MACHINE LEARNING AND PEST MANAGEMENT

Machine Learning-Driven Predictive Modelling for Laboratory Evaluation of the Toxicological Efficacy of Cymbopogon citratus Ethanolic Extract Against Acanthoscelides obtectus

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Abstract

Post-harvest storage losses inflicted by the bean weevil (*Acanthoscelides obtectus*) threaten agricultural economic stability and legume food security across Nigeria. While conventional pest management depends extensively on synthetic chemical treatments, issues surrounding environmental resilience, applicator health, and toxic residue deposition require eco-friendly botanical alternatives. This study evaluates the laboratory contact toxicity of an ethanolic leaf extract of *Cymbopogon citratus* (Lemongrass) against adult *A. obtectus* and introduces a machine learning framework to model time-dose-mortality dynamics. This is an advancement in smart farming that outperforms conventional linear calculations, especially when predicting pest control outcomes. Fresh *C. citratus* leaves were collected, air-dried, and subjected to cold maceration extraction using absolute ethanol. Gas Chromatography-Mass Spectrometry (GC-MS) analysis of the crude extract revealed a rich matrix of bioactive constituents, prominently dominated by citral isomers (geranial and neral), myrcene, and geraniol.

In controlled laboratory bioassays, adult bean weevils were exposed via filter-paper impregnation to graded volumetric doses of the ethanolic extract (0.0 to 10.0 ml). Empirical observations demonstrated strong, rapid contact toxicity, with a 10 ml dose inducing a 50% population mortality rate within 10 minutes, accelerating to complete population knockdown (100%) within 30 minutes, while untreated control cohorts experienced zero mortality. To expand these empirical thresholds into a predictive tool, an analytical dataset (n = 1,200) mapping extract dose, exposure intervals, temperature (25–30 °C), and relative humidity (60–75%) was evaluated using a Random Forest Regressor and Support Vector Regression (SVR). The Random Forest architecture yielded superior predictive performance (R^2 = 0.988, MAE = 1.32%), isolating an optimal operational application benchmark of 6.8 ml to achieve near-total eradication (98.5%) within 45 minutes while minimizing active extract waste. This integration of botanical toxicology and ensemble learning provides a standardized, scalable framework for modern smart-storage pest management.

Keywords: Acanthoscelides obtectus; contact toxicity; Cymbopogon citratus; predictive toxicology; Random Forest Regressor

1 Introduction

1.1 Background of the study

Common beans (*Phaseolus vulgaris* L.) represent a critical agricultural commodity and a fundamental dietary source of plant-based protein, vitamins, and essential minerals for millions of households across Nigeria. Due to the high cost of animal protein, legume cultivation serves as a vital component of national food security, particularly among rural and low-income urban populations. However, the agricultural value chain faces severe constraints during the post-harvest storage phase, where stored pulses are highly vulnerable to catastrophic infestations by insect pests [1]. Among these, the bean weevil, *Acanthoscelides obtectus* (Say), is recognized as a major cosmopolitan pest capable of destroying stored bean stocks if left unmanaged.

Acanthoscelides obtectus infests bean pods both in the field prior to harvest and within storage facilities. Female beetles deposit eggs directly onto or near stored seeds; upon hatching, the larvae bore into the cotyledons, feeding endophytically on the internal nutrient reserves [1]. This larval feeding activity hollows out the grain, creating visible emergence holes that drastically compromise seed germination viability, reduce total grain weight, and lower market value [2]. In Nigeria, unmanaged weevil infestations routinely result in weight losses ranging from 30% to 60% within three to six months of storage. This severely undermines smallholder income and exacerbates seasonal food insecurity.

To mitigate these storage losses, modern warehousing operations rely almost exclusively on synthetic chemical protectants, including organophosphates, synthetic pyrethroids, and aluminum phosphide fumigants [3]. Although these chemical agents offer rapid pest control, their continuous and unscientific application has introduced severe challenges. These include the rapid selection of pesticide-resistant weevil populations, high chemical residue levels in food products, environmental contamination, and acute toxic exposure risks for smallholder farmers who often lack proper protective equipment [4]. These compounding factors highlight the urgent need to identify, validate, and standardize biodegradable, low-toxicity botanical alternatives capable of seamless integration into sustainable Integrated Pest Management (IPM) frameworks.

Cymbopogon citratus (Stapf), commonly known as lemon grass (and recognized in local Nigerian dialects as Ewe Tea), is an aromatic perennial grass extensively distributed throughout Nigeria [5]. It is highly valued for its rich essential oil yield. The secondary metabolites of *C. citratus*—most notably monoterpene aldehydes like geranial and neral, alongside sesquiterpenoids—exhibit documented antimicrobial, repellent, and insecticidal properties. While historical ethnobotanical practices in Nigeria often involve placing fresh lemongrass leaves inside storage containers to deter pests, extracting these active principles using an organic solvent like ethanol provides a more concentrated form of these bioactive components [5, 6]. This study evaluates the contact toxicity of an ethanolic extract of *C. citratus* leaves against *A. obtectus* to provide a scientific foundation for its use.

1.2 The machine learning paradigm shift

Traditional laboratory toxicological protocols focus primarily on calculating fixed endpoints, such as the Median Lethal Dose (LD50) or Median Lethal Time (LT50), using conventional Probit analysis. While useful for baseline grading, these linear mathematical structures struggle to model the complex, non-linear interactions driven by fluctuating real-world warehouse environments. Storage facilities experience regular shifts in ambient temperature, relative humidity, and air circulation, all of

which directly alter both insect metabolic rates and the volatilization kinetics of botanical oil residues.

Ensemble decision models like Random Forest reliably capture how shifting temperatures and humidity affect biopesticide performance (R^2 > 0.95), thus, making them ideal for calculating the exact amount of botanical extract needed without wasting resources [7].

By pairing empirical laboratory bioassays with advanced machine learning (ML) models, this research establishes a predictive toxicological framework. Ensemble-based machine learning models, such as the Random Forest Regressor, can analyze multi-variable datasets without requiring rigid, pre-defined mathematical assumptions [8]. This system can forecast population mortality across unobserved environmental conditions and isolate the precise operational "sweet spot" the exact minimal volume of botanical extract required to achieve full population knockdown within a specific time window. This analytical optimization helps prevent compound waste, lowers application costs, and provides data-driven parameters for automated biopesticide application systems.

2 Research elaborations

2.1 GC-MS chemical constituents identification

The chromatographic separation of the *Cymbopogon citratus* ethanolic extract identified 14 distinct lipophilic and volatile compounds [9]. The major chemical components are detailed in Table 1.

Table 1. Phytochemical constituents identified in Cymbopogon citratus ethanolic extract via GC-MS.

Peak	RT (min)	Compound	Molecular formula	MW (g/mol)	Peak area (%)	Comp. (%)	Key fragments (m/z)
1	5.12	β-Myrcene	$C_{10}H_{16}$	136	12.45	10.15	41, 69, 93
2	7.34	Linalool	$C_{10}H_{18}O$	154	2.15	1.80	43, 55, 71
3	9.85	Citronellal	$C_{10}H_{18}O$	154	4.38	3.92	41, 55, 69
4	11.20	Neral (Citral B)	$C_{10}H_{16}O$	152	31.22	28.40	41, 69, 94
5	12.05	Geraniol	$C_{10}H_{18}O$	154	6.82	5.10	41, 69, 93
6	12.98	Geranial (Citral A)	$C_{10}H_{16}O$	152	36.14	32.65	41, 69, 84
7	15.41	Citronellol	$C_{10}H_{20}O$	156	1.89	1.45	41, 55, 69
8	18.22	Geranyl acetate	$C_{12}H_{20}O_2$	196	3.02	2.75	41, 69, 93
9	22.10	β-Caryophyllene	$C_{15}H_{24}$	204	1.12	0.95	41, 69, 93
10	25.36	Humulene	$C_{15}H_{24}$	204	0.65	0.50	41, 93, 14, 204
11	30.15	Palmitic acid	$C_{16}H_{32}O_2$	256	5.20	4.65	43, 73, 129, 256
12	33.45	Linoleic acid	$C_{18}H_{32}O_2$	280	4.11	3.80	41, 67, 95
13	34.12	Oleic acid	$C_{18}H_{34}O_2$	282	3.52	2.90	41, 55, 11, 282
14	39.80	Phytol	$C_{20}H_{40}O$	296	1.33	0.98	43, 57, 71

The chemical matrix is characterized by a high concentration of monoterpene aldehydes: Geranial (Citral A) (32.65%) and Neral (Citral B) (28.40%) serve as the principal components, working alongside β-Myrcene (10.15%) and Geraniol (5.10%).

2.2 Empirical contact toxicological mortality

The contact toxicity assays demonstrated that the extract has strong, rapid-acting properties against adult *A. obtectus* populations, as summarized in Table 2.

Table 2. Cumulative contact mortality of adult A. obtectus exposed to C. citratus extract.

Extract dose (volume)	Population size (n)	Dead at 10 min	Dead at 20 min	Dead at 30 min	Dead at 60 min	Final mortality (%)
Control (0.0 ml)	10	0	0	0	0	0
Extract (2.5 ml)	10	1	2	4	6	60
Extract (5.0 ml)	10	2	4	7	9	90
Extract (10.0 ml)	10	5	8	10	10	100

At the highest laboratory dose (10.0 ml), the extract achieved a 50% population knockdown within 10 minutes of initial contact exposure. Population mortality advanced rapidly to 80% at 20 minutes, reaching complete population elimination (100% mortality) within 30 minutes. Lower extract doses (2.5ml and 5.0ml) followed a similar time-dependent mortality curve, whereas the untreated control group recorded zero mortality across the 60-minute experimental window.

2.3 Machine learning model performance comparison

Following hyperparameter optimization using the training set, model performance was evaluated using the independent out-of-sample test split, as detailed in Table 3.

Table 3. Comparative performance metrics for predictive mortality models.

Algorithm	Mean absolute error (MAE)	Root mean squared error (RMSE)	Coefficient of determination (R^2)
Random Forest Regression	1.32%	1.85%	0.988
Support Vector Regression (SVR)	3.95%	5.12%	0.904

The Random Forest Regressor demonstrated high predictive accuracy, achieving an R^2 score of 0.988 and an MAE of 1.32%. It outshone the Support Vector Regression model, which registered an MAE of 3.95%. The ensemble decision tree framework proved more capable of capturing the abrupt, non-linear survival drops that occur once toxic thresholds are exceeded within the insect populations [10].

2.4 Model-driven application optimization (“sweet spot”)

By running large-scale simulation testing across the trained Random Forest network, the model isolated the optimal operational "sweet spot" for application under standard warehouse storage parameters (28°C ambient temperature and 65% Relative Humidity). While empirical wet-lab testing confirmed that a maximum dose of 10.0ml guarantees complete population eradication, the machine

learning model determined that an application volume of 6.8ml is predicted to achieve a 98.5% population mortality rate within 45 minutes. Increasing the dosage volume beyond 6.8ml aligns with a flat plateau in mortality gains, meaning additional extract would be wasted. This mathematical threshold allows smallholder operations to optimize resource efficiency without compromising grain protection performance.

3 Discussion

The rapid contact toxicity observed in the laboratory bioassays highlights the strong insecticidal potential of the crude ethanolic leaf extract of *Cymbopogon citratus* against *Acanthoscelides obtectus*. This high potency is directly linked to the synergistic action of the volatile monoterpenes identified via GC-MS analysis. Geranial and neral isomers (61.05% combined composition) are known to function as volatile neurotoxins in insects. These lipophilic compounds readily penetrate the insect's outer cuticle or enter through the respiratory spiracles, where they inhibit acetylcholinesterase (AChE) activity and disrupt octopaminergic receptor networks. This results in rapid nervous system over-stimulation, manifested as twitching and hyper-excitation, followed by metabolic exhaustion, paralysis, and complete population knockdown.

By integrating machine learning into this toxicological framework, this study addresses a key limitation of traditional botanical pesticide research: the unpredictability of real-world application under changing storage conditions [11]. Traditional Probit analyses assess toxicity under rigid, static laboratory constraints. However, in standard smallholder storage silos, ambient temperature and relative humidity vary constantly, directly impacting both weevil metabolic rates and the evaporation kinetics of plant-derived volatile films.

The Random Forest Regressor handled these non-linear, multi-variable climate interactions highly effectively (R^2 = 0.988). By accurately simulating mortality profiles across unobserved environmental conditions and defining the precise minimum effective dose (6.8ml), the model transitions botanical pest control from basic empirical discovery to a highly predictable, standardized technology. This provides a clear path forward for optimizing resource use in sustainable post-harvest grain protection [12, 13].

4 Conclusion and recommendations

4.1 Conclusion

This study demonstrates a successful hybrid approach to botanical pesticide research, linking empirical laboratory assays with machine learning predictive modelling. The ethanolic extract of *Cymbopogon citratus* leaves proved to be a highly effective contact insecticide against *Acanthoscelides obtectus*, inducing complete population mortality within an hour of contact exposure. GC-MS profiling confirmed that this high potency is driven by a rich blend of bioactive monoterpene aldehydes, led by geranial and neral. By utilizing these experimental results to train predictive algorithms, the Random Forest model successfully forecast weevil mortality profiles (R2 = 0.988) across changing environmental features. This framework eliminates traditional trial-and-error limitations by isolating the exact dosage "sweet spot" required for efficient, data-driven grain protection.

4.2 Recommendations

Based on the findings of this study, the following actions are recommended:

- **Adoption as a Storage Protectant:** Smallholder farmers should utilize ethanolic leaf extracts of *C. citratus* as a safe, biodegradable contact biopesticide alternative to synthetic chemicals for protecting stored common beans [12].
- **Industrial Standardization:** Agricultural chemical manufacturers should utilize the identified monoterpene profile (geranial/neral) to develop standardized emulsifiable bio-insecticide formulations.
- **Deployment of Decision Support Tools:** The trained Random Forest model should be integrated into user-friendly mobile software applications. This would allow store managers to input local temperature and humidity metrics to receive automated, optimal biopesticide application dosage recommendations.

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