



Integrated VOC-Based Early Prediction of *Aspergillus flavus* Infection and Aflatoxin B₁ Risk in Maize Kernels



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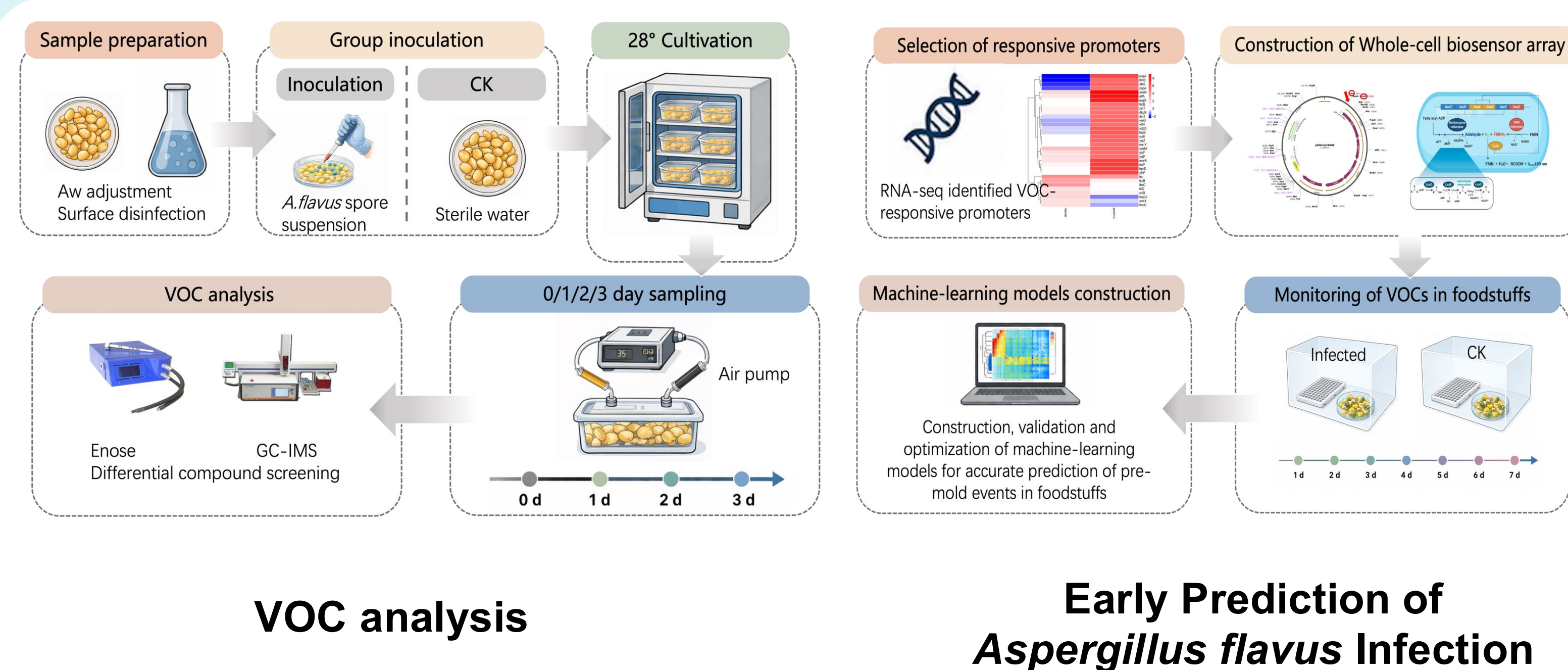
Introduction

- Aflatoxin B₁ (AFB₁), produced by *Aspergillus flavus*, is a potent carcinogen that contaminates maize and peanuts, posing serious health risks and economic losses.
- Early and accurate detection of AFB₁ is critical for food safety, yet conventional methods are often slow, invasive, and unsuitable for real-time monitoring.

Objectives

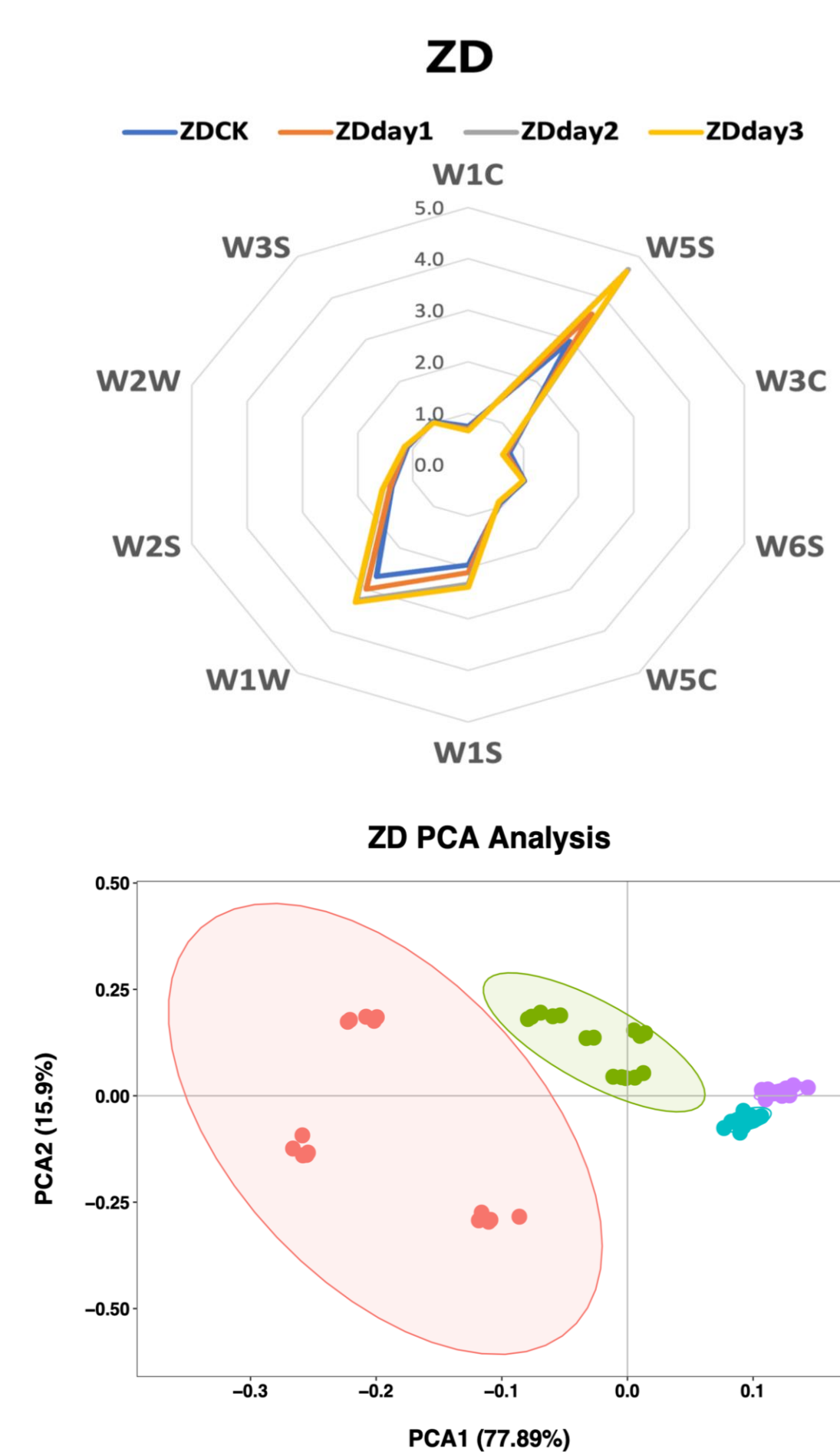
- To integrate electronic nose and GC-IMS VOC fingerprinting, transcriptome-guided whole-cell biosensors, and machine learning regression for non-invasive early prediction of *A. flavus* infection stage and AFB₁ risk in maize and peanut kernels.

Methods



Results and Expectation

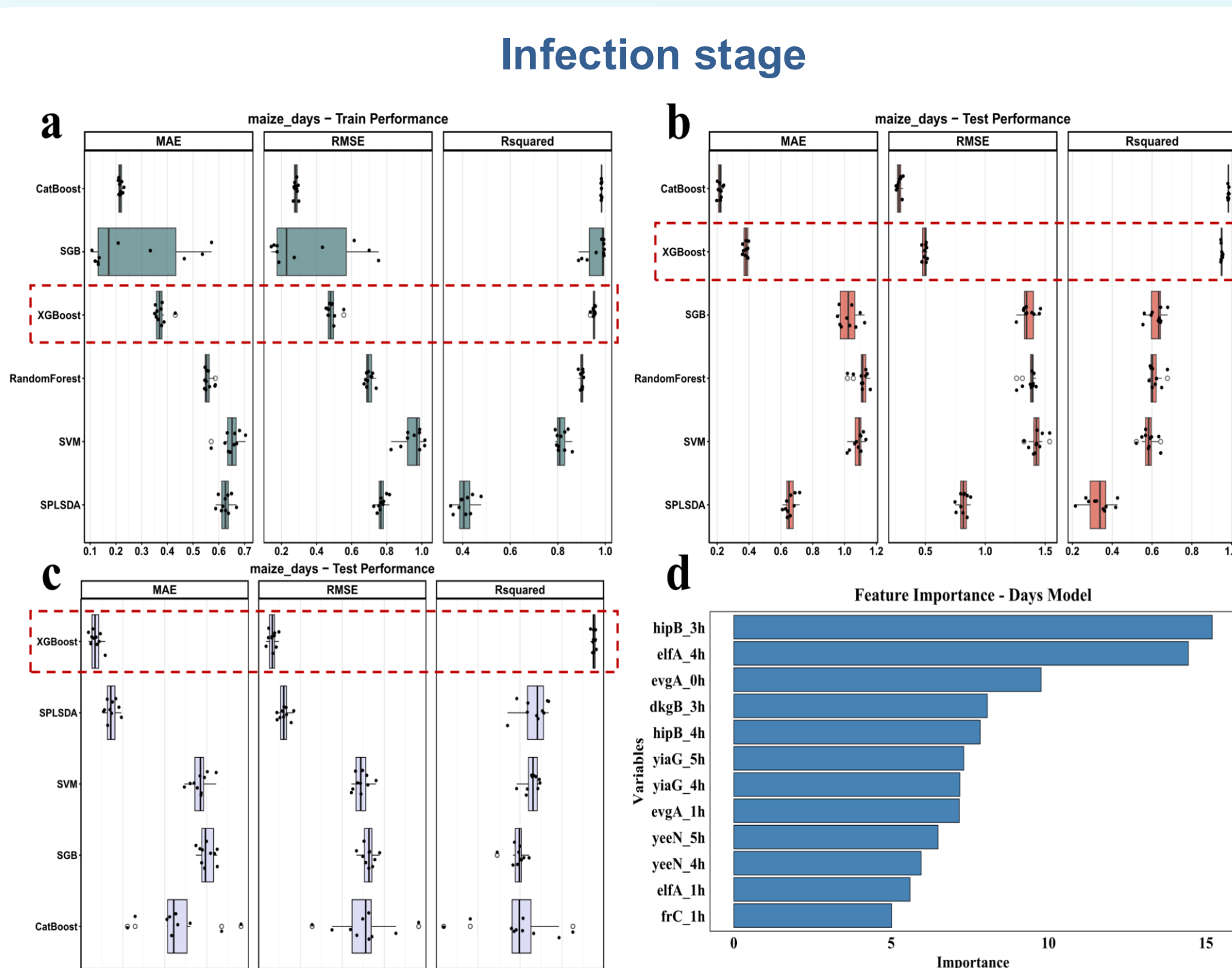
KEY RESULTS -E-NOSE



- E-nose rapidly distinguished infected from non-infected maize samples.
- The strongest sensor responses were observed in W5S (nitrogen oxide compounds) and W1W (terpenes compounds).
- PCA clearly separated control and infected samples in all three cultivars.

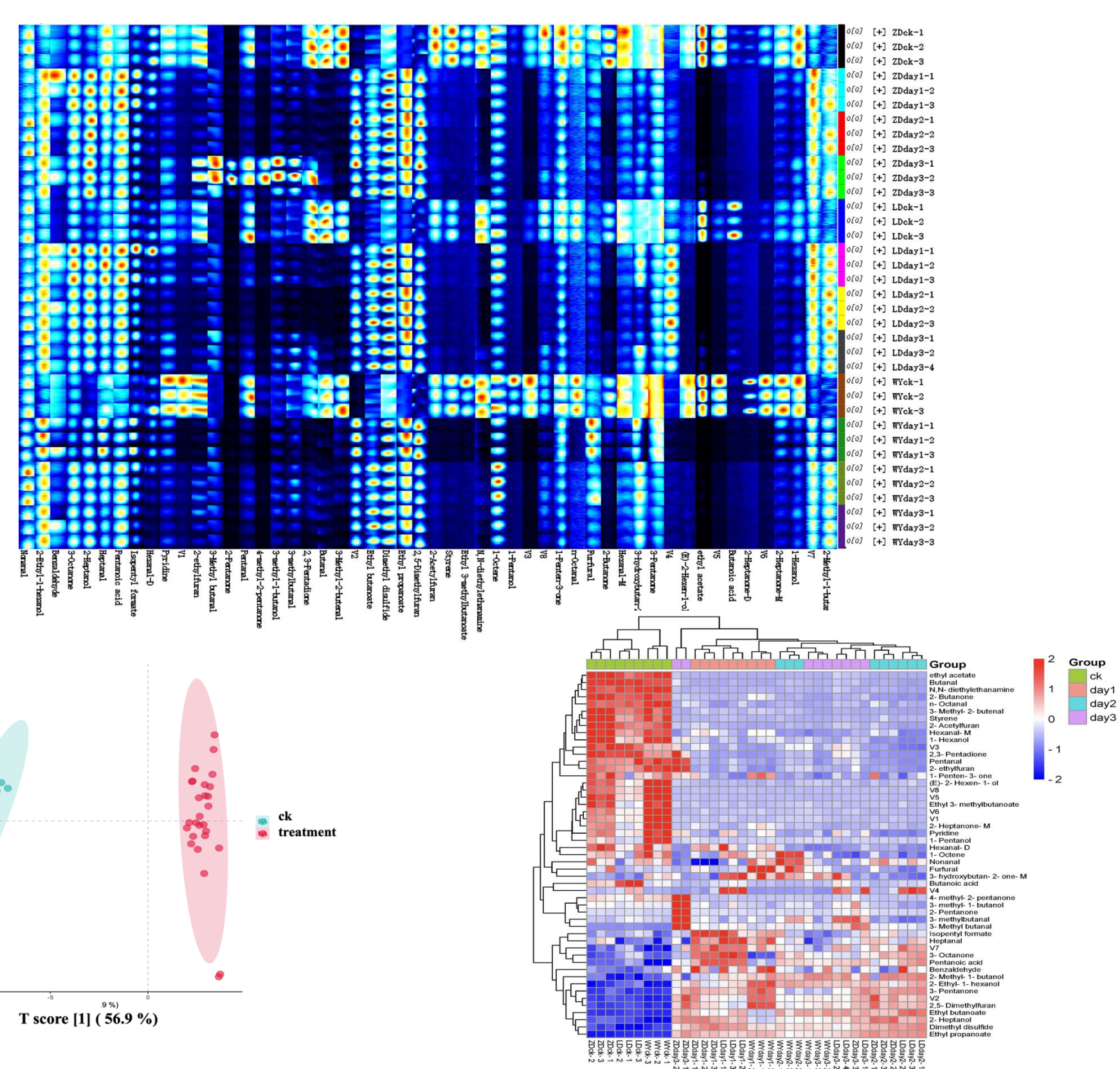
Radar plot of mean sensor responses (ZD cultivar shown as example)

XGBoost consistently achieved superior performance in internal validation, with R² values of 0.94, 0.98 for maize infection staging and AFB₁ quantification, respectively.

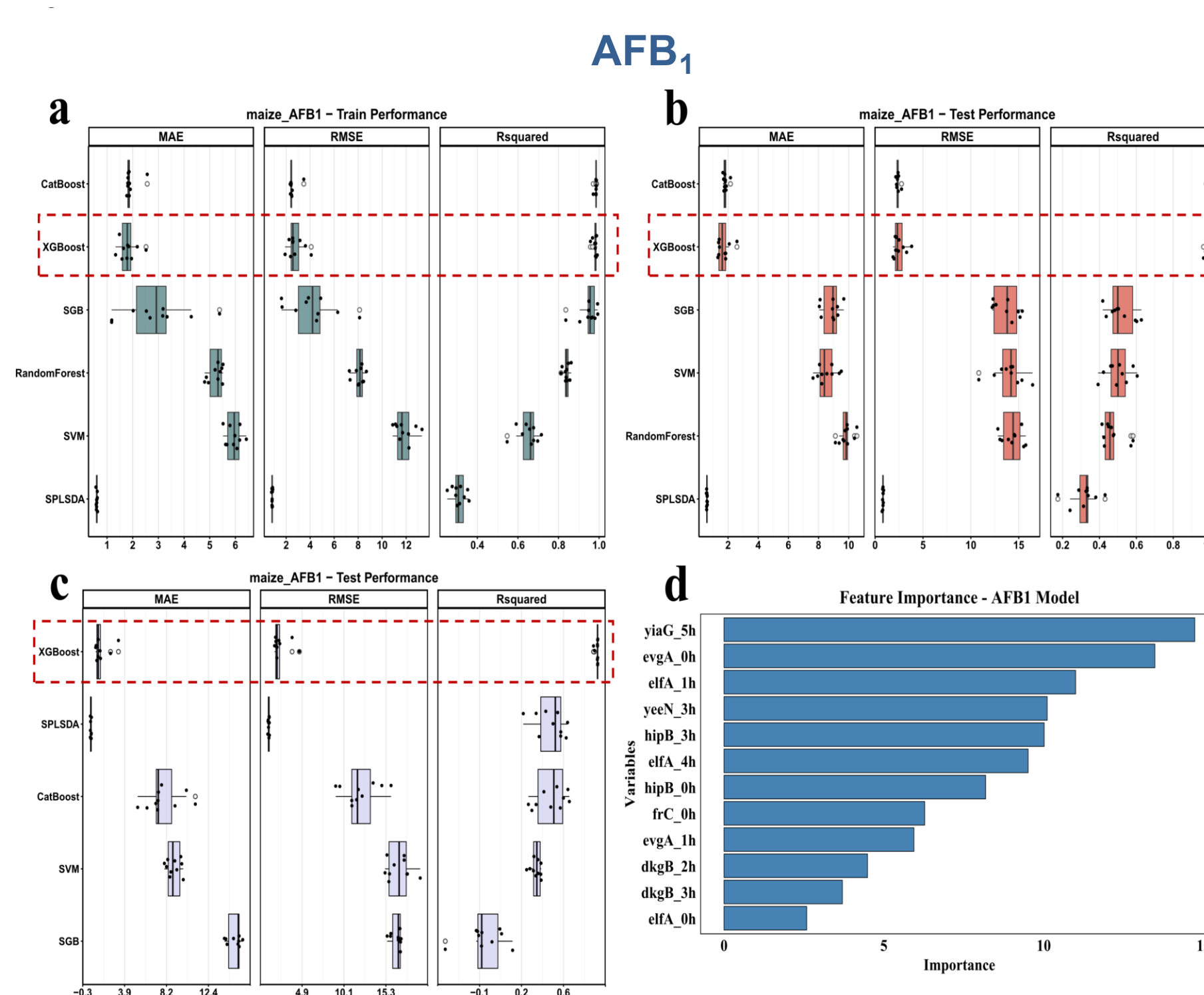


KEY RESULTS -GC-IMS

GC-IMS fingerprint heatmap



- GC-IMS tentatively identified 52 VOCs.
- Major compound classes included esters, alcohols, aldehydes, ketones, and terpenes.
- VOC fingerprints showed clear time-dependent shifts during 1-3 dpi.



The model also maintained strong generalization in external validation using independent *A. flavus* isolates, achieving R² values of 0.92 and 0.91.

Best model: XGBoost

	Infection stage prediction	AFB ₁ prediction
Maize	R ² = 0.94 (internal), 0.92 (external)	R ² = 0.98 (internal), 0.91 (external)

IV. Conclusion

Together, E-nose and GC-IMS offer a rapid, non-destructive strategy for early warning of asymptomatic fungal contamination in maize. Clearly differentiated control and infected samples.

This biosensor-ML platform enables real-time, non-invasive, and quantitative prediction of AFB₁, offering a scalable and cost-effective tool for early aflatoxin risk assessment in post-harvest crops.

