Predictive Design of Renewable Oil-Derived Thermosetting Polymers Using Machine Learning

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Introduction and Background

- Bio-based polymers with predictable thermo-mechanical properties are difficult to design.
- A closed-loop framework integrating **synthetic biology, polymer chemistry, and ML** enables rational engineering of triglyceride-based thermosets.
- Diverse **microbial oils & Vegetable oils** are polymerized with **DVB** and **BMA** to create materials for structure-property analysis.
- Fatty acid features: **chain length, unsaturation, and composition,** are correlated with **Tg, modulus, and crosslink density**.
- ML models trained on composition-property datasets support **forward prediction** and **inverse design** of polymer performance.
- This approach advances **sustainable, high-performance, bio-derived thermosets** for structural and thermal applications.

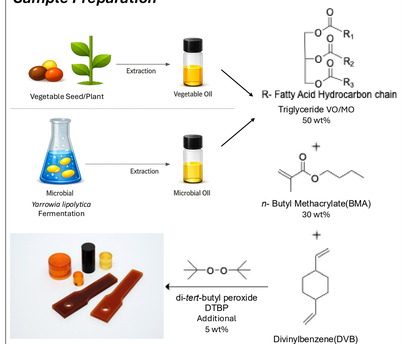
Previous work- Cordova et al, ACS Appl. Polym. Mater. 2021.

Materials

Vegetable Oils

1. TO-Tung Oil
2. AO-Avocado Oil
3. CO-Coconut Oil
4. JO- Joannesia Oil
5. PO- Pequi Oil
6. SoyO-Soybean Oil
7. CorO-Corn Oil
8. CasO- Caster Oil
9. LinO- Linseed Oil
10. SesO- Sesame Oil
11. OliO- Olive Oil
12. GraO- Grapeseed Oil
13. CanO- Canola Oil
14. SunO- Sunflower Oil
15. PeaO-Peanut Oil
16. CotO- Cottonseed Oil
17. MacO- Macadamia Oil
18. RicO- Ricebran Oil
19. SeaO- Sea Buckthron Oil
20. RosO- Rosehip Oil
21. ChiO- Chia Seed Oil
22. ManO- Mango Butter Oil
23. CamO- Camelina Oil
24. PerO- Perilla Seed Oil
25. BabO- Babasu Oil
26. RedO- Red Palm Oil
27. SheO- Shea Butter Oil
28. BitO- Bitter Gourd Oil
29. PalO- Palm Kernel Oil
30. HemO-Hempseed Oil

Sample Preparation



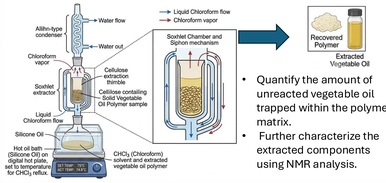
Methods

Transesterification: FAME prep for GC-MS

$$Triglyceride + 3CH_3OH \xrightarrow[2h]{\frac{NaOH}{50^{\circ}C}} 3Fatty\ Acid\ Methyl\ Ester + Glycerol$$

$$C_5H_5(COOR)_3 + 3CH_3OH \rightarrow 3RCOOCH_3 + C_3H_5(OH)_3$$

Soxhlet Extraction: of the Vegetable Oil Polymers over 24h with $CHCl_3$



- Quantify the amount of unreacted vegetable oil trapped within the polymer matrix.
- Further characterize the extracted components using NMR analysis.

Results: Vegetable and Microbial Oil Polymers

	50%	Best%-b
Tung Oil (b-50%)		
Avocado Oil(b-60%)		
Coconut Oil(b-60%)		
Pequi Oil (b-55)		
Joannesia Oil(b-60%)		

	50%	Best%-b
Soybean Oil (b-65%)		
Corn Oil (b-65%)		
Caster Oil (b-50%)		
Linseed Oil (b-60%)		
Sesame Oil (b-65%)		

	50%	Best%-b
Olive Oil (b-60%)		
Grapeseed Oil (b-60%)		
Canola Oil (b-50%)		
Sunflower Oil (b-50%)		
Peanut Oil (b-50%)		

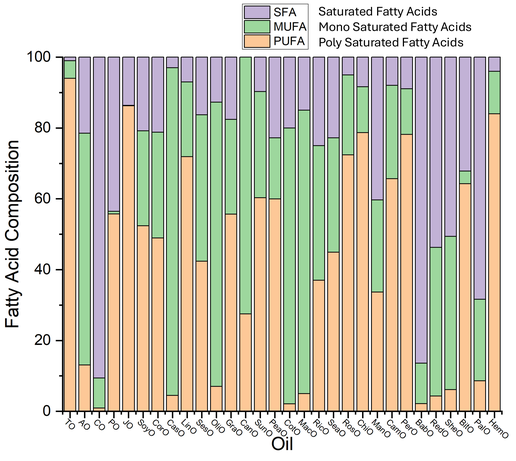
	50%	Best%-b
Cottonseed Oil (b-65%)		
Macadamia Oil (b-65%)		
Ricebran Oil (b-65%)		
Seabuckthorn Oil (b-60%)		
Rosehip Oil (b-70%)		

	50%	Best%-b
Chia seed Oil (b-50%)		
Mango Butter Oil (b-60%)		
Camelina Oil (b-65%)		
Perilla Oil (b-70%)		
Babasu Oil (b-50%)		

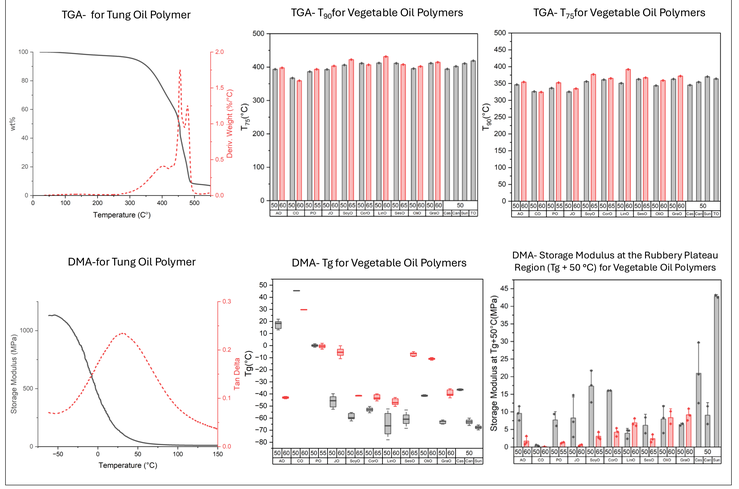
Microbial Oil Polymers	50%
MO10	
MO11	
MO12	
MO13	
MO14	

Results: Fatty Acid Compositions via GC-MS

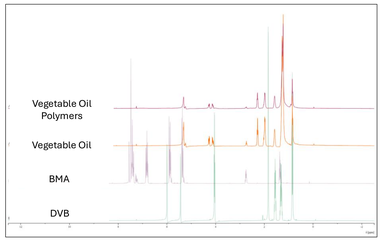
Fatty Acid	Chemical Formula	Molecular Structure
Caprylic(8:0)	$C_8H_{16}O_2$	
Capric/Decanoic(10:0)	$C_{10}H_{20}O_2$	
Lauric(12:0)	$C_{12}H_{24}O_2$	
Myristic(14:0)	$C_{14}H_{28}O_2$	
Palmitic(16:0)	$C_{16}H_{32}O_2$	
Palmitoleic(16:1)	$C_{16}H_{32}O_2$	
Stearic(18:0)	$C_{18}H_{36}O_2$	
Oleic(18:1)	$C_{18}H_{36}O_2$	
Trans-Oleic(18:1 n-9)	$C_{18}H_{36}O_2$	
Linoleic(18:2 n-6)	$C_{18}H_{32}O_2$	
α-eleostearic(18:3 n-6)	$C_{18}H_{30}O_2$	
α-Linolenic(18:3 n-6)	$C_{18}H_{30}O_2$	
Arachidic/Eicosanoic(20:0)	$C_{20}H_{40}O_2$	
Gadoleic (20:1)	$C_{20}H_{38}O_2$	
Arachidonic(20:4n-6)	$C_{20}H_{40}O_2$	
Behenic/ Docosanoic(22:0)	$C_{22}H_{44}O_2$	
Tetracosanoic(24:0)	$C_{24}H_{48}O_2$	
Ricinoleic Acid(C18H34O3)	$C_{18}H_{34}O_3$	
Dihydroxystearic Acid(C18H36O4)	$C_{18}H_{36}O_4$	



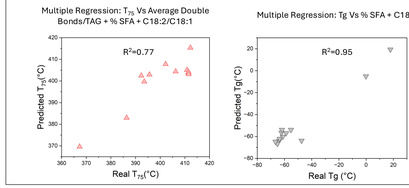
Results: Thermogravimetric(TGA) and Dynamic Mechanical Analysis(DMA)



Results: NMR



Results: Initial ML Approaches



Conclusions and Next Steps

- NMR analysis confirms that Soxhlet extraction yields unreacted vegetable oils with minor traces of unpolymerized BMA.
- Initial machine learning (ML) approaches show promising trends and support moving forward with further model development.

Next Steps

- Expand the dataset by incorporating additional vegetable oil polymer analysis data covering a wider range of fatty acid profiles.
- Include engineered microbial oil polymers from the Alper Lab to improve dataset diversity and model robustness.

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