UNIVERSITY OF CAMBRIDGE

The modern-day blacksmith

Gareth Conduit

Machine learning to

Model datasets where the data is sparse

Exploit property-property relationships

Merge data, computer simulations, and physical laws

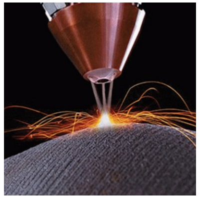
Reduce costly experiments to accelerate discovery

Black box machine learning for materials design

Composition

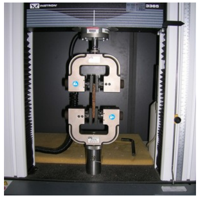
Properties

Defects

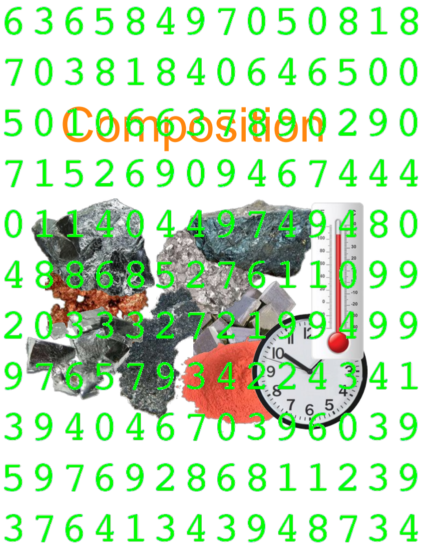


Fatigue

Strength



Train the machine learning

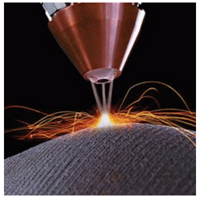


Machine learning predicts material properties

Composition

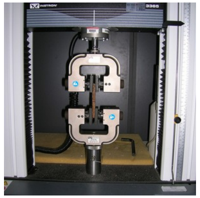
Properties

Defects

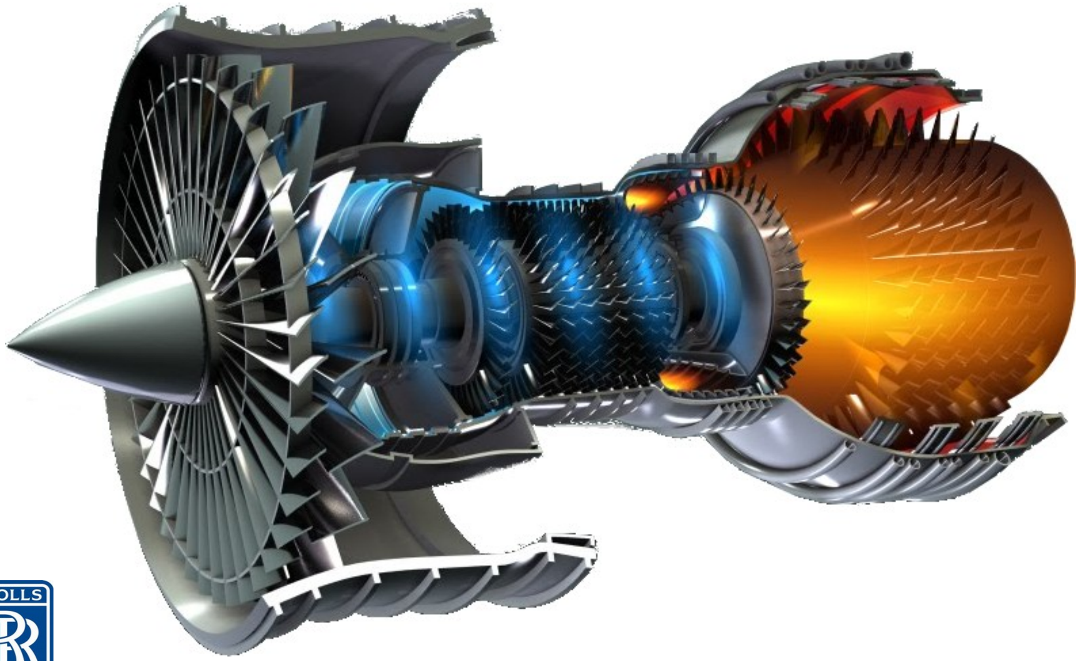


Fatigue

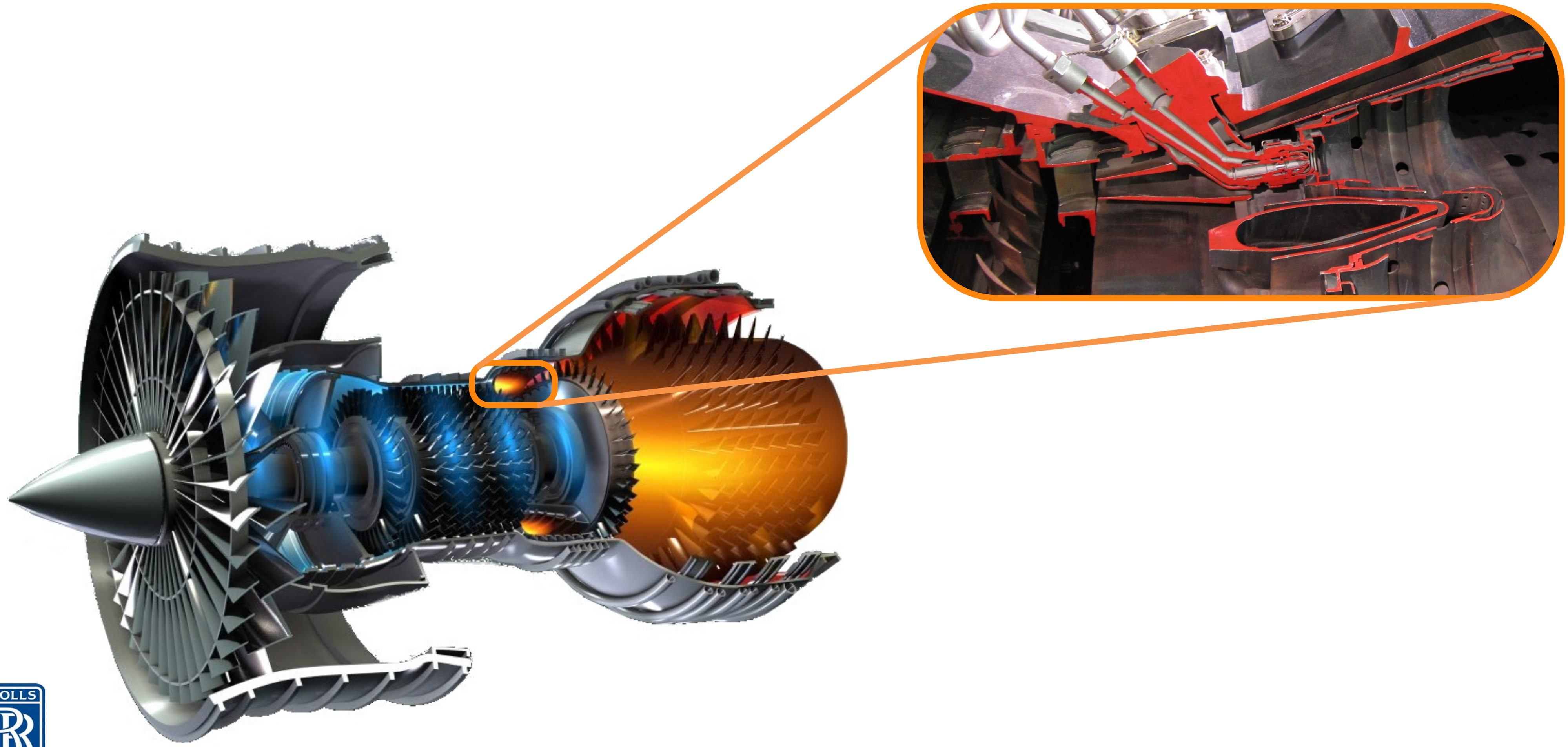
Strength



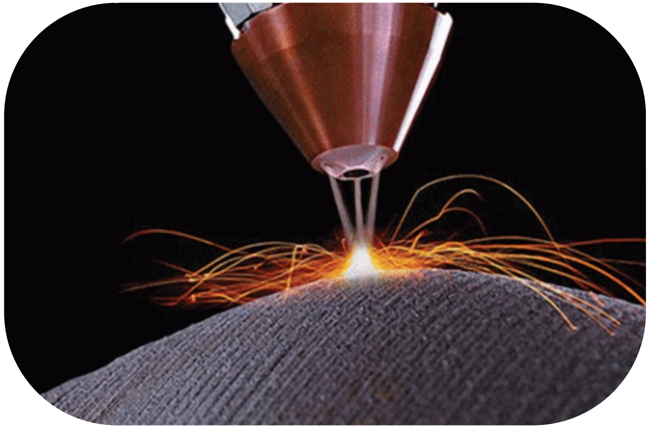
Jet engine schematic



Combustor in a jet engine

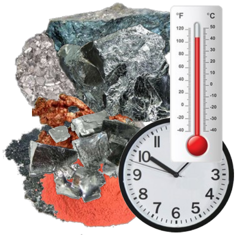


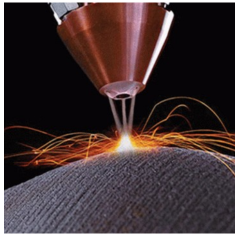
Direct laser deposition



Data available to model defect density

10 entries



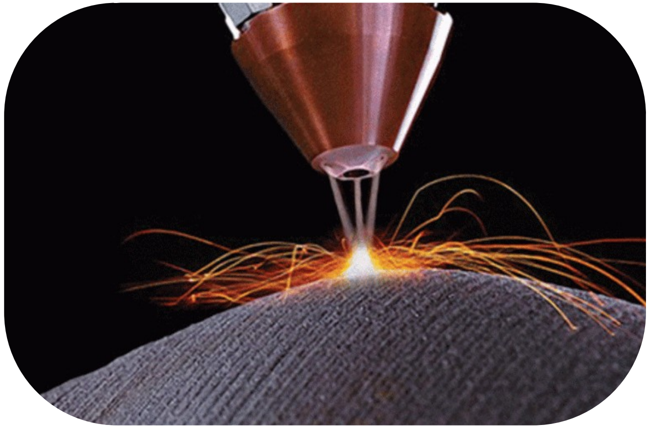


Composition and heat treatment space 30 dimensions

Requires 31 points to fit a hyperplane

Just 10 data entries available to model defect density

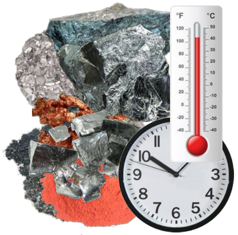
Ability for printing and welding are strongly correlated



Laser

Electricity

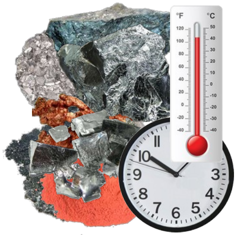
First predict weldability



1000 entries

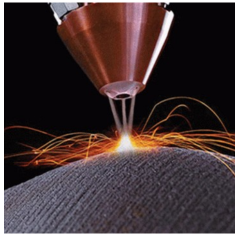
Use 1000 weldability entries to understand complex composition → weldability model

Use weldability to predict defects formed



1000 entries

10 entries

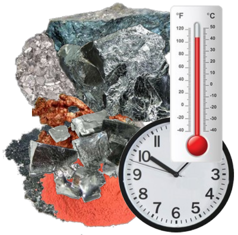


Use 1000 weldability entries to understand complex composition → weldability model

10 defects entries capture the simple weldability → defect relationship

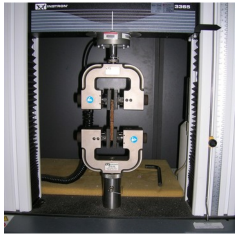
Two interpolations aid composition → defects extrapolation

Use CALPHAD to predict strength



100,000 entries

500 entries



Use 100,000 CALPHAD results to model complex composition → phase behavior

500 strength entries capture the phase behavior → strength relationship

Two interpolations aid the composition → strength extrapolation

Target properties

Elemental cost	< 25 $\$kg^{-1}$
Density	< 8500 kgm^{-3}
γ' content	< 25 wt%
Oxidation resistance	< 0.3 $mgcm^{-2}$
Defects	< 0.15% defects
Phase stability	> 99.0 wt%
γ' solvus	> 1000˚C
Thermal resistance	> 0.04 $K\Omega^{-1}m^{-3}$
Yield stress at 900˚C	> 200 MPa
Tensile strength at 900˚C	> 300 MPa
Tensile elongation at 700˚C	> 8%
1000hr stress rupture at 800˚C	> 100 MPa
Fatigue life at 500 MPa, 700˚C	> 10^5 cycles

Composition and processing variables

Cr 19%

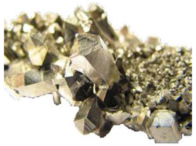
Co 4%

Mo 4.9%

W 1.2%

Zr 0.05%

Nb 3%



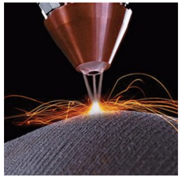
Al 2.9%

C 0.04%

B 0.01%

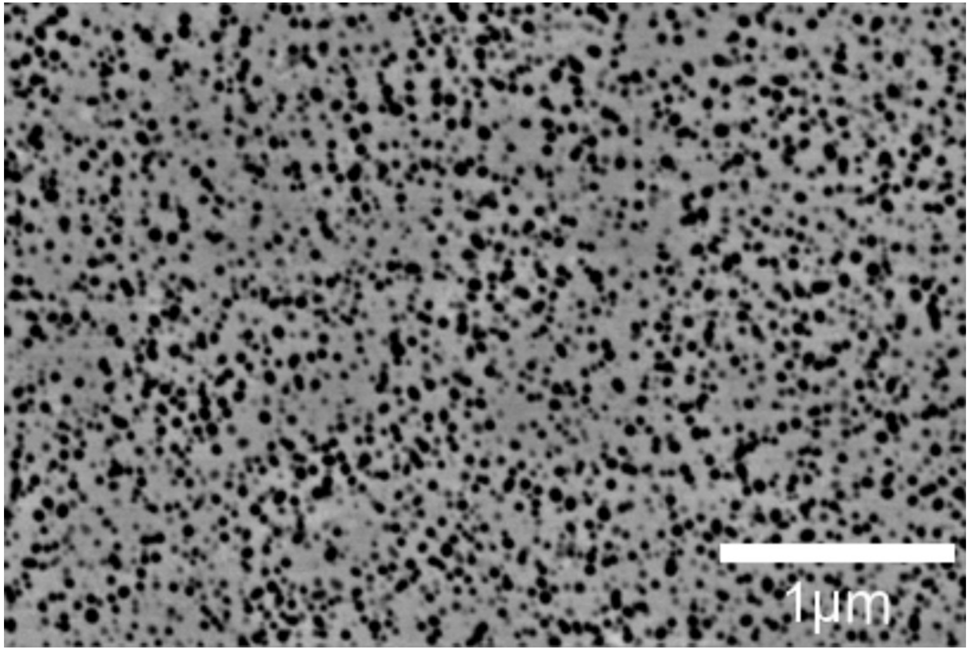
Ni

Expose 0.8

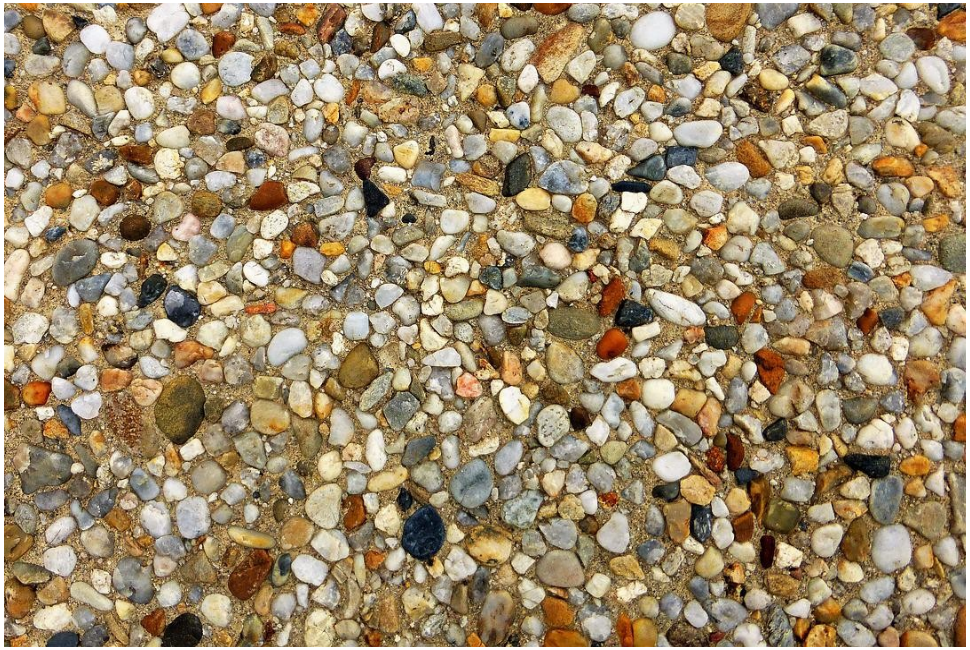


T_{HT} 1300ºC

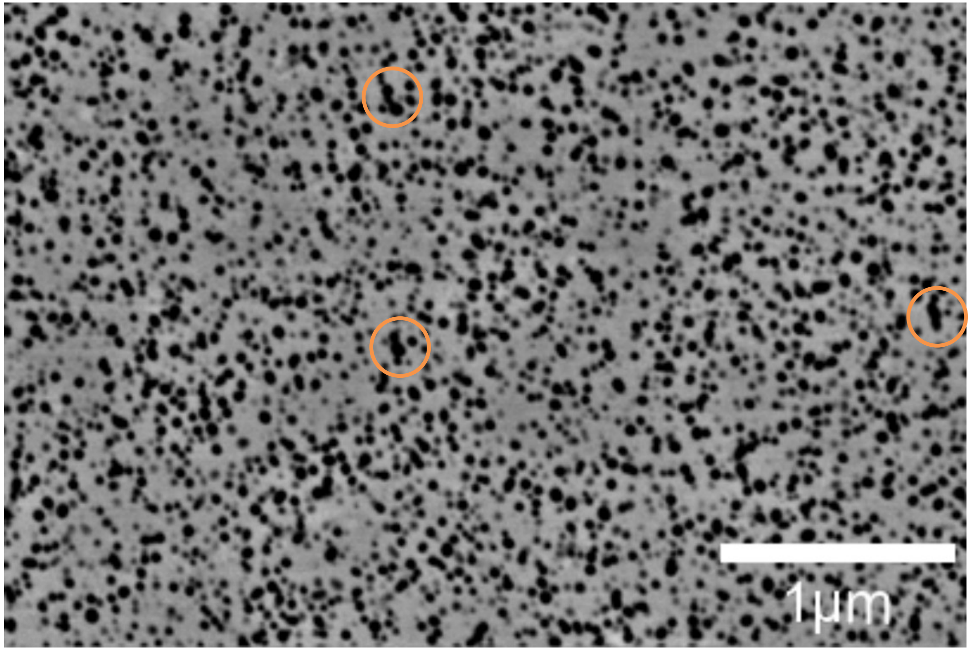
Microstructure



Concrete



Microstructure



Defects target

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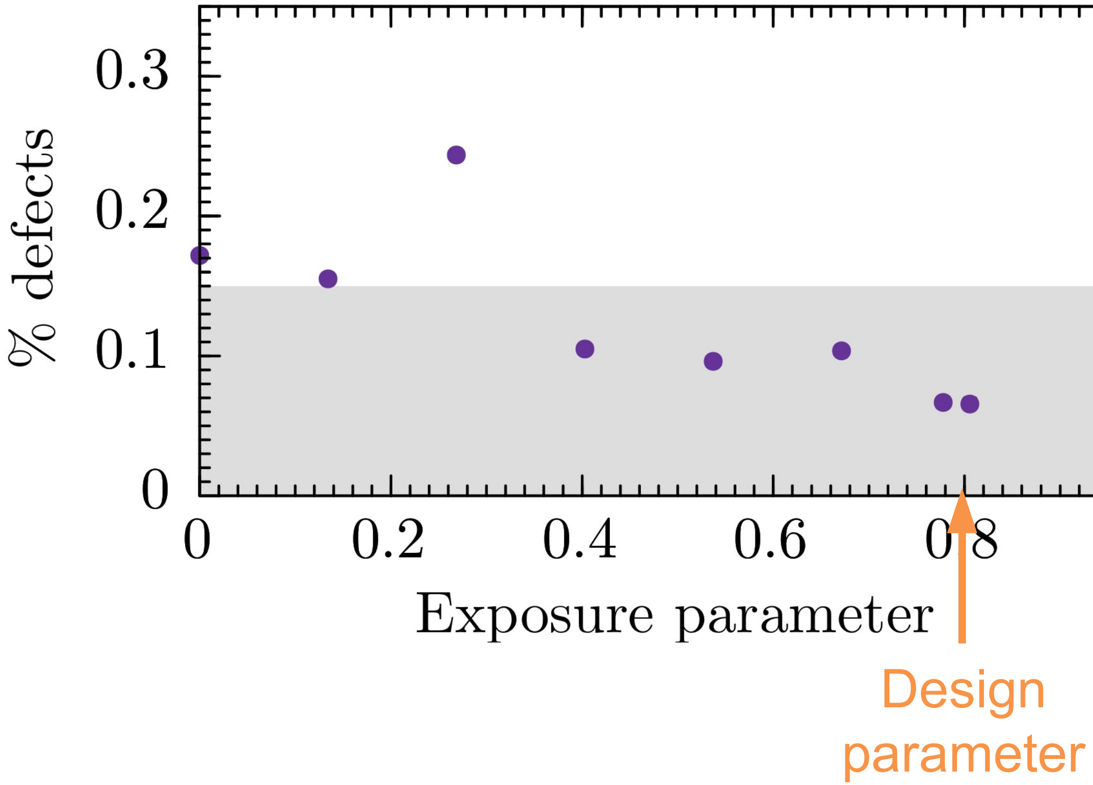
Testing the defect density



Probabilistic neural network identification of an alloy for direct laser deposition
Materials & Design 168, 107644 (2019)

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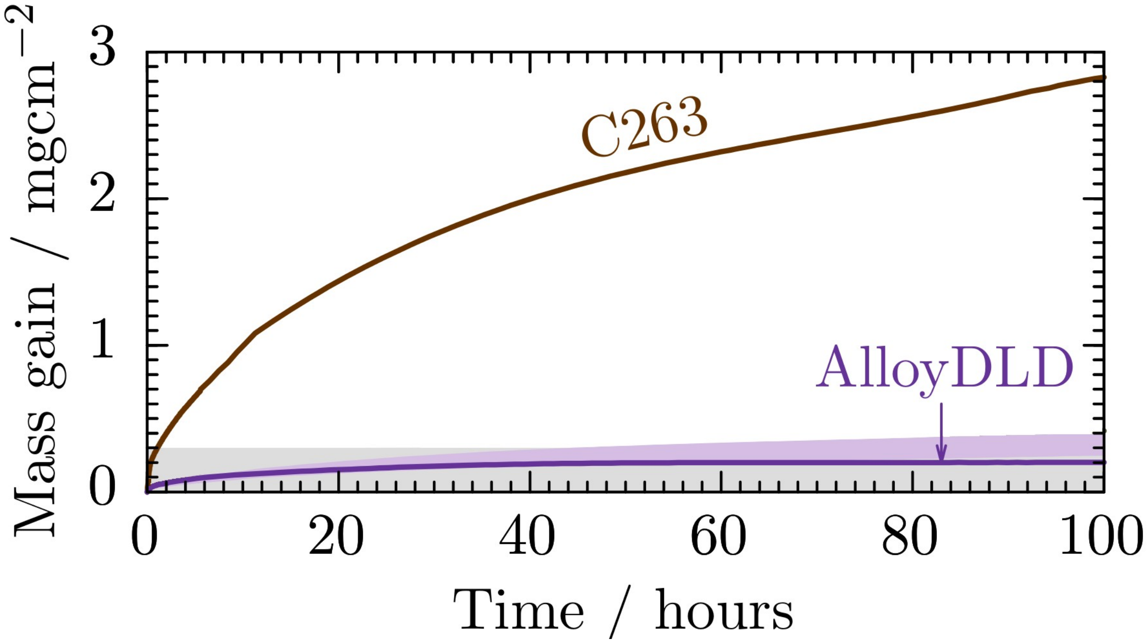
Testing the oxidation resistance



Probabilistic neural network identification of an alloy for direct laser deposition
Materials & Design 168, 107644 (2019)

DOMINO

optibrium

iff

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

The University Of Sheffield. AMRC Advanced Manufacturing Research Centre

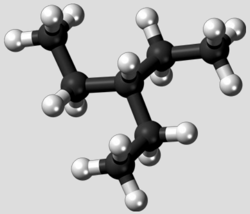
BOEING

Agency for Science, Technology and Research

SINGAPORE

NASA

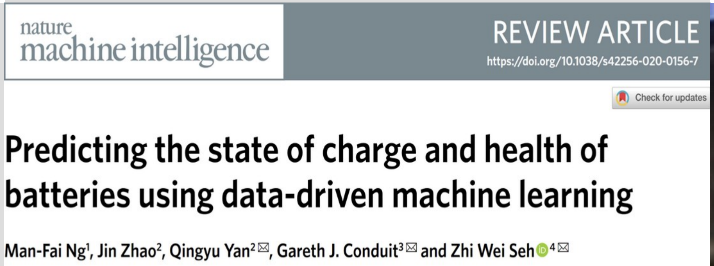
ROLLS ROYCE



Fluid Phase Equilibria
501, 112259 (2019)

Journal of Chemical Physics
153, 014102 (2020)

bp


nature machine intelligence

REVIEW ARTICLE

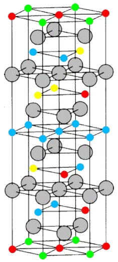
https://doi.org/10.1038/s42256-020-0156-7

Check for updates

Predicting the state of charge and health of batteries using data-driven machine learning

Man-Fai Ng[1], Jin Zhao[2], Qingyu Yan[2], Gareth J. Conduit[3] and Zhi Wei Seh[4]

SAMSUNG



Johnson Matthey
Technology Review
66, 130 (2022)

JM

Development of methodology

2013

Multiple properties for Rolls Royce engines

Development of methodology

2013	2014
Multiple properties for Rolls Royce engines	Property-property correlations with Rolls Royce and BP

Development of methodology

Concurrent materials design

2013	2014	2015
Multiple properties for Rolls Royce engines	Property-property correlations with Rolls Royce and BP	Royal Society University Research Fellowship

Development of methodology

Concurrent materials design

2013	2014	2015	2016
Multiple properties for Rolls Royce engines	Property-property correlations with Rolls Royce and BP	Royal Society University Research Fellowship	Experiment-simulation correlations with Samsung Electronics

Development of methodology

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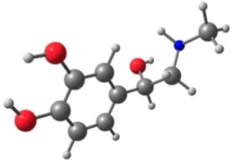
2015

Royal Society University Research Fellowship

2016

Experiment-simulation correlations with Samsung Electronics



2017

Drug discovery study with etherapeutics

Development of methodology

ROLLS ROYCE

ROLLS ROYCE bp

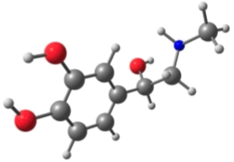
THE ROYAL SOCIETY

Concurrent materials design

UNIVERSITY OF CAMBRIDGE

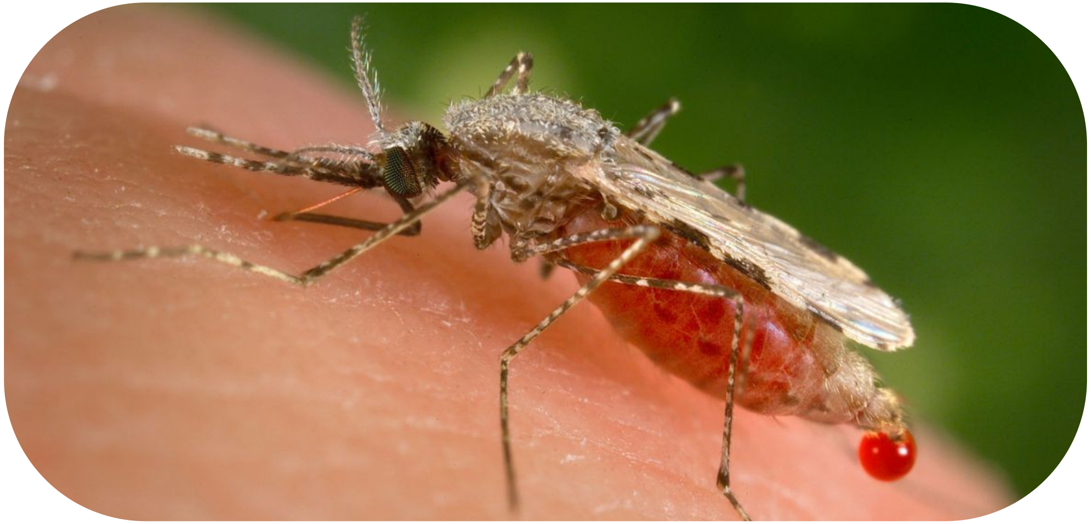
SAMSUNG

therapeutics



2013	2014	2015	2016	2017	2018
Multiple properties for Rolls Royce engines	Property-property correlations with Rolls Royce and BP	Royal Society University Research Fellowship	Experiment-simulation correlations with Samsung Electronics	Drug discovery study with etherapeutics	Founding of Intellegens

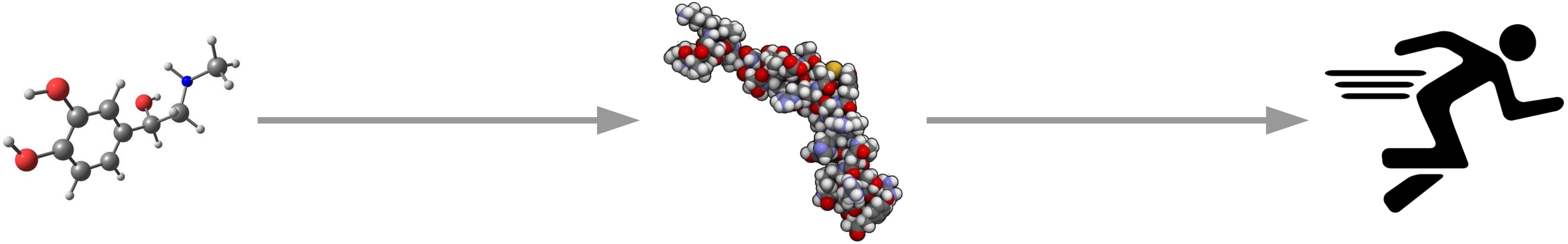
Open Source Malaria contest



OPEN SOURCE MALARIA

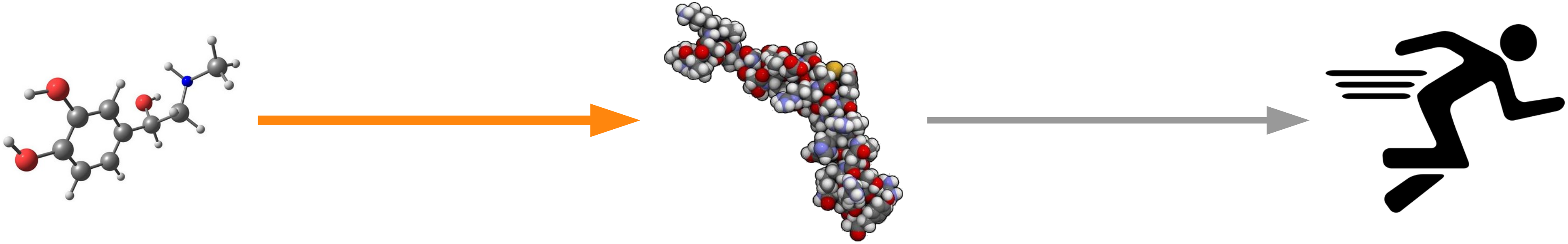
Looking for New Medicines

Action of a drug



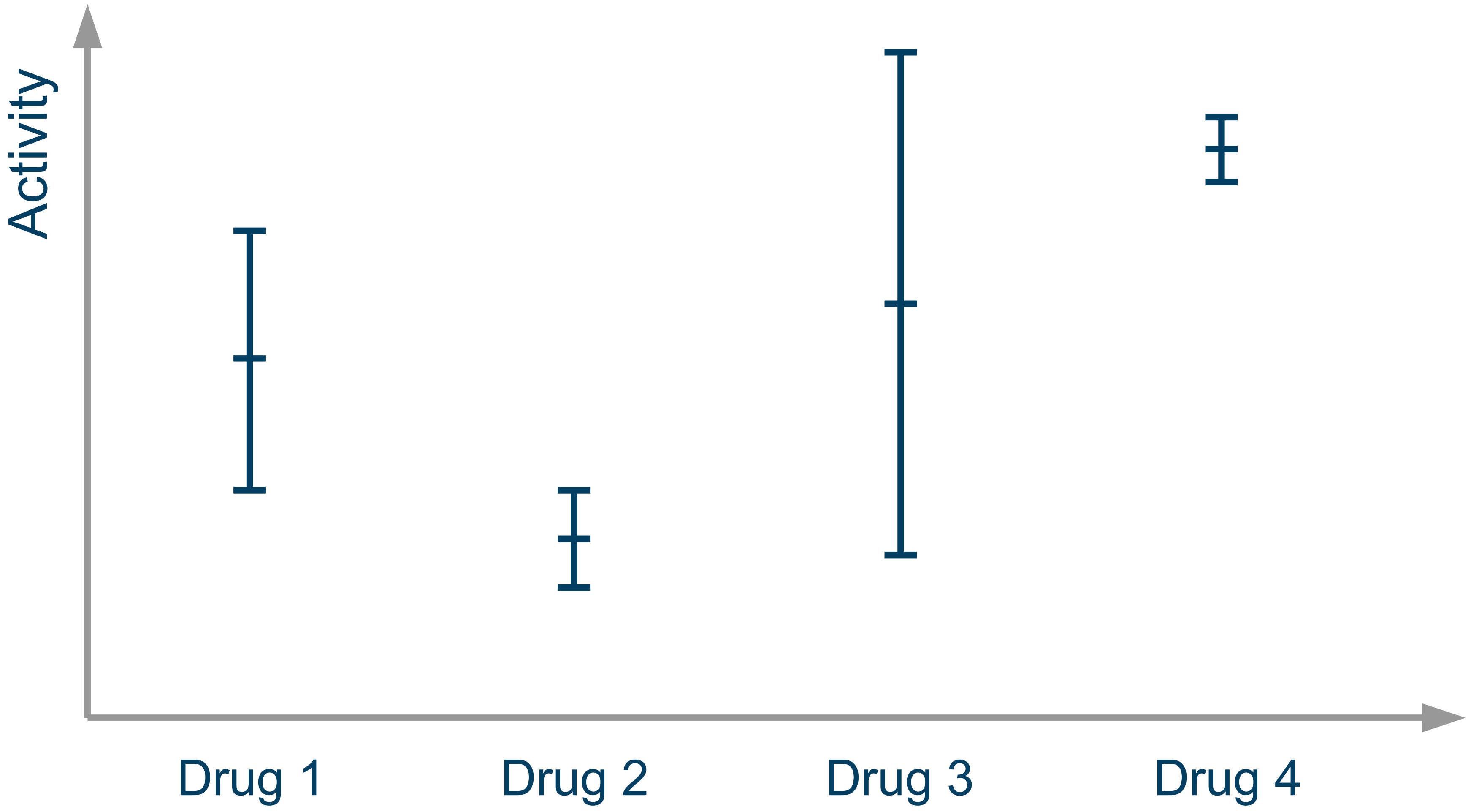
Drug   Protein   Effect

Action of a drug

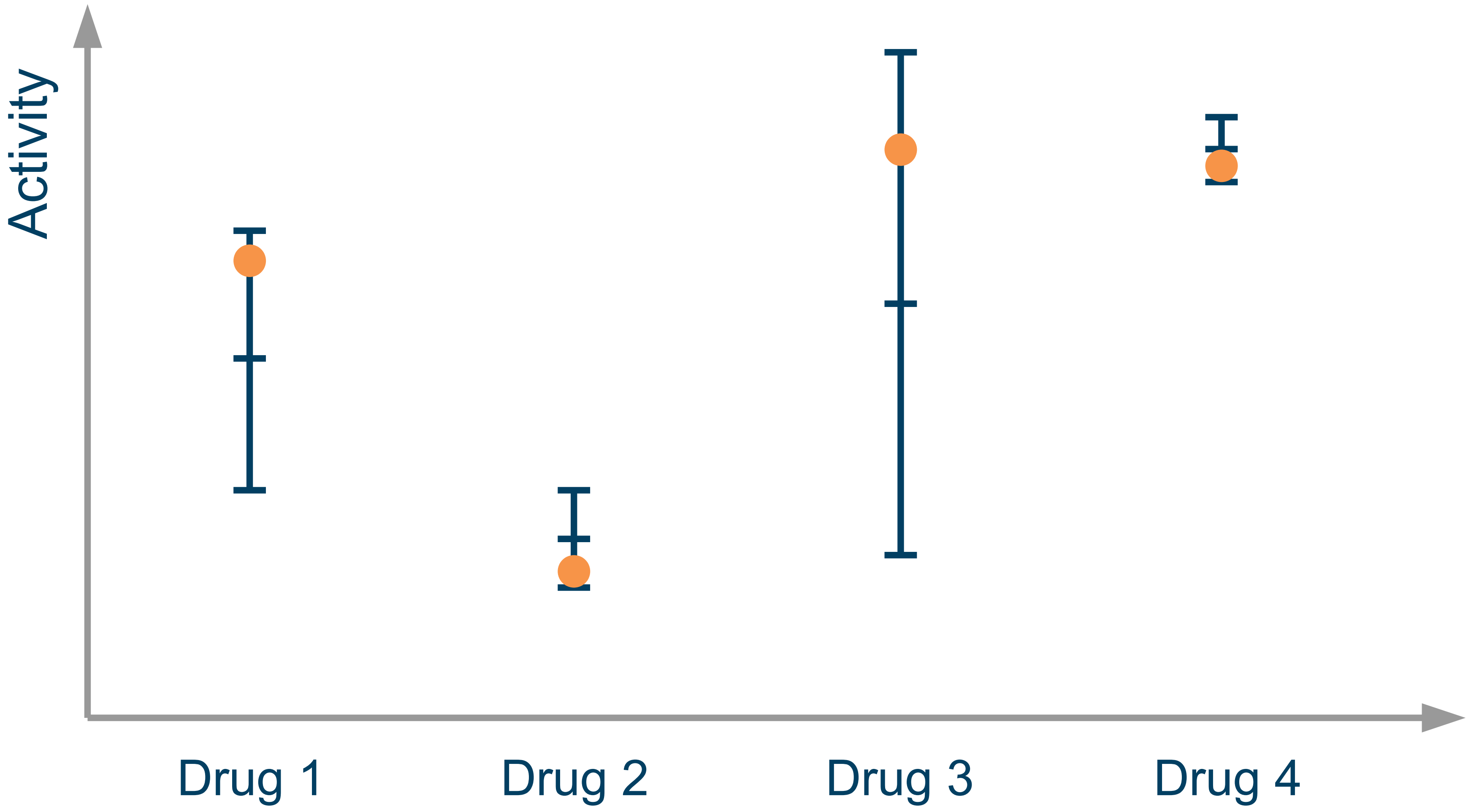


Drug Protein Effect

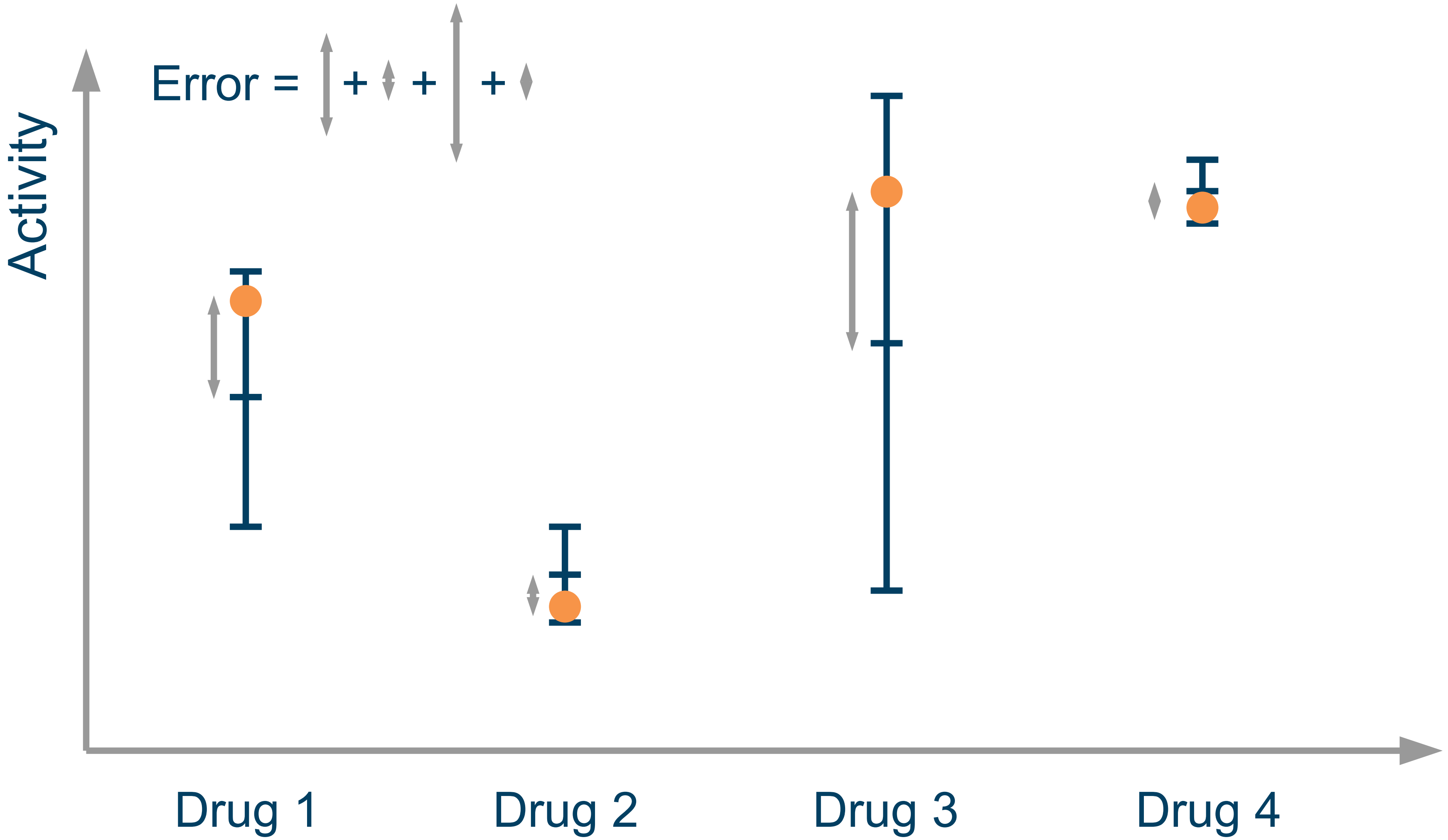
Predictions have an uncertainty



Validation data typically within one standard deviation

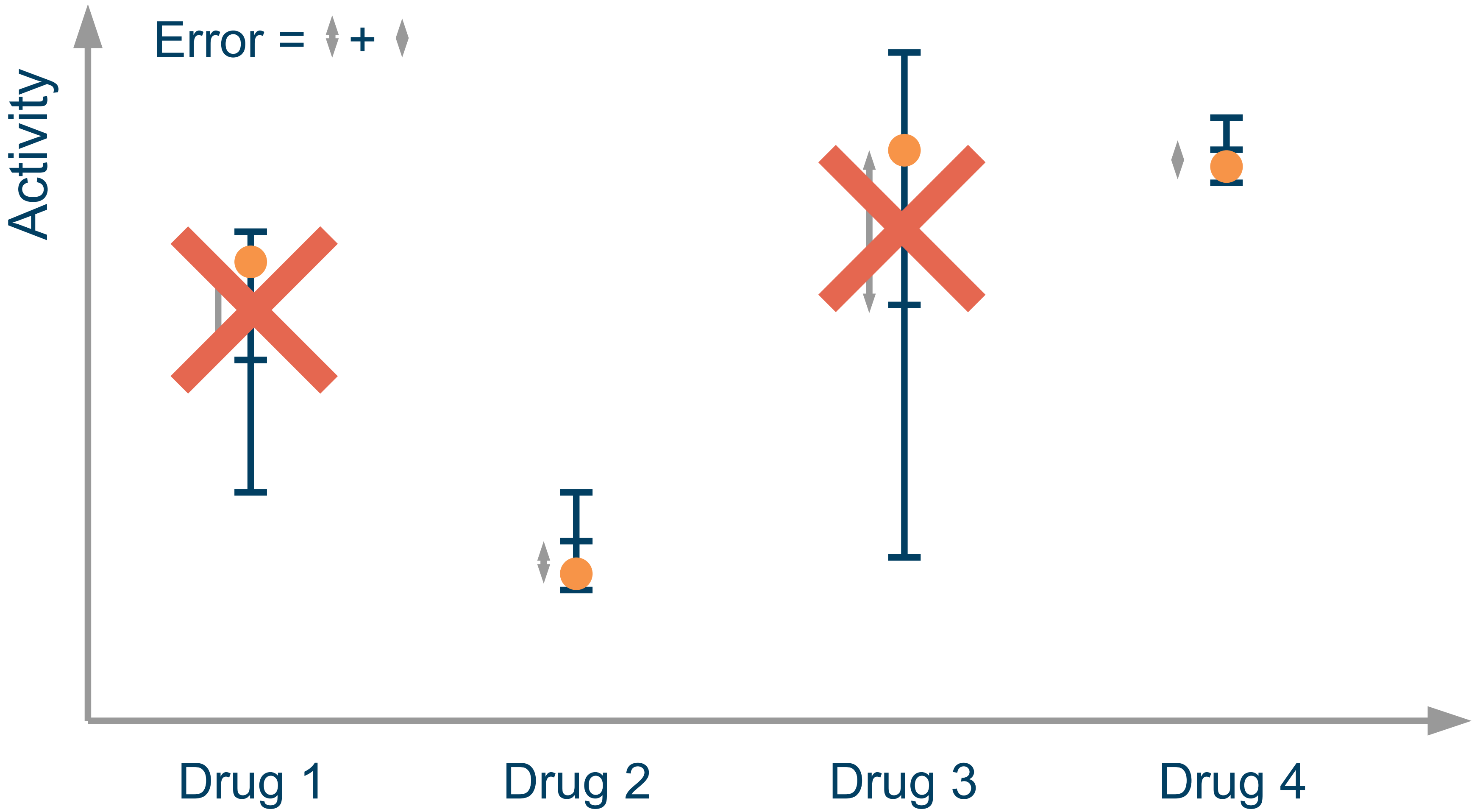


R^2 metric calculated with difference from mean

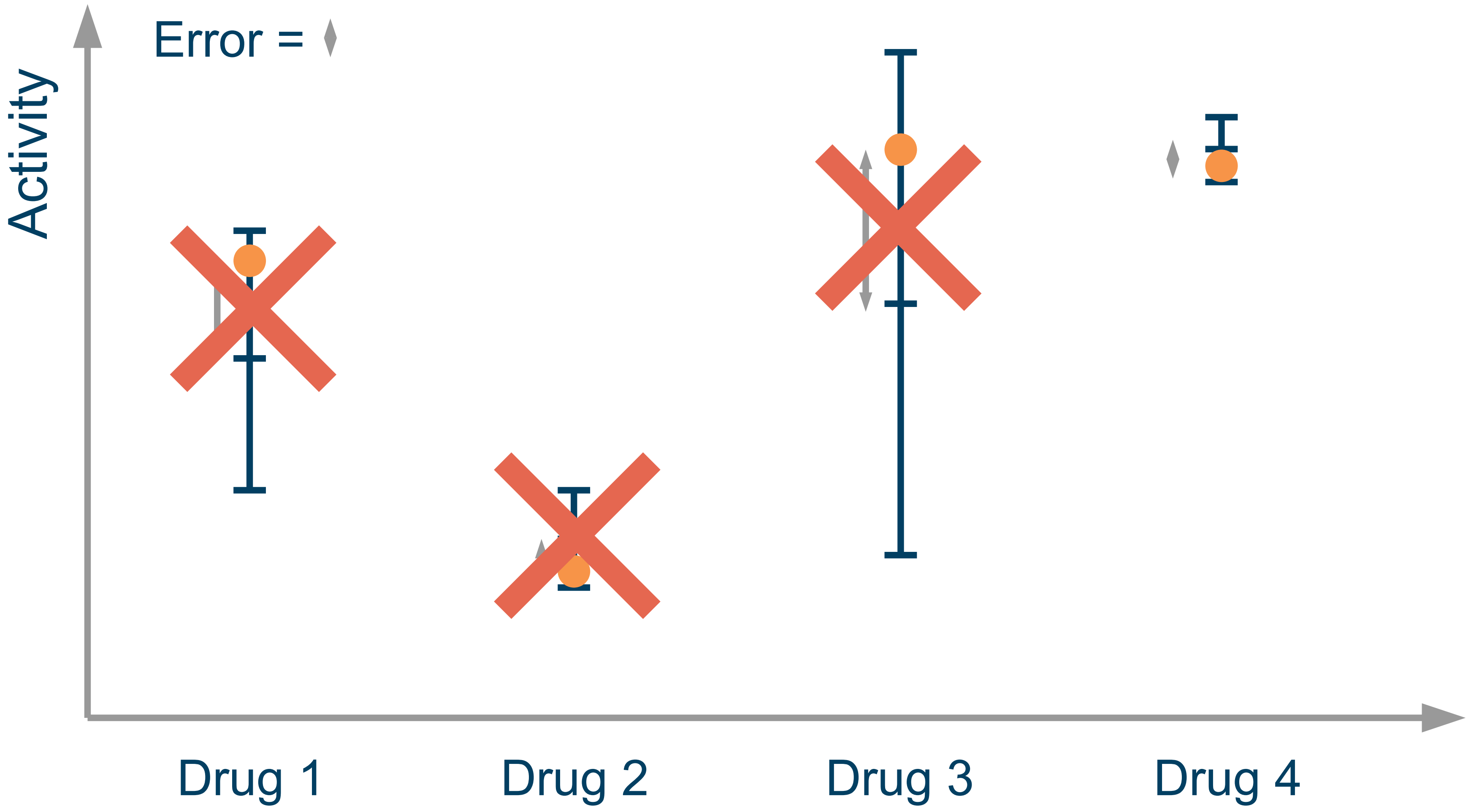


Impute 75% of data with smallest uncertainty

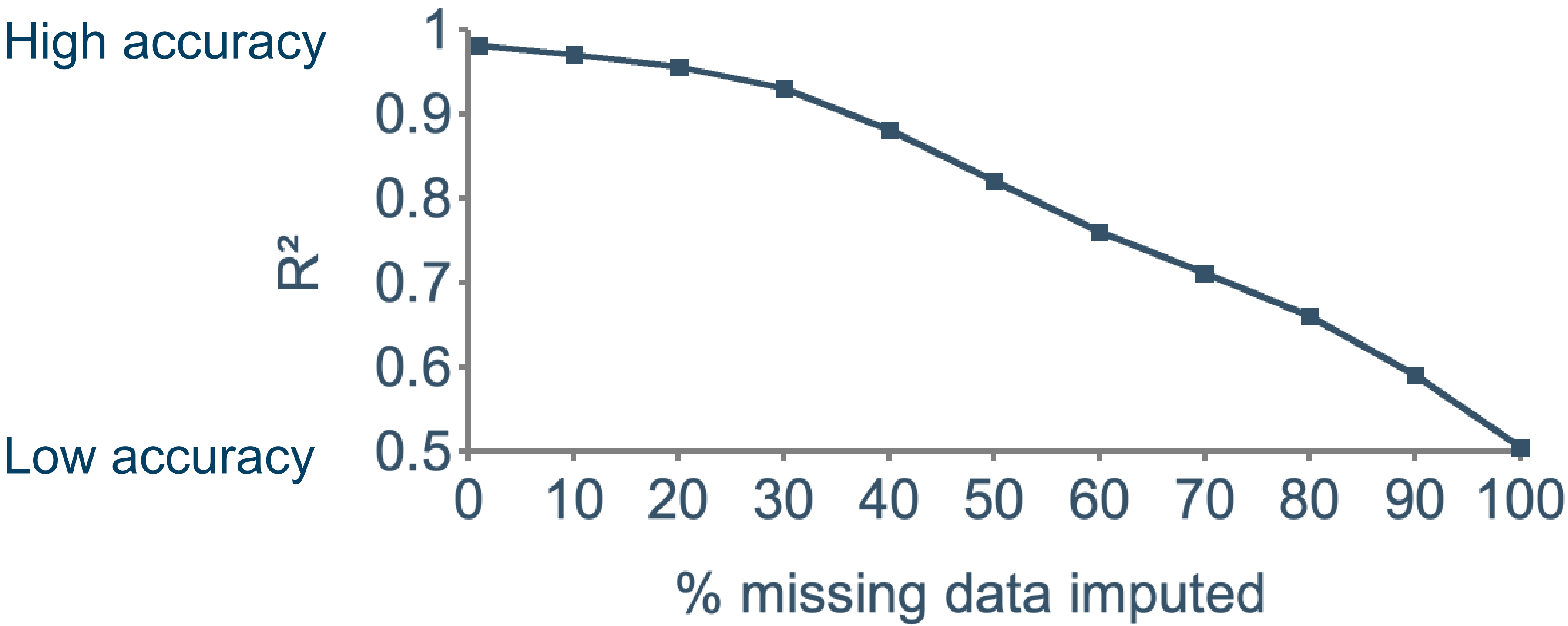
Impute 50% of data with smallest uncertainty



Impute 25% of data with smallest uncertainty



Improved performance by exploiting uncertainty



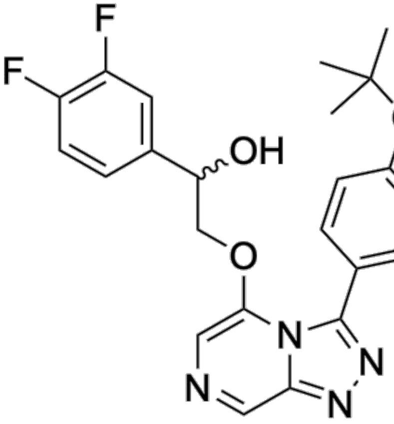
Different drugs can treat the same ailment

Focus on compounds with low uncertainty

High accuracy

Low accuracy

Open Source Malaria experimental validation

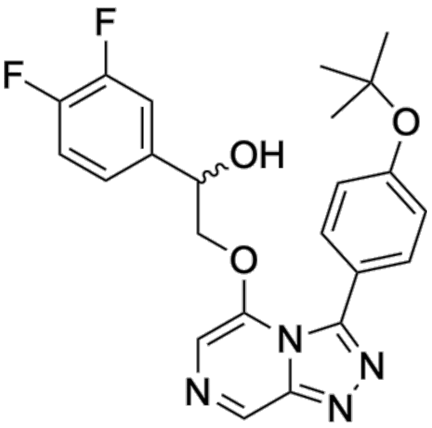


Optibrium & Intellegens

0.647 µM

Journal of Medicinal Chemistry 64, 16450 (2021)

Open Source Malaria other compounds



Optibrium & Intellegens

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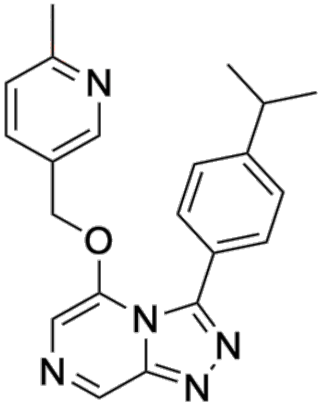
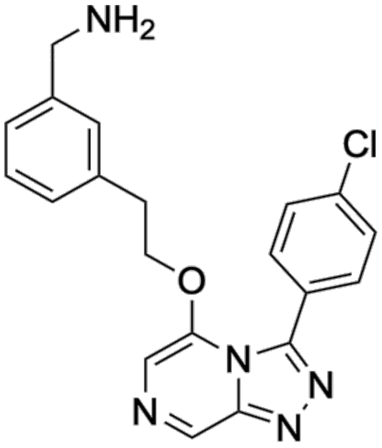


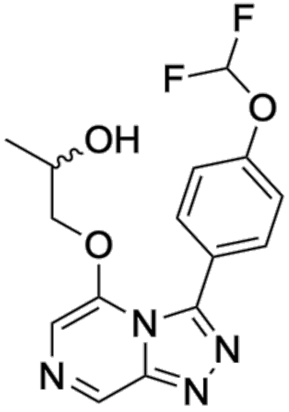
Davy Guan

>25 μM



Exscientia

10.9 μM



Molomics

>25 μM

Journal of Medicinal Chemistry 64, 16450 (2021)

Commercialization

therapeutics

bp

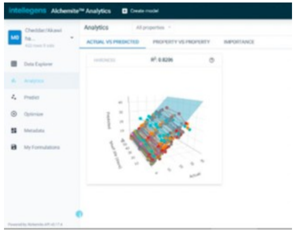
2018

Bring across contracts from University

Commercialization

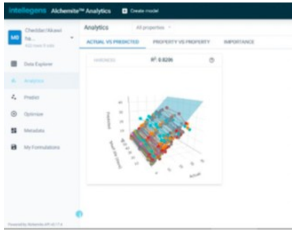
2018	2019
Bring across contracts from University	Consultancy work

Commercialization



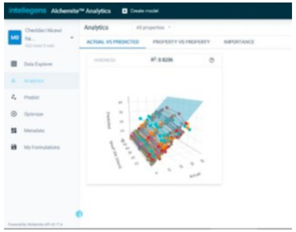
2018	2019	2020
Bring across contracts from University	Consultancy work	Release Alchemite Analytics™ product

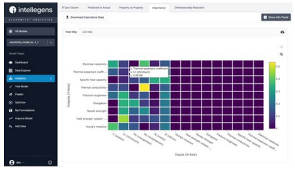
Commercialization



2018	2019	2020	2021
Bring across contracts from University	Consultancy work	Release Alchemite Analytics™ product	Release Cerella™ product with Optibrium

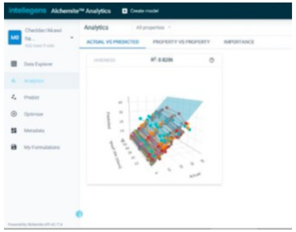
Commercialization

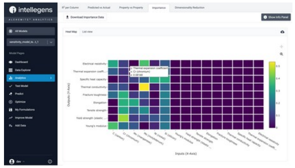




2018	2019	2020	2021	2021
Bring across contracts from University	Consultancy work	Release Alchemite Analytics™ product	Release Cerella™ product with Optibrium	Progress to enterprise licenses

Commercialization





2018	2019	2020	2021	2021	2022
Bring across contracts from University	Consultancy work	Release Alchemite Analytics™ product	Release Cerella™ product with Optibrium	Progress to enterprise licenses	Release product with ANSYS Granta

Summary

Merge computer simulations with experimental data and exploit property-property relationships to circumvent missing data

Designed and experimentally verified alloy for direct laser deposition

Exploited uncertainty to predict drug most probable drug

Generic approach applied to materials, batteries, pharmaceuticals, and beyond

Taken to market through startup Intellegens