



AI-driven development of new sustainable materials

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**Laboratory of
Natural Materials
Technology**

Plastics is a global problem



Developing bioplastics



Developing bioplastics

Bio-derived composites:



Developing bioplastics

Bio-derived composites:
polylactic acid (PLA)



Developing bioplastics

Bio-derived composites:

polylactic acid (PLA)

+ birch lignin



Developing bioplastics

Bio-derived composites:

polylactic acid (PLA)

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+ plasticiser (triethyl citrate TEC)



Developing bioplastics

Bio-derived composites:

polylactic acid (PLA)

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How to find the best material blend?



Objectives

Use AI to sample material formulations and:

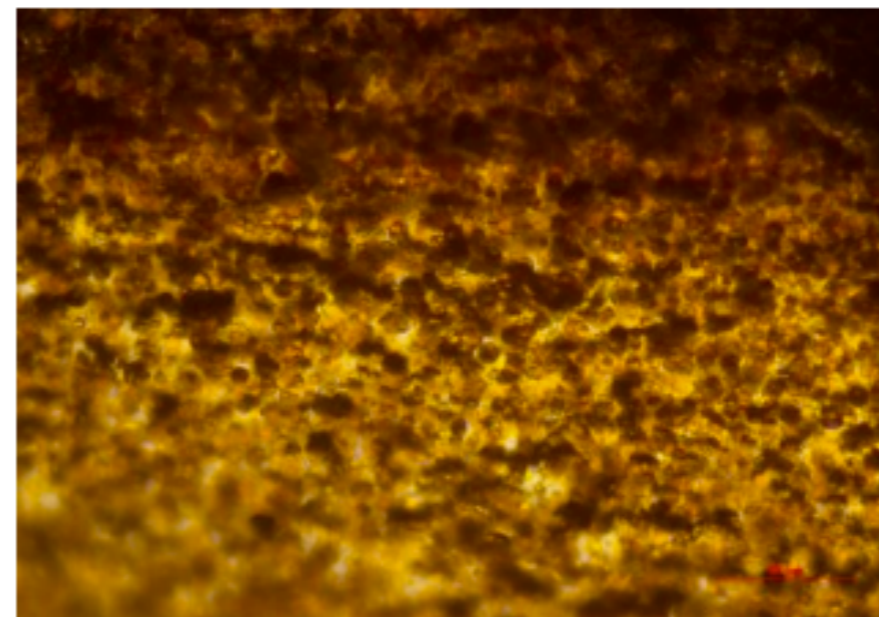
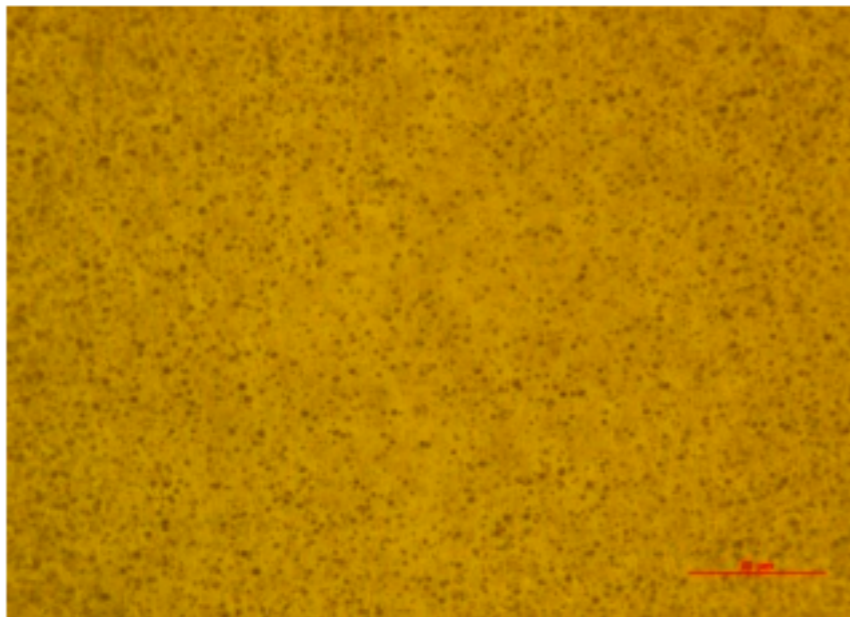
1. **Increase the compatibility** of the mixture
2. Find the mixture with **best elastic properties**

Objectives

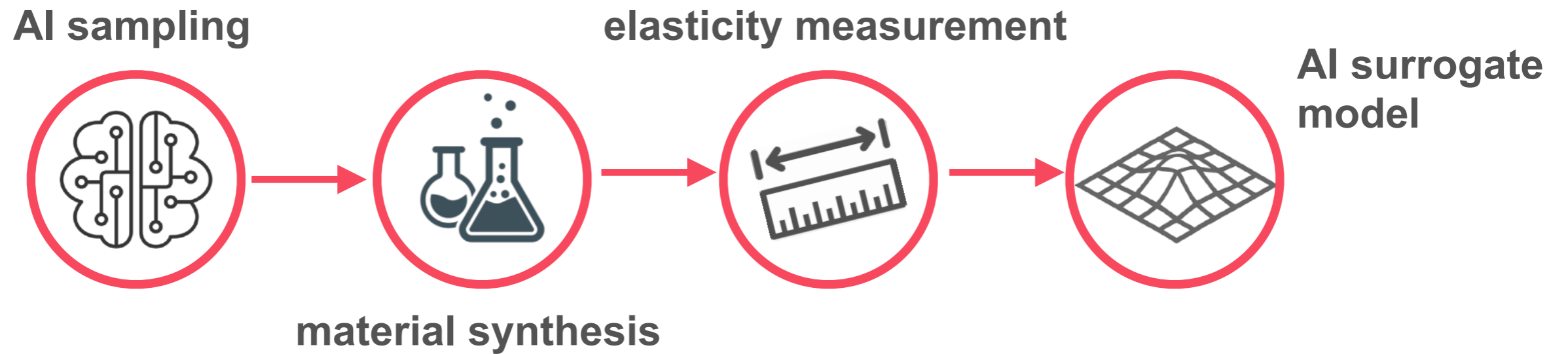
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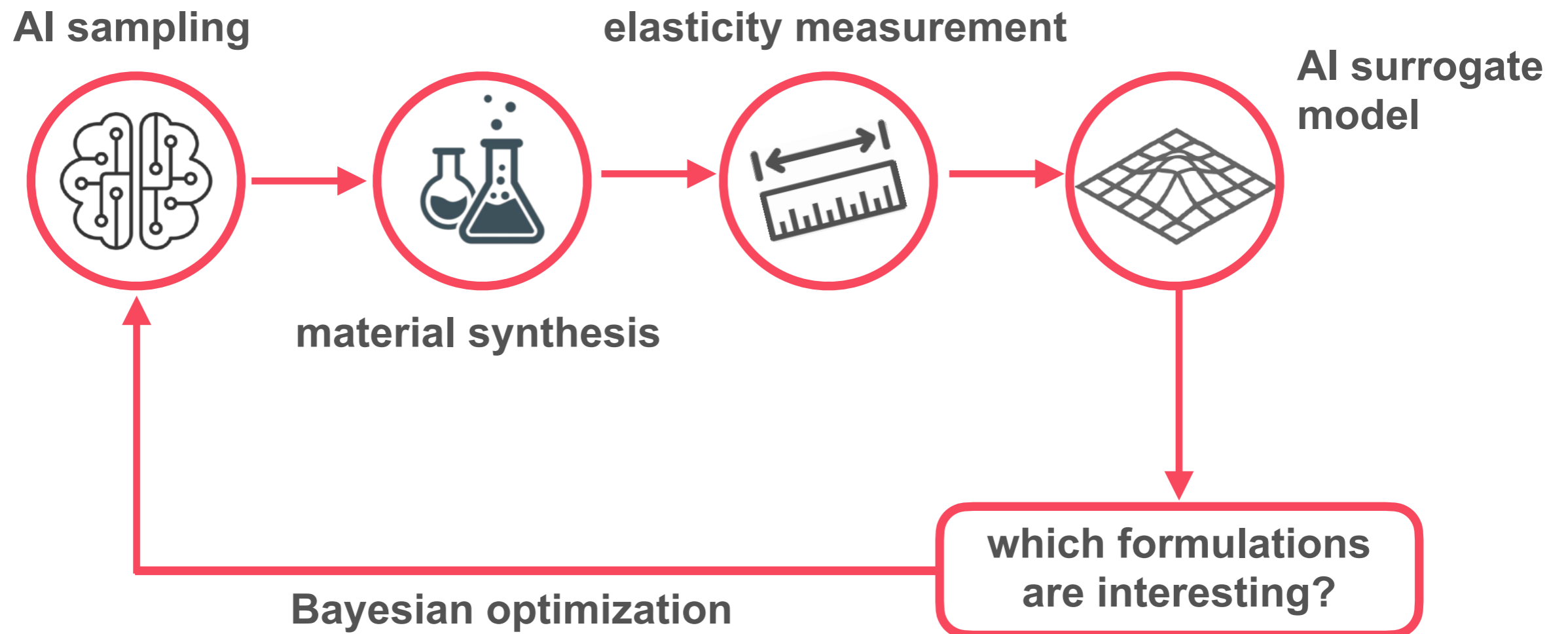
Compatibility of composite blends: microscopy images showing lignin particles



AI-driven experimentation



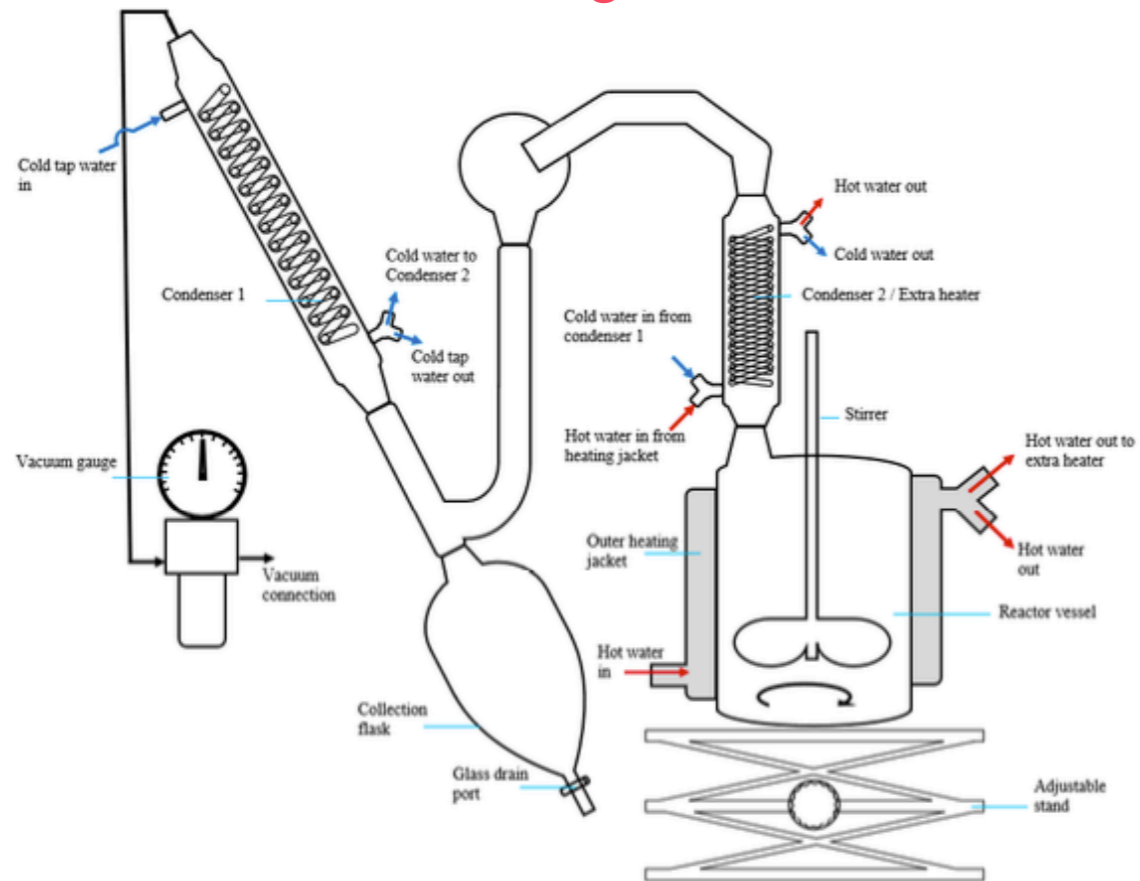
AI-driven experimentation



Methods

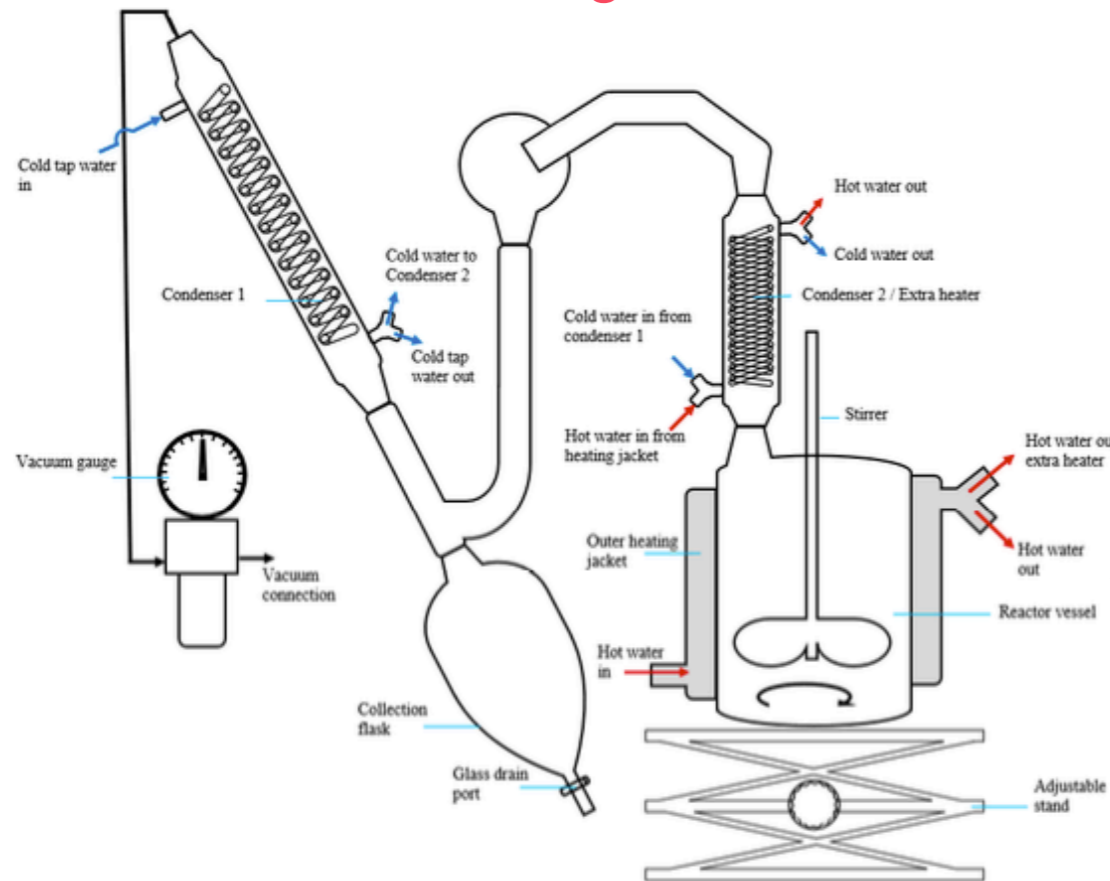
Experimental approach

Reactor design to blend lignin & PLA



Experimental approach

Reactor design
to blend lignin & PLA



birch



Lignin extracted
with MBTE,
fractionated, dried

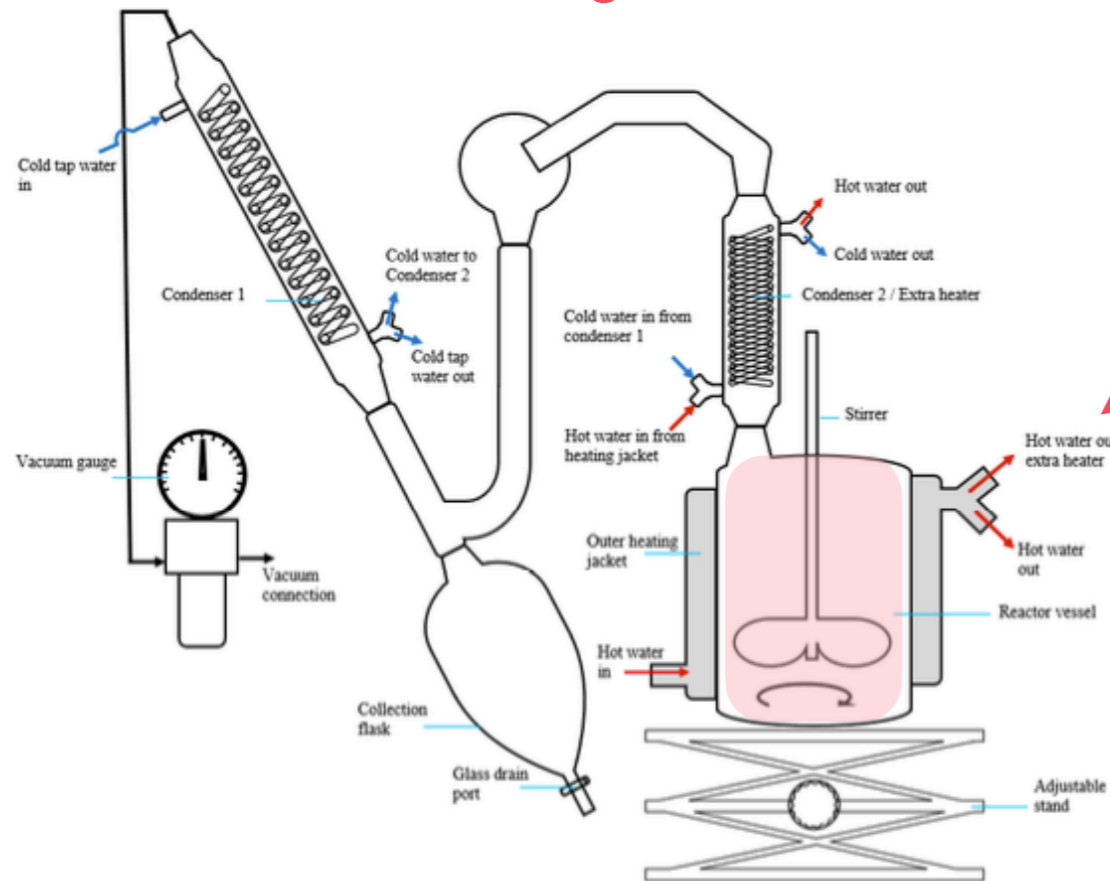
Lignin dissolved
in DCM at RT°

Experimental approach

birch



Reactor design
to blend lignin & PLA



PLA dissolved
in THF at 50°

Lignin dissolved
in DCM at RT°

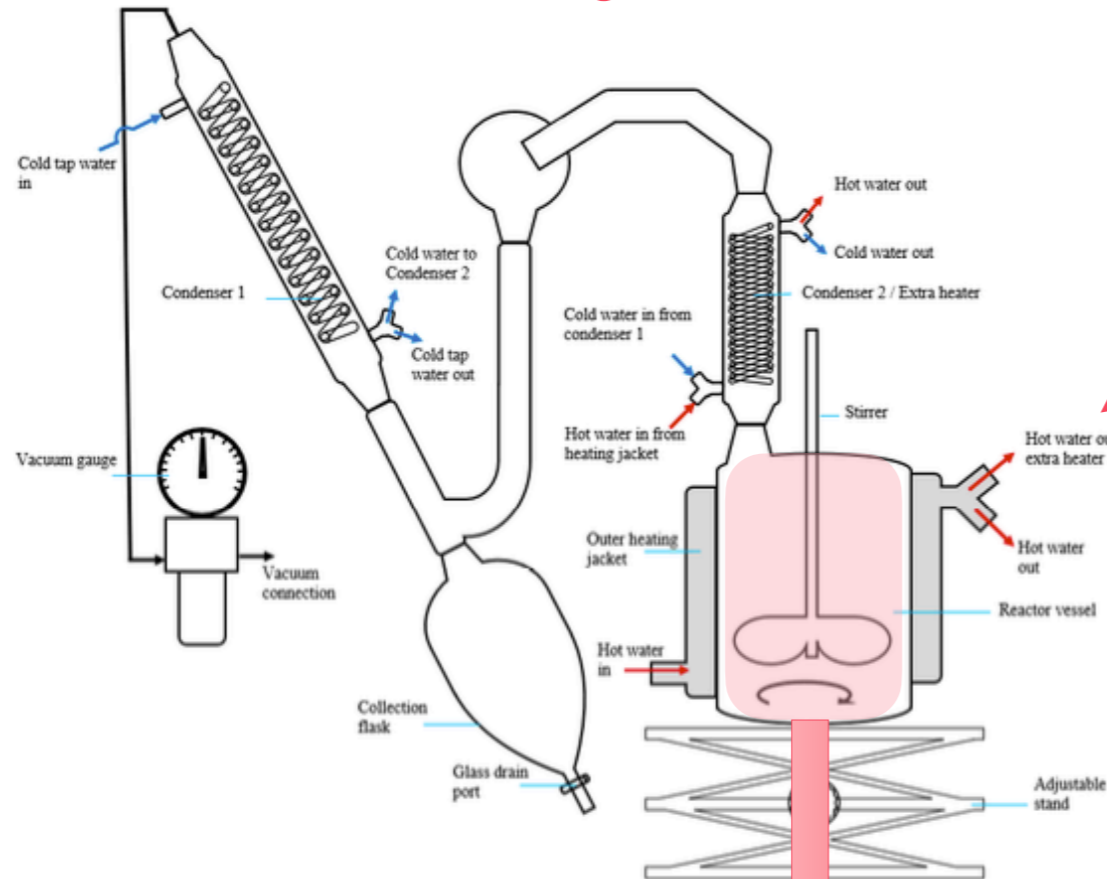
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Experimental approach

birch



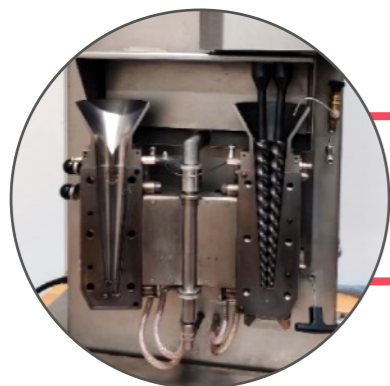
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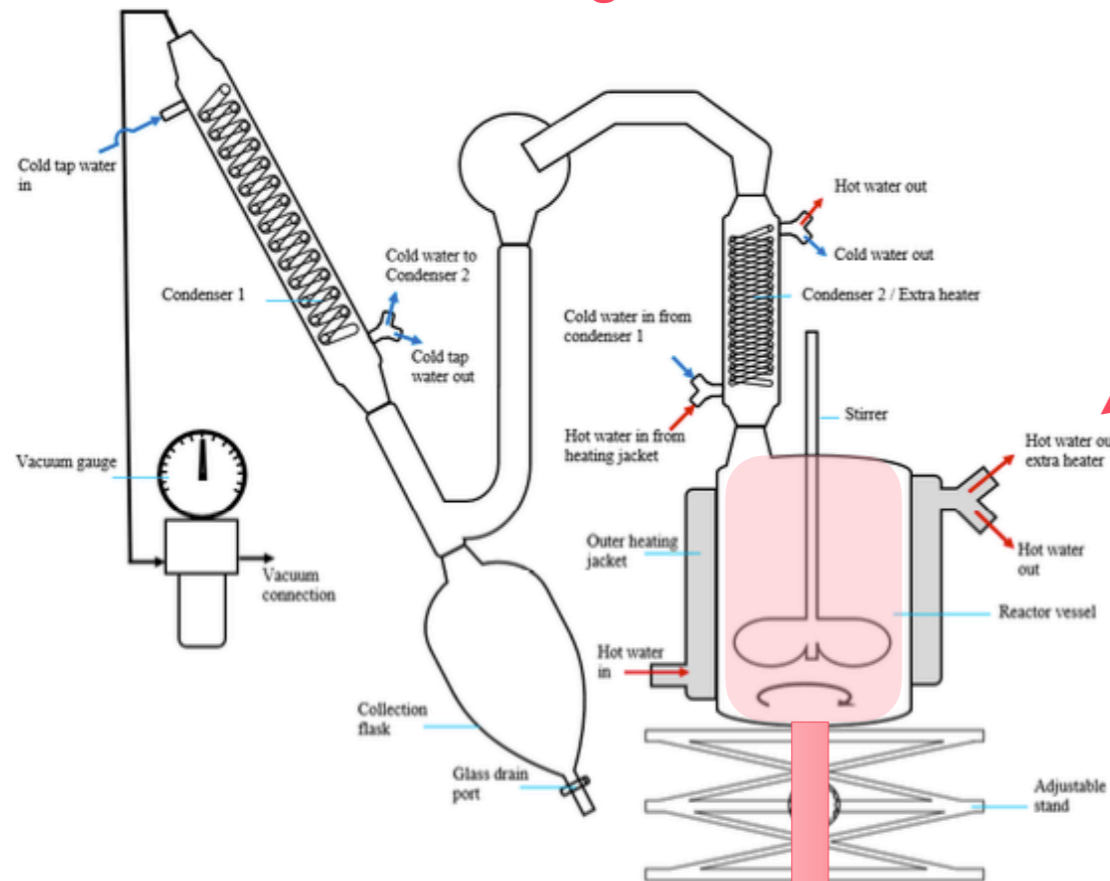
Compounding
with TEC

Experimental approach

birch



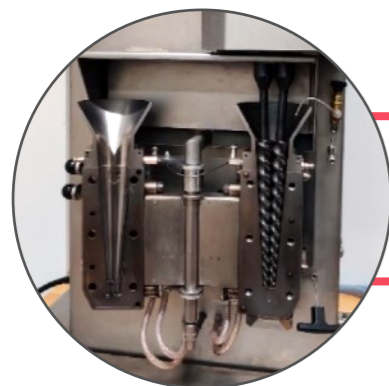
Reactor design
to blend lignin & PLA



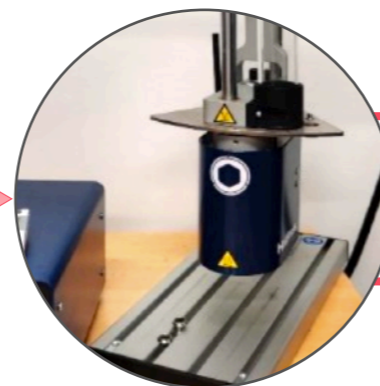
PLA dissolved
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Compounding
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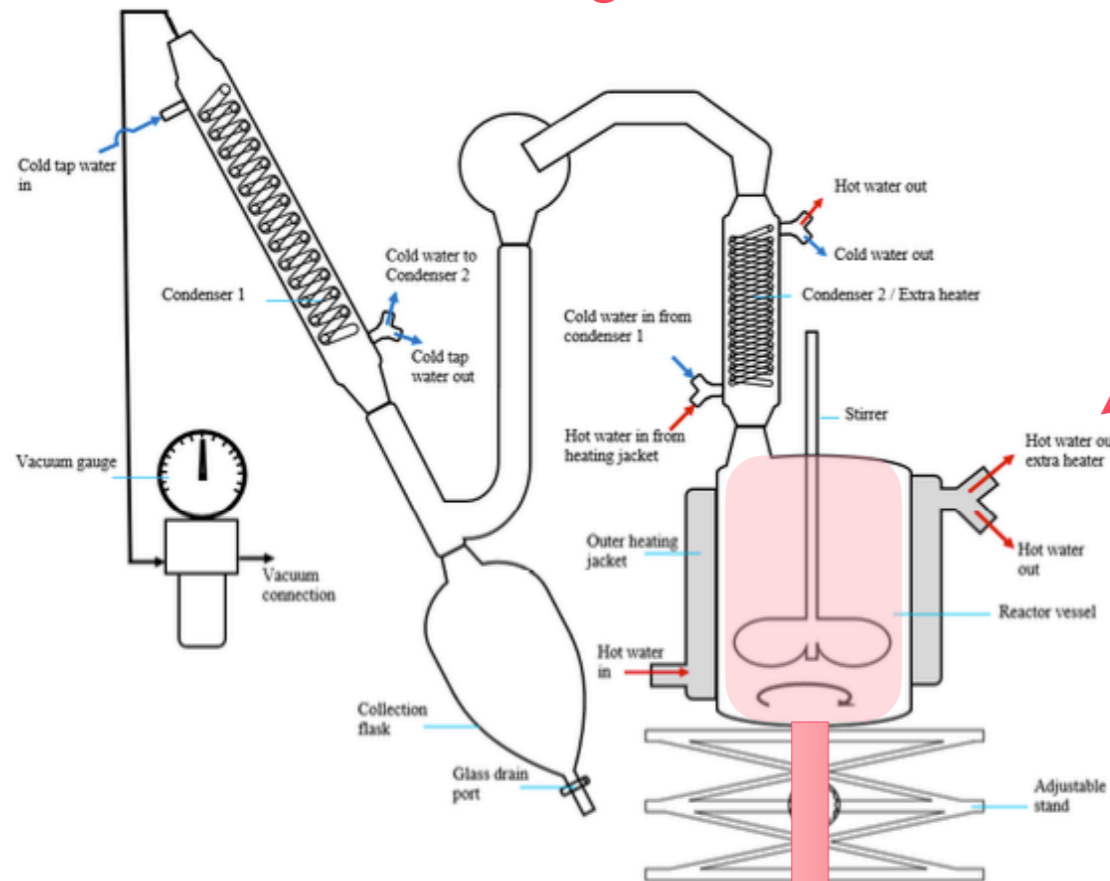
Injection
molding

Experimental approach

birch



Reactor design
to blend lignin & PLA

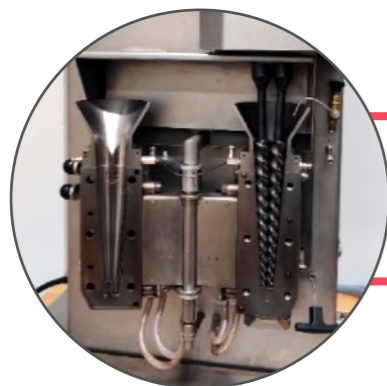


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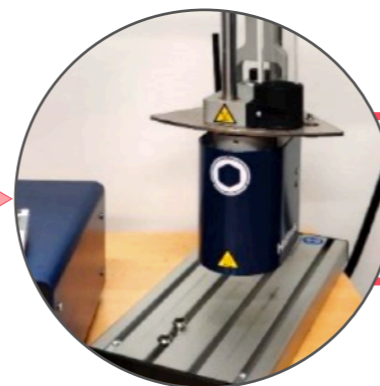
Lignin extracted
with MBTE,
fractionated, dried

Lignin dissolved
in DCM at RT°

sample



Compounding
with TEC



Injection
molding

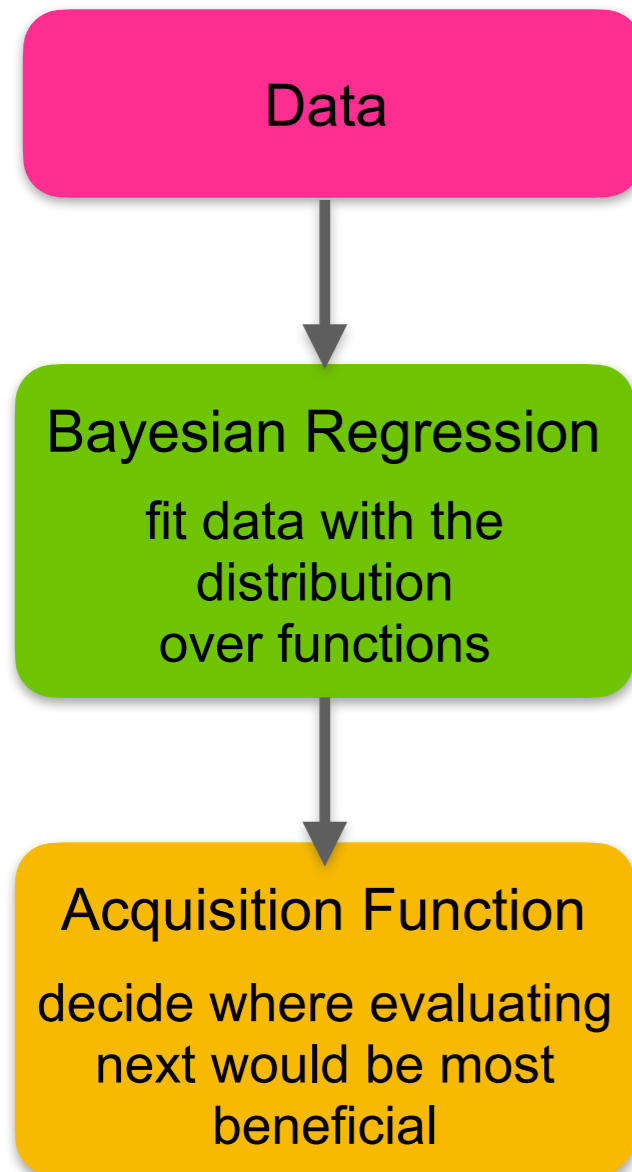


Bayesian optimisation approach

Active (Machine) Learning: “Taking the human out-of-the-loop”

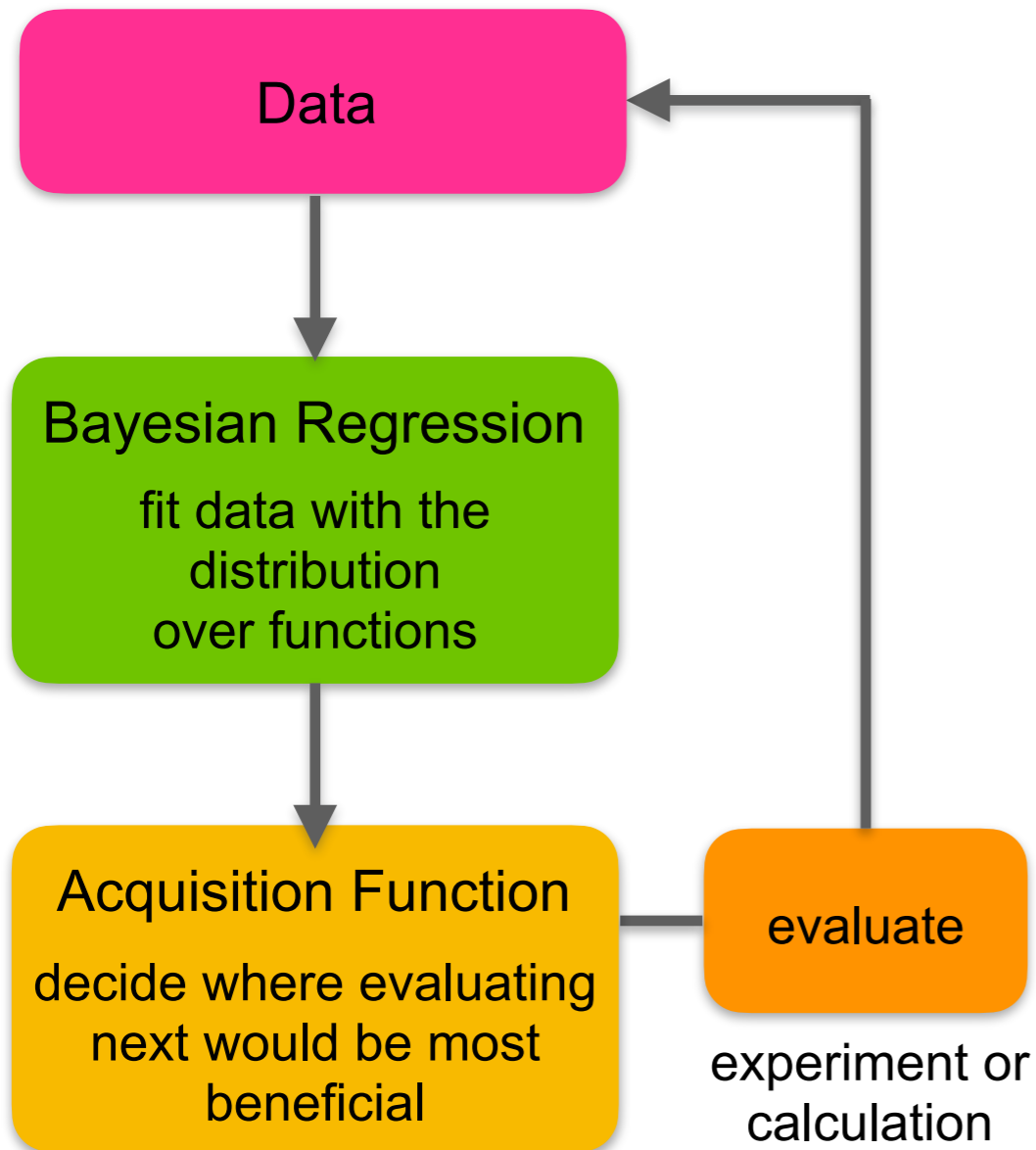
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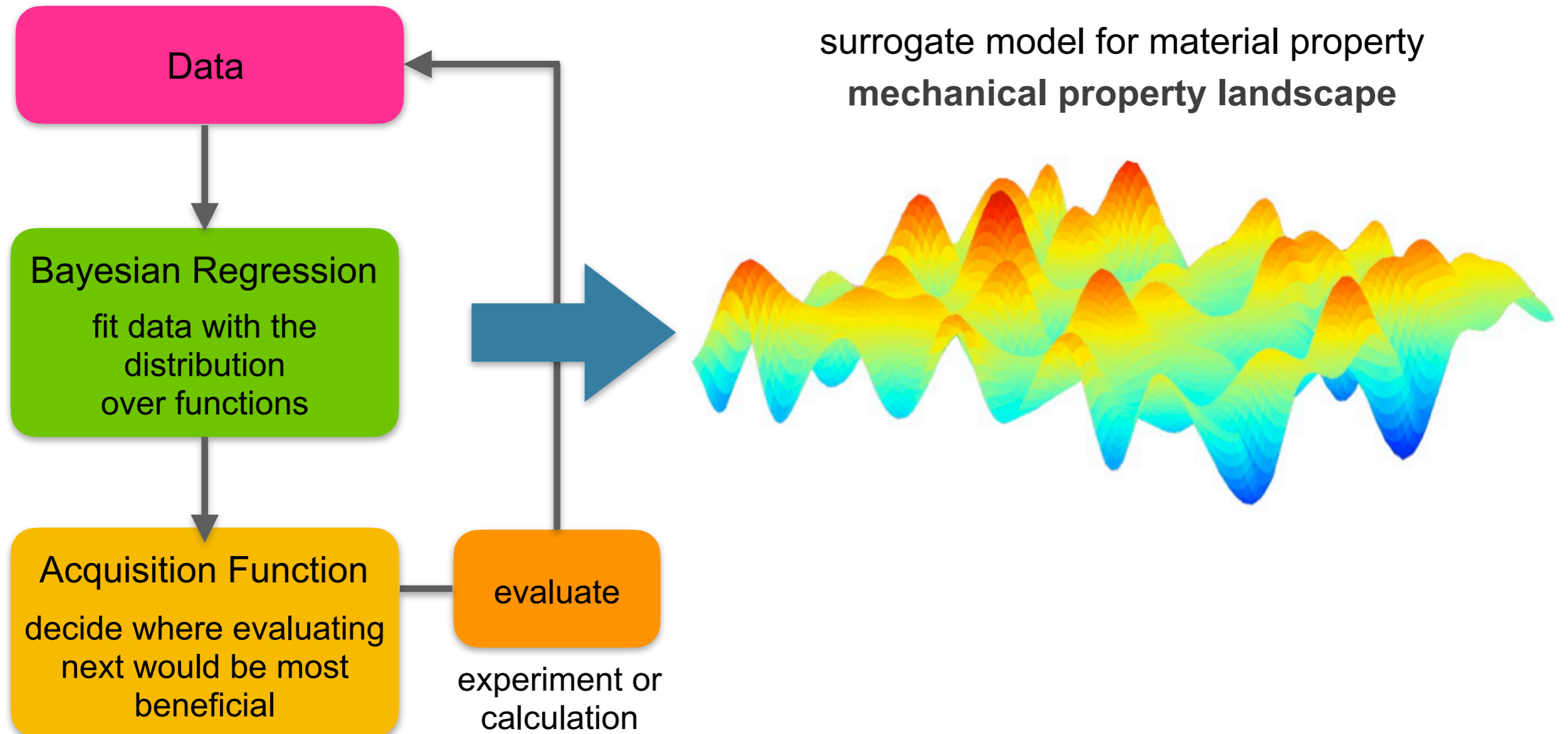
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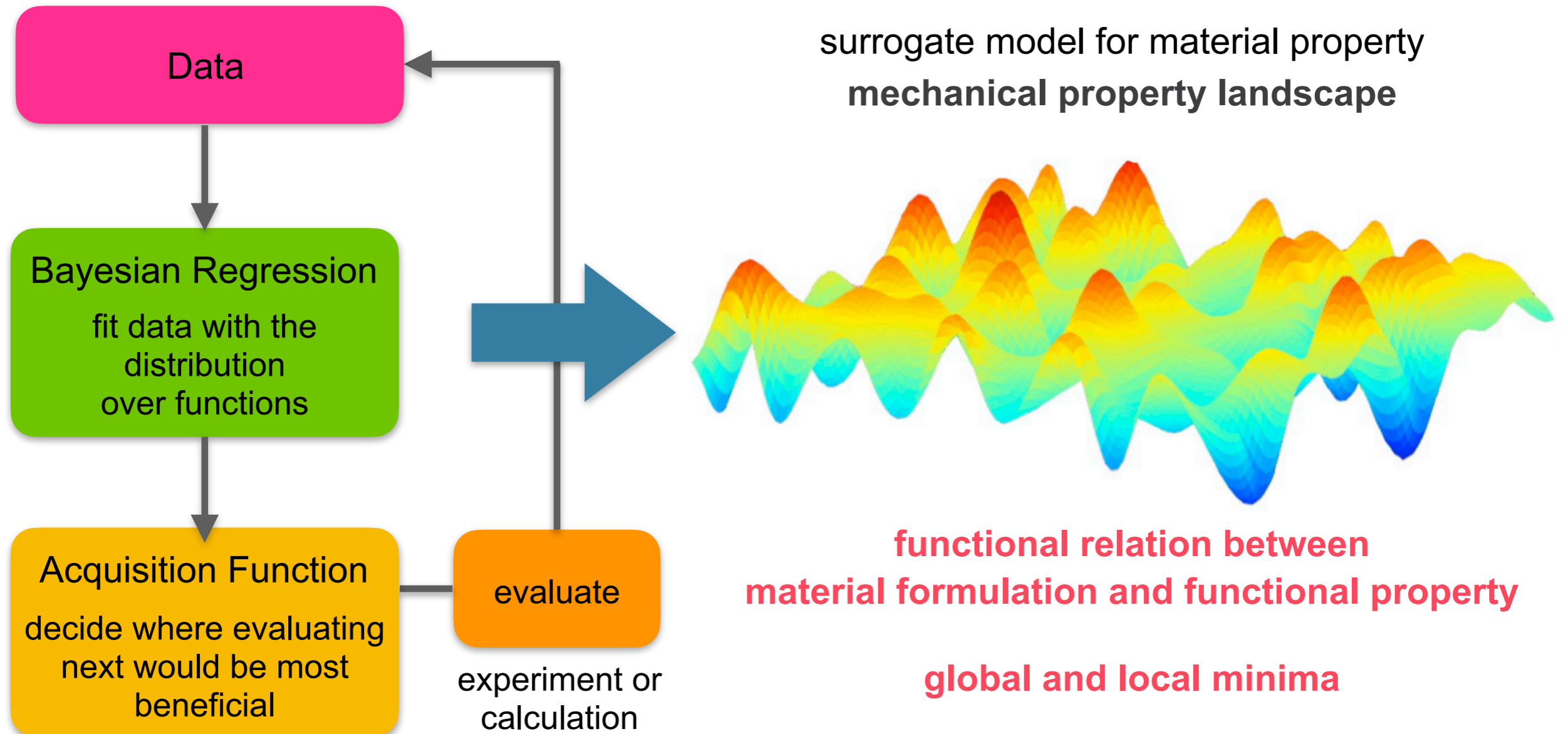
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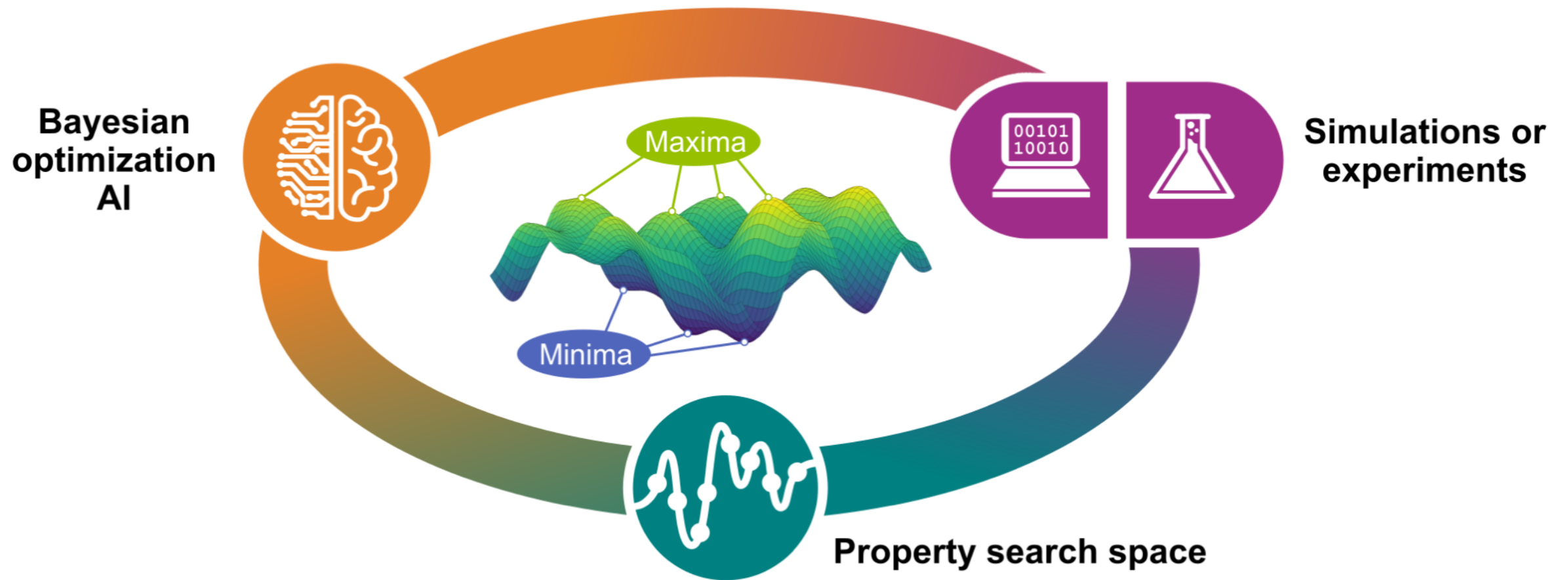


Bayesian optimisation approach

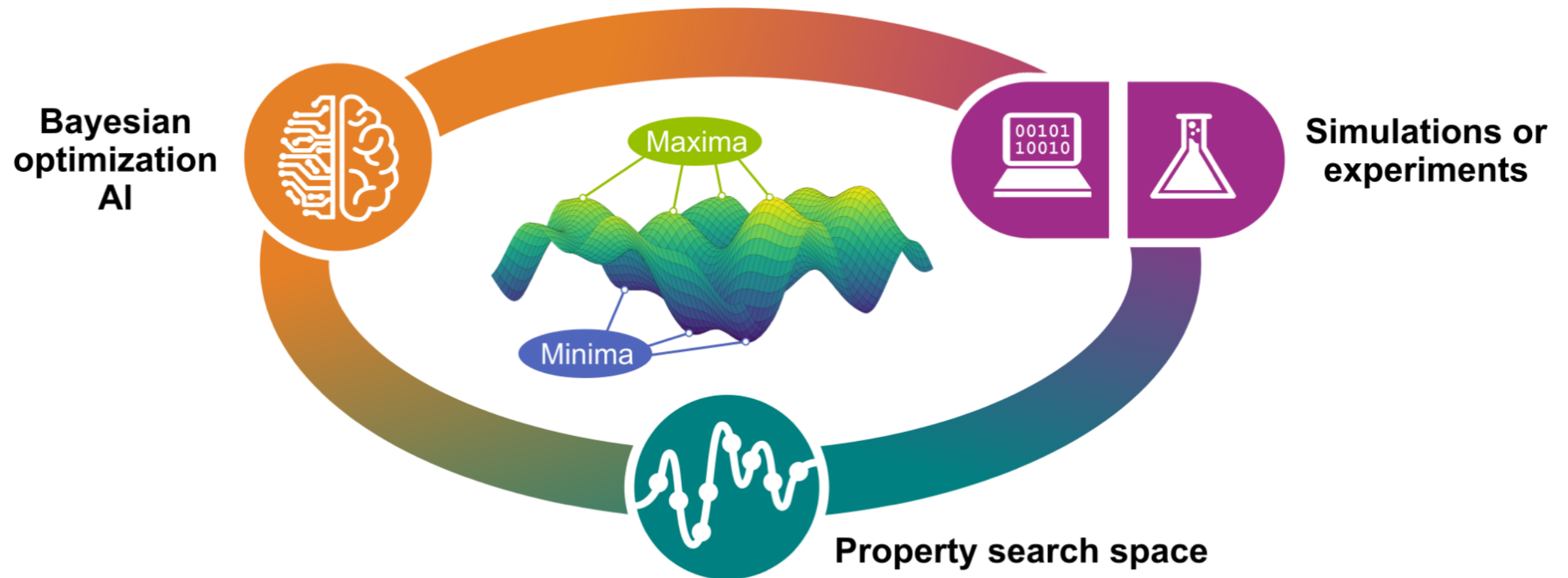
Active (Machine) Learning: “Taking the human out-of-the-loop”



BOSS code

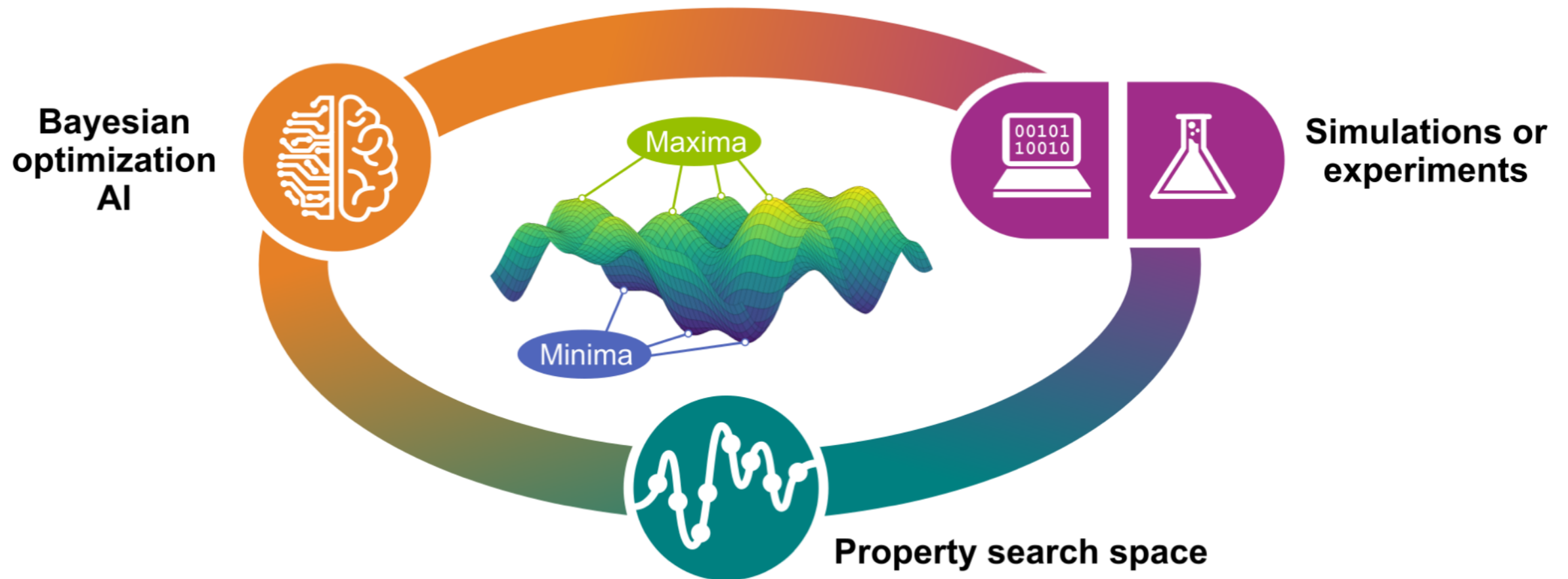


BOSS code



Active machine learning tool for global phase space exploration
Fast inference of extrema for black-box functions.

BOSS code



Active machine learning tool for global phase space exploration
Fast inference of extrema for black-box functions.

Active learning code: www.utu.fi/boss

M. Todorović, M.U. Gutmann, J. Corander and P. Rinke,
npj Comput. Mater. 5, 35 (2019)

Materials formulation space

Key decisions:

1. How much lignin to add into PLA?
2. How much TEC plasticiser to add?

Materials formulation space

Key decisions:

1. How much lignin to add into PLA? → $\frac{\text{lignin}}{\text{PLA}} : 0 - 50\%$
2. How much TEC plasticiser to add?

Materials formulation space

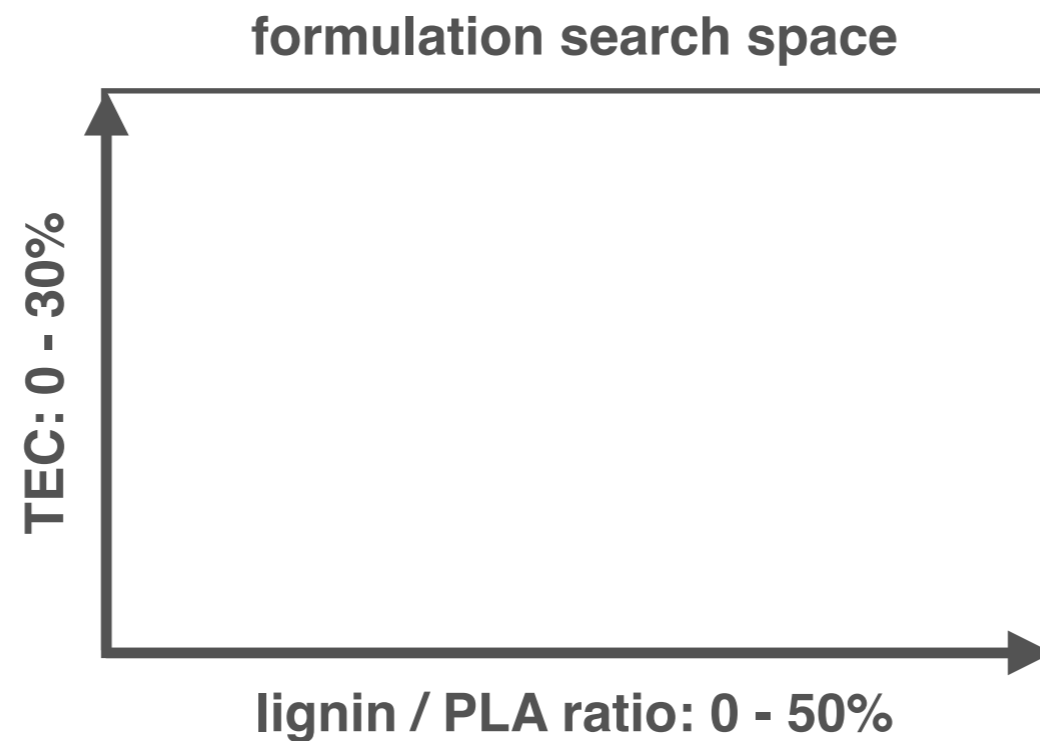
Key decisions:

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2. How much TEC plasticiser to add? → TEC : 0 - 30%

Materials formulation space

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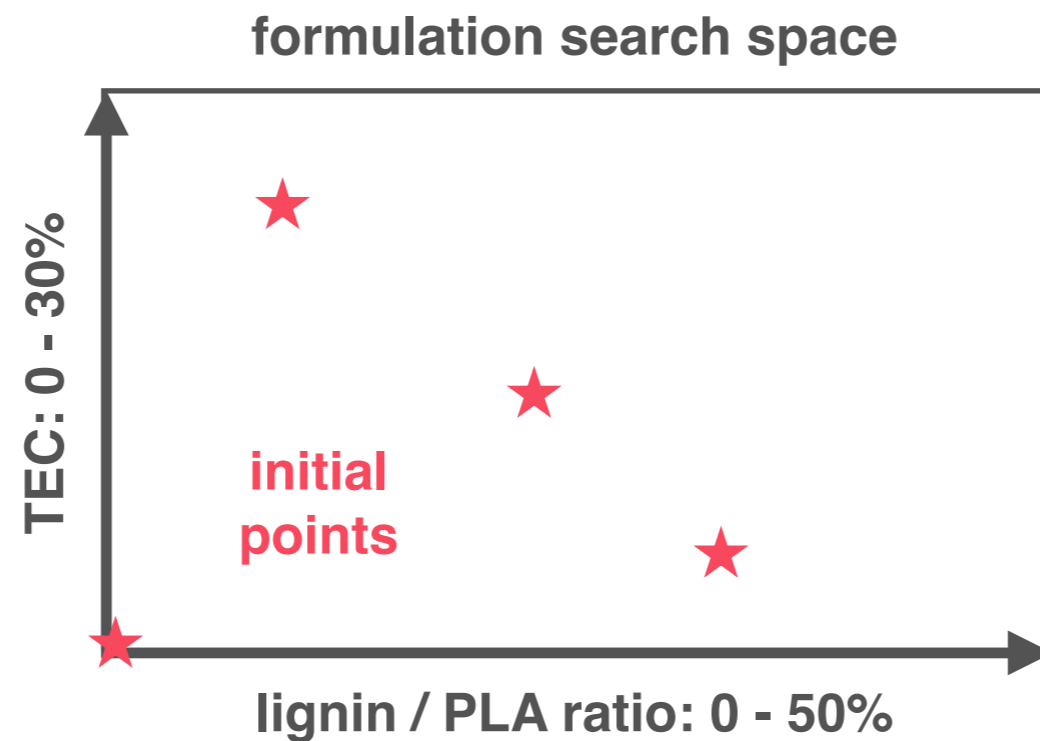
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Materials formulation space

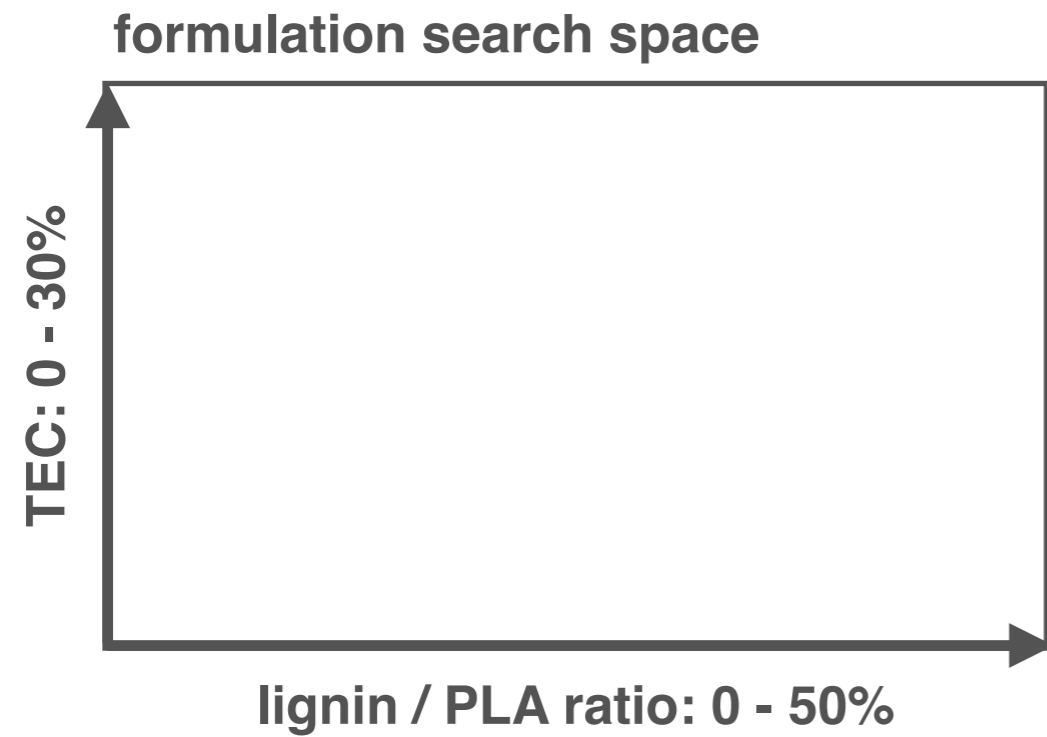
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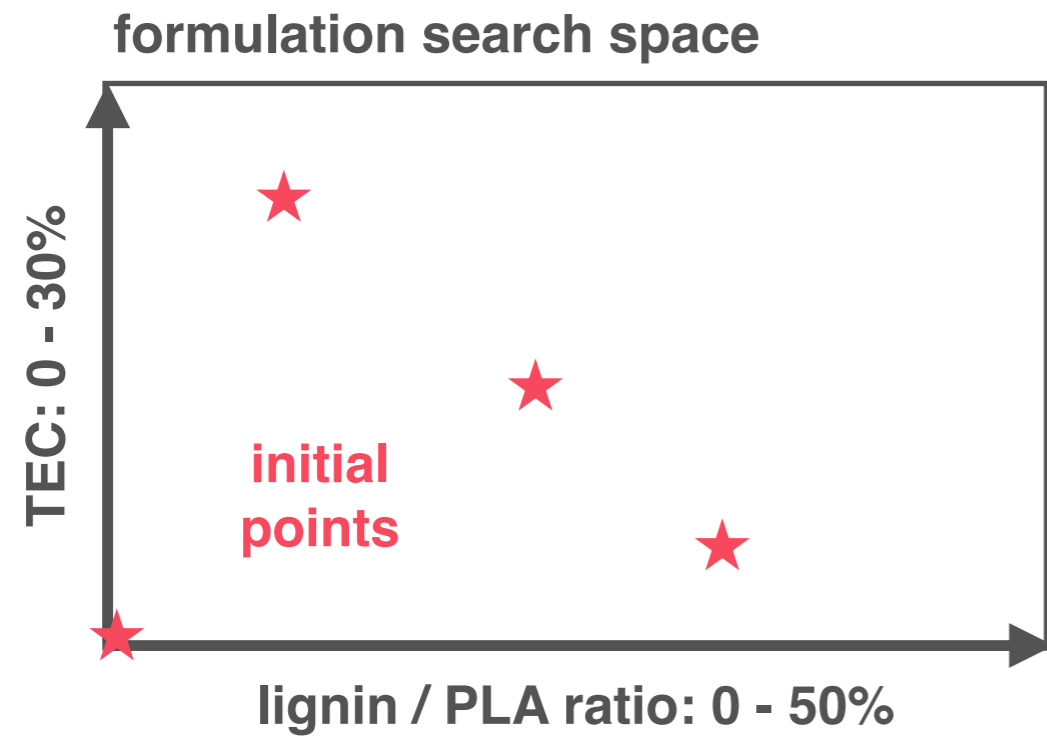


Results

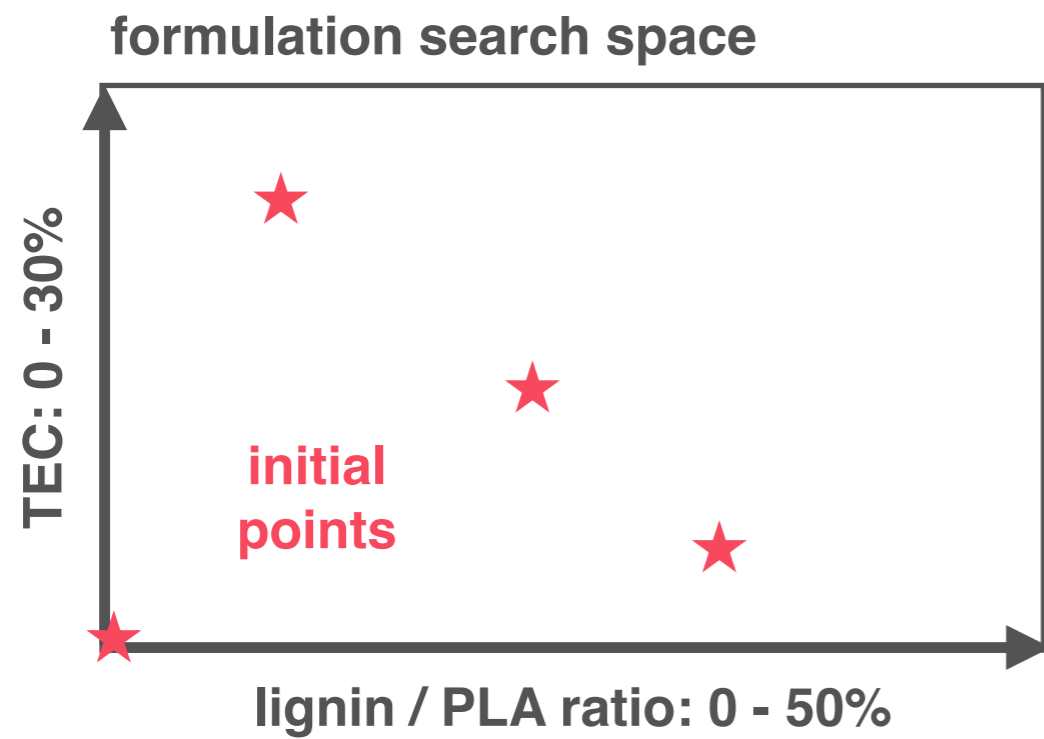
AI workflow in action



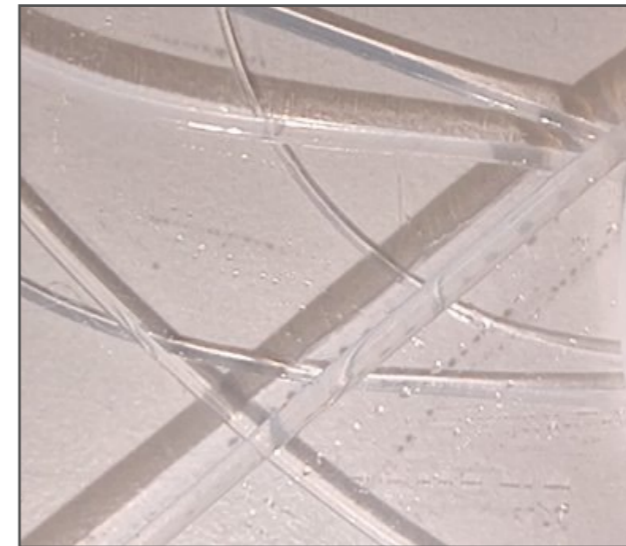
AI workflow in action



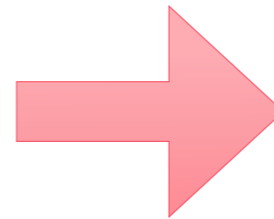
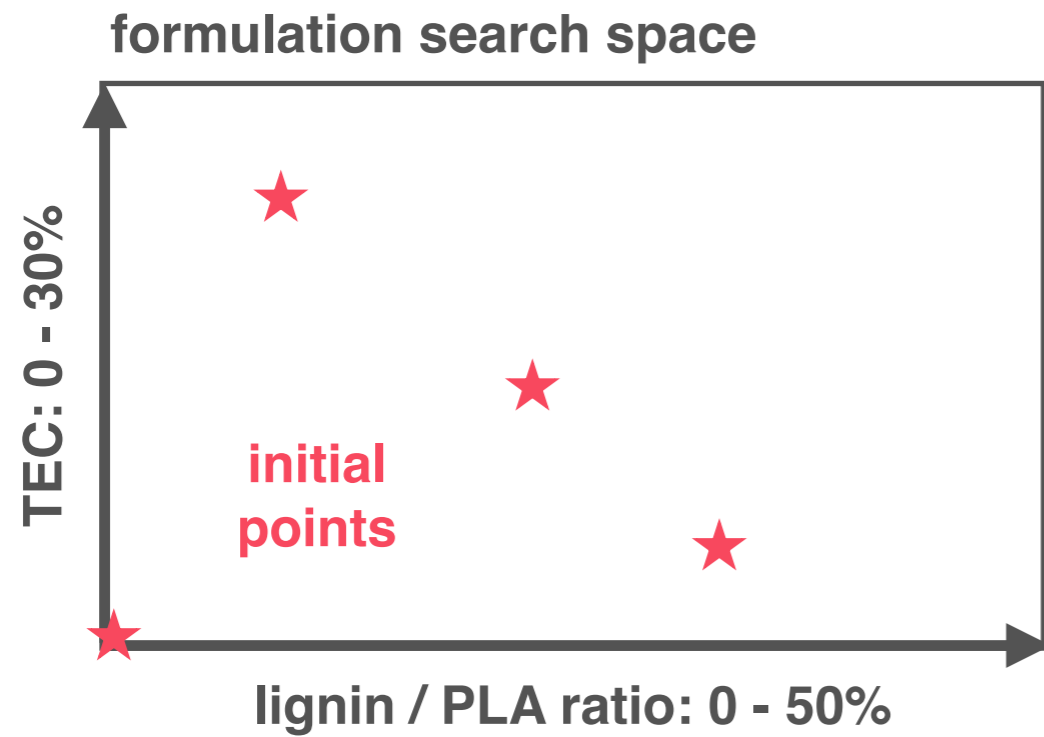
AI workflow in action



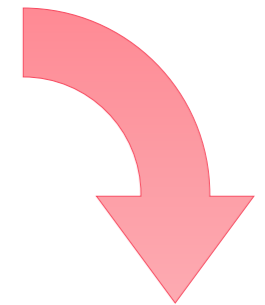
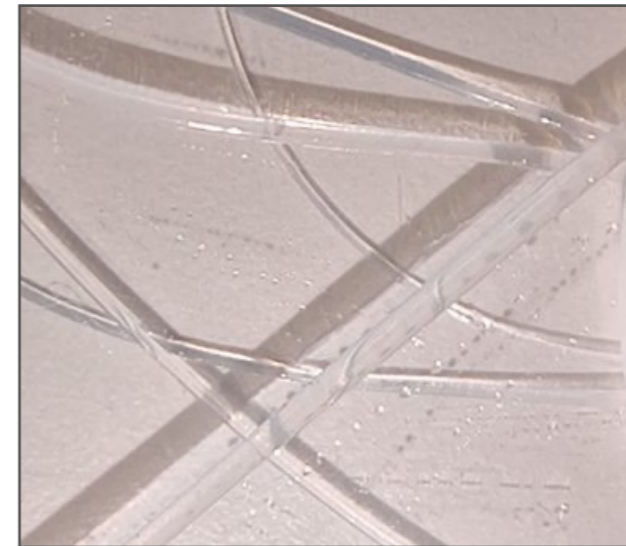
synthesised sample



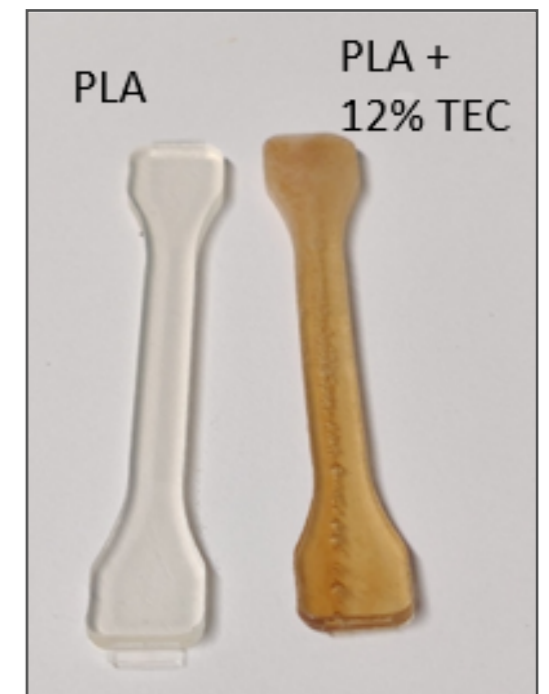
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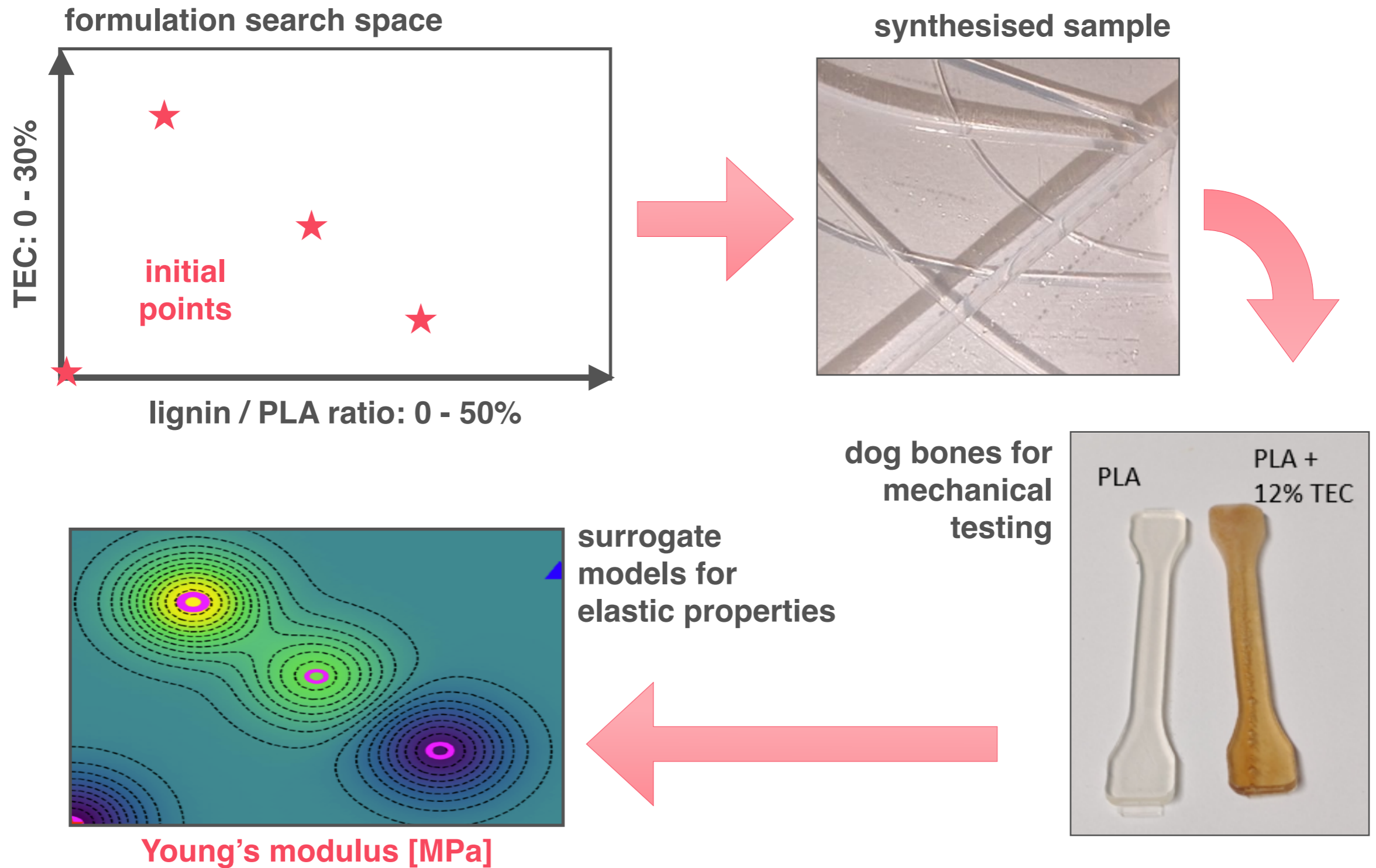
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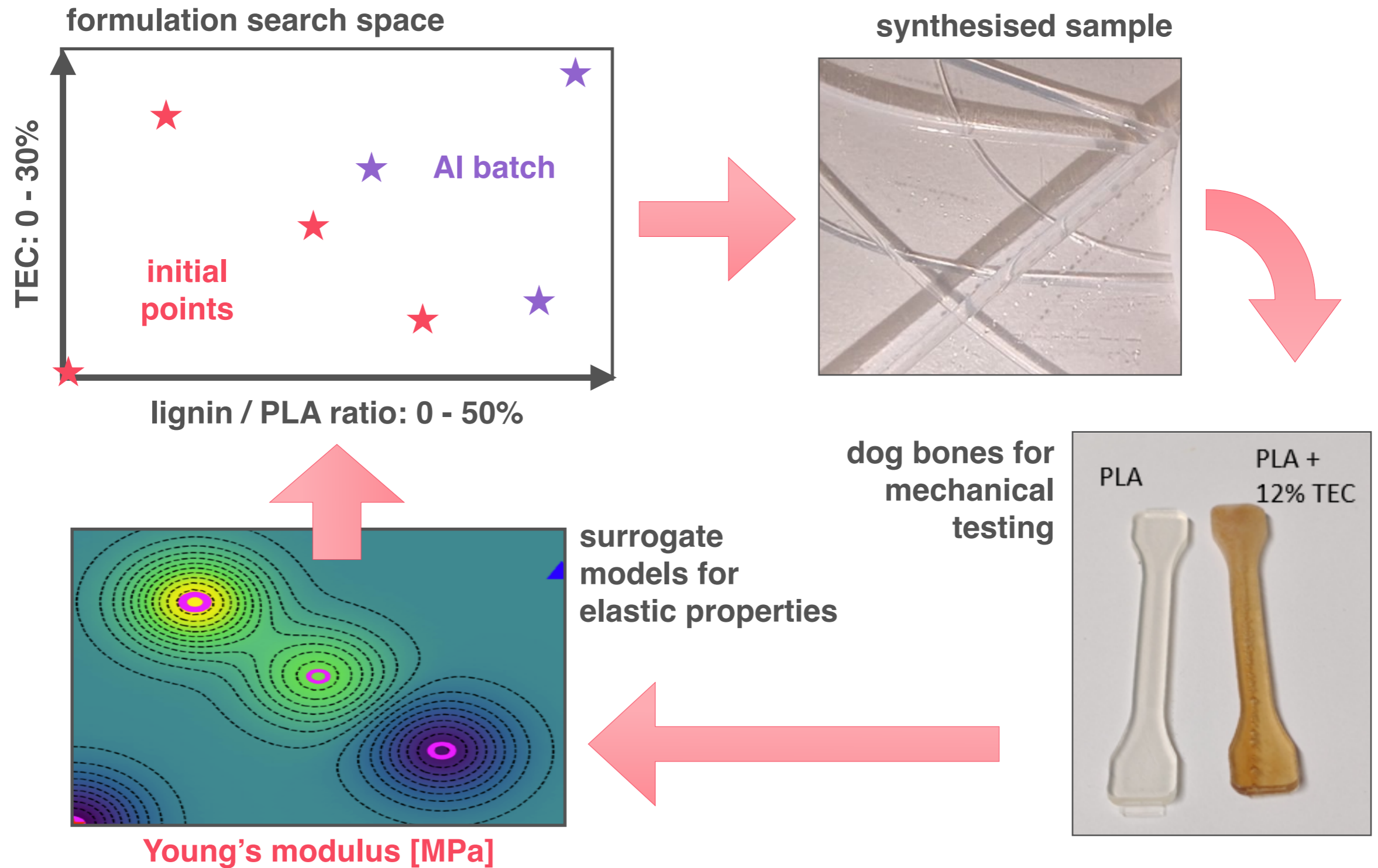
dog bones for
mechanical
testing



AI workflow in action

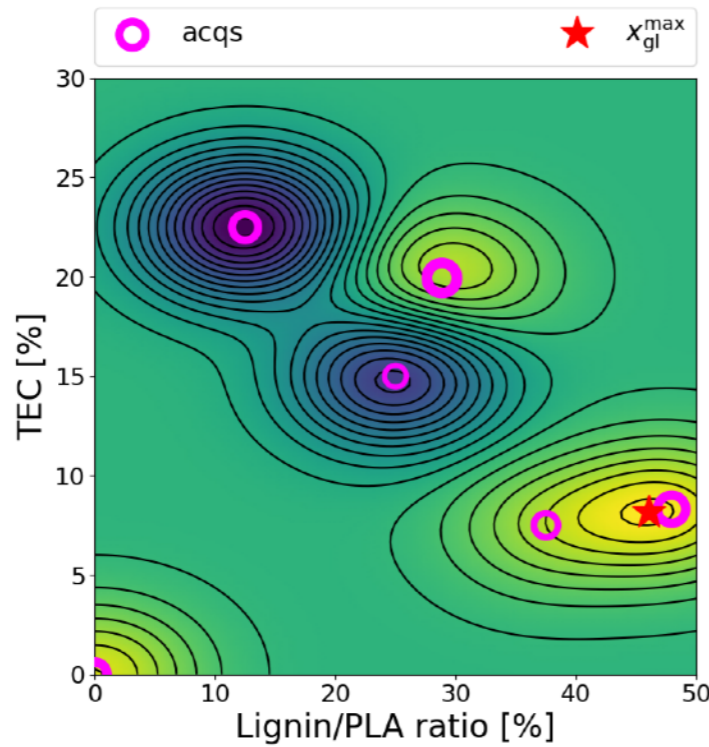


AI workflow in action

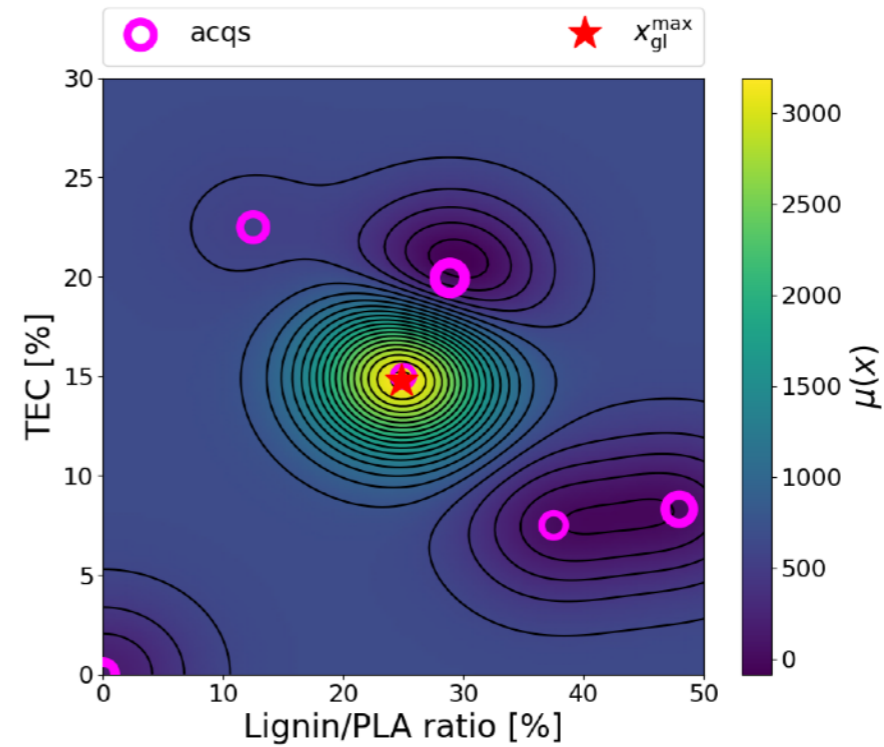


Elastic property surrogate models

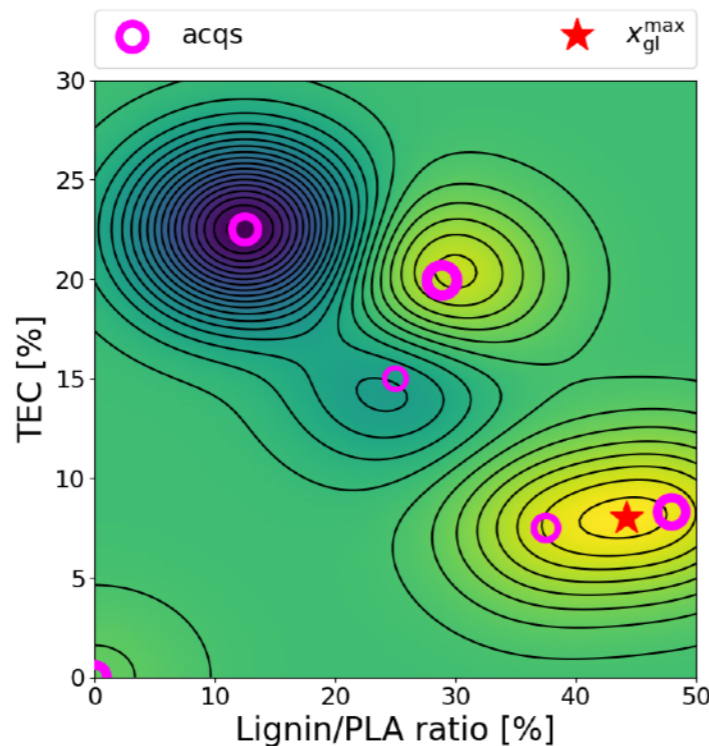
Young's modulus [MPa]



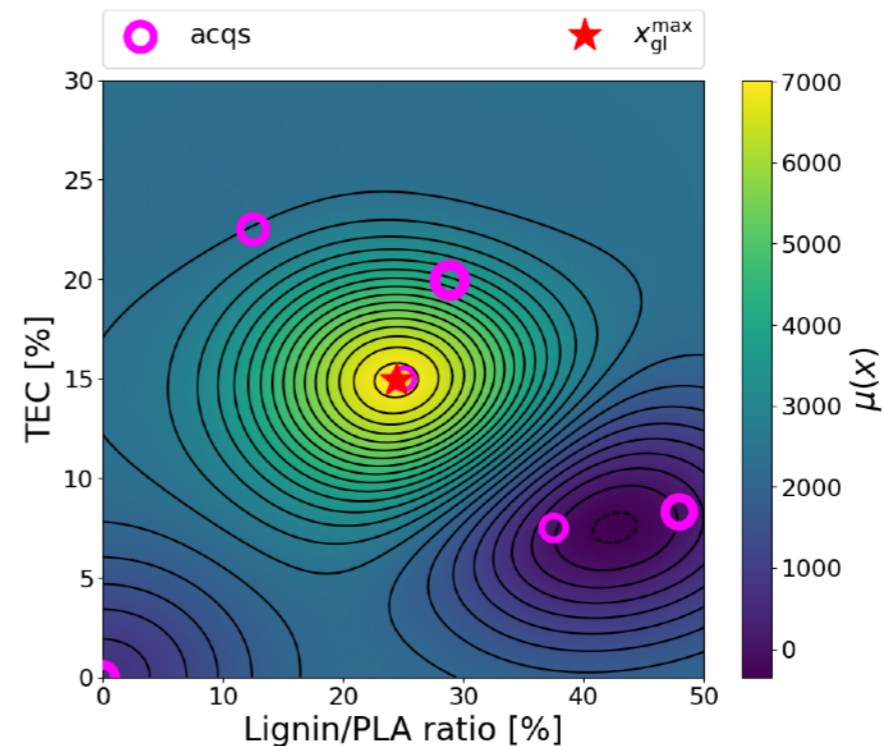
Tensional strength [MPa]



Change in storage modulus $\Delta G'$ [MPa]

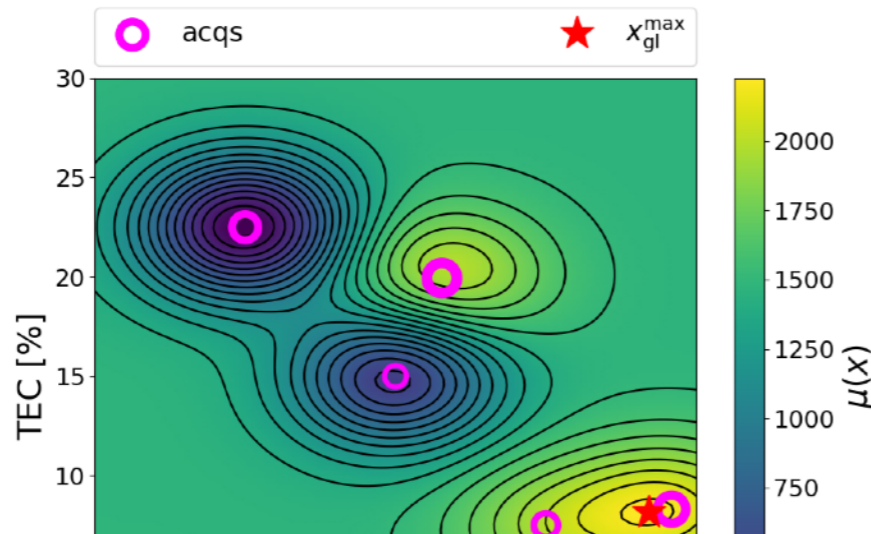


Torsional strength [MPa]

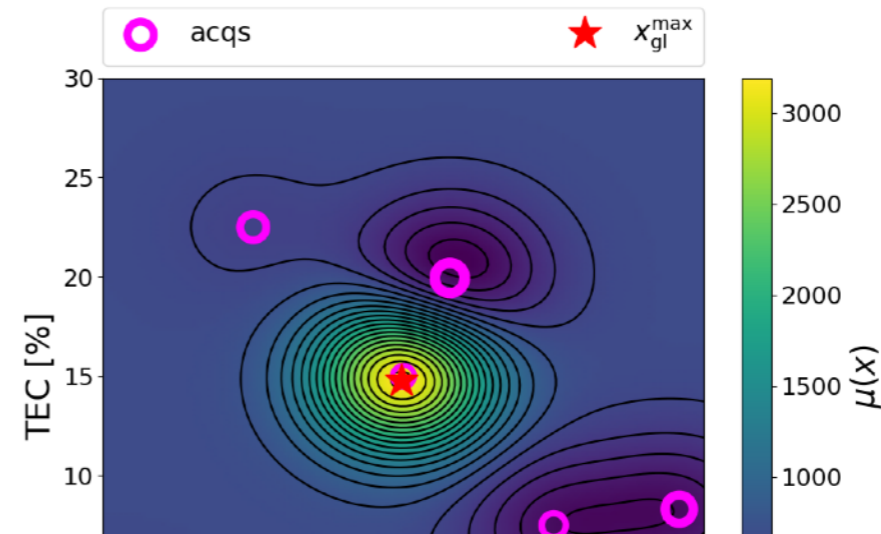


Elastic property surrogate models

Young's modulus [MPa]

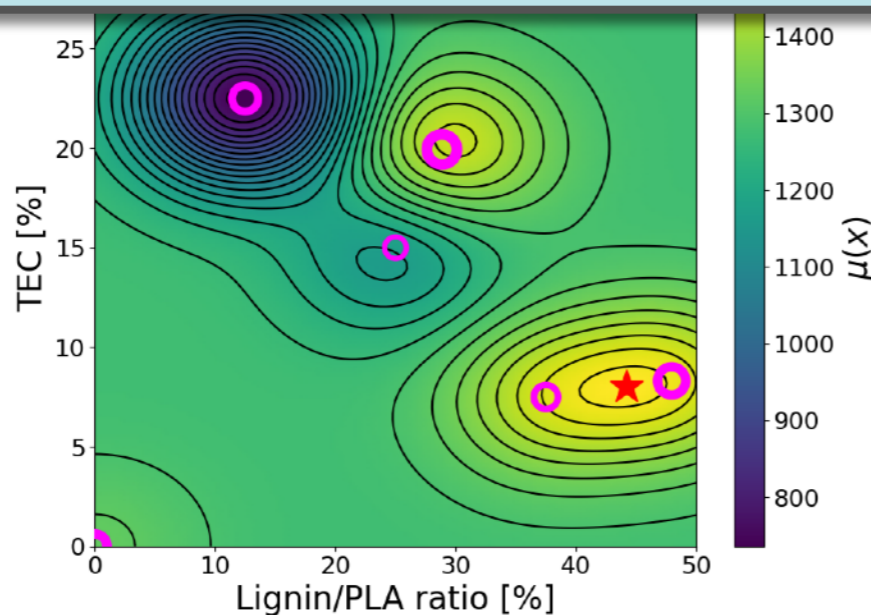


Tensional strength [MPa]

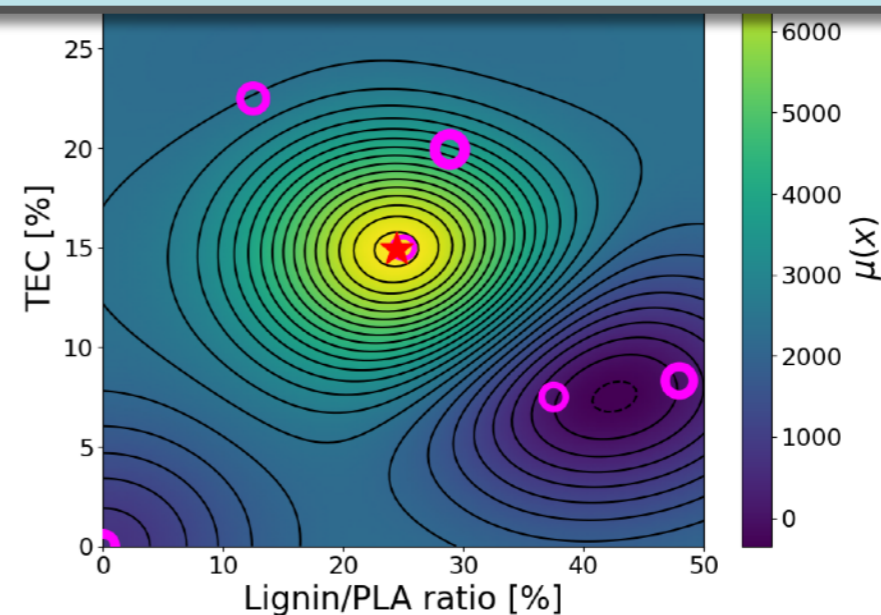


Which materials formulation optimises all mechanical properties?

Change in storage modulus $\Delta G'$ [MPa]

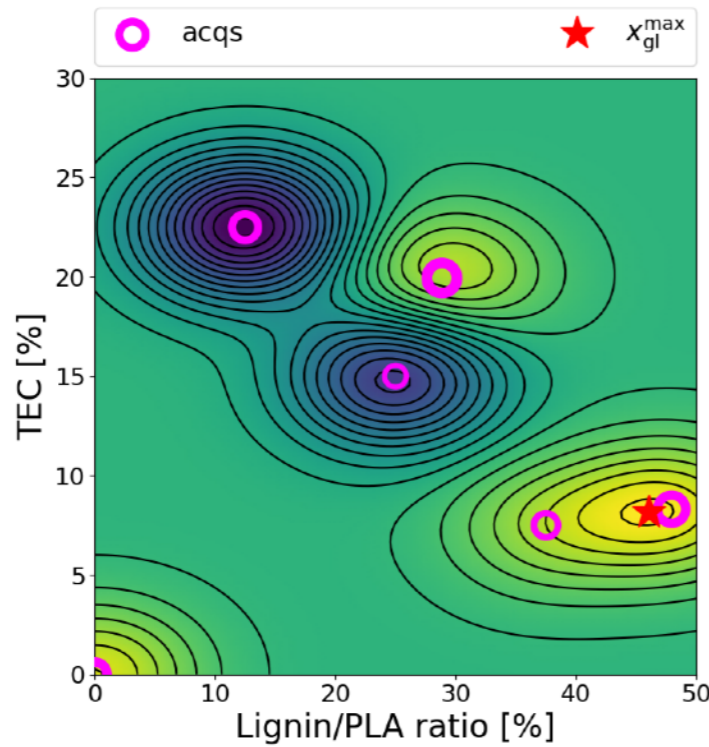


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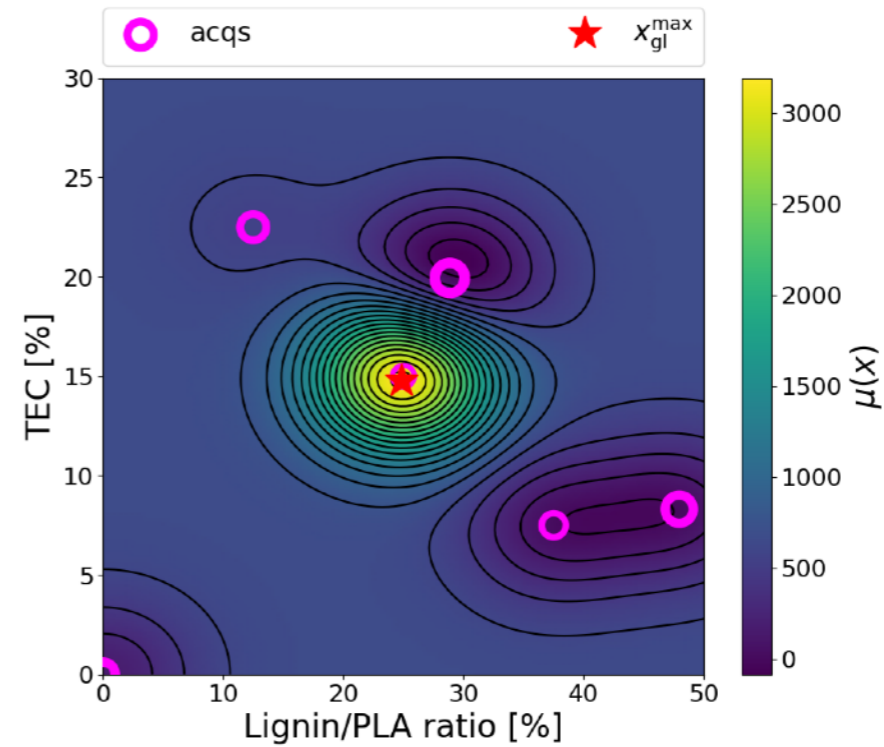


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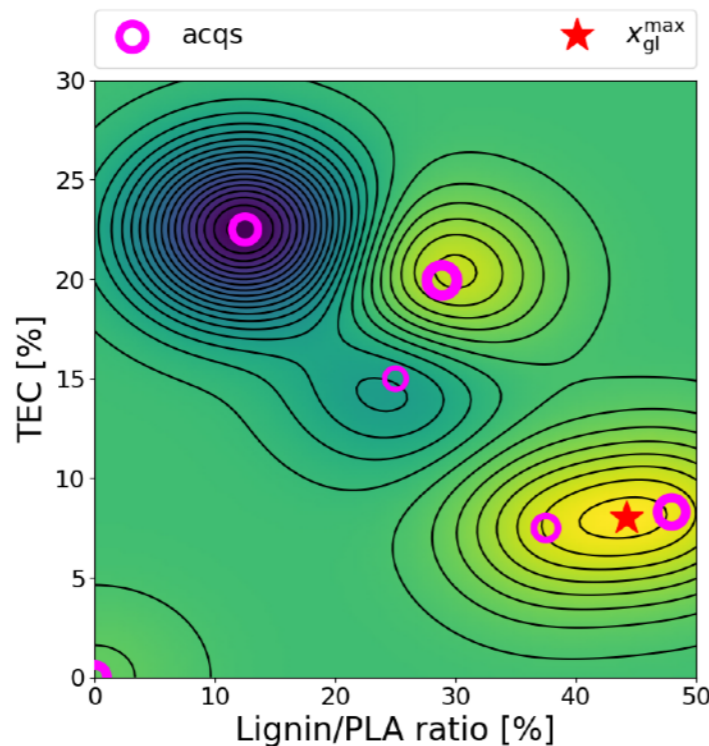
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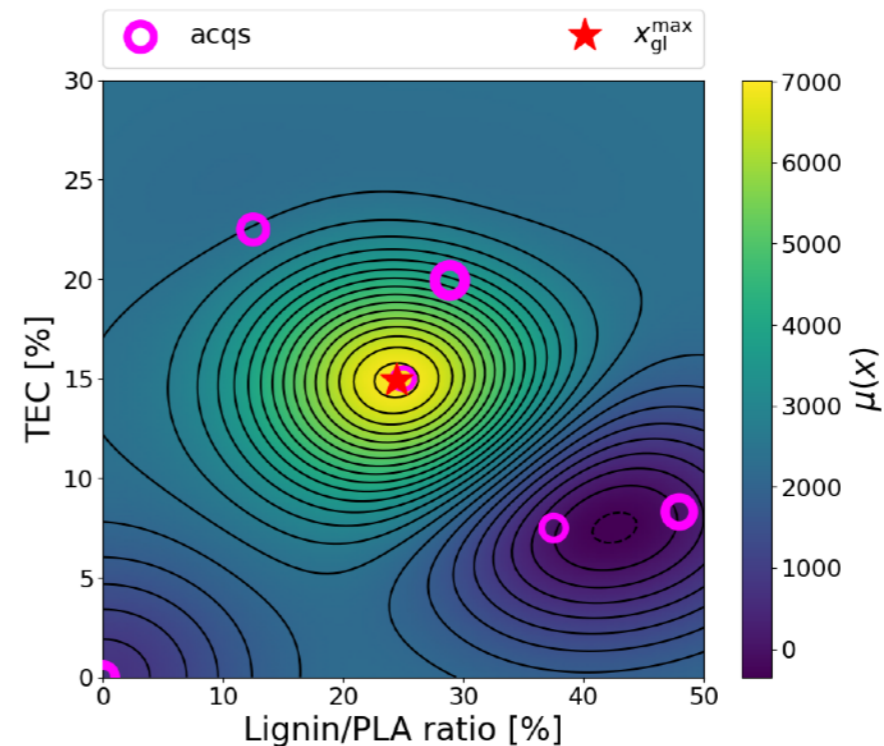
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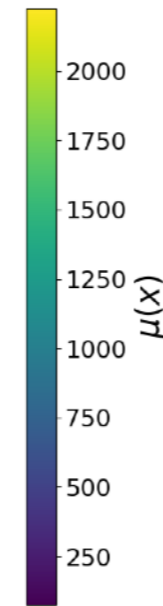
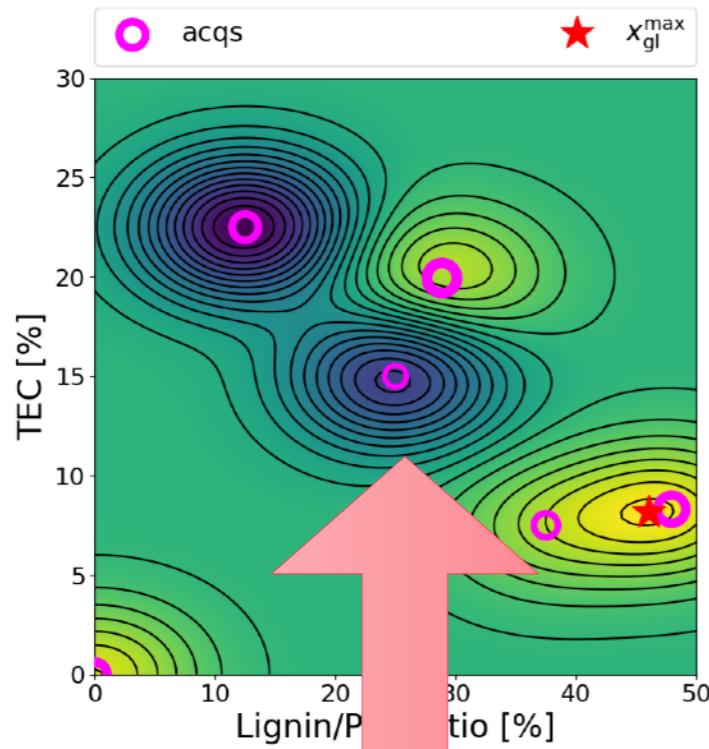


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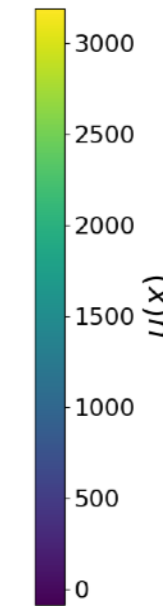
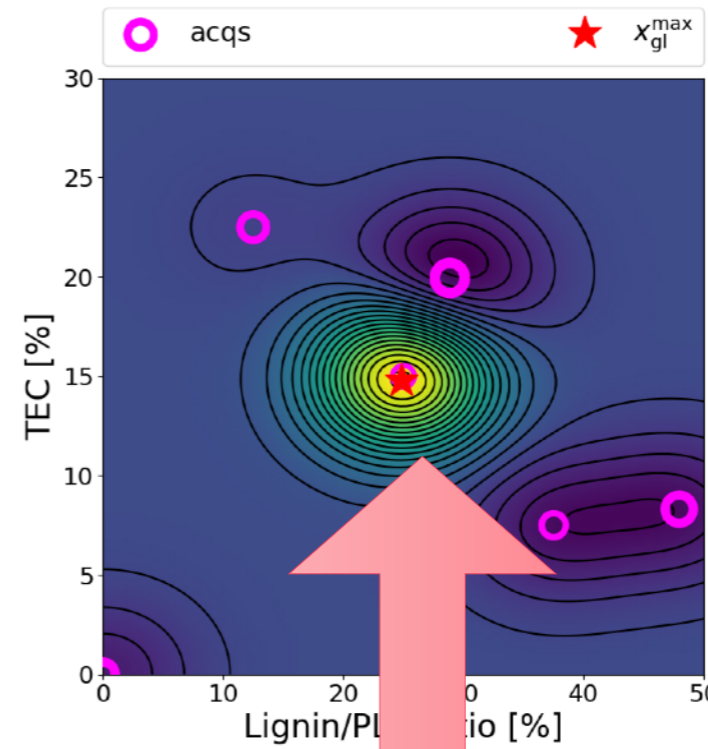


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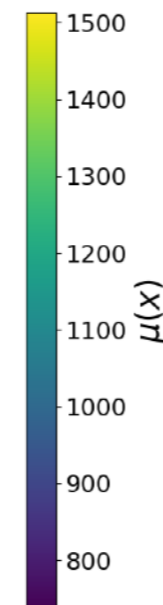
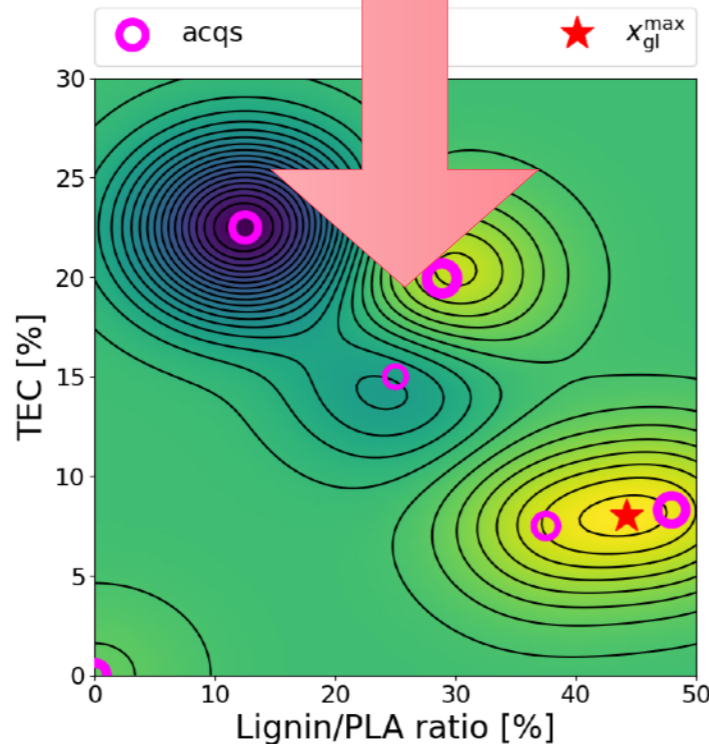
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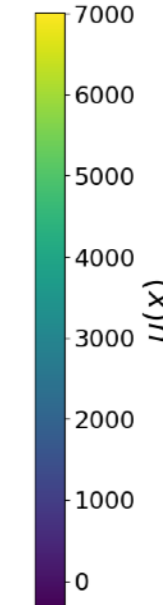
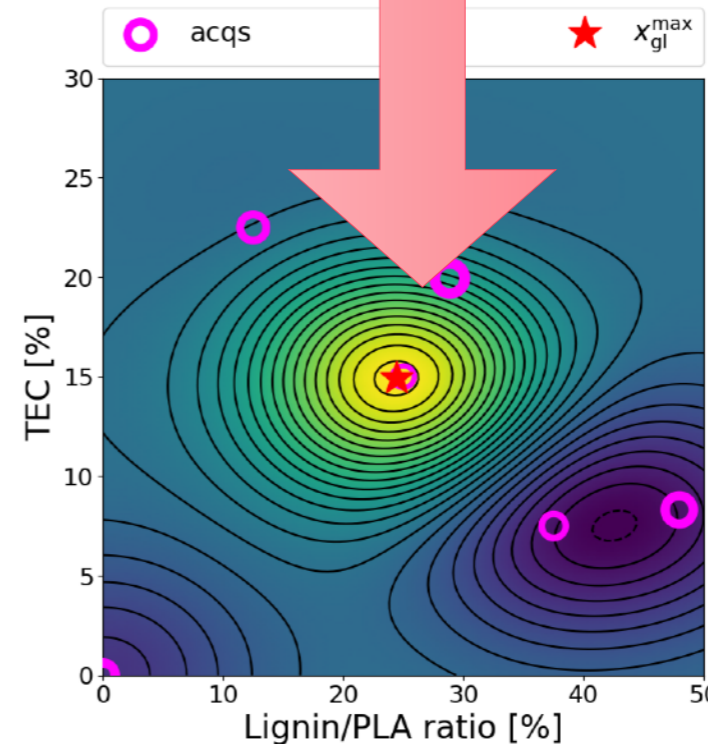
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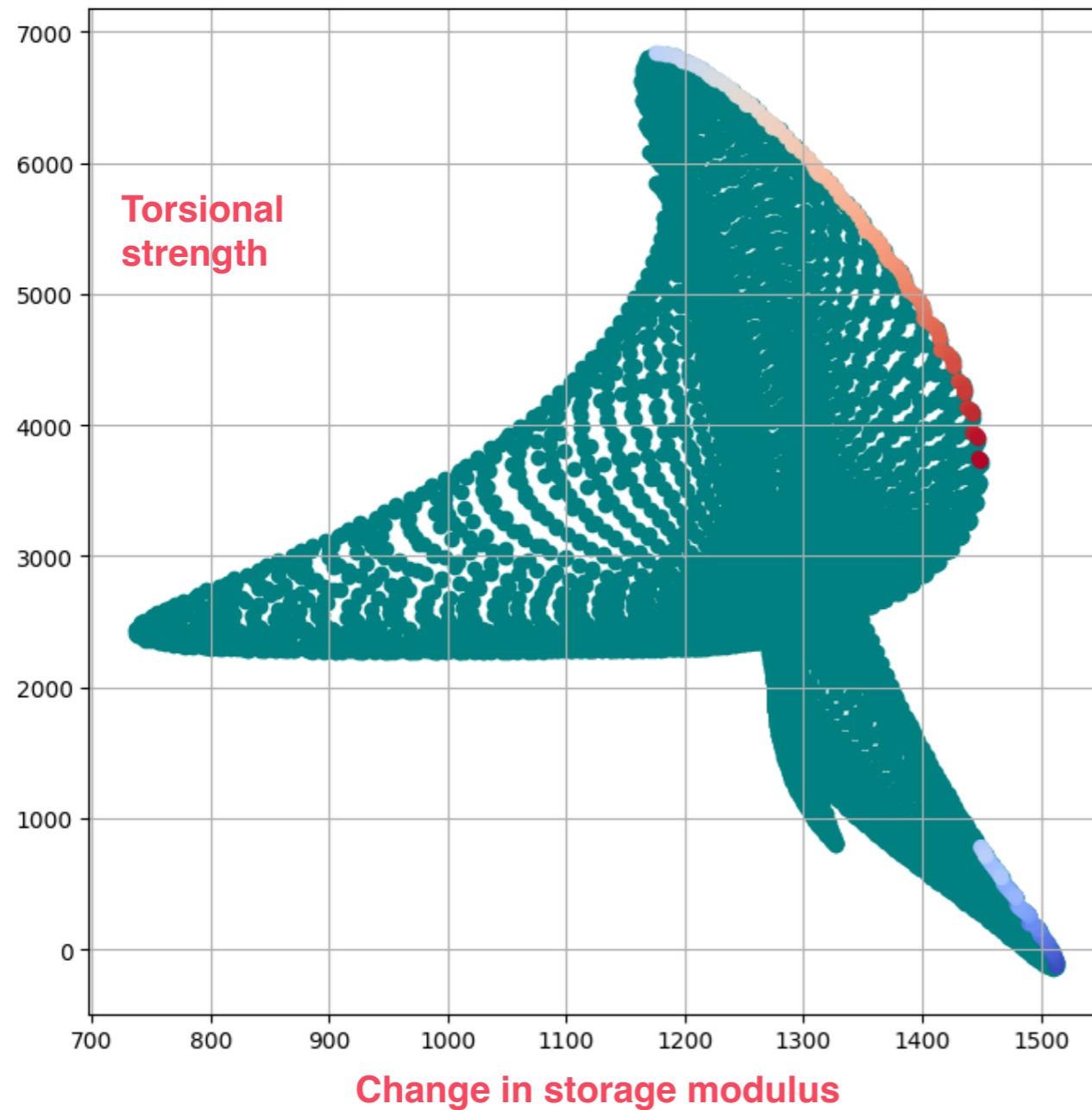


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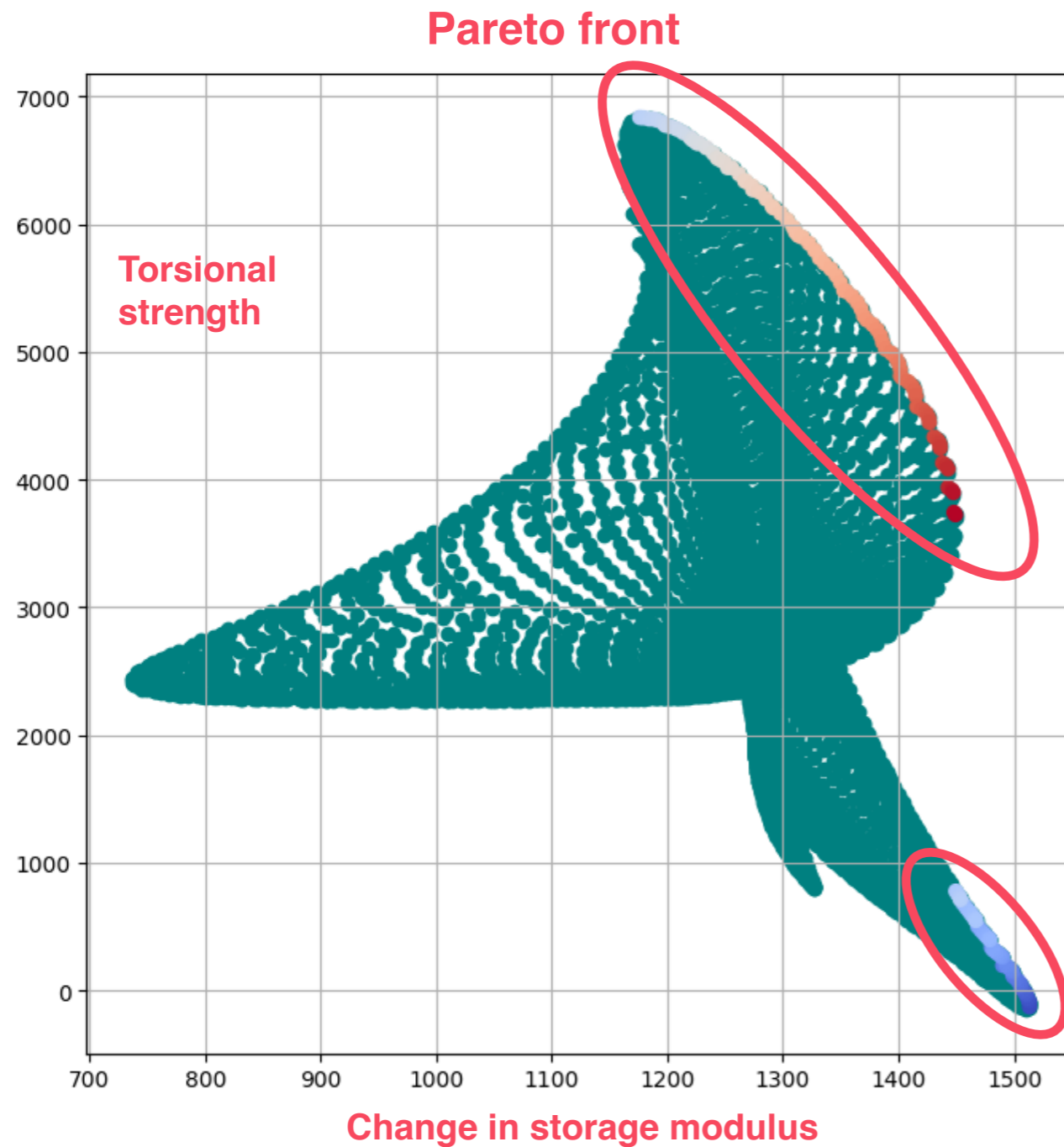


Maximising elastic properties

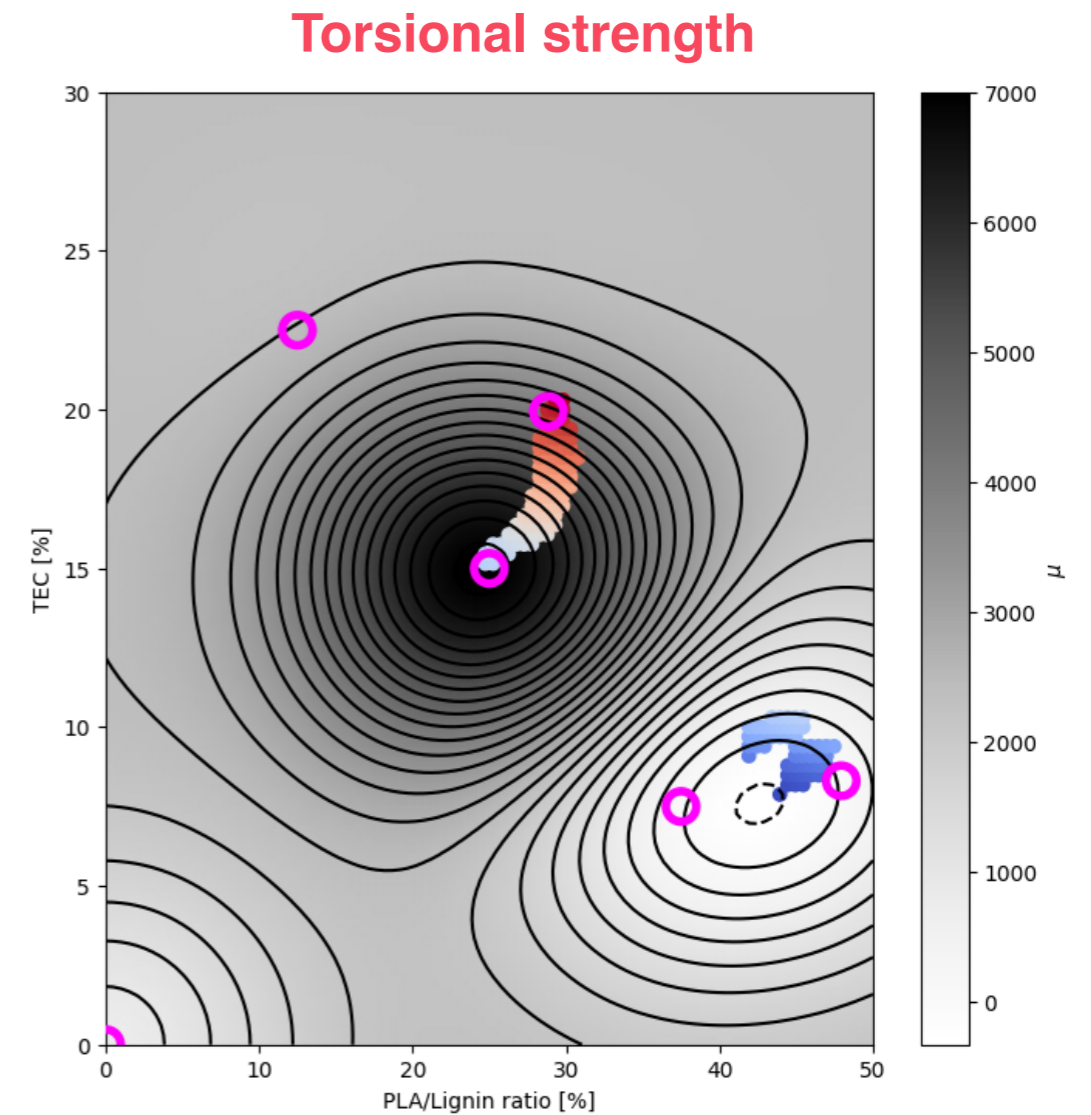
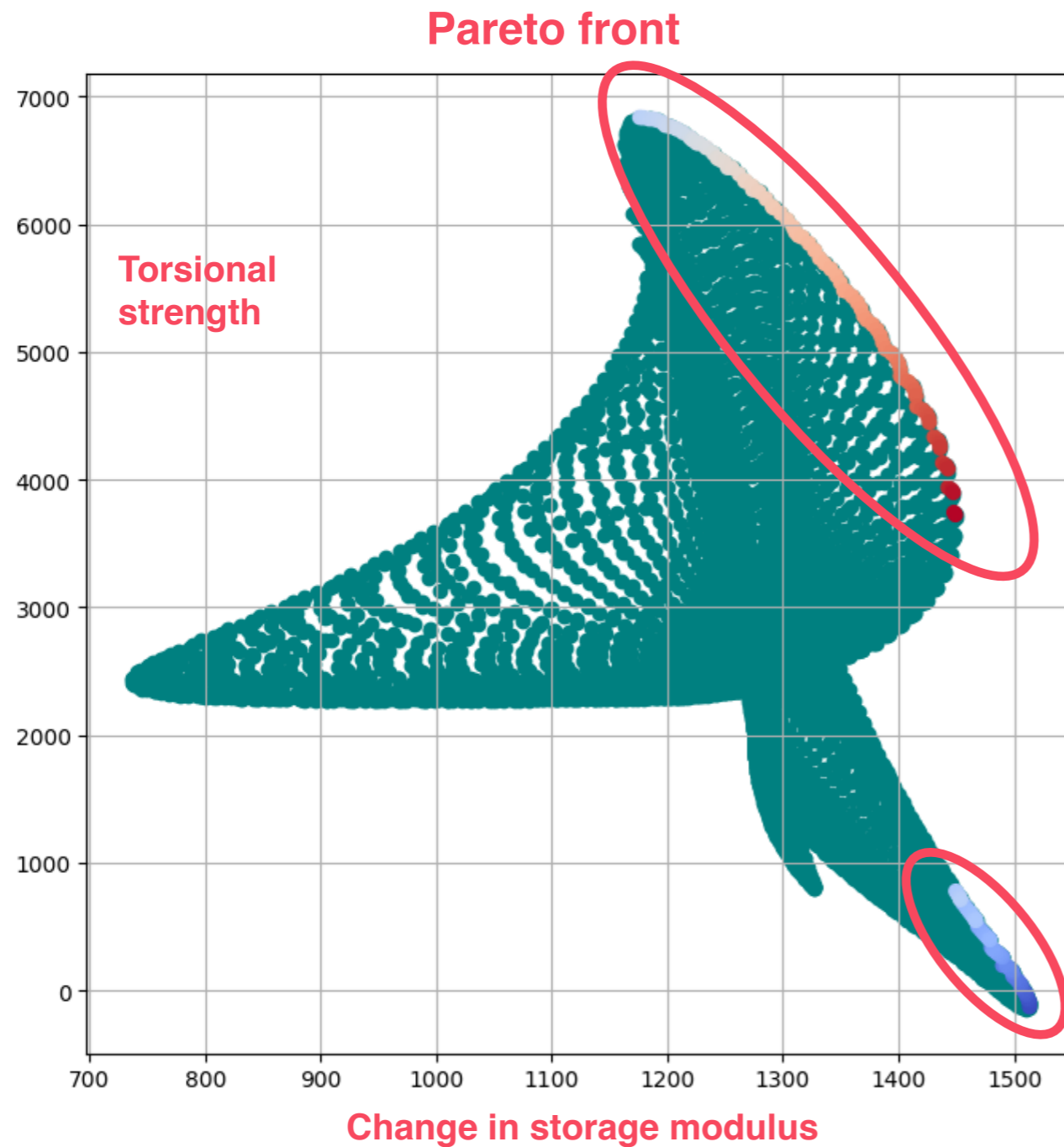
Pareto front



Maximising elastic properties

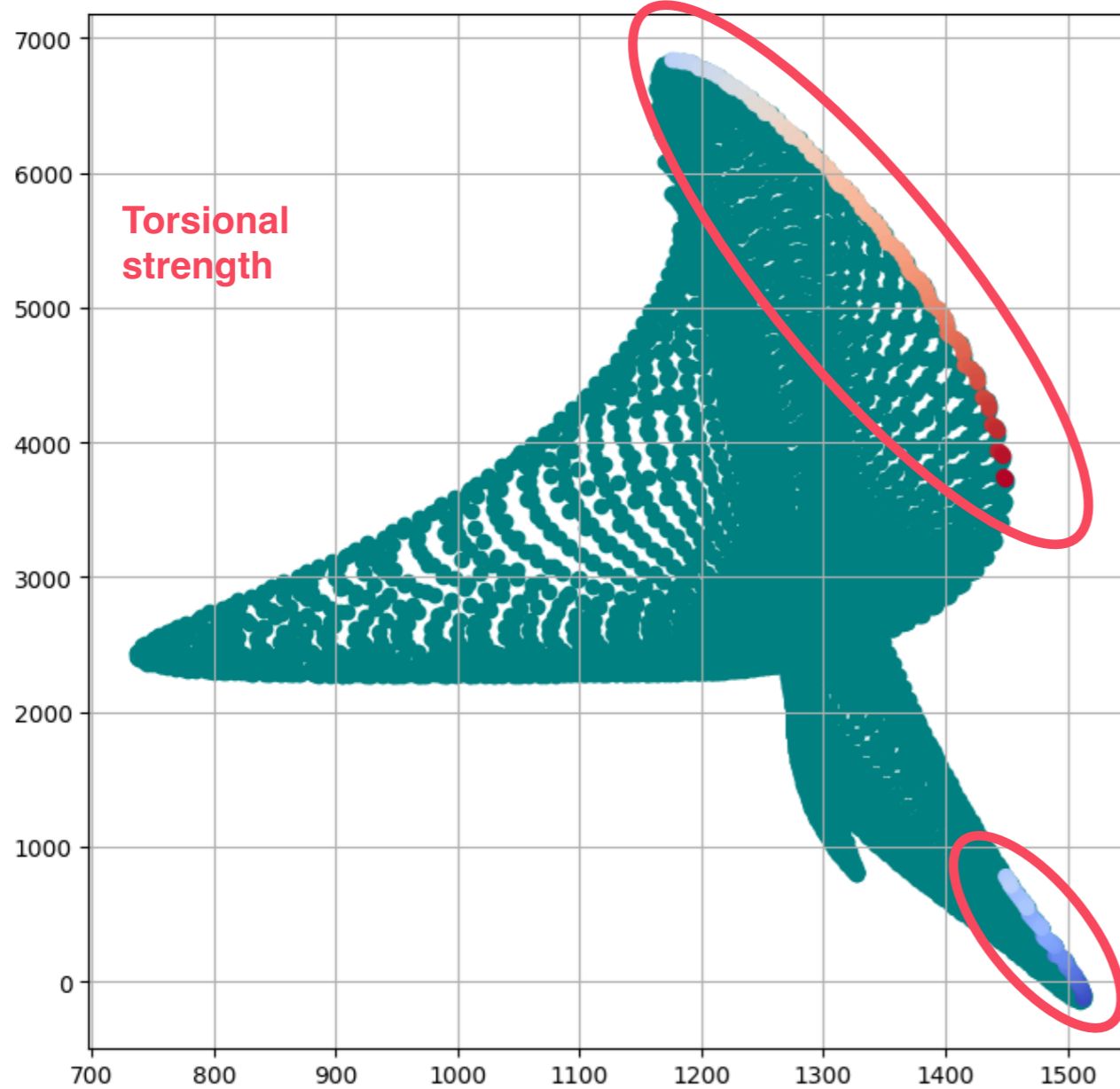


Maximising elastic properties



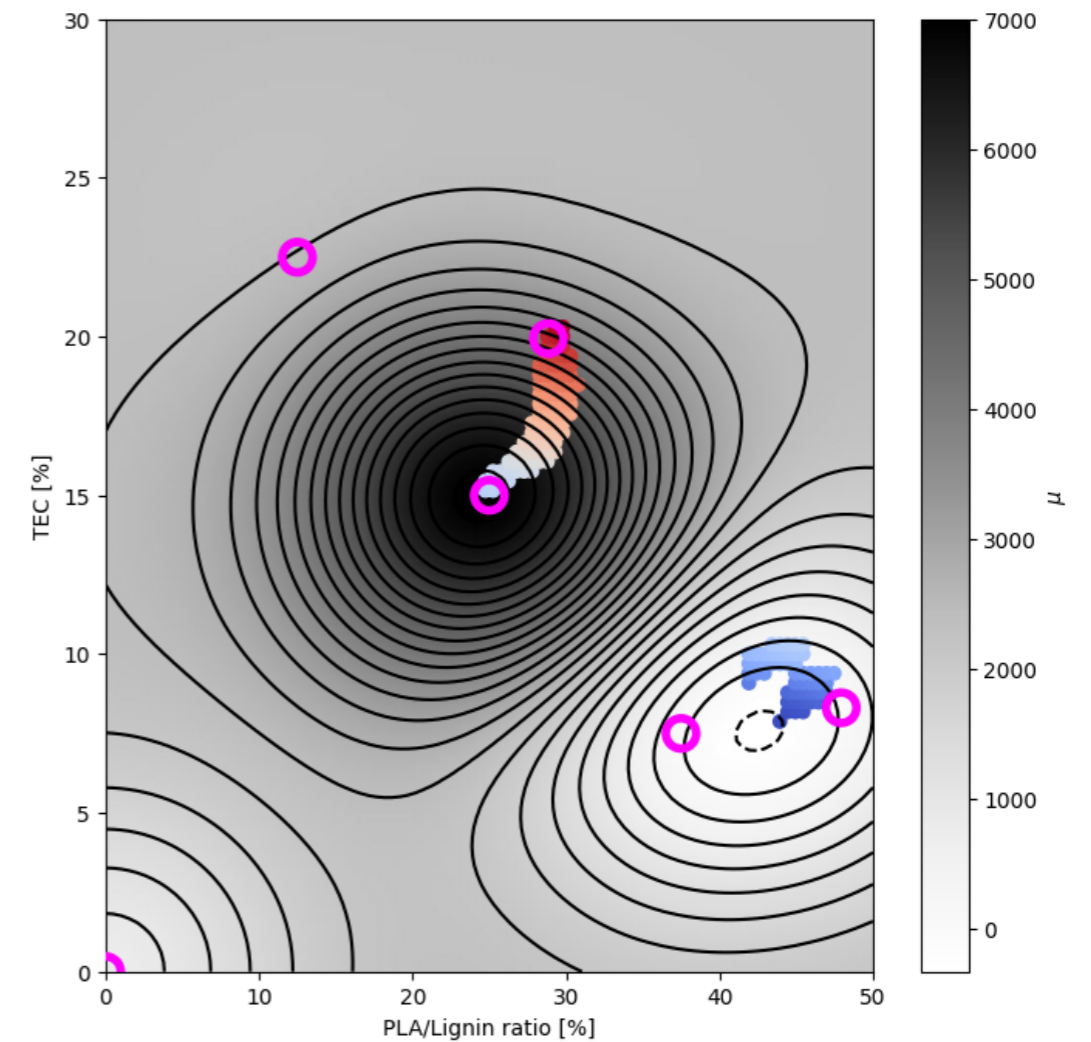
Maximising elastic properties

Pareto front



Change in storage modulus

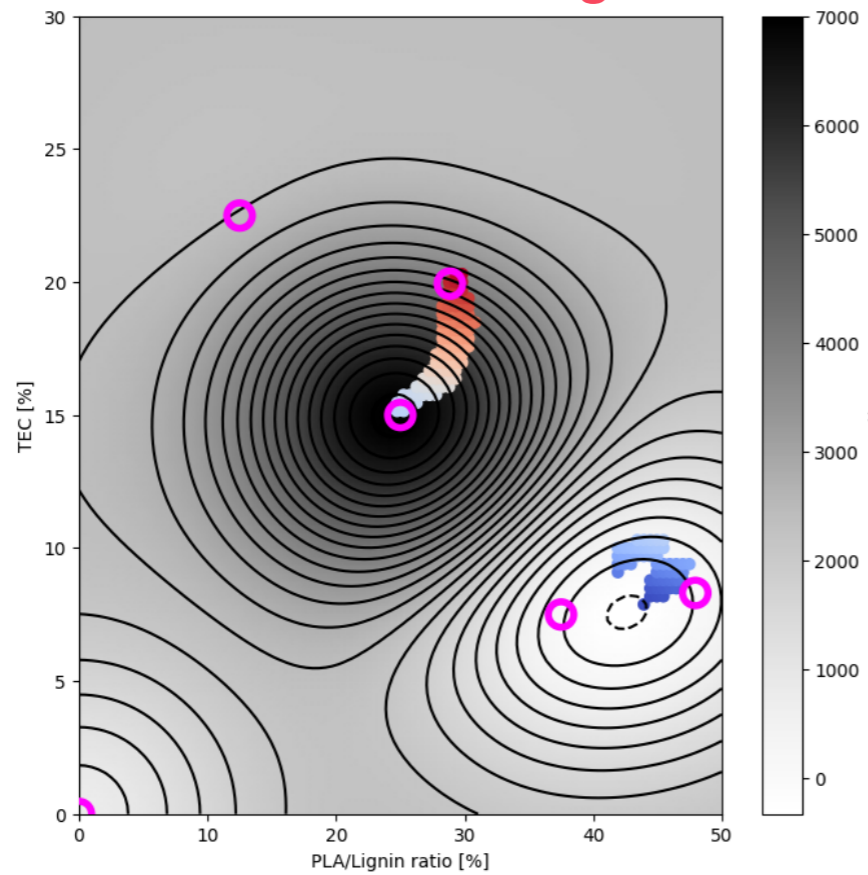
Torsional strength



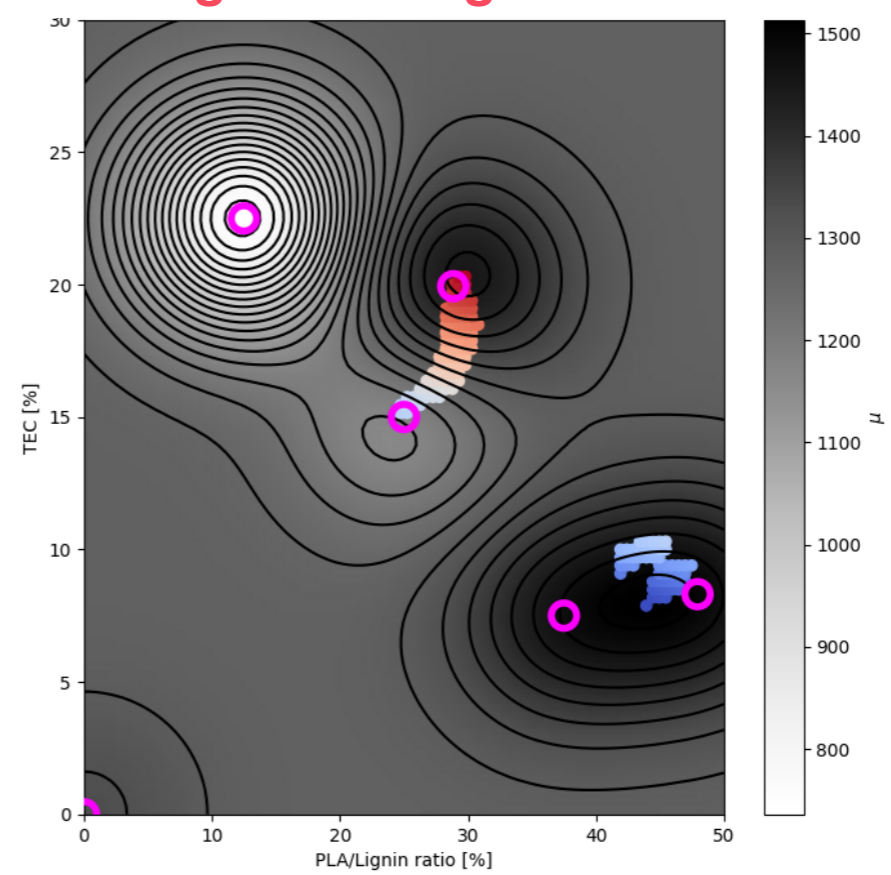
clear optimum found - only 7 experiments

Optimal material formulations

Torsional strength

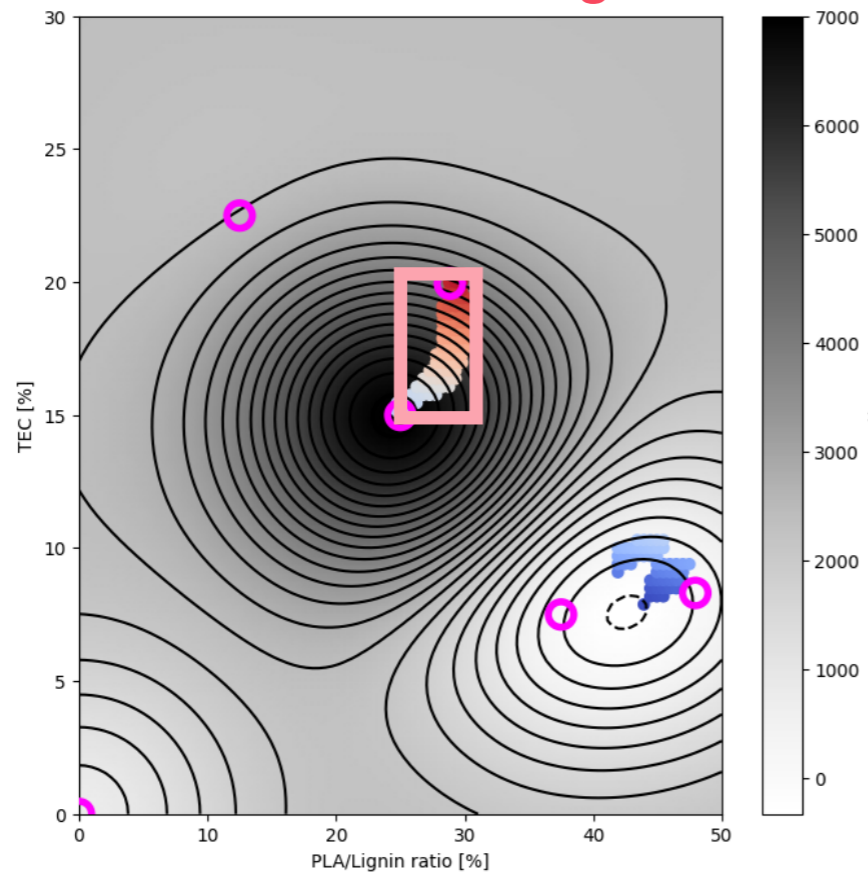


Change in storage modulus

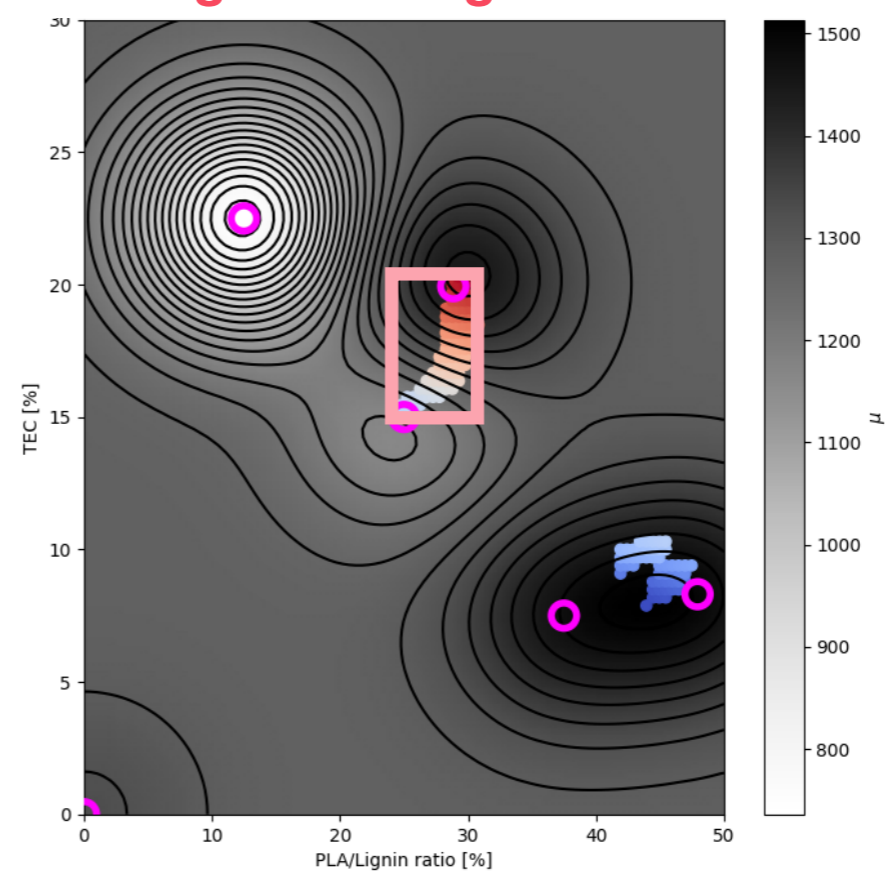


Optimal material formulations

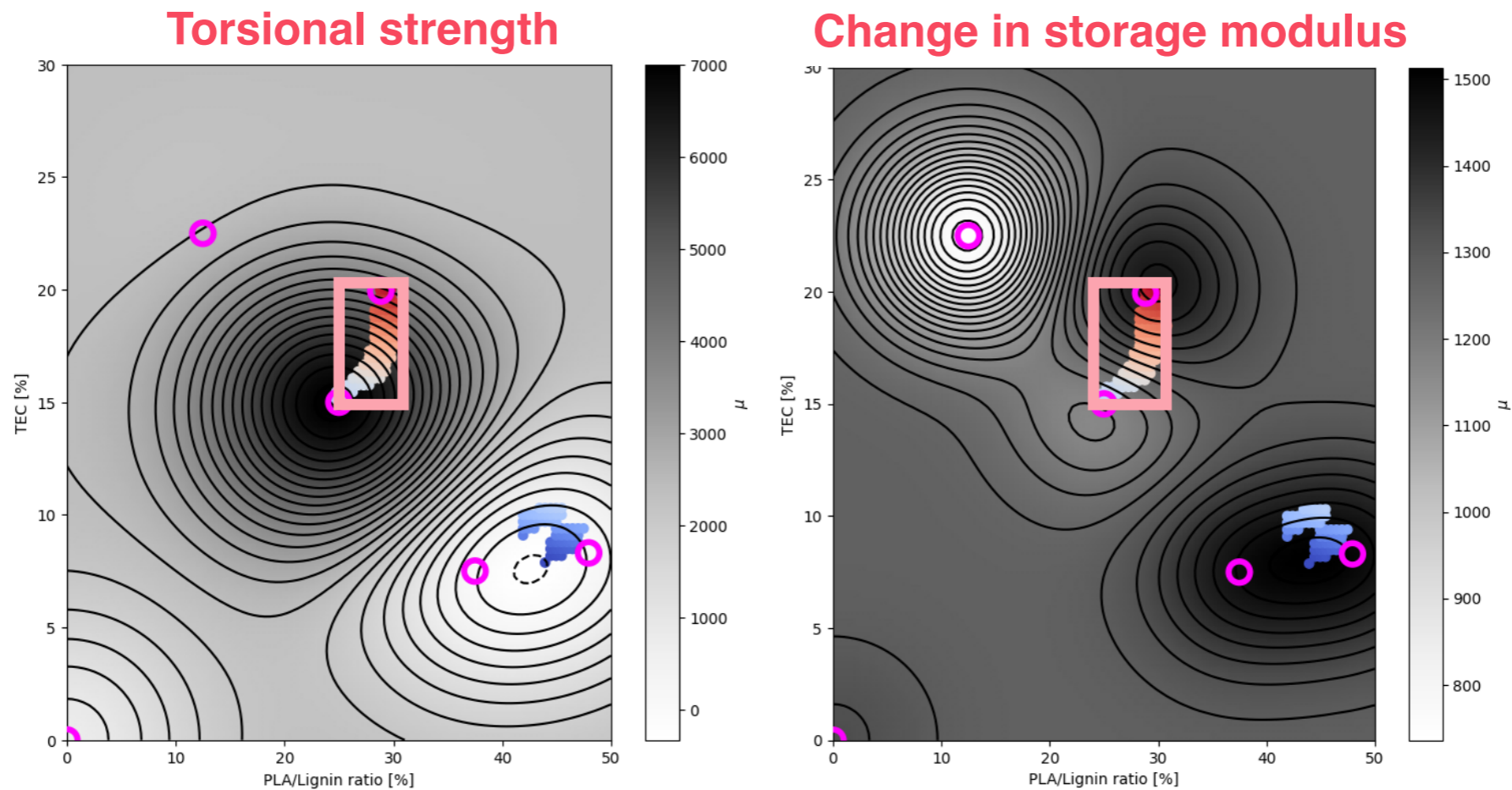
Torsional strength



Change in storage modulus



Optimal material formulations



optimal materials formulation:
25-30% Lignin/PLA ratio + 15-20% TEC

Conclusions & Outlook



Conclusions & Outlook



- designed a computational and experimental methodology

Conclusions & Outlook



- designed a computational and experimental methodology ✓
- determined the formulation with optimal elasticity ✓

MSc Thesis, Tim Salomäki, Åbo Akademi
<https://www.doria.fi/handle/10024/188474>

Conclusions & Outlook



- designed a computational and experimental methodology ✓
- determined the formulation with optimal elasticity ✓
- verifying materials in the laboratory

MSc Thesis, Tim Salomäki, Åbo Akademi
<https://www.doria.fi/handle/10024/188474>

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- considering future steps

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