DOE Bioenergy Technologies Office (BETO) 2023 Project Peer Review

Inverse Bioproduct Design Through Machine Learning and Molecular Simulation

Performance-Advantaged Bioproducts, Bioprocessing Separations, and Plastics

PI: Brandon C. Knott, National Renewable Energy Laboratory

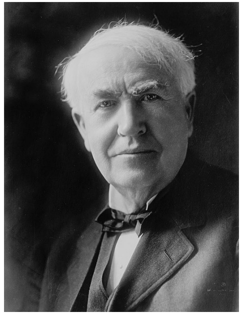
Project overview

Context
In the *quest to design better plastics*, there is a *vast design space*. An Edisonian approach is inefficient; computational tools can accelerate discovery.

History
Project start in 2018 with an initial focus on *performance-advantaged polymers*

Project goal
Predict material properties from molecular structure to facilitate *targeted synthesis* and pave the way for reduced time-to-market of PABPs

This project answers this question:
How effectively can computational methods downselect material candidates from molecular structure?



*I have not failed. I've just found **10,000 ways** that won't work.*

Thomas Alva Edison

Number of Polymers

$10^6 - 10^2 - 10^1 \rightarrow$ **PABP**

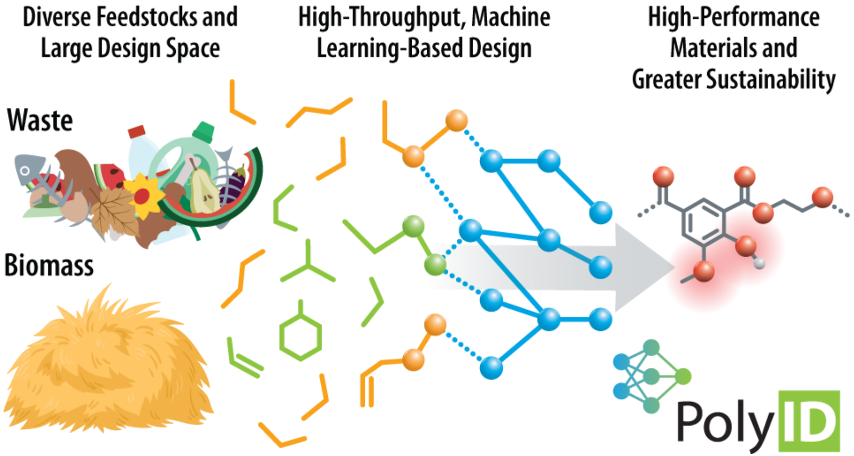
- Synthesis Candidates (PABP Synthesis)
- Machine Learning & Molecular Simulation (Inverse Design)
- Potential Materials

PABP = performance-advantaged bioproduct

1. Approach – key elements

Technical Approach

- Take advantage of the unique chemical functionality of novel building blocks from sugars, lignin-derived aromatic compounds, and more
- Focus on both polymers and small molecule PABPs
- Feed targeted materials to *Synthesis and Analysis of PABP* project
- Collaborate with other BETO projects: Biological Lignin Valorization, Bioconversion of Thermochemical Intermediates, BOTTLE Consortium, Catalytic Upgrading of Pyrolysis Products
- Apply computational tools to identify *industrially relevant technologies* and *guide industry engagement* projects



PABP = performance-advantaged bioproduct

Wilson *et al. In revision.*

1. Approach – key elements

Technical Approach

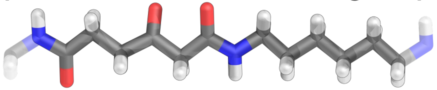
Task 1: Machine Learning (ML)

Build and deploy ML models to vastly reduce design space of potential PABPs via molecular property prediction

Frequent communication, working meetings, development of milestones, sharing results, and joint troubleshooting

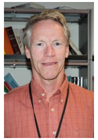
Task 2: Molecular Simulation (MS)

- Develop structure-function relationships and design principles via molecular-level insight
- Augment datasets for training ML models
- Predict performance-advantaged properties



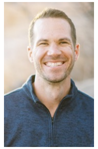
PABP = performance-advantaged bioproduct
ML = machine learning
MS = molecular simulation

Management Plan



Mark Nimlos (ML task lead)
Database development, machine learning for molecular property prediction

Michael Crowley (Former PI)
Macromolecular Simulation, QM/MM, CHARMM, Amber



Brandon Knott (MS task lead, PI)
Molecular dynamics, structure-function elucidation

Leverage expertise in multiple modeling approaches to synergize internally and with partners.

1. Approach – risks and milestones

Risks and mitigation strategies

- **Risk**: low accuracy and throughput
- **Mitigation**: incorporation of additional model features, domain of validity

- **Risk**: low interpretability of ML outputs
- **Mitigation**: molecular simulations can provide molecular insight

- **Risk**: insufficient population of database for certain substructures
- **Mitigation**: augment with additional data, either from experiment or simulation

Major milestones, Go/No-Go Decisions:

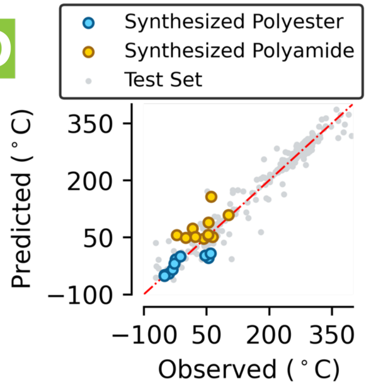
- **FY21**: Predict new polymeric materials via machine learning (PolyID) and down select to ≥5 polymers to be experimentally synthesized and characterized, demonstrating a PABP (joint with *Synthesis and Analysis of PABP* project).
- **FY22 Go/No-Go**: Demonstrate a 10% improvement in accuracy by augmenting ML datasets with molecular simulation generated data (milestone met, “Go”)
- **FY23**: Predict solubility of PET in lignin-derived solvents

- *All milestones have been met on time*
- *Most milestones have resulted in peer-reviewed publications*

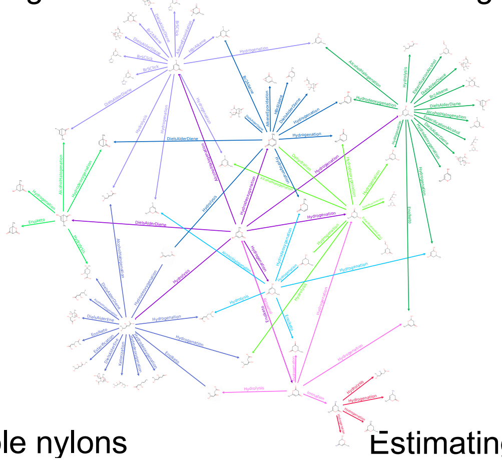
2. Progress and outcomes - outline

Integration of PolyID with synthesis partners

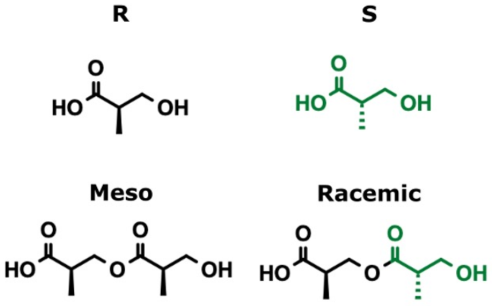
PolyID



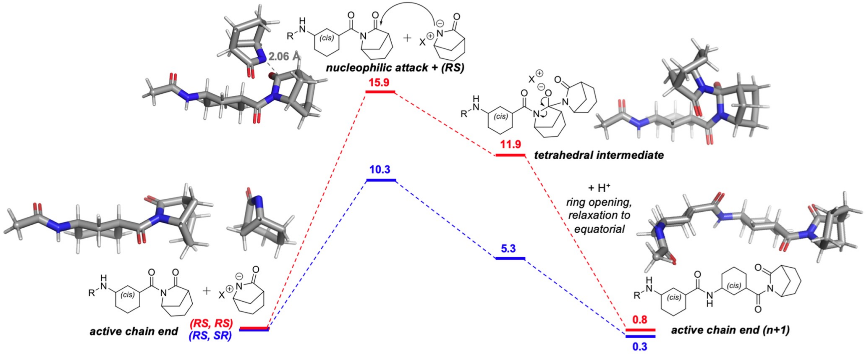
Coupling reaction network generation with machine learning



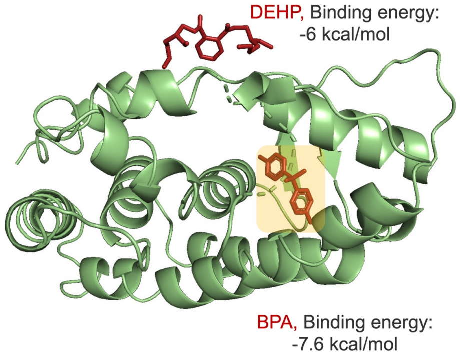
Increasing ML model accuracy by integrating tacticity



Mechanistic insight into recyclable nylons



Estimating toxicity of bio-based plasticizers



2. Progress and outcomes

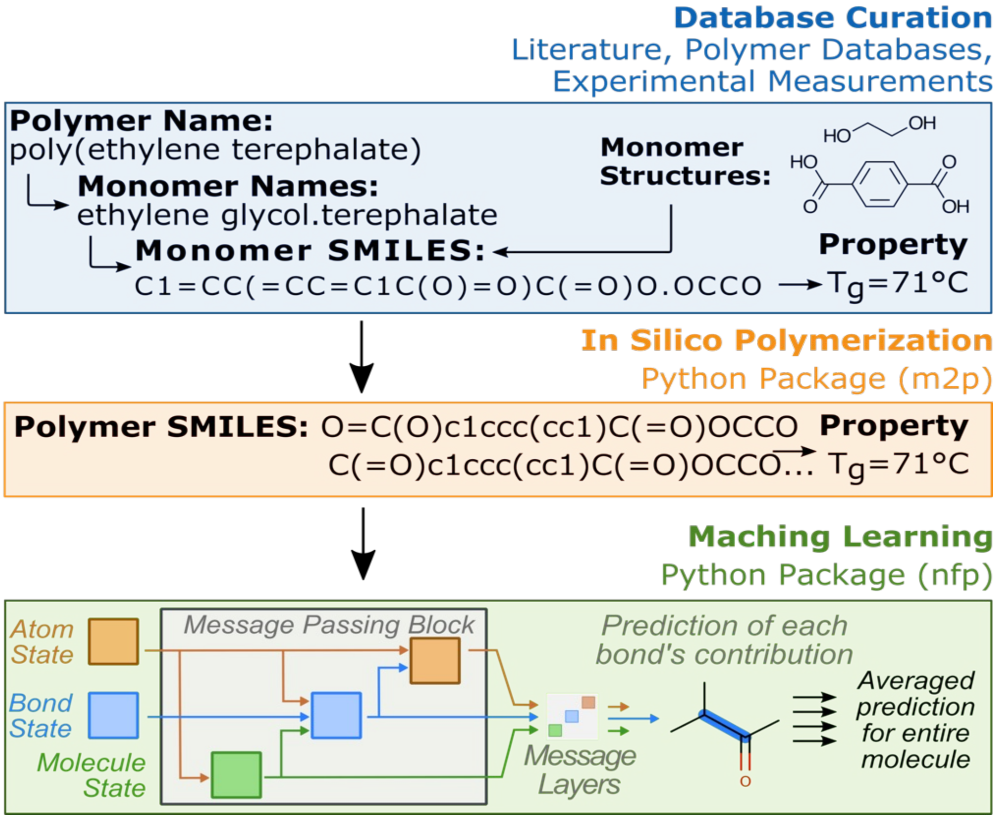
PolyID

PolyID is a machine learning tool for polym

PolyID comprises 3 components:

1. Database - links monomer structure to polymer properties. 1,791 unique polymers.
2. Automated, structure generation (*in silico* polymerization)
3. Message passing neural network for polymer property prediction

   -T_g (glass transition temperature)
   -T_m (melt temperature)
   -Barrier properties (e.g. how readily O_2, CO_2, H_2O, etc. pass through)
   -Mechanical properties (moduli)



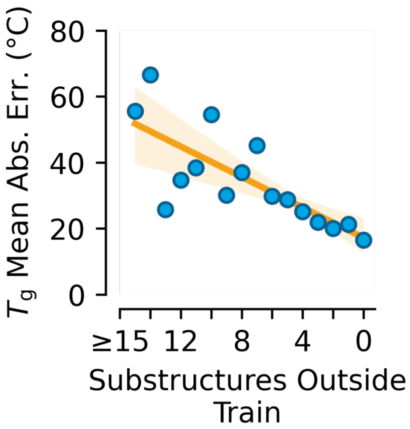
SMILES = simplified molecular input line entry system
m2p = monomers to polymers (python package)
nfp = neural fingerprint (python package)

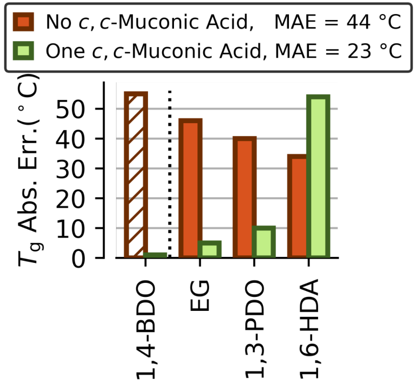
Wilson *et al. In revision.*

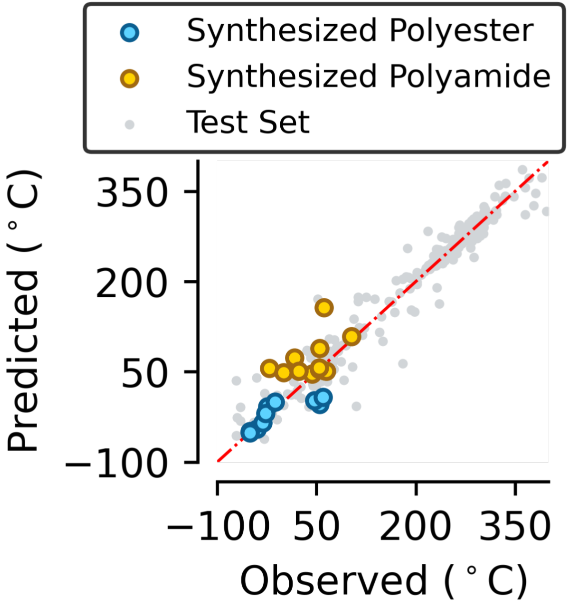
PolyID

ML predictions validated by synthesis of polyesters and polyamides

- Quantifiable relationship between model accuracy and overlap between training/test structures
- Targeted augmentation of database to increase prediction accuracy
- 10 polyesters and 12 polyamides that were not in the database were synthesized and characterized by partner PABP project (*Synthesis and Analysis of PABPs*)



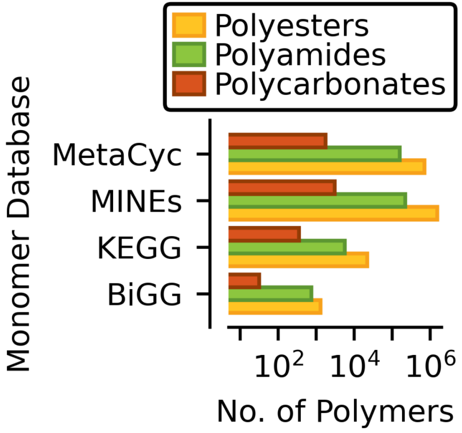




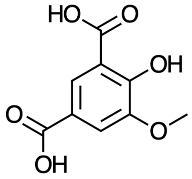
Wilson *et al. In revision.*

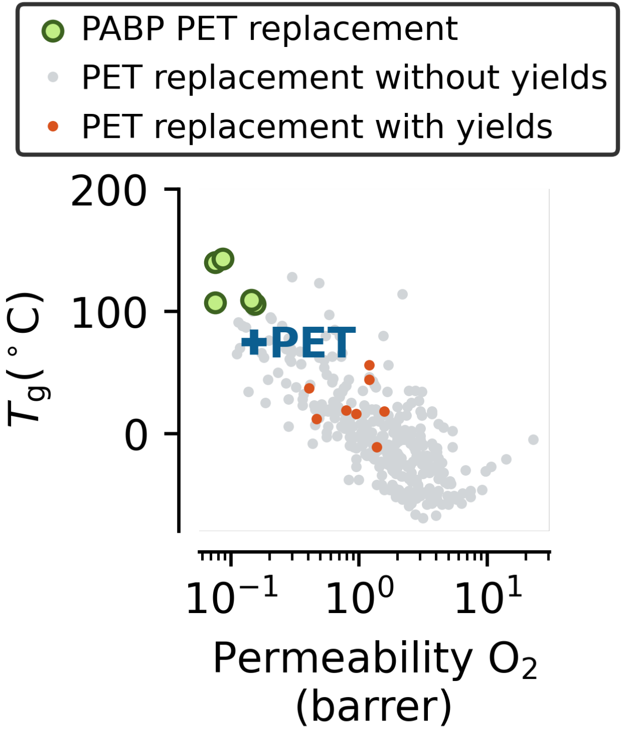
ML vastly reduces the design space for PABP PET replacements

- PABP analog of PET was targeted with a T_g above the boiling point of water and with equivalent or improved O_2 barrier properties
- 5 PABPs predicted from KEGG that met the requirements (green circles), linked to 3 diacids
- 1 polymer synthesized (poly(ethylene 5-carboxyvanillate), PEC), with T_g = 112 C



5-carboxyvanillate





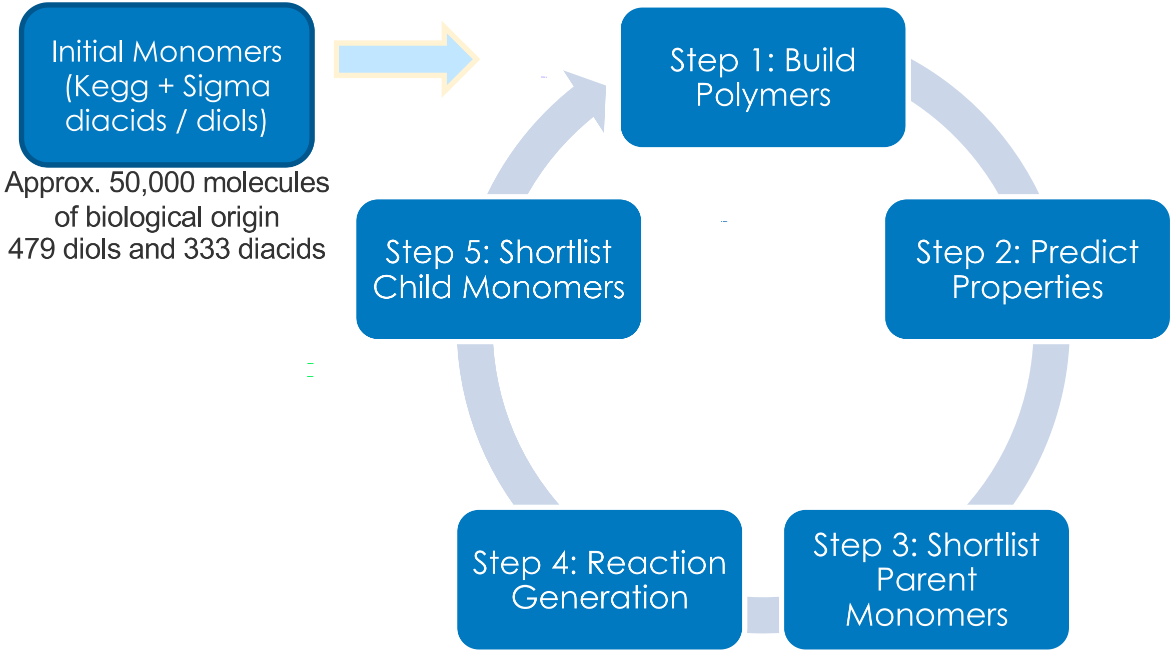
Wilson *et al. In revision.*

PET = poly(ethylene terephthalate)
T_g = glass transition temperature
KEGG = Kyoto Encyclopedia of Genes and Genomes (https://www.genome.jp/kegg/)
ML = machine learning

2. Progress and outcomes – coupled network generation

Coupling reaction network generation with ML for polymer property prediction

- Integration of PolyID[1] and Pickaxe[2] expands discovery space to chemically accessible molecules
- Initial molecules from known biological sources
- Proof of concept performed with optimizing difference of T_m and T_g for diol and diacid polyesters



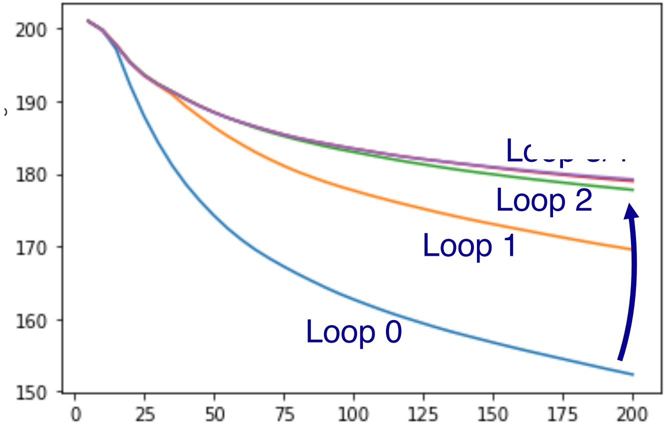
[1] Wilson *et al. In revision.*
[2] https://github.com/tyo-nu/MINE-Database
T_m = melting temperature
T_g = glass transition temperature
KEGG = Kyoto Encyclopedia of Genes and Genomes (https://www.genome.jp/kegg/)

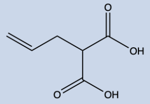
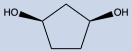
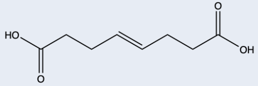
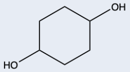
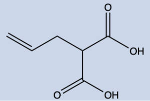
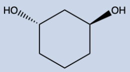
2. Progress and outcomes – coupled network generation

Pickaxe + PolyID predicts PABPs with excellent T_m-T_g

- Network generation coupled with property prediction expands the discovery space
- Increasing network expansion from one generation to two generations leads to faster property convergence and higher properties
- Increasing similarity amongst monomers across loops supports converging properties
- Further improvement of properties can be tuned by further expansion of reaction networks

T_m = melting temperature
T_g = glass transition temperature

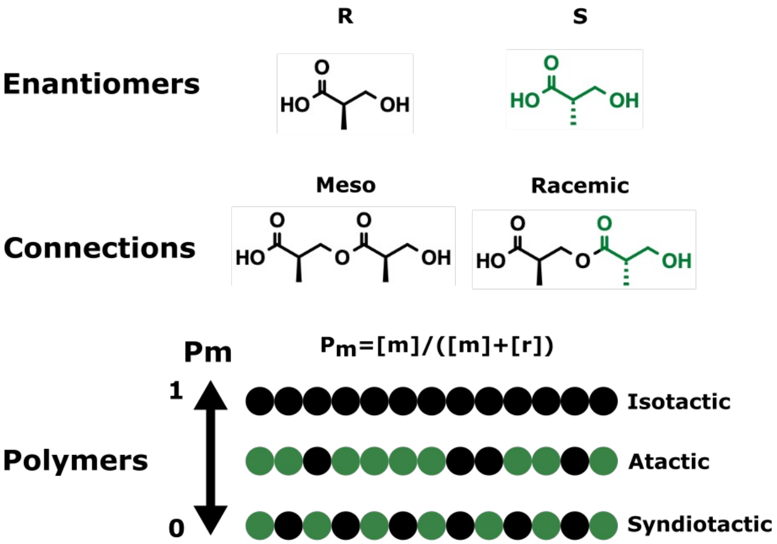


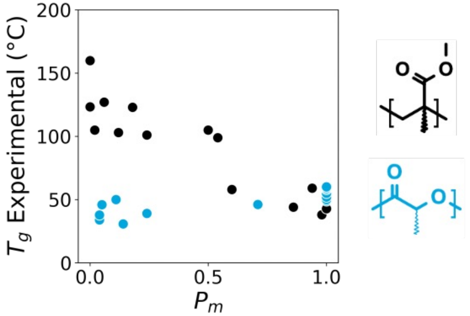
Monomer A	Monomer B	T_m T_g
		201 ⁰C
		201 ⁰C
		201 ⁰C

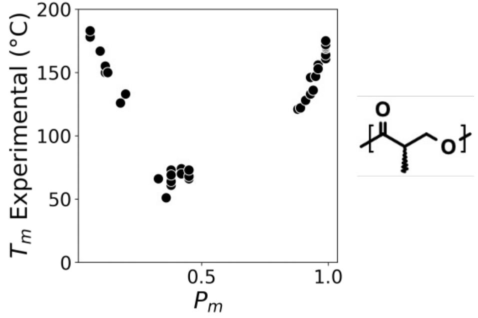
Lopez *et al. In preparation.*

There is significant potential for improvement of existing ML models by incorporating chirality

- Polymers can contain stereochemical information on the pendant groups, known as chirality.
- Chirality can have a significant impact on the properties of polymers.
- Current models do not incorporate chirality for prediction, which can introduce significant error







P_m = probability of a meso linkage
T_m = melting temperature
T_g = glass transition temperature

Shebek *et al. In preparation.*

2. Progress and outcomes – incorporating tacticity

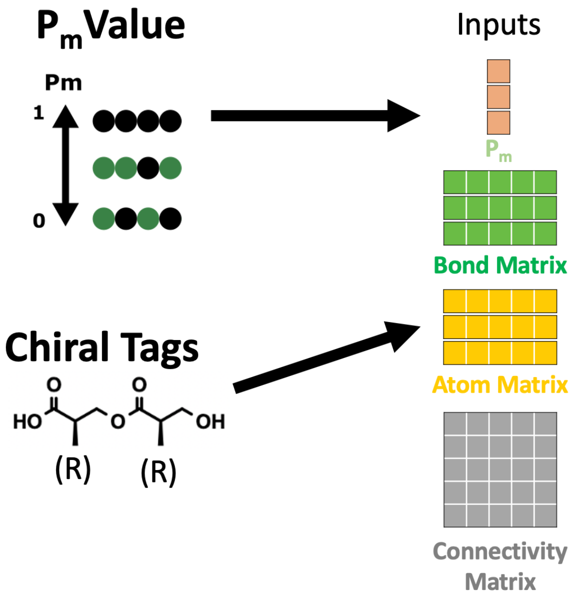
Incorporating chirality improves model predictions

We incorporate chiral information into our model in two ways:

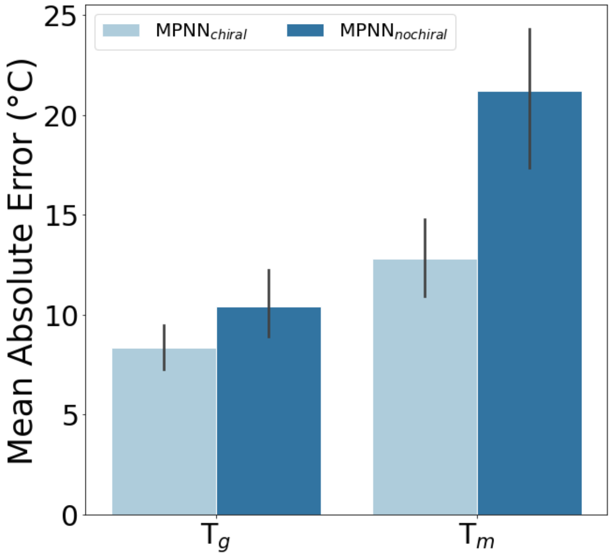
1) P_m (global)

2) Chiral tags (atom-based)

Tacticity incorporation



Including tacticity reduces error



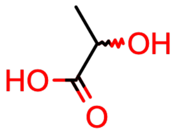
MPNN = Message Passing Neural Net
P_m = probability of a meso linkage
T_m = melting temperature
T_g = glass transition temperature

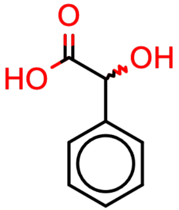
Shebek *et al. In preparation.*

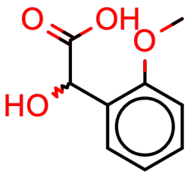
2. Progress and outcomes – incorporating tacticity

Application: PHA replacements for PET

- Many (10^5) possible polymers from KEGG
- Accurately predicted performance for a PHA copolymer (top)
- Predicted an as-yet-uncharacterized novel PHA polymer with high performance (bottom)







Poly(lactic-co-mandelic) Acid

	T_g (°C)		T_m (°C)	
Tacticity	**Pred**	**Exp**	**Pred**	**Exp**
Syndio	71	N/A	195	N/A
Atac	52	54	96	N/A
Iso	71	76	164	N/A

Poly(2-methoxymandelic) acid

	T_g (°C)		T_m (°C)	
Tacticity	**Pred**	**Exp**	**Pred**	**Exp**
Syndio	65	N/A	199	N/A
Iso	75	N/A	197	N/A

Experimental data:
Lukito, B. R., et al. (2021). *Bioresources and Bioprocessing*, *8*(1)
Pedna, A., et al. (2015). *Journal of Applied Polymer Science*, *132*(30)

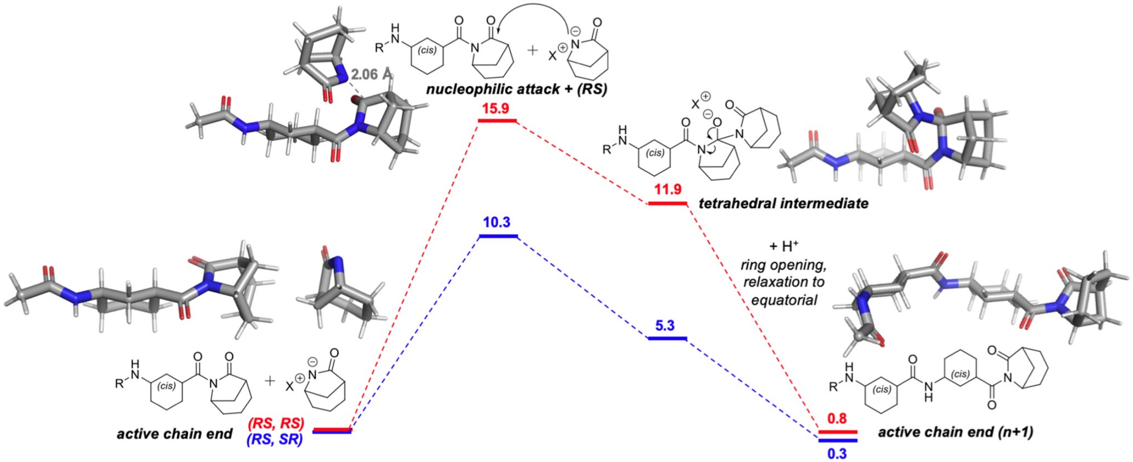
PHA = poly(hydroxyalkanoate)
T_m = melting temperature
T_g = glass transition temperature
KEGG = Kyoto Encyclopedia of Genes and Genomes (https://www.genome.jp/kegg/)

Shebek *et al. In preparation.*

2. Progress and outcomes – mechanistic understanding of redesigned nylons

Atomistic modeling rationalizes mechanisms of polymerization and chemical recyclability

- A novel, hybrid nylon (nylon 4/6) was introduced by partner projects (BOTTLE, PABP) that exhibits:
    - optical clarity
    - high T_g
    - melt processability
    - full chemical recyclability
- We employed density functional theory (DFT) to model the propagation step in order to investigate which stereoselectivity is more kinetically favorable

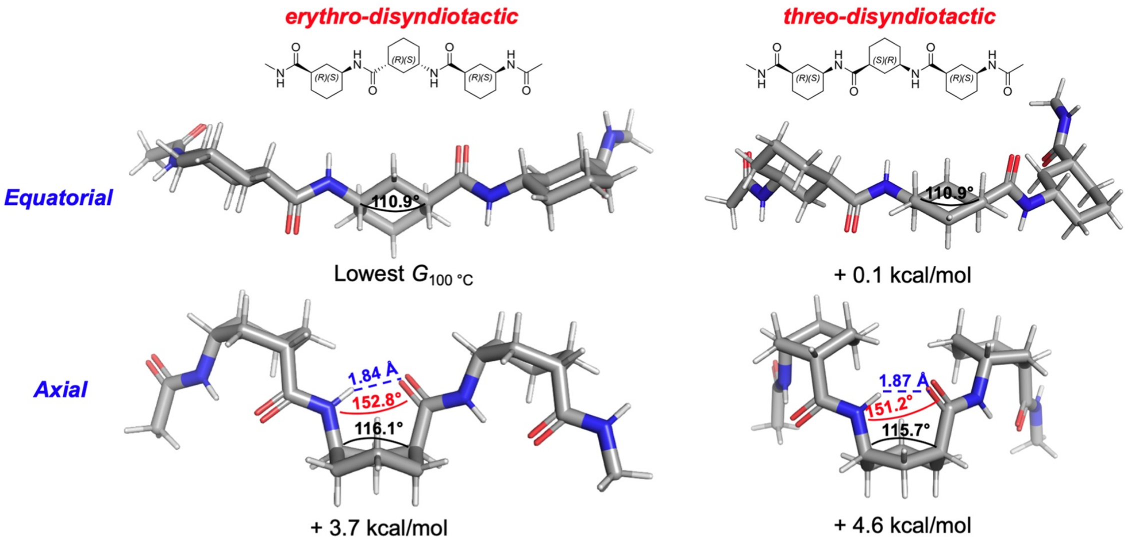


DFT = density functional theory
T_g = glass transition temperature

Cywar *et al. JACS* 2022

Atomistic modeling rationalizes mechanisms of polymerization and chemical recyclability

- A novel, hybrid nylon (nylon 4/6) was introduced by partner projects (BOTTLE, PABP) that exhibits:
    - optical clarity
    - high T_g
    - melt processability
    - full chemical recyclability
- DFT suggests molecular level conformational changes and hydrogen bonding promote nylon 4/6 thermal decomposition (recycling) before melting



DFT = density functional theory
T_g = glass transition temperature

Cywar *et al. JACS* 2022

3. Impact – Publications and code distributions

Publications

- Forthcoming PolyID paper (in review)
- ACS central science I.F. = 18.7
- Green Chemistry I.F. = 11.0

  Toxicity of lignin-derived plasticizers
- JACS JOURNAL OF THE AMERICAN CHEMICAL SOCIETY I.F. = 16.4

  DFT of fully recyclable nylon
- Cell Reports Physical Science I.F. = 7.8

  Structure-function of β ketoadipate-based nylon

I.F. = impact factor

PolyID available as an online tool!

https://polyid.nrel.gov

Code distributions

Monomers to Polymers (m2p)
A simple interface for converting monomers to polymers using SMILES representation.
https://pypi.org/project/m2p

Neural Fingerprint (nfp)
Python-based end-to-end learning on molecular structure.
https://pypi.org/project/nfp

PolyID (polyid)
Framework for building, training, and predicting polymer properties using graph neural networks.
https://pypi.org/project/polyid

3. Impact –Partnerships

Tools developed in this project are being applied to specific polymer classes targeting specific properties collaboratively with companies and DOE partners

KraftHeinz

- **Goal**: Identify polymer candidates with superior barrier performance compared to non-recyclable multi-layer films
- **Other partners**: BOTTLE Consortium

Algix, Patagonia, Tempur Sealy

- **Goal**: develop bio-based non-isocyanate polyurethanes for industrial applications.
- PolyID tool used to map chemical properties of polyurethane precursors
- Several formulas with promising performance were successfully prepared
- **Other partners**: TCF project "Commercialization of biobased non-isocyanate polyurethane"

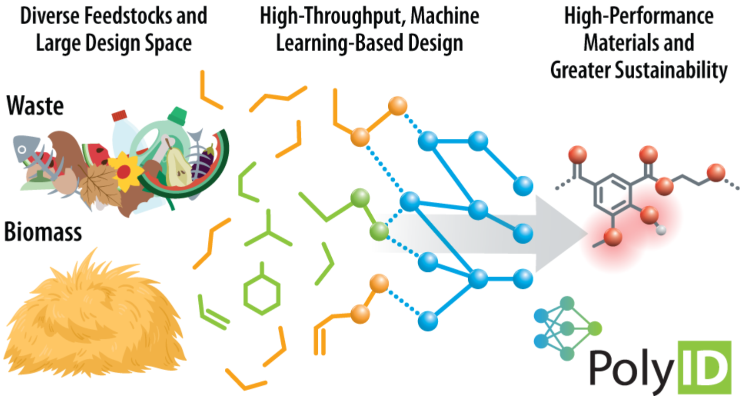
ExxonMobil

- **Goal**: discover polymers that can be produced from anhydrous sugars generated via biomass deconstruction.
- PolyID work initiated in FY22Q2 and completed in FY22Q3
- **Current status**: synthesis based on PolyID predictions initiated in FY23Q2

bottle **(BETO/AMO)**

- **Goal**: Redesign of waste plastics into recycle-by-design materials leveraging Inverse Design tools
- In collaboration with the University of Wisconsin, PolyID is being used to develop bioderived polyesters.

Summary



Wilson *et al. In revision.*

Number of Polymers

10^6 – 10^2 – 10^1 → **PABP**

- Synthesis Candidates (PABP Synthesis)
- Machine Learning & Molecular Simulation (Inverse Design)
- Potential Materials

ML = machine learning
MS = molecular simulation
PABP = performance-advantaged bioproduct

Overview

- Predict material properties from molecular structure to reduce PABP design space, facilitating targeted synthesis

Approach

- Machine learning and molecular simulation to predict novel PABPs and develop structure-function relationships

Progress and outcomes

- PolyID: machine learning tool for polymer property prediction
- Mechanistic insight, rationalization of physical properties, and *in silico* predictions of performance advantages

Impact

- Targeted synthesis of PABPs
- High impact publications
- Public code distribution
- Industrial collaborations leveraging PolyID

Quad chart overview

Timeline

- Active Project Duration: 10/1/2020 – 9/30/2023
- Total Project Duration: 10/1/2017 – 9/30/2023

	FY22 funding	Total Award
DOE Funding	$400,000 (10/01/2021–9/30/2022)	$400,000 – FY23 $1,200,000 – Active Project (FY21-23)

Project Partners

BETO Projects: Synthesis and Analysis of Performance-Advantaged Bioproducts, Biological Lignin Valorization, Bioconversion of Thermochemical Intermediates, BOTTLE Consortium, Catalytic Upgrading of Pyrolysis Products, Commercialization of Biobased Non-Isocyanate Polyurethane (TCF)

University Partners: Northwestern University, Colorado State University, University of Wisconsin-Madison

Project Goal

Accurate computational prediction and structure-function relationships of performance-advantaged bioproducts

End of Project Milestone

Establish and apply a computational method for assessing the suitability of new bio-based solvents for polymer synthesis and processing: Predict solubility of PET in ≥ 25 novel lignin-derived performance-advantaged solvents and benchmark against experimental values.

Funding Mechanism

Bioenergy Technologies Office FY21 AOP Lab Call (DE-LC-000L079) – 2020

TRL at Project Start: 2

TRL at Project End: 4

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Collaborators:
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Kevin Shebek (Northwestern), Lauren Lopez (Northwestern),
Eugene Chen (CSU),
George Huber (University of Wisconsin-Madison)

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BIOENERGY TECHNOLOGIES OFFICE

Q&A

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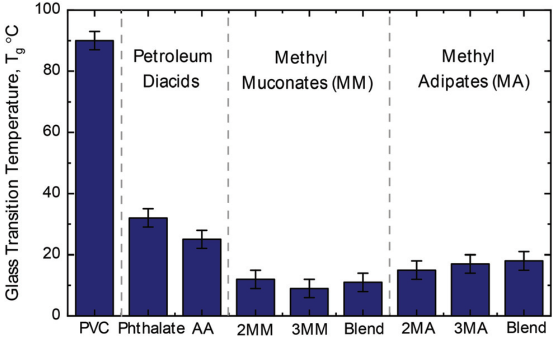
NREL Transforming ENERGY

Additional Slides

2. Progress and outcomes – *in silico* toxicity prediction

Bio-derived plasticizers predicted to exhibit reduced toxicity

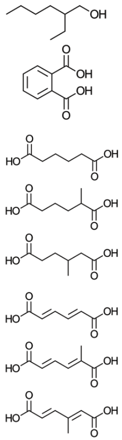
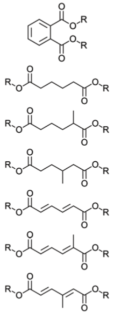
- PABP project partners biologically converted CFP wastewater molecules into performance-advantaged, bio-based plasticizers for PVC
- We utilized the EPA Toxicity Estimation Software Tool (TEST)[1] and Chemical Transformation Simulator (CTS)[2] to predict several health and environmental toxicity metrics and rationalize toxicity via primary metabolic pathways
- Compared to two industry standard plasticizers (DEHP and DEHA), diacid-based plasticizers were predicted to exhibit reduced health and environmental risks



Primary citation:
Henson *et al. Green Chemistry* 2022

Similar contribution in the context of plasticizers derived from oxidative depolymerization of hardwood lignins:
Su *et al. ACS Central Science* 2023

CFP = catalytic fast pyrolysis
PVC = poly(vinyl chloride)
EPA = Environmental Protection Agency
[1] Martin, T. M. T. E. S. T. (Toxicity Estimation Software Tool) Version 5.1, 5.1; U.S. EPA: 2020.
[2] Chemical Transformation Simulator(CTS), Version 1.0 2019.

	Dev. Toxin	Oral Rat Toxicity (mg/kg)	Bioconc. Factor	Aquatic Toxicity (mg/L)
Diacids and Oxoalcohols				
EH	yes	1,720	19.5	31.2
PA	yes	5,130	0.5	29.5
AA	no	4,210	0.2	150
2MA	no	5,950	0.2	103
3MA	no	4,620	0.2	133
MA	no	6,200	0.4	47.1
2MM	yes	5,800	0.3	26.5
3MM	no	5,050	0.3	33.4
Plasticizers				
DEHP	yes	31,000	17.8	0.09
DEHA	no	9,750	53.7	0.48
DEH2MA	no	10,100	61.7	0.32
DEH3MA	no	9,890	63.2	0.31
DEHM	yes	12,700	19.5	0.03
DEH2MM	yes	13,500	9.12	0.02
DEH3MM	yes	13,500	9.12	0.02

Responses to previous reviewers' 2021 comments

- Reviewer comment: "More involvement with industry would be a good addition, although it is encouraging to see an exploration of "Commercialization of Fully Renewable Non-Isocyanate Polyurethanes" with industry such as Sealy, Patagonia, Agilix."

- Reviewer comment: "Key will be to connect to an even greater base of materials experts in industry to tap their insights into structure/property relationships and performance."

  - Response: Industrial engagement / partnership has always been a goal of this project, and as the first reviewer noted, we had some engagement that was reported on in the 2021 Peer Review. Since the last Peer Review, we have since built significantly on those efforts, as noted in the Impact section of our 2023 review. The computational tools developed in the Inverse Design project are applied selectively within this project. This development work is also leveraged significantly in other projects with industrial partners, where they are applied to specific polymer classes, targeting specific properties, and for specific applications.

Responses to previous reviewers' 2021 comments

- Reviewer comments: Not clear why ML ("black box") is superior to simply using molecular / mechanistic simulation tools. ML could be faster, certainly, but such models are often unreliable upon extrapolation of the training date set.
  - Response: The team does not assert that machine learning (“black box”) or molecular simulation is superior because both approaches have their strengths and weaknesses, and leveraging both approaches can provide the greatest outcomes. We are employing machine learning to pare down the immense design space to pass the most promising candidates to our experimental partners. The atomistic simulations are a finer-resolution tool to further pick out promising candidates as well as drive the development of structure-function relationships.

Responses to previous reviewers’ 2021 comments

- Reviewer comments: Results are indicative of good progress and outcomes. There is emphasis on believing that this is going to work supported by rigorous statistical input. It is important to bear in mind that a null hypothesis might be that the predictions have potential to deliver a zero outcome.

  - Response: The team acknowledges the possibility of the null hypothesis. This would be an unfortunate outcome of the research, and the tools developed within this project will help experimental efforts in identifying both promising candidates as well as candidates that are unlikely to be performance advantaged.

Responses to previous reviewers' 2021 comments

- Reviewer comments: It is interesting that the team chose to pursue an alternative to PET rather than targeting ways to make PET more sustainable. This team would also have the means to improve PET, producing greener versions of monomers for PET production. They might consider the (often) prohibitively high cost of introducing new polymers vs improving an existing one.
  - Response: We appreciate the costs and challenges in bringing new materials to the market, and we acknowledge that both more sustainable routes to existing materials (e.g., PET) as well as sustainable replacements will likely be needed to realize a fully circular economy.

Publications, patents, and presentations

Publications

In preparation

Caroline B. Hoyt, Nicholas A. Rorrer, A. Nolan Wilson, Avantika Singh, Scott Nicholson, Robert A. Allen, Gregg T. Beckham. “Bio-based aromatic amines for catalytic naphthoxazine synthesis and effects on ring opening.” In preparation (Target Journal: *Green Chemistry*).

Lauren Lopez, Linda J. Broadbelt, Nolan A. Wilson. “Combining reaction network generation with machine learning for expanded discovery of renewably sourced polymers with performance advantages.” In preparation.

Kevin M. Shebek, Linda J. Broadbelt, Nolan A. Wilson. “Accurate property prediction for chiral polymers via multiple strategies for incorporating tacticity into machine learning predictions.” In preparation.

Under review

A. Nolan Wilson, Peter C. St. John, Daniela H. Marin, Caroline B. Hoyt, Erik G. Rognerud, Mark R. Nimlos, Robin M. Cywar, Nicholas A. Rorrer, Kevin M. Shebek, Linda J. Broadbelt, Gregg T. Beckham, Michael F. Crowley. “PolyID: Artificial intelligence for discovering performance-advantaged and sustainable polymers.” Under review.

Publications, patents, and presentations

2023

Zhi-Ming Su, Jack Twilton, Caroline B. Hoyt, Fei Wang, Lisa Stanley, Heather B. Mayes, Kai Kang, Daniel J. Weix, Gregg T. Beckham, Shannon S. Stahl. “Ni- and Ni/Pd-catalyzed reductive coupling of lignin-derived aromatics to access biobased plasticizers.” *ACS Central Science*. 2023.

2022

Nicholas A. Rorrer, Sandra F. Notonier, Brandon C. Knott, Brenna A. Black, Avantika Singh, Scott R. Nicholson, Christopher P. Kinchin, Graham P. Schmidt, Alberta C. Carpenter, Kelsey J. Ramirez, Christopher W. Johnson, Davinia Salvachúa, Michael F. Crowley, Gregg T. Beckham. "Production of β-ketoadipic acid from glucose in Pseudomonas putida KT2440 for use in performance-advantaged nylons." *Cell Reports Physical Science*. 2022.

William R. Henson, Nicholas A. Rorrer, Alex W. Meyers, Caroline B. Hoyt, Heather B. Mayes, Todd Vander Wall, Rui Katahira, Jared J. Anderson, Brenna A. Black, William E. Michener, Lahiru Jayakody, Davinia Salvachúa, Christopher W. Johnson, Gregg T. Beckham, "Bioconversion of wastewater-derived methyl phenols to methyl muconic acids for use in performance-advantaged bioproducts." *Green Chemistry*. 2022.

Robin M. Cywar, Nicholas A. Rorrer, Heather B. Mayes, Anjani K. Maurya, Christopher J. Tassone, Gregg T. Beckham, Eugene Y.-X. Chen. “Redesigned hydrid nylons with optical clarity and chemical recyclability.” *Journal of the American Chemical Society*. 2022.

Publications, patents, and presentations

Code distributions

Monomers to Polymers (m2p)
A simple interface for converting monomers to polymers using SMILES representation.
https://pypi.org/project/m2p/

Neural Fingerprint (nfp)
Python-based end-to-end learning on molecular structure.
https://pypi.org/project/nfp/

PolyID (polyid)
Framework for building, training, and predicting polymer properties using graph neural networks.
https://pypi.org/project/polyid

Publications, patents, and presentations

Presentations

“Machine learning for prediction of sustainable polymers.” American Chemical Society, Fall 2022 Meeting. Nolan Wilson (presenter), Peter St. John, Mark Nimlos, Mike Crowley.

“Bio-derived, Sustainable Polymers Through End-to-End Learning.” Gordon Research Conference – Computational Materials Science and Engineering. 2022. Nolan Wilson (presenter), Peter St. John, Daniella Marin, Caroline B. Hoyt, Mark Nimlos, Nic Rorrer, Gregg T. Beckham, Mike Crowley.

Publications, patents, and presentations

Provisional Patent Number	Title
63/158,715	Machine Learning for Biopolymers and High-Performance Aromatic Bio-based Polyesters.

ROI Number	Title
	Copolymerized anhydrosugar-based methacrylates with olefins
ROI-22-43	High barrier and compostable films

Software ROI Number	Title
SWR-19-40	“M2P” Monomers to Polymers
SWR-19-13	“NFP” Neural Fingerprints
SWR-21-98	PolyID*

*PolyID^{TM} has been retained as a trademark for the machine learning tool