

# Data-Driven Inverse Design of Electrospun Biomaterials with Controlled Fibre-Diameter Distributions for Tissue Regeneration

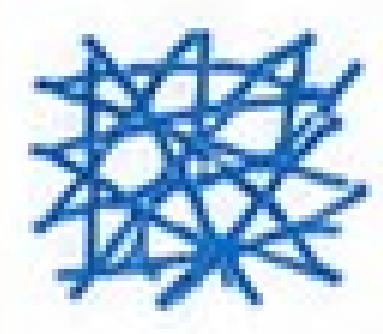
## SpinCastML: an open inverse-design framework for electrospinning

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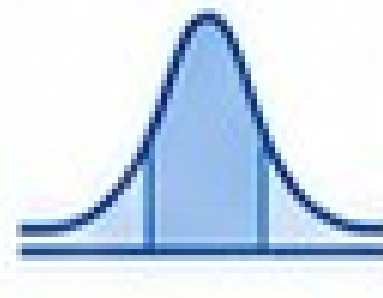
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### 1 INTRODUCTION / RESEARCH OBJECTIVE



Electrospinning can produce biomimetic fibrous scaffolds for tissue regeneration, but design is still largely based on trial-and-error because fibre diameter depends on strongly coupled polymer, solvent, and process variables.



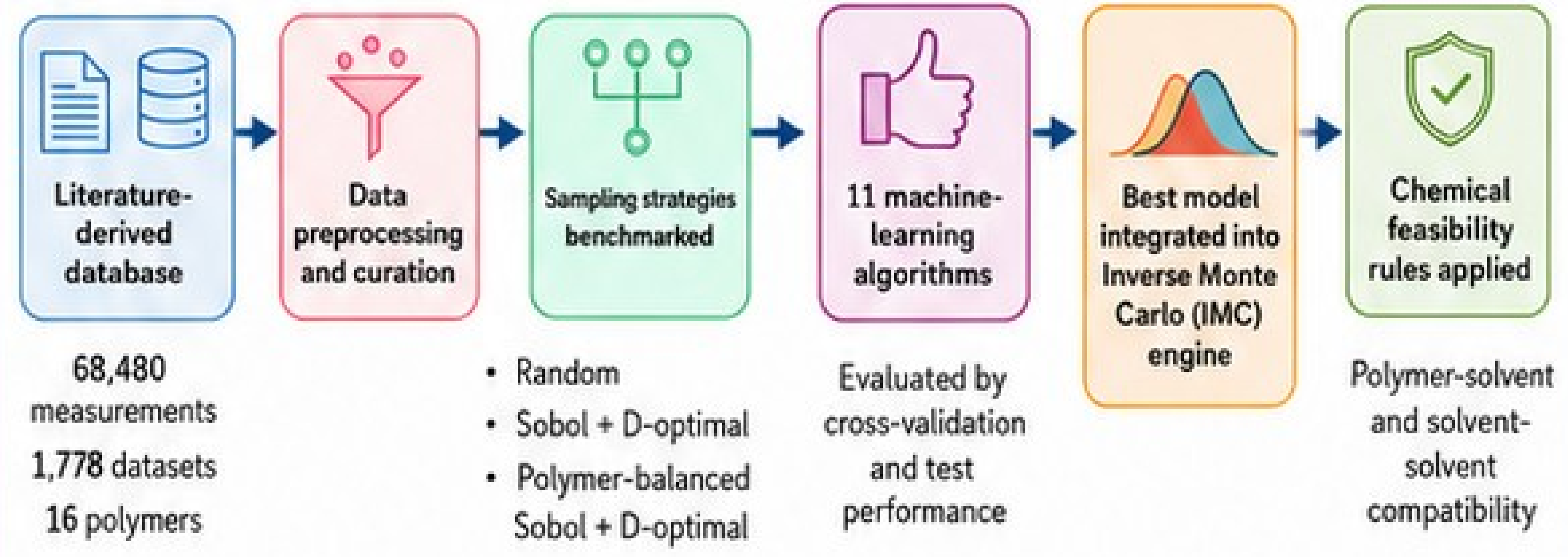
For regenerative biomaterials, controlling the full fibre-diameter distribution is more informative than predicting only a single mean diameter.



**Objective:** develop SpinCastML, an open data-driven and chemically constrained inverse-design framework that predicts and back-calculates feasible electrospinning conditions to achieve target fibre-diameter distributions.

From trial-and-error to probabilistic inverse design

### 2 METHODOLOGY



### 3 MAIN RESULTS

KEY DATA AT A GLANCE

68,480 measurements

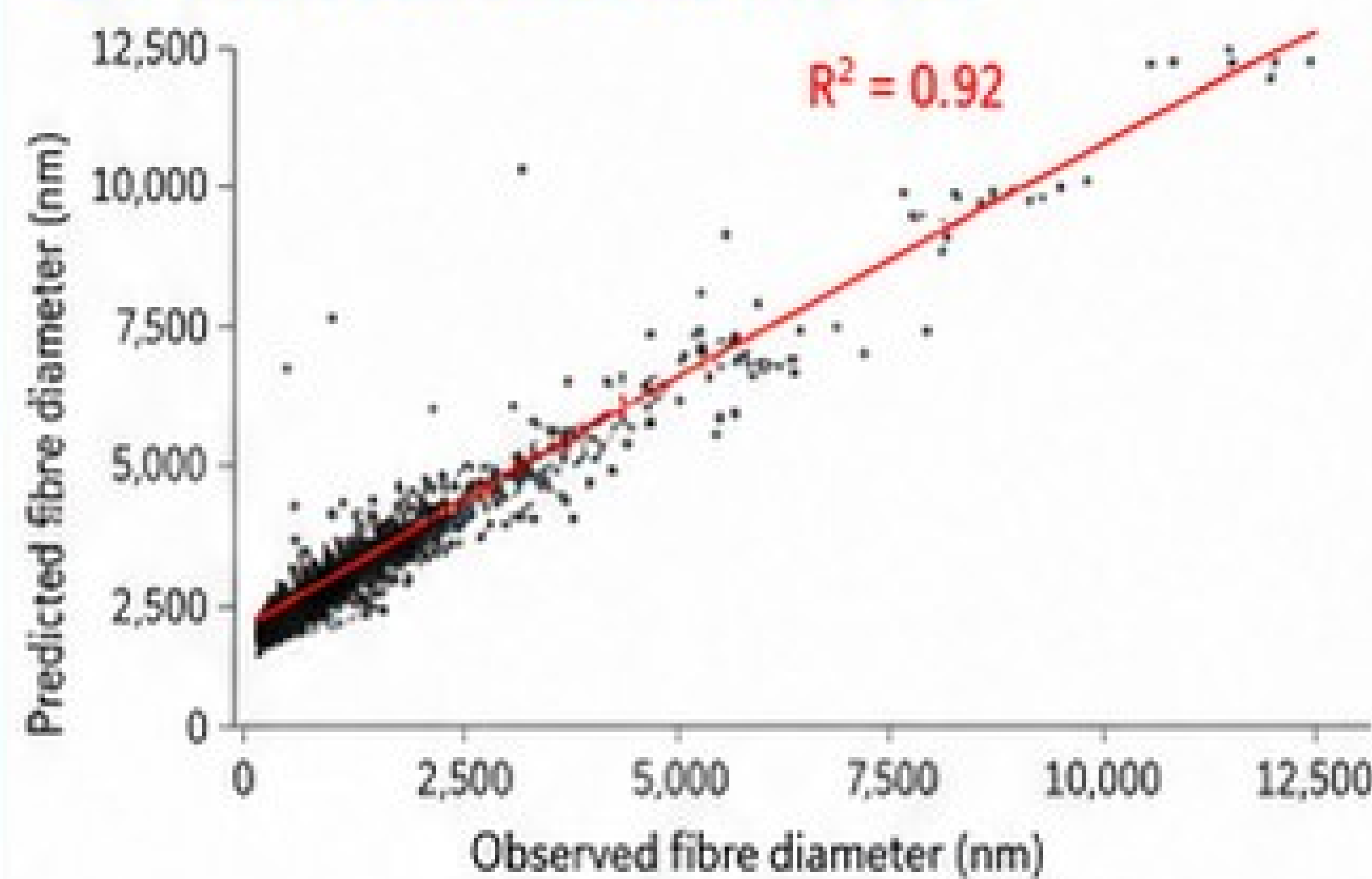
1,778 datasets

16 polymers

11 ML models

Best-performing approach: **Balanced sampling + Cubist**

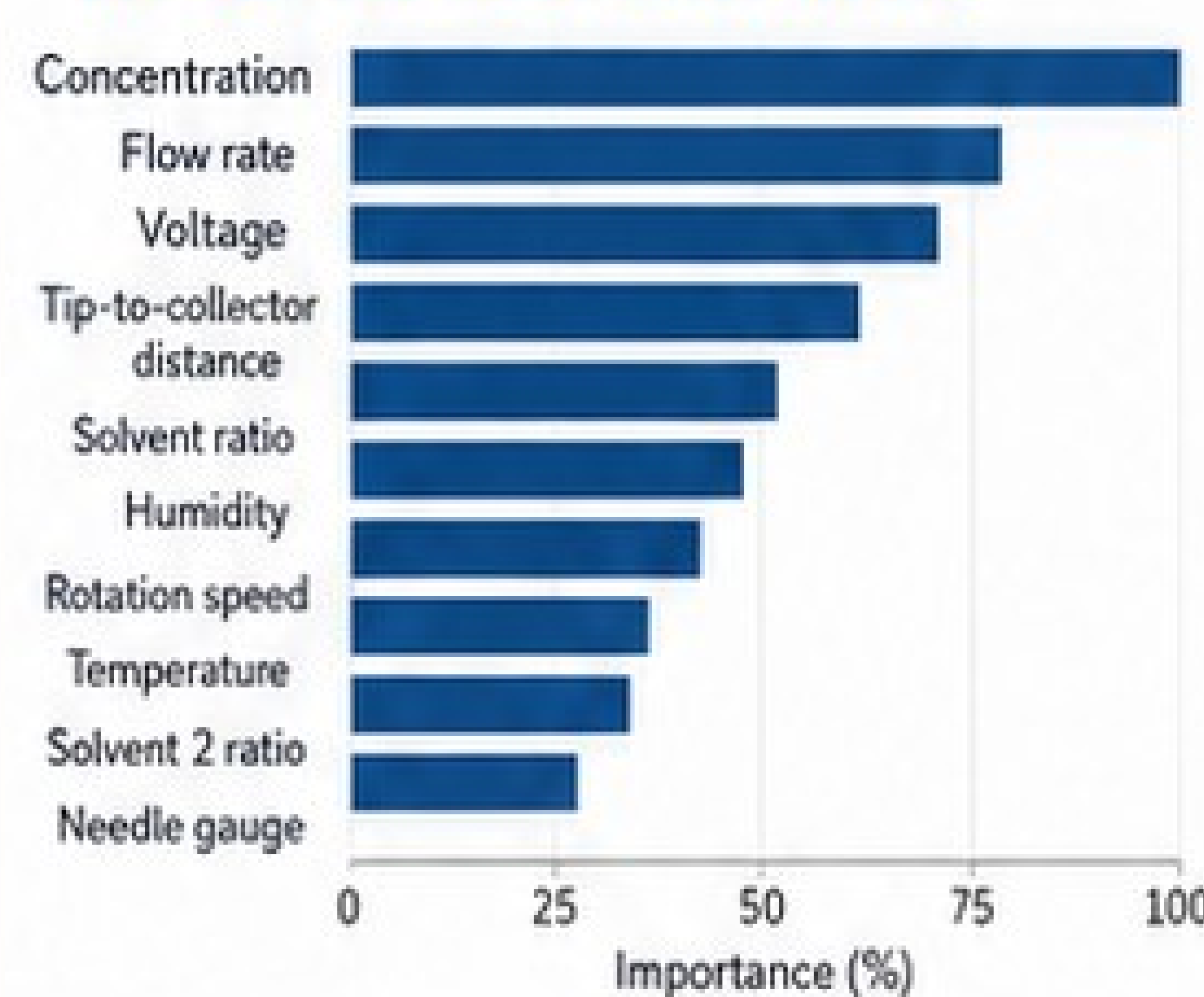
#### 3A. MODEL PERFORMANCE (TEST SET)



$R^2 = 0.92$  | RMSE = 260 nm | MAE = 50 nm

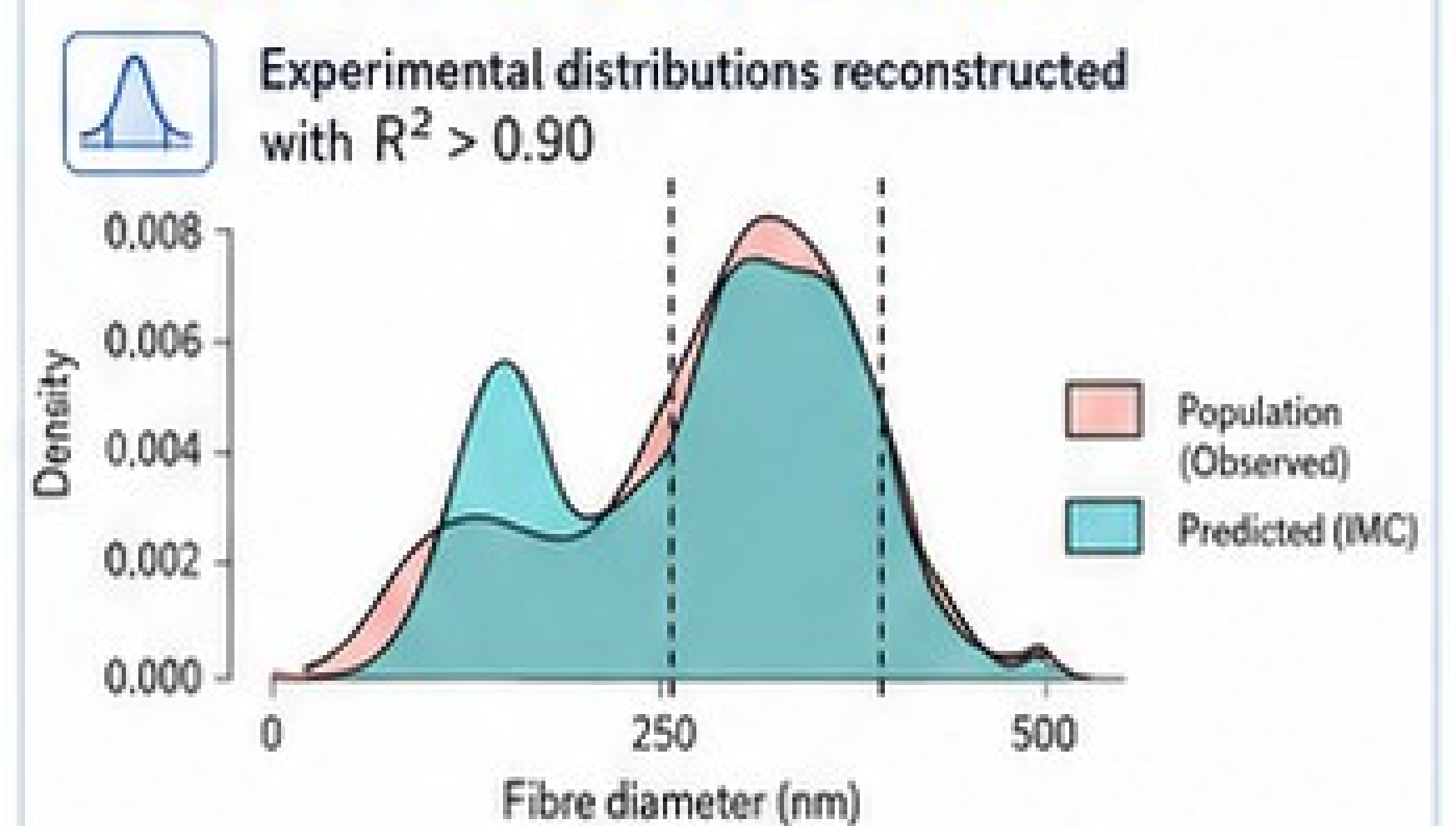
Strong agreement between predicted and observed fibre diameters across the dataset.

#### 3B. FEATURE IMPORTANCE (CUBIST)



Concentration emerged as the dominant predictor, followed by flow rate and voltage.

#### 3C. DISTRIBUTION & SUCCESS PREDICTIONS



Success rates predicted with <1% absolute error across independent systems. Modelled success probabilities align closely with experimental outcomes.

### 4 PROSPECTIVE CASE STUDY / EXPERIMENTAL VALIDATION (PVA)

- Target:  $250 \pm 50$  nm
- IMC generated 20 chemically feasible PVA candidate families.
- Selected formulation:  
12% w/w PVA in water; 22 G needle; 25 kV;  $0.3 \text{ mL h}^{-1}$ ; 10 cm;  $20^\circ \text{C}$ ; 45% RH

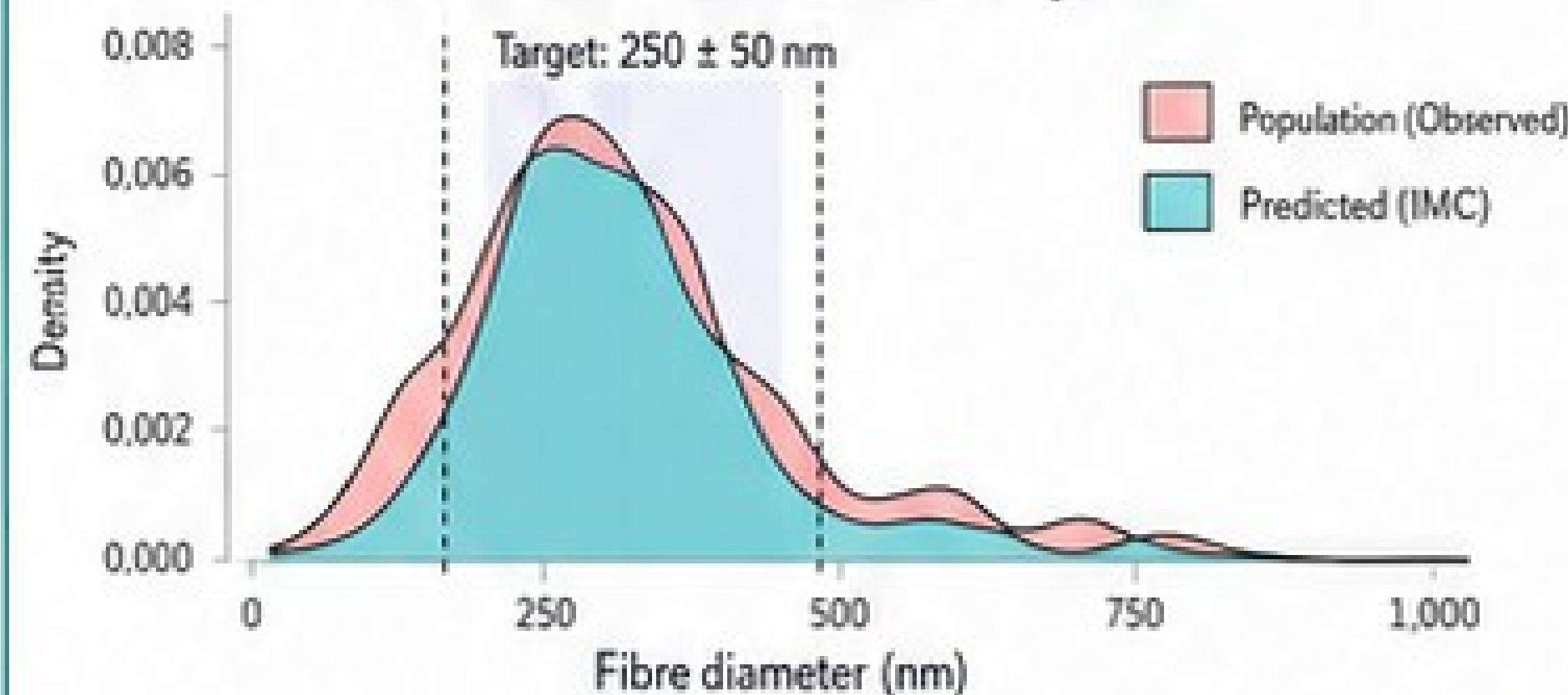
Predicted distribution:  
 $256.94 \pm 121.07$  nm

Observed population distribution:  
 $258.85 \pm 125.72$  nm

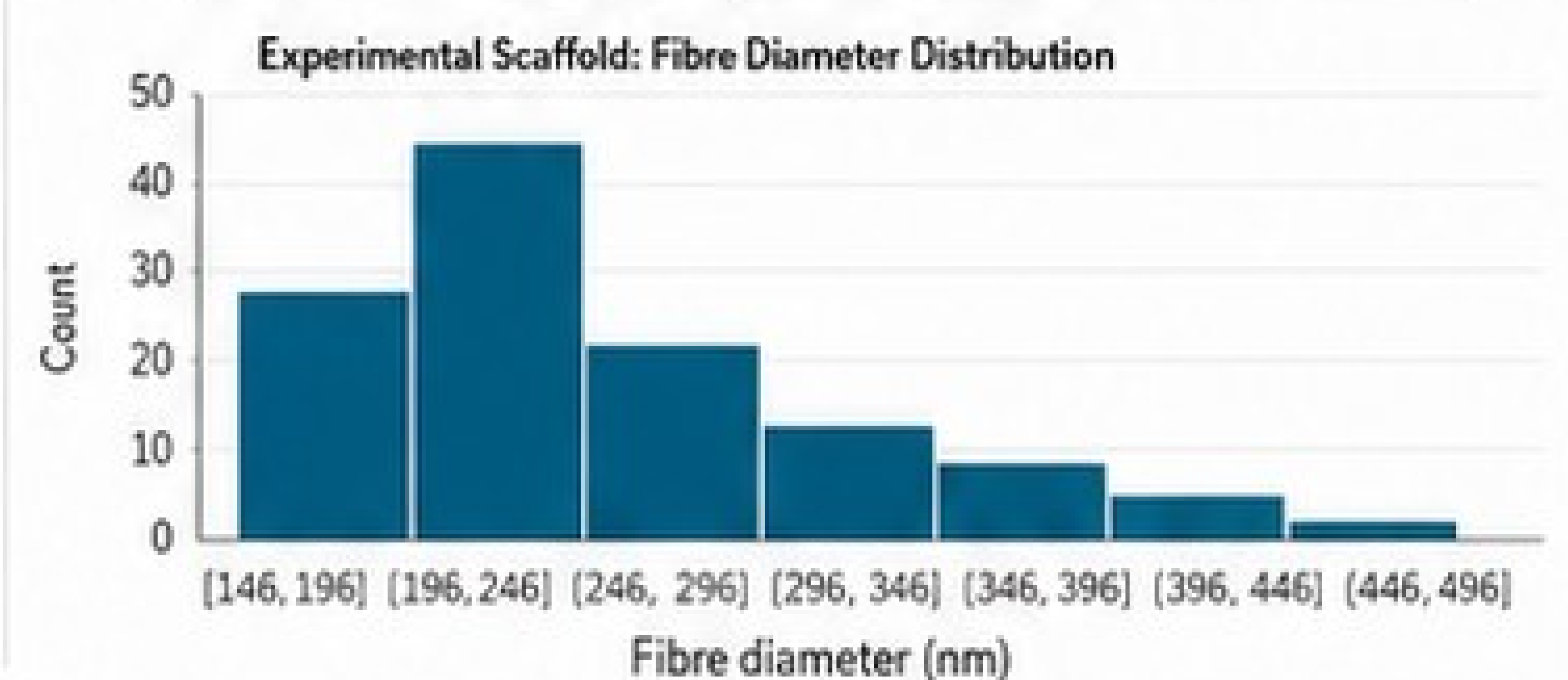
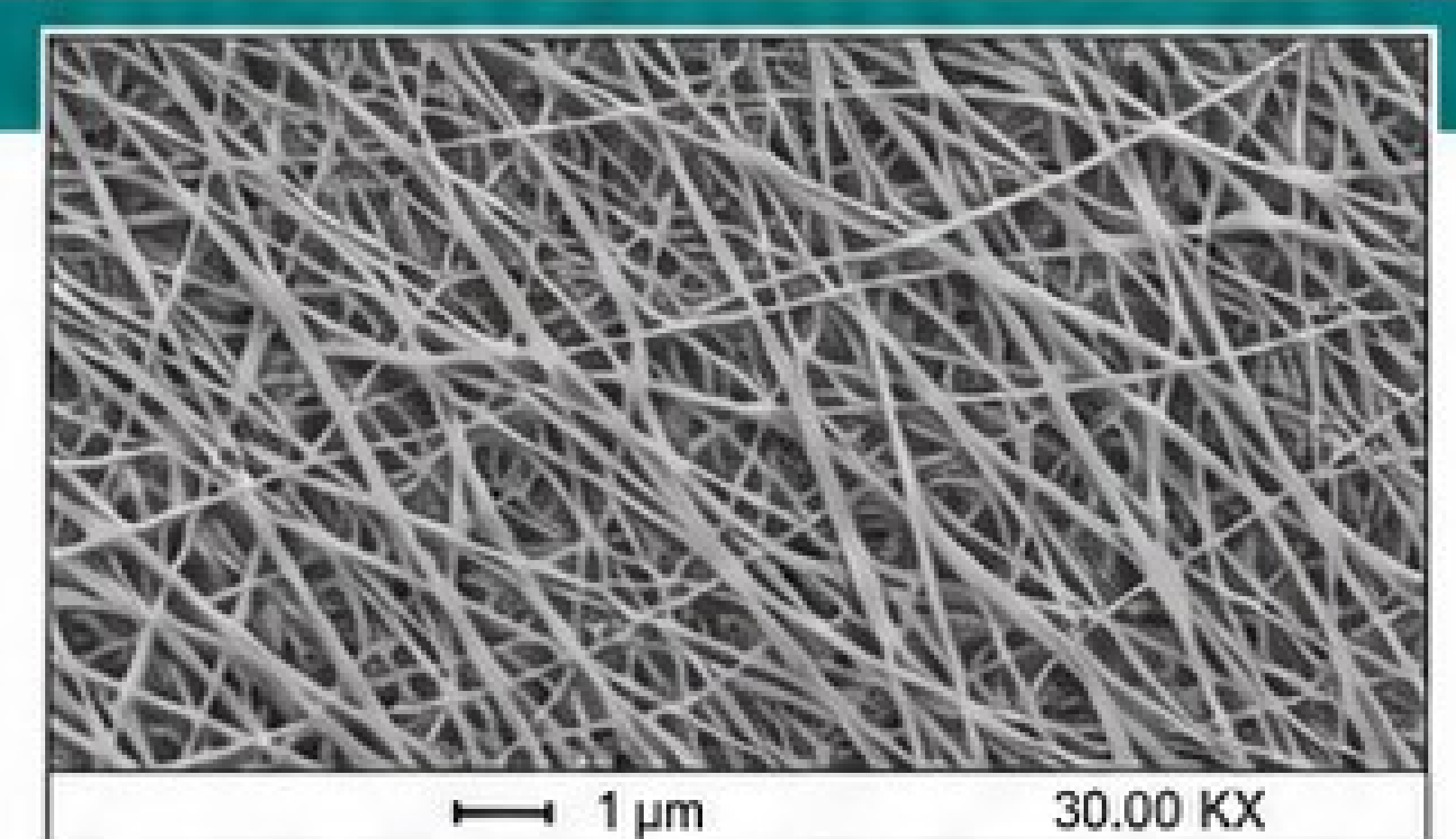
Experimental scaffold:  
 $243.59 \pm 70.39$  nm

The experimentally produced scaffold fell within the target window, confirming the practical feasibility of the inverse-design workflow.

#### PVA Validation: Distribution Comparison



Summary of PVA Validation Results	
Metric	Value (mean $\pm$ SD)
Target window	$250 \pm 50$ nm
Predicted distribution (IMC)	$256.94 \pm 121.07$ nm
Observed population distribution	$258.85 \pm 125.72$ nm
Experimental scaffold	$243.59 \pm 70.39$ nm



### 5 IMPACT / CONCLUSIONS

- SpinCastML reframes electrospinning as a distribution-aware, probabilistic inverse-design problem.
- It returns families of chemically feasible solutions with quantified success probabilities rather than a single fragile optimum.
- The framework can reduce trial-and-error experimentation, improve reproducibility, and support more sustainable biomaterial manufacturing.
- This approach can accelerate the design of electrospun biomaterials for tissue regeneration.

A new paradigm for data-driven design of electrospun regenerative biomaterials.

### 6 TRY SPINCASTML – OPEN APPLICATION



Scan to access the SpinCastML application on Zenodo

DOI: <https://doi.org/10.5281/zenodo.18557969>