

REMOVING PFAS

AND OTHER PROBLEMATIC INGREDIENTS

The drive to replace raw materials being phased out due to regulatory restrictions is a dynamic area of AI application in the chemicals industry.

READ ON FOR

1 HOW DOES IT WORK?



SMILES ENCODING

Computer-readable molecular structure format

2 CASE STUDIES



FEATURE COMPUTATION

Automated analysis of molecular properties



ALTERNATIVE IDENTIFICATION

Rapid discovery of viable substitutes

CITRINE



INFORMATICS

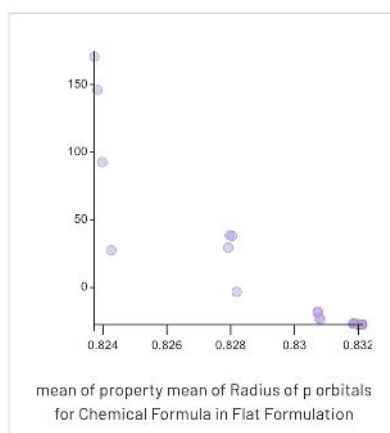
HOW IT WORKS

By leveraging chemical formulas and molecular structures, the Citrine Platform can automatically compute essential "features." This is done by encoding molecular structures using computer-readable formats like SMILES (Simplified Molecular Input Line Entry System). This allows for the computation of various molecular properties, including the number of hydrogen bonds, polarizability, molecular weight, and more.



AI-POWERED ANALYSIS

As AI models analyze these features to determine their significance for achieving target properties, they can efficiently evaluate alternative molecules that possess these key attributes.



RAPID REFORMULATION

By identifying viable substitutes, AI aids companies in reformulating products more swiftly and effectively, accelerating compliance with evolving regulations.

PATENTED TECHNOLOGY

Using Machine Learning to Explore Formulation Recipes with New Ingredients

Patent granted No. 10,984,145 B1

This methodology ranks candidate formulation recipes based on their likelihood of achieving target specifications. These recipes can include previously untested ingredients.

CASE STUDY: REMOVING PFAS IN ADHESIVES

2

YEARS SAVED

Of R&D work on a 5-year project timeline

30

VIABLE CANDIDATES

Narrowed from millions of formulations



THE CHALLENGE

A global materials conglomerate faced mounting pressure to reformulate their pressure-sensitive adhesives product line to exclude PFAS compounds. The challenge involved accelerating product development to comply with increasing regulatory demands around PFAS elimination while maintaining current mechanical performance and navigating a complex formulation space with numerous variables and constraints.

MONTH 1

Trained internal team, reaching autonomy quickly.

1

MONTH 4

Identified breakthrough candidate formulation.

3

MONTH 3

Screened millions of formulations,
narrowed to 30 viable candidates.

2

MONTH 6

Team generated 25 user models,
quadrupled projects and platform
users.

4

CASE STUDY: REFORMULATING PLASTICS FOR SAFETY

REPLACING TOXIC INGREDIENTS WHILE RETAINING TECHNICAL PERFORMANCE

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

COLLABORATING PARTNERS AND FUNDING INSTITUTION



01

THE CHALLENGE

Toxic additives in PVC plastics are becoming increasingly scrutinized and banned, particularly phthalate plasticizers. However, non-toxic replacements have unknown impacts on PVC mechanical performance. The goal: identify PVC formulations that remove phthalates but retain plasticity.

02

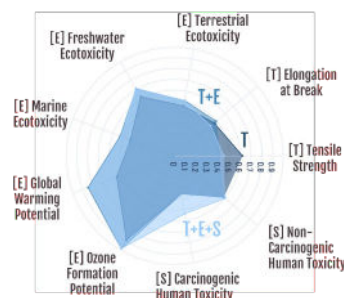
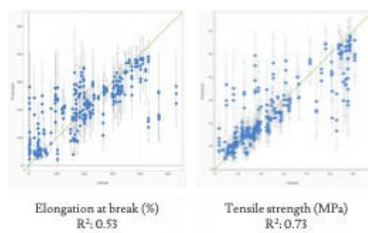
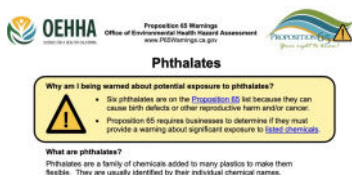
THE PROCESS

- Gathered data on plastic ingredients (plasticizers, fillers, stabilizers, lubricants) and PVC formulations
- Built ML models to **predict mechanical performance and toxicity**
- Optimized plastic formulations** for mechanical performance with and without toxicity constraints

03

THE RESULTS

Quantitative trade-off of technical (T) performance, with and without ecological (E) and societal (S) constraints. Engineers can now determine the cost of satisfying regulations or supply-chain constraints.



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

LEARN MORE ABOUT US

WATCH AN ON DEMAND WEBINAR



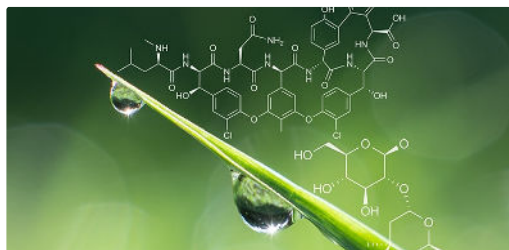
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MEET US

REQUEST A MEETING AND MEET OUR TEAM. OUR SOLUTION ENGINEERS HAVE CHEMICAL INDUSTRY EXPERIENCE AND ARE MOTIVATED TO CAREFULLY ASSESS TECHNOLOGY FIT AND BUSINESS VALUE.

Meet now