

Thermal and barrier properties of poly(3-hydroxybutyrate) nanocomposites: use of experimental data for reliable prediction via machine learning

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Table S.1. Thermal properties of P3HB/SEP/MWCNT/WS₂ bionanocomposites.

SEP (wt%)	MWCNT (wt%)	WS ₂ (wt%)	T _{onset} (°C)	T ₁₀ (°C)	T _{max} (°C)
0	0	0	178	217	219
0	1	0	192	232	235
0	2	0	204	246	247
0	3	0	218	259	263
0	5	0	235	277	279
1	0	0	185	225	225
2	0	0	191	230	232
3	0	0	197	236	239
5	0	0	210	249	251
0	0	1	190	230	233
0	0	2	202	238	239
0	0	3	216	245	248
0	0	5	233	267	272
0	1	1	203	244	244
0	1	2	216	257	261
0	1	4	232	275	278
1	1	0	199	239	240
1	2	0	212	253	255
1	4	0	229	273	274
1	0	1	197	235	237
1	0	2	205	241	243
1	0	4	222	269	270
2	1	0	205	240	241
4	1	0	208	244	246
2	0	1	195	227	232
4	0	1	206	236	238
1	1	1	195	229	231
2	2	1	261	301	315
2	1	2	179	230	297
1	2	2	262	312	343
2	1	1	197	233	237
1	2	1	200	247	269
1	1	2	195	232	235

Table S.2. Barrier properties of P3HB/SEP/MWCNT/WS₂ bionanocomposites.

SEP (wt%)	MWCNT (wt%)	WS ₂ (wt%)	OP (mL $\mu\text{m m}^{-2} \text{day}^{-1}$)	WVP x 10 ¹² (gm ⁻¹ s ⁻¹ Pa ⁻¹)
0	0	0	38046	5.41
0	1	0	34272	4.13
0	2	0	29996	3.34
0	3	0	25671	2.96
0	5	0	22537	2.35
1	0	0	32066	4.02
2	0	0	26578	3.11
3	0	0	20345	2.43
5	0	0	18635	2.07
0	0	1	31723	3.99
0	0	2	24598	2.93
0	0	3	17645	1.97
0	0	5	8669	0.98
0	1	1	22343	2.71
0	1	2	14354	1.84
0	1	4	9334	1.34
1	1	0	25891	2.92
1	2	0	21007	2.21
1	4	0	13982	1.51
1	0	1	20465	2.54
1	0	2	12546	1.67
1	0	4	3323	0.46
2	1	0	20153	2.02
4	1	0	11232	1.19
2	0	1	19645	1.69
4	0	1	5656	0.93
1	1	1	18765	1.76
2	2	1	3567	0.49
2	1	2	2178	0.38
1	2	2	3016	0.45
2	1	1	7891	0.95
1	2	1	9856	1.45
1	1	2	6875	0.83

Table S.3. Scoring results for Lasso regression.

Variable	alpha	Mean test score	STD test score	Mean train score	STD train score
OP	0.010	-2.243E+07	1.449E+07	-1.095E+07	2.011E+06
	0.028	-2.243E+07	1.449E+07	-1.095E+07	2.011E+06
	0.077	-2.243E+07	1.449E+07	-1.095E+07	2.011E+06
	0.215	-2.243E+07	1.449E+07	-1.095E+07	2.011E+06
	0.599	-2.243E+07	1.449E+07	-1.095E+07	2.011E+06
	1.668	-2.243E+07	1.448E+07	-1.095E+07	2.011E+06
	4.642	-2.241E+07	1.447E+07	-1.095E+07	2.011E+06
	12.915	-2.238E+07	1.444E+07	-1.095E+07	2.011E+06
	35.938	-2.230E+07	1.434E+07	-1.096E+07	2.010E+06
	100	-2.212E+07	1.413E+07	-1.102E+07	2.005E+06
WVP	0.010	-3.351E-01	2.362E-01	-1.513E-01	3.216E-02
	0.028	-3.409E-01	2.732E-01	-1.560E-01	3.158E-02
	0.077	-3.938E-01	4.176E-01	-1.921E-01	2.747E-02
	0.215	-7.749E-01	9.951E-01	-4.615E-01	2.644E-02
	0.599	-1.695E+00	1.270E+00	-1.458E+00	2.095E-01
	1.668	-1.750E+00	1.233E+00	-1.604E+00	2.851E-01
	4.642	-1.750E+00	1.233E+00	-1.604E+00	2.851E-01
	12.915	-1.750E+00	1.233E+00	-1.604E+00	2.851E-01
	35.938	-1.750E+00	1.233E+00	-1.604E+00	2.851E-01
	100	-1.750E+00	1.233E+00	-1.604E+00	2.851E-01
T _{onset}	0.010	-2.778E+02	1.582E+02	-1.890E+02	3.221E+01
	0.028	-2.778E+02	1.581E+02	-1.890E+02	3.221E+01
	0.077	-2.778E+02	1.579E+02	-1.890E+02	3.221E+01
	0.215	-2.782E+02	1.579E+02	-1.893E+02	3.219E+01
	0.599	-2.813E+02	1.620E+02	-1.915E+02	3.204E+01
	1.668	-2.882E+02	1.790E+02	-2.058E+02	3.274E+01
	4.642	-3.516E+02	2.978E+02	-2.723E+02	2.697E+01
	12.915	-4.482E+02	3.146E+02	-4.377E+02	7.315E+01
	35.938	-4.485E+02	3.143E+02	-4.403E+02	7.587E+01
	100	-4.485E+02	3.143E+02	-4.403E+02	7.587E+01
T ₁₀	0.010	-3.083E+02	1.585E+02	-1.944E+02	3.169E+01
	0.028	-3.082E+02	1.586E+02	-1.944E+02	3.169E+01
	0.077	-3.080E+02	1.591E+02	-1.944E+02	3.169E+01
	0.215	-3.077E+02	1.608E+02	-1.947E+02	3.168E+01
	0.599	-3.089E+02	1.687E+02	-1.969E+02	3.160E+01
	1.668	-3.116E+02	1.983E+02	-2.111E+02	3.225E+01
	4.642	-3.583E+02	3.196E+02	-2.744E+02	3.131E+01
	12.915	-5.047E+02	3.591E+02	-4.866E+02	9.268E+01
	35.938	-5.129E+02	3.612E+02	-5.092E+02	9.150E+01
	100	-5.129E+02	3.612E+02	-5.092E+02	9.150E+01

Variable	alpha	Mean test score	STD test score	Mean train score	STD train score
$T_{\max}$	0.010	-4.773E+02	3.007E+02	-3.213E+02	6.057E+01
	0.028	-4.770E+02	3.007E+02	-3.213E+02	6.057E+01
	0.077	-4.763E+02	3.005E+02	-3.213E+02	6.057E+01
	0.215	-4.745E+02	3.002E+02	-3.216E+02	6.057E+01
	0.599	-4.717E+02	3.002E+02	-3.238E+02	6.058E+01
	1.668	-4.809E+02	3.094E+02	-3.405E+02	6.077E+01
	4.642	-5.476E+02	3.907E+02	-4.374E+02	5.991E+01
	12.915	-7.656E+02	5.427E+02	-7.497E+02	1.343E+02
	35.938	-7.947E+02	5.412E+02	-7.911E+02	1.428E+02
	100	-7.947E+02	5.412E+02	-7.911E+02	1.428E+02

Scoring criteria: negative mean square error.

Table S.4. Extended polynomial regression results for the prediction of the barrier and thermal properties: CV – cross-validation mean value; STD – Standard Deviation; Split – best split value obtained.

Degree	Output variable	MSE (CV)	MSE STD (CV)	MAE (CV)	MAE STD (CV)	R ² (CV)	R ² STD (CV)	MSE (Split)	MAE (Split)	R ² (Split)
2	OP	6.167E+06	2.951E+06	2.087E+03	5.500E+02	7.860E-01	4.559E-02	9.166E+06	2.517E+03	8.134E-01
2	WVP	3.070E-02	1.851E-02	1.280E-01	4.536E-02	9.132E-01	5.924E-02	7.790E-02	1.970E-01	8.872E-01
2	T _{onset}	3.320E+02	3.337E+02	1.374E+01	7.973E+00	-4.791E-01	1.887E+00	2.046E+02	1.040E+01	-1.772E-01
2	T ₁₀	3.986E+02	2.883E+02	1.565E+01	6.099E+00	-1.818E-01	7.165E-01	2.575E+02	1.371E+01	-1.527E-01
2	T _{max}	8.199E+02	6.104E+02	2.183E+01	8.504E+00	-1.440E+00	1.659E+00	5.603E+02	1.882E+01	-9.732E-01
3	OP	6.554E+07	6.175E+07	6.360E+03	3.206E+03	-2.854E+00	5.098E+00	1.016E+08	6.839E+03	-1.068E+00
3	WVP	2.924E-01	2.180E-01	3.555E-01	1.116E-01	-2.135E-02	8.310E-01	4.478E-02	1.691E-01	9.351E-01
3	T _{onset}	1.458E+04	1.200E+04	7.082E+01	3.057E+01	-8.896E+01	9.060E+01	2.780E+03	3.525E+01	-1.499E+01
3	T ₁₀	1.073E+04	8.307E+03	6.358E+01	2.111E+01	-4.104E+01	2.884E+01	1.996E+03	3.227E+01	-7.937E+00
3	T _{max}	4.834E+03	3.473E+03	4.898E+01	2.356E+01	-2.100E+01	2.354E+01	4.330E+03	3.740E+01	-1.425E+01
4	OP	6.853E+08	6.657E+08	1.510E+04	5.901E+03	-2.195E+01	1.411E+01	2.104E+08	8.305E+03	-3.284E+00
4	WVP	3.440E+00	3.368E+00	8.396E-01	4.824E-01	-4.708E+00	4.045E+00	4.066E+00	1.202E+00	-4.891E+00
4	T _{onset}	1.696E+04	3.097E+04	4.706E+01	4.260E+01	-5.348E+01	8.779E+01	1.341E+03	2.206E+01	-6.713E+00
4	T ₁₀	1.480E+04	2.679E+04	4.699E+01	3.879E+01	-3.862E+01	6.953E+01	2.778E+03	3.065E+01	-1.144E+01
4	T _{max}	1.151E+04	1.768E+04	5.057E+01	3.105E+01	-2.986E+01	4.338E+01	1.001E+03	2.446E+01	-2.524E+00

Table S.5. Extended SVM results for the prediction of the barrier and thermal properties: std – Standard Deviation.

Variable	parameters	Test		Train	
		mean	std	mean	std
OP	{'C': 0.1, 'kernel': 'linear'}	0.7	0.1	0.8	0.0
		27	64	95	46
	{'C': 0.1, 'kernel': 'rbf'}	0.4	0.1	0.6	0.1
		87	73	09	70
	{'C': 1, 'kernel': 'linear'}	0.8	0.1	0.9	0.0
		47	48	43	36
	{'C': 1, 'kernel': 'rbf'}	0.7	0.0	0.9	0.0
		67	84	33	23
WVP	{'C': 10, 'kernel': 'linear'}	0.9	0.0	0.9	0.0
		27	90	71	23
	{'C': 10, 'kernel': 'rbf'}	0.8	0.1	1.0	0.0
		07	27	00	00
	{'C': 0.1, 'kernel': 'linear'}	0.7	0.2	0.9	0.0
		67	35	04	42
	{'C': 0.1, 'kernel': 'rbf'}	0.5	0.0	0.5	0.0
		40	80	39	19
T _{onset}	{'C': 1, 'kernel': 'linear'}	0.8	0.0	0.9	0.0
		87	93	42	19
	{'C': 1, 'kernel': 'rbf'}	0.8	0.1	0.9	0.0
		07	79	42	19
	{'C': 10, 'kernel': 'linear'}	0.8	0.0	1.0	0.0
		87	93	00	00
	{'C': 10, 'kernel': 'rbf'}	0.7	0.1	1.0	0.0
		33	52	00	00
T ₁₀	{'C': 0.1, 'kernel': 'linear'}	0.5	0.1	0.7	0.0
		73	55	78	74
	{'C': 0.1, 'kernel': 'rbf'}	0.5	0.2	0.5	0.1
		20	40	89	30
	{'C': 1, 'kernel': 'linear'}	0.6	0.1	0.7	0.0
		40	96	49	88
	{'C': 1, 'kernel': 'rbf'}	0.6	0.2	0.8	0.0
		40	65	84	39
	{'C': 10, 'kernel': 'linear'}	0.6	0.1	0.7	0.0
		40	96	98	65
	{'C': 10, 'kernel': 'rbf'}	0.6	0.2	0.9	0.0
		80	04	52	52
	{'C': 0.1, 'kernel': 'linear'}	0.7	0.1	0.8	0.0
		73	37	55	45
	{'C': 0.1, 'kernel': 'rbf'}	0.5	0.0	0.5	0.0
		40	80	39	19
	{'C': 1, 'kernel': 'linear'}	0.6	0.2	0.8	0.0
		93	00	55	54
	{'C': 1, 'kernel': 'rbf'}	0.7	0.1	0.9	0.0
		60	96	42	19

$T_{\max}$	{'C': 10, 'kernel': 'linear'}	0.7	0.2	0.8	0.0
		20	04	75	78
	{'C': 10, 'kernel': 'rbf'}	0.8	0.2	1.0	0.0
		00	19	00	00
	{'C': 0.1, 'kernel': 'linear'}	0.7	0.1	0.8	0.0
		73	37	84	42
	{'C': 0.1, 'kernel': 'rbf'}	0.5	0.0	0.5	0.0
		40	80	39	19
	{'C': 1, 'kernel': 'linear'}	0.8	0.1	0.8	0.0
		00	26	65	39
	{'C': 1, 'kernel': 'rbf'}	0.8	0.0	0.9	0.0
		80	98	23	49
	{'C': 10, 'kernel': 'linear'}	0.8	0.0	0.8	0.0
		40	80	84	52
	{'C': 10, 'kernel': 'rbf'}	0.8	0.1	0.9	0.0
		80	60	81	23

Table S.6. Extended SVM results for the prediction of the barrier and thermal properties: std – Standard Deviation. (Part I)

Variable	C	epsilon	Test		Train	
			mean	std	mean	std
WVP	0.1	0.01	-1.558E+00	9.622E-01	-1.212E+00	2.019E-01
	0.1	0.1	-1.520E+00	9.330E-01	-1.219E+00	2.072E-01
	0.1	0.5	-1.554E+00	9.198E-01	-1.235E+00	2.138E-01
	0.1	1	-1.457E+00	9.259E-01	-1.342E+00	2.187E-01
	1	0.01	-4.511E-01	5.118E-01	-1.348E-01	3.735E-02
	1	0.1	-4.762E-01	5.178E-01	-1.334E-01	3.639E-02
	1	0.5	-5.799E-01	5.295E-01	-2.658E-01	3.092E-02
	1	1	-9.321E-01	6.779E-01	-6.491E-01	6.792E-02
	10	0.01	-1.415E-01	1.093E-01	-9.939E-04	1.143E-03
	10	0.1	-2.317E-01	1.957E-01	-8.846E-03	3.414E-04
	10	0.5	-4.887E-01	4.268E-01	-1.699E-01	5.643E-03
	10	1	-8.779E-01	6.346E-01	-4.725E-01	2.530E-02
	100	0.01	-1.401E-01	1.108E-01	-1.012E-04	1.936E-06
	100	0.1	-2.317E-01	1.957E-01	-8.846E-03	3.414E-04
	100	0.5	-4.887E-01	4.268E-01	-1.699E-01	5.643E-03

	100	1	-8.779E-01	6.346E-01	-4.725E-01	2.530E-02
T_{onset}	0.1	0.01	-4.756E+02	4.953E+02	-4.562E+02	1.115E+02
	0.1	0.1	-4.758E+02	4.951E+02	-4.559E+02	1.113E+02
	0.1	0.5	-4.777E+02	4.955E+02	-4.550E+02	1.107E+02
	0.1	1	-4.795E+02	4.967E+02	-4.557E+02	1.105E+02
	1	0.01	-4.477E+02	4.789E+02	-4.070E+02	1.061E+02
	1	0.1	-4.490E+02	4.804E+02	-4.069E+02	1.061E+02
	1	0.5	-4.547E+02	4.874E+02	-4.070E+02	1.064E+02
	1	1	-4.613E+02	4.972E+02	-4.085E+02	1.073E+02
	10	0.01	-3.397E+02	4.232E+02	-2.068E+02	8.497E+01
	10	0.1	-3.392E+02	4.234E+02	-2.071E+02	8.506E+01
	10	0.5	-3.368E+02	4.223E+02	-2.084E+02	8.563E+01
	10	1	-3.368E+02	4.190E+02	-2.103E+02	8.638E+01
	100	0.01	-5.799E+02	6.659E+02	-3.810E+01	2.633E+01
	100	0.1	-5.776E+02	6.633E+02	-3.802E+01	2.641E+01
	100	0.5	-5.676E+02	6.512E+02	-3.761E+01	2.648E+01
	100	1	-5.615E+02	6.412E+02	-3.737E+01	2.636E+01

Table S.6. Extended SVM results for the prediction of the barrier and thermal properties: std – Standard Deviation. (Part II)

Variable	C	epsilon	Test		Train	
			mean	std	mean	std
T_{10}	0.1	0.01	-5.834E+02	6.922E+02	-5.451E+02	1.438E+02
	0.1	0.1	-5.832E+02	6.924E+02	-5.456E+02	1.440E+02
	0.1	0.5	-5.825E+02	6.929E+02	-5.478E+02	1.451E+02
	0.1	1	-5.827E+02	6.952E+02	-5.505E+02	1.461E+02
	1	0.01	-5.396E+02	6.641E+02	-4.878E+02	1.361E+02
	1	0.1	-5.396E+02	6.642E+02	-4.883E+02	1.365E+02
	1	0.5	-5.394E+02	6.651E+02	-4.913E+02	1.384E+02
	1	1	-5.443E+02	6.719E+02	-4.941E+02	1.388E+02
	10	0.01	-4.362E+02	5.942E+02	-2.580E+02	1.113E+02
	10	0.1	-4.356E+02	5.932E+02	-2.579E+02	1.113E+02
	10	0.5	-4.323E+02	5.874E+02	-2.580E+02	1.116E+02
	10	1	-4.261E+02	5.779E+02	-2.582E+02	1.115E+02
	100	0.01	-5.303E+02	6.065E+02	-4.695E+01	3.274E+01
	100	0.1	-5.315E+02	6.073E+02	-4.688E+01	3.268E+01
	100	0.5	-5.350E+02	6.117E+02	-4.651E+01	3.227E+01

	100	1	-5.381E+02	6.140E+02	-4.542E+01	3.102E+01
	0.1	0.01	-9.535E+02	1.173E+03	-9.022E+02	2.488E+02
	0.1	0.1	-9.535E+02	1.173E+03	-9.022E+02	2.488E+02
	0.1	0.5	-9.534E+02	1.173E+03	-9.023E+02	2.489E+02
	0.1	1	-9.466E+02	1.163E+03	-9.009E+02	2.506E+02
	1	0.01	-8.888E+02	1.104E+03	-8.336E+02	2.469E+02
	1	0.1	-8.901E+02	1.106E+03	-8.338E+02	2.465E+02
	1	0.5	-8.957E+02	1.118E+03	-8.328E+02	2.431E+02
	1	1	-8.931E+02	1.114E+03	-8.292E+02	2.410E+02
T _{max}	10	0.01	-6.332E+02	8.541E+02	-4.757E+02	1.728E+02
	10	0.1	-6.337E+02	8.547E+02	-4.760E+02	1.728E+02
	10	0.5	-6.355E+02	8.576E+02	-4.758E+02	1.722E+02
	10	1	-6.423E+02	8.698E+02	-4.782E+02	1.715E+02
	100	0.01	-4.838E+02	6.161E+02	-1.171E+02	4.294E+01
	100	0.1	-4.814E+02	6.132E+02	-1.172E+02	4.312E+01
	100	0.5	-4.613E+02	5.805E+02	-1.179E+02	4.469E+01
	100	1	-4.407E+02	5.454E+02	-1.183E+02	4.648E+01

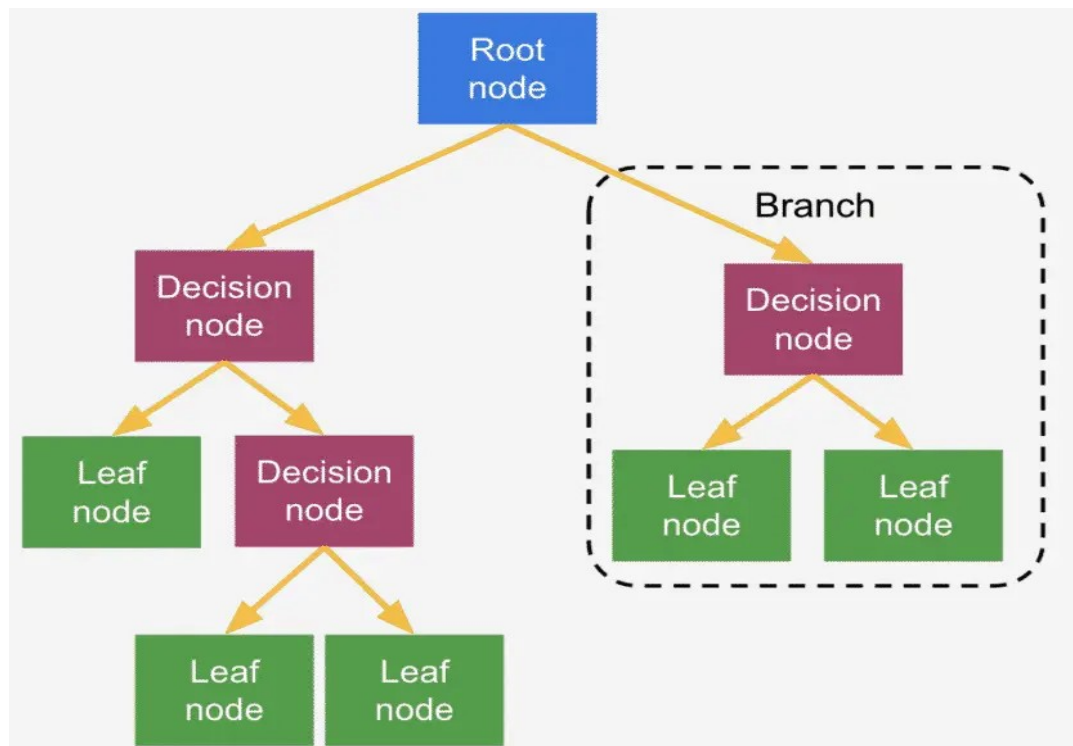


Figure S1. Schematic representation of the decision tree model including its main concepts

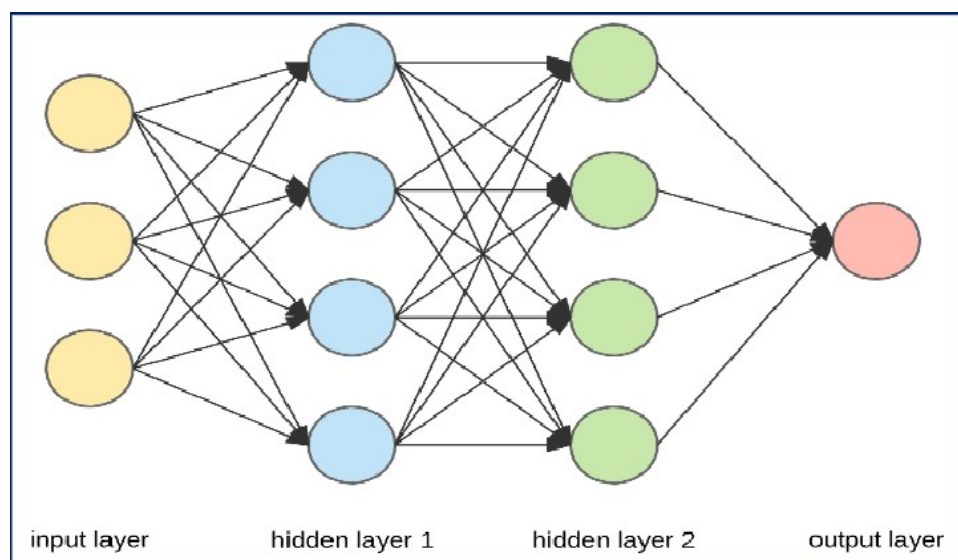


Figure S2. Schematic representation of the ANN model with two hidden layers

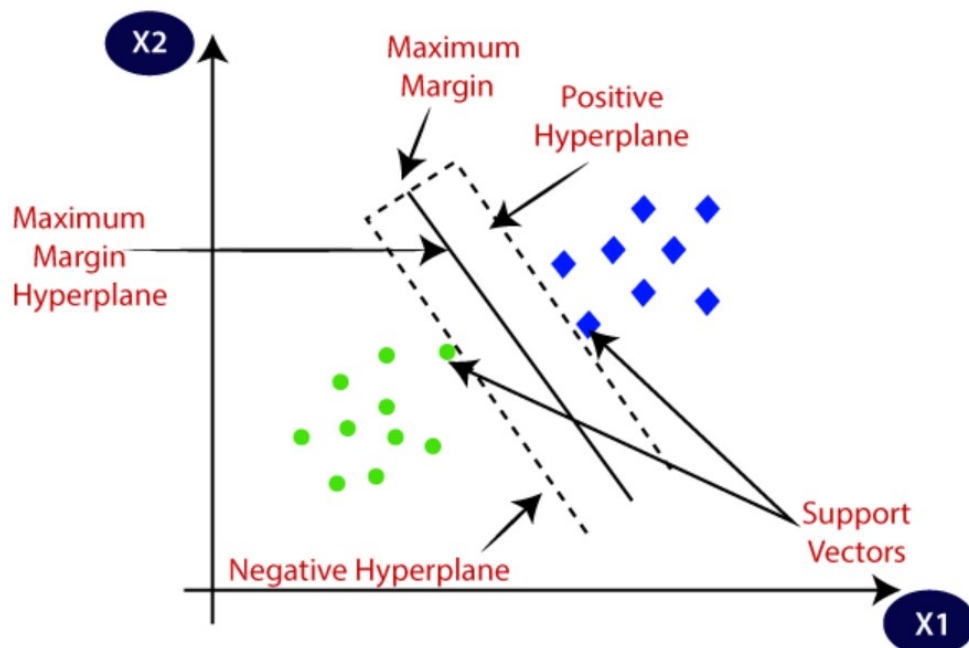


Figure S3. Schematic representation of the SVM model. A decision hyperplane with maximal margin separates every sample into two classes. The support vector is the sample point on the margin hyperplane.

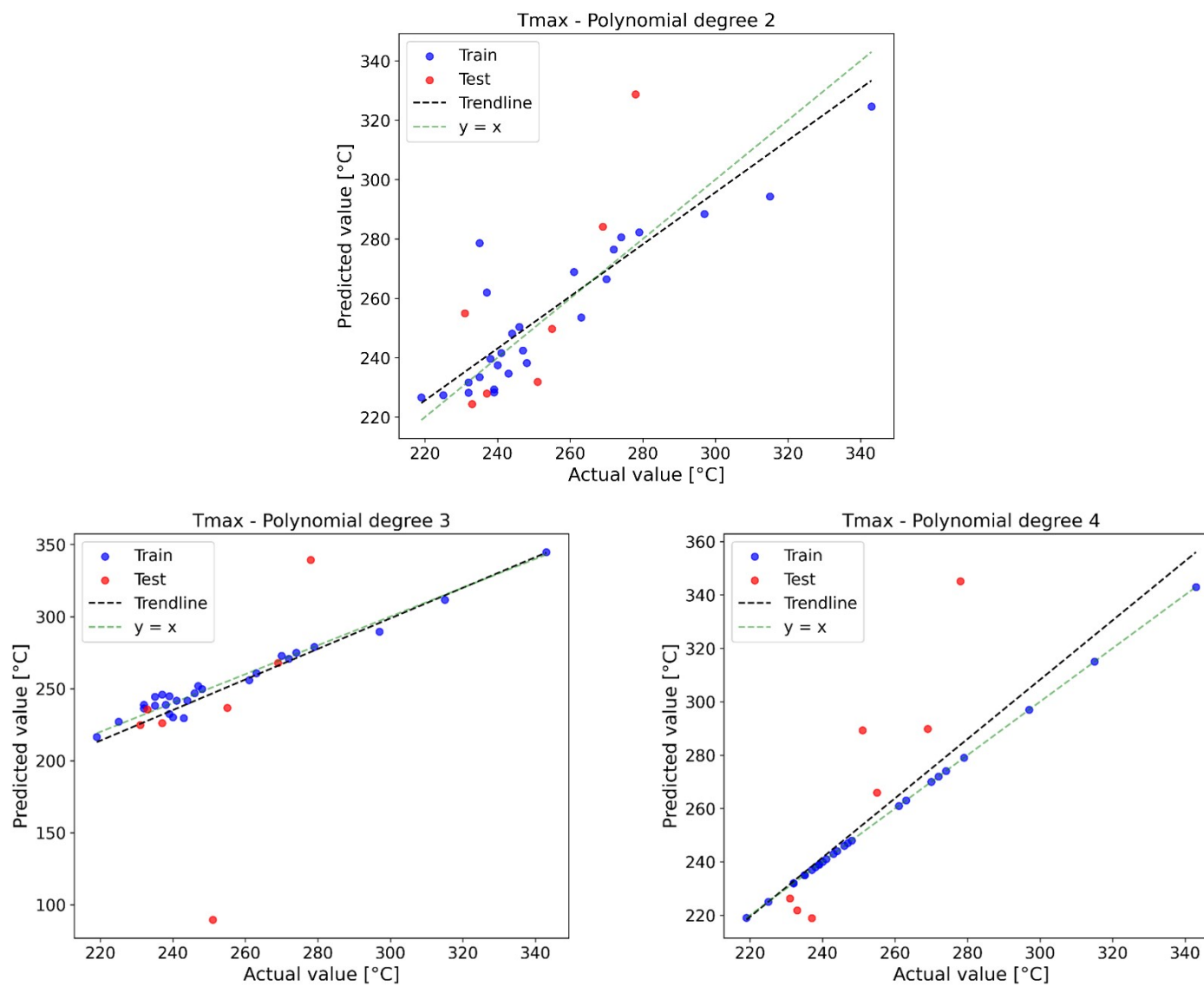


Figure S4. Comparative representation of polynomial regression models of three degrees for $T_{\max}$.

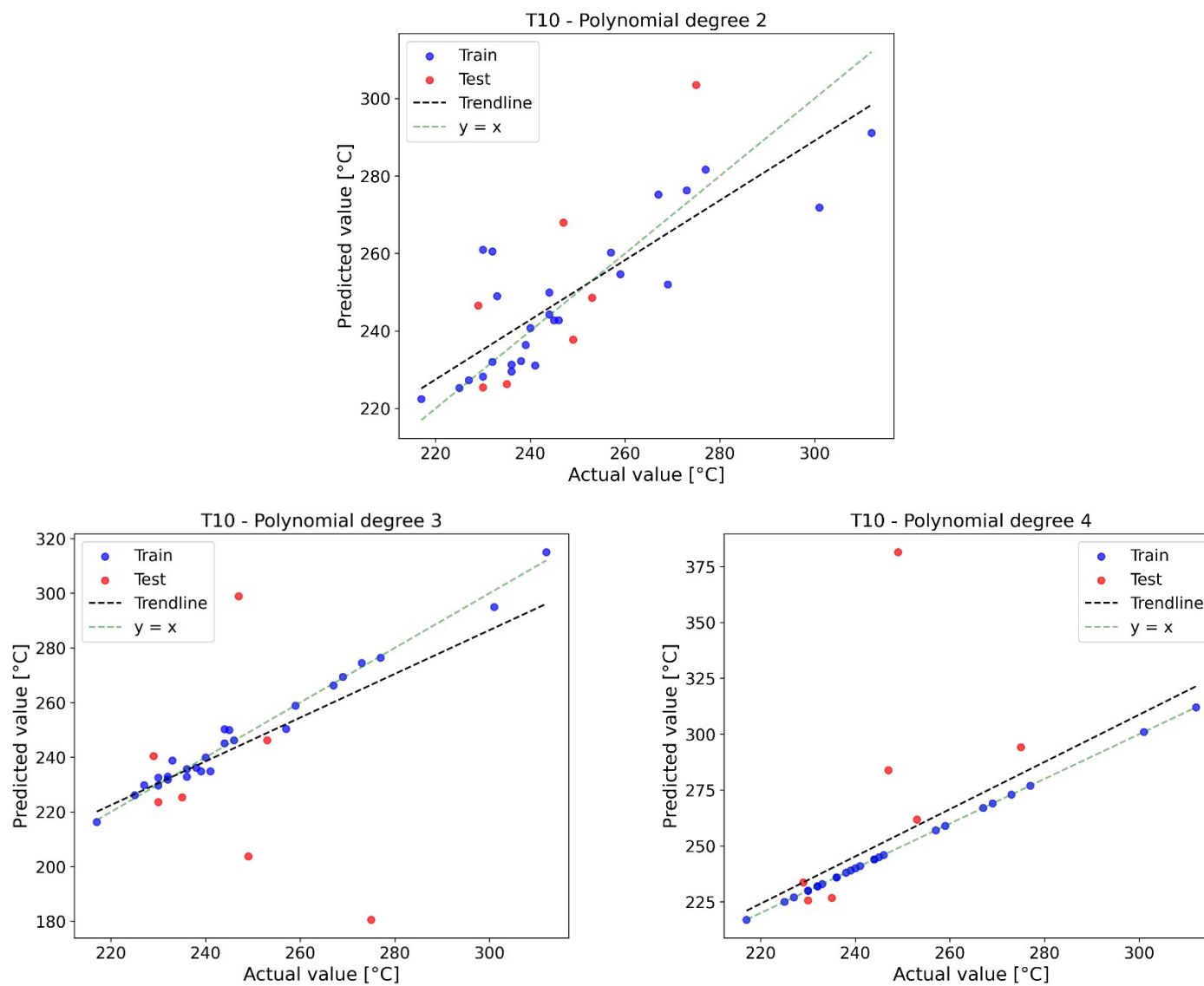


Figure S5. Comparative representation of polynomial regression models of three degrees for T₁₀.

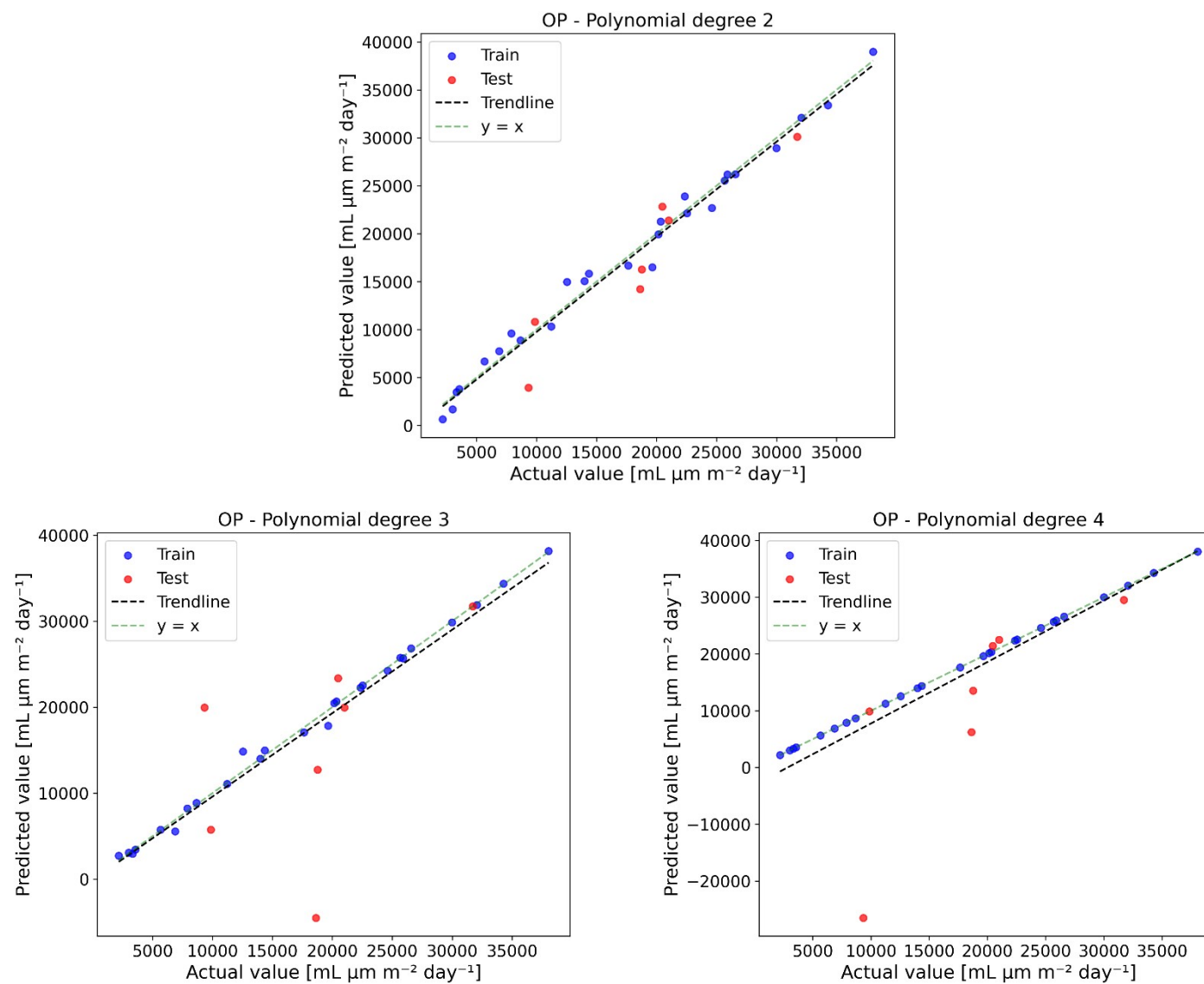


Figure S6. Comparative representation of polynomial regression models of three degrees for OP.

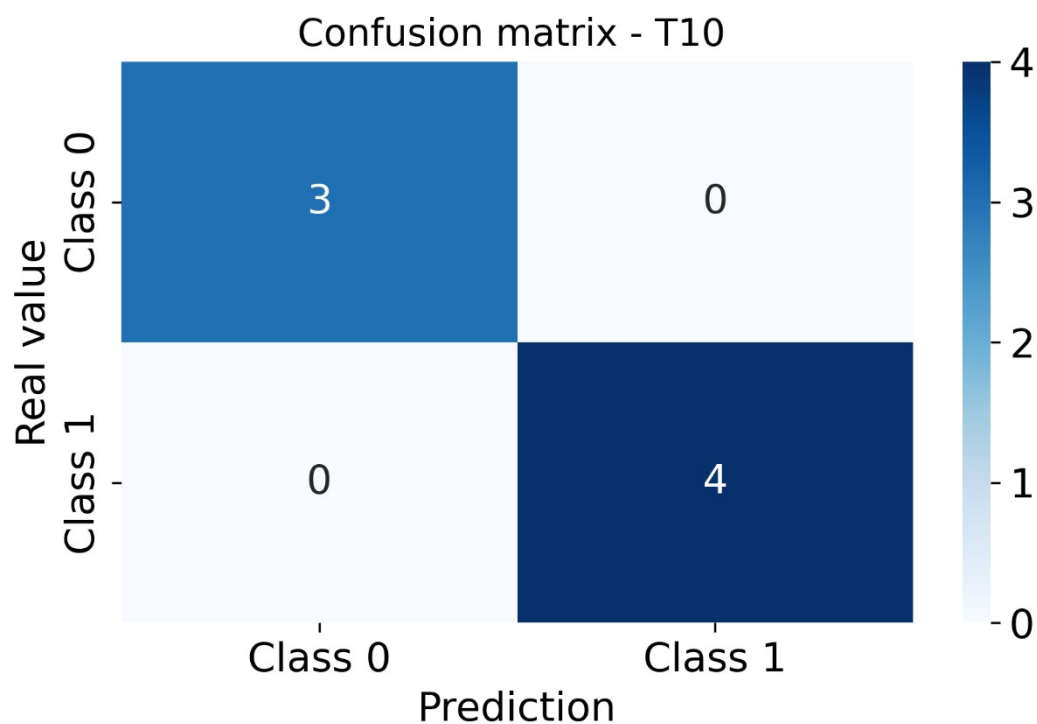


Figure S7. Confusion matrices for Support Vector Machine method results for T_{10} .

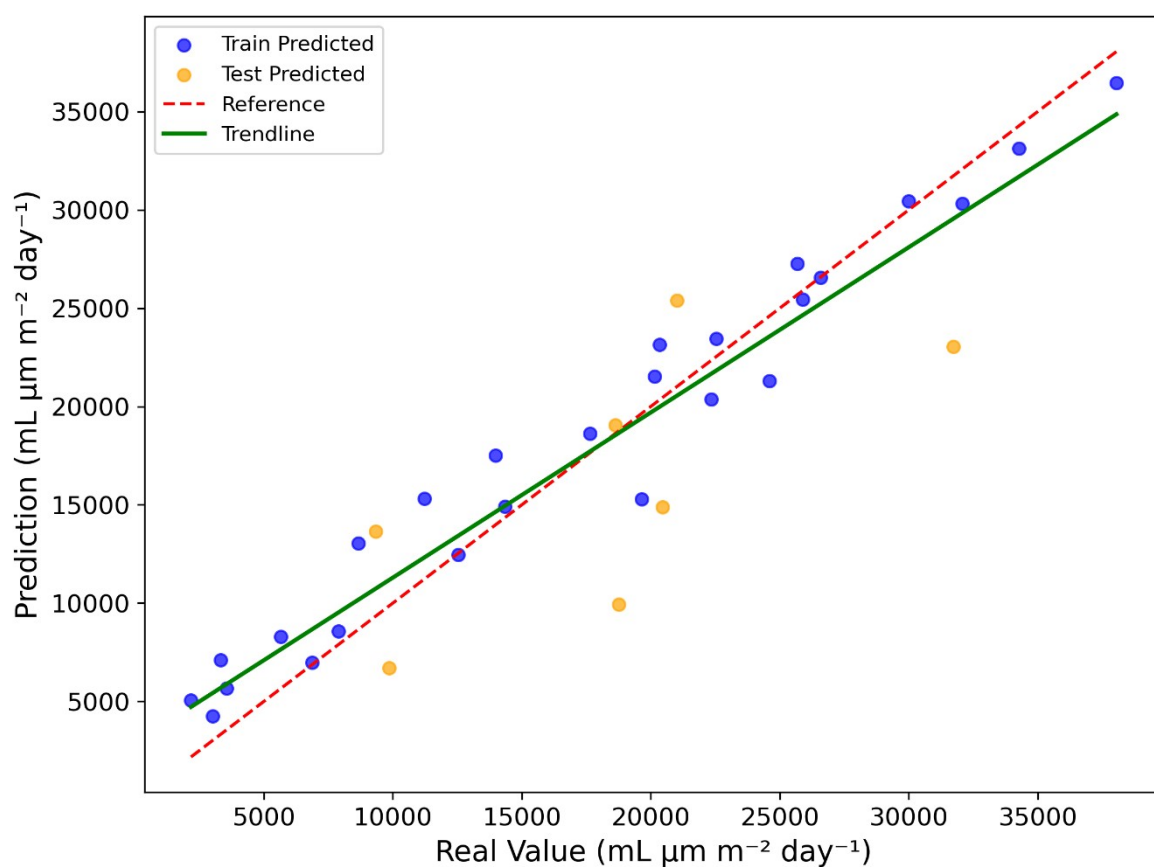


Figure S8. Predicted values using Random Forest model vs experimental values for OP.

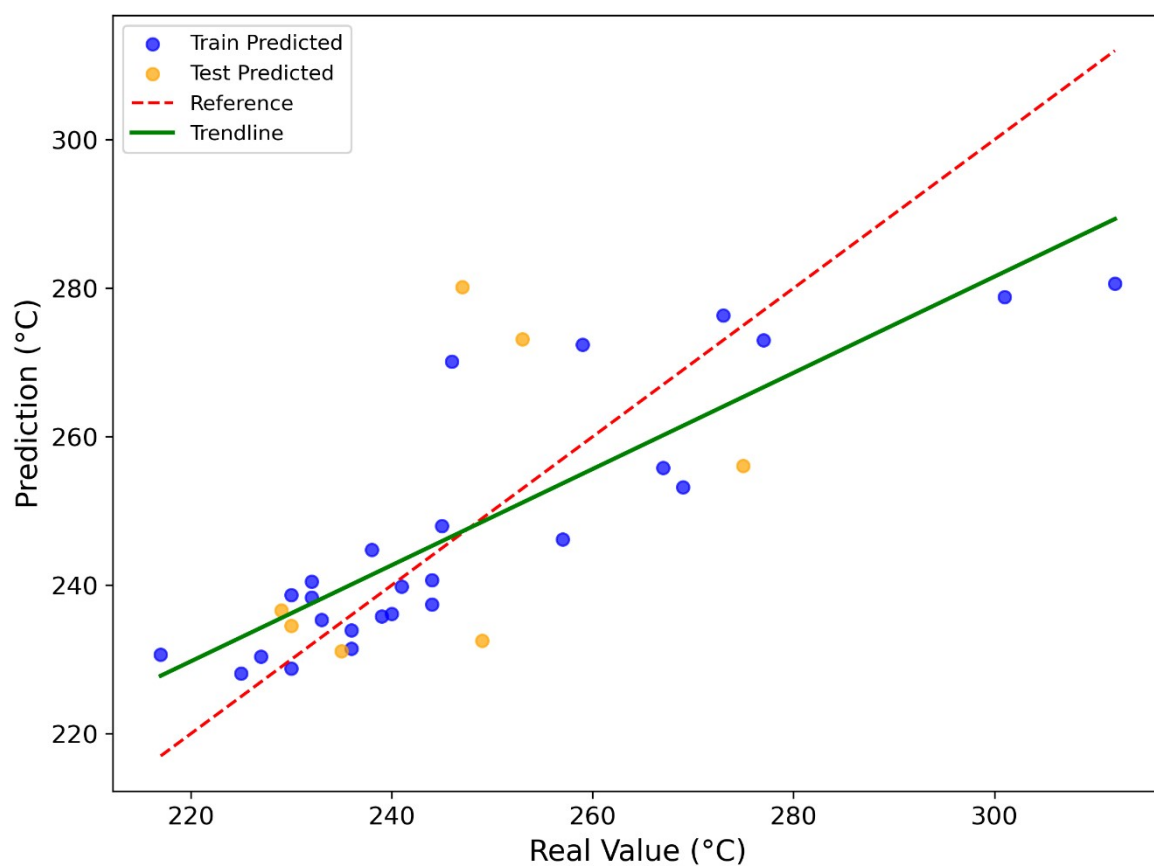


Figure S9. Predicted values using Random Forest model vs experimental values for T_{10} .

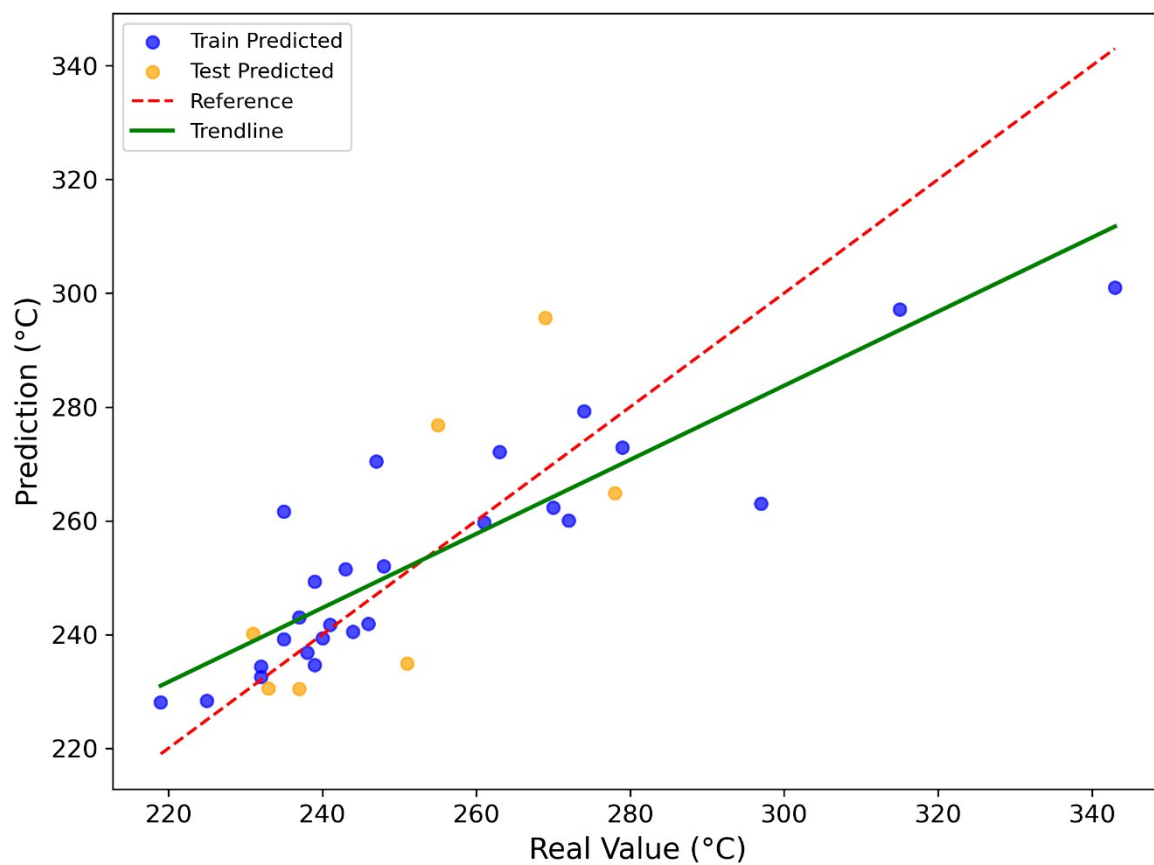


Figure S10. Predicted values using Random Forest model vs experimental values for T_{max} .

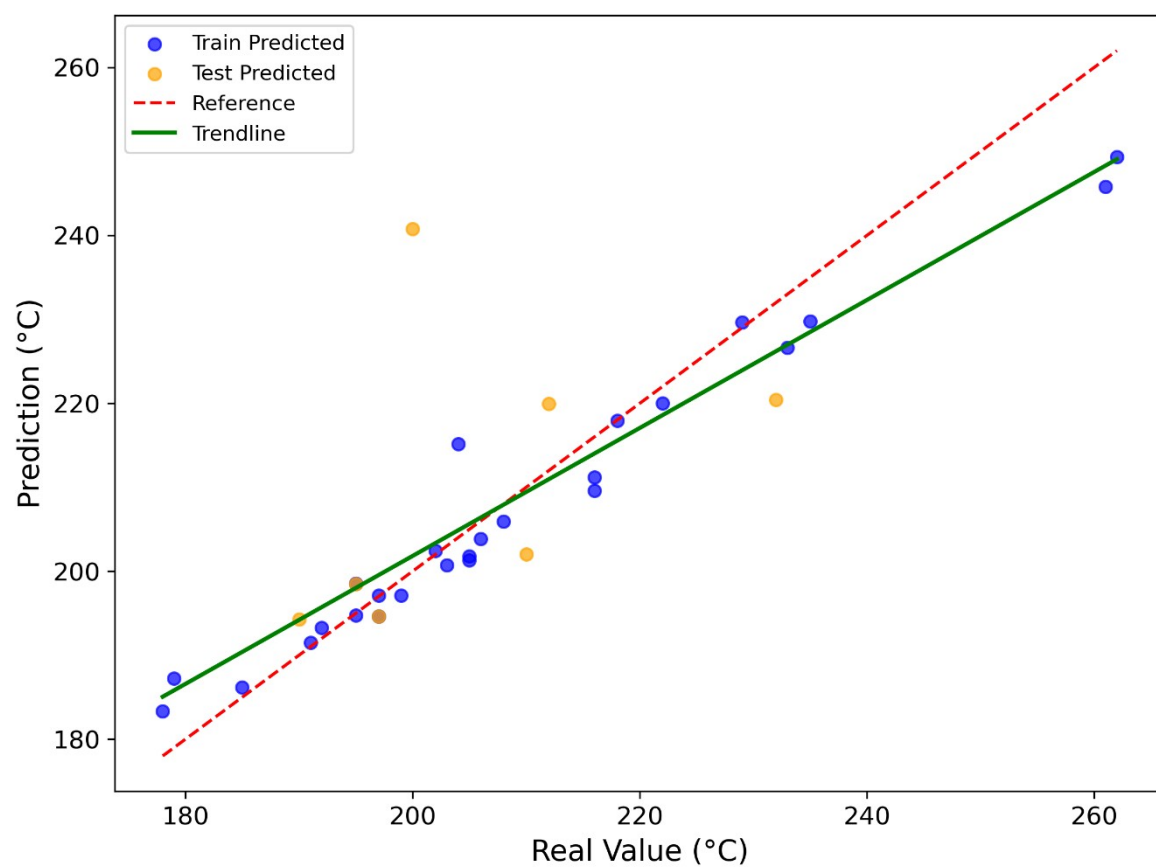


Figure S11. Predicted values using Random Forest model vs experimental values for T_{onset} .