Accelerating Formulation of Adhesives and Thermal Interfaces with AI

Marco Musto

Citrine Informatics. Senior Research Scientist

Adhesives & Bonding Expo 2024

Stuttgart, DE, 5th December

Overview of Citrine

CITRINE INFORMATICS

AI FOR PRODUCT DEVELOPMENT, PRODUCTION, AND SALES

- Founded in 2013
- Global team across Americas & EU
- Corporate & academic clients / collaborators
- Cloud-based SaaS materials informatics platform

OUR CLIENTS ARE GETTING RESULTS WITH AI TODAY

LyondellBasell | Rolls-Royce
Solvay | Eastman
B. Braun | Saint-Gobain
EMD Electronics | Arkema
Grace | Morrow
Braskem | AGC

4 of the top 10 global Chemicals companies

4 of the top 10 global Adhesives & Sealants companies

2 of the top 10 global Personal Care & Beauty companies

REMOVING PFAS FROM ADHESIVES

A global materials conglomerate successfully reformulated an adhesive to exclude PFAS and saved **2 years** of R&D work on a 5-year project.

The Problem

- Accelerate product development in response to regulatory demands
- Pressure sensitive adhesive excluding PFAS, same performance
- Unable to achieve critical breakthroughs using internal resources

The Process

- Launched a pilot project in first month to reach autonomy
- Within first quarter, assessed **millions of ingredient combinations**,
- In the following 2 months, single user generated 25 new models autonomously.

The Outcome

- First breakthrough candidate identified in 4 months
- Customer team estimates to have saved **2 years of R&D work** on a project that would typically be 5 years.
- Customer planned data integration alongside rapid enterprise expansion

FROM ZERO DATA TO ON-TARGET LOCALIZED FORMULATIONS IN 5 MONTHS

Korean national composites champion develops carbon fiber additives using local ingredients on new capital equipment in 5 months.

The Problem

- Starting from scratch with new locally-sourced ingredients on new processing equipment.
- No historical data available.
- Hit the same performance criteria as competitor products.

The Process

- Create & synthesize initial grid of 20 experiments.
- Build AI model on 20 training data points with formulation-specific featurization.
- Compare AI-generated candidates with those suggested by traditional R&D process.

The Outcome

- **5 months from zero data** to successful recipes.
- The first AI model performed **4X better than traditional** R&D approaches

BETTER TAILOR-MADE POLYMER FORMULATIONS - QUICKER

21% increase in fiber reinforced plastic mechanical performance in just 10 months

The Customer

- A multinational producer of specialty chemicals.
- Wanted to create differentiated products more quickly.

The Problem

- Increase the mechanical properties of a fiber reinforced plastic, while maintaining the rest of its property profile.
- Trillions of potential recipes.
- Citrine identified that there was high process variability between R&D sample batches

The Process

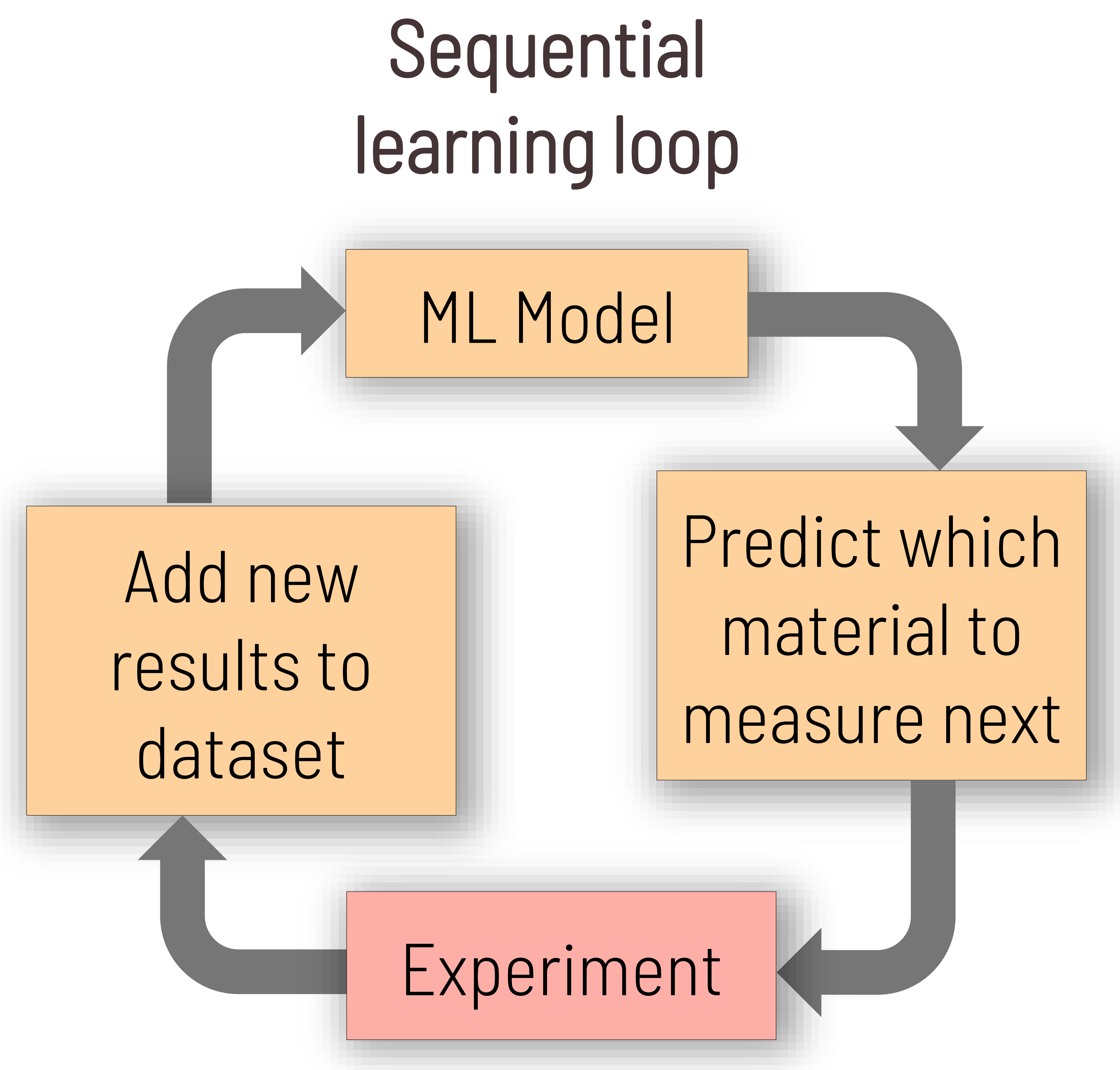
- A sequential learning approach was used.
- Programmatic normalization of results from batch to batch was instituted.

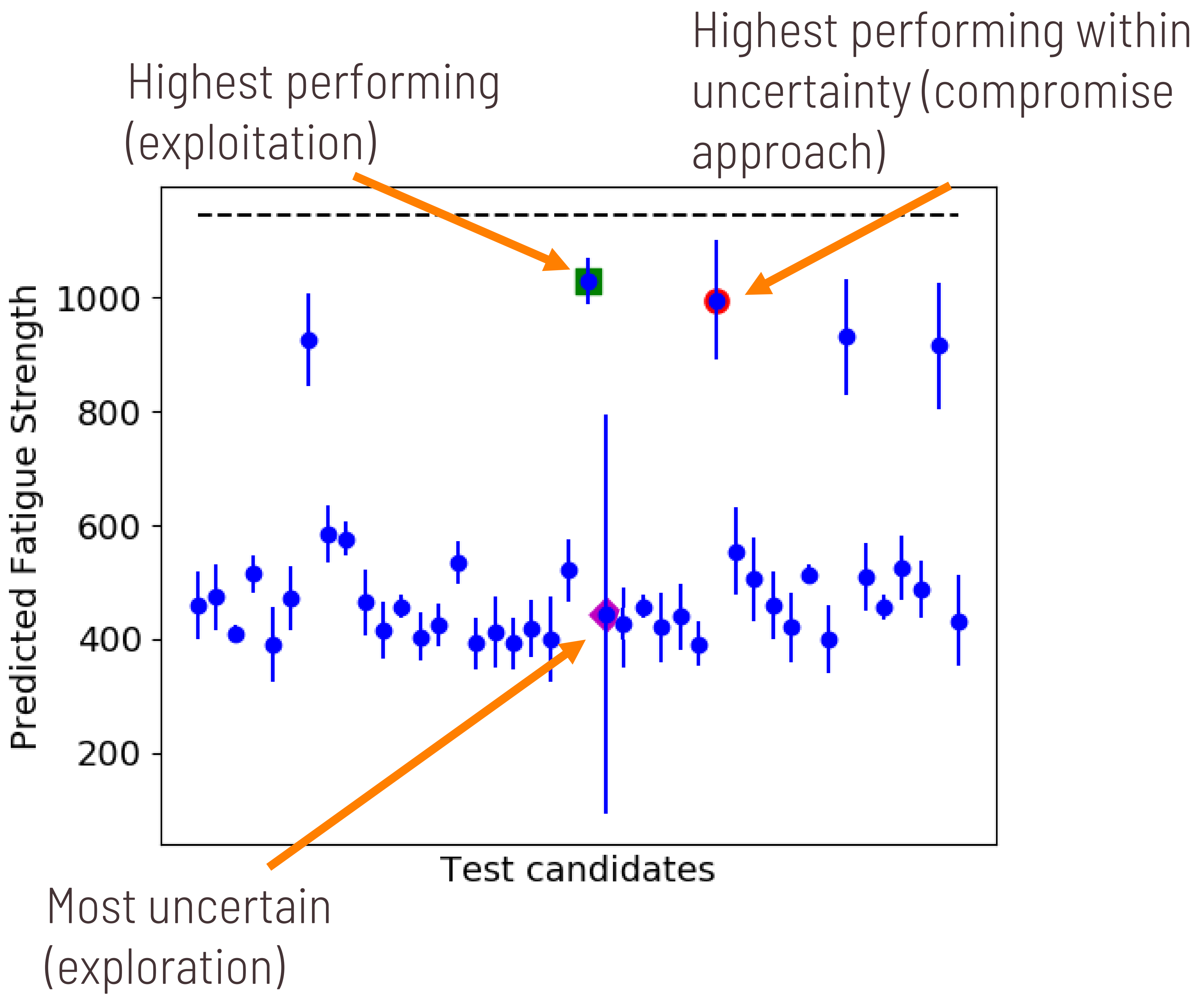
The Outcome

- In just 10 months a **21% increase of mechanical properties** was achieved.
- Process variability was better handled and accounted for, leading to a **reduction in performance uncertainty by 58%**

SEQUENTIAL LEARNING: UNCERTAINTY-DRIVEN OPTIMIZATION

Optimization of model and/or design performance





Ling, et al. High-dimensional materials and process optimization using data-driven experimental design with well-calibrated uncertainty estimates. Integrating Materials and Manufacturing Innovation 6 (2017): 207-217

Borg, et al. Quantifying the performance of machine learning models in materials discovery. Digital Discovery 2.2 (2023): 327-338.

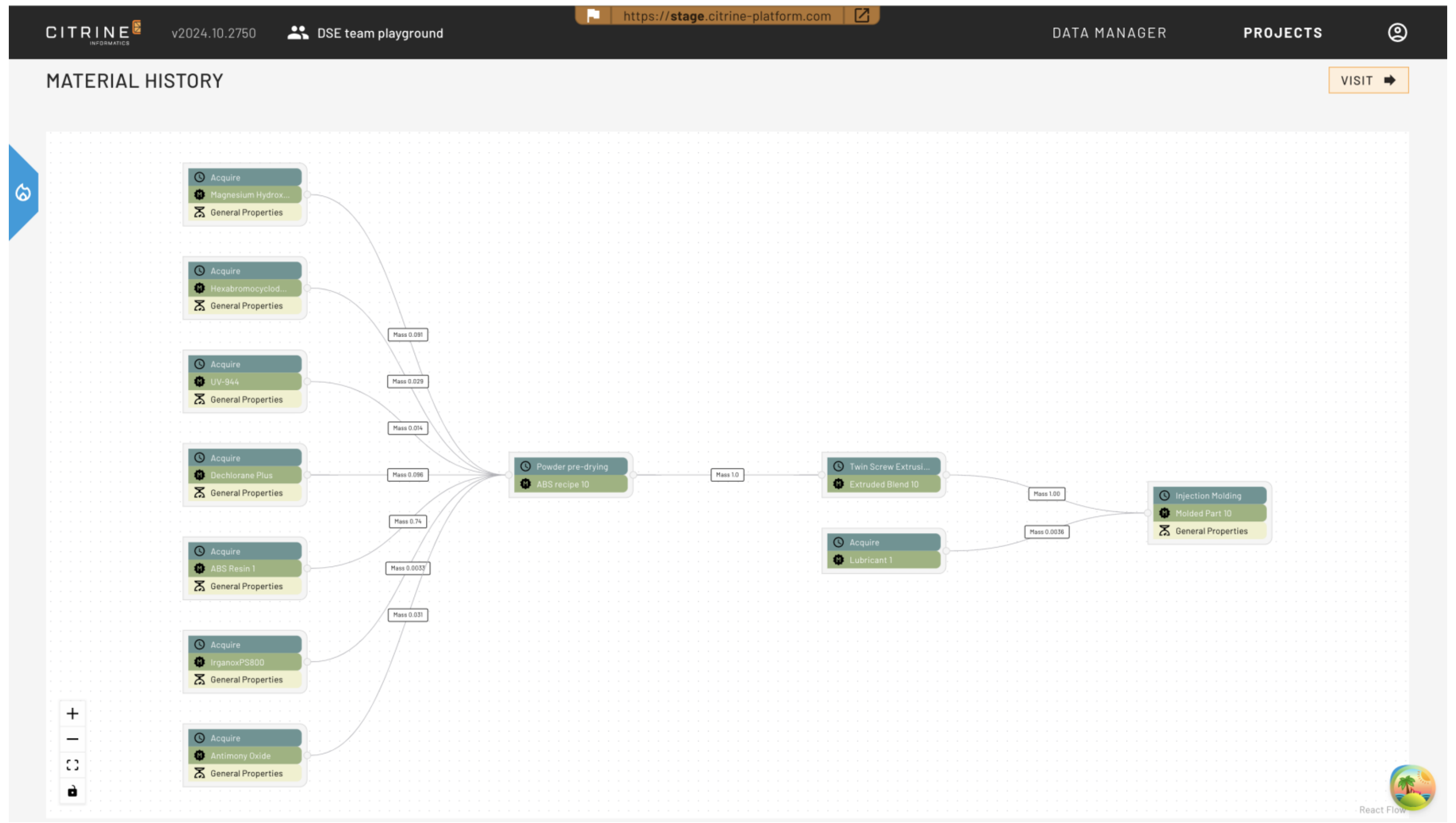
THE CITRINE PLATFORM: AI-GUIDED MATERIALS DEVELOPMENT

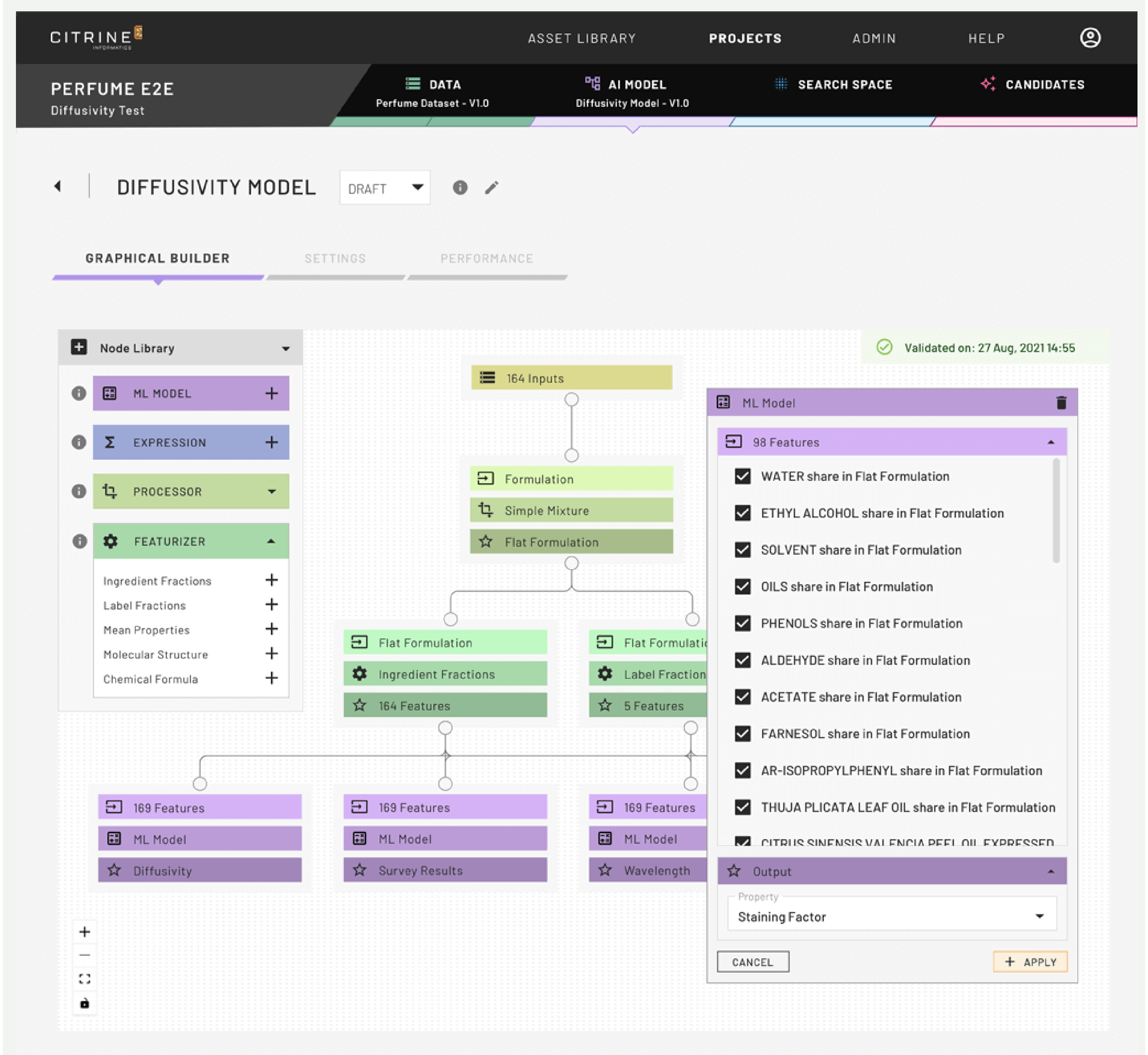
Data Infrastructure → AI Models → Search Space → Materials Optimization

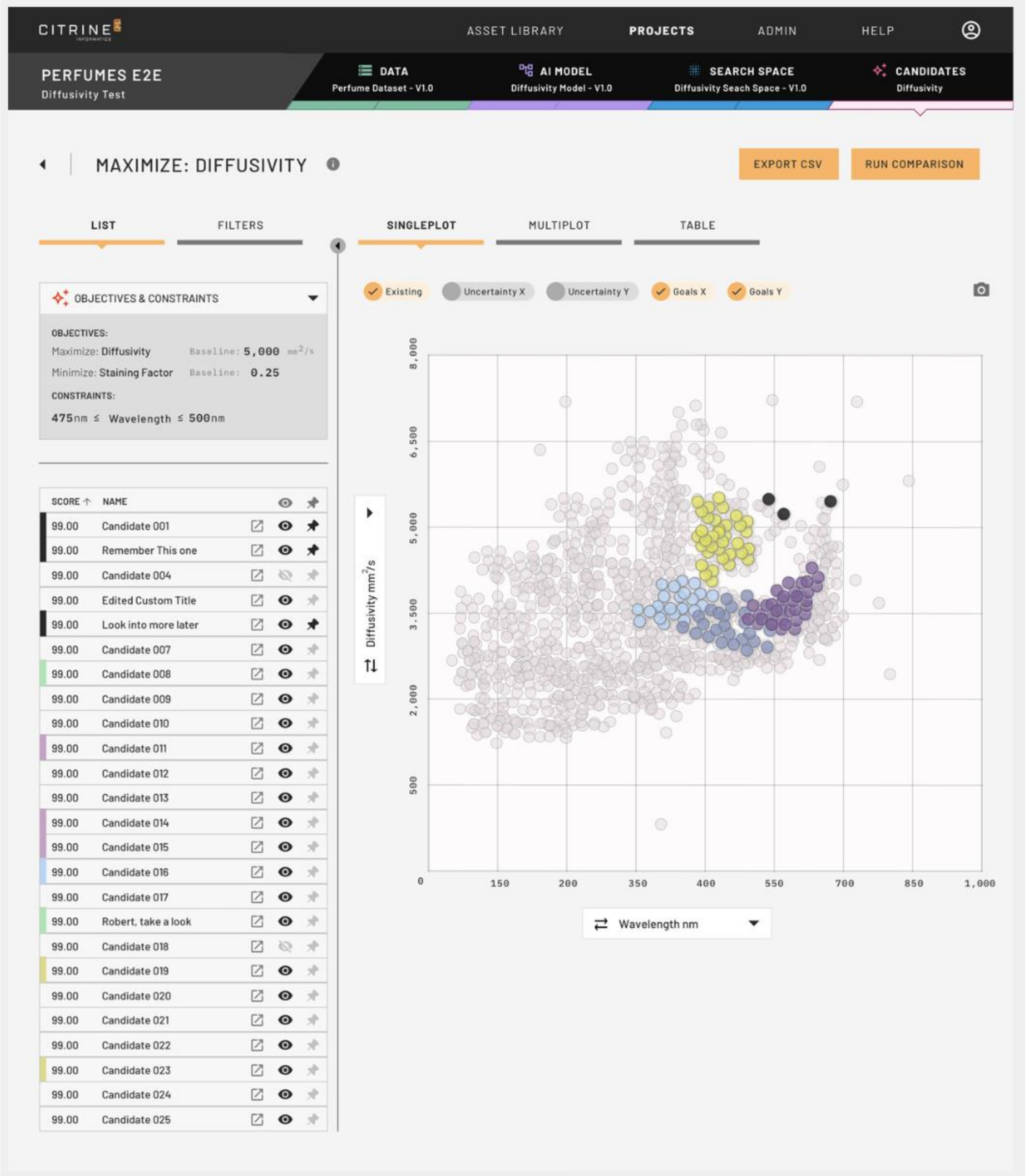
Manage material data

Featurize data, build and test models

Construct search spaces and make candidate predictions







Case Studies

DOME 4.0

SIEMENS

Digital Open Marketplace Ecosystem 4.0

"A scalable, semantically interoperable, ecosystem of ***marketplaces and data spaces*** *to transform data and information into knowledge and intelligence assets [...] within the high-economic-impact* ***materials*** *and* ***manufacturing*** *sectors."*

9 B2B showcases

- Chemistry Knowledge Graph - Marine, Air Quality And Nanoparticles
- Lightweight Construction - Fibre Reinforced Plastics
- Polymer Additives For Corrosion Protection
- Structural Adhesives: Fatigue Life
- Production Equipment And Service Catalogues
- Turnkey Services And Custom Workflows Integrating Simulations And Data
- Formulated Consumer Products
- Semantic Analytics Of Manufacturing Assets
- Virtual Development Of Composite Materials

CMCL innovations · Fraunhofer · netcompany intrasoft · Alma Mater Studiorum Università di Bologna · EPFL · UKRI · SIEMENS · UCL Institute for Materials Discovery · UNIRESEARCH · SINTEF · BOSCH · Cambridge Nanomaterials Technology Ltd

FATIGUE OF STRUCTURAL ADHESIVES UNDER STRESS CONCENTRATIONS

Materials:

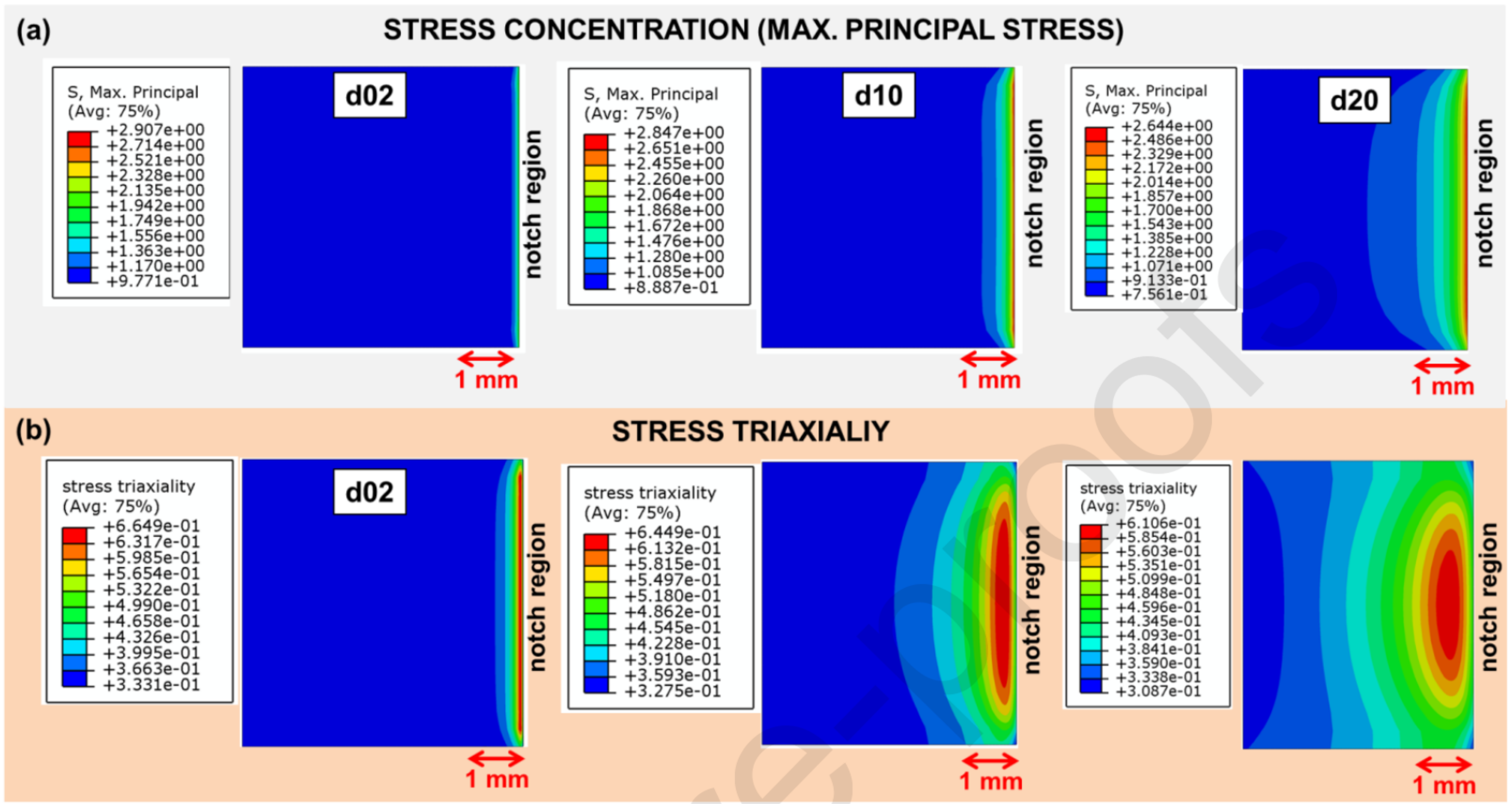
- DGEBA epoxy:
  - PU toughened
  - Rubber toughnede

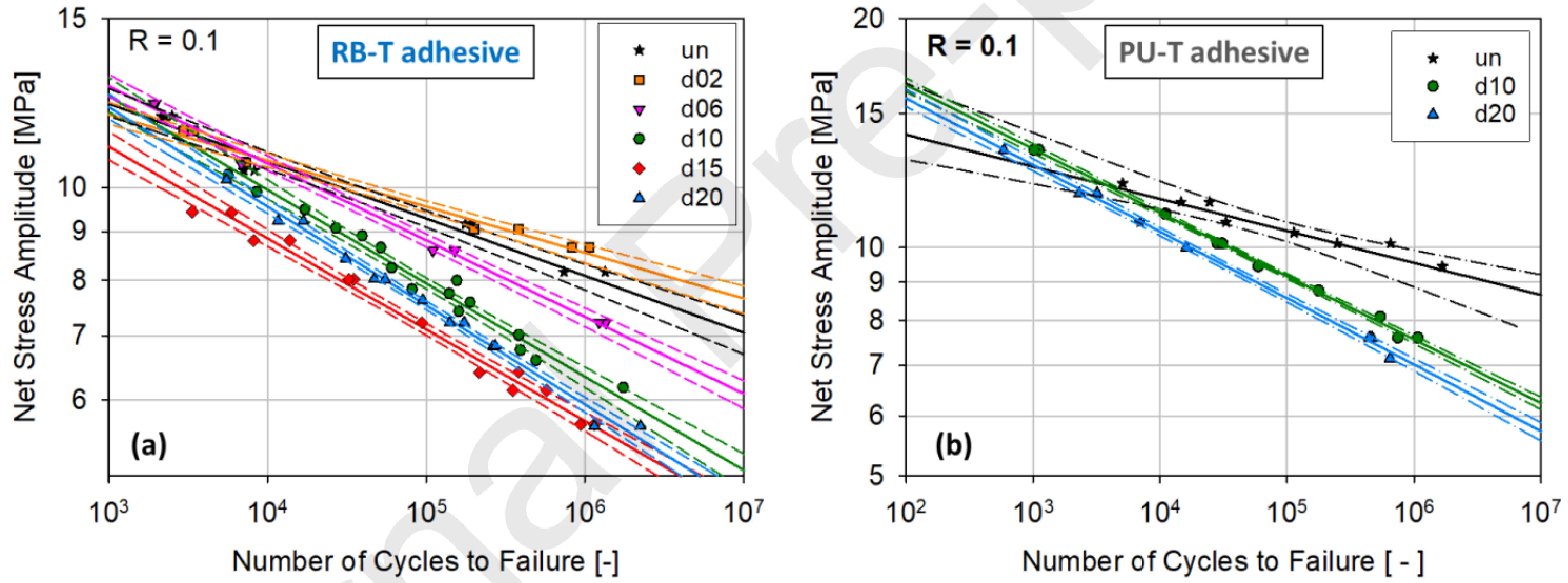
Geometry:

- Stress concentration Factors (analytical)
- Gradient effects length scale:

Fatigue Behaviour:

- S-N curves
- Damage evolution (stiffness loss)



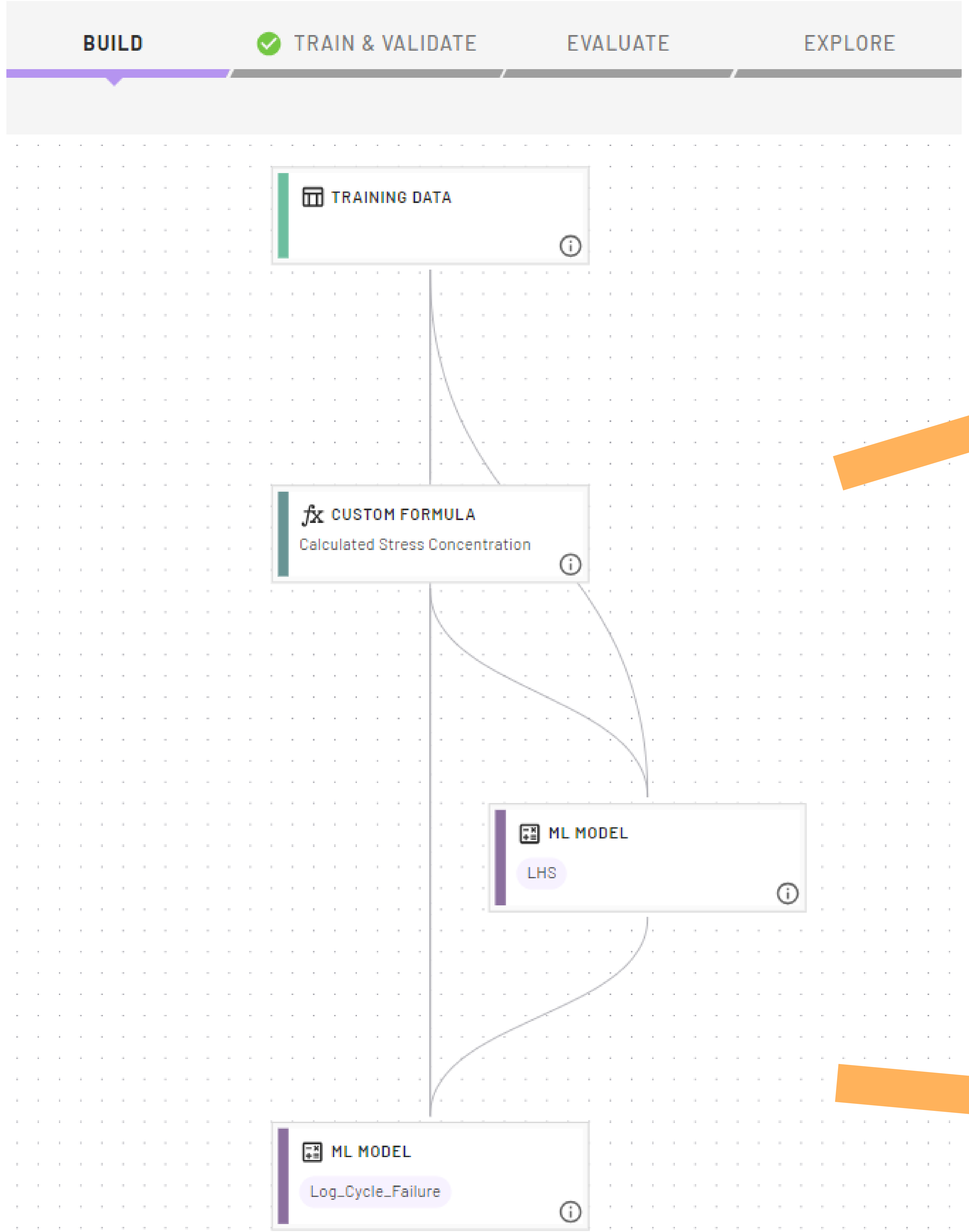


Figs. 4 and 5 from [1].

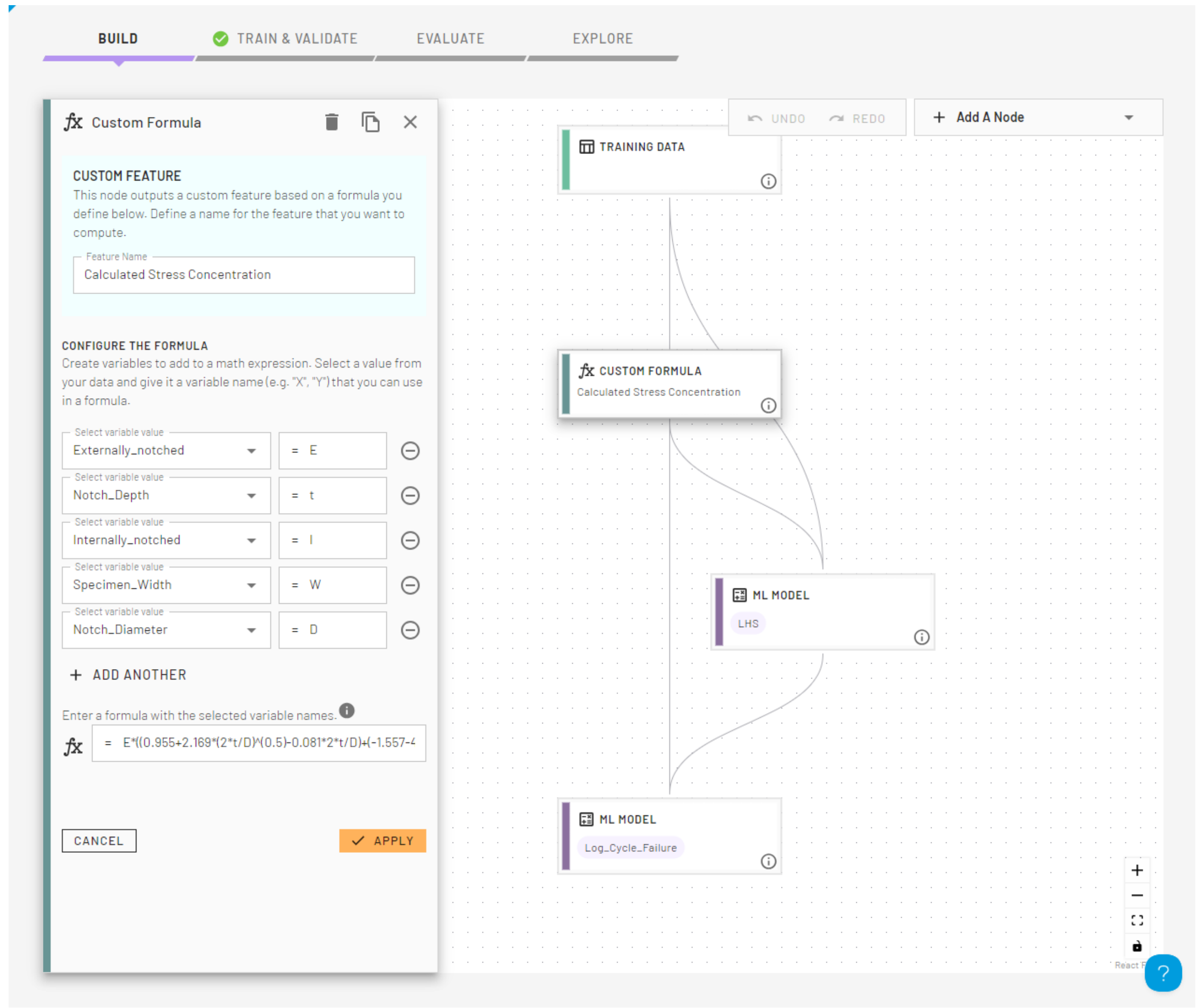
[1] "Fatigue of structural adhesives under stress concentrations: notch effect on fatigue strength, crack initiation and damage evolution", V.C. Beber, B. Schneider, Internation Journal of Fatigue 140 (2020)

[2] "Advancements in predicting the fatigue lifetime of structural adhesive joints " https://blogs.sw.siemens.com/simcenter/advancements-in-predicting-the-fatigue-lifetime-of-structural-adhesive-joints/

CITRINE ML MODEL



Domain Knowledge

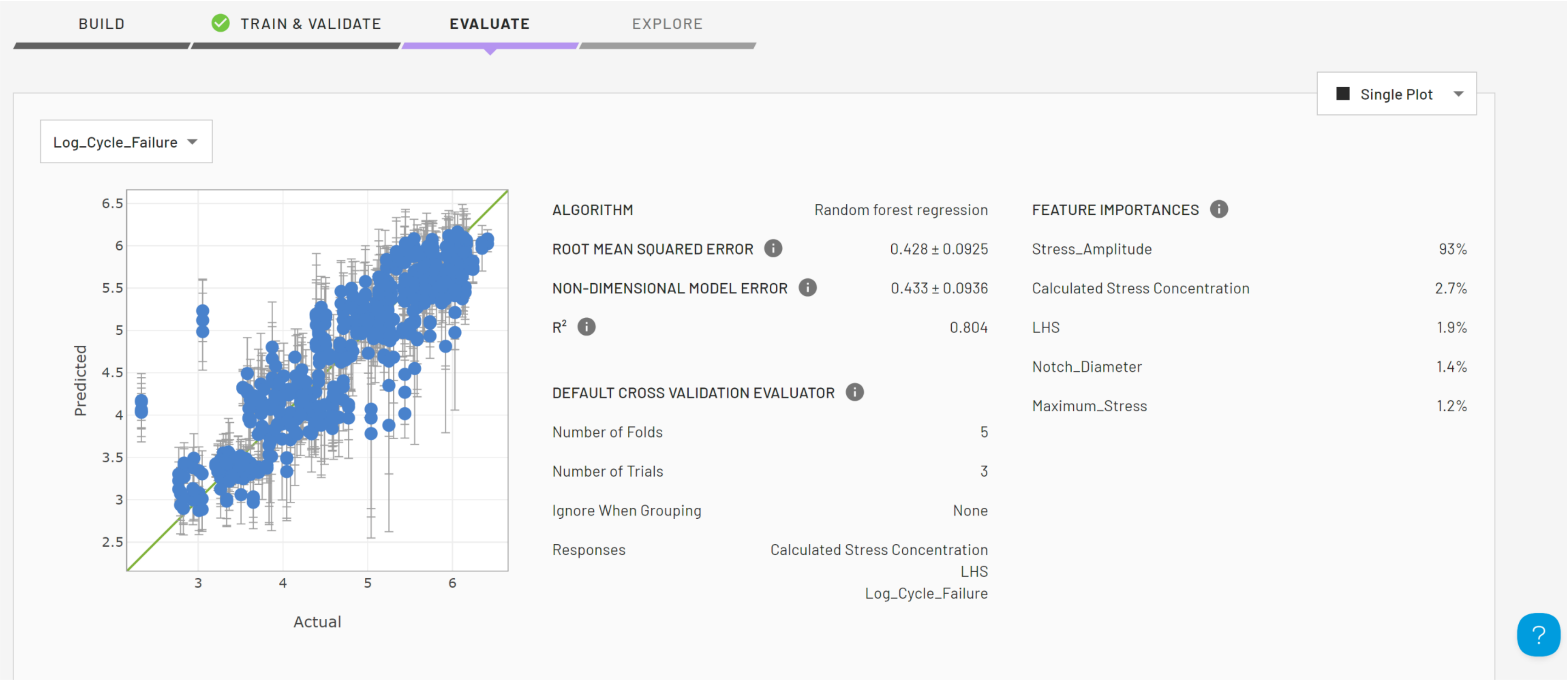


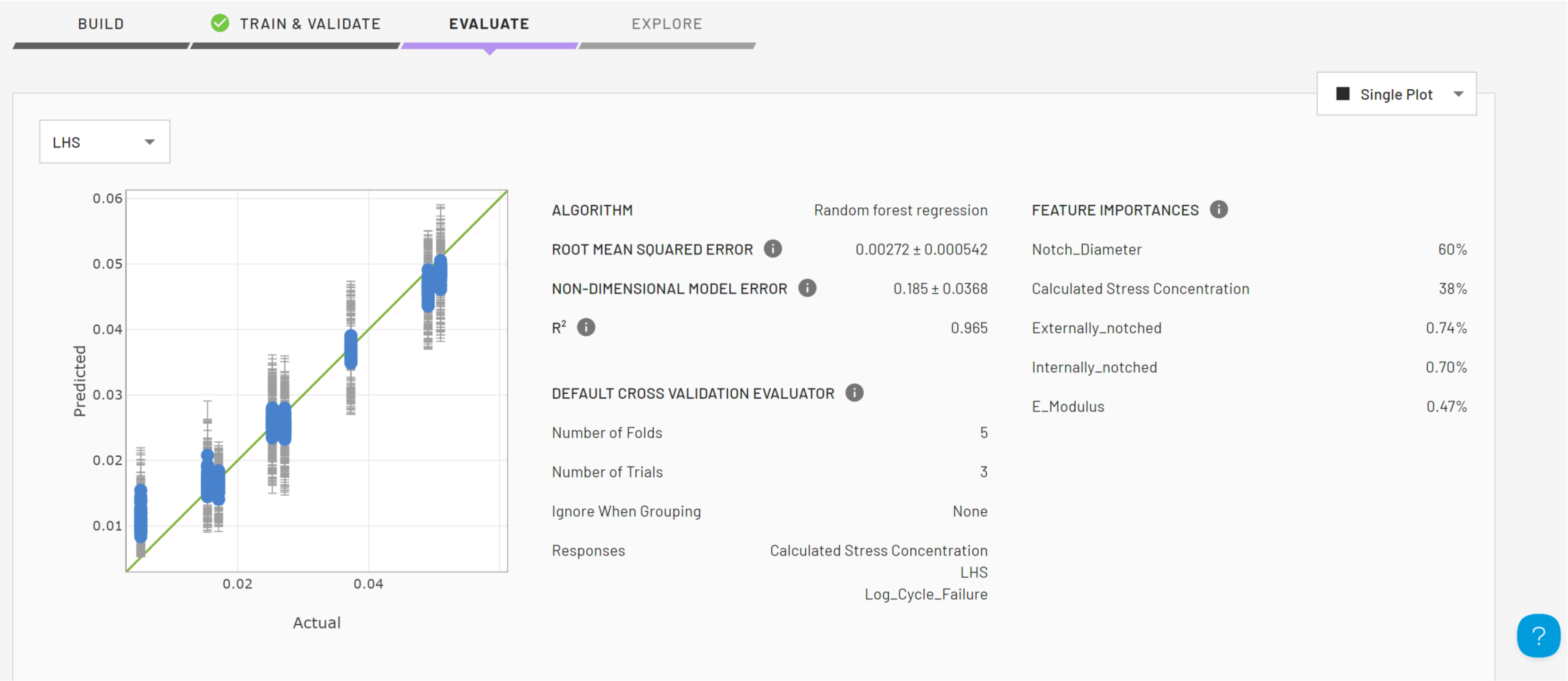
Surrogate Modelling of intermediate variables

ML Output

- Handling multiple length scales, from molecular descriptions to surrogate modelling of structural behaviour
- Efficiently incorporate pre-existing domain knowledge

CITRINE MODEL RESULTS

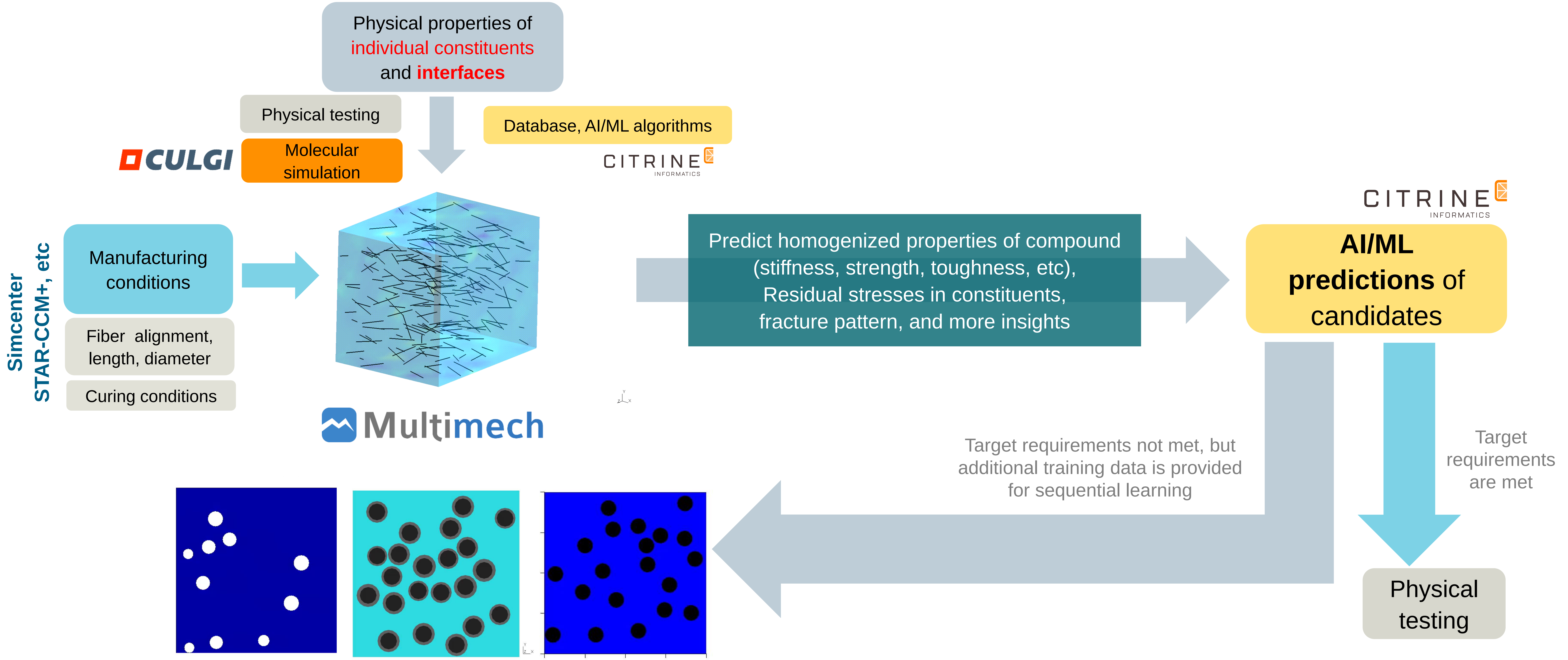




- ML model can serve as a virtual testing environment
- Can be used to improve formulations and/or notch geometry – “Candidate Generation”
- Transferability to other geometries and or chemistries

INTEGRATION OF MULTISCALE MODELS WITH AI/ML

SIEMENS



"Materials informatics accelerates customer tailored composite material design"
https://blogs.sw.siemens.com/simcenter/material-informatics-accelerates-customer-tailored-composite-material-design/

Thank you

Marco Musto mmusto@citrine.io

BETTER CUSTOMIZED SOLUTIONS FOR COMPANIES MANUFACTURING WITH COMPOSITES

AI-driven physics-based modelling

The Customer

- **Siemens, Sabic** and Citrine Informatics worked together as part of "Virtual Development of Composite Materials" in DOME 4.0.
- https://dome40.eu/

The Problem

- End customers need to determine the correct ratio of PP and glass fiber for a particular application.
- This takes many expensive experiments and may not result in a working solution.
- The DOME 4.0 (Digital Open Marketplace Ecosystem 4.0), project also aimed to create a digital platform connecting materials data sources along a value chain.

The Process

- Historical data was used to create a model of mechanical properties of GFRP dependent on raw material ratios, processing parameters, and design.
- The model was used to suggest experiments that could then be simulated.
- Those that were successful in simulation could then be physically tested.

The Outcome

- Customers are given more accurate recommendations faster for masterbatch and polymer ratios.
- The feasibility of new applications can be assessed without physical tests.
- Additional insights into innovative combinations of resin and reinforcement can be gained without physical tests.

https://blogs.sw.siemens.com/simcenter/material-informatics-accelerates-customer-tailored-composite-material-design/

BETTER CUSTOMIZED SOLUTIONS FOR COMPANIES MANUFACTURING WITH COMPOSITES

AI-driven physics-based modelling

The Customer

- **Siemens, Sabic** and Citrine Informatics worked together as part of "Virtual Development of Composite Materials" in DOME 4.0.
- https://dome40.eu/

The Problem

- End customers need to determine the correct ratio of PP and glass fiber for a particular application.
- This takes many expensive experiments and may not result in a working solution.
- The DOME 4.0 (Digital Open Marketplace Ecosystem 4.0), project also aimed to create a digital platform connecting materials data sources along a value chain.

The Process

- Historical data was used to create a model of mechanical properties of GFRP dependent on raw material ratios, processing parameters, and design.
- The model was used to suggest experiments that could then be simulated.
- Those that were successful in simulation could then be physically tested.

The Outcome

- Customers are given more accurate recommendations faster for masterbatch and polymer ratios.
- The feasibility of new applications can be assessed without physical tests.
- Additional insights into innovative combinations of resin and reinforcement can be gained without physical tests.

https://blogs.sw.siemens.com/simcenter/material-informatics-accelerates-customer-tailored-composite-material-design/

MIND OVER MATTER: SOCIORESILIENT MATERIALS DESIGN

PIs: Christine Ortiz (MIT) and Ellan Spero (MIT, Station1)

- Building capabilities for the new field of socioresilient materials design, combining traditional structure-property-processing-performance paradigms, circular design principles, emergent computational capabilities, and humanistic and social sciences methodologies.
- Developing software tools, novel metrics, datasets, and computational methods to enable *practical* integration of socioresilient concepts into existing materials design workflows.

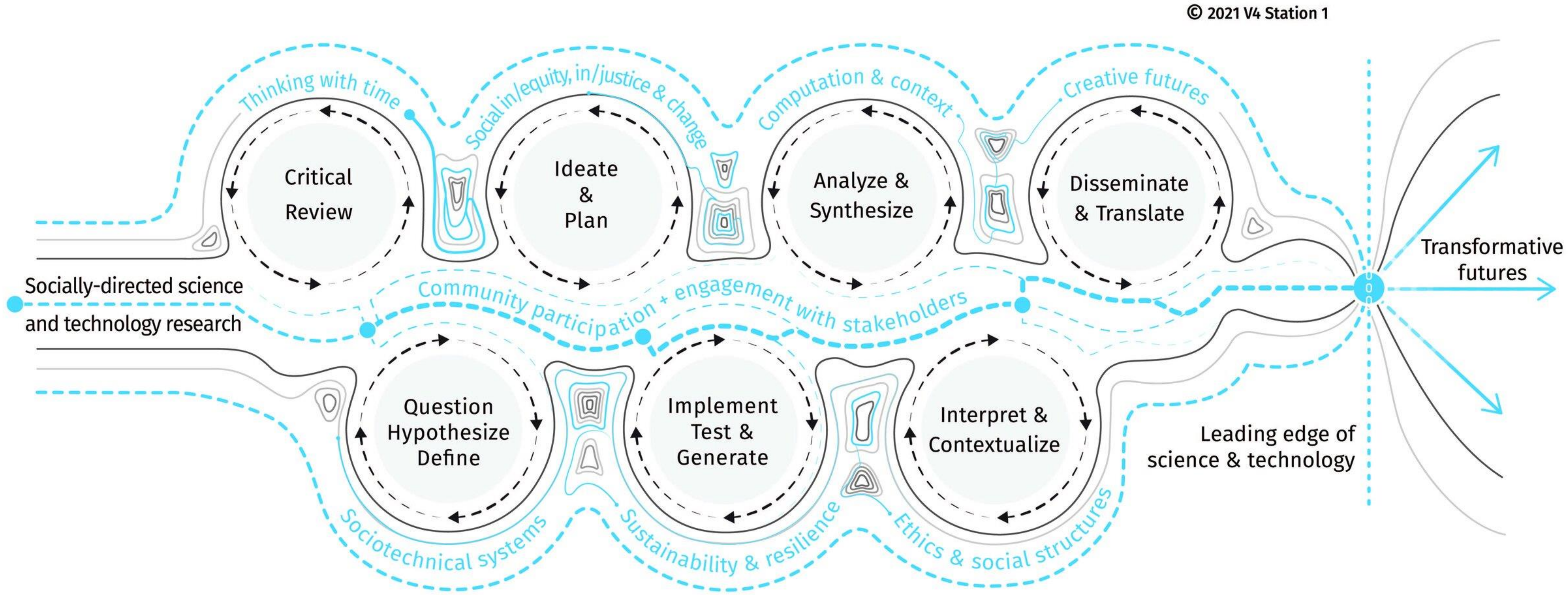
Massachusetts Institute of Technology

STATION 1 SOCIALLY-DIRECTED SCIENCE AND TECHNOLOGY

Swansea University Prifysgol Abertawe

Cornell University

CITRINE INFORMATICS



Spero, E. F., & Ortiz, C. (2021) *Diseña*, (18), Article 1.

Award# ITE-2236190
TIP C-Accel, PM Linda Molnar

CONSIDER PLASTIC DESIGN

Plastics are complex formulations consisting of many ingredients

Component	Function	Typical amount	Examples
Polymer resin(s)	The "plastic" in plastic	100 g	PVC, PS, ABS, PET
Plasticizer	Processability, flexibility	0 – 100 phr#	Phthalates, Adipates, Nitriles
Stabilizer	Stabilization against heat, light	0 – 10 phr	Pb-based (phased out), Ca/Cd/Zn/Sn stearates/dialkyls
Filler	Reduce cost, improve properties like stiffness, flammability, …	0 – 100x phr	$CaCO_3$, mica, wollastonite, glass fibers
Lubricant	Reduce sticking to equipment surfaces while processing	0 – 2 phr	Paraffin wax, oils

#phr = parts per hundred resin, a unit commonly used in the plastics/formulation industry

Other common additives include flame retardants, antistatics, pigments, curing agents, …

Currently, some additives consist of toxic chemicals that are being phased out.

PVC METRICS: TECHNICAL (T), ENVIRONMENTAL(E), AND SOCIETAL(S)

Consider increasingly difficult design metrics and compare results

T

- Tensile strength
- Elongation at break

T+E

- Tensile strength
- Elongation at break

- Ecotoxicity (terrestrial, freshwater, marine)
- Global warming potential
- Ozone formation potential

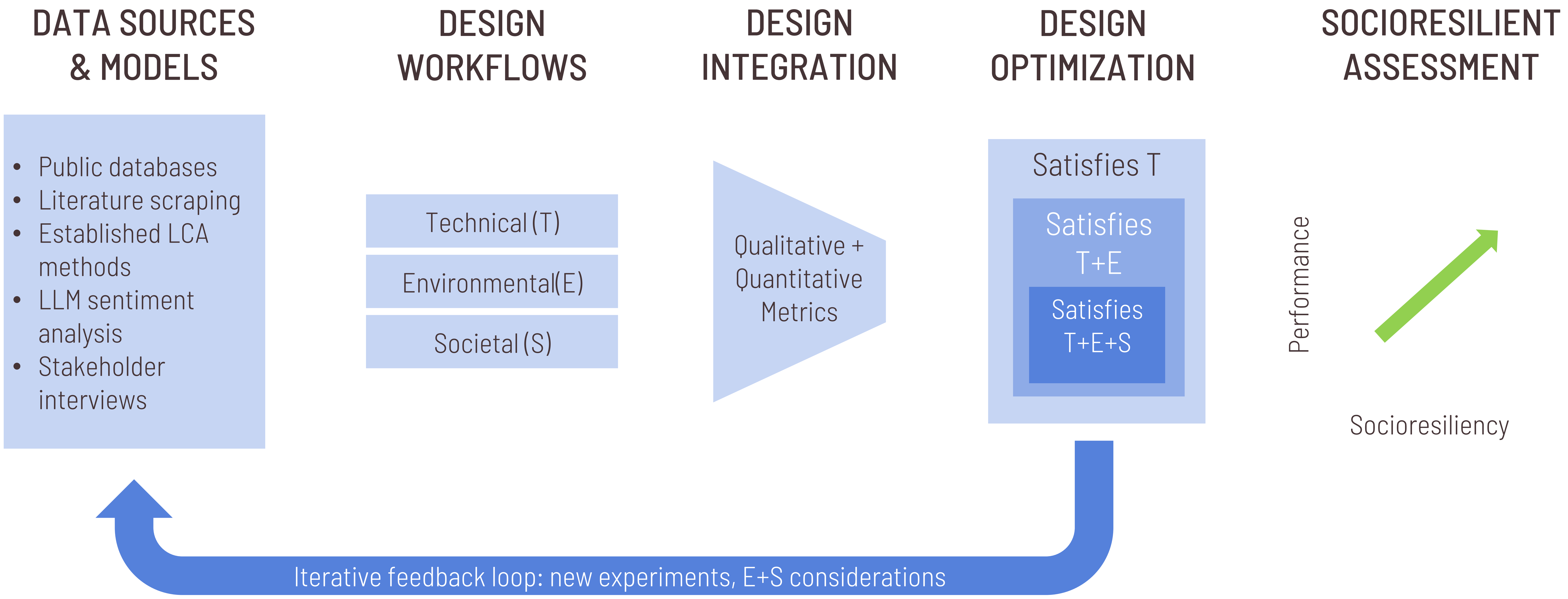
T+E+S

- Tensile strength
- Elongation at break

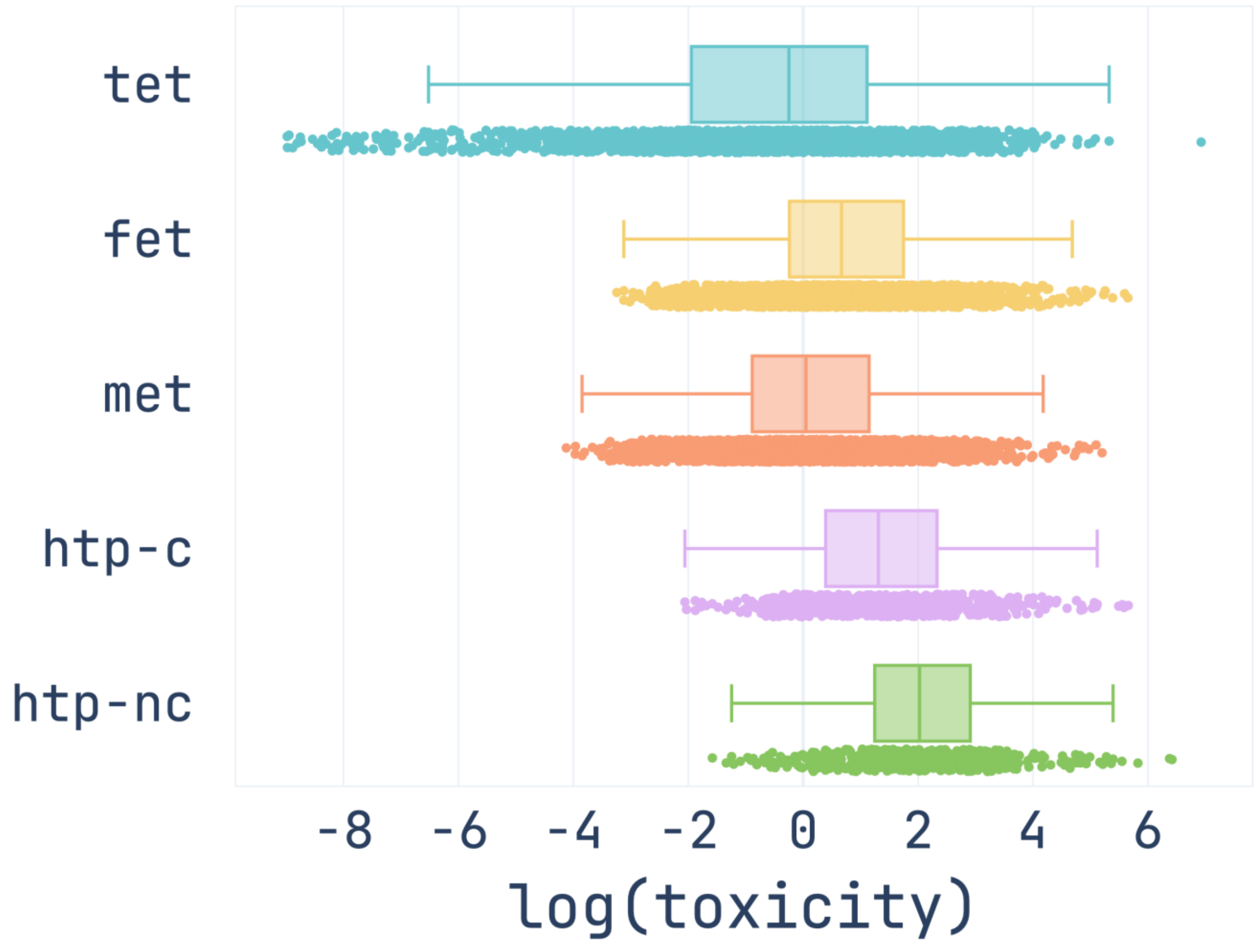
- Ecotoxicity (terrestrial, freshwater, marine)
- Global warming potential
- Ozone formation potential

- Human toxicity (carcinogenic, non-carcinogenic)

SOCIORESILIENT MATERIALS DESIGN FRAMEWORK

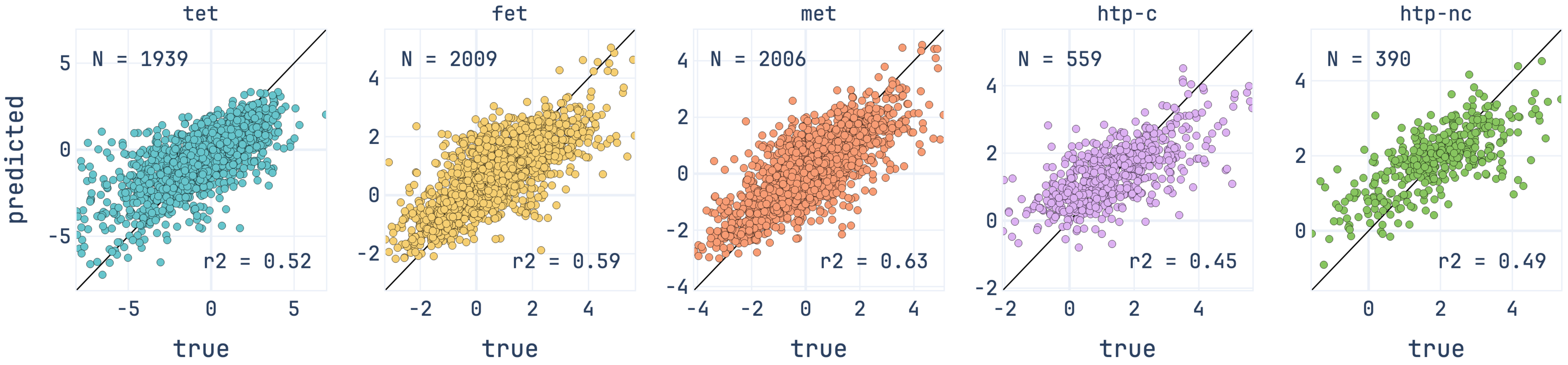


ReCiPe2016 TOXICITY: MODELS (v1)



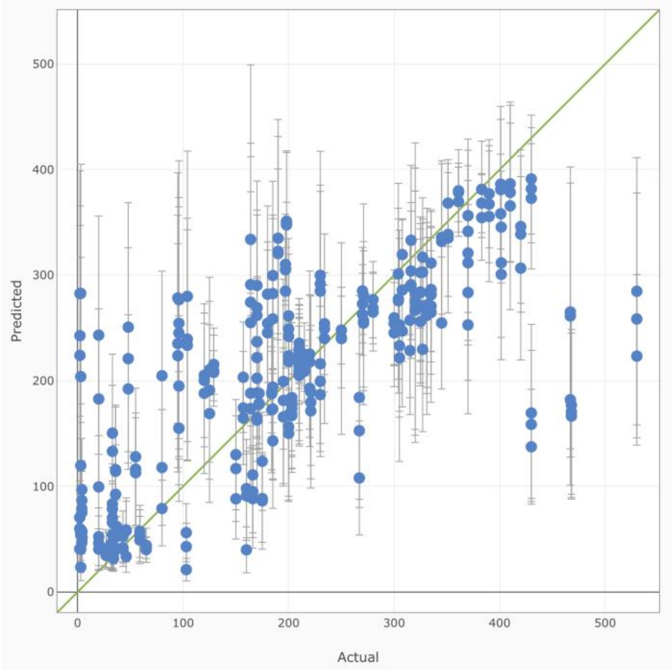
1. SMILES → QSAR-style fingerprints (deepchem.RDKitDecriptors)
2. For each toxicity type:
   a. Drop examples with NaN values
   b. Transform $y \rightarrow \log_{10}(y)$
   c. Drop examples with $Z_{modified}(y) \geq 3.5$
   d. 5-fold random test/train split
   e. Train RF regressor (lolopy) on held-in
   f. Test RF regressor on held-out

(tet) Terrestrial ecotoxicity
(fet) Freshwater ecotoxicity
(met) Marine ecotoxicity
(htp-c) Human carcinogenic toxicity
(htp-nc) Human noncarcinogenic toxicity

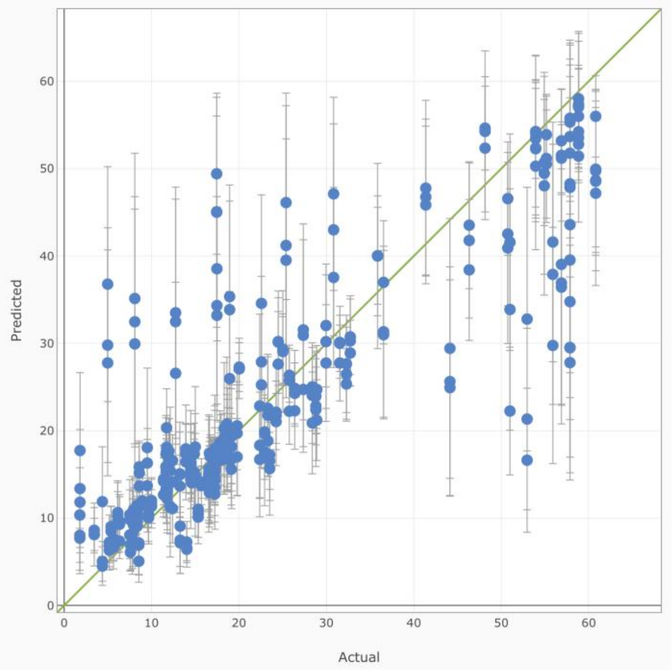


PVC [T] DESIGN: EXAMPLE

Target property models under 5-fold cross-validation

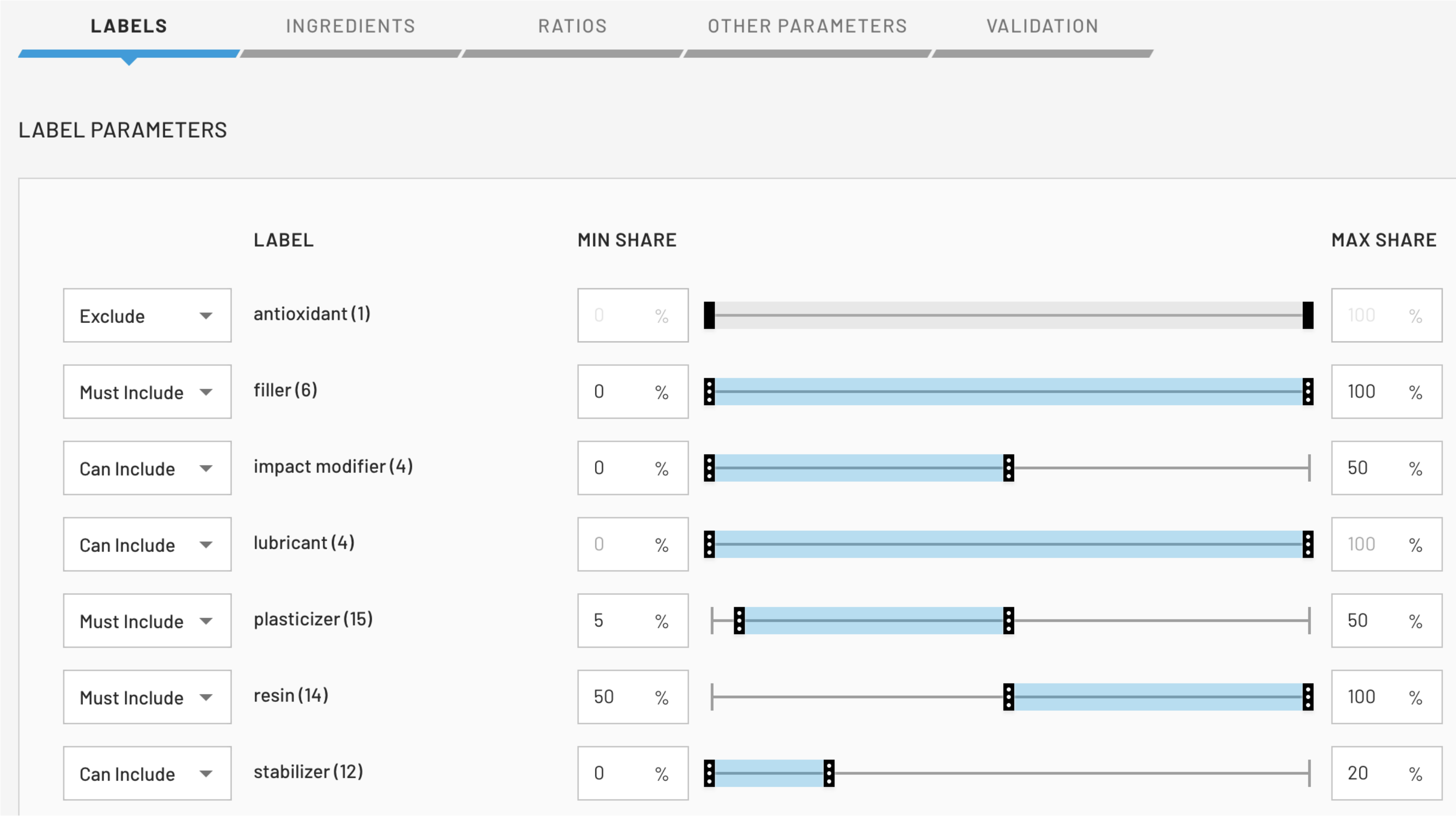


Elongation at break (%)
R^2: 0.53



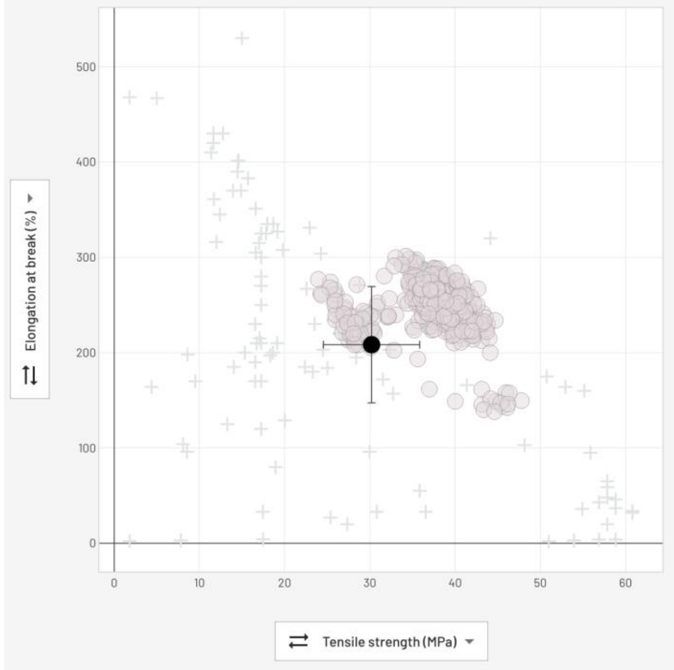
Tensile strength (MPa)
R^2: 0.73

Search space to generate reasonable candidates



Candidate scoring

Sample candidate target property distribution

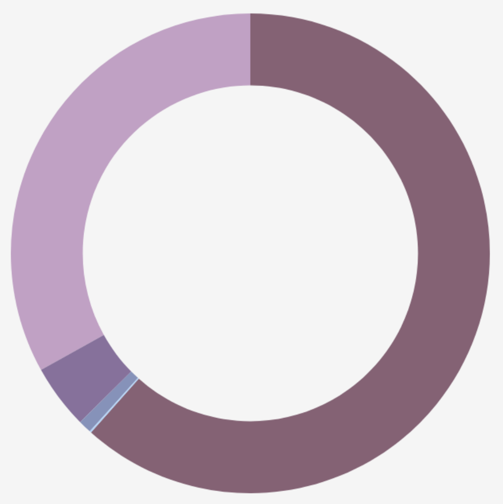


Sample candidate predicted output performance

TENSILE STRENGTH 30 ± 6 MPa	MAX
ELONGATION AT BREAK (%) 208 ± 61	MAX

Sample candidate PVC formulation composition

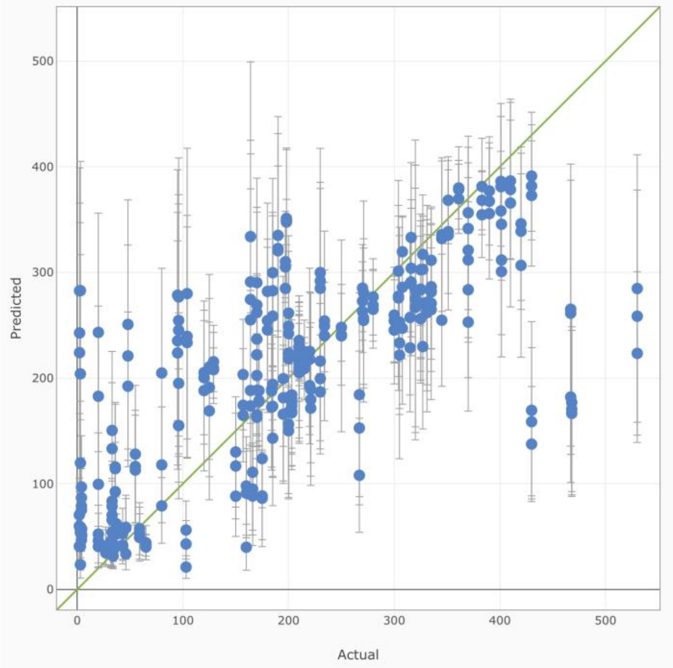
LABEL	% OF TOTAL
resin	94.7%
plasticizer	5.34%



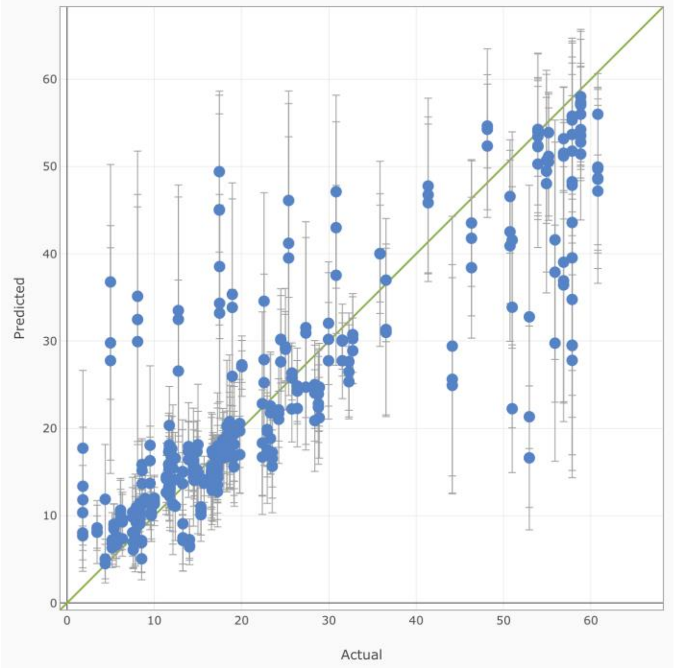
INGREDIENT	% OF TOTAL
Polyvinyl chloride, PVC	61.588%
Polyvinyl butyral, PVB	33.072%
Dioctyl phthalate, DOP	4.346%
Polyurethane	0.886%
Butyl benzyl phthalate	0.107%

PVC [T+E] DESIGN: EXAMPLE

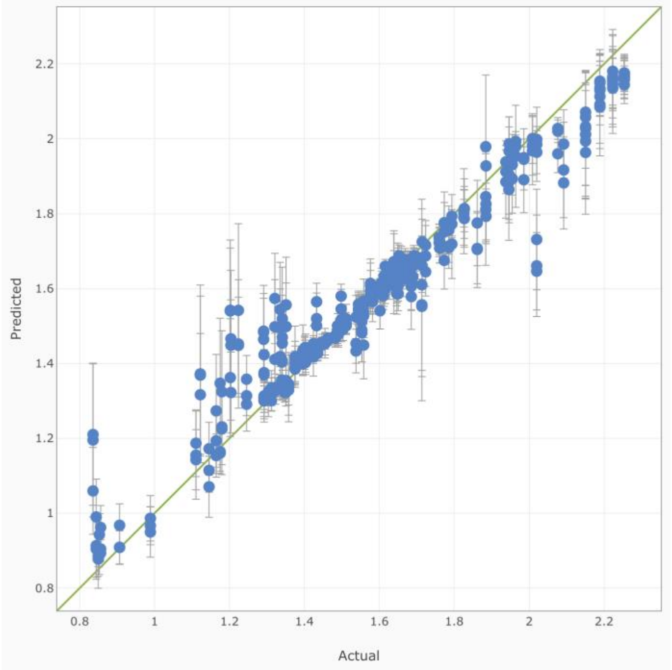
Target property models under 5-fold cross-validation



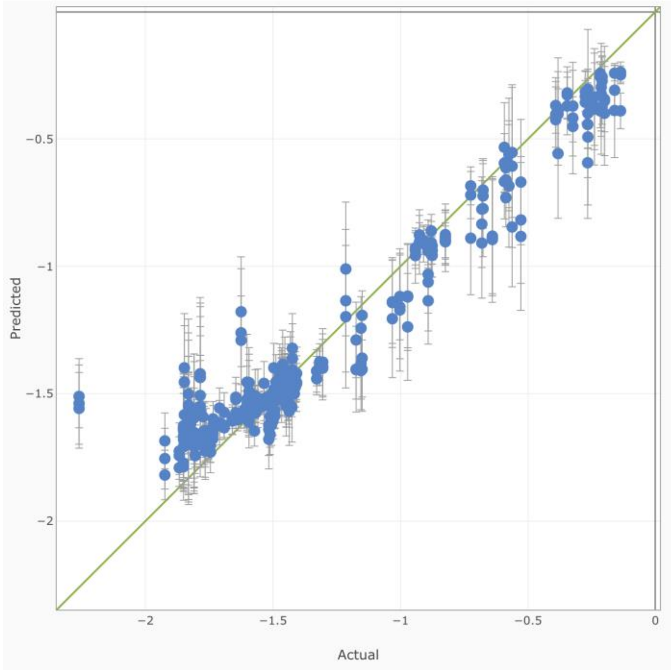
Elongation at break (%)
R^2: 0.53



Tensile strength (MPa)
R^2: 0.73



HTP-nc
R^2: 0.95



TET
R^2: 0.93

Candidate scoring

OBJECTIVES & CONSTRAINTS

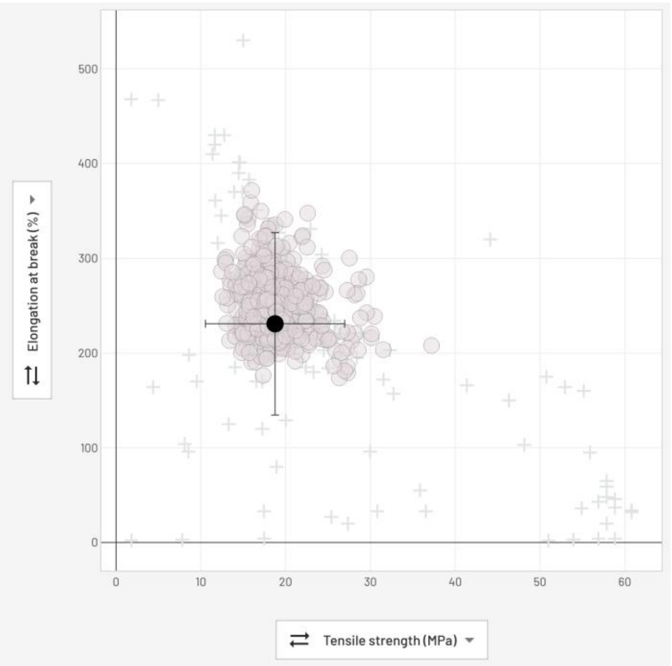
OBJECTIVES:
- Tensile strength > 20 MPa
- Elongation at break (%) > 100
- tet < -1
- fet < 0
- met < -0.5
- htp-c < 1
- htp-nc < 1

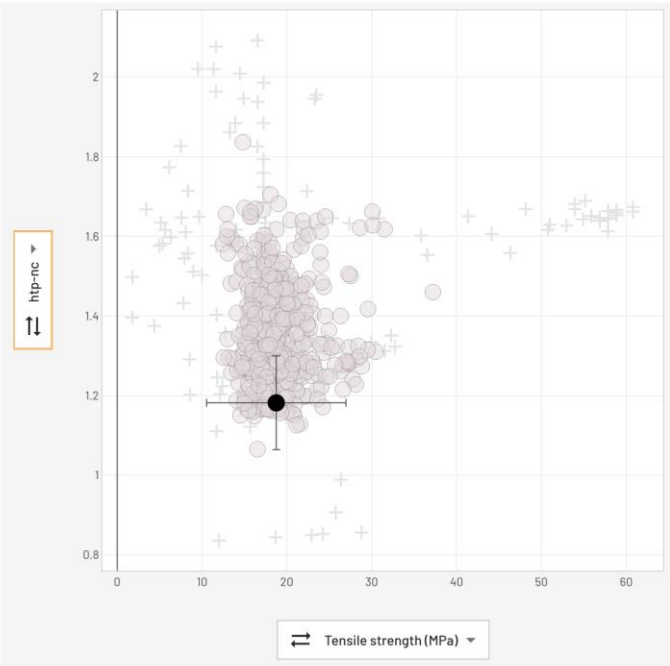
CONSTRAINTS:
No constraints selected

SCORE TYPE:
Likelihood of Improvement

CORRELATED SCORING:
- Elongation at break (%), Tensile strength
- fet, htp-nc, htp-c, met
- tet

Sample candidate target property distribution



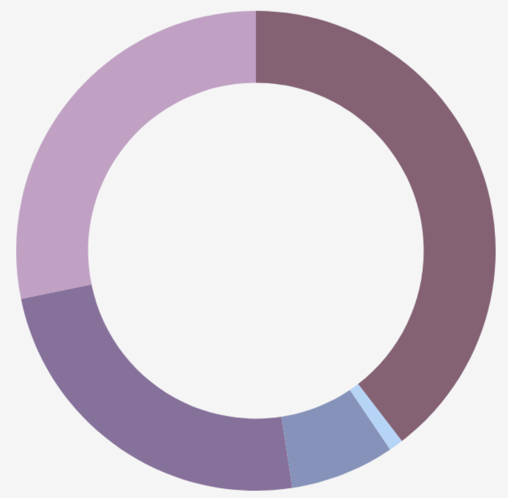


Sample candidate predicted output performance

TENSILE STRENGTH	19 ± 8 MPa	MAX
ELONGATION AT BREAK (%)	231 ± 96	MAX
TET	-1.07 ± 0.20	MIN
FET	-0.10 ± 0.12	MIN
MET	-0.46 ± 0.11	MIN
HTP-C	0.78 ± 0.13	MIN
HTP-NC	1.18 ± 0.12	MIN

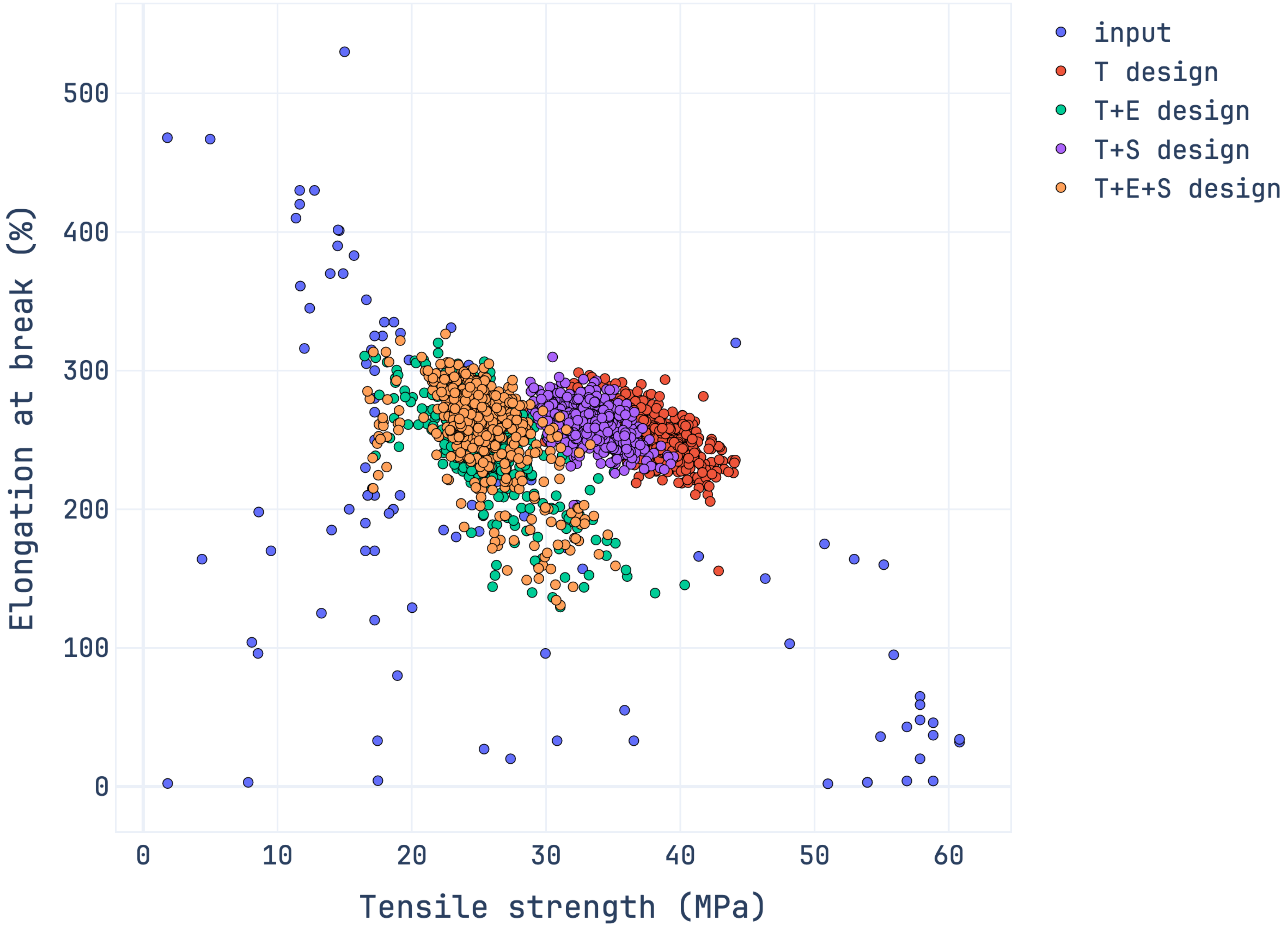
Sample candidate PVC formulation composition

LABEL	% OF TOTAL
resin	67.8%
filler	24.2%
plasticizer	7.98%

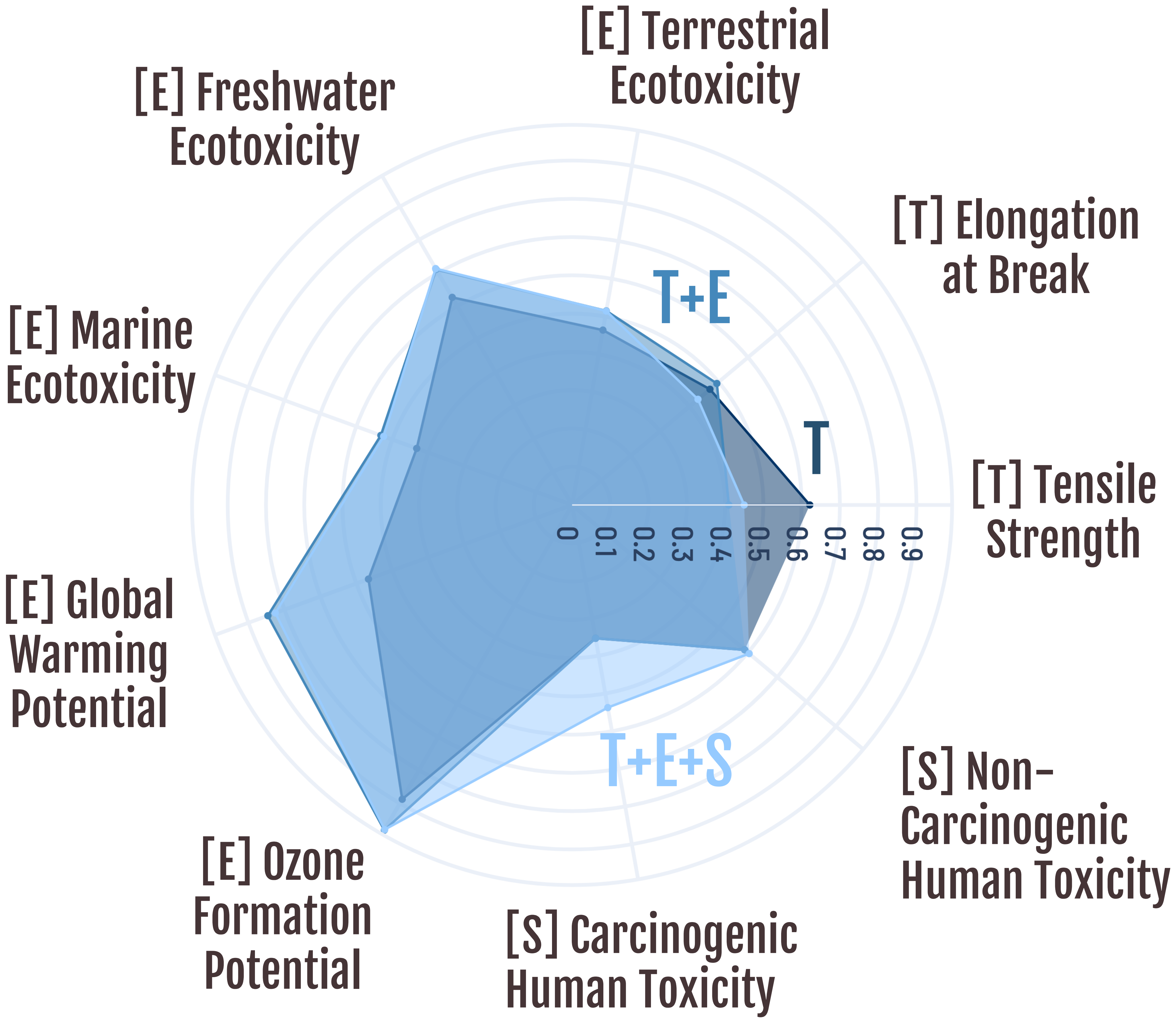


INGREDIENT	% OF TOTAL
Polyvinyl chloride, PVC	39.584%
Styrene in S/ACN copolymer	28.219%
Carbon black	24.212%
Butyl benzyl phthalate	7.029%
Dibutyl terephthalate, DBTP	0.955%

VISUALIZING T+E+S DESIGN TRADEOFFS



Visualizing the Pareto frontier of performance metrics of candidates from different design goals



Normalized properties, higher is better (e.g., less toxic)

SUMMARY

- ML can support formulation and characterization of complex polymer systems
- Use cases include, among other:
  - Optimal formulation
  - Tuning to novel customer specification
  - Ingredient replacement (*e.g.* regulatory concerns / supply chain optimization)
- The Citrine Platform is designed to efficiently support R&D work:
  - No-code approach
  - Possibility to add own domain knowledge
  - Can incorporate inputs at various length scales, from molecular descriptions to structural computations

LLM

CITRINE | Catalyst

The digital assistant for the materials and chemicals industry helping teams work more effectively

CITRINE CATALYST

Digital assistant RAG to accelerate product development

LITERATURE
Curated, Relevant, Public Journal Articles

INTERNAL DOCUMENTS
Securely uploaded

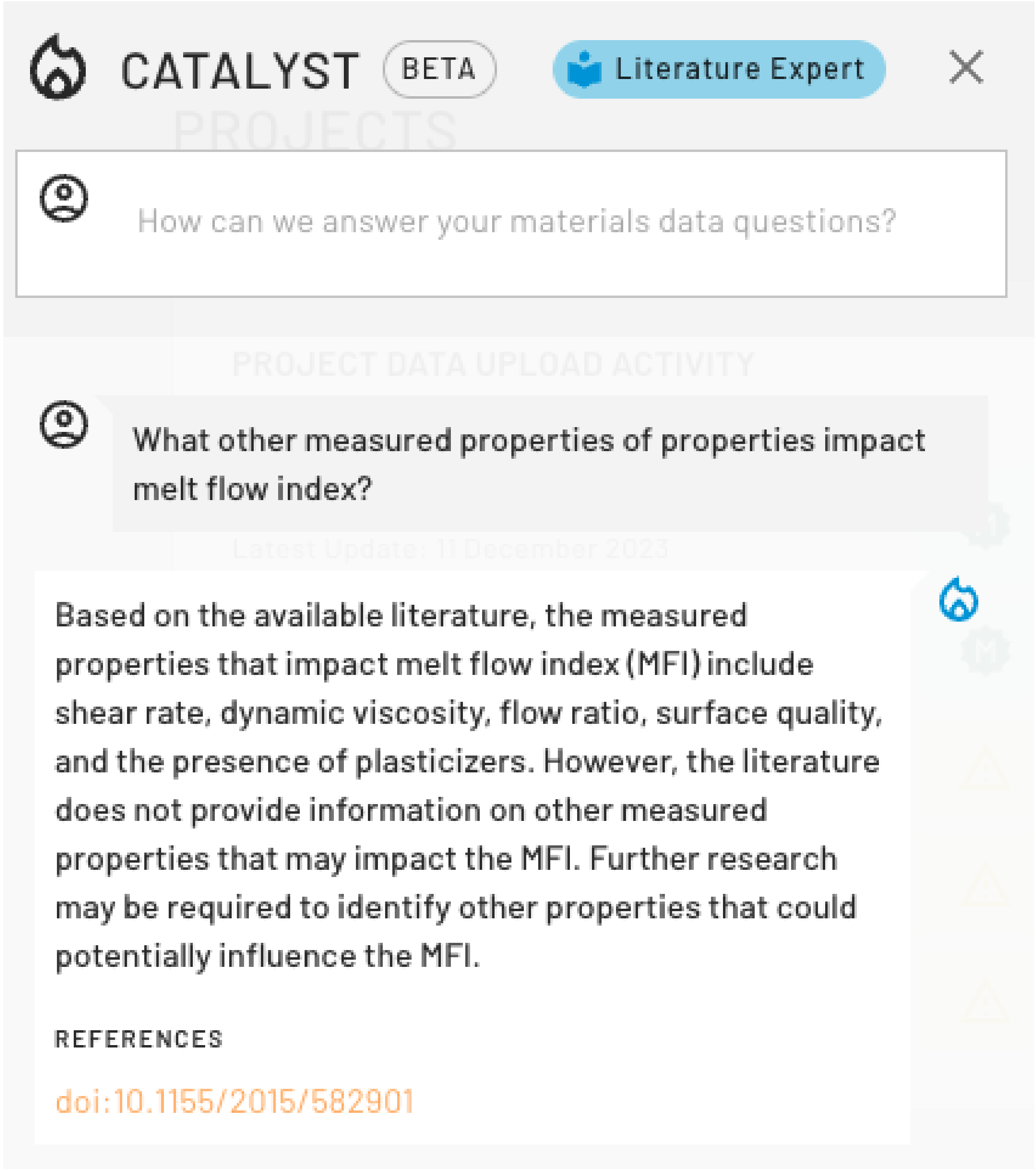
- Project reports
- Consumer research
- Product Catalogue
- Safety Data Sheets
- Experimental Procedures
- Test results
- Internal Knowledge Base

Use natural language to ask questions

CITRINE CATALYST: Knowledge Assistant

Receive response in natural language

- Draw on trusted sources
- Quickly answer your question without bothering a colleague
- Easily access a variety of company documents



OUR CUSTOMERS' DATA ARE NOT PERFECT

In fact, almost all our customers need help cleaning their data to get it AI-ready

Thermo Fisher SCIENTIFIC

SAFETY DATA SHEET

Creation Date 26-Sep-2009 **Revision Date** 24-Dec-2021 **Revision Number** 5

1. Identification

Product Name	**Acetylsalicylic acid**
Cat No. :	**AC158180000; AC158180025; AC158180500; AC158185000**
CAS No	50-78-2
Synonyms	2-Acetoxybenzoic acid
Recommended Use	Laboratory chemicals.
Uses advised against	Food, drug, pesticide or biocidal product use.

Details of the supplier of the safety data sheet

Company
Fisher Scientific Company
One Reagent Lane
Fair Lawn, NJ 07410
Tel: (201) 796-7100

Acros Organics
One Reagent Lane
Fair Lawn, NJ 07410

Emergency Telephone Number For information **US** call: 001-800-ACROS-01 / **Europe** call: +32 14 57 52 11
Emergency Number **US:**001-201-796-7100 / **Europe:** +32 14 57 52 99
CHEMTREC Tel. No.**US:**001-800-424-9300 / **Europe:**001-703-527-3887

2. Hazard(s) identification

Classification
This chemical is considered hazardous by the 2012 OSHA Hazard Communication Standard (29 CFR 1910.1200)

Acute oral toxicity	Category 4
Combustible dust	Yes

Label Elements

Signal Word
Warning

Hazard Statements
May form combustible dust concentrations in air
Harmful if swallowed

X-Materials Analytical Lab Hall Measurement

ID: MATX-BM-M004
Request ID: X9PY4T

Probe Resistance	3.1 ohm	Current	0.1 mA
Gas Flow Rate	1 L/min	Field Strength	5 T

	A	B
1		**Processing**
2	**recipe 0**	The formulation was stirred at a speed of 500 RPM for 30 minutes in a glass vessel. The reaction temperature was set at 70¬∞C and the total volume of the vessel was 2 liters
3	**recipe 1**	The stir speed was set to 600 RPM and the stir time was 45 minutes. The formulation was prepared in a stainless steel vessel at a reaction temperature of 80¬∞C. The total volume of the vessel was 3 liters
4	**recipe 2**	The formulation process involved stirring at 700 RPM for 1 hour in a ceramic vessel. The reaction temperature was maintained at 90¬∞C and the vessel had a total volume of 4 liters
5	**recipe 3**	Stirring was carried out at a speed of 800 RPM for 1.5 hours in a glass vessel. The reaction temperature was 100¬∞C and the total volume of the vessel was 5 liters
6	**recipe 4**	The formulation was stirred at 900 RPM for 2 hours in a stainless steel vessel. The reaction temperature was set at 110¬∞C and the vessel's total volume was 6 liters
7	**recipe 5**	The stir speed was set to 1000 RPM and the stir time was 2.5 hours. The formulation was prepared in a ceramic vessel at a reaction temperature of 120¬∞C. The total volume of the vessel was 7 liters
8	**recipe 6**	The formulation process involved stirring at 1100 RPM for 3 hours in a glass vessel. The reaction temperature was maintained at 130¬∞C and the vessel had a total volume of 8 liters
9	**recipe 7**	Stirring was carried out at a speed of 1200 RPM for 3.5 hours in a stainless steel vessel. The reaction temperature was 140¬∞C and the total volume of the vessel was 9 liters
10	**recipe 8**	The formulation was stirred at 1300 RPM for 4 hours in a ceramic vessel. The reaction temperature was set at 150¬∞C and the vessel's total volume was 10 liters
11	**recipe 9**	The stir speed was set to 1400 RPM and the stir time was 4.5 hours. The formulation was prepared in a glass vessel at a reaction temperature of 160¬∞C. The total volume of the vessel was 11 liters
12	**recipe 10**	The formulation process involved stirring at 1500 RPM for 5 hours in a stainless steel vessel. The reaction temperature was maintained at 170¬∞C and the vessel had a total volume of 12 liters
13	**recipe 11**	Stirring was carried out at a speed of 1600 RPM for 5.5 hours in a ceramic vessel. The reaction temperature was 180¬∞C and the total volume of the vessel was 13 liters
14	**recipe 12**	The formulation was stirred at 1700 RPM for 6 hours in a glass vessel. The reaction temperature was set at 190¬∞C and the vessel's total volume was 14 liters
15	**recipe 13**	The stir speed was set to 1800 RPM and the stir time was 6.5 hours. The formulation was prepared in a stainless steel vessel at a reaction temperature of 200¬∞C. The total volume of the vessel was 15 liters
16	**recipe 14**	The formulation process involved stirring at 1900 RPM for 7 hours in a ceramic vessel. The reaction temperature was maintained at 210¬∞C and the vessel had a total volume of 16 liters
17	**recipe 15**	Stirring was carried out at a speed of 2000 RPM for 7.5 hours in a glass vessel. The reaction temperature was 220¬∞C and the total volume of the vessel was 17 liters
18	**recipe 16**	The formulation was stirred at 2100 RPM for 8 hours in a stainless steel vessel. The reaction temperature was set at 230¬∞C and the vessel's total volume was 18 liters
19	**recipe 17**	The stir speed was set to 2200 RPM and the stir time was 8.5 hours. The formulation was prepared in a ceramic vessel at a reaction temperature of 240¬∞C. The total volume of the vessel was 19 liters
20	**recipe 18**	The formulation process involved stirring at 2300 RPM for 9 hours in a glass vessel. The reaction temperature was maintained at 250¬∞C and the vessel had a total volume of 20 liters
21	**recipe 19**	Stirring was carried out at a speed of 2400 RPM for 9.5 hours in a stainless steel vessel. The reaction temperature was 260¬∞C and the total volume of the vessel was 21 liters
22	**recipe 20**	The formulation was stirred at 2500 RPM for 10 hours in a ceramic vessel. The reaction temperature was set at 270¬∞C and the vessel's total volume was 22 liters
23	**recipe 21**	The stir speed was set to 2600 RPM and the stir time was 10.5 hours. The formulation was prepared in a glass vessel at a reaction temperature of 280¬∞C. The total volume of the vessel was 23 liters
24	**recipe 22**	The formulation process involved stirring at 2700 RPM for 11 hours in a stainless steel vessel. The reaction temperature was maintained at 290¬∞C and the vessel had a total volume of 24 liters
25	**recipe 23**	Stirring was carried out at a speed of 2800 RPM for 11.5 hours in a ceramic vessel. The reaction temperature was 300¬∞C and the total volume of the vessel was 25 liters
26	**recipe 24**	The formulation was stirred at 2900 RPM for 12 hours in a glass vessel. The reaction temperature was set at 310¬∞C and the vessel's total volume was 26 liters
27	**recipe 25**	The stir speed was set to 3000 RPM and the stir time was 12.5 hours. The formulation was prepared in a stainless steel vessel at a reaction temperature of 320¬∞C. The total volume of the vessel was 27 liters
28	**recipe 26**	The formulation process involved stirring at 3100 RPM for 13 hours in a ceramic vessel. The reaction temperature was maintained at 330¬∞C and the vessel had a total volume of 28 liters
29	**recipe 27**	Stirring was carried out at a speed of 3200 RPM for 13.5 hours in a glass vessel. The reaction temperature was 340¬∞C and the total volume of the vessel was 29 liters
30	**recipe 28**	The formulation was stirred at 3300 RPM for 14 hours in a stainless steel vessel. The reaction temperature was set at 350¬∞C and the vessel's total volume was 30 liters

Technical Data Sheet

LYB LyondellBasell

***Accucomp* ABS892BL**
Acrylonitrile Butadiene Styrene
LyondellBasell Industries
Engineering Plastics

General	
Material Status	• Commercial: Active
Availability	• North America
Features	• High Heat Resistance
Forms	• Pellets

Physical	**Nominal Value (English)**	**Nominal Value (SI)**	**Test Method**
Density / Specific Gravity	1.05	1.05 g/cm³	ASTM D792
Melt Mass-Flow Rate (MFR) (200°C/5.0 kg)	0.80 g/10 min	0.80 g/10 min	ASTM D1238
Mechanical	**Nominal Value (English)**	**Nominal Value (SI)**	**Test Method**
Tensile Modulus	247000 psi	1700 MPa	ASTM D638
Tensile Strength			ASTM D638
Yield	7540 psi	52.0 MPa	
Break	5510 psi	38.0 MPa	
Tensile Elongation			ASTM D638
Yield	4.0 %	4.0 %	
Break	20 %	20 %	
Flexural Modulus	377000 psi	2600 MPa	ASTM D790
Flexural Strength	10400 psi	72.0 MPa	ASTM D790
Impact	**Nominal Value (English)**	**Nominal Value (SI)**	**Test Method**
Notched Izod Impact	6.9 ft·lb/in	370 J/m	ASTM D256
Hardness	**Nominal Value (English)**	**Nominal Value (SI)**	**Test Method**
Rockwell Hardness (R-Scale)	104	104	ASTM D785
Thermal	**Nominal Value (English)**	**Nominal Value (SI)**	**Test Method**
Deflection Temperature Under Load			ASTM D648
66 psi (0.45 MPa), Unannealed	208 °F	98.0 °C	
264 psi (1.8 MPa), Unannealed	180 °F	82.0 °C	

Notes

These are typical property values not to be construed as specification limits.

Processing Techniques

Specific recommendations for resin type and processing conditions can only be made when the end use, required properties and fabrication equipment are known.

Product Storage and Handling

- Product should be stored in dry conditions at temperatures below 50°C and protected from UV-light
- Improper storage may bring damage to the packaging and can negatively affects on the quality of this product
- Keep material completely dry for good processing

Company Information

For further information regarding the LyondellBasell company, please visit http://www.lyb.com/.

Disclaimer

Information in this document is accurate to the best of our knowledge at the date of publication. The document is designed to provide users general information for safe handling, use, processing, storage, transportation, disposal and release and does not constitute any warranty or quality specification, either express or implied, including any warranty of merchantability or fitness for any particular purpose. Users shall determine whether the product is suitable for their use and can be used safely and legally.

In addition to any prohibitions of use specifically noted in this document, LyondellBasell may further prohibit or restrict the sale of its products into certain applications. For further information, please contact a LyondellBasell representative.

Page: 1 of 2
LyondellBasell

www.lyondellbasell.com
Publish Date: 2023-12-14

SCIENTIFIC DATA

EXAMPLE 1: SAFETY DATA SHEETS

A wealth of information, trapped in unstructured PDFs

Sigma-Aldrich.

www.sigmaaldrich.com

SAFETY DATA SHEET

according to Regulation (EC) No. 1907/2006

Version 6.9
Revision Date 27.10.2023
Print Date 05.12.2023
GENERIC EU MSDS - NO COUNTRY SPECIFIC DATA - NO OEL DATA

SECTION 1: Identification of the substance/mixture and of the company/undertaking

1.1 Product identifiers

Product name	:	Acetophenone
Product Number	:	W200905
Brand	:	Aldrich
Index-No.	:	606-042-00-1
REACH No.	:	01-2119533169-37-XXXX
CAS-No.	:	98-86-2

1.2 Relevant identified uses of the substance or mixture and uses advised against

Identified uses : Laboratory chemicals, Manufacture of substances

1.3 Details of the supplier of the safety data sheet

Company	:	Sigma-Aldrich Pte Ltd (Co. Registration No. 199403788W) 2 Science Park Drive #05-01/12 Ascent Building SINGAPORE 118222 SINGAPORE
Telephone	:	+65 6890 6633
Fax	:	+65 6890 6639
E-mail address	:	TechnicalService@merckgroup.com

1.4 Emergency telephone

Emergency Phone # : 1-800-262-8200

ThermoFisher SCIENTIFIC

SAFETY DATA SHEET

Creation Date 26-Sep-2009 Revision Date 24-Dec-2021 Revision Number 5

1. Identification

Product Name	**Acetylsalicylic acid**
Cat No. :	**AC158180000; AC158180025; AC158180500; AC158185000**
CAS No	50-78-2
Synonyms	2-Acetoxybenzoic acid
Recommended Use	Laboratory chemicals.
Uses advised against	Food, drug, pesticide or biocidal product use.

Details of the supplier of the safety data sheet

Company
Fisher Scientific Company
One Reagent Lane
Fair Lawn, NJ 07410
Tel: (201) 796-7100

Acros Organics
One Reagent Lane
Fair Lawn, NJ 07410

Emergency Telephone Number For information **US** call: 001-800-ACROS-01 / **Europe** call: +32 14 57 52 11
Emergency Number **US**:001-201-796-7100 / **Europe:** +32 14 57 52 99
CHEMTREC Tel. No.**US**:001-800-424-9300 / **Europe**:001-703-527-3887

2. Hazard(s) identification

Classification
This chemical is considered hazardous by the 2012 OSHA Hazard Communication Standard (29 CFR 1910.1200)

Acute oral toxicity	Category 4
Combustible dust	Yes

Label Elements

Signal Word
Warning

Hazard Statements
May form combustible dust concentrations in air
Harmful if swallowed

SAFETY DATA SHEET

Airgas
an Air Liquide company

Ethyl Chloride

Section 1. Identification

GHS product identifier	:	Ethyl Chloride
Chemical name	:	chloroethane
Other means of identification	:	Ethane, chloro-; Ethyl chloride; Muriatic ether; Monochloroethane; Hydrochloric ether; ether hydrochloric; 1-CHLOROETHANE; Ethyl chloride (Chloroethane); ethane, chloro; Monochlorethane; R 160
Product type	:	Liquefied gas
Product use	:	Synthetic/Analytical chemistry.
Synonym	:	Ethane, chloro-; Ethyl chloride; Muriatic ether; Monochloroethane; Hydrochloric ether; ether hydrochloric; 1-CHLOROETHANE; Ethyl chloride (Chloroethane); ethane, chloro; Monochlorethane; R 160
SDS #	:	001023
Supplier's details	:	Airgas USA, LLC and its affiliates 259 North Radnor-Chester Road Suite 100 Radnor, PA 19087-5283 1-610-687-5253
24-hour telephone	:	1-866-734-3438

Section 2. Hazards identification

OSHA/HCS status	:	This material is considered hazardous by the OSHA Hazard Com (29 CFR 1910.1200).
Classification of the substance or mixture	:	FLAMMABLE GASES - Category 1 GASES UNDER PRESSURE - Liquefied gas CARCINOGENICITY - Category 2 AQUATIC HAZARD (LONG-TERM) - Category 3

GHS label elements

Hazard pictograms :

Signal word	:	Danger
Hazard statements	:	Extremely flammable gas. Contains gas under pressure; may explode if heated. Suspected of causing cancer. Harmful to aquatic life with long lasting effects. May cause frostbite. May displace oxygen and cause rapid suffocation. May form explosive mixtures with air.

Precautionary statements

General	:	Read and follow all Safety Data Sheets (SDS'S) before use. Rea Keep out of reach of children. If medical advice is needed, have label at hand. Close valve after each use and when empty. Use cylinder pressure. Do not open valve until connected to equipme Use a back flow preventative device in the piping. Use only equip materials of construction. Always keep container in upright positi suspected leak area with caution.
Prevention	:	Obtain special instructions before use. Wear protective gloves. V clothing. Wear eye or face protection. Keep away from heat, hot flames and other ignition sources. No smoking. Avoid release to

Date of issue/Date of revision : 5/5/2020 Date of previous issue : 2/23/2018 V

avantor
delivered by VWR

Safety Data Sheet

according to Regulation (EC) No. 1907/2006 (REACH)

Revision date: 06.05.2022 *Version: 7.2* *Print date: 06.05.2022*

SECTION 1: Identification of the substance/mixture and of the company/undertaking

1.1 Product identifier

Trade name/designation:	Chrysene
Product No.:	12300
CAS No.:	218-01-9
Index No.:	601-048-00-0
EU REACH No.:	A registration number is not available for this substance as the substance or its use is exempted from registration according to REACH Article 2 or the annual tonnage does not require a registration.
Other means of identification:	1,2-Benzophenanthrene, Benzo[a]phenanthrene

1.2 Relevant identified uses of the substance or mixture and uses advised against

Relevant identified uses: General chemical reagent

1.3 Details of the supplier of the safety data sheet

Ireland

VWR International Ltd.

Street	Orion Business Campus, Northwest Business Park
Postal code/City	Ballycoolin, Dublin 15
Telephone	+353 1 8822222
Telefax	+353 1 8822333
E-mail (competent person)	SDS@avantorsciences.com

1.4 Emergency phone number

Telephone +44 (0) 1270 502894 (CareChem24)

*This SDS for user in JP - Not correspond to the regulation of other countries.

TCI
TOKYO CHEMICAL INDUSTRY CO., LTD.

Azelaic Acid Revision number: 2 Revision date: 03/04/2023 Page 1 of 4
Revision date: 03/04/2023

SAFETY DATA SHEET

ION
: Azelaic Acid
: A1318
TOKYO CHEMICAL INDUSTRY CO., LTD.
4-10-2, Nihonbashi-honcho, Chuo-ku, Tokyo 103-0023, Japan
lepartment: Global Business Department
+81-3-5640-8872
+81-3-5640-8902
globalbusiness@TCIchemicals.com
ber: 2

ENTIFICATION
of the substance or mixture
AZARDS Not classified
ZARDS
e damage/eye irritation Category 2B
NTAL HAZARDS Not classified
ts
r hazard symbols None
Warning
ments Causes eye irritation
y statements
on] Wash hands and face thoroughly after handling.
e] IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing. If eye irritation persists: Get medical advice or attention.

N/INFORMATION ON INGREDIENTS
xture: Substance
Azelaic Acid
>98.0%(GC)(T)
123-99-9
1,7-Heptanedicarboxylic Acid , Nonanedioic Acid
nula: $C_9H_{16}O_4$
h Official Gazettes Reference Number
: (2)-878
Official announcement chemistry substance.

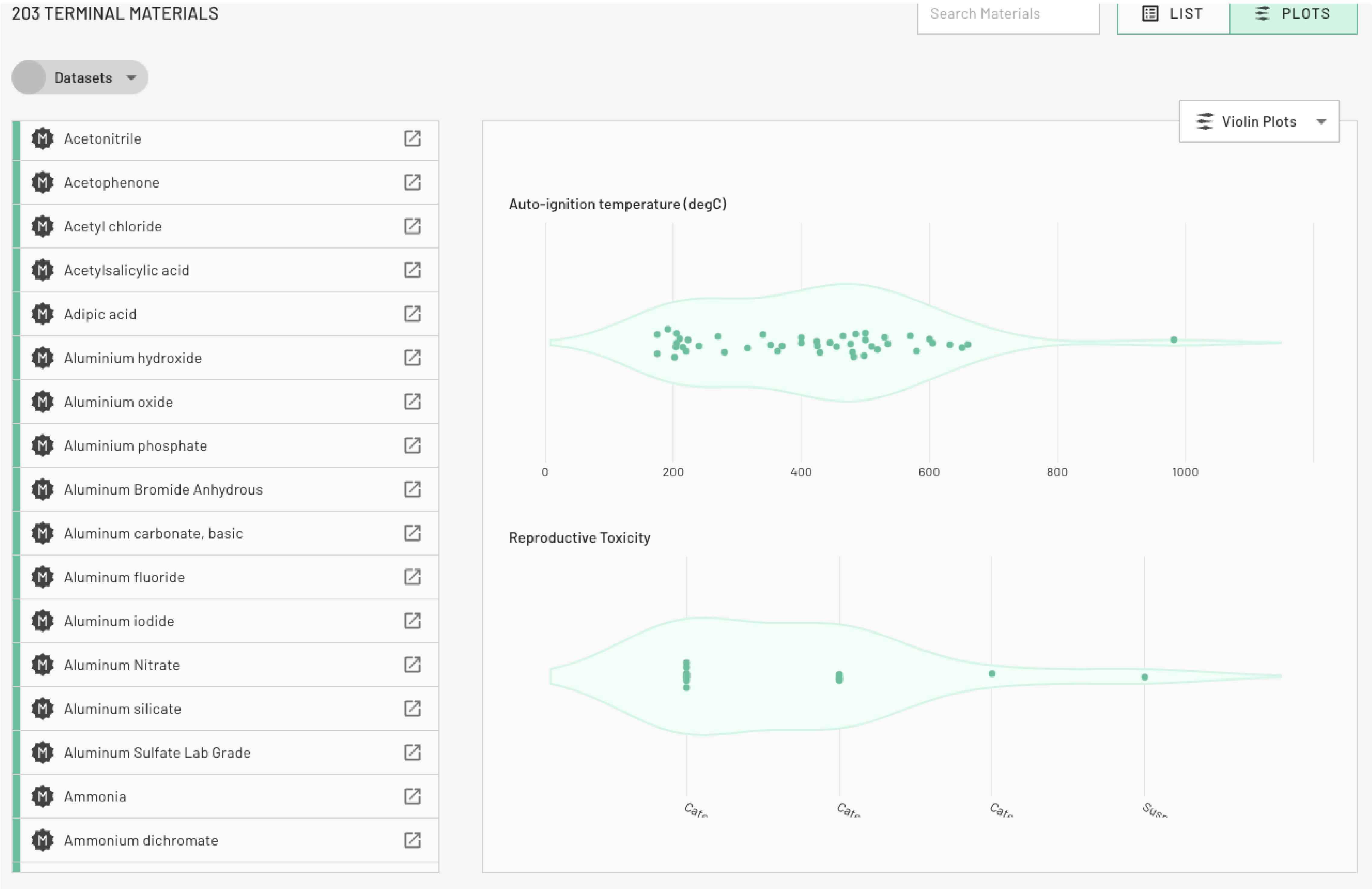
EASURES
Remove victim to fresh air and keep at rest in a position comfortable for breathing. Get medical advice/attention if you feel unwell.
Remove/Take off immediately all contaminated clothing. Rinse skin with water/shower. If skin irritation or rash occurs: Get medical advice/attention.
Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing. If eye irritation persists: Get medical advice/attention.
Get medical advice/attention if you feel unwell. Rinse mouth.
first-aiders: A rescuer should wear personal protective equipment, such as rubber gloves and air-tight goggles.

ition
stance or mixture
to Regulation (EC) No 1272/2008
ory 4), H302
H319
atements mentioned in this Section, see Section 16.

Page 1 of 14
MilliporeSigma in the US and

EXAMPLE 1: SAFETY DATA SHEETS

Citrine can automatically parse and normalize your SDS PDFs



MATERIAL: Acetylsalicylic acid

DESCRIPTION

generated from SDS

MEASURED PROPERTIES

Melting point	[136, 140] °C
Odor	odorless
Physical State	Powder Solid
Color	white
Relative density	1.4
Molecular weight	180 g/mol
pH	3.5
Acute toxicity, oral	Category 4
Flash point	250 °C
CAS number	50-78-2
Auto-ignition temperature (degC)	500 °C

SUMMARY

- LLMs are a transformative technology, and they WILL impact the materials and chemicals industry
- Citrine is utilizing LLMs across our Platform to accelerate customer workflows and improve the user experience
- New capabilities to be announced soon

- Interested in learning more or collaborating? mmusto@citrine.io

EXAMPLE 2: PROCESSING INFORMATION

Often, how a process was performed is stored as long-form text.

For effective AI, key single-value metrics must be extracted.

	A	B
1		**Processing**
2	**recipe 0**	The formulation was stirred at a speed of 500 RPM for 30 minutes in a glass vessel. The reaction temperature was set at 70¬∞C and the total volume of the vessel was 2 liters
3	**recipe 1**	The stir speed was set to 600 RPM and the stir time was 45 minutes. The formulation was prepared in a stainless steel vessel at a reaction temperature of 80¬∞C. The total volume of the vessel was
4	**recipe 2**	The formulation process involved stirring at 700 RPM for 1 hour in a ceramic vessel. The reaction temperature was maintained at 90¬∞C and the vessel had a total volume of 4 liters
5	**recipe 3**	Stirring was carried out at a speed of 800 RPM for 1.5 hours in a glass vessel. The reaction temperature was 100¬∞C and the total volume of the vessel was 5 liters
6	**recipe 4**	The formulation was stirred at 900 RPM for 2 hours in a stainless steel vessel. The reaction temperature was set at 110¬∞C and the vessel's total volume was 6 liters
7	**recipe 5**	The stir speed was set to 1000 RPM and the stir time was 2.5 hours. The formulation was prepared in a ceramic vessel at a reaction temperature of 120¬∞C. The total volume of the vessel was 7 lite
8	**recipe 6**	The formulation process involved stirring at 1100 RPM for 3 hours in a glass vessel. The reaction temperature was maintained at 130¬∞C and the vessel had a total volume of 8 liters
9	**recipe 7**	Stirring was carried out at a speed of 1200 RPM for 3.5 hours in a stainless steel vessel. The reaction temperature was 140¬∞C and the total volume of the vessel was 9 liters
10	**recipe 8**	The formulation was stirred at 1300 RPM for 4 hours in a ceramic vessel. The reaction temperature was set at 150¬∞C and the vessel's total volume was 10 liters
11	**recipe 9**	The stir speed was set to 1400 RPM and the stir time was 4.5 hours. The formulation was prepared in a glass vessel at a reaction temperature of 160¬∞C. The total volume of the vessel was 11 liters
12	**recipe 10**	The formulation process involved stirring at 1500 RPM for 5 hours in a stainless steel vessel. The reaction temperature was maintained at 170¬∞C and the vessel had a total volume of 12 liters
13	**recipe 11**	Stirring was carried out at a speed of 1600 RPM for 5.5 hours in a ceramic vessel. The reaction temperature was 180¬∞C and the total volume of the vessel was 13 liters
14	**recipe 12**	The formulation was stirred at 1700 RPM for 6 hours in a glass vessel. The reaction temperature was set at 190¬∞C and the vessel's total volume was 14 liters
15	**recipe 13**	The stir speed was set to 1800 RPM and the stir time was 6.5 hours. The formulation was prepared in a stainless steel vessel at a reaction temperature of 200¬∞C. The total volume of the vessel was
16	**recipe 14**	The formulation process involved stirring at 1900 RPM for 7 hours in a ceramic vessel. The reaction temperature was maintained at 210¬∞C and the vessel had a total volume of 16 liters
17	**recipe 15**	Stirring was carried out at a speed of 2000 RPM for 7.5 hours in a glass vessel. The reaction temperature was 220¬∞C and the total volume of the vessel was 17 liters
18	**recipe 16**	The formulation was stirred at 2100 RPM for 8 hours in a stainless steel vessel. The reaction temperature was set at 230¬∞C and the vessel's total volume was 18 liters
19	**recipe 17**	The stir speed was set to 2200 RPM and the stir time was 8.5 hours. The formulation was prepared in a ceramic vessel at a reaction temperature of 240¬∞C. The total volume of the vessel was 19 lit
20	**recipe 18**	The formulation process involved stirring at 2300 RPM for 9 hours in a glass vessel. The reaction temperature was maintained at 250¬∞C and the vessel had a total volume of 20 liters
21	**recipe 19**	Stirring was carried out at a speed of 2400 RPM for 9.5 hours in a stainless steel vessel. The reaction temperature was 260¬∞C and the total volume of the vessel was 21 liters
22	**recipe 20**	The formulation was stirred at 2500 RPM for 10 hours in a ceramic vessel. The reaction temperature was set at 270¬∞C and the vessel's total volume was 22 liters

EXAMPLE 2: PROCESSING INFORMATION

Often, how a process was performed is stored as long-form text.

For effective AI, key single-value metrics must be extracted.

	A	B	C	D	E	F
1		**Stir Speed (RPM)**	**Stir Time (hr)**	**Vessel Type (category)**	**Reaction Temperature (degC)**	**Vessel total Volume (L)**
2	**recipe 0**	500	0.5	glass	70	2
3	**recipe 1**	600	0.75	stainless steel	80	3
4	**recipe 2**	700	1	ceramic	90	4
5	**recipe 3**	800	1.5	glass	100	5
6	**recipe 4**	900	2	stainless steel	110	6
7	**recipe 5**	1000	2.5	ceramic	120	7
8	**recipe 6**	1100	3	glass	130	8
9	**recipe 7**	1200	3.5	stainless steel	140	9
10	**recipe 8**	1300	4	ceramic	150	10
11	**recipe 9**	1400	4.5	glass	160	11
12	**recipe 10**	1500	5	stainless steel	170	12
13	**recipe 11**	1600	5.5	ceramic	180	13
14	**recipe 12**	1700	6	glass	190	14
15	**recipe 13**	1800	6.5	stainless steel	200	15
16	**recipe 14**	1900	7	ceramic	210	16
17	**recipe 15**	2000	7.5	glass	220	17
18	**recipe 16**	2100	8	stainless steel	230	18
19	**recipe 17**	2200	8.5	ceramic	240	19
20	**recipe 18**	2300	9	glass	250	20
21	**recipe 19**	2400	9.5	stainless steel	260	21
22	**recipe 20**	2500	10	ceramic	270	22

EXAMPLE 3: DIVERGENT FORMS

Often, forms change over times and people customize templates to suit their needs making programmatic data extraction unscalable.

X-Labs Analytical Lab

Sample	MATX-BM-M009
Measurement	Hall

Probe Resistance (ohm)	4.3
Gas Flow Rate (L/min)	1
Gas	Ar
Probe Material	W
Current (mA)	0.1
Field Strength (T)	5
Position	1
Magnet Reversal	trur

```
         X-LABS DATA FORM
====================================
material_uid               MATX-BM-M011
Measurement                Hall
Probe Resistance (ohm)     6.9
Gas Flow Rate (L/min)      1
Gas Type                   Ar
Probe Material             W
Current (mA)               0.1
Field Strength (T)         5
Sample Position            2
Magnet Reversal            True
```

X-Materials Analytical Lab
Hall Measurement

ID: MATX-BM-M004
Request ID: X9PY4T

Probe Resistance	3.1 ohm	Current	0.1 mA
Gas Flow Rate	1 L/min	Field Strength	5 T
Gas Type	Ar	Sample Position	1
Probe Material	W	Magnet Reversal	True

EXAMPLE 3: DIVERGENT FORMS

Often, forms change over times and people customize templates to suit their needs making programmatic data extraction unscalable.

X-Labs Analytical Lab

Sample MATX-BM-M009

Probe Resistance (ohm) 4.3

	A	B	C	D	E	F	G	H	I	J
1	Sample ID	Measurement Name	Probe Resistance (ohm)	Gas Flow Rate (L/min)	Gas Type	Probe Material	Current (mA)	Field Strength (T)	Sample Position	Magnet Reversal
2	MATX-BM-M011	Hall	6.9	1	Ar	W	0.1	5	2	TRUE
3	MATX-HP-M001	Hall	2.3	1	Ar	W	0.1	5	1	TRUE
4	MATX-HP-M036	Hall	2.5	1	Ar	W	0.1	5	2	TRUE
5	MATX-BM-M009	Hall	4.3	1	Ar	W	0.1	5	1	TRUE
6	MATX-BM-M004	Hall	3.1	1	Ar	W	0.1	5	1	TRUE

Current (mA) 0.1
Field Strength (T) 5
Sample Position 2
Magnet Reversal True

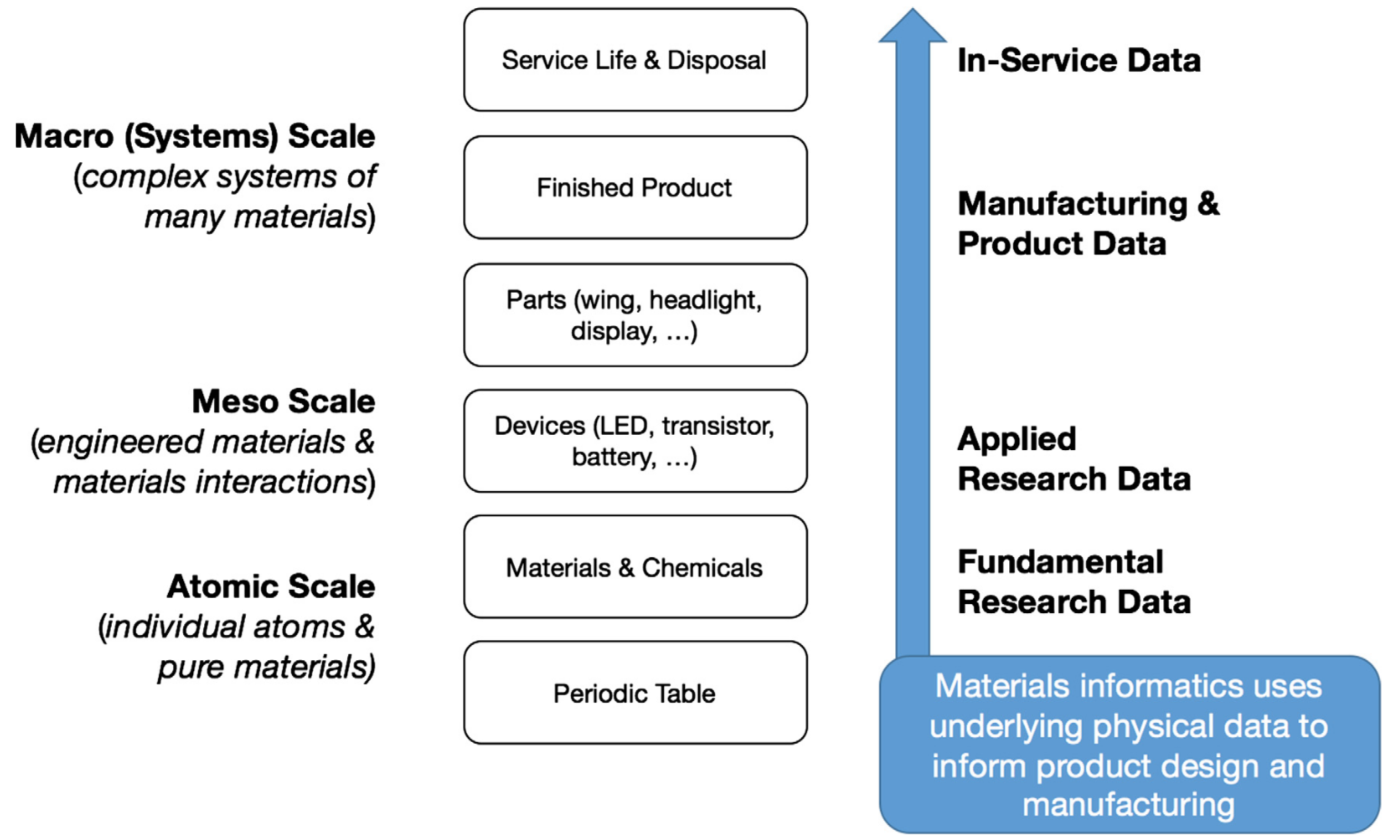
Request ID: X9PY4T

Probe Resistance	3.1 ohm	Current	0.1 mA
Gas Flow Rate	1 L/min	Field Strength	5 T
Gas Type	Ar	Sample Position	1
Probe Material	W	Magnet Reversal	True

Data Management and AI at Scale

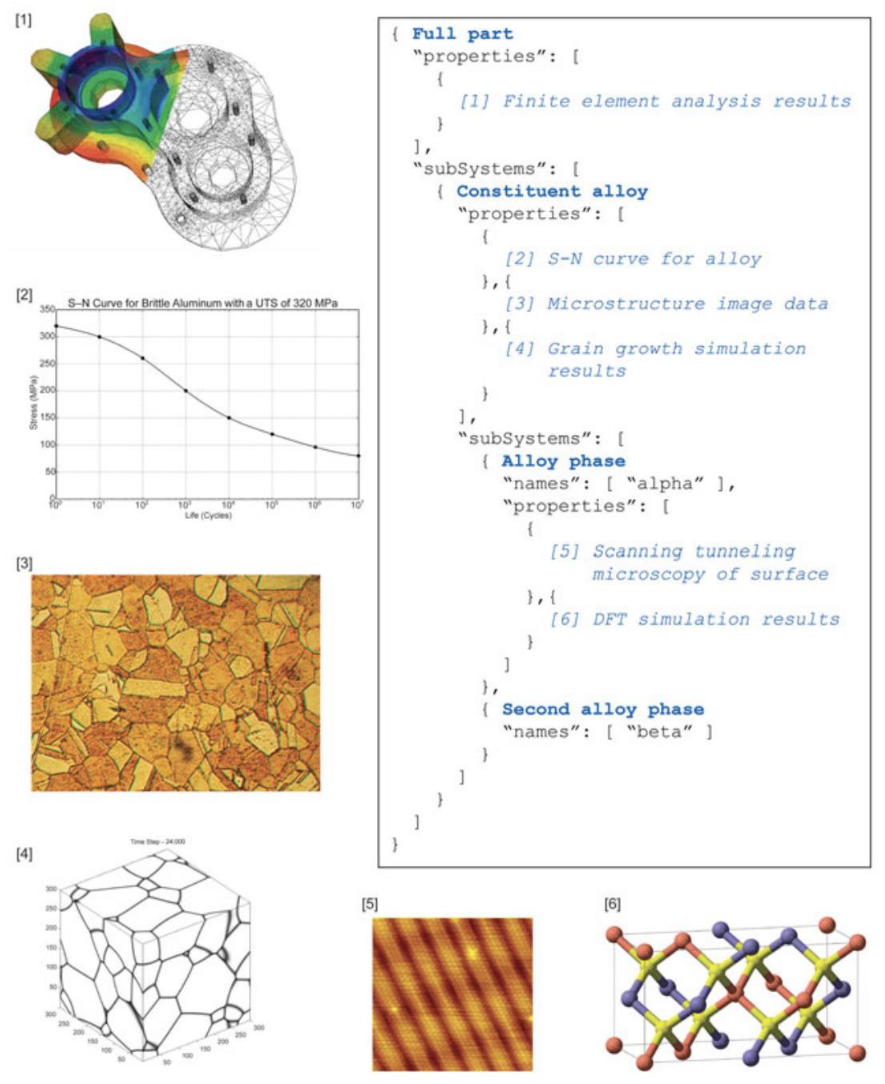
SETTING THE VISION: AI AT SCALE

Integrating Material Informatics across multiple scales



Multiple dimensions:

- "vertical", from constituents to structure
- "horizontal", promoting re-usability of AI models on different applications
- Beyond: LCA, socioresilience, etc.



Left: "Beyond bulk single crystals: A data format for all materials structure- property-processing relationships", K. Michel, B. Meredig, MRS Bulleting, Vol. 41, 2016
Right: "Industrial materials informatics: Analyzing large-scale data to solve applied problems in R&D, manufacturing, and supply chain,
", B. Meredig, Current Opinion in Solid State and Materials Science , 2017

SCALE AND REUSE WITHIN PRODUCT DEVELOPMENT

Current state: a single expert, carefully assigned

Surface Energy Expert

Project 1
Lubricants

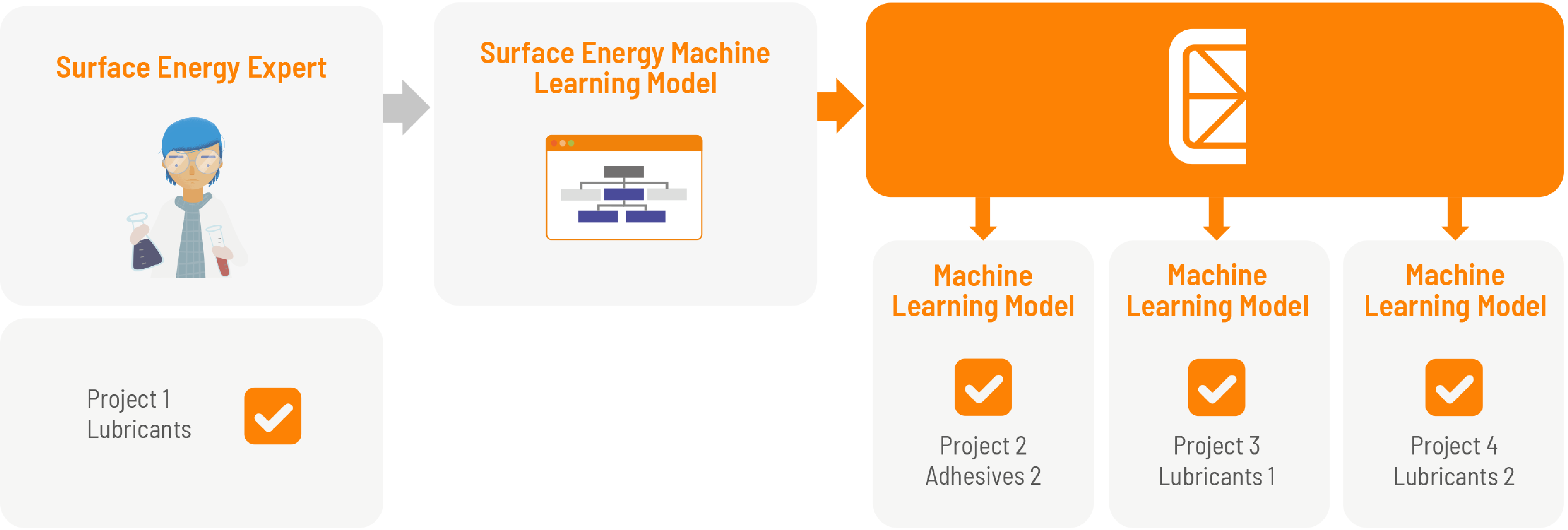
✓

Project 2
Adhesives

X

SCALE AND REUSE WITHIN PRODUCT DEVELOPMENT

Future state: expert knowledge, shared across similar projects

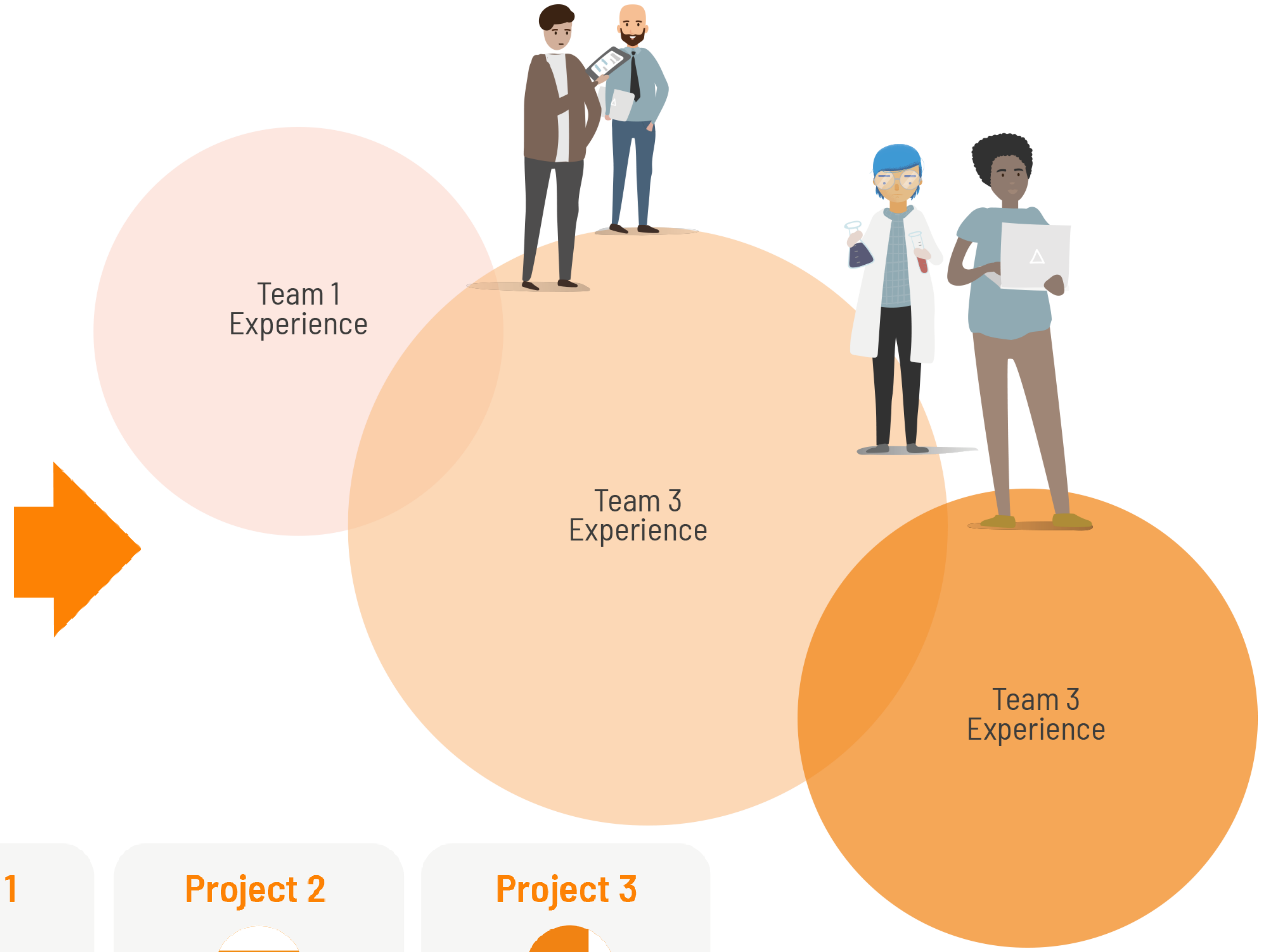


SCALE AND REUSE WITHIN R&D

Current state: use of ingredients and processes limited by experience and bias

Glass filled Nylon for Electric Vehicle market

Available ingredients, processes and parameter ranges



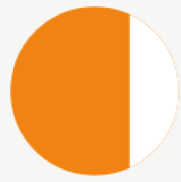
Project 1

Glass Filled Nylon for BMW

Project 2

Arc resistant Nylon for Tesla

Project 3

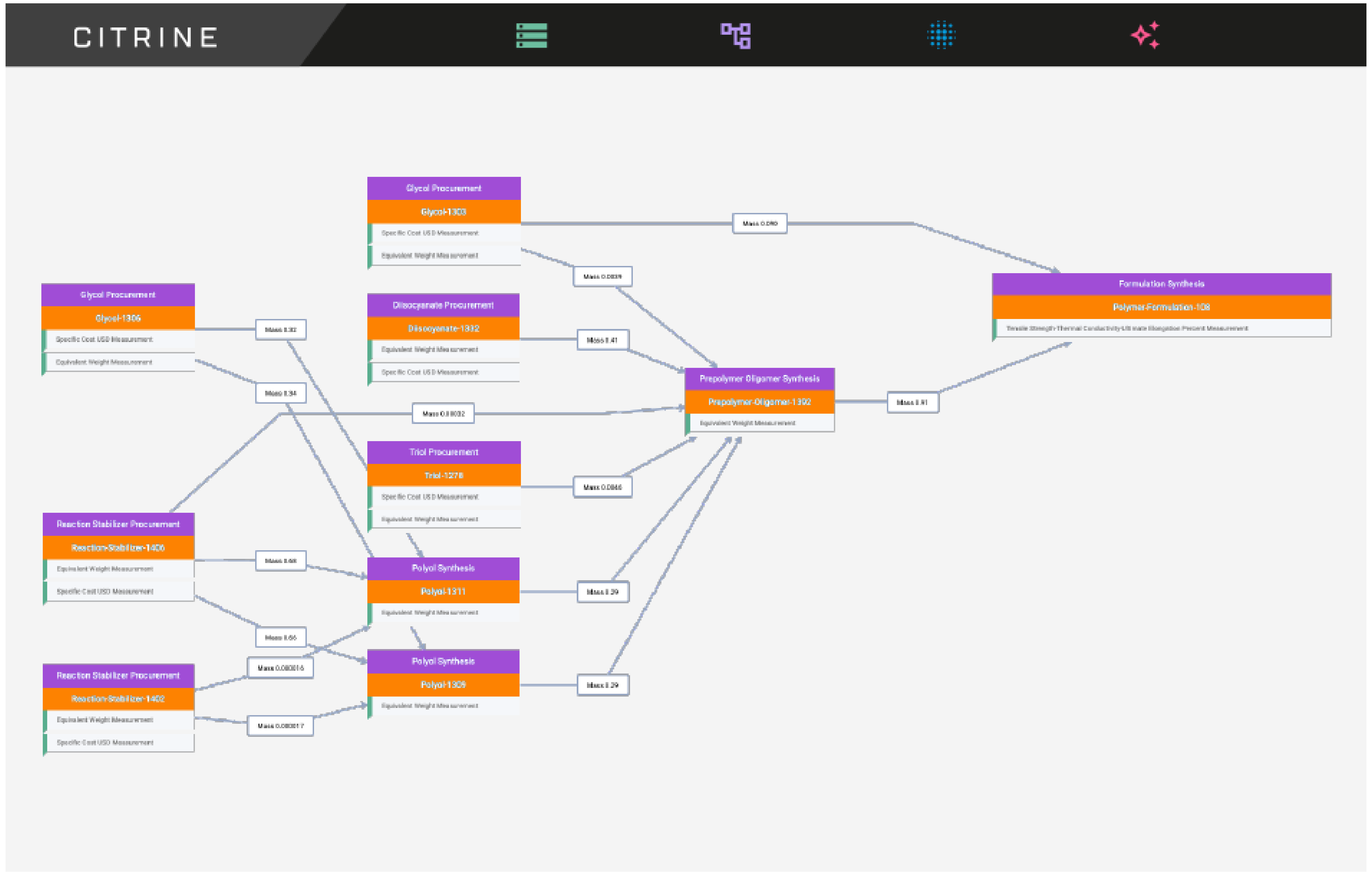


Corrosion Optimized HDPE for Oil and Gas

FAIR R&D DATA IS POSSIBLE

Entropy is real and must be combated

- Balance Flexibility and Structure
  - Directed acyclic graph of Materials, Processes, Measurements and Ingredients
  - If materials share a common precursor, that shared heritage can be represented
- Enforce Standards
  - Unless standards are created and enforced, they will not be followed
  - Allow for and incentivize data structuring over time.
- Reward work
  - Researchers should be incentivized to put in the work needed for FAIR data



HISTORICAL DATA SYSTEMS

We've been Using Computers to Store Scientific Data for Over 50 years

Before Data Capture Systems:

- All hand-written notes.
- Rooms filled with filing cabinets, notebooks, and lookup cards

1973: LIMS are first discussed!

- ASTM-Organized Conference
- Focused on Lab Automation

In 1976 the focus has shifted to automated analyses

- Applications and Laboratory Automation
- Specific sessions around specific types of experimentations (and let the data silos begin!)

In the late 1970's to early 1980's we started to see relational databases being used to store

1982 LIMS hit the market! (and the abbreviation is used)

- Perkin-Elmer: 'LIMS 2000'
- Purvis Systems: 'Turnkey LIMS'
- Spectrogram Corporation: `LMIS`

By 1995 there are >= 42 LIMS on the market

Gerst A. Gibbon. A brief history of LIMS. (32)1, (1996) p. 1-5

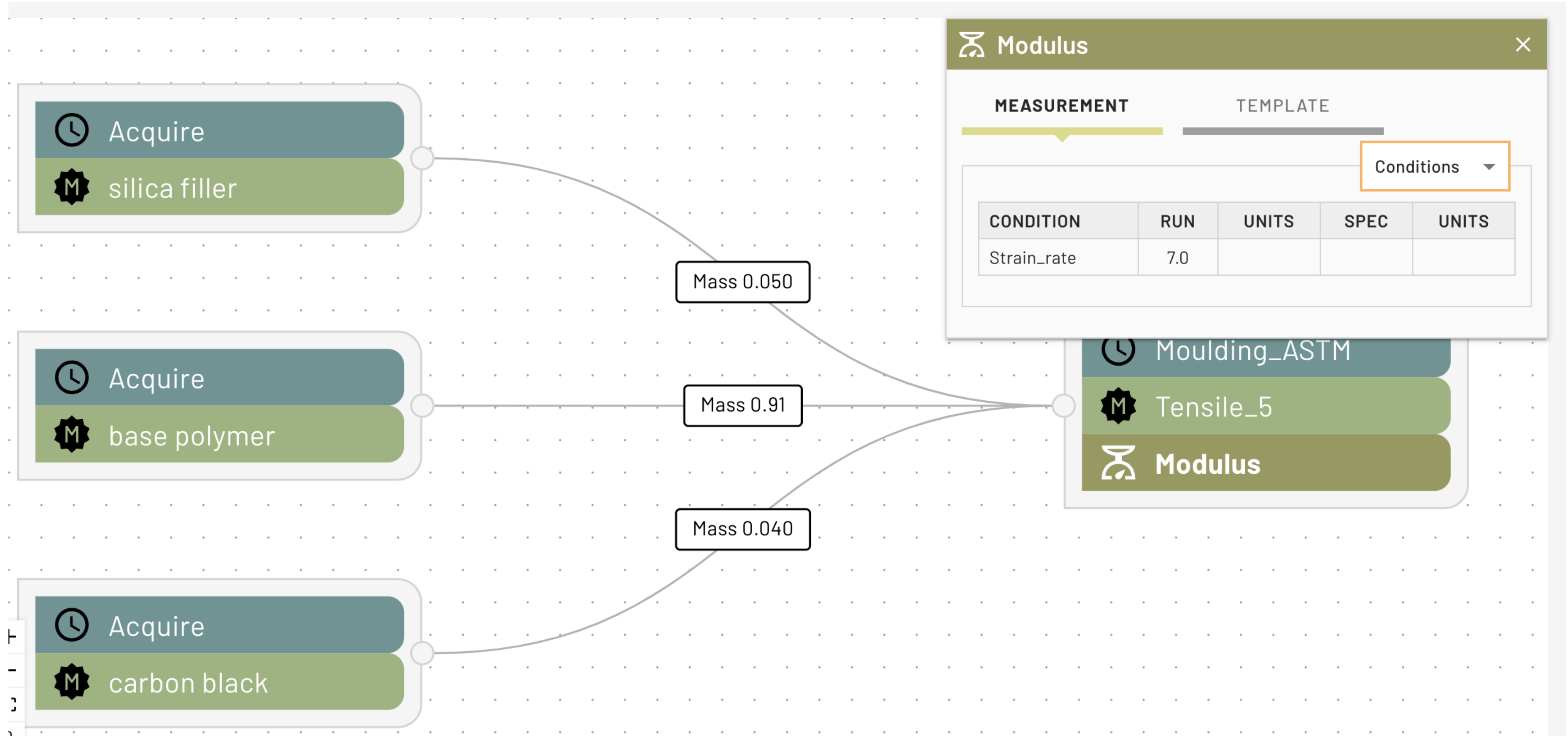
CHANGING DATA USES MEANS CHANGING NEEDS

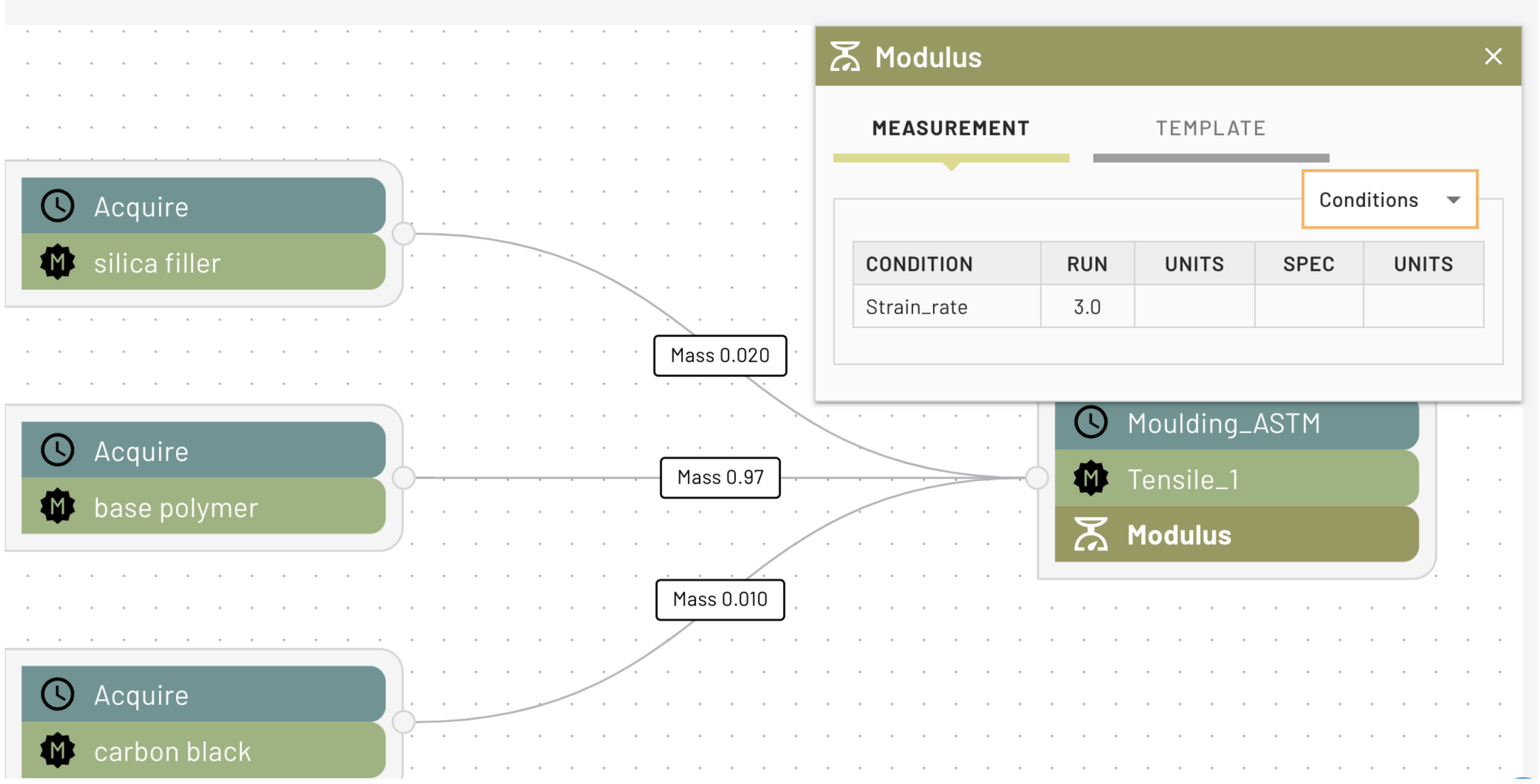
Digitalization is only step one for using R&D data in AI.

- **Materials Informatics relies on data** to power AI models, which can then be used to predict properties from formulations, processing information, and measurement conditions.
- Both measured **properties *and* "input" data** (formulations, processing information) **need to be available** for the same samples
- Additionally, **"failed" experiments should be recorded** to train the model what does *not* work
- Data from various datasets should be **interoperable** to enable transfer learning and bolster data volume
- Single-point-metrics or **AI-interpretable data** (e.g., SEM image) should be programmatically available
- **Data volume should be measure of # of unique high-quality samples**/data points not gigabytes

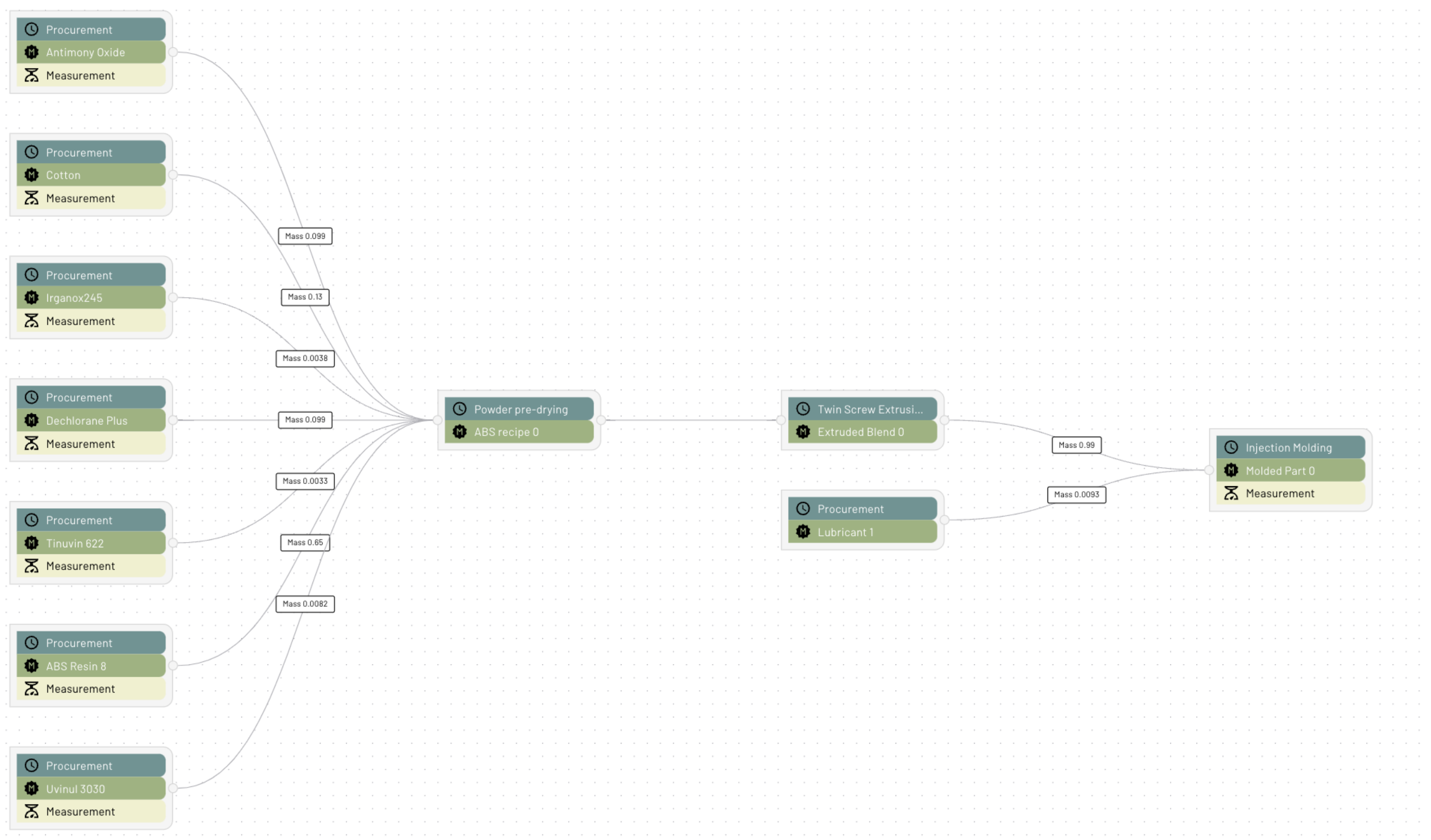
DATA CHALLENGES: MEAUSUREMENT CONDITIONS

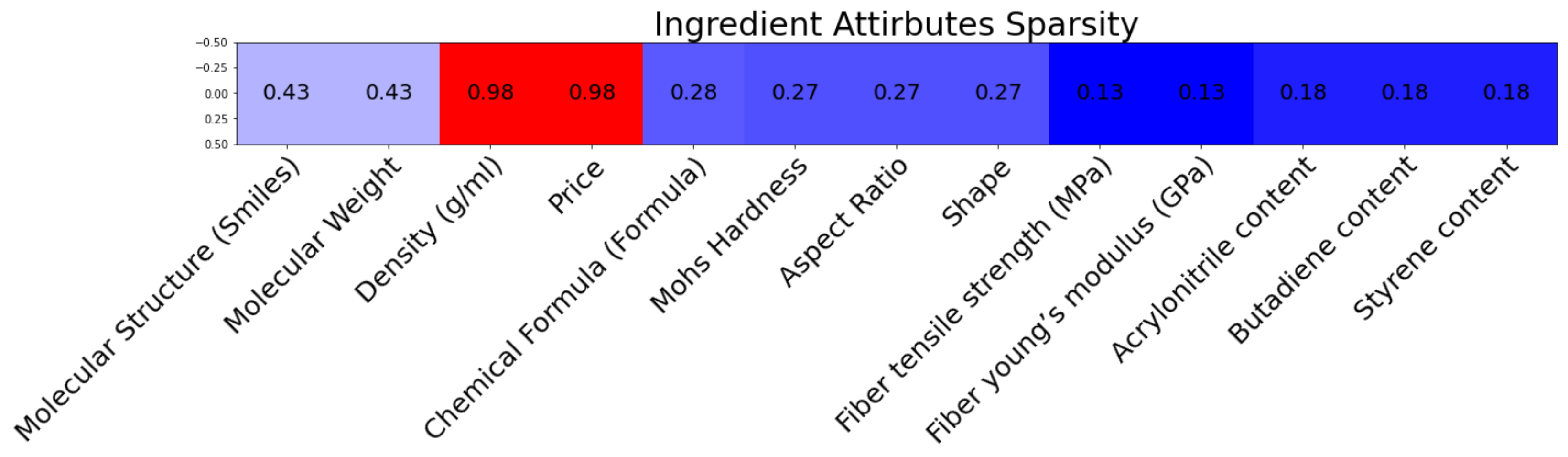
- Need to be able to describe in "AI friendly" fashion:
- Same nominal property measured under different standards and/or conditions
- Same nominal property measured with different equipment



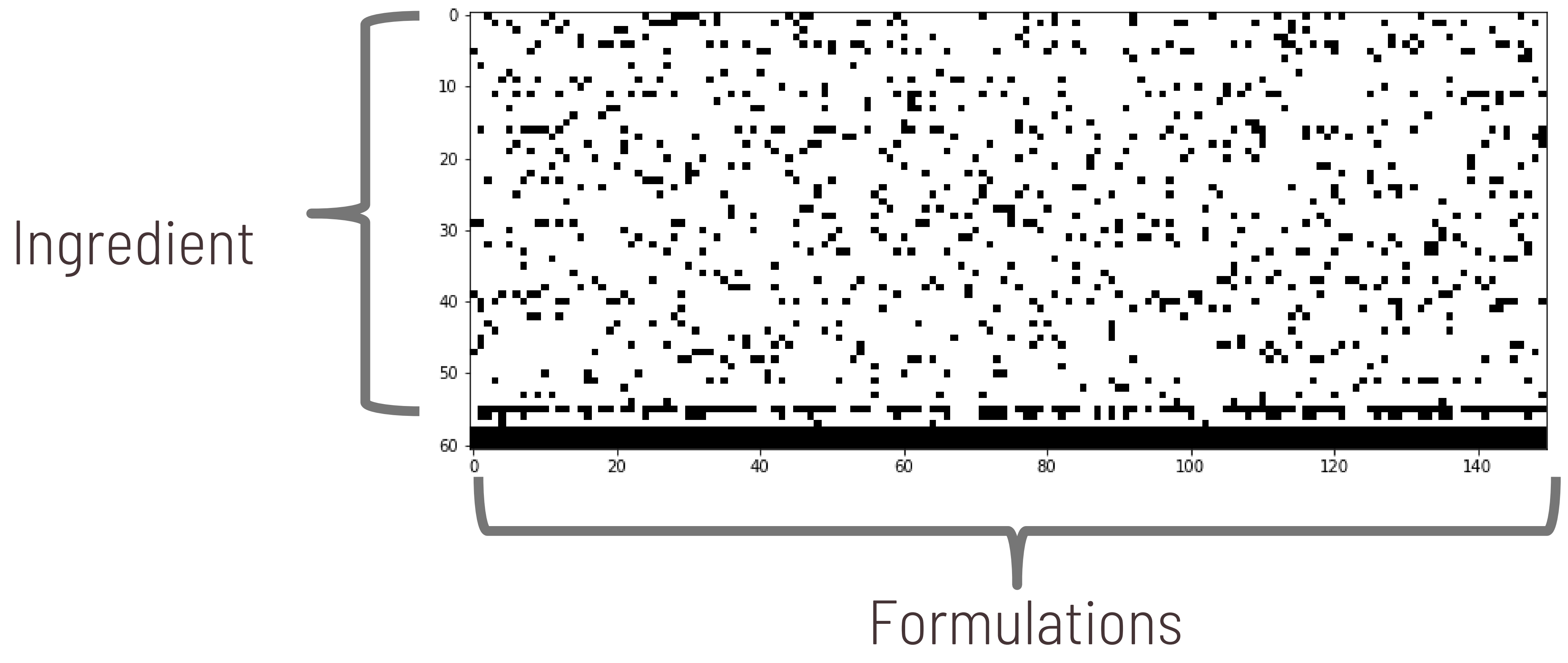


DATA CHALLENGES: SPARSITY





Sparsity for ingredients' properties



"Sparsity matrix" for first mixing step

- Sparsity can be common even in domain-specific datasets
- It is inherent in datasets attempting to bridge applications