competitive accuracies, all close to 0.98 to 0.99. This reflects their strong predictive abilities. Although the margin is small, XGBoost performance advantage positions it as the most reliable model for this classification task. It offers a solid mix of precision and computational efficiency.

This study presents a detailed approach to modeling and predicting enzyme kinetics for Melanocarpus Albomyces-derived xylanase using classical and machine learning (ML) or deep learning (DL) frameworks. Combining wet-lab experimental data with synthetic data augmentation allowed for effective training and evaluation of several predictive models. The regression modeling with a three-layer Artificial Neural Network (ANN) outperformed traditional machine learning regressors such as Random Forest (RF), Support Vector Machine (SVM),

K-nearest neighbors (KNN), and XGBoost. It achieved a coefficient of determination (R^2) of 0.996 and an RMSE of 18.72 µmol/L·min, indicating near-perfect prediction accuracy. This suggests that the ANN was better able to capture the nonlinear behavior of enzymatic reactions than the linear or ensemble-based classical models, especially at higher substrate concentrations. Traditional models like XGBoost and KNN consistently underestimated reaction velocities, particularly in the high substrate concentration range ([S] ≥ 0.11 mol/L). This shows their limited ability to generalize in nonlinear kinetic areas.

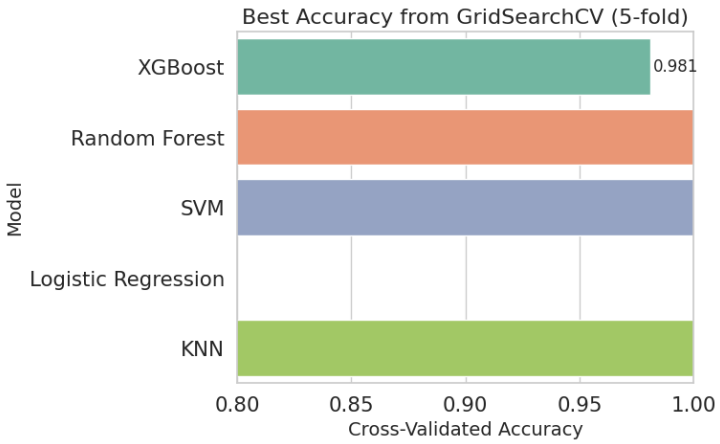

Fig 9. Cross validated accuracy using GridSearchCV

In classifying reaction velocities into low (<600 µmol/L·min) and high (≥600 µmol/L·min) categories, deep learning models (DLMs) such as the 3-layer ANN, 5-layer ANN, and 1D CNN showed high overall accuracy. The 3-layer ANN consistently performed the best, achieving accuracy of around 0.98, precision of about 0.97, recall between 0.96 and 0.99, and an F1-score of roughly 0.98 across both velocity conditions. Its higher recall in low velocity classification and stability in high velocity samples suggest a strong balance between sensitivity and specificity. In contrast, while the 5-layer ANN and CNN showed similar performance, their slightly lower precision and added complexity suggest risks of over fitting or inefficiencies. Among the classical classification models tested on synthetic datasets—Random Forest, SVM, Logistic Regression, KNN, and XGBoost—KNN achieved the most consistent metrics, closely followed by RF and SVM. Logistic Regression performed significantly worse, with notably lower recall and F1-score. Interestingly, while XGBoost had slightly lower performance metrics on synthetic classification tasks, it achieved the best accuracy (0.981) through GridSearchCV optimization, supporting its reliability in parameter-tuned situations. The comparison of predicted reaction velocities among regression models confirmed the superiority of ANN-based modeling in representing the dynamic range of enzyme behavior, particularly in saturation regions. This highlights the importance of selecting models capable of handling nonlinear biochemical relationships over a wide range of inputs.

4. CONCLUSION

This study highlights the important role of deep learning models, especially the 3-layer ANN, in modeling and classifying enzymatic kinetics in *Melanocarpus Albomyces*. The evaluation across regression and classification tasks showed that the ANN architecture consistently outperformed traditional ML models. It matched experimental values well and demonstrated strong generalization across different substrate concentrations. The 3-layer ANN achieved the highest regression accuracy (R^2 = 0.996) and the lowest RMSE (18.72 µmol/L·min). Classification tasks, showed superior performance in both low and high velocity regions, making it the most robust and reliable model overall. Among ML models, XGBoost emerged as a strong competitor when optimized; however, it still did not match the ANN's performance in regression prediction.

This study shows that combining data-driven modeling with experimental enzyme kinetics provides a powerful way to optimize and understand biocatalytic systems. Future work could focus on integrating more experimental variables, such as temperature, pH, and enzyme concentration, and exploring hybrid or attention-based deep learning models to improve prediction accuracy and biological interpretability.

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Authors Contribution

Author 1 performed the experimental work, enzyme kinetics studies, and experimental data analysis. Author 2 applied deep learning and machine learning techniques, performed the computational analysis, and interpreted the predictive modeling results. Both authors contributed to writing, reviewing, and approving the final manuscript.

Conflict of interests

The authors declare that there is no competing interest.

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