

Temporal Profiling of Structure–Property Relationships in Biodegradable Polymers via NMR-Driven Data Science

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Supplementary research

Cluster analysis of tensile properties and degradability

To examine the relationship between tensile properties and degradation behavior in biodegradable polyesters, mass loss was compared with three mechanical parameters: Young's modulus, strain at break, and maximum stress (Fig. S1). Among these metrics, strain at break showed the most consistent inverse relationship with degradation behavior, with more ductile materials exhibiting slower mass loss, whereas brittle samples degraded more rapidly (Fig. S1A). This trend suggests an empirical relationship between macroscopic deformation capability and mass loss behavior, rather than directly reflecting molecular accessibility under environmental conditions.

In contrast, stiffness and strength related parameters (Young's modulus and maximum stress; Figs. S1B, C) did not exhibit monotonic relationships with mass loss, indicating that degradation behavior cannot be reliably predicted by these metrics alone. For instance, PBS_2_2 and PBS_1_1 showed low mass loss despite high stiffness and strength, implying that crystalline structure and other microstructural factors also jointly influence environmental stability. Consistent with this interpretation, unsupervised clustering based on tensile parameters and degradation behavior separated the materials into two groups: ductile, slowly degrading polymers and brittle, rapidly degrading ones. Although derived from a different analytical perspective, this clustering pattern broadly agrees with segmental mobility trends identified by TD-NMR. Furthermore, in line with previous studies, higher crystallinity in PBS and PBSA was associated with reduced mass loss (Fig. 2), likely due to restricted diffusion of water molecules and enzymes¹.

Overall, from a mechanical standpoint, this analysis shows a consistent

negative relationship between mass loss and tensile properties, especially as seen by strain at break. The purpose of this clustering analysis is to provide an intuitive comparative perspective across different polyester systems, offering context and reference for further time course NMR-based research.

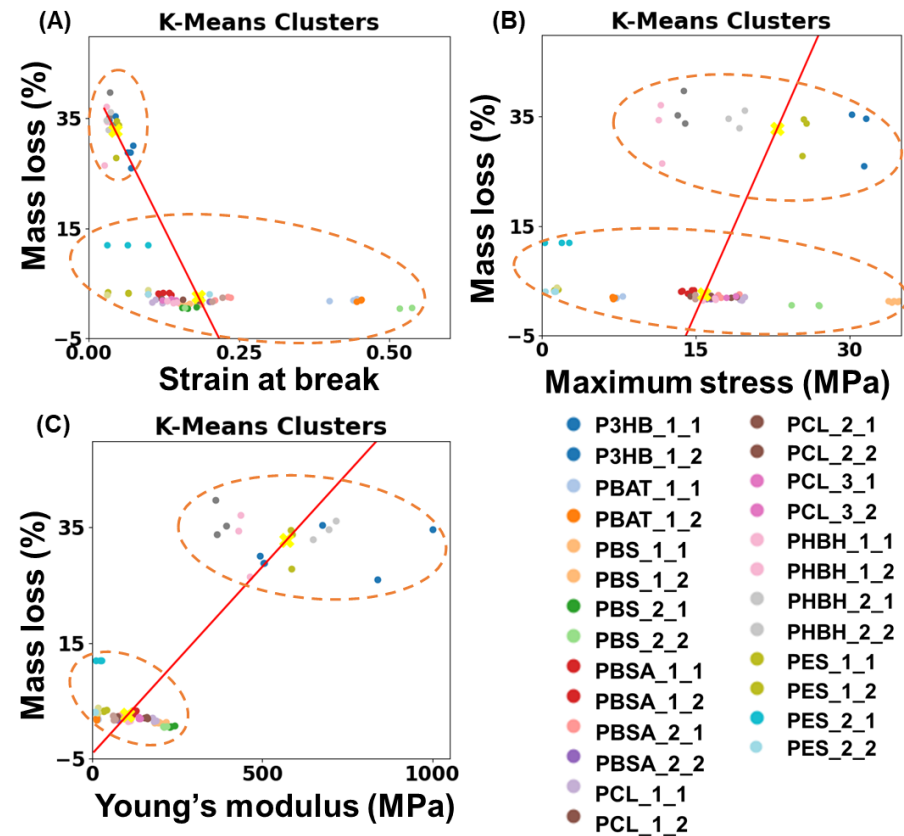


Fig. S1. Clustered plots showing the correlations between mass loss rate and tensile properties related parameters of biodegradable polymers over a 30-day period. (A) Relationship between strain at break and mass loss, (B) Relationship between maximum stress and mass loss, and (C) Relationship between Young's modulus and mass loss.

Multi-feature random forest prediction analysis

Before implementing deep learning, we built a random forest regression analysis was first performed using quantitative features extracted directly from TD-NMR relaxation measurements to determine whether experimentally attainable features could predict polymer attributes. Specifically, numerical features derived from MSE, DQ, and MAPE based T_2 relaxation curves were used as input variables to predict mass loss, young's modulus, strain at break, maximum stress, glass transition temperature (T_g), melting temperature (T_m), and crystallization temperature (T_c) for seven representative polymers (Fig. S2 and S3)

The random forest model based on these TD-NMR-derived relaxation

60 features achieved accurate prediction of polymer mass loss, with a coefficient
61 of determination (R^2) of 0.81. Among the three pulse sequences, features
62 derived from DQ measurements exhibited relatively high importance scores,
63 indicating that relaxation components associated with constrained segmental
64 motion contributed substantially to the prediction of mass loss behavior.
65 Concurrently, MSE-derived characteristics had a considerable impact on model
66 predictions, particularly those describing rapid and diverse relaxation behavior.
67 Such characteristics are commonly associated with movable amorphous
68 regions and moderately mobile segments, which have been connected to
69 polymer degradation processes in previous research². In this dataset, higher
70 early-time signal intensities in the MSE relaxation curves were frequently
71 associated with faster mass loss. Overall, these results indicate that
72 quantitative features extracted from TD-NMR relaxation measurements, even
73 in the absence of explicit chemical structure information, can provide useful
74 predictive information for degradation behavior.

75 Beyond mass loss, TD-NMR-derived relaxation features also showed
76 good performance in predicting tensile properties-related mechanical
77 properties, including Young's modulus, strain at break, and maximum stress.
78 When using features derived from DQ relaxation measurements, all three
79 mechanical properties were predicted with high accuracy, with Young's modulus
80 achieving a coefficient of determination (R^2) of 0.92 (Fig. S2C). Similar
81 predictive performance was observed for strain at break and maximum stress
82 (Figs. S2E and S2G). The relatively weak prediction observed for the thermal
83 history index (THI) ($R^2 = 0.34$, Fig. S3) reflects its strong dependence on
84 processing history and DSC-specific thermal protocols, which are only indirectly
85 related to the NMR-derived initial state features used here. As a result, THI is
86 less predictable within the present framework than thermal parameters more
87 directly associated with intrinsic chain mobility (Fig.S3). These results suggest
88 that relaxation components associated with constrained segmental motion
89 carry substantial importance in the prediction of mechanical properties within
90 the present dataset. DQ signals are particularly sensitive to restricted
91 segmental mobility, which is commonly observed in physically constrained or
92 relatively ordered regions. Accordingly, the corresponding relaxation features
93 are statistically associated with structural characteristics relevant to stiffness
94 and failure behavior.

95 In addition to DQ-derived features, MSE-derived relaxation features
96 supplement stiffness-related performance predictions, owing to their sensitivity
97 to heterogeneous relaxation behavior and mixed segment motion states³.
98 Furthermore, MAPE-derived characteristics have a larger role in predicting
99 strain at break. Given that the MAPE pulse sequence emphasizes fast-relaxing,
100 highly mobile segments, its inclusion in the model implies that features
101 associated with chain flexibility provide additional information for extensibility
102 prediction, supplementing the rigidity-related features captured by DQ
103 experiments.

The TD-NMR relaxation features recovered from the DQ, MSE, and MAPE pulse sequences form a compact feature set suited for random forest-based prediction of polymer mass loss and tensile properties-related parameters. In this work, random forest analysis is utilized as an analytical tool to assess the relative relevance and relationships of various characteristics in prediction. The relationship between model prediction performance and the information included in various pulse sequences implies that TD-NMR-derived segmental motion characteristics serve as a connection between molecular-scale relaxation behavior and macroscopic material properties.

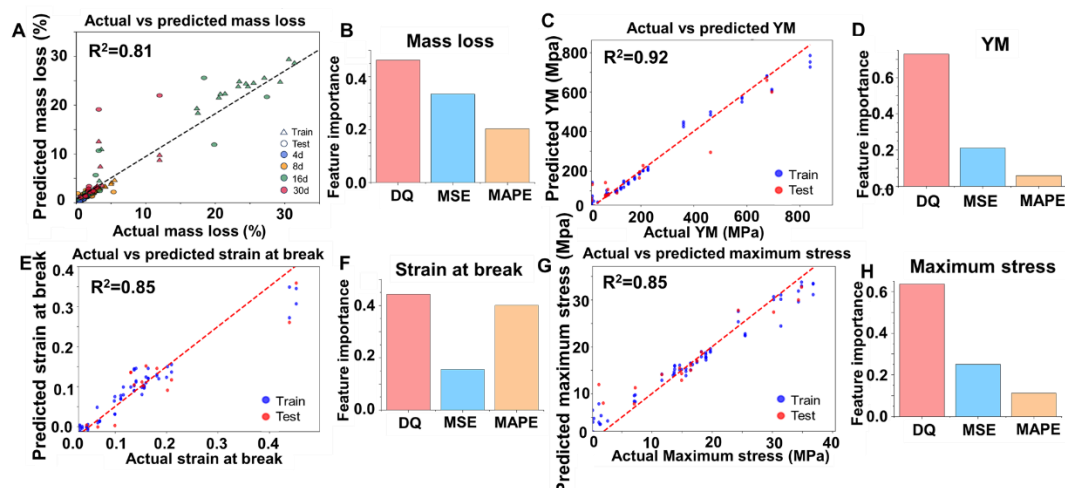


Fig. S2 Random Forest regression analysis. (A, C, E, G) Regression prediction plot for degree of characterization, and (B, D, F, H) feature importance analysis of multiple polymers. (Young's modulus is abbreviated as YM)

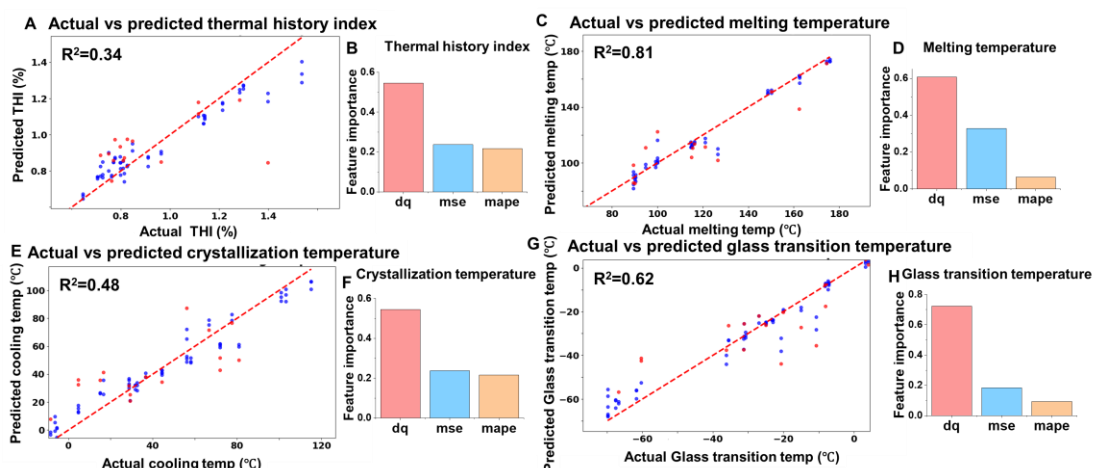
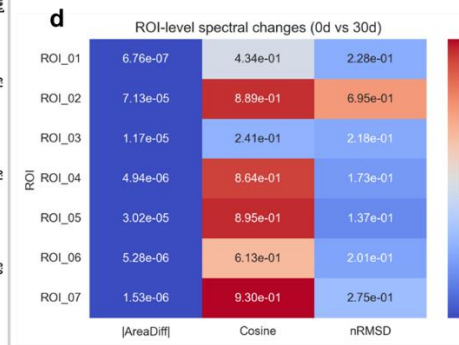
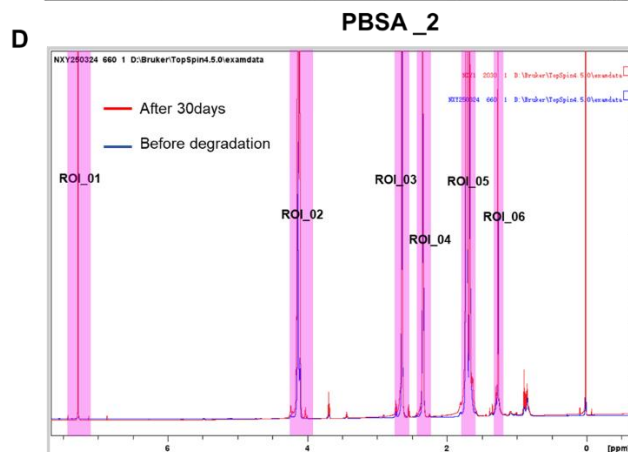
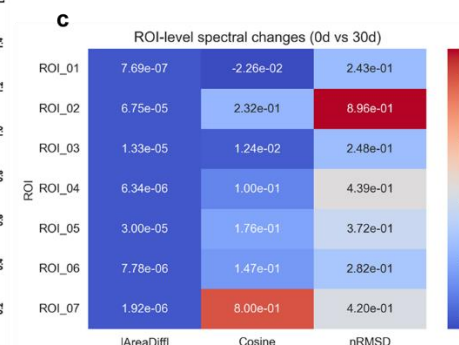
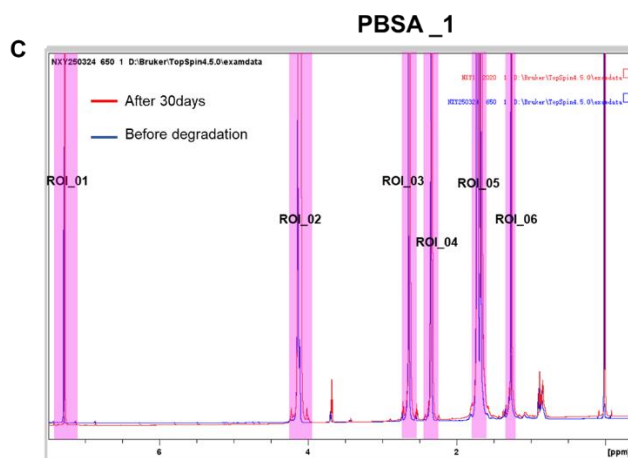
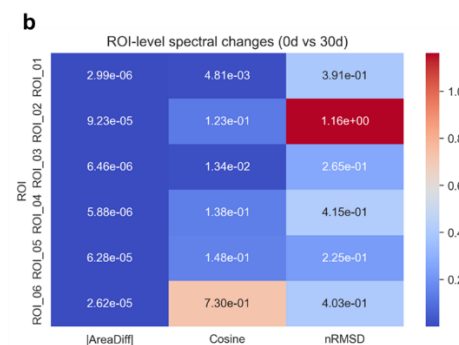
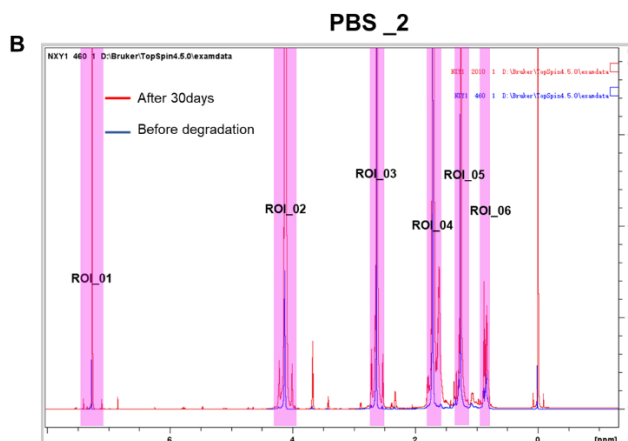
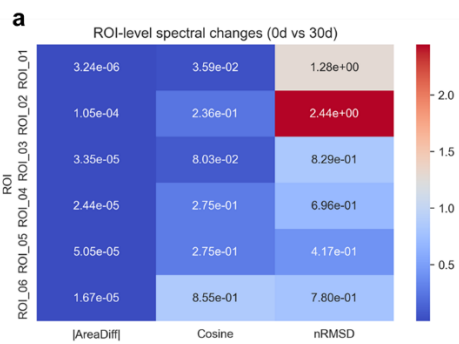
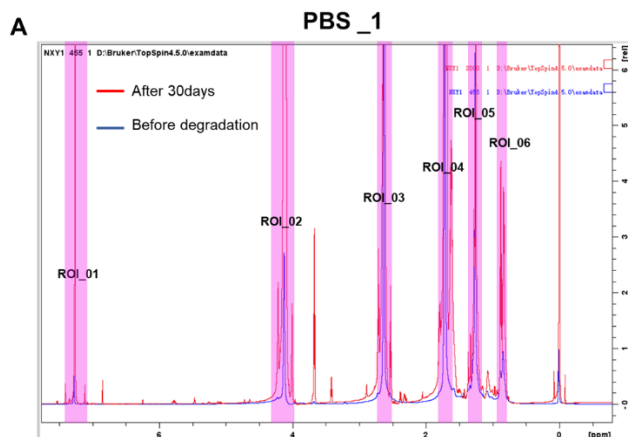
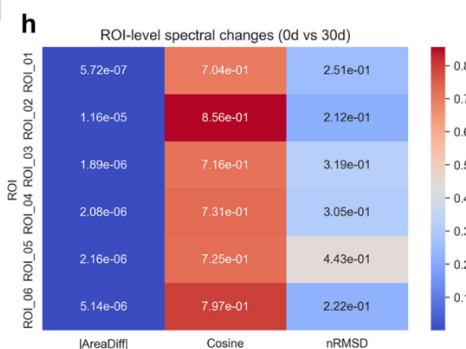
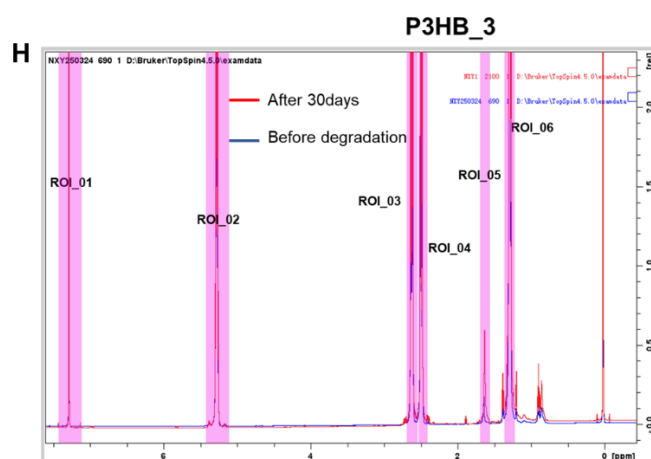
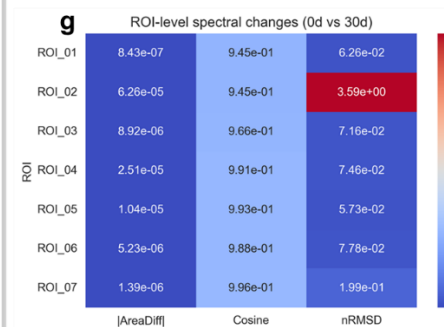
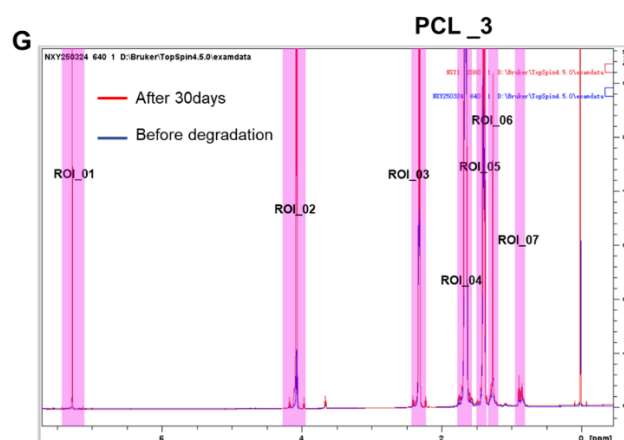
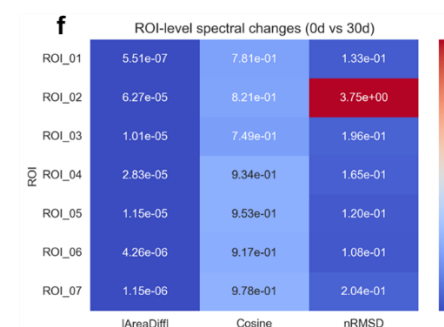
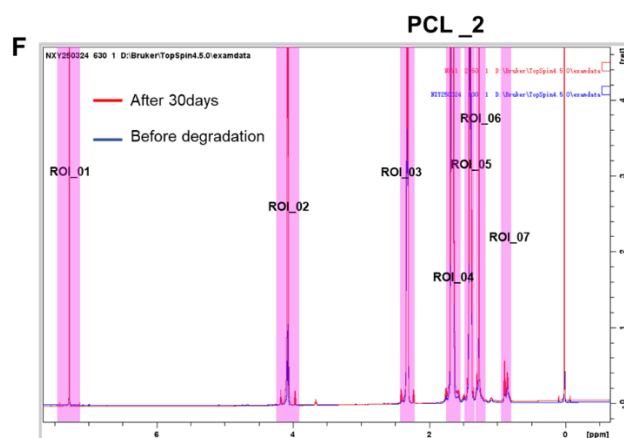
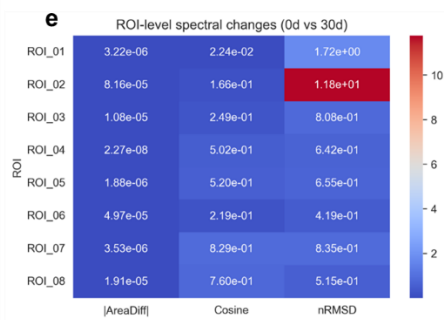
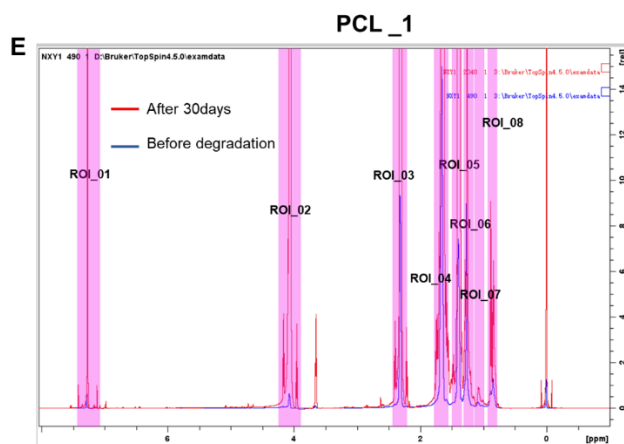
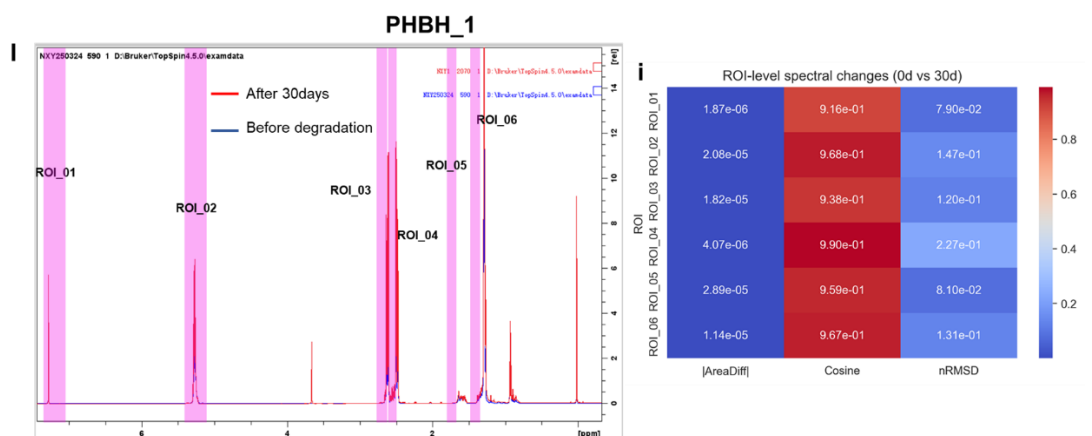


Fig. S3 Random Forest regression analysis. (A)–(H) Scatter plots show the correlation between actual and predicted values for (A) thermal history index ($R^2 = 0.34$), (C) melting temperature ($R^2 = 0.81$), (E) crystallization temperature ($R^2 = 0.48$), and (G) glass transition temperature ($R^2 = 0.62$). Red dashed lines represent ideal correlations ($y = x$). (B, D, F, H) Corresponding bar charts indicate feature importance for each prediction. Train data : red, Test data : blue.

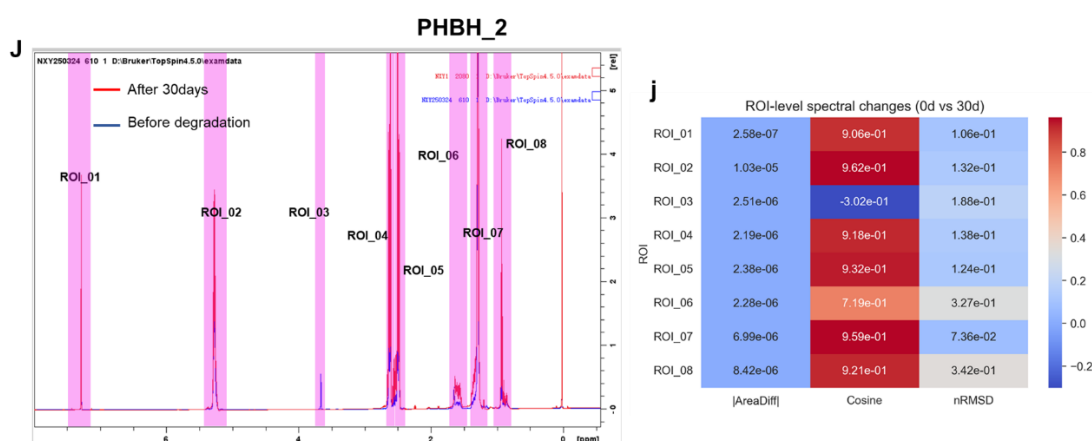




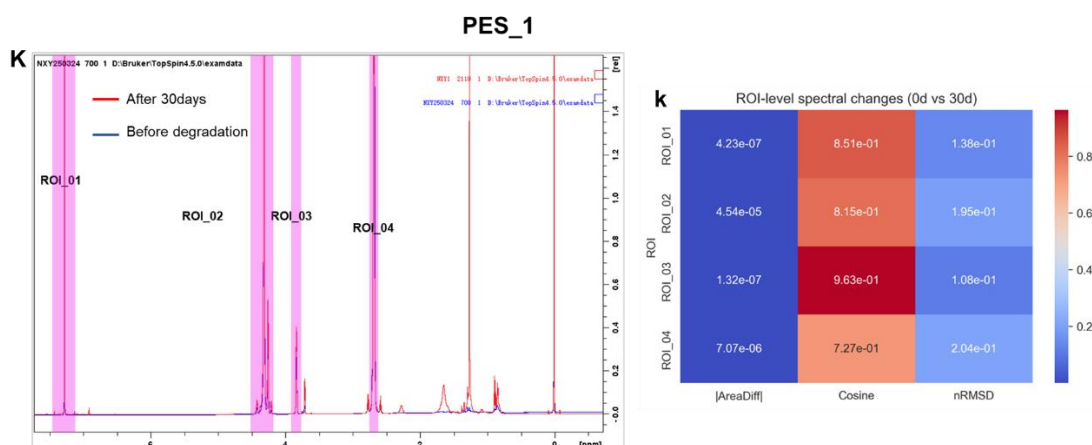
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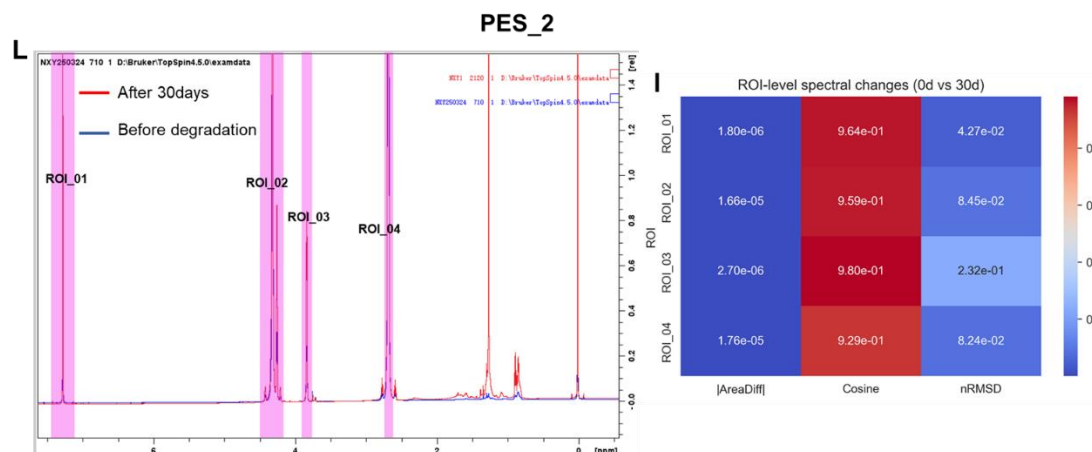
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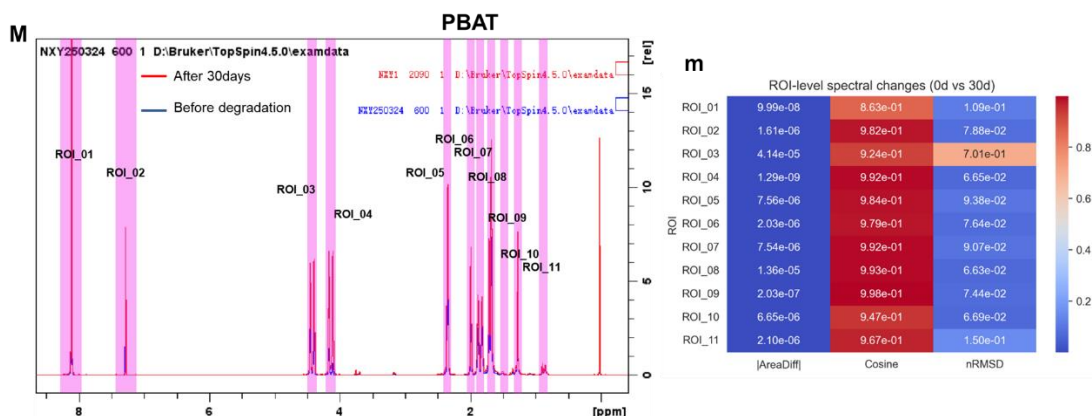


Fig. S4 Comparison of polymers' ^1H NMR spectra before degradation (blue) and after 30 days of exposure (red). Shaded regions indicate predefined regions of interest (ROIs) used for quantitative comparison. The heatmap summarizes ROI-level spectral changes between 0 and 30 days based on absolute area difference, cosine similarity, and normalized root mean square deviation (nRMSD).

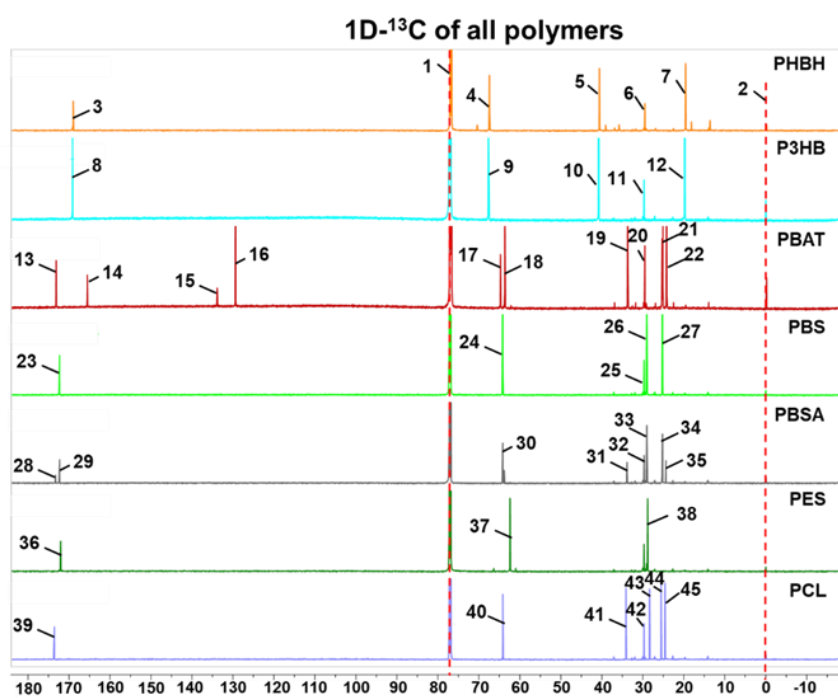


Fig. S5 Chemical-structure features captured by ^{13}C NMR spectra. From bottom to top: PHBH, P3HB, PBAT, PBS, PBSA, PES, PCL. The x-axis represents chemical shift (δ , ppm).

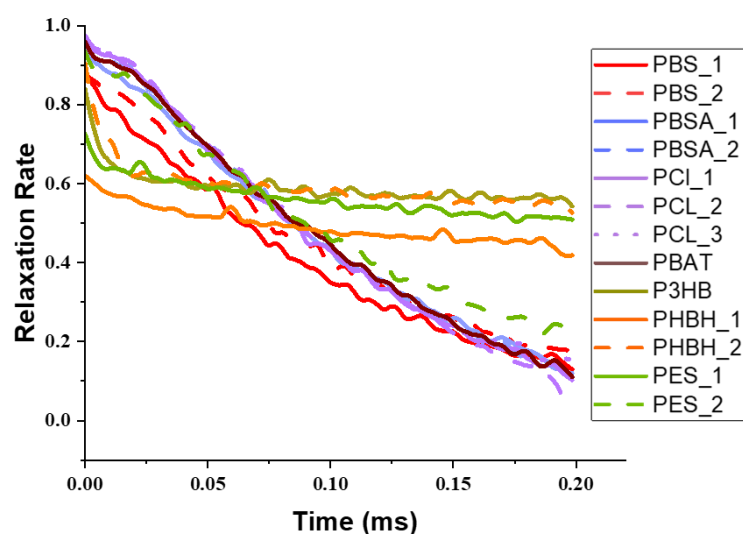


Fig. S6 MAPE (TD-NMR) denoise smoothing curve of all polymers. Each curve represents one polymer sample, with color coding corresponding to polymer types as indicated on the right. Polymer name_x denote different distinct grades or formulations of polymers (Table S2).

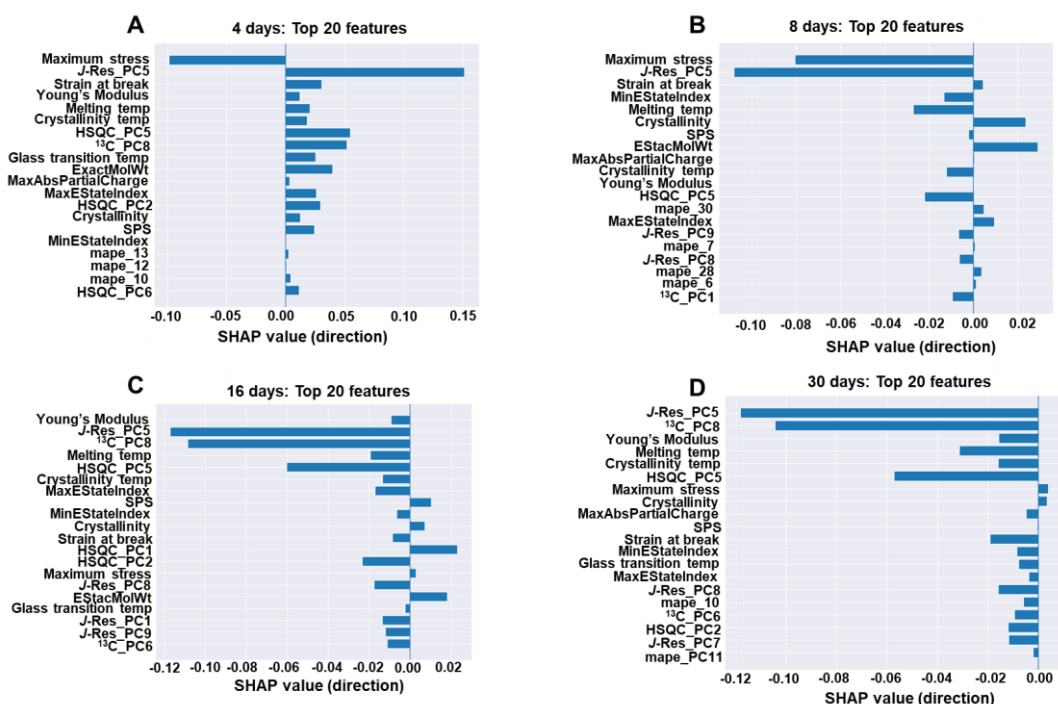


Fig. S7 Visualization of CNN-derived negative SHAP values reveals stage-specific inhibitory feature contributions in polymers mass loss.

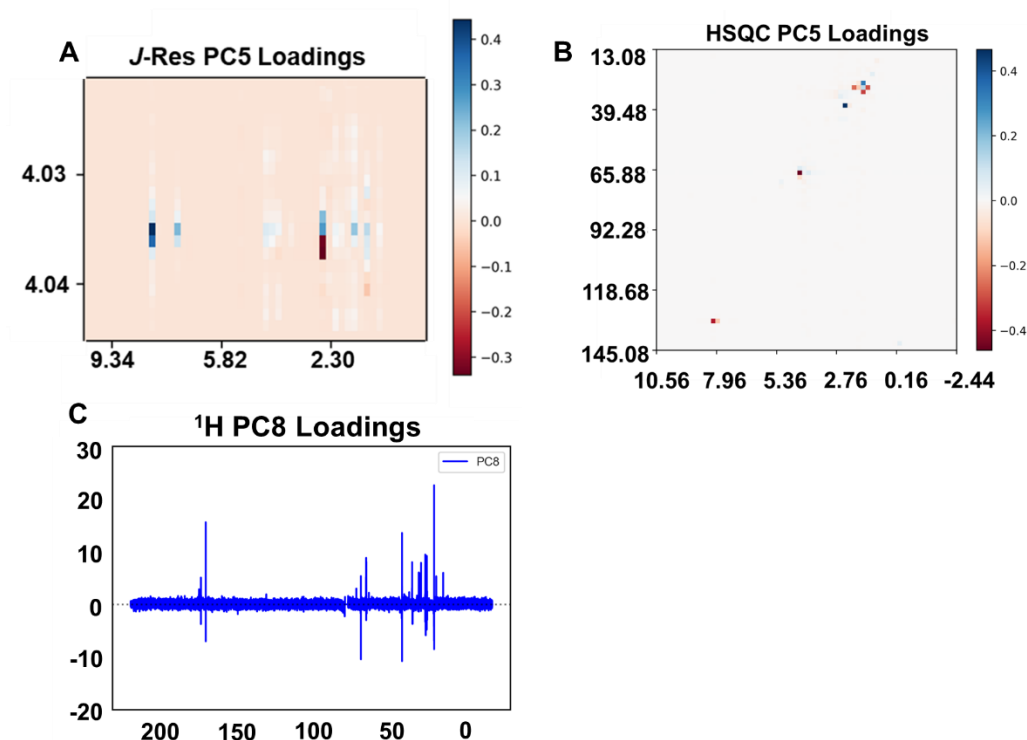


Fig. S8 Principal component loadings of *J*-Res/HSQC/¹H spectra inputs with SHAP-informed feature highlights. (A) *J*-Res PC5 loadings, (B) HSQC PC5 loadings and (C) ¹H PC8 loadings. Numbered peaks indicate SHAP-informed high-importance features. Color bars represent loading values, where blue indicates positive contribution and red indicates negative contribution to *J*-Res PC5 and HSQC PC5.

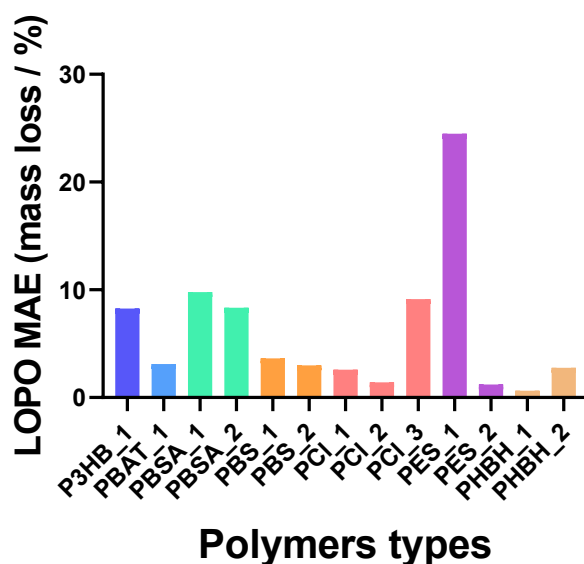


Fig. S9 Comparison of model performance under random splitting and leave-one-polymer-out (LOPO) validation.

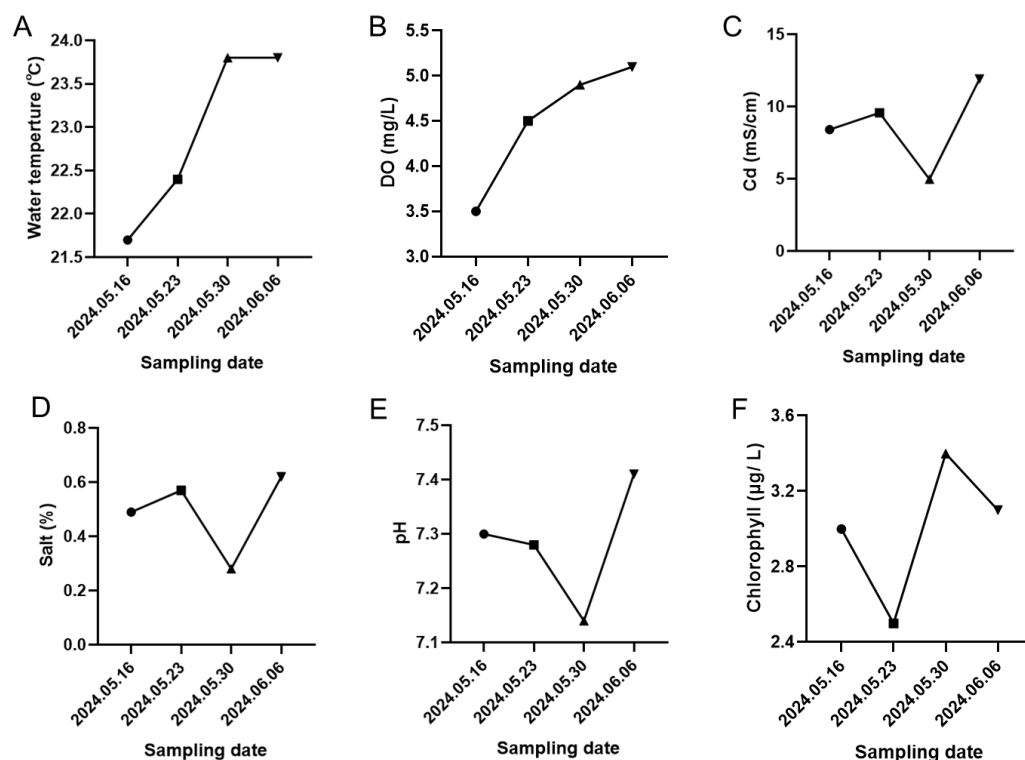


Fig. S10 Water environmental parameters during the degradation experiment: (A) water temperature, (B) dissolved oxygen (DO), (C) Cd, (D) salinity, (E) pH, and (F) chlorophyll concentration. Measurements were performed weekly throughout the experimental period.

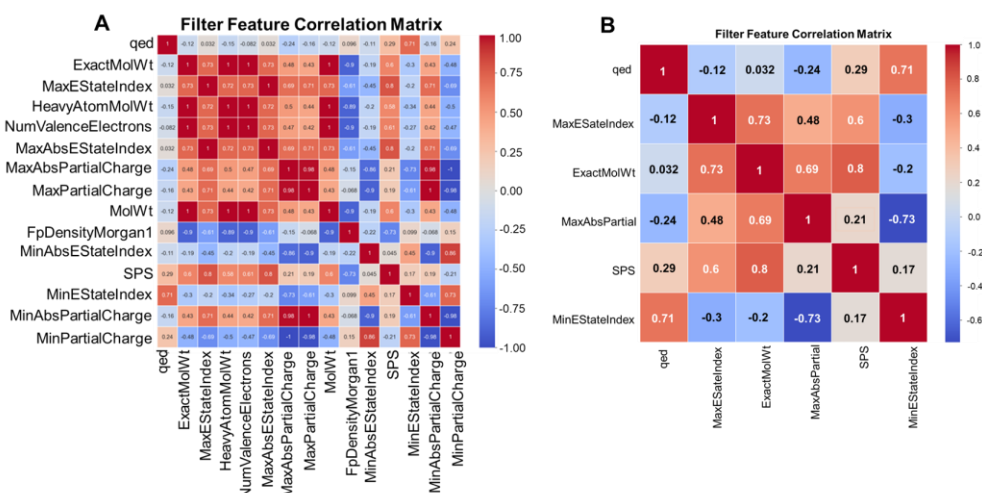


Fig. S11 Correlation matrices of selected RDKit features. (A) Correlation between RDKit features and target properties. (B) Low inter-feature correlation among the selected six features.

Polymer	Chemical Structure
Poly(butylene succinate) PBS	
Poly(butylene succinate-co-butylene adipate) PBSA	
Poly(ε-caprolactone) PCL	
Poly(3-hydroxybutyrate-co-3-hydroxyhexanoate) PHBH	
Poly(3-hydroxybutyrate) P3HB	
Poly(butylene adipate-co-terephthalate) PBAT	
Poly(ethylene succinate) PES	

Table S2 Thermal and Structural Descriptors of Polymers

Polymers name	Crystallization temperature ($T_c/^{\circ}\text{C}$)		Mw (g/mol)	Glass transition temperature ($T_g/^{\circ}\text{C}$)	Backbone/ End Group (BB/EG, %)	Melting temperature ($T_m/^{\circ}\text{C}$)
PBS_1	Low	29	-	-15	1.15×10^1	115
	High	72	-	-15	1.15×10^1	115
PBS_2	Low	29	-	-20	1.22×10^1	115
	High	72	-	-25	1.22×10^1	116
PBSA_1	Low	5	-	-36	1.25×10^1	89
	High	44	-	-31	1.25×10^1	90
PBSA_2	Low	5	-	-21	1.29×10^1	89
	High	44	-	-11	1.29×10^1	90
PCL_1	Low	-6	2.50×10^4	-70	6.10×10^0	62
	High	33	2.50×10^4	-70	6.10×10^0	65
PCL_2	Low	-9	8.00×10^4	-67	8.20×10^0	61
	High	29	8.00×10^4	-60	8.20×10^0	61
PCL_3	Low	-6	3.70×10^4	-62	8.70×10^0	63
	High	32	3.70×10^4	-68	8.70×10^0	63
PES_1	Low	17	1.00×10^4	-27	6.10×10^0	100
	High	58	1.00×10^4	-23	6.10×10^0	100
PES_2	Low	-31	1.00×10^4	-31	7.20×10^0	95
	High	-23	1.00×10^4	-23	7.20×10^0	99
PHBH_1	Low	-8	-	-8	1.52×10^1	162
	High	-7	-	-7	1.52×10^1	163
PHBH_2	Low	-8	-	-8	9.10×10^0	150
	High	-7	-	-7	9.10×10^0	148
P3HB	Low	4	-	-4	3.48×10^1	175
	High	3	-	3	3.48×10^1	176
PBAT	Low	-31	-	-31	1.08×10^1	121
	High	36	-	-36	1.08×10^1	127

Table S3 Selected RDKit Descriptors Relevant to Polymer Properties

Polymer name	qed	ExactMol Weight	MaxEState Index	MaxAbs Partial Charge	SPS	MinEState Index
PBS	3.32×10^{-1}	1.76×10^2	1.06×10^1	4.8×10^{-1}	9.42×10^0	-1.19×10^0
PBAT	3.74×10^{-1}	3.04×10^2	1.13×10^1	4.7×10^{-1}	1.04×10^1	-2.2×10^{-1}
PCL	4.25×10^{-1}	1.16×10^2	9.71×10^0	4.0×10^{-1}	9.13×10^0	2.5×10^{-1}
PBSA	2.94×10^{-1}	3.08×10^2	1.06×10^1	4.8×10^{-1}	9.29×10^0	-1.19×10^0
PHBH	5.44×10^{-1}	2.76×10^2	1.07×10^1	4.7×10^{-1}	9.58×10^0	-1.3×10^{-1}
PES	3.06×10^{-1}	1.32×10^2	1.02×10^1	4.6×10^{-1}	8.56×10^0	-6.0×10^{-1}
P3HB	5.07×10^{-1}	1.16×10^2	1.05×10^1	4.7×10^{-1}	9.50×10^0	-1.2×10^{-1}

Table S4 Experimental Toughness of Polymers

Polymers name	T_c	Young's modulus (MPa)	Strain at break	Maximum stress (MPa)
PBS_1	Low	1.94×10^2	1.50×10^{-1}	3.40×10^1
	High	1.96×10^2	1.60×10^{-1}	3.50×10^1
PBS_2	Low	2.28×10^2	1.60×10^{-1}	3.70×10^1
	High	2.08×10^2	1.50×10^{-1}	2.40×10^1
PBSA_1	Low	1.11×10^2	1.40×10^{-1}	1.50×10^1
	High	1.25×10^2	1.20×10^{-1}	1.40×10^1
PBSA_2	Low	7.80×10^1	2.10×10^{-1}	1.70×10^1
	High	7.70×10^1	2.00×10^{-1}	1.60×10^1
PCL_1	Low	1.77×10^2	1.10×10^{-1}	2.00×10^1
	High	1.54×10^2	1.60×10^{-1}	1.90×10^1
PCL_2	Low	7.30×10^1	1.80×10^{-1}	1.60×10^1
	High	6.60×10^1	1.30×10^{-1}	1.50×10^1
PCL_3	Low	1.36×10^2	1.40×10^{-1}	1.90×10^1
	High	1.06×10^2	1.40×10^{-1}	1.60×10^1
PES_1	Low	1.77×10^1	6.60×10^{-2}	1.20×10^1
	High	1.37×10^1	3.10×10^{-2}	2.70×10^1
PES_2	Low	1.50×10^1	3.10×10^{-2}	1.20×10^0
	High	3.80×10^1	9.90×10^{-2}	1.90×10^0
PHBH_1	Low	4.64×10^2	2.60×10^{-2}	1.17×10^1
	High	3.61×10^2	3.60×10^{-2}	1.38×10^1
PHBH_2	Low	6.95×10^2	2.90×10^{-2}	1.82×10^1
	High	5.82×10^2	4.70×10^{-2}	2.55×10^1
P3HB	Low	6.76×10^2	4.40×10^{-2}	3.02×10^1
	High	8.39×10^2	6.90×10^{-2}	3.14×10^1
PBAT	Low	1.40×10^1	4.40×10^{-1}	7.20×10^0
	High	1.30×10^1	4.50×10^{-1}	7.10×10^0

Table S5 NMR HSQC Structure Information for All Polymers

ID	Polymers name	¹³ C (ppm)	¹ H (ppm)	Multiplicity	Assignment	Structural unit
1	-	77.19	7.26			CDCl ₃
2	-	140.00	0.00			TMS
3	PHBH	70.60	5.23	q	α-CH	3HH
4		67.70	5.25	q	α-CH	3HB
5		39.29	2.46	dd/m	β-CH ₂	3HB
6		40.82	2.59	dd/m	β-CH ₂	3HB
7		40.90	2.48	dd/m	β-CH ₂	3HH
8		19.80	1.27	d	γ-CH ₃	3HB
9		29.80	1.23	t	ε-CH ₂	3HH
10		35.90	1.54	s	ω-CH ₃	3HH
11		13.80	0.93	s	CH ₃	3HH terminal
12	P3HB	67.90	5.24	q	α-CH	3HB
13		41.00	2.59	dd	β-CH ₂	3HB
14		40.80	2.45	dd	β-CH ₂	3HB
15		19.80	1.24	d	γ-CH ₃	3HB
16	PBAT	129.70	8.10	s	CH	Terephthalate
17		65.01	4.40-4.47	m	O-CH ₂	BDO-TPA
18		65.01	4.32-4.40	m	β-CH ₂	BDO-TPA
19		64.00	4.16-4.05	m	O-CH ₂	BDO-Adipate
20		33.80	2.27-2.41	t	α-CH ₂	Adipate
21		25.35	1.98	t	β-CH ₂	Adipate
22		25.40-	1.64-1.95	m	γ-CH ₂	Adipate
23		24.50	1.62	t	δ-CH ₂ -O	BDO
24	PBS	64.20	4.10	t	α-CH ₂	BDO
25		28.80	2.60	t	α-CH ₂	Succinate
26		25.30	1.68	t	γ-CH ₂	Succinate
27		29.70	1.23	t	β-CH ₂	BDO
28	PBSA	64.20	4.10	t	α-CH ₂	BDO
29		29.20	2.61	t	α-CH ₂	Succinate
30		33.80	2.34	t	α-CH ₂	Adipate
31		25.30	1.70	t	β-CH ₂	Succinate
32		30.10	1.27	m	γ-CH ₂ /δ-CH ₂	Adipate
33	PES	62.50	4.28	t	O-CH ₂	EG, terminal
34		66.50	4.26	t	O-CH ₂	EG, internal
35		61.40	3.79	t	CH ₂ -O	EG
36		28.84	2.67	t	β-CH ₂	Succinate
37	PCL	64.40	4.03	t	α-CH ₂	Triplet
38		34.20	2.31	t	ε-CH ₂	Triplet
39		28.40	1.65	t	δ-CH ₂	Triplet
40		25.80	1.40	t	γ-CH ₂	Triplet
41		29.80	1.28	t	β-CH ₂	Triplet

Table S6 NMR J-Res Structure Information for All Polymers

ID	Polymers name	¹ H shift (ppm)	J-coupling (Hz)	Multiplicity	Assignment	Structural unit
1	-	7.24	-1.27-2.41	-	-	CDCl ₃
2	-	0.00	-2.70-4.25	-	-	TMS
3	PHBH	5.23	-10.76-12.32	dd	α-CH	3HB/3HH
4		2.60-2.64	-12.82-17.16	t/m	-CH ₂ -OH	3HH
5		2.46-2.59	-15.25-13.45	t/q	β-CH ₂	3HH
6		1.27	-7.78-10.46	d/q	γ-CH ₃	3HB
7		0.90-0.94	-8.35-9.89	d	σ-CH ₃	3HH
8	P3HB	5.24	-16.24-18.41	dd	α-CH	3HB
9		2.59-2.63	-13.82-18.35	t/q	β-CH ₂	3HB
10		2.50-2.45	-15.97-15.11	t	β-CH ₂	3HB
11		1.24	-10.55-11.90	d/q	γ-CH ₃	3HB
12	PBAT	8.10	-3.60-4.44	d	CH	Terephthalate
13		4.46	-1.03-2.52	m	O-CH ₂	BDO-TPA
14		4.39	-7.32-8.77	dd/t	β-CH ₂	BDO-TPA
15		4.16	-7.14-8.58	t	O-CH ₂	BDO-Adipate
16		2.34	-0.89-2.38	m	α-CH ₂	Adipate
17		1.98	-2.09-3.85	m	β-CH ₂	Adipate
18		1.69	-8.08-9.44	t/q	γ-CH ₂	Adipate
19		1.28	-2.73-4.15	m	δ-CH ₂ -O	BDO
20	PBS	4.10	-7.57-0.010	t	α-CH ₂	BDO
21		2.64	-6.37-8.94	t/q	α-CH ₂	Succinate
22		1.73	-9.51-10.65	t	β-CH ₂	Succinate
23		1.27	-1.14-2.76	m	β-CH ₂	BDO
24	PBSA	4.10	-6.79-8.50	t	α-CH ₂	BDO
25		2.60	-4.77-7.57	t/m	α-CH ₂	Succinate
26		2.34	-0.67-2.21	m	α-CH ₂	Adipate
27		1.70	-7.03-8.68	t	β-CH ₂	Succinate
29		1.27	-1.13-2.99	m	γ-CH ₂ /δ-CH ₂	Adipate
30	PES	4.28	-4.43-5.96	t	O-CH ₂	EG, terminal
31		4.26	-4.93-6.39	t	O-CH ₂	EG, internal
32		2.67	-4.54-7.46	t/q	α-CH ₂	Succinate
33	PCL	4.03	-7.78-9.23	t	α-CH ₂	Caprolactone
34		2.31	-10.37-11.59	dd/t	ε-CH ₂	Caprolactone
35		1.63-1.69	-16.41-17.79	dd	δ-CH ₂	Caprolactone
36		1.42-1.47	-16.64-17.90	dd	γ-CH ₂	Caprolactone
37		1.28	-1.34-2.98	m	β-CH ₂	Caprolactone

Table S7 1D ^{13}C NMR Structure Information for All Polymers

ID	Polymers name	^{13}C (ppm)	Multiplicity	Assignment	Structural unit
1	-	77.14	-	-	CDCl_3
2	-	0	-	-	TMS
3	PHBH	169.20	s	$\text{C}=\text{O}$	3HB / 3HH
4		67.70	q	$\alpha\text{-CH}$	3HB
5		40.90	t	$\beta\text{-CH}_2$	3HH
6		29.80	t	$\varepsilon\text{-CH}_2$	3HH
7		19.80	d	$\gamma\text{-CH}_3$	3HB
8	P3HB	169.10	s	$\text{C}=\text{O}$	3HB
9		67.90	q	$\alpha\text{-CH}$	3HB
10		40.80	t	$\beta\text{-CH}_2$	3HB
11		29.80	d	$\beta\text{-CH}_3$	3HB
12		19.80	d	$\gamma\text{-CH}_3$	3HB
13	PBAT	173.50	s	$\text{C}=\text{O}$	Adipate
14		165.80	s	$\text{C}=\text{O}$	Terephthalate
15		134.10	s	Aromatic C	TPA
16		129.70	d	CH	Terephthalate
17		65.10	m	O-CH_2	BDO-TPA
18		64.00	m	O-CH_2	BDO-Adipate
19		33.80	t	$\alpha\text{-CH}_2$	Adipate
20		29.60	t	$\beta\text{-CH}_2$	Adipate
21		25.60	m	$\gamma\text{-CH}_2$	Adipate
22		24.50	t	$\delta\text{-CH}_2\text{-O}$	BDO
23	PBS	172.30	s	$\text{C}=\text{O}$	Succinate
24		64.20	t	$\alpha\text{-CH}_2$	BDO
25		29.70	t	$\beta\text{-CH}_2$	BDO
26		29.00	t	$\beta\text{-CH}_2$	Succinate
27		25.30	m	$\gamma\text{-CH}_2$	Succinate
28	PBSA	173.70	s	$\text{C}=\text{O}$	Adipate
29		172.40	t	$\text{C}=\text{O}$	Succinate
30		64.20	t	$\alpha\text{-CH}_2$	BDO
31		33.80	t	$\alpha\text{-CH}_2$	Adipate
32		29.72	t	$\gamma/\delta\text{-CH}_2$	Adipate
33		29.20	t	$\gamma/\delta\text{-CH}_2$	Adipate
34		25.30	t	$\beta\text{-CH}_2$	Succinate
35		24.50	t	$\beta\text{-CH}_2$	BDO
36	PES	172.20	s	$\text{C}=\text{O}$	Succinate
37		62.50	m	O-CH_2	EG
38		28.84	t	$\beta\text{-CH}_2$	Succinate
39	PCL	173.50	s	$\text{C}=\text{O}$	Caprolactone
40		64.34	t	$\alpha\text{-CH}_2$	Caprolactone
41		34.20	t	$\varepsilon\text{-CH}_2$	Caprolactone
42		29.80	t	$\beta\text{-CH}_2$	Caprolactone
43		28.40	m	$\gamma\text{-CH}_2$	Caprolactone
44		25.70	t	$\beta/\alpha\text{-CH}_2$	Caprolactone
45		24.58	t	$\text{CH}_2\text{-OH}$	Caprolactone

Table S8 Abbreviations and Corresponding Multiplicity Terms Used in NMR Spectra.

Abbreviation	Full name
t	triplet
q	quartet
dd	doublet of doublets
dq	doublet of quartets
m	multiplet

Reference

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