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Artículo Científico

Improving kinetic model fitting for total titratable acidity in bananas using genetic algorithms

Mejora del ajuste del modelo cinético de la acidez titulable total en bananos mediante algoritmos genéticos

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Abstract

This research aimed to automate the fitting of kinetic models using genetic algorithms (GAs) to optimize the estimation of kinetic parameters—the reaction rate constant (k) and the initial value of total titratable acidity (TTA, C_0)—and enhance predictive accuracy. Experimental data were collected from bananas (*Musa paradisiaca* L.) at ripening stage 2 on Von Loesecke scale, measuring TTA at specific intervals, and three kinetic models—zero-order, first-order, and second-order—were fitted. For optimization, Python-based GA was used to minimize the mean squared error (MSE) and evaluate performance based on R2, AIC, and BIC. Results indicated that while the zero-order model provided the best statistical fit (R2 = 0.918, lowest AIC and BIC), validation on unseen data favored the second-order model, which exhibited superior predictive accuracy (test R2 = 0.9349, lowest test MSE). The integration of GAs enhanced the robustness of kinetic fitting by effectively navigating parameter space and avoiding local minima, outperforming traditional optimization methods, demonstrating their ability to refine parameter estimation and improve model generalization. Future research should explore hybrid models that combine mechanistic kinetic equations with machine learning techniques (e.g., neural networks, or support vector regression), to better capture the biochemical processes underlying acidity changes in bananas.

Keywords: **ripening kinetics, genetic algorithms, parameter estimation, post-harvest modeling, TTA decreasing, food quality.**

Resumen

Esta investigación tuvo como objetivo automatizar el ajuste de modelos cinéticos mediante algoritmos genéticos (AG) para optimizar la estimación de los parámetros cinéticos — constante de velocidad de reacción (k) y valor inicial de la acidez total titulable (ATT, C_0)—, y mejorar la precisión predictiva. Se obtuvieron datos de ATT de plátanos (*Musa paradisiaca* L.) en etapa 2 de maduración, según la escala de Von Loesecke, y se ajustaron los modelos cinéticos de orden cero, de primer y segundo orden. Se implementó AG en Python para minimizar el error cuadrático medio (MSE) y evaluar el desempeño en función de R^2, AIC y BIC. Los resultados muestran mejor ajuste (R^2 = 0.918, menor AIC y BIC) en el modelo de orden cero, mientras que la validación con datos no vistos favoreció al de segundo orden (R^2 = 0.9349, menor MSE). La integración de AG mejoró la robustez del ajuste cinético, demostrando mejor estimación de parámetros y la generalización del modelo. Investigaciones futuras deberían explorar modelos que combinan ecuaciones cinéticas mecanicistas con técnicas de aprendizaje automático (por ejemplo, redes neuronales o regresión de vectores de soporte), para capturar mejor los procesos bioquímicos subyacentes a los cambios de acidez en plátanos.

Palabras clave: **cinética de maduración, algoritmos genéticos, estimación de parámetros, modelado poscosecha, disminución de TTA, calidad de los alimentos.**

1. Introduction

The kinetic analysis allows for monitoring and predicting food quality changes during storage, making it highly valuable in food research and industry. By using kinetic models to study parameters like total titratable acidity (TTA), scientists can quantify quality loss and establish shelf-life based on the degradation of food products (Contreras-López *et al*., 2022; Poonnakasem *et al.*, 2018; Olivera *et al.*, 2013). These models effectively describe changes in texture and color in various foods, providing insights into degradation rates and the effects of environmental factors (Yang and Xu, 2021; Jaimez-Ordaz *et al.*, 2019). Additionally, integrating kinetic models with sensory evaluations and quality assessments enables the development of comprehensive tools for quality management, helping the industry meet regulatory standards and consumer expectations (Kaczmarek and Muzolf-Panek, 2021; Stangierski *et al.*, 2019; Guo *et al.*, 2018). This predictive capability ensures product quality, enhances consumer satisfaction, and supports the industry's commitment to safety, innovation, and sustainability by reducing postharvest losses and improving resource efficiency through informed decision-making. TTA, in particular, is a relevant quality indicator because it reflects changes in organic acid content. These changes influence flavor, freshness perception, and microbial stability and are directly associated with ripeness and senescence (Odediran *et al.*, 2023; De Souza *et al.*, 2022). However, despite the growing interest in modeling quality changes in fruits, limited studies have focused on automating the parameter optimization process using genetic algorithms (GAs) specifically for titratable acidity kinetics in climacteric fruits. This study addresses this gap by presenting a replicable and structured computational framework for fitting kinetic models, applied to bananas as a representative system.

Bananas (*Musa sapientum* L.) are an excellent model for studying food systems due to their high perishability and the extensive biochemical changes they undergo during storage. As climacteric fruits, bananas continue ripening after harvest, with processes such as starch breakdown into simple soluble sugars and increased soluble pectin contributing to fruit softening and flavor enhancement (Dos Santos *et al.*, 2019; Kaka *et al.*, 2019; Zomo *et al.*, 2015). Organic acids, such as malic acid, fluctuate throughout the ripening process, initially increasing and subsequently declining as senescence approaches, which is closely linked to TTA (Gutierrez-Aguirre *et al.*, 2023; Coelho De Queiroz *et al.*, 2019), as malic acid—the predominant acid in bananas—is progressively metabolized through enzymatic decarboxylation and transamination reactions. During ripening, increased activity of enzymes such as NADP-malic enzyme and malate dehydrogenase contributes to malic acid degradation, reducing the total acid content and decreasing TTA (Zhou *et al.*, 2023; Onik *et al.*, 2019). These chemical transformations also involve changes in pH and Total Soluble Solids (TSS), both critical quality attributes during ripening. The gradual reduction in acidity, alongside an increase in TSS and sugar content, imparts the characteristic sweetness and flavor of ripe bananas, making them more appealing to consumers (Nguyen *et al.*, 2023; Aquino *et al.*, 2017; Zomo *et al.*, 2015). Additionally, the interplay between pH and the catalytic activity of cell wall enzymes can influence the fruit's texture, color, and stability during storage. Monitoring these biochemical changes—such as variations in pH, TSS, color, firmness, and TTA—allows for understanding ripening dynamics, optimizing postharvest treatments, and extending the shelf-life of bananas (Novita *et al.*, 2024; Dos Santos *et al.*, 2019).

Several studies have demonstrated that TTA is closely related to other physicochemical parameters during fruit ripening and storage. In bananas, TTA has shown a direct correlation with TSS during early ripening stages, and an inverse correlation with firmness and skin color development, reflecting progressive senescence (Coelho De Queiroz *et al.*, 2019; Aquino *et al.*, 2017). TTA also tends to decline after an initial increase, indicating metabolic transformations such as the conversion of organic acids and sugar accumulation. Similar relationships have been reported in other climacteric fruits, where TTA is inversely associated with pH and firmness, and directly with respiration rate and ethylene production (Odediran *et al.*, 2023). These correlations highlight the role of TTA as an integrative indicator of postharvest quality. Therefore, improving the prediction of TTA through kinetic modeling contributes to a better understanding of ripening dynamics in banana and similar fruit systems.

Performance metrics such as coefficient of determination (R^2), Mean Squared Error (MSE), Akaike Information Criterion (AIC), and Bayesian Information Criterion (BIC) are determinants for evaluating the quality of kinetic model fitting by balancing accuracy and simplicity. R^2 quantifies the variance explained by the model, with higher values indicating better fit (De-Graft H., 2017), while MSE measures the average squared residual error, with lower values reflecting improved accuracy (Collenteur, 2021). AIC and BIC, on the other hand, penalize model complexity to prevent overfitting, with AIC favoring models that balance fit and parameter usage and BIC imposing stricter penalties to promote simplicity (Hoekstra *et al.*, 2023; Corrales *et al.*, 2015). Together, these metrics ensure robust model selection, where R^2 and MSE assess goodness-of-fit, and AIC and BIC enhance interpretability and generalizability. The integrated use of these criteria has been theoretically supported in model selection literature (Vrieze, 2012), and applied in food systems such as drying kinetics modeling (Souza *et al.*, 2019). More recently, their continued relevance has been demonstrated in predictive modeling and longitudinal data analysis across various disciplines (Hoekstra *et al.*, 2023; Zhang & Meng, 2023).

Kinetic models, including zero-order, first-order, and second-order, are frequently used in food science to understand and model quality product changes, allowing preservation optimization. Also, these models enable describing the flavor development and evaluating nutrient stability (Contreras-López *et al.*, 2022; Hazrat *et al.*, 2022; Buehler and Mesbah, 2016). While these models have broad applications, traditional parameter estimation methods like ordinary least squares (OLS) face limitations, including assumptions of error normality and challenges in parameter identifiability for nonlinear systems (Chai *et al.*, 2024; Manzhula *et al.*, 2024). Advanced techniques, such as Bayesian optimization, provide robust alternatives for addressing these challenges and improving model validation (Luciano and Svoboda, 2024; Taylor *et al.*, 2023; Jorayev *et al.*, 2022). These techniques have demonstrated significant predictive accuracy and efficiency advantages, particularly in systems with complex or non-linear behaviors. For instance, Bayesian optimization has been shown to reduce the number of required evaluations by over 90 % compared to grid or random search methods, while improving convergence toward optimal solutions (Taylor *et al.*, 2023). Additionally, in multi-objective optimization scenarios, Bayesian approaches have increased parameter estimation accuracy, such as conversion and yield in chemical processes, by up to 10–20 %, while reducing processing times by several hours (Jorayev *et al.*, 2022). These outcomes support the relevance of Bayesian optimization in enhancing the reliability and performance of predictive models in food and biological systems.

GAs are automated tools for kinetic model fitting in food science, offering advantages over traditional methods like ordinary least squares (OLS). Inspired by natural selection, GAs evolve populations of candidate solutions through operations such as selection, crossover, and mutation, iteratively optimizing model parameters based on a defined fitness function (Xu, 2022; Fischer *et al.*, 2021). Unlike gradient-based approaches, which are often limited by local minima and sensitivity to outliers such as OLS, GAs explore complex, multidimensional parameter spaces globally by maintaining diverse solution populations and evaluating multiple performance metrics simultaneously (Wrzecionek *et al.*, 2021; Turgut, 2018; Umbarkar *et al.*, 2015), ensuring a thorough search for the global optimum (Wrzecionek *et al.*, 2021; Zarejousheghani *et al.*, 2016). This robustness has enabled the successful application of GAs in modeling nonlinear and multistep reaction kinetics, including optimized kinetic parameters for enzymatic biodiesel production (Zarejousheghani *et al.*, 2016)., and polycondensation and triglyceride epoxidation reactions (Kousaalya *et al.*, 2019).

In food-related applications, GAs have been used to optimize fermentation kinetics in cocoa processing, where they effectively estimated key parameters such as the maximum specific growth rate (μmax) and saturation constants (Ks), yielding reliable predictions of metabolite production and supporting process scale-up and control (López-Pérez *et al.*, 2018). Additionally, they are increasingly applied in food engineering tasks such as thermal degradation modeling, drying optimization, and process control (Koop *et al.*, 2024). GAs have also been employed to model the polycondensation of citric acid with glycerol, a reaction relevant to developing edible coatings and biodegradable food packaging matrices. These examples highlight the flexibility and robustness of GAs in modeling complex reaction systems in food science (Wrzecionek *et al.*, 2021).

GAs and other predictive tools have been increasingly employed to model post-harvest changes' kinetics in climacteric and non-climacteric fruits under controlled temperatures. These methods help predict quality attributes, optimize storage protocols, and explore the genetic basis of post-harvest traits. Tools such as artificial neural networks, fuzzy logic, adaptive neuro-fuzzy inference systems, and GAs have been applied to model parameters like chilling injury, moisture loss, and firmness (Salehi, 2020). Predictive models have also distinguished ripening behaviors in melons and tracked changes in texture and physiology during storage (Tijskens *et al.*, 2008). In blueberries, GAs have supported breeding strategies by identifying traits linked to superior post-harvest quality (Casorzo *et al.*, 2024), while in barley, they have been used to monitor fungal development (Wawrzyniak, 2023). In climacteric fruits, strategies to delay ethylene-driven ripening have benefited from physiological, molecular, and computational approaches, reinforcing the utility of predictive modeling for quality control (Alonso-Salinas *et al.*, 2024). Altogether, these studies highlight the growing relevance of GAs and machine learning in post-harvest quality prediction across plant systems.

It is hypothesized that the automation of kinetic model fitting using genetic algorithms enables more efficient parameter estimation and allows for accurate modeling of TTA decreasing in bananas during post-harvest ripening.

Based on the above, this study aimed to model the decrease in TTA in bananas (*Musa paradisiaca* L.) by automating the fitting of zero-order, first-order, and second-order kinetic models. A Python script was developed to implement GAs, which optimized the kinetic parameters—initial TTA (C_0) and reaction rate constant (k)—by minimizing the MSE between experimental and predicted values. Model performance was assessed using R^2, AIC, and BIC to explore a broader solution space and enhance the predictive capacity of kinetic analysis.

2. Materials and methods

2.1 Samples

The bananas (*Musa paradisiaca* L., Cavendish variety) used in this study were sourced from the central supply market of Pachuca de Soto, Hidalgo, Mexico. The fruits were selected based on visual uniformity (color and size), corresponding to ripening stage 2 of the Von Loesecke scale (Khodabakhshian and Baghbani, 2021), indicative of early post-harvest ripening, and were used without prior washing, peeling, or chemical treatment. The samples were transported to the laboratory in a tray without packaging or refrigeration, approximately five minutes after purchase.

2.2 Experimental conditions and storage setup

The experiment was conducted in the common-use laboratory of the Área Académica de Química at the Universidad Autónoma del Estado de Hidalgo, Mexico. Whole, unpeeled bananas were placed directly on clean laboratory work tables, maintaining a 30 cm separation between fruits to promote adequate airflow and avoid physical contact. Although no specialized monitoring equipment was installed, ambient temperature and relative humidity were recorded using publicly available internet-based data corresponding to the study location. These environmental conditions averaged

21 ± 1 °C and 57 ± 1 % relative humidity throughout the 16-day storage period. While direct verification was not possible, the laboratory environment remained stable, and the primary objective focused on modeling TTA degradation, making the referenced data appropriate for contextualizing the storage conditions.

During the storage period, the fruits progressed naturally from ripening stage 2 to stages beyond 7 on the Von Loesecke scale. By the end of the 16-day period, the bananas exhibited brown to black peels, a very soft pulp and signs of fermentation, such as an alcoholic odor. These characteristics are consistent with late senescence under non-refrigerated conditions. Despite these advanced changes, TTA was successfully measured at all time points, enabling a continuous and reliable kinetic analysis throughout the study.

2.3 Total Titratable Acidity

The bananas' TTA was measured in triplicate at specific time intervals: days 0, 1, 2, 3, 6, 7, 8, 9, 10, 13, 14, 15, and 16. These systematic measurements tracked changes in acidity over time, offering valuable insights into the ripening process.

TTA was determined by titration with 0.01 mol/L NaOH after macerating the samples in distilled water, following the procedure described in previous researches (García-Curiel *et al.*, 2023; Barreto Ferreira and Faria Freitas, 2019). The titration was performed using a 50 mL manual glass burette (PYREX®, Corning Inc., USA, 2020) held in place with a burette clamp on a universal stand. The Erlenmeyer flask (PYREX®, Corning Inc., USA, 2020) containing the sample and a magnetic stir bar was placed on a magnetic stirrer with hot plate (Thermo Scientific® Cimarec™+, Waltham, MA, USA, 2020), operating at 400 rpm to ensure constant mixing under ambient conditions. All volumetric glassware used was previously calibrated. The results were expressed as grams of malic acid per 100 grams of banana.

Although no separate reproducibility test was performed, all determinations were conducted under uniform laboratory conditions using the same equipment and operator, ensuring procedural consistency appropriate to the modeling scope of the study.

2.4. Kinetic modeling of total titratable acidity in bananas

2.4.1 Data preparation

The TTA data for bananas was collected and organized by time intervals. To ensure consistency and reliability, the TTA measurements for each time point were averaged, resulting in a representative dataset for kinetic modeling.

2.4.2 Kinetic models

Three kinetic models—zero-order, first-order, and second-order — were employed to describe the changes in TTA over time (Table 1). In these models, $Q(t)$ represents the critical quality attribute, which is the TTA at time t (in days), while Q_0 denotes the initial TTA, and k is the rate constant characterizing the speed of the reaction (Contreras-López *et al.*, 2022). Each model was fitted to the averaged dataset using the OLS method.

The observed TTA values were compared with the predictions generated by each kinetic model through scatter plots of the experimental data overlaid with the corresponding model predictions. For the zero-order model (Eq. (1)), TTA was plotted directly against time. In contrast, the first-order model (Eq. (2)) used the natural logarithm of TTA ($\ln(Q(t))$ plotted against time, and the second-order model (Eq. (3)) represented the reciprocal of TTA ($1/Q(t)$) plotted against time.

Table 1. Kinetic models and their equations.
Tabla 1. Modelos cinéticos y sus ecuaciones.

Model	Mathematical expression	Eq.
Zero-order	$Q(t) = Q_0 - k \cdot t$	**(1)**
First-order	$lnQ(t) = Q_0 \cdot e^{-k \cdot t}$	**(2)**
Second-order	$Q(t) = \frac{1}{1 + Q_0 \cdot k \cdot t}$	**(3)**

2.4.3 Model evaluation

The statistical summaries for each model were generated, including parameter estimates, standard errors, and goodness-of-fit metrics such as R^2.

2.5. Automated optimization and evaluation of kinetic models

2.5.1. Data splitting and optimization

The data preparation was carried out as described earlier, following the steps for calculating TTA values from the experimental data. Subsequently, the kinetic models outlined in Table 1 described the TTA changes over time, forming the basis for parameter optimization and model evaluation.

The dataset was divided into training (80 %) and test (20 %) subsets using random splitting to ensure the robustness of the model evaluation process. The optimization of kinetic parameters, namely k (reaction rate constant) and Q_0 (initial TTA), was performed using a genetic algorithm implemented with the DEAP library in Python. This algorithm aimed to minimize the MSE between the observed and predicted TTA values. Initially, a population of candidate solutions, each representing potential values of k and Q_0, was generated. The fitness of each individual was evaluated through an objective function based on the Eq. (4) (Dong *et al.*, 2017).

$$MSE = \frac{1}{n}\sum_{i=1}^{n}\left(Q_{observed,i} - Q_{predicted,i}\right)^2 \qquad \textbf{Eq. (4)}$$

Subsequently, genetic operators, including selection, crossover, and mutation, were iteratively applied to evolve the population over 100 generations or until convergence. This iterative process enabled the exploration of a vast parameter space, ensuring the identification of the optimal set of kinetic parameters for each model.

2.5.2. Model evaluation

The performance of each kinetic model was evaluated using multiple metrics to assess accuracy and complexity. The MSE was calculated to quantify the average squared difference between the observed ($Q_{observed}$) and predicted ($Q_{predicted}$) values, providing a measure of the model's prediction error (Eq. (4)).

The R^2 was used to measure the proportion of variance in the observed data explained by the model, indicating its goodness of fit. Higher values of R^2 suggested better predictive performance.

The AIC was also computed to evaluate the trade-off between model fit and complexity. It was calculated as described in Eq. (5) (Vaga *et al.*, 2014; Zhang and Meng, 2023).

$$AIC = n \cdot ln(MSE) + 2 \cdot k \qquad \textbf{Eq. (5)}$$

where n represents the number of data points, MSE is the mean squared error, and k is the number of parameters in the model.

The BIC was also calculated to incorporate the effect of sample size on model complexity. The BIC was calculated as described in Eq. (6) (Zhang and Meng, 2023; Brewer *et al.*, 2016).

$$BIC = n \cdot ln(MSE) + k \cdot ln(n) \qquad \textbf{Eq. (6)}$$

These metrics allowed for a comprehensive and balanced evaluation of the models. While the MSE and R^2 assessed predictive accuracy, the AIC and BIC penalized unnecessary complexity (Brewer *et al.*, 2016; Corrales *et al.*, 2015). They ensured simpler models were favored for comparable accuracy and identified the most robust and efficient kinetic model for describing TTA dynamics.

The kinetic modeling and optimization procedures were implemented using the Python programming language (version 3.12.2) within the Visual Studio Code integrated development environment (IDE, version 1.96.2). Anaconda (version 25.1.1) was employed as the package and environment manager to ensure compatibility and reproducibility across dependencies. The analysis relied on several Python libraries: 'pandas' (2.2.3) for data handling, 'numpy' (1.26.4) for numerical operations, 'matplotlib' (3.9.1) and 'plotly' (5.22.0) for data visualization, 'scipy' (1.15.1) and 'statsmodels' (0.14.2) for statistical modeling, 'sklearn' (1.6.1) for model evaluation metrics, and 'deap' (1.4) for implementing genetic algorithms.

The analysis was performed on a personal computer running Linux Mint 22 "Wilma" (Ubuntu 24.04 base) with Cinnamon desktop environment (version 6.2.9) and kernel 6.8.0-58-generic, using a 64-bit x86_64 architecture and GCC compiler version 13.3.0. This configuration ensured the computational efficiency and reproducibility of the modeling and optimization processes.

The dataset, containing time and TTA values and the analysis scripts, will be publicly available on a GitLab repository (https://gitlab.com/FoodChem-DataSci-Lab/kinetic-analysis-banana). This repository will enable interested researchers and practitioners to download, analyze, and implement the methodology for their studies or extend it to similar applications. This openness fosters transparency, reproducibility, and collaborative kinetic modeling and optimization advancements.

2.6 Comparative analysis of model performance

To evaluate the effectiveness of the GAs-based optimization in improving kinetic model fitting, a comparative analysis was performed between models fitted using traditional methods (Trad) and those optimized with GAs. Four performance metrics were analyzed: R^2, AIC, and BIC.

Quantitative comparisons were conducted using percentage and absolute differences between the values obtained by each fitting method. The percentage improvement in model accuracy was assessed by changes in R^2 and MSE, calculated using Eqs. (7) - (9), as follows:

$$\%\Delta R^2 = \left(R^2_{GAs} - \frac{R^2_{Trad}}{R^2_{Trad}}\right) \cdot 100 \quad \textbf{Eq. (7)}$$

$$\Delta AIC = AIC_{Trad} - AIC_{GAs} \quad \textbf{Eq. (8)}$$

$$\Delta BIC = BIC_{Trad} - BIC_{GAs} \quad \textbf{Eq. (8)}$$

3. Results and discussion

Fig. 1 presents the experimental data of TTA in bananas alongside the fitted curves for three kinetic models: zero-order, first-order, and second-order. The zero-order model, shown in the left panel, assumes a constant rate of TTA degradation over time, resulting in a linear decline in TTA. This model provides the best statistical fit, with an R^2 value of 0.918 and an adjusted R^2 of 0.910 (Table 2). It exhibits the lowest AIC (−104.0) and BIC (−102.9), indicating that it is the most parsimonious model. The estimated rate constant (k) is −0.0024 day^{-1}, suggesting a steady and uniform decrease in TTA regardless of its initial concentration. This behavior, visible as a straight line in Fig. 1a, is characteristic of zero-order kinetics and reflects a linear behavior, where the rate of change remains constant over time. In this context, it suggests that the overall decrease in acidity, as reflected by TTA, proceeds at a uniform rate regardless of the fruit's evolving biochemical composition.

The first-order model, shown in the middle panel, follows an exponential decay function, assuming that the rate of change in TTA is proportional to its current value. This model also shows a strong fit, with an R^2 of 0.913 and an adjusted R^2 of 0.905. However, its AIC (−47.67) and BIC (−46.54) values are higher than those of the zero-order model, suggesting that it may be less efficient in explaining the observed variability. The estimated rate constant (k) is -0.0204 day^{-1}, indicating a more rapid decline in TTA at the beginning of storage. As seen in Figure 1b, this behavior reflects a dynamic in which the processes contributing to acidity loss are initially more active and gradually slow down, as expected in a first-order process. The enzymatic conversion of organic acids such as malic or citric acid into sugars or intermediate metabolites during ripening may explain this trend. Previous studies have shown that enzymes like malate dehydrogenase are transcriptionally regulated throughout ripening and contribute to the decline in TTA as part of a coordinated metabolic shift (García-Gómez *et al.*, 2020; Gao *et al.*, 2018; González-Agüero *et al.*, 2016).

The second-order model, presented in the right panel, was fitted using the inverse of TTA against time. Although this model achieves a relatively high R^2 value of 0.899, it has the weakest fit among the three, as indicated by the lowest adjusted R^2 (0.890). Furthermore, its AIC (10.13) and BIC (11.26) are higher than those of the other models, making it the least suitable for describing TTA degradation in bananas from a statistical standpoint. The positive rate constant (k = 0.1744 day^{-1}) suggests a nonlinear behavior in which the decrease in TTA progressively slows over time. This deceleration may reflect a cumulative or saturable pattern of acidity loss, potentially associated with the gradual depletion of acid-related compounds and the downregulation of metabolic activity involved in acid transformation. Although the model does not provide the best fit, its structure may be indicative of a more complex physiological process. This interpretation is supported by studies in climacteric fruits such as peach, mango, and tomato, which have shown that the decline in TTA during ripening slows as a result of both substrate depletion and reduced activity of organic acid-related enzymes (X. Jiang *et al.*, 2023; Zhao *et al.*, 2019; Batista-Silva *et al.*, 2018; Rooban *et al.*, 2016).

On the whole, the comparison of model performance indicates that the zero-order model best represents the experimental data, supported by the highest R^2, the lowest AIC and BIC values, and a consistent linear trend. Although the first-order model also shows a good fit, its higher information criteria values suggest a less parsimonious description of the observed TTA changes. The second-order model, despite offering a biologically plausible framework for complex degradation dynamics, demonstrated a weaker statistical fit and higher prediction uncertainty. Therefore, a zero-order kinetic model appears to provide the most appropriate and statistically robust representation of titratable acidity degradation in bananas during ripening under the evaluated conditions. However, to improve the precision of parameter estimation and overcome potential limitations associated with traditional fitting methods, GAs were employed.

The experimental TTA values obtained in this study (ranging from 0.45 to 0.90 g of malic acid per 100 g of banana) are consistent with those reported in previous studies on climacteric fruits. For instance, a comparable decline in malic acid content during postharvest storage of bananas under physical treatments has been reported (Zhou *et al.*, 2023), while TTA values between 0.60 and 1.20 g of malic acid per 100 g of pulp have been documented for 'Maçã' bananas stored at room temperature (Dos Santos *et al.*, 2019). These comparisons support the physiological plausibility of the observed data and validate the modeling approach applied in this study.

Table 2. Kinetic model comparison for total titratable acidity.
Tabla 2. Comparación de modelos cinéticos para la acidez total titulable.

Model	R^2	Adjusted R^2	F-statistic	AIC	BIC	Intercept (C_0)	Rate constant (k)
Zero Order	0.918	0.91	122.6	−104	−102.9	0.1385	−0.0024
First Order	0.913	0.905	114.9	−47.67	−46.54	−1.9699	−0.0204
Second Order	0.899	0.89	98.28	10.13	11.26	7.1008	0.1744

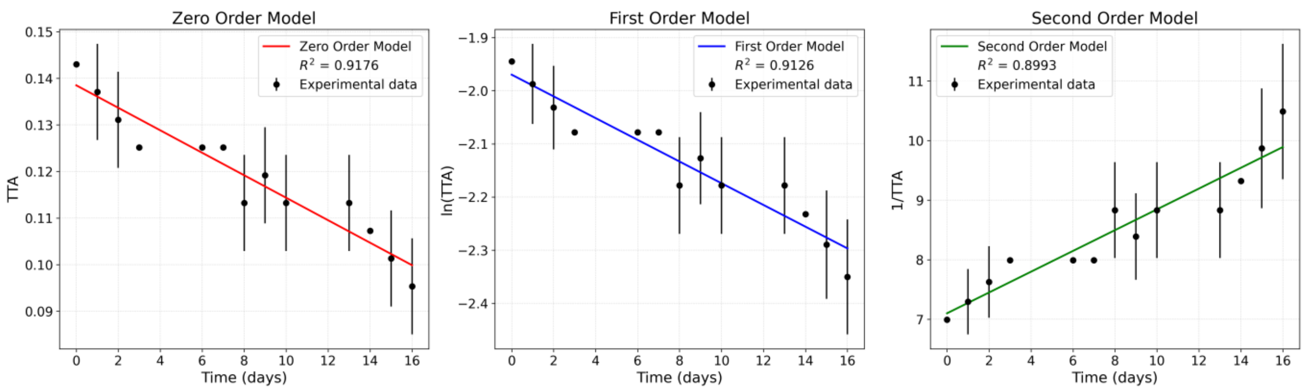

Figure 1. Kinetic model fitting for total titratable acidity (TTA) in bananas using classical models. TTA: Total titratable acidity, expressed as g of malic acid per 100 g of banana. Error bars represent the standard deviation of three replicates.
Figura 1. Ajuste del modelo cinético para la acidez titulable total (TTA) en plátanos utilizando modelos clásicos. TTA: Acidez titulable total, expresada como g de ácido málico por 100 g de plátano. Las barras de error representan la desviación estándar de tres réplicas.

Fig. 2 shows the predictive performance of three kinetic models—zero-order, first-order, and second-order fitted to the TTA in bananas using genetic algorithms. This provides a more reliable assessment of model generalization, avoiding over-fitting to the training data. The left panel represents the zero-order model, which maintains a linear decline in TTA with a train R^2 of 0.9120 and a test R^2 of 0.9126. Despite exhibiting a low MSE in the training set (1.1874×10^{-5}), its test MSE increases to 2.6915×10^{-5}, suggesting a slight decrease in predictive accuracy (Table 3).

The middle panel presents the first-order model, where the decay follows an exponential trend. This model demonstrates improved predictive performance, with a test R^2 of 0.9246, outperforming the zero-order model in predictive capacity. The test MSE decreases to 2.3204×10^{-5}, further supporting its higher predictive reliability. Additionally, the first-order model has a slightly higher AIC (−108.5263) and BIC (−107.9211) than the zero-order model, indicating a modest increase in model complexity without significant over-fitting.

The right panel illustrates the second-order model with the highest test R^2 (0.9349) and the lowest test MSE (2.0029×10^{-5}), indicating that it provides the best predictive performance among the three models. Although its train R^2 (0.8933) is slightly lower than the other models, the improved test results suggest better generalization. However, its AIC (−107.4819) and BIC (−106.8768) are higher than those of the zero- and first-order models, indicating that this model is statistically less parsimonious despite its predictive strength.

These results highlight the importance of train-test validation when evaluating kinetic models for decreasing TTA. This step allows the model's generalization ability to be assessed beyond the dataset used for calibration. Without this step, a model may exhibit excellent statistical fit (e.g., high R^2, low AIC) but fail to predict unseen data reliably, potentially leading to over-fitting and poor real-world applicability. In this study, validation revealed that although the zero-order model fitted the training data best, the second-order model showed superior predictive performance, emphasizing the need for this evaluation step (Sivakumar *et al.*, 2024; Pandey *et al.*, 2020). The initial analysis (Fig. 1) suggested that a zero-order kinetic model best represented TTA loss. However, when tested on unseen data, the second-order model demonstrated superior predictive performance. This indicates that the degradation of TTA may follow a more complex mechanism than a simple linear or exponential decay, warranting further exploration of higher-order or mechanistic models.

Table 3. Predictive performance of kinetic models for total titratable acidity.
Tabla 3. Rendimiento predictivo de modelos cinéticos para la acidez total titulable.

Model	Train MSE	Test MSE	AIC	BIC	Train R^2	Test R^2	Optimized k	Optimized C_0
Zero Order	1.1874×10^{-5}	2.6915×10^{-5}	−109.4115	−108.8064	0.912	0.9126	0.0024	0.1372
First Order	1.2973×10^{-5}	2.3204×10^{-5}	−108.5263	−107.9211	0.9039	0.9246	0.02	0.1382
Second Order	1.4401×10^{-5}	2.0029×10^{-5}	−107.4819	−106.8768	0.8933	0.9349	0.167	0.1391

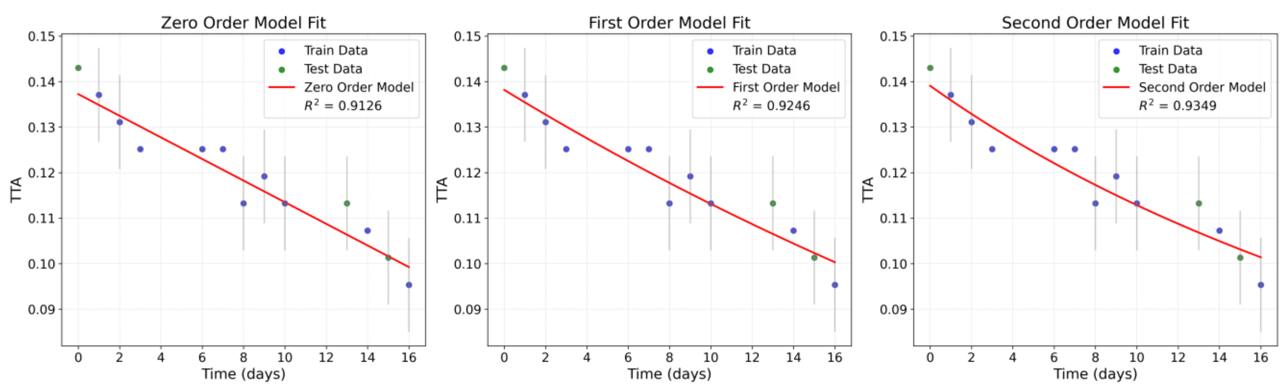

Figure 2. Kinetic model fits for total titratable acidity (TTA) in bananas using genetic algorithms: Training and test data. TTA: Total titratable acidity, expressed as g of malic acid per 100 g of banana. Error bars represent the standard deviation of three replicates.
Figura 2. Ajustes del modelo cinético para la acidez titulable total (TTA) en plátanos mediante algoritmos genéticos: datos de entrenamiento y prueba. TTA: Acidez titulable total, expresada como g de ácido málico por 100 g de plátano. Las barras de error representan la desviación estándar de tres réplicas.

The results in Figs. (1) and (2) emphasize the necessity of selecting an appropriate kinetic model to describe the decreasing of TTA in bananas. While the zero-order model initially exhibited the best statistical fit based on R^2, AIC, and BIC values (Fig. 1), its predictive performance on unseen data was lower than that of the other models, as indicated by an increase in test MSE (2.6915×10^{-5}) (Table 3), which suggests that although the zero-order model is parsimonious, it may not fully capture the complexity of TTA degradation.

The first-order model demonstrated improved predictive performance, with a higher test R^2 (0.9246) and a lower test MSE (2.3204×10^{-5}) than the zero-order model, indicating that an exponential decay assumption better reflects the initial decline in TTA. However, the second-order model achieved the best predictive results, with the highest test R^2 (0.9349) and the lowest test MSE (2.0029×10^{-5}), suggesting that the degradation process involves more complex mechanisms. Nevertheless, its higher AIC and BIC values indicate an increased model complexity that may limit its practical application.

To quantify the improvement achieved through GAs-based optimization, a comparative analysis was conducted using R^2, AIC, and BIC values from the traditional and optimized models. The first-order model showed the most significant increase in explanatory power, with a 1.27 % increase in R^2 (from 0.913 to 0.9246), while the second-order model exhibited a 3.99 % improvement (from 0.899 to 0.9349). Although the R^2 of the zero-order model decreased slightly by 0.59 % (from 0.918 to 0.9126), it still retained strong performance.

In terms of model parsimony, all three models showed clear improvements after optimization. The AIC was reduced by 5.41, 60.86, and 117.61 units for the zero-, first-, and second-order models, respectively. Similarly, the BIC values were lowered by 5.91, 61.38, and 118.14 units, confirming that GA optimization enhanced the balance between model fit and complexity across all models.

Among the models evaluated using GAs optimization, the second-order model yielded the highest coefficient of determination ($R^2 = 0.9349$) and the lowest MSE on the test data, suggesting that its nonlinear structure better captured the dynamics of TTA decline over time. This is also evident in Fig. 2, where the fitted curve for the second-order model closely follows the experimental points throughout the ripening period.

The kinetic parameters obtained in this study, particularly the initial TTA ($C_0 = 0.1391$ g of malic acid/100 g) and the rate constant for the second-order model ($k = 0.167$ day^{-1}), fall within the ranges reported in previous studies on banana ripening under ambient conditions. For instance, titratable acidity values ranging from 0.60 to 1.20 g of malic acid per 100 g of pulp have been documented for 'Maçã' bananas (Dos Santos *et al.*, 2019), while values between 0.34 and 0.73 % have been reported for different banana cultivars depending on ripening stage (Aquino *et al.*, 2017). Additionally, acidity values in 'Prata Anã' bananas showed similar declining patterns during storage at 23 ± 2 °C (Aquino *et al.*, 2017). The observed decrease in acidity in these studies aligns with the nonlinear decay pattern captured by the second-order model in this work. These similarities support the physiological plausibility of the fitted model and reinforce the value of GAs-based parameter optimization for capturing complex postharvest transformations in climacteric fruits.

Results highlight the advantages of GAs in kinetic fitting, as they facilitate a more robust exploration of the parameter space and mitigate local minima issues associated with traditional methods like OLS (Lei *et al.*, 2018; Zarejousheghani *et al.*, 2016). The ability of GAs to optimize multiple performance metrics, including R^2, MSE, AIC, and BIC, provides a comprehensive framework for model selection (Xue *et al.*, 2023). Furthermore, their automated nature enhances efficiency and reproducibility, allowing for a systematic evaluation of complex kinetic models without extensive manual intervention (Chakrabarti *et al.*, 2013).

The observed discrepancy between statistical fit and predictive performance underscores the necessity of train-test validation in kinetic modeling. While the zero-order model may appear optimal based on training data, its reduced accuracy in test predictions suggests it oversimplifies the degradation process. Conversely, despite its greater complexity, the second-order model provides a more accurate representation of TTA degradation, reinforcing the need for robust optimization techniques like GAs to improve parameter estimation reliability (Razdan *et al.*, 2023).

Thus, integrating GAs in kinetic modeling enhances parameter estimation accuracy and model reliability. Although the zero-order model remains a practical option due to its simplicity, the predictive superiority of the second-order model suggests that TTA degradation follows a more intricate mechanism. Future studies could explore hybrid or mechanistic models to refine this understanding, leveraging GAs' adaptability to gain deeper insights into food degradation kinetics.

From a chemical perspective, while a zero-order kinetic model accurately describes the observed TTA degradation in the dataset, a second-order approach may better capture the underlying biochemical complexities when applied to unseen data. This discrepancy suggests that the apparent linear decline in TTA could arise from the interplay of multiple biochemical processes, which, when analyzed individually, exhibit nonlinear behavior. Banana ripening is a complex process driven by various biochemical reactions, including the degradation of organic acids, influenced by factors such as enzymatic activity, cellular respiration, and ethylene production (Zhou *et al.*, 2023; Thakur *et al.*, 2019).

Enzymatic activity plays a central role in TTA decreasing, with malic enzymes facilitating the breakdown of malic acid, the predominant organic acid in bananas (Zhou *et al.*, 2023). This contributes to the overall decline in acidity, particularly in the early stages of ripening. Ethylene, an autocatalytic hormone, further accelerates acid degradation by regulating the transcription of genes associated with organic acid metabolism, including those coding for malate dehydrogenase and NADP-malic enzyme (Wei *et al.*, 2023; Cordenunsi-Lysenko *et al.*, 2019). Additionally, ethylene modulates other ripening-related processes such as starch-to-sugar conversion, softening, and changes in pigment synthesis, all of which influence the biochemical environment in which acid degradation occurs. Cellular respiration also consumes organic acids to generate energy, reducing TTA levels and reinforcing the link between ripening intensity and acidity loss (Ton Nu and Kobayashi, 2020). Together, these factors suggest that the degradation process is not strictly linear, but rather results from multiple overlapping reactions operating at different rates throughout ripening. The superior predictive performance of the second-order model in validation tests reinforces the idea that TTA decreasing follows a more intricate pattern, consistent with a dynamic and evolving metabolic context (X. Jiang *et al.*, 2023; Zhao *et al.*, 2019).

While the experimental data's statistical analysis is a zero-order kinetic model for TTA degradation in bananas, predictive validation suggests that a second-order approach may better represent the biochemical processes' complexity. Further studies incorporating mechanistic models or hybrid approaches may provide deeper insights into the dynamic changes in acidity during banana ripening.

Integrating GAs into kinetic modeling refines parameter estimation and broadens the applicability of predictive models in food science. By leveraging these advanced optimization techniques, researchers can develop more robust models that account for variability in storage conditions and biochemical interactions (Zhong and Tian, 2011). Future research should explore combining data-driven machine-learning methods with mechanistic models to enhance predictive accuracy and adaptability (Kousaalya *et al.*, 2019). Such advancements will contribute to more effective post-harvest management strategies, ultimately improving food quality and reducing economic losses in the industry (Zhong and Tian, 2011).

These results underscore the methodological contribution of this study. Although genetic algorithms (GAs) have been previously applied in food-related modeling tasks, such as optimizing parameters in reaction kinetics or enhancing classification accuracy (Nirere *et al.*, 2023; Ozbuyukkaya *et al.*, 2021; Rivera *et al.*, 2020), to date, no studies have been found that focus on their application to model acidity changes in climacteric fruits. In this study, the use of GAs led to improved fitting of the kinetic models, particularly in the second-order model, where the predictive R^2 increased to 0.9349 and the AIC and BIC values decreased significantly compared to traditional methods. These improvements align with the broader literature that highlights the ability of GAs to explore complex parameter spaces and reduce prediction error in non-linear systems. Thus, the present results contribute novel evidence supporting the integration of GAs in postharvest acidity modeling and reinforce their potential for improving the reliability of kinetic predictions in perishable fruit systems.

4. Conclusion

This study successfully automated the fitting of kinetic models to describe TTA degradation in bananas using GAs. Among the three evaluated models, the zero-order kinetic model exhibited the best statistical fit on training data ($R^2 = 0.9120$; AIC = −109.41; BIC = −108.81). However, test validation revealed that the second-order model achieved superior predictive performance (test $R^2 = 0.9349$; test MSE = 2.00×10^{-5}), suggesting that the degradation process follows a more complex mechanism than initially assumed.

These results emphasize the value of train-test validation to avoid overfitting and highlight the ability of GAs to enhance parameter estimation and generalization in food kinetic modeling. Despite the promising results, the study is limited by the scope of the data (single temperature, fixed ripening stage, and no cross-validation), which could be addressed in future studies.

Future research should consider expanding the experimental design to include varying temperature and humidity conditions, extended storage periods, and larger datasets to improve model robustness and generalizability. Additionally, although this study was conceptual and methodological, focused on developing a replicable optimization framework, the practical usefulness of the GA-optimized models could be further strengthened through experimental validation using independent samples or external post-harvest conditions. Future work should also explore hybrid modeling approaches, such as those combining mechanistic kinetic equations with machine learning techniques (e.g., neural networks or support vector regression), better to capture the biochemical processes underlying banana acidity changes. Moreover, applying this methodology to other perishable fruits or complementary biochemical quality markers, such as texture, soluble solids, or vitamin degradation, represents a promising avenue for advancing postharvest quality modeling and supporting data-driven decision-making in the food industry.

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Conflict of Interest statement

The authors declare no conflicts of interest.

5. References

Alonso-Salinas, R., López-Miranda, S., Pérez-López, A. J., & Acosta-Motos, J. R. (2024). Strategies to Delay Ethylene-Mediated Ripening in Climacteric Fruits: Implications for Shelf Life Extension and Postharvest Quality. *Horticulturae*, 10(8): 840. https://doi.org/10.3390/horticulturae10080840

Aquino, C. F., Salomão, L. C. C., Cecon, P. R., Siqueira2, D. L. D., & Ribeiro, S. M. R. (2017). Physical, Chemical and Morphological Characteristics of Banana Cultivars Depending on Maturation Stages. *Revista Caatinga*, 30(1): 87–96. https://doi.org/10.1590/1983-21252017v30n110rc

Bao, Y., Zhou, Z., Lu, H., Luo, Y., & Shen, H. (2013). Modelling quality changes in S ongpu mirror carp (C*yprinus carpio*) fillets stored at chilled temperatures: Comparison between A rrhenius model and log-logistic model. *International Journal of Food Science & Technology*, 48(2): 387–393. https://doi.org/10.1111/j.1365-2621.2012.03200.x

Batista-Silva, W., Nascimento, V. L., Medeiros, D. B., Nunes-Nesi, A., Ribeiro, D. M., Zsögön, A., & Araújo, W. L. (2018). Modifications in Organic Acid Profiles During Fruit Development and Ripening: Correlation or Causation? *Frontiers in Plant Science*, 9: 1689. https://doi.org/10.3389/fpls.2018.01689

Brewer, M. J., Butler, A., & Cooksley, S. L. (2016). The relative performance of AIC, AICC and BIC in the presence of unobserved heterogeneity. *Methods in Ecology and Evolution*, 7(6): 679–692. https://doi.org/10.1111/2041-210X.12541

Buehler, E. A., & Mesbah, A. (2016). Kinetic Study of Acetone-Butanol-Ethanol Fermentation in Continuous Culture. *PLOS ONE*, 11(8): e0158243. https://doi.org/10.1371/journal.pone.0158243

Casorzo, G., Ferrão, L. F., Adunola, P., Tavares Flores, E., Azevedo, C., Amadeu, R., & Munoz, P. R. (2024). Understanding the genetic basis of blueberry postharvest traits to define better breeding strategies. *G3: Genes, Genomes, Genetics*, 14(9): jkae163. https://doi.org/10.1093/g3journal/jkae163

Chai, K., Xia, W., Shen, R., Luo, G., Cheng, Y., Su, W., & Su, A. (2024). Optimization of heterogeneous continuous flow hydrogenation using FTIR inline analysis: A comparative study of multi-objective

Bayesian optimization and kinetic modeling. *Chemistry*. https://doi.org/10.26434/chemrxiv-2024-m0kf5

Chakrabarti, A., Miskovic, L., Soh, K. C., & Hatzimanikatis, V. (2013). Towards kinetic modeling of genome-scale metabolic networks without sacrificing stoichiometric, thermodynamic and physiological constraints. *Biotechnology Journal*, 8(9): 1043–1057. https://doi.org/10.1002/biot.201300091

Coelho De Queiroz, L. G., Oliveira De Jesus, M., Aguiar, F. S., Paraizo, E. A., Soares, M. D. C., Da Silva Pinheiro, J. M., Mizobutsi, G. P., Mendes Rodrigues, M. L., & Santos, T. C. (2019). Influence of Different 'Prata-Anã' Banana Bunch Ages on Post-Harvest Quality. *Journal of Experimental Agriculture International*, 1–14. https://doi.org/10.9734/jeai/2019/v36i130227

Collenteur, R. A. (2021). How Good Is Your Model Fit? Weighted Goodness-of-Fit Metrics for Irregular Time Series. *Groundwater*, 59(4): 474–478. https://doi.org/10.1111/gwat.13111

Contreras-López, E., Jaimez-Ordaz, J., Ugarte-Bautista, I., Ramírez-Godínez, J., González-Olivares, L. G., García-Curiel, L., & Pérez-Flores, J. G. (2022). Use of image analysis to determine the shelf-life of an apple compote with wine. *Food Science and Technology*, 42, e04122. https://doi.org/10.1590/fst.04122

Cordenunsi-Lysenko, B. R., Nascimento, J. R. O., Castro-Alves, V. C., Purgatto, E., Fabi, J. P., & Peroni-Okyta, F. H. G. (2019). The Starch Is (Not) Just Another Brick in the Wall: The Primary *Metabolism of Sugars During Banana Ripening. Frontiers in Plant Science*, 10: 391. https://doi.org/10.3389/fpls.2019.00391

Corrales, J. D., Munilla, S., & Cantet, R. J. C. (2015). Polynomial order selection in random regression models via penalizing adaptively the likelihood. *Journal of Animal Breeding and Genetics*, 132(4): 281–288. https://doi.org/10.1111/jbg.12130

De Souza, F. G., De Araújo, F. F., Orlando, E. A., Rodrigues, F. M., Chávez, D. W. H., Pallone, J. A. L., Neri-Numa, I. A., Sawaya, A. C. H. F., & Pastore, G. M. (2022). Characterization of Buritirana (*Mauritiella armata*) Fruits from the Brazilian Cerrado: Biometric and Physicochemical Attributes, Chemical Composition and Antioxidant and Antibacterial Potential. *Foods*, 11(6): 786. https://doi.org/10.3390/foods11060786

De-Graft H., A. (2017). The Effect of Outliers on the Performance of Akaike Information Criterion (AIC) and Bayesian Information Criterion (BIC) in Selection of an Asymmetric Price Relationship. *Russian Journal of Agricultural and Socio-Economic Sciences*, 65(5): 32–37. https://doi.org/10.18551/rjoas.2017-05.05

Dong, F., Zhang, Y., & Yang, J. (2017). Attention-based Recurrent Convolutional Neural Network for Automatic Essay Scoring. Proceedings of the 21st Conference on Computational Natural Language Learning (CoNLL 2017), 153–162. https://doi.org/10.18653/v1/K17-1017

Dos Santos, E. X., Santana, P. J. A., Diniz, A. C. C., Sanches, A. G., & Cordeiro, C. A. M. (2019). Postharvest technologies in the ripening of 'Maçã' bananas stored in ambient condition. *Amazonian Journal of Plant Research*, 3(1): 290–297. https://doi.org/10.26545/ajpr.2019.b00036x

Fischer, S. H., De Oliveira, J. A. A., Mumford, J. D., & Kell, L. T. (2021). Using a genetic algorithm to optimize a data-limited catch rule. *ICES Journal of Marine Science*, 78(8): 3013–3014. https://doi.org/10.1093/icesjms/fsab070

Gao, L., Zhao, S., Lu, X., He, N., Zhu, H., Dou, J., & Liu, W. (2018). Comparative transcriptome analysis reveals key genes potentially related to soluble sugar and organic acid accumulation in watermelon. *PLOS ONE*, 13(1): e0190096. https://doi.org/10.1371/journal.pone.0190096

García-Curiel, L., Pérez-Flores, J. G., Contreras-López, E., Pérez-Escalante, E., & Hernández-Hernández, A. A. (2023). Anthocyanin content prediction in frozen strawberry puree. *Italian Journal of Food Science*, 35(2): 88–97. https://doi.org/10.15586/ijfs.v35i2.2315

García-Gómez, B. E., Salazar, J. A., Nicolás-Almansa, M., Razi, M., Rubio, M., Ruiz, D., & Martínez-Gómez, P. (2020). Molecular Bases of Fruit Quality in Prunus Species: An Integrated Genomic, Transcriptomic, and Metabolic Review with a Breeding Perspective. *International Journal of Molecular Sciences*, 22(1): 333. https://doi.org/10.3390/ijms22010333

González-Agüero, M., Tejerina Pardo, L., Zamudio, M., Contreras, C., Undurraga, P., & Defilippi, B. (2016). The Unusual Acid-Accumulating Behavior during Ripening of Cherimoya (*Annona cherimola* Mill.) is Linked to Changes in Transcription and Enzyme Activity Related to Citric and Malic Acid Metabolism. *Molecules*, 21(5): 398. https://doi.org/10.3390/molecules21050398

Guo, Z., Ge, X., Yu, Q. L., Han, L., Zhao, H., & Cao, H. (2018). Quality predictive models for bovine liver during storage and changes in volatile flavors. *International Journal of Food Properties*, 21(1): 2452–2468. https://doi.org/10.1080/10942912.2018.1522330

Gutierrez-Aguirre, B. R., Llave-Davila, R. E., Olivera-Montenegro, L. A., Herrera-Nuñez, E., & Marzano-Barreda, L. A. (2023). Effect of Potassium Permanganate as an Ethylene Scavenger and Physicochemical Characterization during the Shelf Life of Fresh Banana (*Musa paradisiaca*). *International Journal of Food Science*, 2023: 1–7. https://doi.org/10.1155/2023/4650023

Hazrat, M. A., Rasul, M. G., Khan, M. M. K., Ashwath, N., Silitonga, A. S., Fattah, I. M. R., & Mahlia, T. M. I. (2022). Kinetic Modelling of Esterification and Transesterification Processes for Biodiesel Production Utilising Waste-Based Resource. *Catalysts*, 12(11): 1472. https://doi.org/10.3390/catal12111472

Hoekstra, R. H. A., Epskamp, S., Nierenberg, A., Borsboom, D., & McNally, R. J. (2023). Testing similarity in longitudinal networks: The Individual Network Invariance Test (INIT). *PsyArXiv*. https://doi.org/10.31234/osf.io/ugs2r

Jaimez-Ordaz, J., Pérez-Flores, J. G., Castañeda-Ovando, A., González-Olivares, L. G., Añorve-Morga, J., & Contreras-López, E. (2019). Kinetic parameters of lipid oxidation in third generation (3G) snacks and its influence on shelf-life. *Food Science and Technology*, 39(1): 136–140. https://doi.org/10.1590/fst.38917

Jiang, W., Zhang, M., He, J., & Zhou, L. (2004). Regulation of 1-MCP-Treated Banana Fruit Quality by Exogenous Ethylene and Temperature. *Food Science and Technology International*, 10(1): 15–20. https://doi.org/10.1177/1082013204042189

Jiang, X., Liu, K., Peng, H., Fang, J., Zhang, A., Han, Y., & Zhang, X. (2023). Comparative network analysis reveals the dynamics of organic acid diversity during fruit ripening in peach (*Prunus persica* L. Batsch). *BMC Plant Biology*, 23(1): 16.

Jorayev, P., Russo, D., Tibbetts, J. D., Schweidtmann, A. M., Deutsch, P., Bull, S. D., & Lapkin, A. A. (2022). Multi-objective Bayesian optimisation of a two-step synthesis of p-cymene from crude sulphate turpentine. *Chemical Engineering Science*, 247: 116938. https://doi.org/10.1016/j.ces.2021.116938

Kaczmarek, A., & Muzolf-Panek, M. (2021). Prediction of Thiol Group Changes in Minced Raw and Cooked Chicken Meat with Plant Extracts—Kinetic and Neural Network Approaches. *Animals*, 11(6): 1647. https://doi.org/10.3390/ani11061647

Kaka, A. K., Kumar, E. A., Ibupoto, K. A., Chattha, A. H., Soomro, S. A., Mangio, H. U. R., Junejo, S. A., Soomro, A. H., Khaskheli, S. G., & Kaka, S. K. (2019). Effect of hot water treatments and storage period on the quality attributes of banana (*Musa sp.*) fruit. *Pure and Applied Biology*, 7(4). https://doi.org/10.19045/bspab.2018.700195

Khodabakhshian, R., & Baghbani, R. (2021). Classification of bananas during ripening using peel roughness analysis—An application of atomic force microscopy to food process. *Journal of Food Process Engineering*, 44(11): e13857. https://doi.org/10.1111/jfpe.13857

Koop, L., Ramos, N. M. D. V., Bonilla-Petriciolet, A., Corazza, M. L., & Voll, F. A. P. (2024). A Review of Stochastic Optimization Algorithms Applied in Food Engineering. *International Journal of Chemical Engineering*, 2024: 1–31. https://doi.org/10.1155/2024/3636305

Kousaalya, A. B., Beyene, S. D., Ayalew, B., & Pilla, S. (2019). Epoxidation Kinetics of High-Linolenic Triglyceride Catalyzed by Solid Acidic-Ion Exchange Resin. *Scientific Reports*, 9(1): 8987. https://doi.org/10.1038/s41598-019-45458-8

Lei, Z., Zhang, Y., & Cui, P. (2018). Investigate the kinetics of coke solution loss reaction with an alkali metal as a catalyst based on the improved genetic algorithm. *International Journal of Coal Science & Technology*, 5(4): 430–438. https://doi.org/10.1007/s40789-017-0176-z

López-Pérez, P. A., Cuervo-Parra, J. A., Robles-Olvera, V. J., Del C Rodriguez Jimenes, G., Pérez España, V. H., & Romero-Cortes, T. (2018). Development of a Novel Kinetic Model for Cocoa Fermentation Applying the Evolutionary Optimization Approach. *International Journal of Food Engineering*, 14(5–6): 20170206. https://doi.org/10.1515/ijfe-2017-0206

Luciano, G., & Svoboda, R. (2024). Simulation and non-linear optimization of kinetic models for solid-state processes. *Modelling and Simulation in Materials Science and Engineering*, 32(3): 035014. https://doi.org/10.1088/1361-651X/ad2788

Manzhula, V., Dyvak, M., & Zabchuk, V. (2024). The Improved Method for Identifying Parameters of Interval Nonlinear Models of Static Systems. *International Journal of Computing*, 23(1): 19-25. https://doi.org/10.47839/ijc.23.1.3431

Mírian L. F. Freitas & T. H. B. F. (2019). Production, physical, chemical and sensory evaluation of dried banana (*Musa cavendish*). *Emirates Journal of Food and Agriculture*, 31(2):102–108. https://doi.org/10.9755/ejfa.2019.v31.i2.1912

Nguyen, V. P., Tran, H. X. N., & Phan, T. L. K. (2023). Effect of pre-treatments on qualities and storage life of banana dried by using solar dryer dome. *IOP Conference Series: Earth and Environmental Science*, 1155(1): 012020. https://doi.org/10.1088/1755-1315/1155/1/012020

Nirere, A., Sun, J., Kama, R., Atindana, V. A., Nikubwimana, F. D., Dusabe, K. D., & Zhong, Y. (2023). Nondestructive detection of adulterated wolfberry (*Lycium Chinens*) fruits based on hyperspectral imaging technology. *Journal of Food Process Engineering*, 46(4): e14293. https://doi.org/10.1111/jfpe.14293

Novita, M., Husna, N. E., & Alfiana, D. (2024). The Use of Chitosan and Beeswax Coatings on Berangan Banana (*Musa paradisiaca*) in Different Maturity Stages. *IOP Conference Series: Earth and Environmental Science*, 1290(1): 012049. https://doi.org/10.1088/1755-1315/1290/1/012049

Odediran, A., Yu, J., & Gu, S. (2023). The effect of layers of high tunnel covering and soil mulching on tomato fruit quality. *Journal of the Science of Food and Agriculture*, 103(14): 7176–7186. https://doi.org/10.1002/jsfa.12805

Olivera, D. F., Bambicha, R., Laporte, G., Cárdenas, F. C., & Mestorino, N. (2013). Kinetics of colour and texture changes of beef during storage. *Journal of Food Science and Technology*, 50(4): 821–825. https://doi.org/10.1007/s13197-012-0885-7

Onik, J. C., Xie, Y., Duan, Y., Hu, X., Wang, Z., & Lin, Q. (2019). UV-C treatment promotes quality of early ripening apple fruit by regulating malate metabolizing genes during postharvest storage. *PLOS ONE*, 14(4): e0215472. https://doi.org/10.1371/journal.pone.0215472

Ozbuyukkaya, G., Parker, R. S., & Veser, G. (2022). Determining robust reaction kinetics from limited data. *AIChE Journal*, 68(3): e17538. https://doi.org/10.1002/aic.17538

Pandey, S. K., Rathee, D., & Tripathi, A. K. (2020). Software defect prediction using K-PCA and various kernel-based extreme learning machine: An empirical study. *IET Software*, 14(7): 768–782. https://doi.org/10.1049/iet-sen.2020.0119

Poonnakasem, N., Laohasongkram, K., Chaiwanichsiri, S., & Prinyawiwatkul, W. (2018). Changes in physicochemical properties and starch crystallinity of sponge cake containing HPMC and extra virgin coconut oil during room temperature storage. *Journal of Food Processing and Preservation*, 42(5): e13600. https://doi.org/10.1111/jfpp.13600

Razdan, N. K., Lin, T. C., & Bhan, A. (2023). Concepts Relevant for the Kinetic Analysis of Reversible Reaction Systems. *Chemical Reviews*, 123(6): 2950–3006. https://doi.org/10.1021/acs.chemrev.2c00510

Rivera, E. C., Summerscales, R. L., Tadi Uppala, P. P., & Kwon, H. J. (2020). Electrochemiluminescence Mechanisms Investigated with Smartphone-Based Sensor Data Modeling, Parameter Estimation and Sensitivity Analysis. *ChemistryOpen*, 9(8): 854–863. https://doi.org/10.1002/open.202000165

Rooban, R., Shanmugam, M., Venkatesan, T., & Tamilmani, C. (2016). Physiochemical changes during different stages of fruit ripening of climacteric fruit of mango (*Mangifera indica* L.) and non-climacteric of fruit cashew apple (*Anacardium occidentale* L.). *Journal of Applied and Advanced Research*, 1(2): 53–58. https://doi.org/10.21839/jaar.2016.v1i2.27

Salehi, F. (2019). Recent Advances in the Modeling and Predicting Quality Parameters of Fruits and Vegetables during Postharvest Storage: A Review. *International Journal of Fruit Science*, 20(3): 506–520. https://doi.org/10.1080/15538362.2019.1653810

Sivakumar, M., Parthasarathy, S., & Padmapriya, T. (2024). Trade-off between training and testing ratio in machine learning for medical image processing. *PeerJ Computer Science*, 10: e2245. https://doi.org/10.7717/peerj-cs.2245

Souza, D. G., Resende, O., Moura, L. C. D., Ferreira Junior, W. N., & Andrade, J. W. D. S. (2019). Drying Kinetics of the Sliced Pulp of Biofortified Sweet Potato (*Ipomoea batatas* L.). *Engenharia Agrícola*, 39(2): 176–181. https://doi.org/10.1590/1809-4430-eng.agric.v39n2p176-181/2019

Stangierski, J., Weiss, D., & Kaczmarek, A. (2019). Multiple regression models and Artificial Neural Network (ANN) as prediction tools of changes in overall quality during the storage of spreadable processed Gouda cheese. *European Food Research and Technology*, 245(11): 2539–2547. https://doi.org/10.1007/s00217-019-03369-y

Taylor, C. J., Felton, K. C., Wigh, D., Jeraal, M. I., Grainger, R., Chessari, G., Johnson, C. N., & Lapkin, A. A. (2023). Accelerated Chemical Reaction Optimization Using Multi-Task Learning. *ACS Central Science*, 9(5): 957–968. https://doi.org/10.1021/acscentsci.3c00050

Thakur, R., Pristijono, P., Bowyer, M., Singh, S. P., Scarlett, C. J., Stathopoulos, C. E., & Vuong, Q. V. (2019). A starch edible surface coating delays banana fruit ripening. *LWT*, 100: 341–347. https://doi.org/10.1016/j.lwt.2018.10.055

Tijskens, L. M. M., Dos Santos, N., Obando-Ulloa, J. M., Moreno, E., Schouten, R. E., García-Mas, J., Monforte, A. J., & Fernández-Trujillo, J. P. (2008). First Attempts of Linking Modelling, Postharvest Behaviour and Melon Genetics. *Acta Horticulturae*, 802: 401–408. https://doi.org/10.17660/ActaHortic.2008.802.53

Ton Nu, P. T., & Kobayashi, T. (2020). Nylon-6–Mordenite Composite Membranes for Adsorption of Ethylene Gas Released from Chiquita Bananas. *Industrial & Engineering Chemistry Research*, 59(17): 8212–8222. https://doi.org/10.1021/acs.iecr.9b06149

Turgut, H. (2018). Artificial Intelligence Algorithms Inspired By Life Sciences. *Journal of the Turkish Chemical Society Section A: Chemistry*, 5(3): 1233–1238. https://doi.org/10.18596/jotcsa.471300

Umbarkar, A. J., Joshi, M. S., & Sheth, P. D. (2015). Dual Population Genetic Algorithm for Solving Constrained Optimization Problems. *International Journal of Intelligent Systems and Applications*, 7(2): 34–40. https://doi.org/10.5815/ijisa.2015.02.05

Vaga, S., Bernardo-Faura, M., Cokelaer, T., Maiolica, A., Barnes, C. A., Gillet, L. C., Hegemann, B., Van Drogen, F., Sharifian, H., Klipp, E., Peter, M., Saez-Rodriguez, J., & Aebersold, R. (2014). Phosphoproteomic analyses reveal novel cross-modulation mechanisms between two signaling pathways in yeast. *Molecular Systems Biology*, 10(12): 767. https://doi.org/10.15252/msb.20145112

Vrieze, S. I. (2012). Model selection and psychological theory: A discussion of the differences between the Akaike information criterion (AIC) and the Bayesian information criterion (BIC). *Psychological Methods,* 17(2): 228–243. https://doi.org/10.1037/a0027127

Wawrzyniak, J. (2023). Predictive Assessment of Mycological State of Bulk-Stored Barley Using B-Splines in Conjunction with Genetic Algorithms. *Applied Sciences*, 13(9): 5264. https://doi.org/10.3390/app13095264

Wei, W., Yang, Y., Wu, C., Kuang, J., Chen, J., Lu, W., & Shan, W. (2023). MaMADS1–MaNAC083 transcriptional regulatory cascade regulates ethylene biosynthesis during banana fruit ripening. *Horticulture Research*, 10(10): uhad177. https://doi.org/10.1093/hr/uhad177

Wrzecionek, M., Matyszczak, G., Bandzerewicz, A., Ruśkowski, P., & Gadomska-Gajadhur, A. (2021). Kinetics of Polycondensation of Citric Acid with Glycerol Based on a Genetic Algorithm. *Organic Process Research & Development*, 25(2): 271–281. https://doi.org/10.1021/acs.oprd.0c00492

Xu, T. (2022). Reflection on Randomness from an Interdisciplinary Perspective. SHS Web of Conferences, 148: 02001. https://doi.org/10.1051/shsconf/202214802001

Xue, H., Qi, T., Su, W., Wu, K.-J., & Su, A. (2023). Heterogeneous Continuous Flow Hydrogenation of Hexafluoroacetone Trihydrate and Its Kinetic Modeling. *Industrial & Engineering Chemistry Research*, acs.iecr.3c00291. https://doi.org/10.1021/acs.iecr.3c00291

Yang, J., & Xu, Y. (2021). Prediction of fruit quality based on the RGB values of time–temperature indicator. *Journal of Food Science*, 86(3): 932–941. https://doi.org/10.1111/1750-3841.15518

Zarejousheghani, F., Kariminia, H., & Khorasheh, F. (2016). Kinetic modelling of enzymatic biodiesel production from castor oil: Temperature dependence of the Ping Pong parameters. *The Canadian Journal of Chemical Engineering*, 94(3): 512–517. https://doi.org/10.1002/cjce.22408

Zhang, Y., & Meng, G. (2023). Simulation of an Adaptive Model Based on AIC and BIC ARIMA Predictions. *Journal of Physics: Conference Series*, 2449(1): 012027. https://doi.org/10.1088/1742-6596/2449/1/012027

Zhao, X., Yuan, X., Chen, S., Fu, D.-Q., & Jiang, C.-Z. (2019). Metabolomic and Transcriptomic Analyses Reveal That a MADS-Box Transcription Factor TDR4 Regulates Tomato Fruit Quality. *Frontiers in Plant Science*, 10: 792. https://doi.org/10.3389/fpls.2019.00792

Zhong, W., & Tian, Z. (2011). Application of Genetic Algorithm in Chemical Reaction Kinetics. *Applied Mechanics and Materials*, 79: 71–76. https://doi.org/10.4028/www.scientific.net/AMM.79.71

Zhou, X., Cheng, J., Sun, J., Guo, S., Guo, X., Chen, Q., Wang, X., Zhu, X., & Liu, B. (2023). Effect of Red Visible Lighting on Postharvest Ripening of Bananas via the Regulation of Energy Metabolism. *Horticulturae*, 9(7): 840. https://doi.org/10.3390/horticulturae9070840

Zomo, S. A., Ismail, S. M., Jahan, M. S., Kabir, K., & Kabir, M. H. (2015). Chemical Properties and Shelf Life of Banana (*Musa sapientum* L.) as Influenced by Different Postharvest Treatments. *The Agriculturists*, 12(2): 06–17. https://doi.org/10.3329/agric.v12i2.21725