intellegens

DATA - DRIVEN DISCOVERY

7 examples of how materials & chemicals companies innovate using Alchemite machine learning

1. Alloys in aerospace
2. Batteries
3. Antimalarial drug discovery
4. 3D printing
5. Data validation
6. Forging hammers
7. Alkanes for lubricants

Alloys in aerospace

Challenge

Alloys must have good performance at **high temperatures**

Commercial superalloys do not have the **optimal balance of properties**

Long and **iterative** research and development process is expensive

Solution

Machine learning tool **Alchemite**

Augment **experimental data** with **thermodynamic predictions**

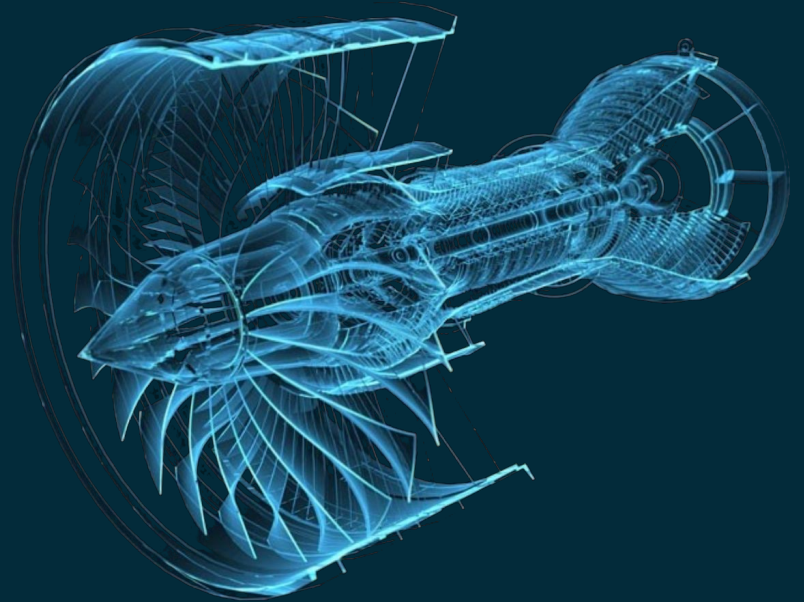Incorporate **uncertainty** to design alloys with the highest likelihood to **meet design targets**

Outcome

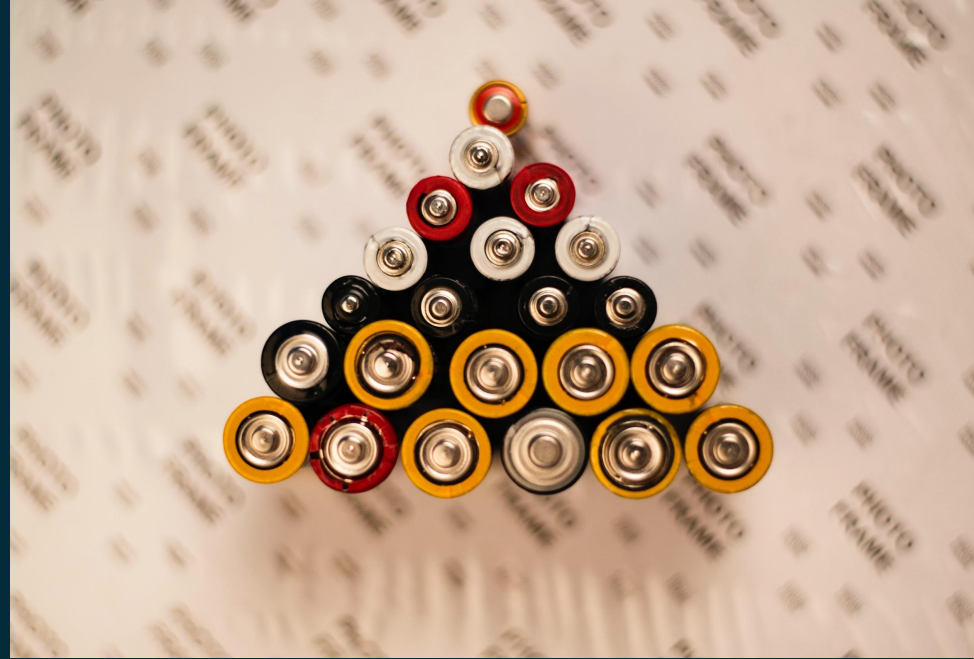New nickel-base superalloy
that met **11** targets

Properties were
experimentally verified

Reduced development **cost**
by £10m

Batteries

Challenge

Performance, cost, and safety of batteries will drive the development of **electric vehicles**

Materials and **battery management** system can both be improved by machine learning

Further research into battery chemistries requires **more complicated** battery dynamics

Solution

Machine learning to design the **cathode**, **anode**, and **electrolyte**

Predictive models for **battery management** systems to alleviate range anxiety

Outcome

Ran virtual experiments to **focus the search** for new materials

Reduced development and fabrication **costs** while improving key battery metrics

Predict remaining useful life, state of health, and state of charge

Antimalarial drug discovery

Challenge

Identify a new molecule against a novel **antimalarial** mechanism of action

Available data covers multiple assays, but only a **small fraction** have been measured

Solution

In blind test Alchemite **accurately predicted** activity of compounds against novel mechanisms of action
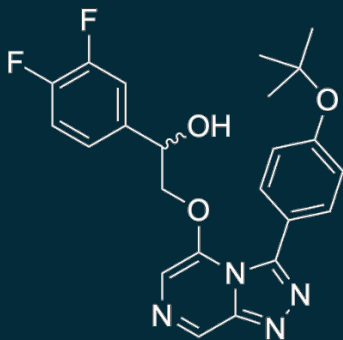
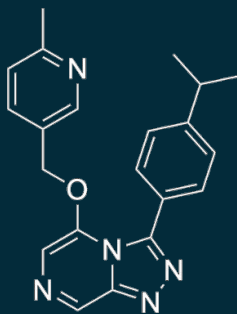**Outperforms** conventional QSAR and other machine learning models

Outcome

Alchemite confidently predicted a compound generated automatically by Optibrium's StarDrop™ software
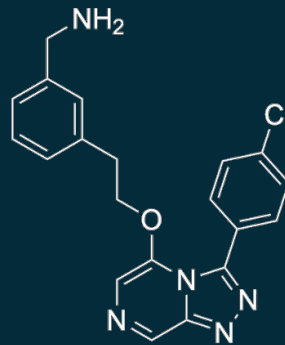
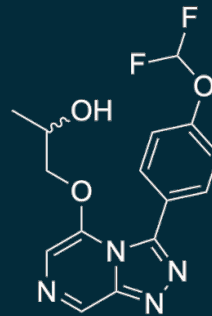Compound synthesised and tested by OSM group, only entry that demonstrated **potency against the target**
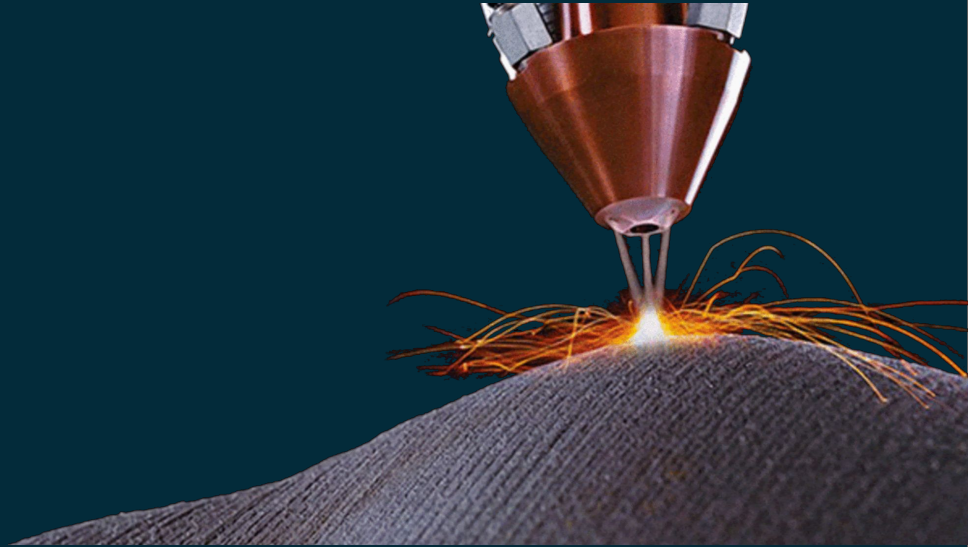

Optibrium/Intellegens
0.647 µM

Davy Guan
>25 µM

Exscientia
10.9 µM

Molomics
>25 µM

3D printing

Challenge

Additive manufacturing is a **new process** that requires **new materials**

Ability to print materials is **poorly understood**

Direct laser deposition (a 3D printing method) has only been applied to **ten** nickel alloys

Solution

Alchemite exploited **property-property** relationships to capture of new insights

Juxtaposed historical **welding** and sparse **direct laser deposition** data

Optimized alloy for direct laser deposition and also fulfil other target properties
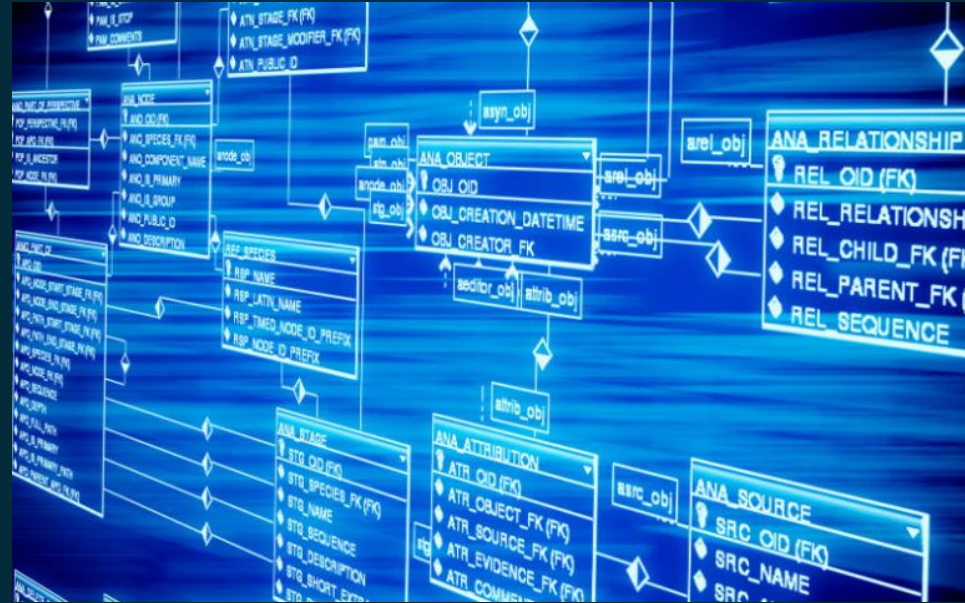
Outcome

Alloy for direct laser deposition **experimentally verified**

Alchemite **saved 15 years** worth of development

Data validation

Challenge

Companies that sell curated databases must have efficiently **identified** and **fixed** all erroneous entries

Errors in central database misguides research programs and will lead to **inaccurate** machine learning

Triage data introduced to a central database

Solution

Alchemite models all available data

Automatically identifies **unexpected** values to **focus attention** where additional investigation is most effective

Outcome

Identified errors including typos, errors, or genuine outliers

Automate tool to **triage** submitted data

Forging hammers

Challenge

Forging hammers wear and degrade through repeated use, can they be made more durable?

Machine learning explores **new alloys** to improve strength at elevated temperature

Solution

Augment **experimental data** with **thermodynamic models**

Incorporate **uncertainty** to propose molybdenum-base alloys with the highest likelihood to meet **design targets**

Alchemite suggests new precipitate chemistry with improved properties
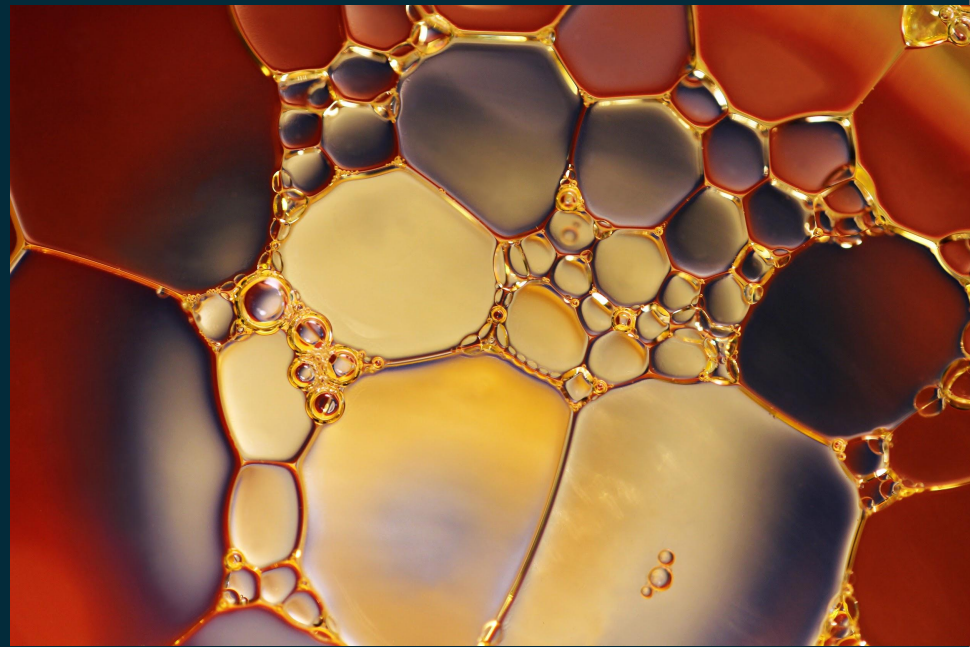
Outcome

New molybdenum-base alloys found with **5-fold** reduction in experimental time and cost

Improve molybdenum-base hammers **lifetime by 30%**, reducing deployment cost and factory downtime

# Alkanes for lubricants

Challenge

Lubricants need to be optimized for new applications such as electric vehicles

Lubricants contain **hydrocarbon** molecules

Predicting the properties of hydrocarbons facilitates the development of base oils

Solution

Exploit **property-property** correlations augmented by computer simulations to predict physical properties
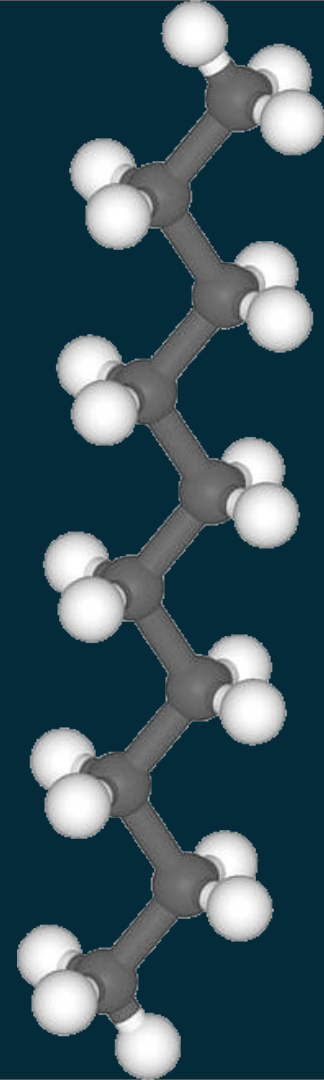
Outcome

Alchemite accelerated the identification of optimal hydrocarbons **tenfold**

Alchemite estimated intractable properties including **shear viscosity** five-times more accurately than other methods

Summary

Alchemite adds value to **sparse** data problems by exploiting **property-property** correlations

Juxtapose results from **different methods**

Significant saving in **reduced cost** and **accelerated** discovery

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