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SUPPLEMENTARY INFORMATION

Predicting Inflammatory Response of Biomimetic Nanofibre Scaffolds for Tissue Regeneration Using Machine Learning and Graph Theory

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STable 1. Physico-chemical characteristics (pore diameter, fibre diameter, water contact angle, and Young's modulus) of scaffolds, levels of TNF-α measured after 24 hours, ruffling index, and main phenotypes observed of macrophages.

Nanoscaffolds	Pore diameter /(µm)	Fibre diameter/ (µm)	Water contact angle/ (°)	Young's modulus/ (MPa)	Concentration of TNF-α/(pg/ml)	Ruffling index	Phenotype
Polyhydroxybutyrate (PHB)/kappa-carrageenan (KCG)							
100/0	1.9 ± 0.7	1.3 ± 0.4	126 ± 1	518.2 ± 36.5	803.9 ± 56.4	2.8 ± 0.1	M1
90/10	1.2 ± 0.6	0.9 ± 0.5	120 ± 1.9	271.7 ± 58.9	1123.7 ± 36.9	1.9 ± 0.3	M1
80/20	0.9 ± 0.3	0.7 ± 0.5	107 ± 1.3	160.5 ± 32.8	947.0 ± 141.7	2.1 ± 0.2	M1
70/30	1.1 ± 0.5	0.7 ± 0.5	104 ± 0.9	90.6 ± 10.9	631.2 ± 151.2	2.6 ± 0.2	M1
Poly(hydroxybutyrate-*co*-valerate (PHBV)/KCG							
100/0	0.8 ± 0.3	0.4 ± 0.1	112 ± 1	197.2 ± 44.6	784.6 ± 58.8	2.6 ± 0.1	M1
90/10	1.0 ± 0.5	0.7 ± 0.2	73.6 ± 2.8	160 ± 14.8	1345.5 ± 63.6	0.2 ± 0.1	M1
80/20	0.9 ± 0.3	0.6 ± 0.2	62.4 ± 0.5	111.7 ± 22.2	1293.0 ± 67.8	0.2 ± 0.1	M1
70/30	1.0 ± 0.5	0.5 ± 0.2	57.8 ± 1.7	108.5± 6.8	865.6 ± 35.3	0.2 ± 0.1	M0
Polydioxanone (PDX)/fucoidan (FUC)							
100/0	0.2 ± 0.06	0.3 ± 0.1	32.1 ± 0.0	73.8 ± 7.6	261.1 ± 57.9	2.9 ± 0.1	M1
90/10	0.2 ± 0.08	0.2 ± 0.07	32.1 ± 0.0	69.6 ± 8.4	854.5 ± 47.9	1.7 ± 0.1	M1
80/20	0.2 ± 0.1	0.2 ± 0.05	32.1 ± 0.0	38.1 ± 3.9	644.8 ± 67.5	0.9 ± 0.1	M1
70/30	0.2 ± 0.1	0.2 ±0.05	32.1 ± 0.0	35 ± 11.3	1079.6 ± 2.1	1.2 ± 0.2	M1
PDX/KCG							
100/0	2.0 ± 0.7	1.1 ± 0.3	32.1 ± 0.0	73.8 ± 7.6	537.0 ± 125.2	2.5 ± 0.1	M1
90/10	1.6 ± 0.5	1.0 ± 0.2	32.1 ± 0.0	72 ± 6.5	376.7 ± 76.6	3.0 ± 0.0	M1
80/20	1.5 ± 0.6	0.9 ± 0.2	32.1 ± 0.0	42.6 ±6.3	258.9 ± 49.9	1.2 ± 0.5	M0
70/30	0.9 ± 0.3	0.5 ± 0.2	32.1 ± 0.0	38.2 ± 5.5	504.5 ± 62.1	0.3 ± 0.2	M0

PDX/PHBV							
100/0	1.1 ± 0.4	0.4 ± 0.1	32.1 ± 0.0	73.8 ± 7.6	196.5 ± 16.7	1.6 ± 0.3	M1
90/10	1.7 ± 0.6	1.0 ± 0.3	32.1 ± 0.0	95.6 ± 11.6	722.3 ± 37.3	1.6 ± 0.7	M1
80/20	1.2± 0.4	0.7 ± 0.3	105.1 ± 2.2	72.9 ± 6.9	1210.5 ± 61.8	0.2 ± 0.1	M1
70/30	1.2 ± 0.5	0.6 ± 0.2	119.6 ± 2.5	100.4 ± 18.3	675.2 ± 63.8	2.4 ± 0.2	M0
PDX/polysucrose (PSuc)							
100/0	8.9 ± 5.4	1.0 ± 0.04	32.1 ± 0.0	51.8 ± 10.3	219.4 ± 49.7	2.9 ± 0.1	M0
90/10	6.2 ± 4.2	0.8 ± 0.1	32.1 ± 0.0	43.0 ± 10.4	296.1 ± 90.0	3.0 ± 0.1	M1
80/20	5.1 ± 2.8	0.8 ± 0.03	32.1 ± 0.0	31.5 ± 5.2	230.1 ± 88.1	2.8 ± 0.1	M1
70/30	4.1 ± 3.2	0.7 ± 0.06	32.1 ± 0.0	83.2 ± 23.9	202.6 ± 41.6	2.9 ± 0.0	M1
60/40	3.6 ± 2.3	0.7 ± 0.03	32.1 ± 0.0	58.2 ± 27.5	151.2 ± 11.8	3.0 ± 0.0	M1
50/50	3.4 ± 2.5	0.6 ± 0.04	32.1 ± 0.0	33.0 ± 2.0	226.9 ± 57.9	2.9 ± 0.0	M1
Poly-L-lactide(PLLA)/ PSuc							
100/0	5.7 ± 3.3	1.0 ± 0.05	141.3 ± 2.0	235 ± 15	163.7 ± 29.9	2.0 ± 0.0	M2
90/10	4.2 ± 2.5	0.9 ± 0.1	135.1 ± 1.6	109 ± 8.7	149.0 ± 24.8	2.8 ± 0.0	M2
80/20	3.9 ± 2.4	0.8 ± 0.03	134.0 ± 0.7	114.3 ± 4.0	168.7 ± 36.3	2.4 ± 0.1	M1
70/30	2.9 ± 2.0	0.7 ± 0.04	126.3 ± 4.7	85.7 ± 5.9	173.1 ± 15.9	2.4 ± 0..3	M1
60/40	2.01 ± 0.8	0.7 ± 0.01	132.9 ± 1.1	90.7 ± 5.5	245.6 ± 55.6	2.4 ± 0.7	M1
50/50	2.4 ± 1.5	0.6 ± 0.02	81.6 ± 9.5	99.3 ± 31.6	240.3 ± 61.0	1.3 ± 0.1	M1
PLLA/cellulose acetate (CA)							
0/100	0.83 ± 0.3	0.7 ± 0.08	134.4 ± 1.8	90.4 ± 15.3	180.9 ± 26.9	0.4 ± 0.0	M1
100/0	5.7 ± 3.3	1.0 ± 0.3	140.7 ± 1.8	235.4 ± 14.8	163.7 ± 29.9	2.0 ± 0.0	M1
30/70	3.5 ± 1.1	0.6 ± 0.2	119.5 ± 0.9	58.9 ± 3.3	140.7 ± 12.8	1.0 ± 0.0	M1
50/50	2.0 ± 0.6	0.5 ± 0.2	117.3 ± 1.3	104.4 ± 13.8	170.7 ± 3.3	1.8 ± 0.0	M1

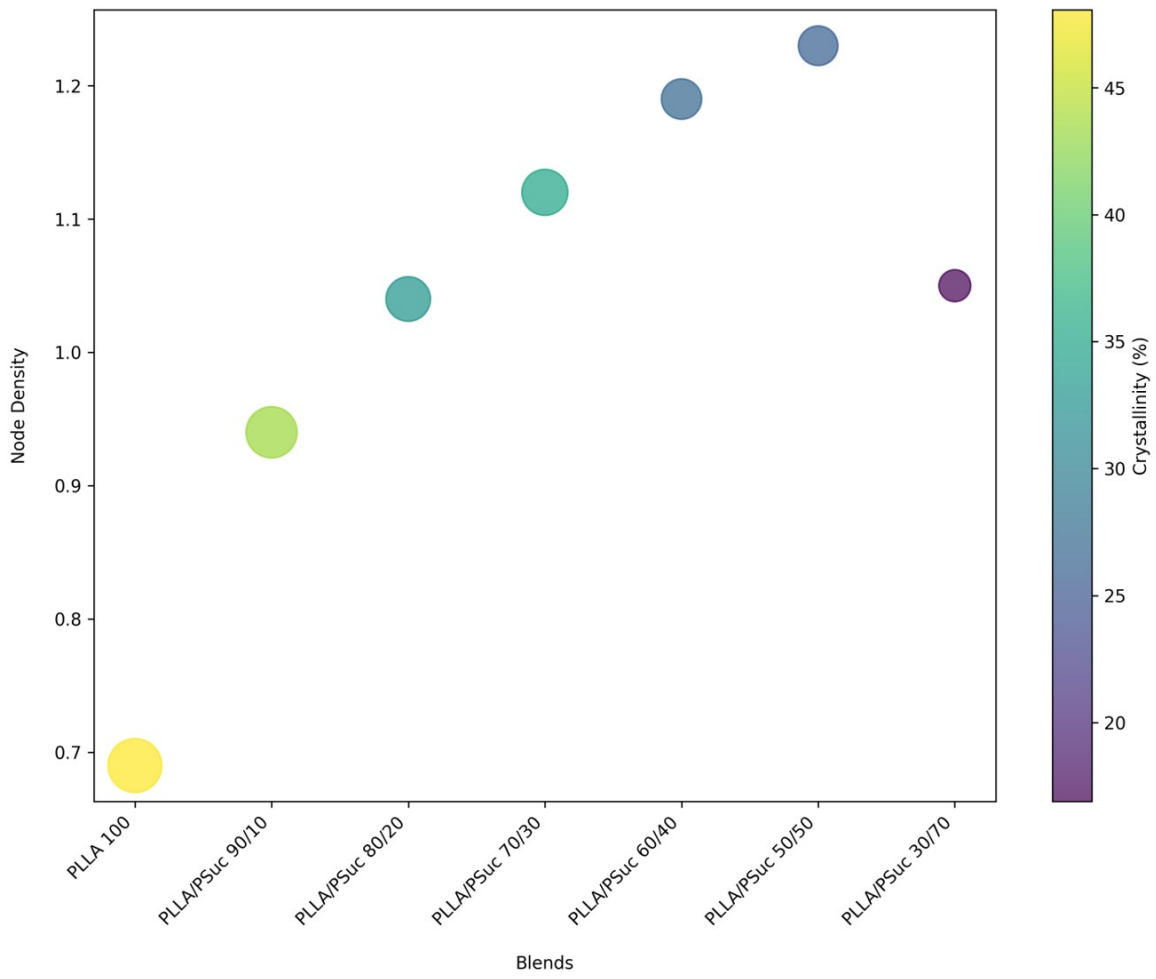
PLLA/cellulose							
0/100	1.5 ± 0.6	0.3 ± 0.1	25.0 ± 0.0	162.3 ± 21.3	280.3 ± 7.0	2.8 ± 0.0	M1
30/70	3.5 ± 1.0	0.6 ± 0.2	25.0 ± 0.0	95.7 ± 6.7	330.7 ± 27.2	2.9 ± 0.0	M1
50/50	2.3 ± 0.5	0.3 ± 0.07	25.0 ± 0.0	102.6 ± 72.8	338.0 ± 102.0	2.9 ± 0.0	M1
PDX/CA							
100/0	8.9 ± 5.4	1.2 ± 0.5	32.1 ± 0.0	51.8 ±10.3	239.4 ± 61.9	2.6 ± 0.0	M1
30/70	4.8 ± 2.1	0.8 ± 0.3	32.1 ± 0.0	134.5 ± 15.5	300.0 ± 28.1	2.3 ± 0.0	M1
50/50	2.2 ± 0.5	0.6 ± 0.2	32.1 ± 0.0	65.7 ± 14.0	298.9 ± 15.8	2.8 ± 0.0	M1
Poly(D,L-lactic acid) PDLLA/CA							
70/30	2.9 ± 0.9	0.4 ± 0.1	130.4 ± 1.3	66.9 ± 8.9	197.4 ± 9.9	1.0 ± 0.0	M1
50/50	2.4 ± 0.5	0.4 ± 0.1	123.6 ± 0.4	89.2 ± 10.3	270.7 ± 30.2	1.0 ± 0.0	M0
PDLLA/cellulose							
0/100	5.7 ± 3.3	1.0 ± 0.1	128.6 ± 0.8	168.3 ± 16.4	280.3 ± 7.0	2.8 ± 0.0	M1
30/70	2.2 ± 0.4	0.4 ± 0.1	25.0 ± 0.0	48.4 ± 20.8	350.9 ± 104.7	3.0 ± 0.0	M1
50/50	1.9 ± 0.5	0.3 ± 0.1	25.0 ± 0.0	135.1 ± 41.7	346.8 ± 61.9	2.9 ± 0.0	M1

STable 2. Hyperparameters used for each regression model.

Regression model	Best values
Support Vector regression	Kernel: rbf, C: 100, Epsilon: 0.1, Gamma: scale
Random Forest regression	n_estimators: 200, max_depth: 15, min_samples_split: 2
Lasso regression	Alpha: 0.01
Ridge regression	Alpha: 0.01
Decision Tree regression	max_depth: 10, min_samples_split: 4, Criterion: mse
k-Nearest Neighbors regression	n_neighbors: 5, Weights: distance, Distance metric (p): 2 (Euclidean distance)

STable 3. Quantitative comparison of macrophage morphology and texture features between M0 and M1 phenotypes identified from a batch of SEM images. The table presents key morphological and texture parameters, including cell area, eccentricity, circularity, mean intensity, and texture features (Zernike, Haralick, and Gabor), for both phenotypes. Data are expressed as mean ± standard deviation. Statistical differences (P-values) between M0 and M1 macrophages are indicated for each feature.

Feature	M0 Macrophages	M1 Macrophages	P-value
Number of cells	6	8	-
Average cell area (μm²)	295 ± 45	455 ± 75	0.025
Shape (eccentricity)	0.30 ± 0.05	0.70 ± 0.07	< 0.001
Mean intensity	110 ± 20	200 ± 35	0.032
Circularity	0.94 ± 0.08	0.50 ± 0.12	< 0.001
Zernike shape features	0.43 ± 0.14	0.35 ± 0.10	0.086
Haralick texture features	2.20 ± 0.45	3.10 ± 0.70	0.018
Gabor texture features	1.75 ± 0.55	2.60 ± 0.85	0.015



SFig. 1. Bubble chart showing the relationship between node density and crystallinity for different PLLA/PSuc blends. The colour of the bubbles indicates the percentage of crystallinity, with darker colours representing lower crystallinity values. Larger bubbles indicate lower node density, highlighting the inverse relationship between node density and crystallinity for different PLLA/PSuc blends.