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# Alchemite™ Analytics

## Machine Learning for materials and chemicals discovery

## Why conventional AI falls short

AI is transforming the world but **conventional AI requires complete data to be available to train accurate models**. Traditional methods exist for managing experimental data; however, they result in discarding data and simple averaging techniques, resulting in models that are unreliable.

**90%**
reduction in experiments

**£10 million**
saved in R&D costs

**15 years**
of research saved

## Applications

- Alloys
- Predictive maintenance
- Drug Design
- Chemicals
- Batteries
- Rubber
- Polymers
- Composites
- Plastics
- Glass
- Food & beverage
- Manufacturing
- Process optimization
- Superalloys
- Construction chemicals
- Cosmetics
- Healthcare
- Oil and Gas

# Alchemite™ Engine

Historical experimental data provides a valuable resource for innovative companies to learn from and deliver improved future processes. **Alchemite™ is a suite of machine learning tools that allows for the simple aggregation of data that can be both sparse and noisy**, typical of experimental data, to generate deep learning models quickly and easily delivering predictive models that learn from all available data.

## Reduce costs

Reduce costs both in terms of the number of experiments that need to be performed and optimize experiments to minimize the need for expensive components or processes

## Validate data

Identify erroneous data and impute missing data with a level of accuracy

## Guide experiments

Model generated can be queried for the next best set of experiments in order to improve understanding of area

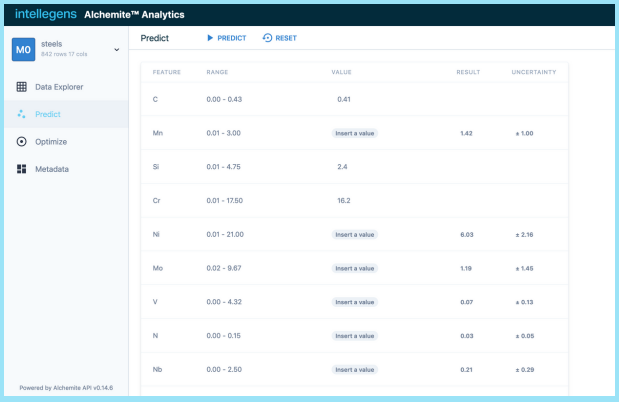
## Optimize formulations

Generate new formula with multiple target properties and understand the effect that altering each subset of ingredients will have

**Integrate the Alchemite™ Engine via an API into your existing software**

# Alchemite™ Analytics Platform

Easily build models to understand the accuracy of your predictions




Alchemite™ Analytics is an easy-to-use optimization tool with a user interface that enables experimentation, understanding and visualization of the implications of real-time process parameter modifications.

## Optimization tool

Obtain the operating and process parameters required to fulfill a target

## Predict mode

Predict missing properties from within your dataset

## Parameter modification

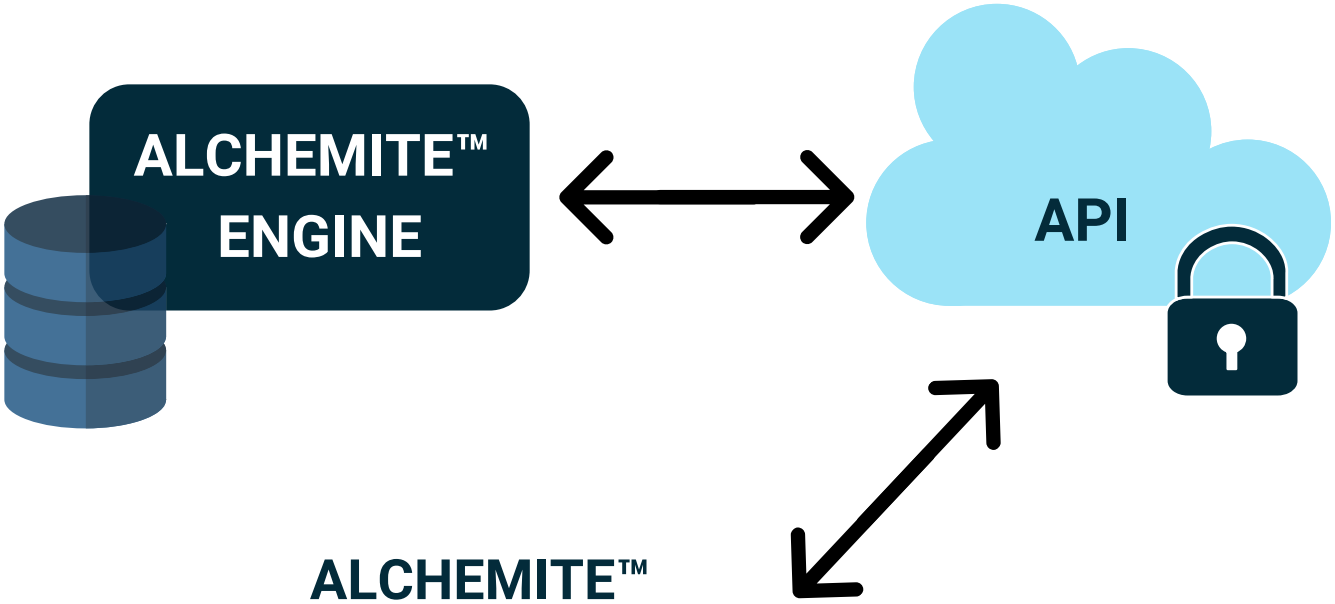
Take full control over all aspects and parameters of your experiments

## Validation

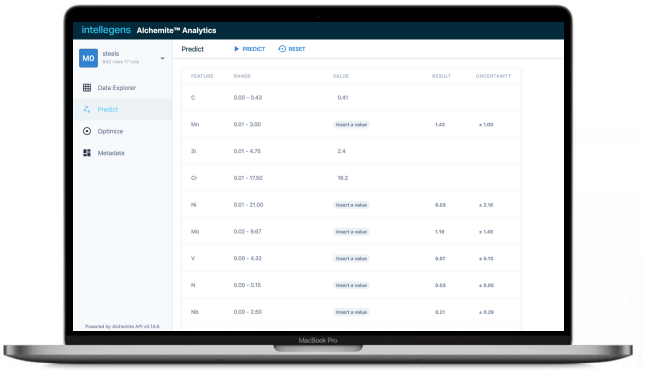
Check the accuracy and quality of data

## Virtual Experiments

Visualize the outcome of time-varying virtual experiments




## ALCHEMITE™ ANALYTICS




**Build models with your data using the Alchemite™ Engine via the well-documented API or the Alchemite™ Analytics platform to guide experiments and accelerate R&D**

# Case studies

## Additive Manufacturing

**Challenge:** To date, very few materials have been fully experimentally verified going through these processes, severely restricting the application of the technology to wider fields of use.

**Current approach:** Expert-led approach. Materials discovery is a long and iterative process.

**Solution:** Used historical welding data combined with the sparse data from direct laser deposition (an AM approach) to optimize this AM process and broaden its application to new processing variables, saving 15 years of research.

## Alloy steels

**Advantages**: Chromium makes steel corrosion resistant and hard

**Disadvantages:** Chromium is toxic, environmentally unfriendly, and expensive

**Challenge:** Design a new steel with the same physical properties but with less Chromium

**Current heuristic approach:** Industry experts, duplicate historic mixes

**Solution:** Tool to run "virtual experiments" to simulate low-chromium steels, whilst maintaining physical targets

## Drug discovery

**Challenge:** Available bioactivity data is sparse. For all the assay endpoints that are available, only a very small proportion of the possible compound-assay combinations have actually been measured in practice

**Current approach:** Traditional machine learning methods cannot directly utilize assay information as input because bioactivity data sets are often incomplete

**Solution:** The predictive accuracy of Alchemite outperforms the leading approaches and uses just 20% of computing resource

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Want to learn more about how our AI technology can be applied to your specific needs? Contact us at info@intellegens.ai

## About Intellegens

Intellegens has developed a unique artificial intelligence engine, Alchemite™ for training neural networks from incomplete, sparse, and noisy data, typical of real-world data. The technique was first developed at the University of Cambridge where it has been used to develop several superalloys, guide the design of new drugs and help optimise battery pack design. The tool is now being used to solve a wide range of real world industrial process problems where rare but valuable data can be used to improve real world industrial processes leading to reduced costs and environmental impact. For more information, please visit intellegens.ai.

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