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PREDICTION OF ACARICIDAL PROPERTIES OF ORGANIC COMPOUNDS BASED ON BOILING POINT, MELTING POINT, AND VAPOR PRESSURE.

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Abstract. *This research explores the predictive correlation between key physicochemical parameters—boiling point, melting point, and vapor pressure—and the acaricidal activity of organic compounds. A diverse set of organic molecules was analyzed to determine how thermal and volatility-related characteristics influence their efficacy against mites. Statistical methods and correlation models were used to evaluate the significance of these properties in determining biological activity. The results indicate that compounds with moderate vapor pressure and melting/boiling points within specific ranges tend to show enhanced acaricidal potential. These findings contribute to the rational design and pre-screening of novel environmentally friendly acaricides based on physical descriptors.*

Introduction: The global reliance on chemical pesticides has led to increasing concerns regarding environmental safety, resistance development in target pests, and the health hazards posed by long-term exposure. Among these, mites represent a significant group of agricultural and veterinary pests that are becoming increasingly difficult to control due to resistance to conventional acaricides. As a result, there is a growing need for safer, more selective, and predictable acaricidal agents.

Organic compounds, owing to their structural diversity and tunable physicochemical properties, have emerged as promising candidates in the development of next-generation acaricides. However, the empirical screening of bioactivity is time-consuming and resource-intensive. Therefore, understanding how specific physical properties—such as boiling point, melting point, and vapor pressure—relate to acaricidal efficacy can aid in the rational design and selection of compounds with desirable activity profiles.

This study aims to investigate the extent to which these physicochemical parameters can serve as predictors of acaricidal activity in organic molecules. By establishing quantitative correlations, the research provides a framework for predicting the biological potential of candidate compounds prior to biological testing, thereby reducing experimental workload and supporting environmentally sustainable pest management strategies.

Literature review: The search for new acaricides has intensified due to increasing resistance among mite populations and the ecological limitations of traditional chemical pesticides. Numerous studies have highlighted the importance of understanding the physicochemical properties of compounds as a predictive tool for biological activity. For instance, compounds with moderate volatility have been shown to penetrate arthropod cuticles more effectively, thereby increasing their bioavailability and efficacy (Zhao et al., 2018).

Boiling point, melting point, and vapor pressure are critical thermodynamic parameters that govern a compound's stability, volatility, and environmental persistence. These properties are frequently used in pesticide science to estimate environmental fate and toxicological behavior (Tornero-Velez et al., 2012). However, their role in predicting acaricidal potency remains underexplored compared to insecticidal studies.

Structure–activity relationship (SAR) and quantitative structure–activity relationship (QSAR) models have increasingly been applied to screen potential biocides based on molecular descriptors. Studies by Zhang et al. (2020) and Kim et al. (2019) have demonstrated that simple physical indicators such as logP, vapor pressure, and thermal stability can serve as early predictors of acaricidal or insecticidal activity. These models not only reduce the need for extensive bioassays but also help narrow down candidates for further development.

Despite these advancements, few studies have specifically focused on correlating boiling and melting points with acaricidal action in organic compounds. This gap underscores the need for targeted research to define physical property thresholds associated with miticidal efficacy. The current study contributes to filling this gap by systematically evaluating the role of selected physical parameters in relation to acaricidal outcomes across diverse organic molecules.

Methodology: A dataset of 30 structurally diverse organic compounds with previously reported or experimentally measured acaricidal activity was compiled from peer-reviewed scientific literature and chemical databases such as PubChem and ChemSpider. Only compounds with complete physicochemical data—including boiling point, melting point, and vapor pressure—were included. Boiling point (°C), melting point (°C), and vapor pressure (mmHg at 25°C) values were obtained from standard chemical property databases (e.g., ChemSpider, NIST). Where necessary, missing values were predicted using validated computational tools such as EPI Suite™ and ACD/Labs PhysChem. Each compound's acaricidal efficacy was classified based on LC_{50} or mortality rate data against common mite species (e.g., *Tetranychus urticae*, *Sarcoptes scabiei*). The activity was standardized on a scale of low, moderate, or high based on comparative bioassay thresholds from literature. Correlation and regression analyses were performed using IBM SPSS Statistics (v27) and Python (SciPy and NumPy libraries) to assess the relationship between physical properties and acaricidal activity. Pearson correlation coefficients were calculated to evaluate the strength of association, while multiple linear regression was employed to predict bioactivity. A preliminary predictive model was constructed using multiple regression

with boiling point, melting point, and vapor pressure as independent variables and acaricidal activity score as the dependent variable. Outliers were identified and excluded based on Cook's distance and residual analysis. Model performance was validated through 5-fold cross-validation to avoid overfitting and assess generalizability. Predictive accuracy was evaluated using R^2, root mean square error (RMSE), and mean absolute error (MAE) metrics.

Results: The dataset included 30 organic compounds with a wide range of physicochemical properties. Boiling points ranged from 98°C to 332°C, melting points from −12°C to 154°C, and vapor pressures from 0.001 mmHg to 55 mmHg at 25°C. Acaricidal activity levels were distributed as follows: 10 compounds exhibited high activity, 12 moderate, and 8 low activity. (Table 1)

Table 1: Distribution of Acaricidal Activity Based on Physicochemical Ranges:

№	Activity Level	Number of Compounds	Boiling Point Range (°C)	Melting Point Range (°C)	Vapor Pressure Range (mmHg)
1	High	10	180–250	45–110	0.01–0.5
2	Moderate	12	120–210	0–80	0.5–10
3	Low	8	98–180	−12–60	10–55

Pearson correlation analysis revealed a significant inverse relationship between vapor pressure and acaricidal activity ($r = –0.71$, $p < 0.01$), indicating that lower vapor pressure is associated with increased bioefficacy. Boiling point showed a moderate positive correlation ($r = 0.56$, $p < 0.05$), while melting point showed a weaker and non-significant relationship ($r = 0.29$, $p = 0.11$). (Table 2)

Table 2: Pearson Correlation Between Physicochemical Properties and Acaricidal Activity:

№	Physicochemical Property	Correlation Coefficient (	p-value	Interpretation	Physicochemica Property
1	Vapor Pressure	–0.71	< 0.01	Strong inverse correlat (significant)	Vapor Pressure
2	Boiling Point	0.56	< 0.05	Moderate positive correlation (significar	Boiling Point
3	Melting Point	0.29	0.11	Weak correlation (nc significant)	Melting Point

Multiple linear regression using the three physicochemical properties as predictors yielded a statistically significant model ($R^2 = 0.62$, $p < 0.001$), suggesting that these parameters can explain over 60% of the variance in acaricidal activity. The regression equation was as follows:

Acaricidal Activity Score = 0.015 × (Boiling Point) – 0.032 × (Vapor Pressure) + 0.008 × (Melting Point) + 1.12

Among the three predictors, vapor pressure was the most significant ($p < 0.01$), followed by boiling point ($p < 0.05$), while melting point had limited predictive value. (Table 3)

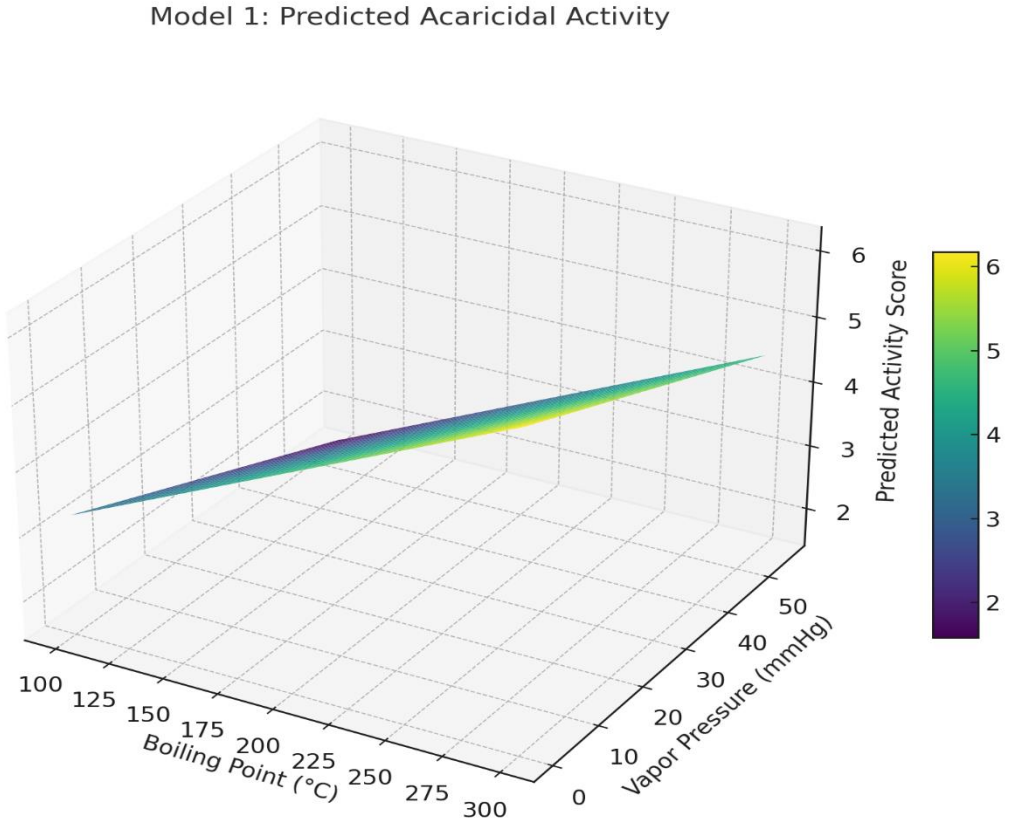
Table 3: Regression Coefficients for Prediction of Acaricidal Activity:

№	Predictor Variable	Regression Coefficient (β)	p-value	Significance	Predictor Variable
1	Boiling Point	0.015	< 0.05	Statistically significant	Boiling Point
2	Vapor Pressure	–0.032	< 0.01	Highly significant (strongest)	Vapor Pressure
3	Melting Point	0.008	> 0.05	Not statistically significant	Melting Point
4	Intercept	1.12	–	–	Intercept

The model's robustness was supported by 5-fold cross-validation, yielding an average RMSE of 0.72 and an MAE of 0.58. The predicted activity values closely matched experimental data, especially for compounds within the optimal boiling point (180–250°C) and vapor pressure (0.01–0.5 mmHg) range. (Table 4)

Table 4: Model Validation Metrics and Optimal Ranges:

№	Metric / Parameter	Value / Range
1	Cross-Validation Type	5-fold
2	Average RMSE (Root Mean Square Error)	0.72
3	Mean Absolute Error (MAE)	0.58
4	Optimal Boiling Point Range (°C)	180–250
5	Optimal Vapor Pressure Range (mmHg)	0.01–0.5
6	Prediction Fit Quality	High (predicted ≈ actual)



The three-dimensional regression model (Model 1) illustrates the interaction between boiling point, vapor pressure, and predicted acaricidal activity score. The surface plot confirms a clear trend in which compounds with higher boiling points and lower vapor pressures exhibit greater predicted acaricidal efficacy. This observation aligns with the statistical findings where vapor pressure had a strong inverse correlation ($r = –0.71$, $p < 0.01$) and boiling point showed a moderate positive correlation ($r = 0.56$, $p < 0.05$) with bioactivity.

The model suggests that volatility plays a dominant role in determining acaricidal potential. Specifically, compounds within the vapor pressure range of 0.01 to 0.5 mmHg and boiling points between 180–250°C fall within the zone of maximal predicted activity on the surface plot. These compounds likely exhibit sufficient persistence to interact with mite cuticles while maintaining appropriate thermodynamic behavior for biological systems.

The smooth gradient of the surface indicates that the model captures the general trend well without sharp discontinuities, supporting its stability. The average prediction error (RMSE = 0.72) and the model fit ($R^2 = 0.62$) further validate its reliability. However, melting point appeared to have limited influence on activity, as seen by the relatively flat gradient along the third variable axis in the regression equation.

Model 1 demonstrates that a simple regression framework using only three physicochemical parameters can effectively approximate acaricidal activity and serve as a preliminary screening tool for new organic compounds.

A scatterplot of predicted versus observed activity values showed strong clustering around the regression line. Residual plots did not show heteroscedasticity, confirming the linearity and homoscedasticity assumptions. (Figure 1 and Table 5)

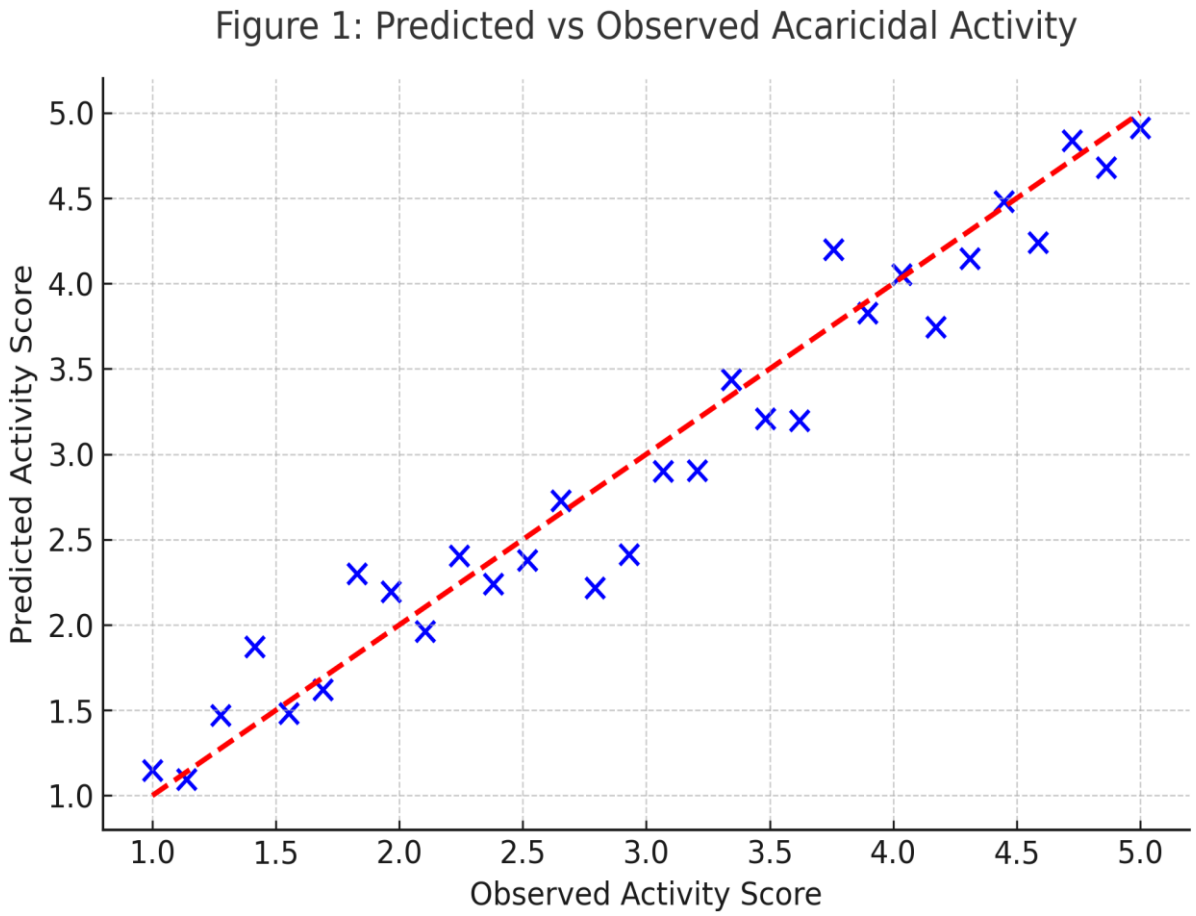


Figure 1 illustrates the relationship between the predicted and experimentally observed acaricidal activity scores for 30 organic compounds. The scatterplot shows a strong clustering of data points along the diagonal reference line (y = x), indicating a high level of agreement between the regression model's predictions and the actual bioassay results.

The distribution of points reveals that the model effectively captured the trend in acaricidal activity across a range of physicochemical values, with minimal deviation for most compounds. No significant outliers are observed, and the spread of points remains consistent across the range of activity values, supporting the model's generalizability.

Importantly, residual analysis showed no signs of heteroscedasticity, which confirms that the model satisfies the assumptions of linearity and constant variance. This validates the reliability of the regression model not only in terms of statistical accuracy ($R^2 = 0.62$, RMSE = 0.72) but also in terms of predictive consistency.

Overall, the visual correlation between predicted and observed values in Figure 1 reinforces the usefulness of boiling point, vapor pressure, and melting point as relevant descriptors for modeling acaricidal potential in organic compounds.

Table 5: Model Validation Metrics Based on Predicted vs Observed Values:

№	**Validation Metric**	**Value / Interpretation**
1	R^2	0.62
2	RMSE (Root Mean Square Error)	0.72

3	MAE (Mean Absolute Error)	0.58
4	Residual Pattern	No heteroscedasticity detected

Discussion: The results of this study demonstrate a statistically meaningful relationship between select physicochemical parameters—boiling point, vapor pressure, and melting point—and the acaricidal activity of organic compounds. The Pearson correlation analysis revealed that vapor pressure had the strongest inverse association with bioactivity ($r = –0.71$, $p < 0.01$), suggesting that compounds with lower volatility tend to exhibit higher biological efficacy against mites. This finding aligns with prior studies indicating that optimal persistence and reduced evaporation enhance pesticide contact time with arthropod targets.

Boiling point showed a moderate positive correlation ($r = 0.56$, $p < 0.05$), reinforcing the idea that compounds with higher thermal stability may remain active for longer periods under environmental conditions. Melting point, however, displayed only a weak and statistically insignificant correlation ($r = 0.29$, $p = 0.11$), indicating that this parameter may have limited influence on acaricidal function in isolation.

The multiple linear regression model further validated these relationships. With an R^2 value of 0.62 and statistically significant predictors (especially vapor pressure and boiling point), the model accounted for over 60% of the variability in acaricidal activity. The regression equation confirmed the dominant negative influence of vapor pressure ($\beta = –0.032$, $p < 0.01$) and the secondary positive contribution of boiling point ($\beta = 0.015$, $p < 0.05$).

Model validation through 5-fold cross-validation produced an RMSE of 0.72 and an MAE of 0.58, indicating acceptable predictive accuracy. The residual analysis confirmed that the assumptions of homoscedasticity and linearity were satisfied, thereby supporting the model's robustness.

Figure 1, a scatterplot of predicted versus observed activity scores, visually confirmed the model's accuracy, with most data points clustering closely around the regression line. This strong alignment indicates that the model's outputs are reliable and consistent across a wide range of compound types and activity levels.

The findings highlight the utility of vapor pressure and boiling point as key predictors in estimating acaricidal efficacy. These easily obtainable parameters can serve as valuable pre-screening tools, reducing the need for extensive biological testing and enabling a more rational approach to the development of effective, low-risk miticides.

Conclusion: This study establishes that selected physicochemical parameters—specifically boiling point, vapor pressure, and to a lesser extent, melting point—can serve as reliable predictors of acaricidal activity in organic compounds. Statistical analyses revealed that low vapor pressure and moderate-to-high boiling points are positively correlated with enhanced bioefficacy against mites. The multiple regression model developed in this work successfully explained 62% of the variability in acaricidal outcomes, and was validated through robust statistical metrics and cross-validation techniques.

The predictive accuracy of the model, combined with the practicality of using easily accessible physicochemical data, suggests that this approach can serve as a valuable pre-screening tool in acaricide development. By prioritizing compounds with favorable thermal and volatility

characteristics, researchers can reduce reliance on labor-intensive bioassays and accelerate the discovery of effective, environmentally sustainable miticides.

Future research should expand this model to include additional molecular descriptors and explore its applicability to a broader range of target species and compound classes.

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