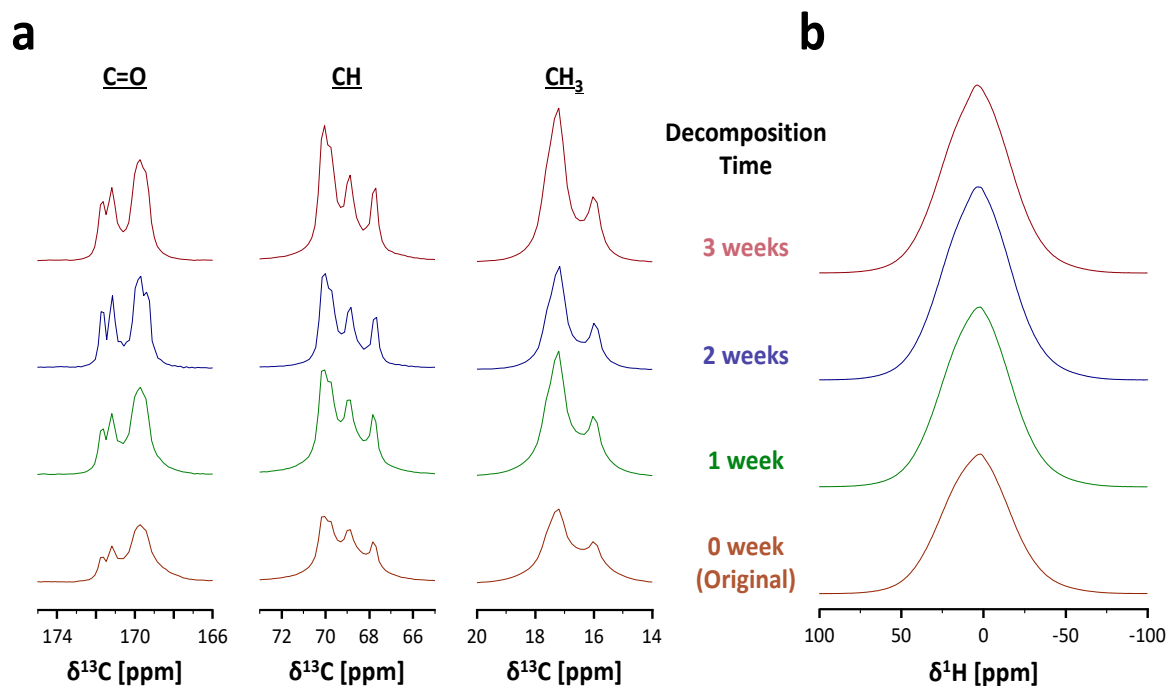# Supplementary Materials: Decomposition Factor Analysis Based on Virtual Experiments throughout Bayesian Optimization for Compost-Degradable Polymers

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Figure 1. Stacked plot of (a) cross-polarization and magic angle spinning (13C-CP/MAS) spectra and (b) 1H wide-line nuclear magnetic resonance (NMR) spectra of sample S/A during the compost-degradation experiments. (a) also shows the carbonyl group (C=O), methine group (CH), and methyl group (CH3).
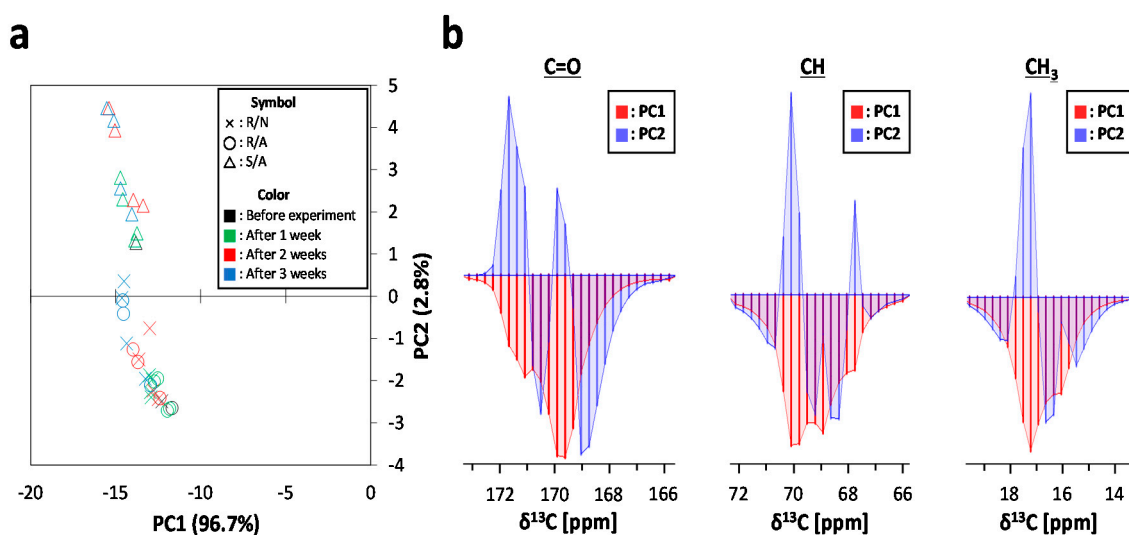
Figure S2. Principal component analysis (PCA) using the 13C-CP/MAS spectra of polylactic acid (PLA). (a) PCA scores, symbolized by sample name and colored by each decomposition period. (b) PCA loadings, colored red for PC1 and blue for PC2. (b) also shows the carbonyl group (C=O), methine group (CH), and methyl group (CH3). Details of samples are listed in Table S1.
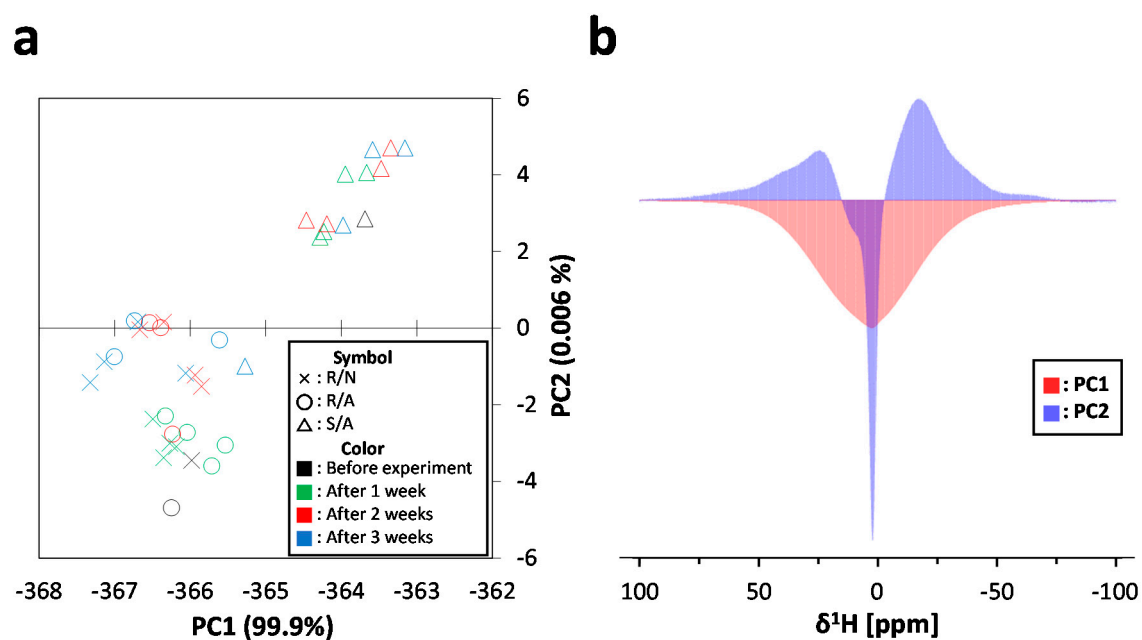
Figure S3. PCA using the 1H wide-line NMR spectra of PLA. (a) PCA scores, symbolized by sample name and colored by decomposition period. (b) PCA loadings, colored red for PC1 and blue for PC2. Details of samples are listed in Table S1.

a   **b**
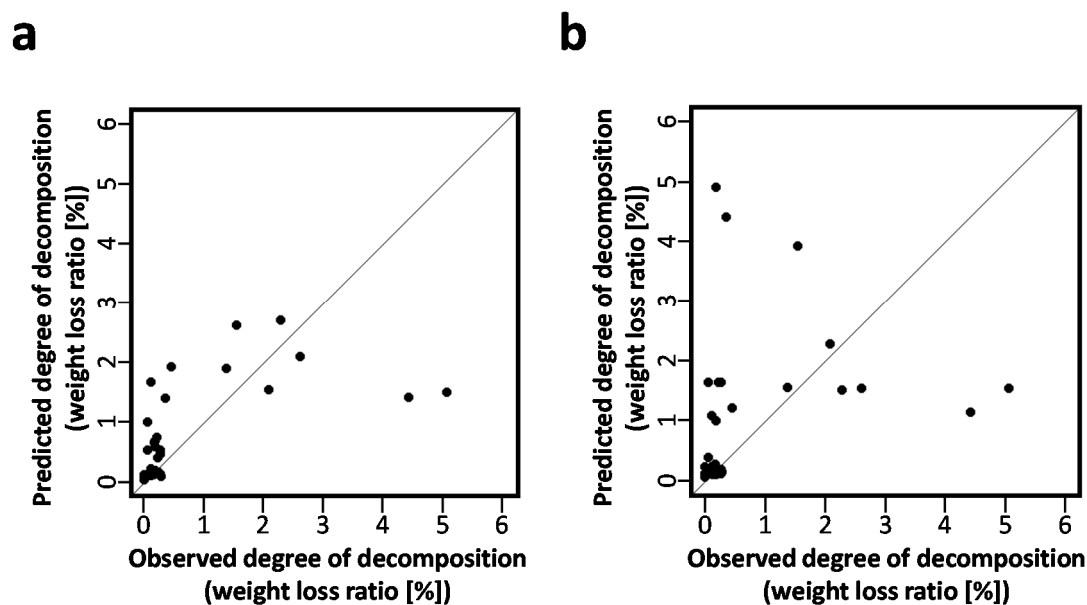
Figure S4. The results of predictive modeling of the degree of decomposition using weight-loss ratio, analytical values, experimental conditions, and PCA scores of 13C-CP/MAS spectra. (a) A bivariate plot of the observed and predicted weight-loss ratio of validation data. The predictive model was constructed by random forest (RF) machine learning. The coefficient of determination (R2) is 0.38 and root mean square error (RMSE) is 0.76%. (b) A bivariate plot of the observed and predicted weight-loss ratio of the validation data. The predictive model was constructed using XGBoost machine learning algorithm. R2 is 0.08 and RMSE is 1.30%.

a   **b**
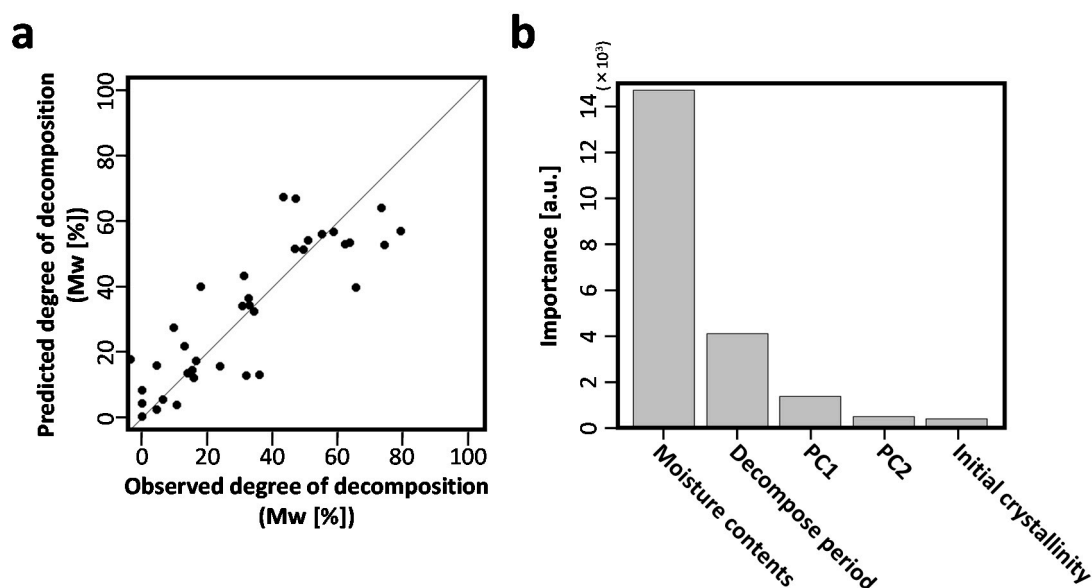
Figure S5. The results of predictive modeling of the degree of decomposition using weight average molecular weight (Mw), analytical values, experimental conditions, and PCA scores of 1H wide-line NMR spectra by RF machine learning. (a) A bivariate plot of the observed and predicted Mw of validation data. R2 is 0.73 and RMSE is 12.42%. (b) Bar chart of importance in the decomposition degree predictive model. Details of PC1 and PC2 scores used for machine learning are shown in Figure S3.

Table 1. List of PLA samples molded by the press-molding machine.

Sample name*	Cooling condition after pressing	Anneal treatment		Initial crystallinity
		Temperature	Time	
R/N	At room temperature	—	—	3.3%
R/A	At room temperature	110°C	15 minutes	25.4%
S/A	To stand still after stopping heater	110°C	56 hours	46.1%

* R, rapid cool; S, slow cool; N, non-annealed; A, annealed