AROPHA

Use Case

Accelerate Persistence Screening of Biopolymers for Compostable Products

Precision and efficiency in predicting biodegradation profiles using ArophaAI

Goal

Predict biodegradation profile of a biopolymer to ensure it can be sufficiently biodegraded when it enters industrial compost environments and will meet certification requirements for advertised compostability profile.

Challenge

Determining the biodegradation rate for a single polymer under lab-scale compost conditions is a variable, complex process. It typically requires multiple iterations of experimental testing which take 12-24 weeks and has high costs associated with testing. When examining many different polymers, it becomes time-prohibitive and costly to test all possible options in the lab.

Solution

Utilize an expert-trained AI model in ArophaAI that captures the structure-biodegradation relationship for the polymer and models the breakdown of the polymer under standard or custom test conditions.

ArophaAI can use novel applications of AI models to read polymer compositions and infer the biodegradation rate of substances outside the original training set.

The model can be used to quickly screen through a large range of target polymers to identify structures with a high likelihood of meeting physical testing requirements, freeing up laboratory resources, reducing development costs, and minimizing time-intensive, iterative testing cycles.

21564 Alexander Road, Bedford, OH 44146 USA
sales@aropha.com | https://www.aropha.com | +1 (440) 252-5235

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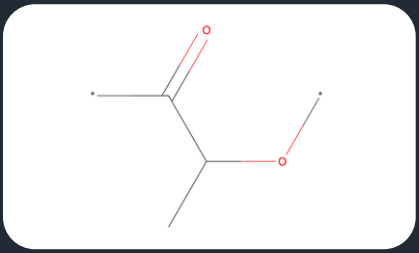
Example



Experiment Design:

Monomer SMILES	Deg. of Polymerization	Morphology	Thickness (mm)	Method	End Point (Day)
*OC(C)C(*)=O	100	Double sided layer	1	ISO 14855	180

Poly(lactic acid): PLA

Polylactic acid is a thermoplastic polyester (or polyhydroxyalkanoate) that has become the most consumed bioplastic in the world, accounting for ~26% of total bioplastic demand in 2023. It has a wide range of use cases from 3D printed filaments to varying consumer goods; although it is mainly used for short-lived, disposable packaging which is often aimed at being compostable. In this example, we examine one PLA homopolymer with the intent of determining if it is a good candidate to make compostable products.

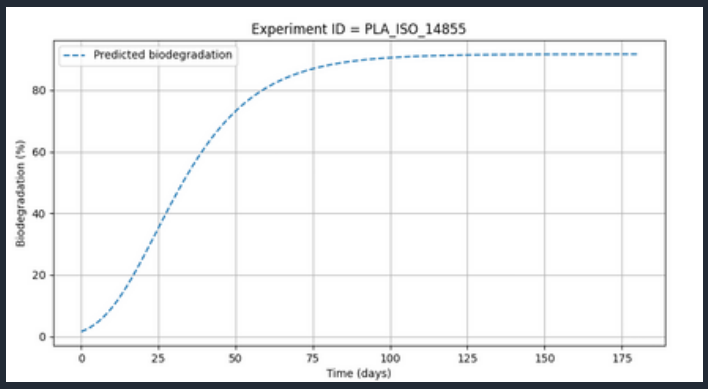
InChIKey: BSABBBMNWQWLLU-UHFFFAOYSA-N

SMILES: *OC(C)C(*)=O

*denotes binding site

Results

When we want to determine if something will biodegrade in industrial compost conditions, we can use a standard test method, ISO 14855. A common passing threshold for this test is achieving 90% biodegradation within a test duration of 6 months. PLA is commonly known as an industrial compostable biopolymer; however, different PLA variations can have vastly different mechanical, and environmental, properties. In the case of this structure, it showed nearly 92% degradation over 180 days, meaning it is likely a good candidate to keep pursuing for use in compostable products.



Biodegradation Achieved: 91.6% in 180 Days

Meets Passing Requirements : Yes

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