

# Predicting Biochar-Mediated Cadmium Immobilization in Agricultural Soils Using *Explainable Machine Learning*: A Circular Approach to Food Safety

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## 01 · BACKGROUND

Cadmium (Cd) contamination in agricultural soils poses critical risks to food safety. Biochar from organic waste has emerged as a promising amendment for heavy metal immobilization, supporting circular waste valorization while improving soil quality in contaminated agroecosystems.

### Research Gap

Predicting biochar effectiveness is complex due to non-linear interactions among soil physicochemical properties, amendment characteristics, and plant dynamics. Explainable ML models are essential to guide practical decisions in contaminated agricultural systems.

### Objectives

- Evaluate cocoa-husk biochar for reducing Cd bioavailability in soils with *Phaseolus vulgaris*
- Monitor soil dynamics (pH, EC, CEC, TC, TN) over 44 days
- Build an explainable ML framework for Cd prediction
- Quantify driver contributions via SHAP permutation analysis

## 02 · EXPERIMENTAL DESIGN

A Biochar act. + Phosphorus

B Biochar act. + Phosphate

C Soil + Phosphorus

D Soil + Phosphate

E Control (unamended)

5 treatments · 44-day monitoring · biweekly sampling · *Lolium multiflorum* as phytoremediator

## 03 · ML PIPELINE

01 Feature engineering — Day, Treatment, OM%

02 Grouped cross-validation by replicate

03 MLP Regressor — pH & EC (128→64→32)

04 SHAP permutation importance analysis

Python 3, scikit-learn, SHAP

MLP Regressor, pandas

### WHY pH & EC AS OUTPUTS?

Alkaline pH (pH>7) promotes Cd-carbonate and Cd-phosphate precipitation, drastically reducing plant-available fractions. EC integrates ionic strength, nutrient release, and amendment dissolution — together the two most diagnostic real-time indicators of biochar-driven Cd immobilization.

## 04 · SOIL PHYSICOCHEMICAL DYNAMICS (44 DAYS)

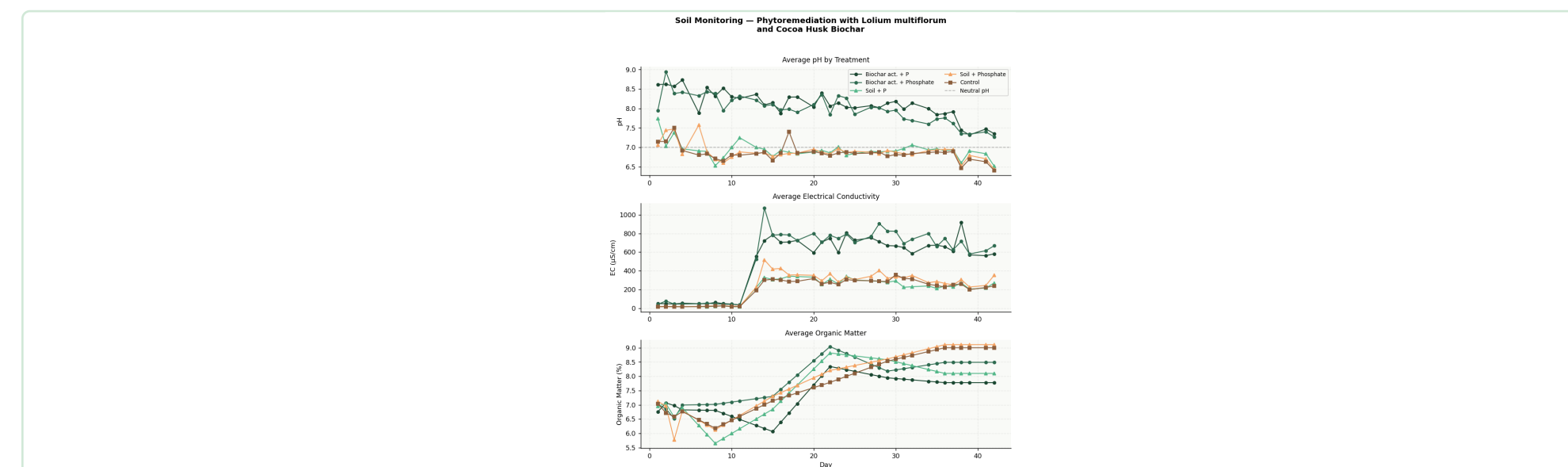


Fig. 1 — Average pH, EC, and organic matter across five treatments over 44 days. Biochar-amended treatments (A & B) consistently maintained alkaline pH (>8.0) and elevated EC, sustaining conditions highly favorable for complete Cd immobilization throughout the entire experimental period.

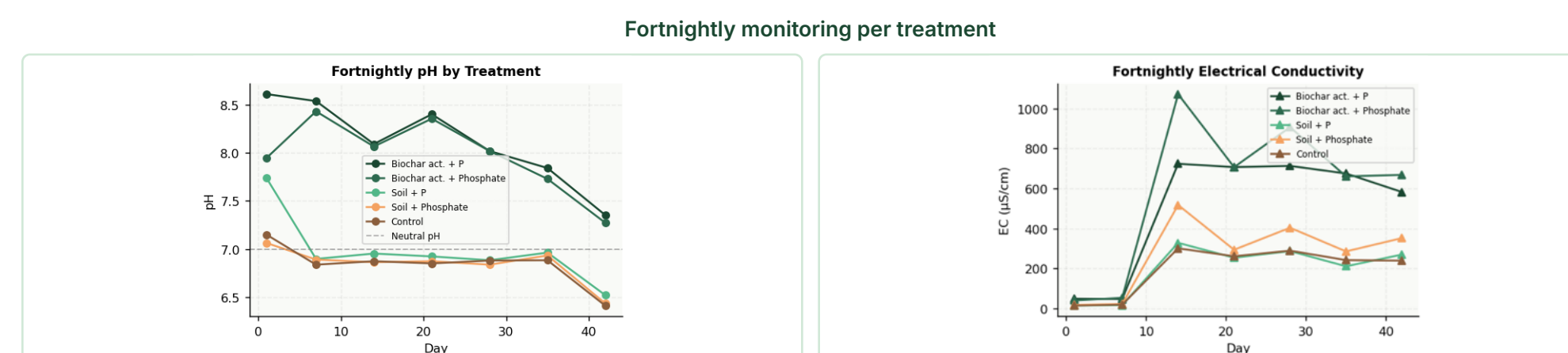


Fig. 2 — Fortnightly pH. Treatments A & B sustained alkaline conditions (pH>8) critical for Cd precipitation and reduced plant uptake risk across all 44 days.

## 05 · ANN MODEL RESULTS

0.834  
R<sup>2</sup> — pH

0.908  
R<sup>2</sup> — EC

0.290  
RMSE pH

81.7  
RMSE EC MS/CM

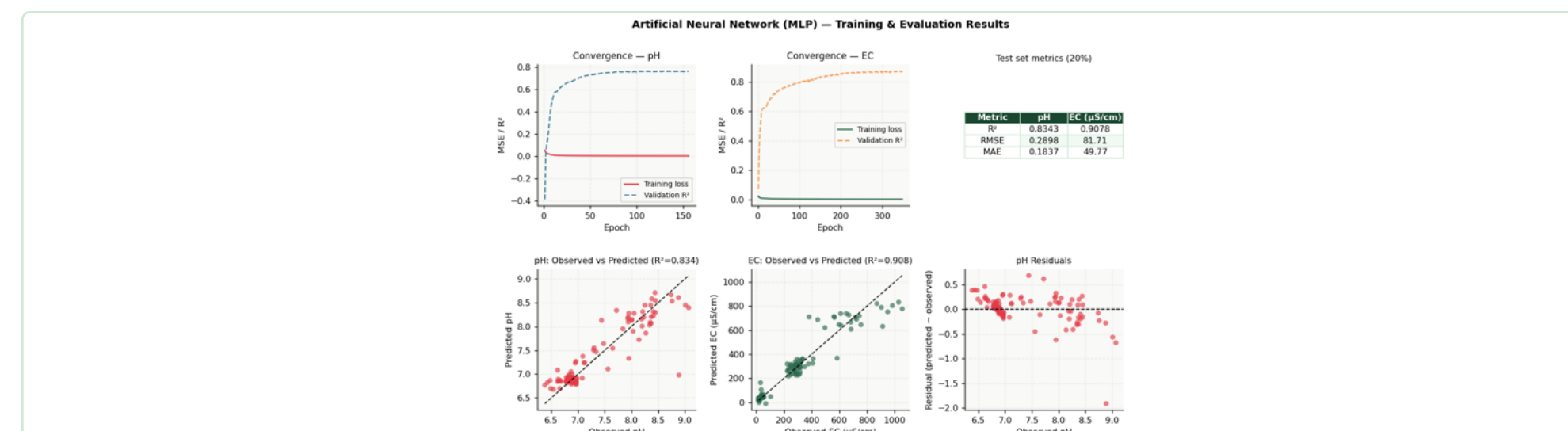


Fig. 4 — Training convergence and observed vs. predicted for pH ( $R^2=0.834$ ) and EC ( $R^2=0.908$ ). Residual analysis confirms well-calibrated, unbiased predictions across the full experimental range.

## 06 · PREDICTIONS BY TREATMENT & SHAP IMPORTANCE

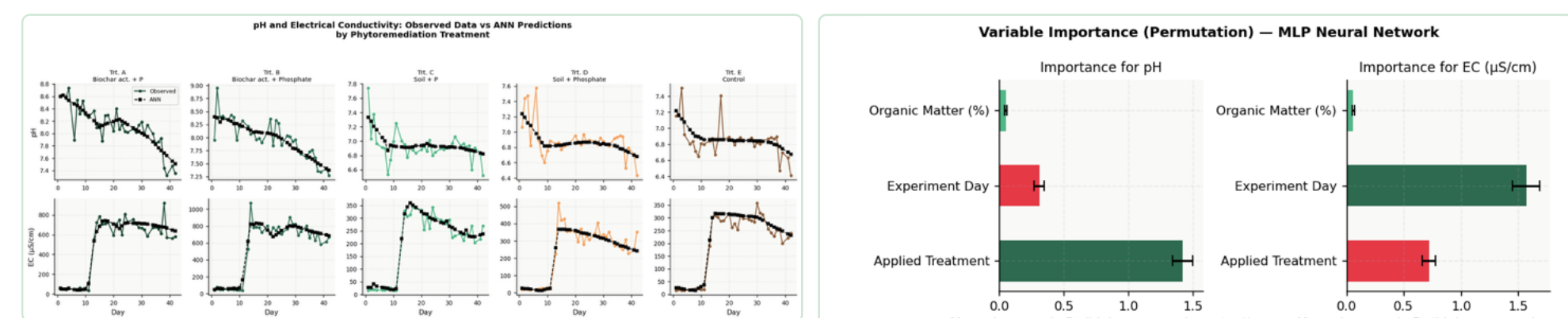


Fig. 5 — Observed vs. ANN predictions for pH (top) and EC (bottom) by treatment. Strong temporal generalization across all amendment scenarios.

Fig. 6 — SHAP importance. Treatment type dominates pH ( $\Delta R^2=1.4$ ); experiment day controls EC ( $\Delta R^2=1.6$ ). Amendment composition governs baseline; time drives ion mobility.

## 07 · KEY QUANTITATIVE FINDINGS

0%

Cd Bioavailability in Soil

undetectable throughout all 44 days — every treatment

~90%

Cd Removed via Plant Tissue

accumulated in *L. multiflorum* above-ground biomass

~10%

Cd Retained in Soil

immobilized by biochar after full phytoextraction cycle

## 08 · PLANT BIOMASS RESPONSE

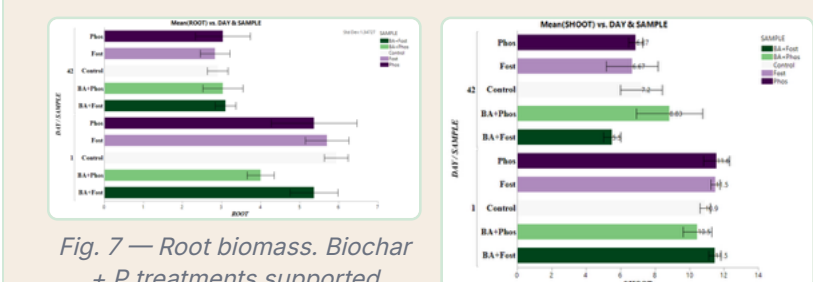


Fig. 7 — Root biomass. Biochar + P treatments supported greatest root development, consistent with improved soil fertility and reduced Cd phytotoxicity.

Fig. 8 — Shoot biomass. Reduced Cd phytotoxicity translated into improved above-ground production and higher phytoextraction capacity per harvest cycle.

### CRITICAL RESULT — CD BIOAVAILABILITY

Soil Cd bioavailability was zero across all treatments throughout all 44 days. Even without biochar (C-E), plant uptake and soil buffering prevented measurable soluble Cd in soil solution — a paramount finding for food safety risk assessment.

### MLP ARCHITECTURE: 128 → 64 → 32

Three hidden layers with ReLU activations, trained up to 348 epochs. Inputs: experimental day, treatment code, and interpolated organic matter (%). Validated on 20% holdout (108 samples) using grouped k-fold CV stratified by replicate to prevent data leakage.

## 09 · CONCLUSIONS

- Zero soil Cd bioavailability**  
Biochar completely immobilized soil Cd across all 44 days, eliminating soluble cadmium risk regardless of amendment type applied.
- Dominant shoot phytoextraction**  
*L. multiflorum* accumulated ~90% of total Cd in above-ground biomass, offering a harvestable circular remediation pathway for contaminated soils.
- High-accuracy ML model**  
MLP achieved  $R^2>0.83$  for pH and  $R^2>0.90$  for EC without empirical parameterization, generalizing robustly across all replicates.
- SHAP-guided optimization**  
Treatment type governs pH; temporal dynamics drive EC — enabling interpretable, site-specific optimization of biochar application and dosing.
- Scalable circular economy framework**  
Waste-derived biochar coupled with explainable AI delivers a replicable decision-support tool that simultaneously advances soil health, food safety, and organic waste valorization at the agroecosystem scale.

## 10 · CIRCULAR ECONOMY PATHWAY

- Cocoa husk organic waste
- Activated biochar production
- Soil Cd immobilization (0% bioavailability)
- ~90% Cd uptake in harvestable biomass
- Safer food crops · Restored soil quality

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## REFERENCE

Serrano, M. F. et al. (2023). Phosphorus-Loaded Biochar-Assisted Phytoremediation to Immobilize Cd, Cr, and Pb in Soils. *ACS Omega*. <https://doi.org/10.1021/ACSOMEGA.3C07433>