UNIVERSITY OF CAMBRIDGE

intellegens

Applied machine learning

AI recipes for a digital kitchen

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Alchemite™ machine learning

Use case of Alchemite™ by Intellegens machine learning in Yili

Applications of generic Alchemite™ to formulation design

Introducing Alchemite™ applied machine learning

Developed at University of Cambridge

Key use cases: chemicals, materials, life sciences, and manufacturing

Innovative method extracts value from sparse, noisy data to solve complex, high-dimensional problems

Focus on ease-of-deployment for immediate return on investment

Collaboration with Yili

working with Matthias Eisner

Ultra heat treatment (UHT) whipping cream

Shelf Life	Physical stability up to 9 months
Yield	How foamy is it (overrun)?
Whipping time	How long does it take to get a strong whipped cream?

Formulation problem

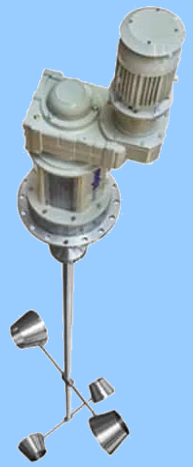
Ingredients

Cream fat, protein
10 stabilizers
14 emulsifiers

Find alternatives
Reduce embedded CO_2
Ensure health / safety
Minimise cost

Processes

Homogenization



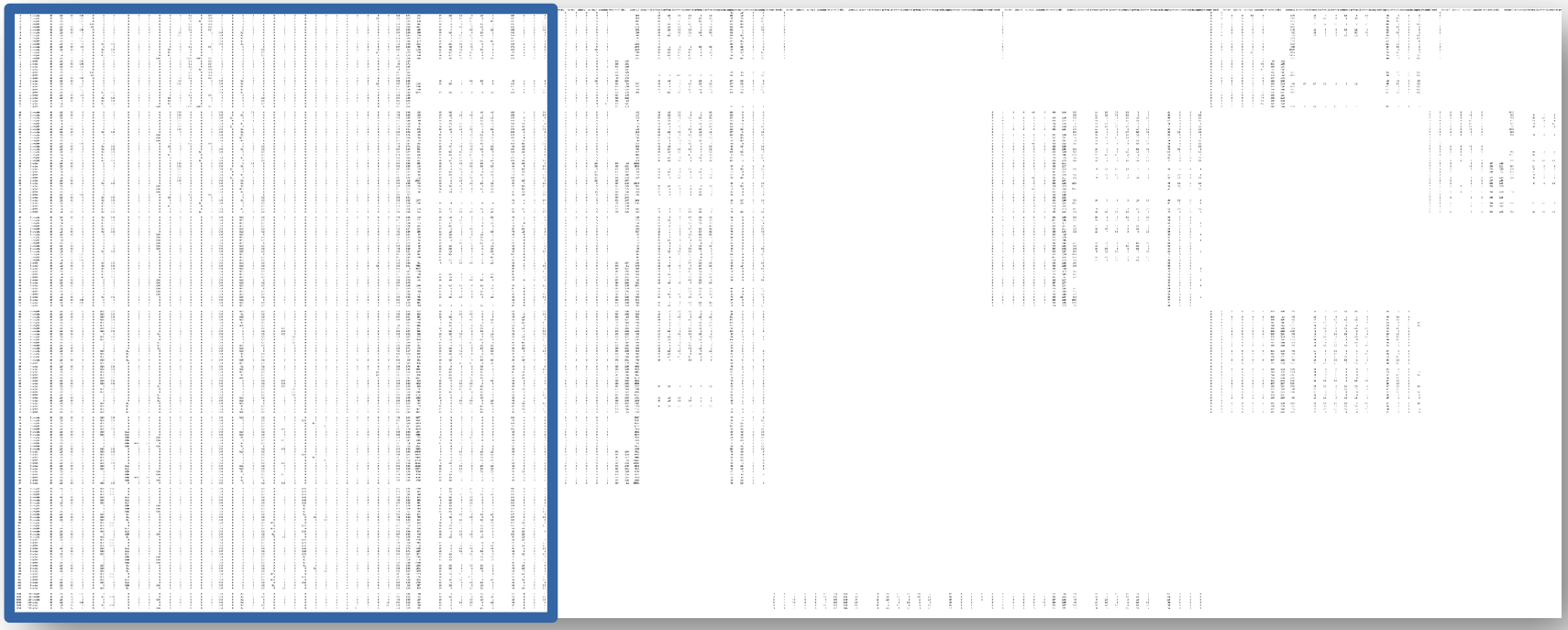
Minimise energy / CO_2
Ensure health / safety
Minimise cost
Minimise time

Properties

Fat rise, color, separation, pouring…
Whipping time, yield, shape stability
Application metrics

Maximise performance
Market requirements
Maximise shelf-life

Data

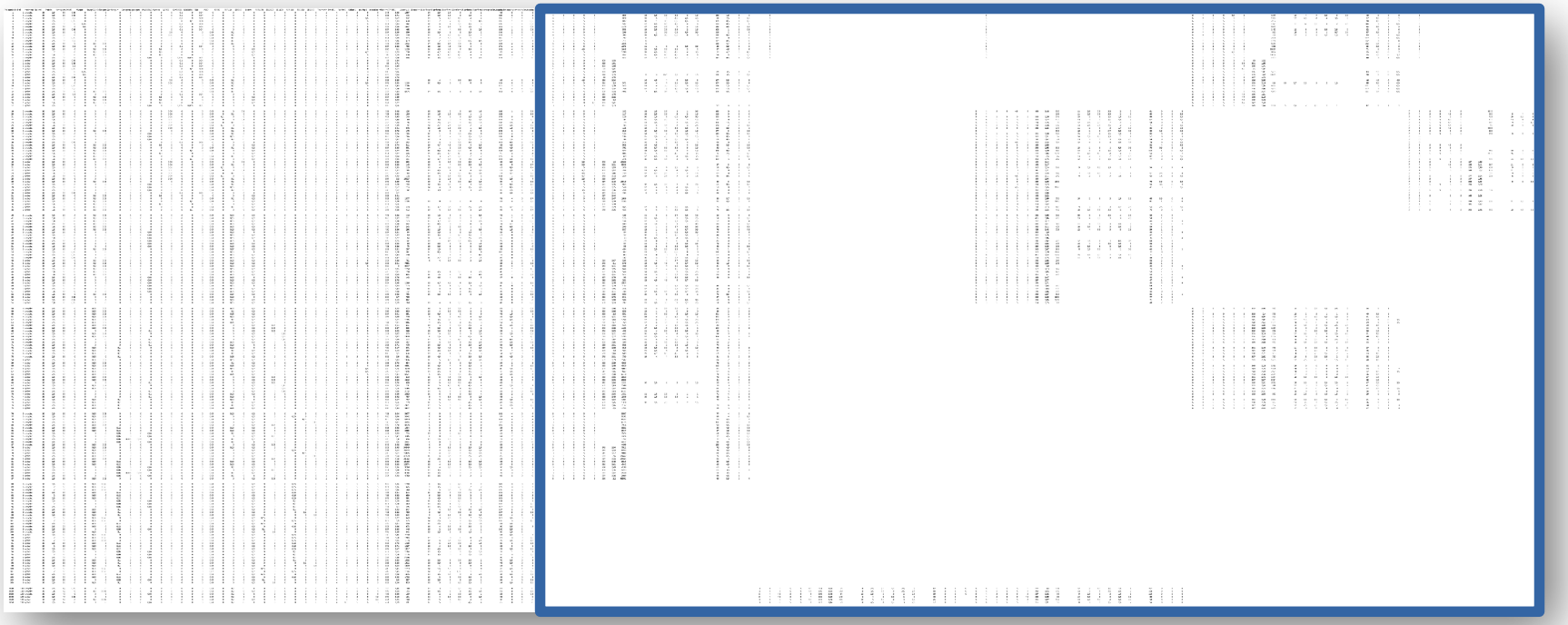


Input usually complete

- raw cream
- process
- storage

Data

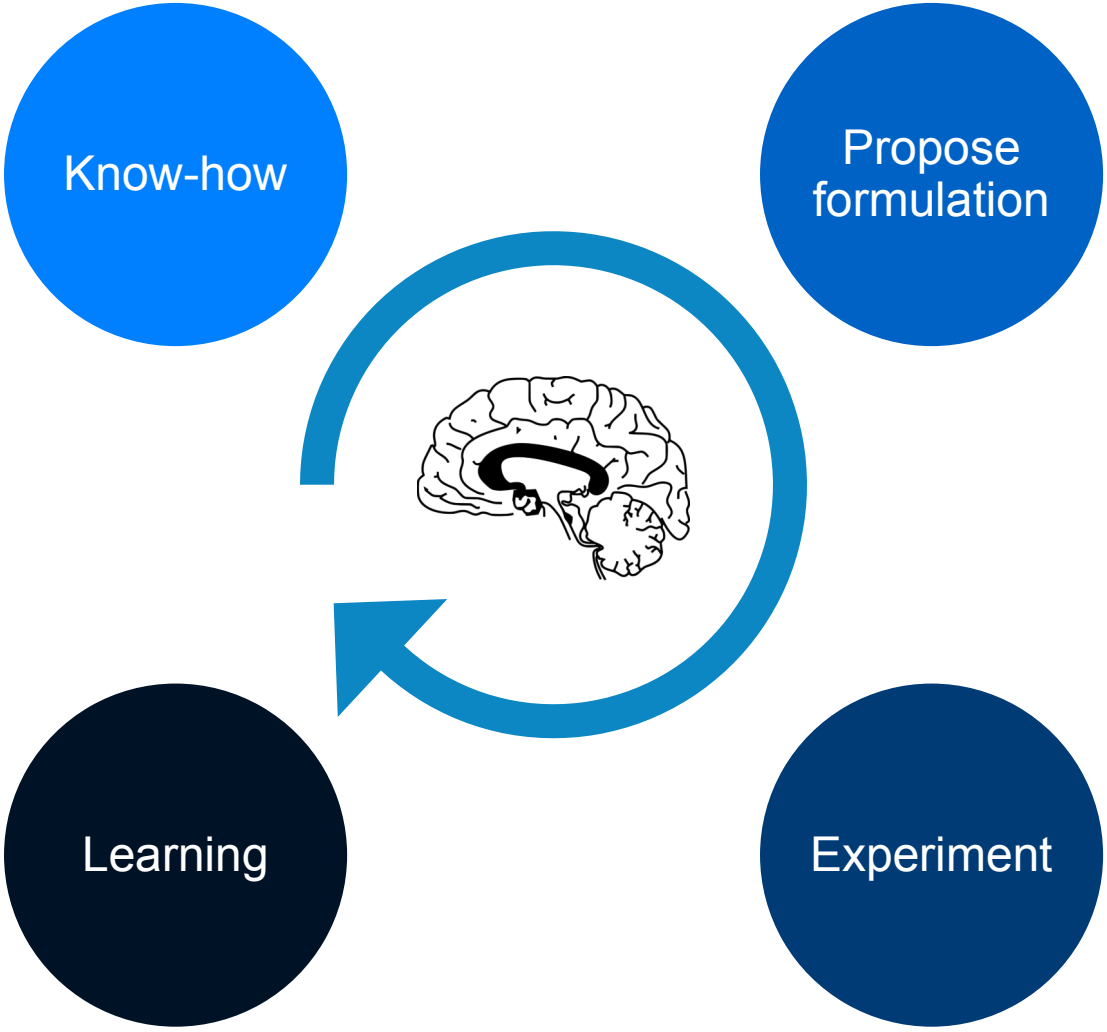
~15000 entries



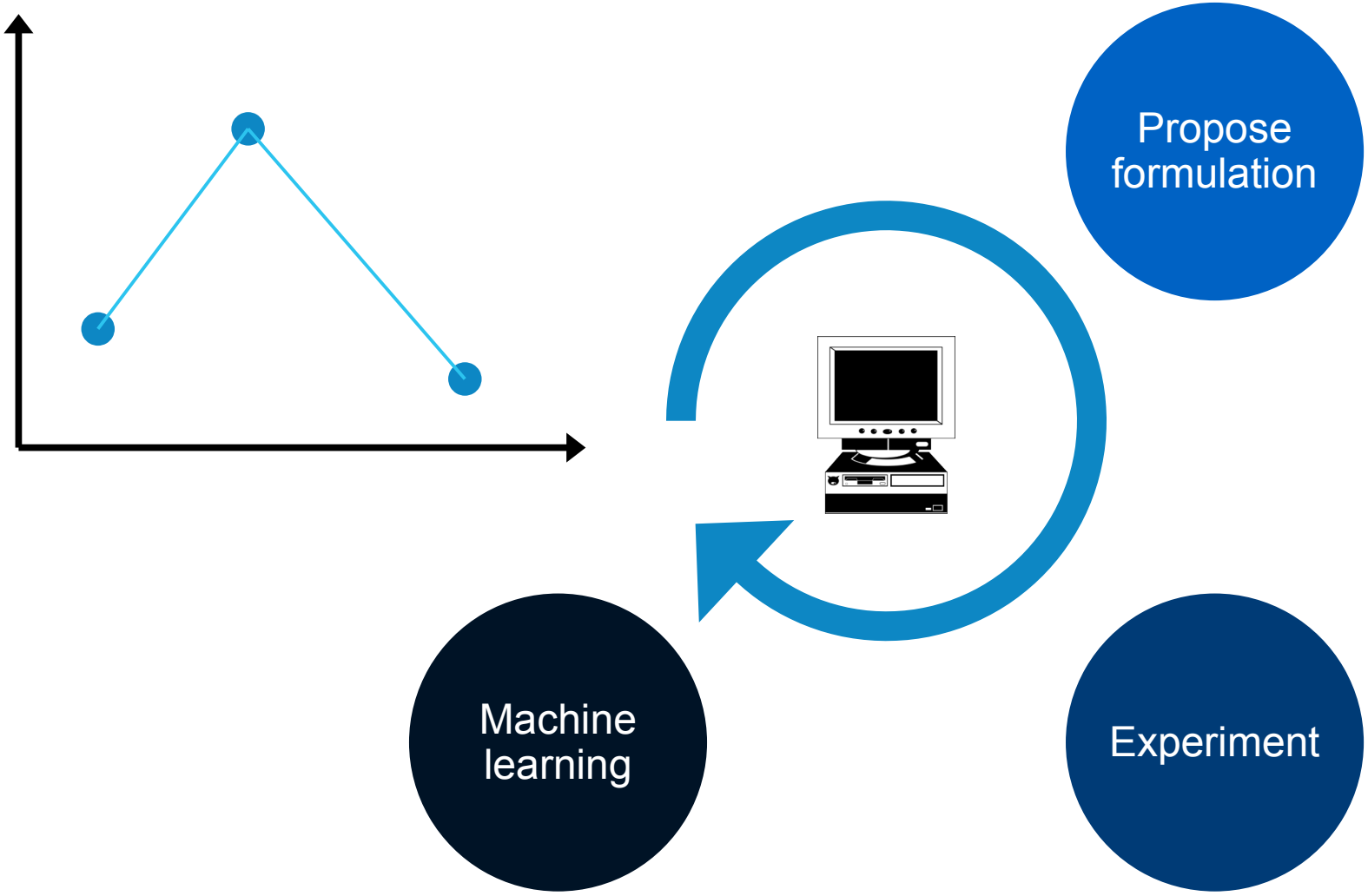
Output measurement normally monthly, but

- some batches still in progress
- some batches stopped (too bad results)
- inconsistent intervals (month 1, 2, 3, 6, 9)

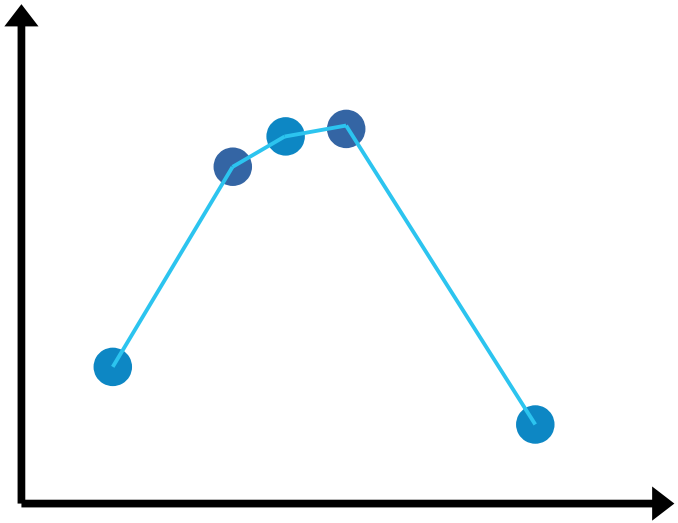
Contemporary approach to the formulation problem



Machine learning approach to the formulation problem



Machine learning approach to the formulation problem

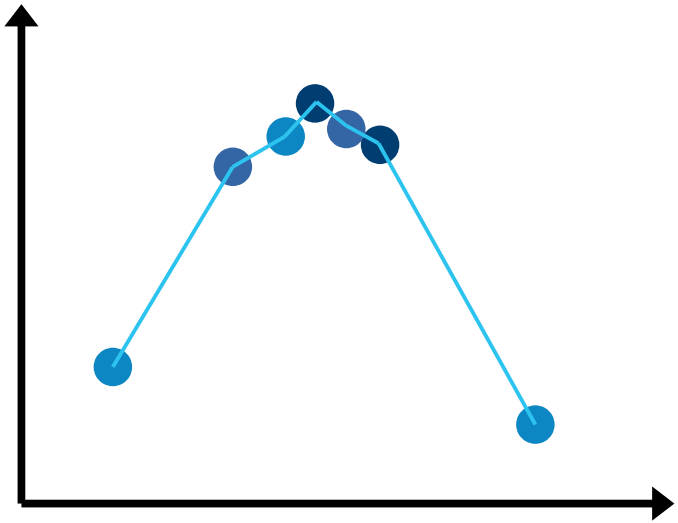


Propose formulation

Machine learning

Experiment

Machine learning approach to the formulation problem



Propose formulation

Machine learning

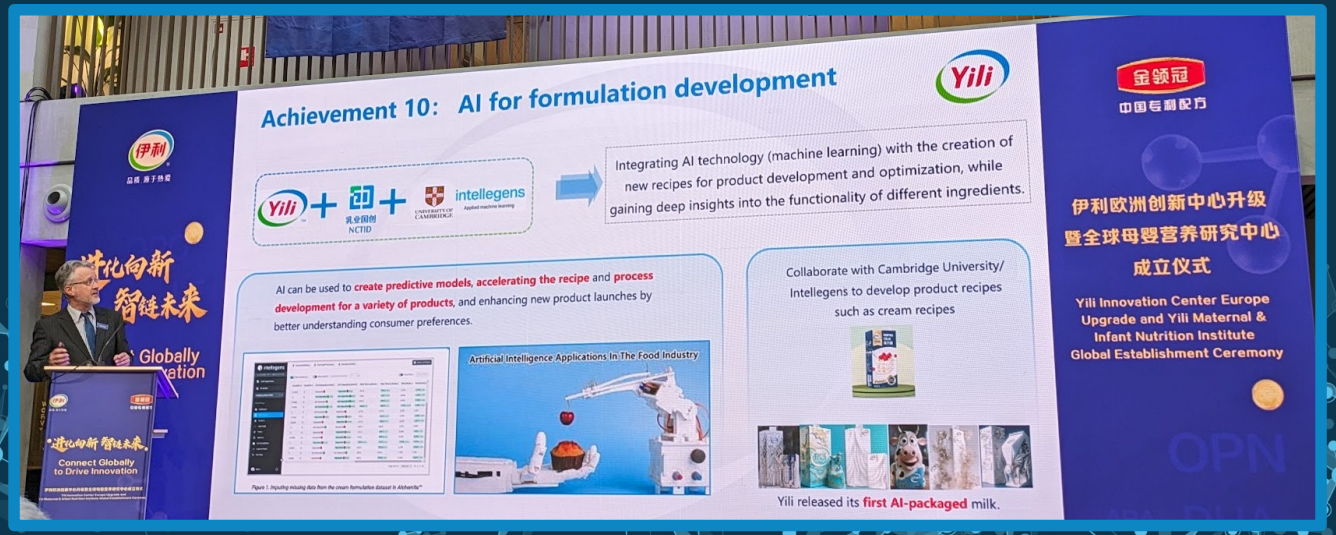
Experiment

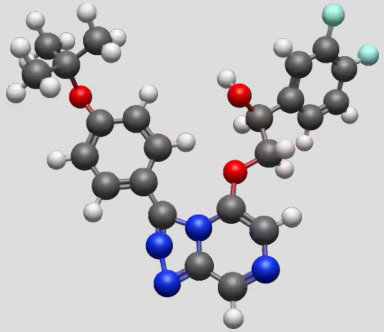
Alchemite™ design of experiments cut R&D time and cost at Yili

Determine important ingredients and process parameters

Mechanistic insights and (un-)expected cross correlations

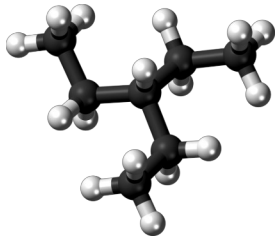
Webinar alongside Matthias Eisner on 13 December 2022





J. of Chem. Info. & Model. **60**, 2848 (2020)
Applied AI Letters **2**, e31 (2021)
Journal of Medicinal Chemistry **64**, 16450 (2021)
Molecular Pharmaceutics **19**, 1488 (2022)

Journal of Computer-Aided Molecular Design **35**, 112501140 (2021)

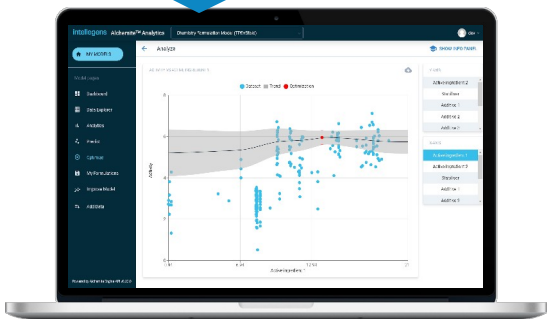


Fluid Phase Equilibria **501**, 112259 (2019)
Journal of Chemical Physics **153**, 014102 (2020)

Webinar and white paper (2023)

Intellegens offers the Alchemite™ product family

Scientists & engineers
Fast start, easy-to-use, visual



Option to deploy models

Data scientists
Add to your ML toolkit

Optional connectors

- *Lab systems*
- *Software & scripts*
- Sharing & collaboration

Alchemite™ Analytics

Deep data insights on your desktop
Guide experiments, predict, design, optimize

Alchemite™ Engine

Integrate into your workflow (API, Python)
Advanced configuration, enterprise deployment

Alchemite™ Success

Apply Intellegens deep learning expertise
Advice to your data science team or full project management

Alchemite™ design of experiments cuts R&D time and cost at Yili

Serves as template for data-driven development

Generic approach applied to many physical, chemical, and biological sciences