UNIVERSITY OF CAMBRIDGE

The modern-day blacksmith

Gareth Conduit

Model sparse datasets

Exploit property-property relationships

Merge data, computer simulations, and physical laws

Reduce costly experiments to accelerate discovery

Commercialized as Alchemite™ by Intellegens

Black box machine learning for materials design

Composition

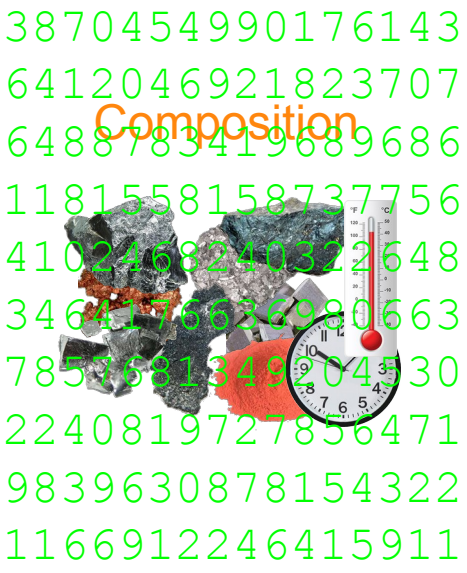
Properties

Defects

Fatigue

Strength

Train the machine learning



Machine learning predicts material properties

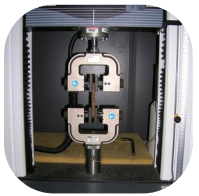
Composition

Properties

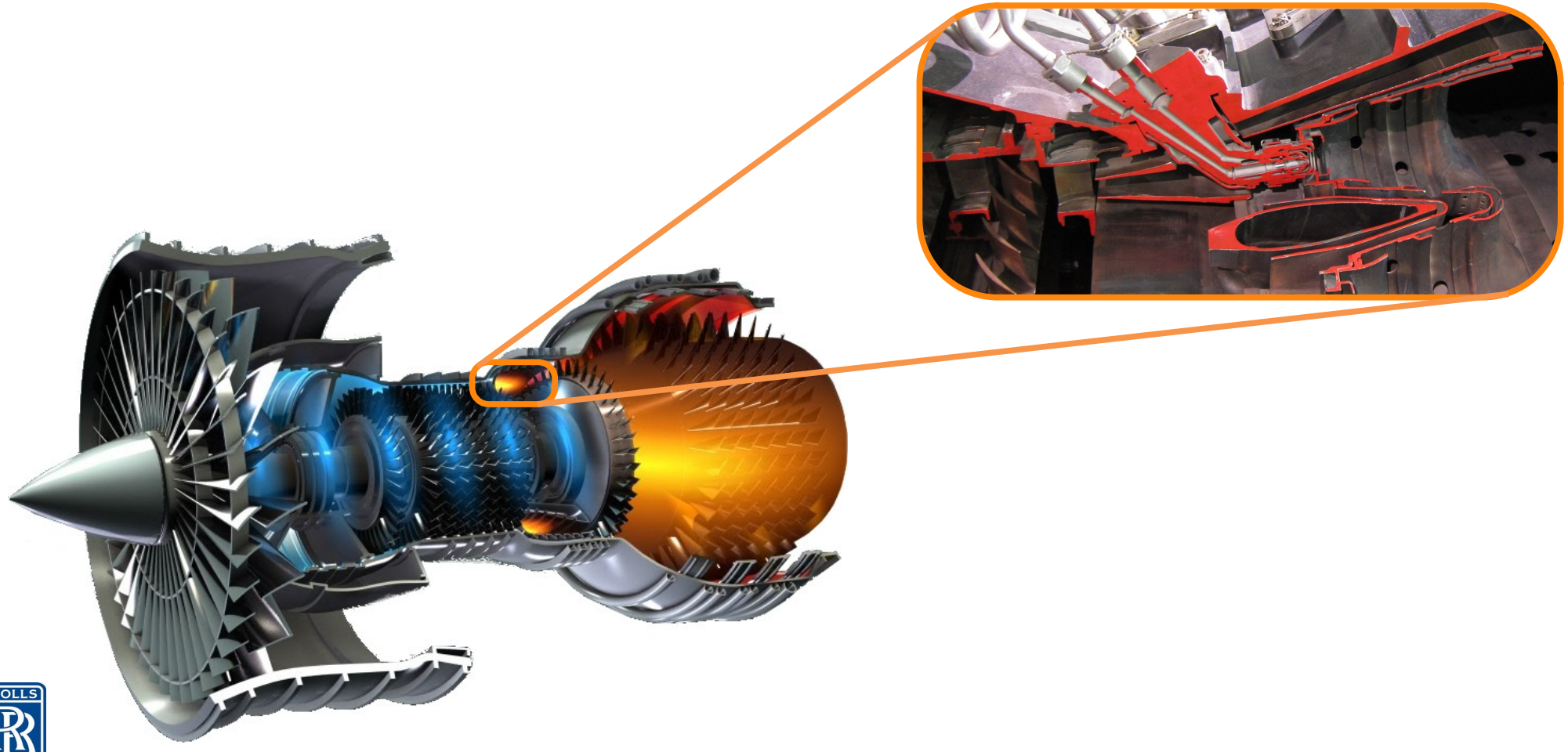
Defects

Fatigue

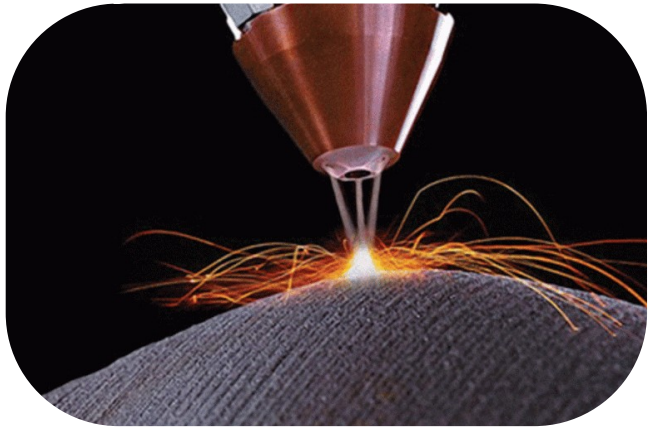
Strength



Combustor in a jet engine



Defects form during printing



Laser

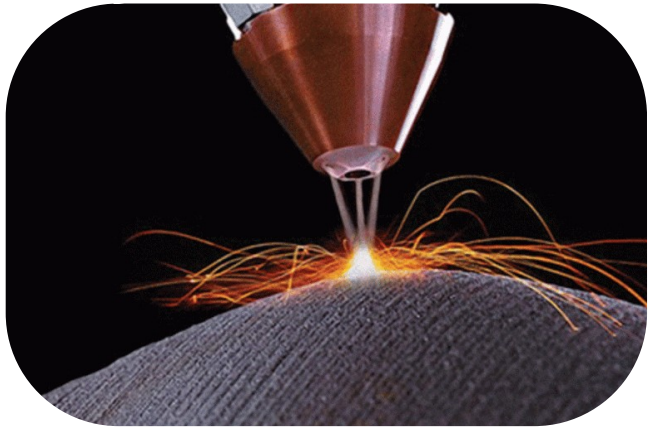
Data available to model defect density

Composition and heat treatment space 30 dimensions

Requires 31 points to fit a hyperplane

Just 10 data entries available to model defect density

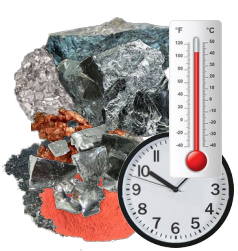
Ability for printing and welding are strongly correlated



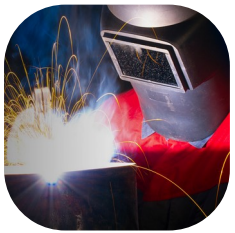
Laser

Electricity

First predict weldability

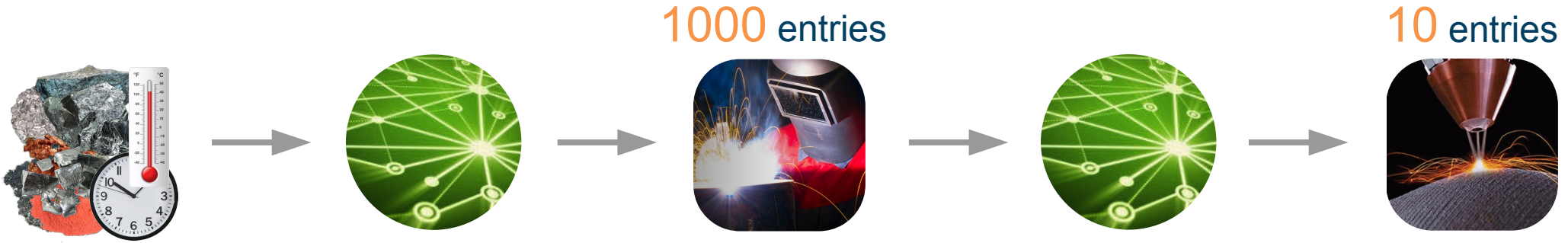


1000 entries



Use 1000 weldability entries to understand complex composition → weldability model

Use weldability to predict defects formed



Use 1000 weldability entries to understand complex composition → weldability model

10 defects entries capture the simple weldability → defect relationship

Two interpolations give composition → defects extrapolation

Use CALPHAD to predict strength

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%

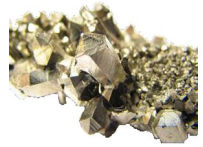
Co 4%

Mo 4.9%

W 1.2%

Zr 0.05%

Nb 3%



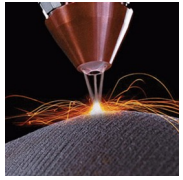
Al 2.9%

C 0.04%

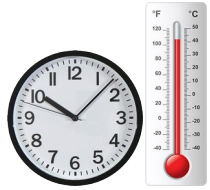
B 0.01%

Ni

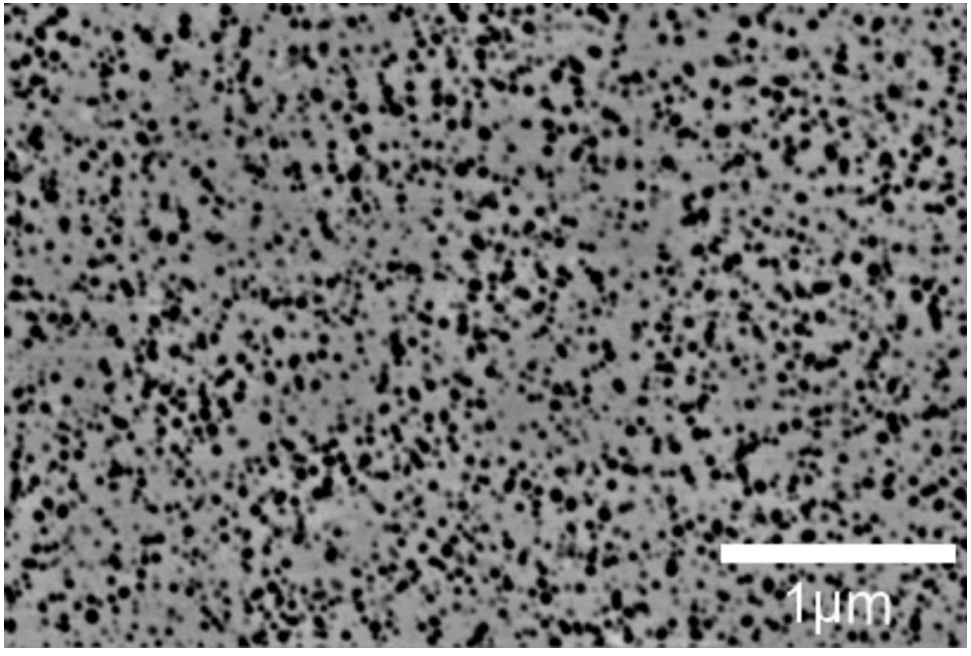
Expose 0.8



T_{HT} 1300ºC

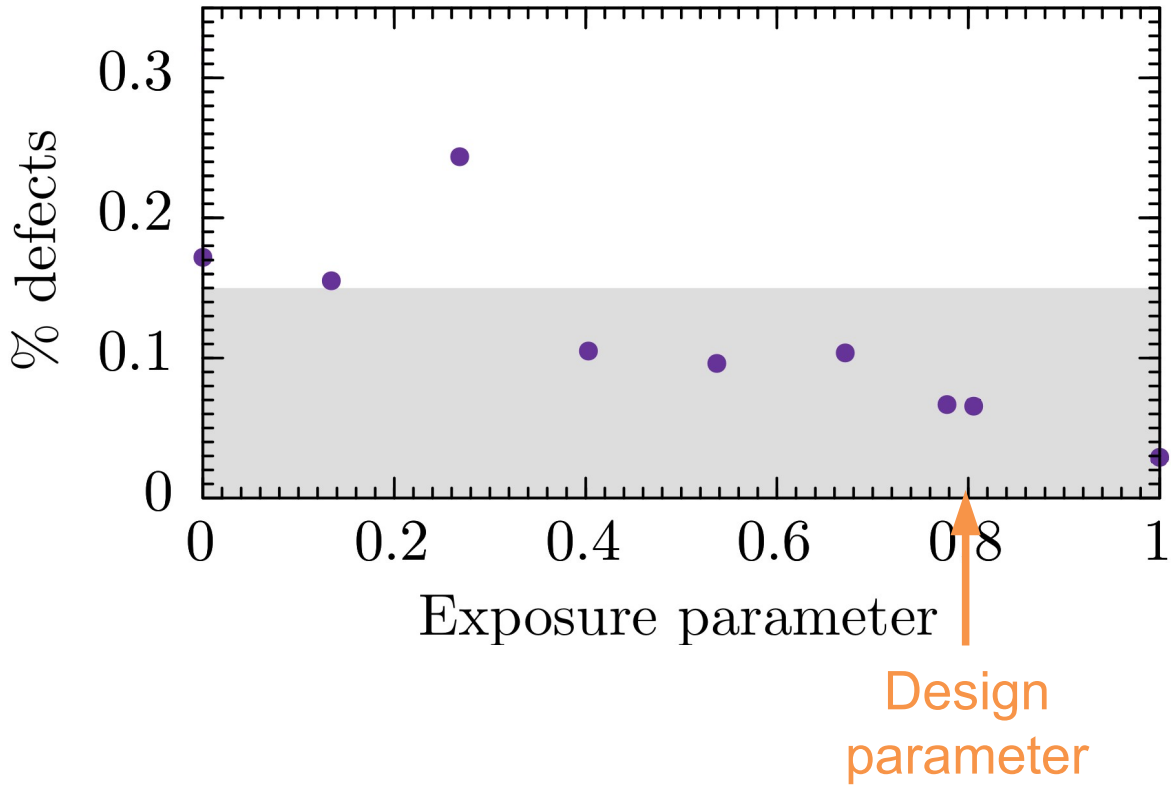


Microstructure



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

Testing the defect density



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)

NASA

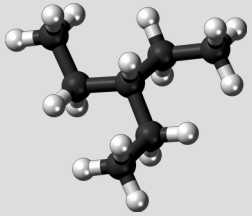
NASA Technical Memorandum 20220008637 (2022)

BOEING

The University Of Sheffield. AMRC Advanced Manufacturing Research

Agency for Science, Technology and Research SINGAPORE

ROLLS ROYCE



Fluid Phase Equilibria **501**, 112259 (2019)

Journal of Chemical Physics **153**, 014102 (2020)

bp

nature machine intelligence

REVIEW ARTICLE

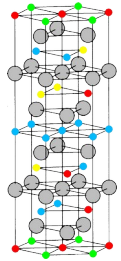
https://doi.org/10.1038/s42256-020-0156-7

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

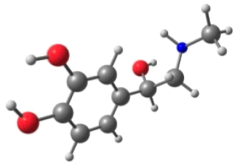
Development of methodology

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

Development of methodology

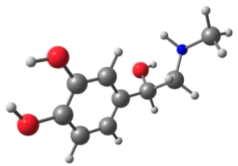
Concurrent materials design



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

Development of methodology

Concurrent materials design



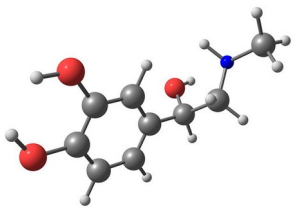
2013	2014	2015	2016	2017	2018
Multiple properties for Rolls Royce engines	Property-property correlations with Rolls Royce and BP	Royal Society University Research Fellowship	Experiment-simulation correlations with Samsung	Drug discovery study with etherapeutics	Founding of Intellegens

Open Source Malaria contest

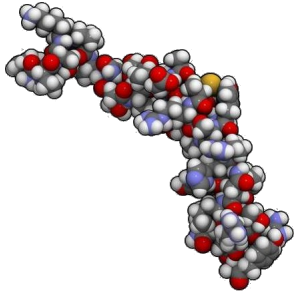
OPEN SOURCE MALARIA

Looking for New Medicines

Action of a drug



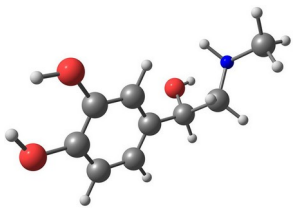
Drug



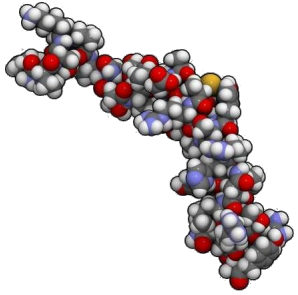
Protein

Effect

Action of a drug



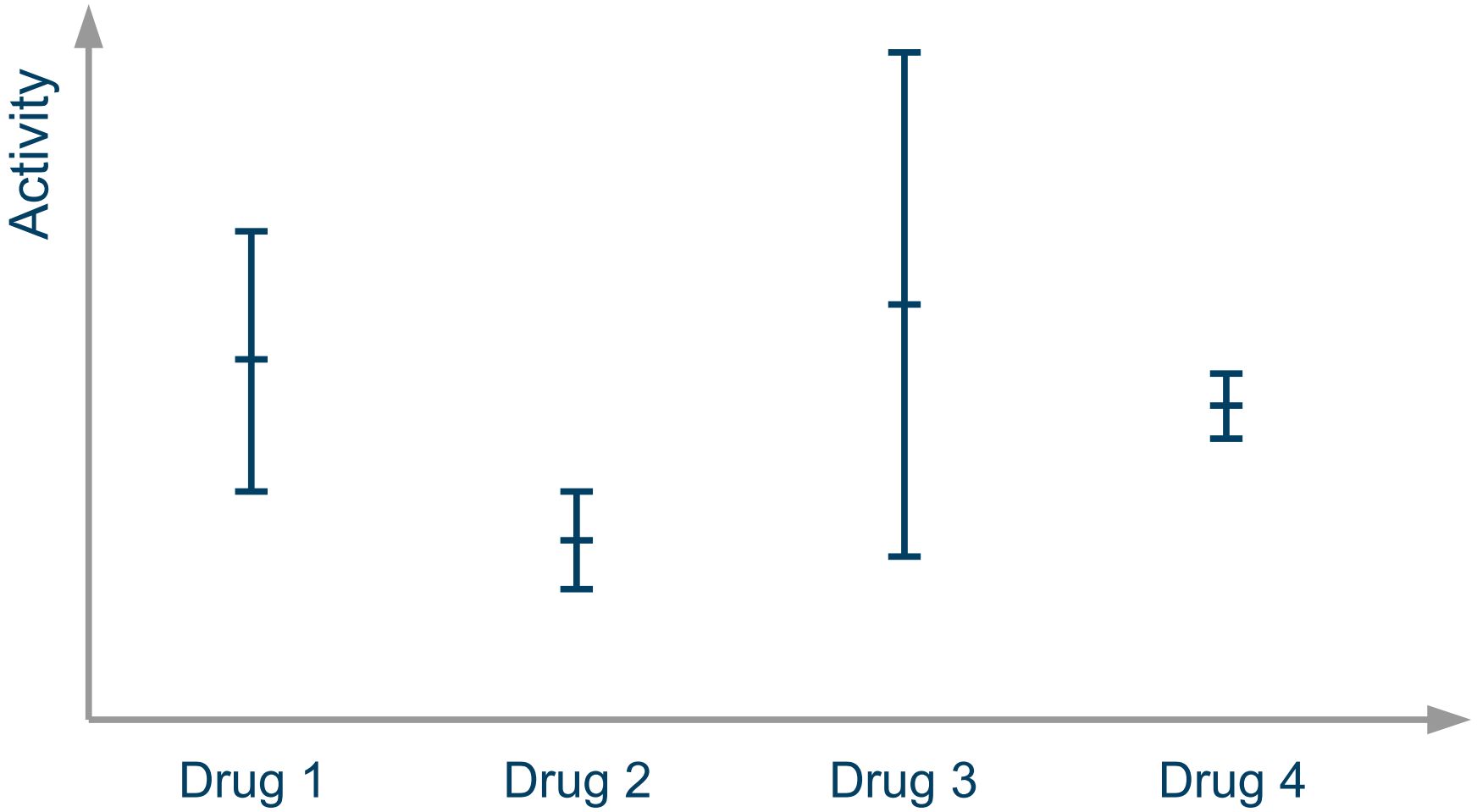
Drug



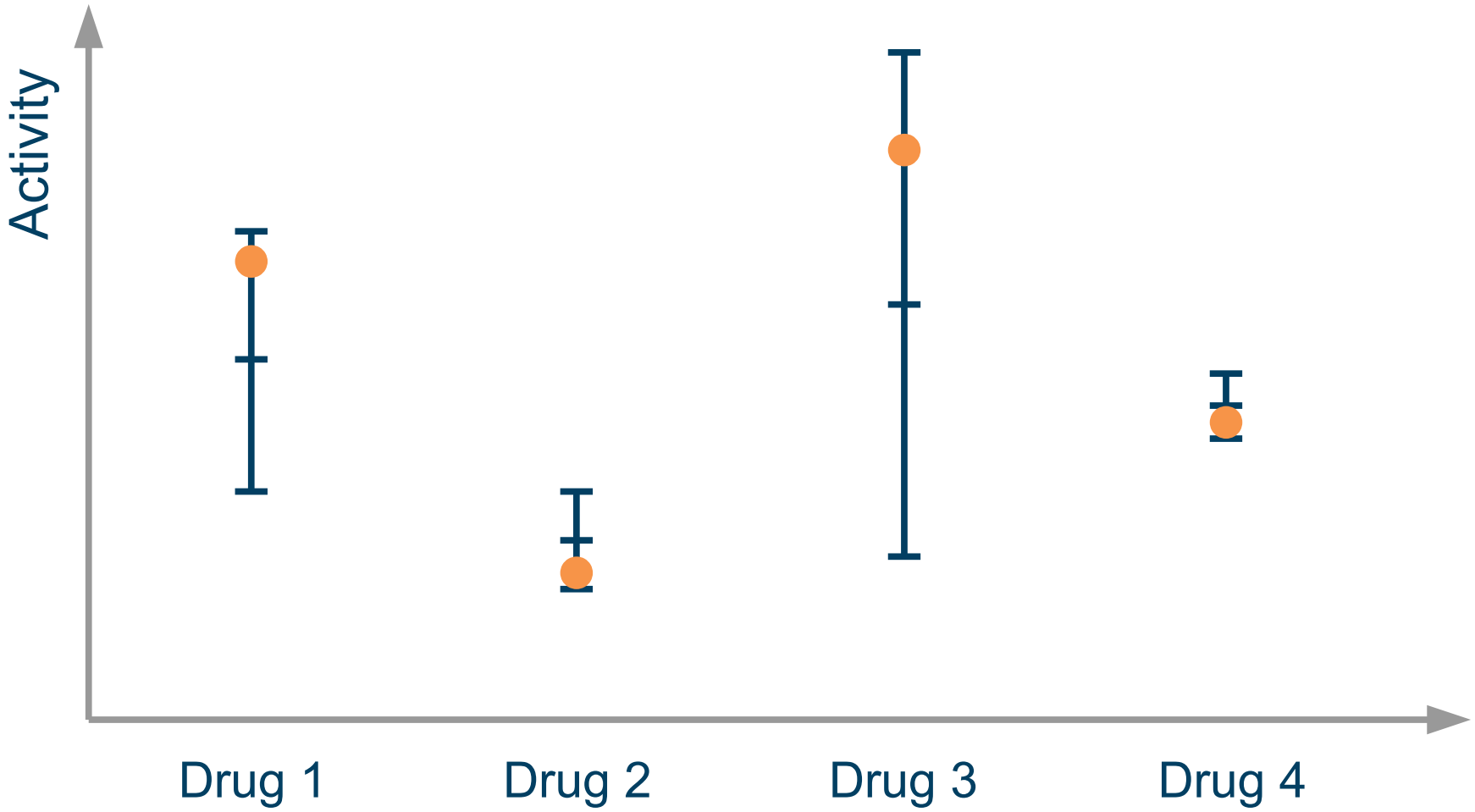
Protein

Effect

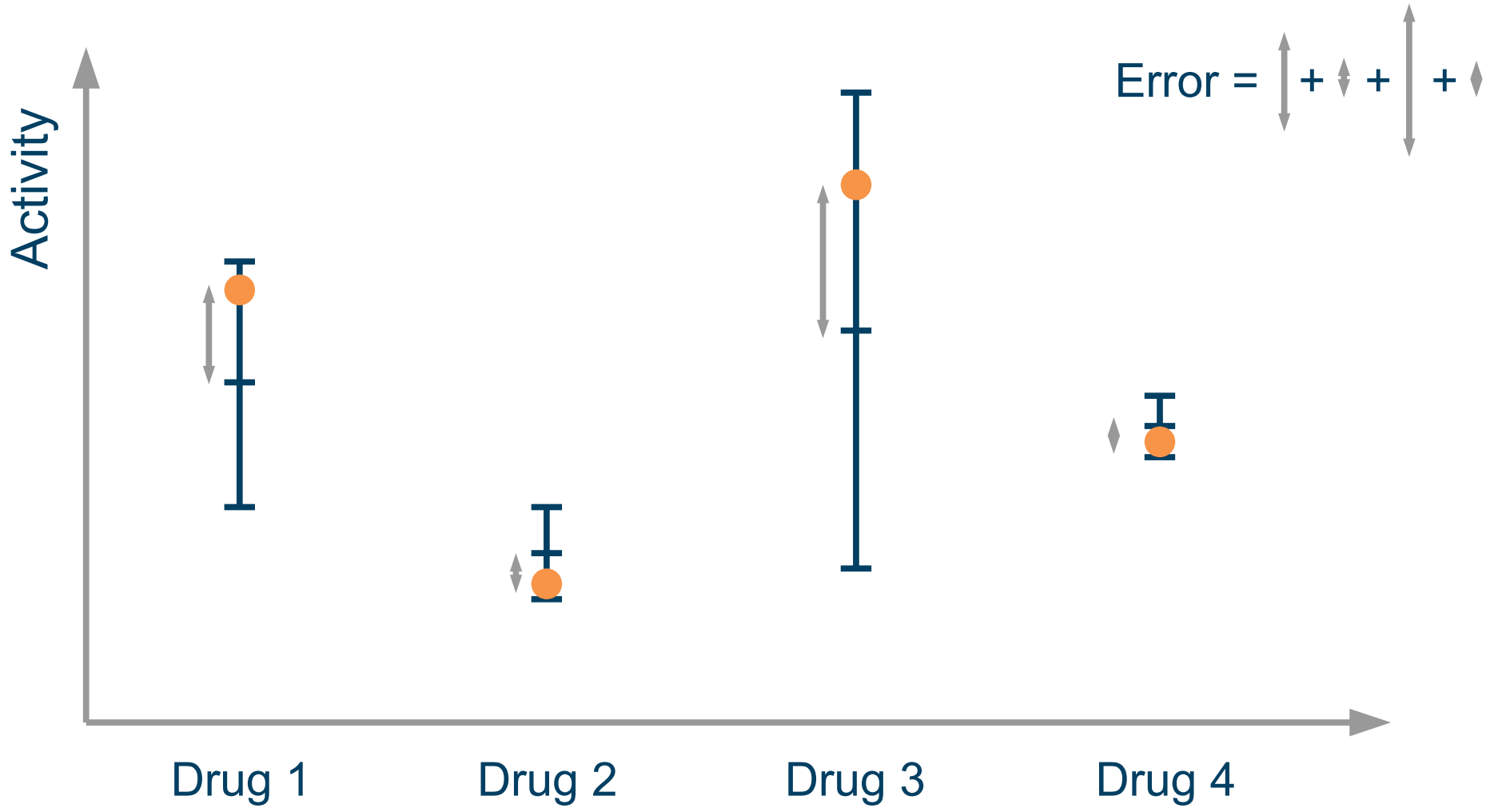
Predictions have an uncertainty



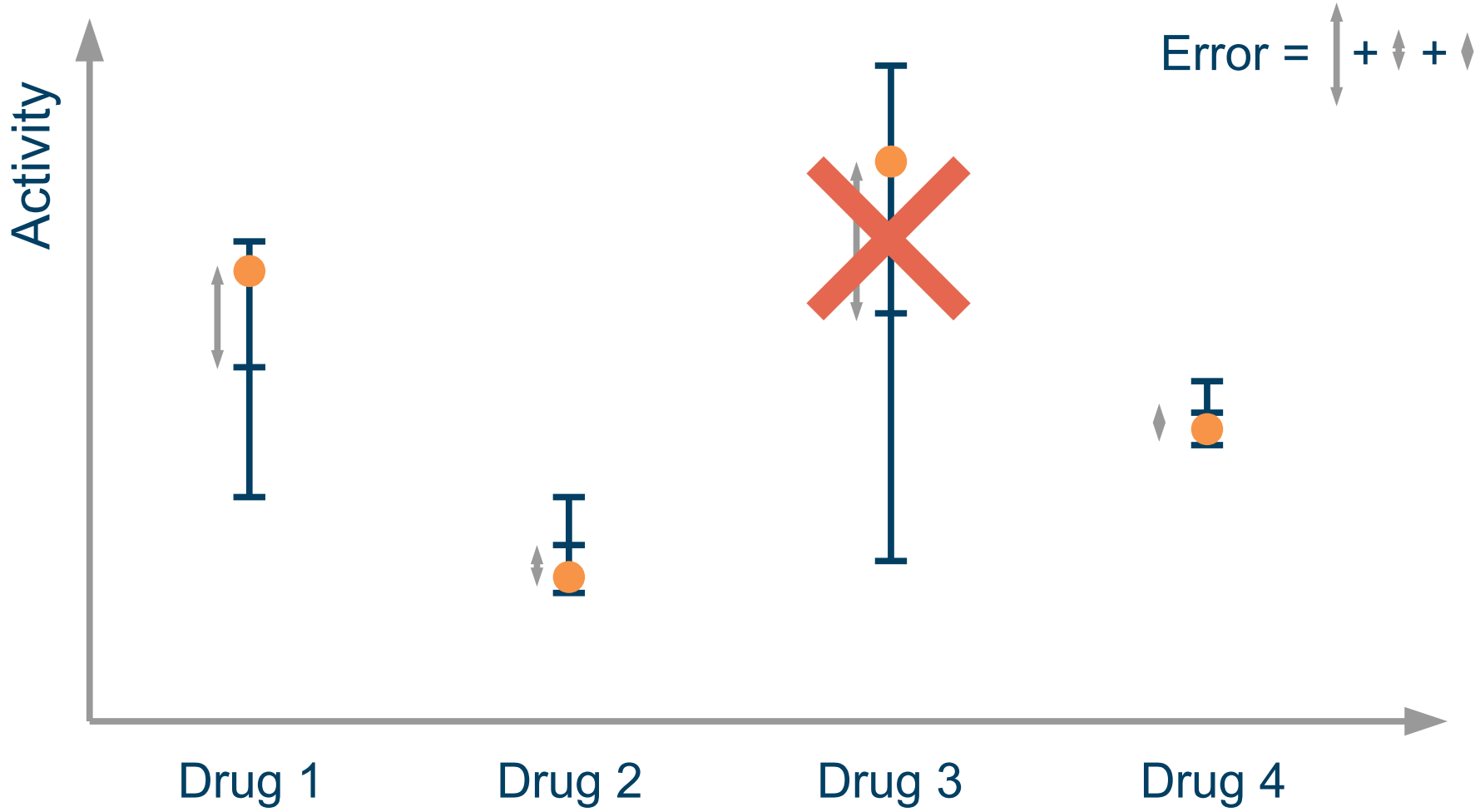
Validation data typically within one standard deviation



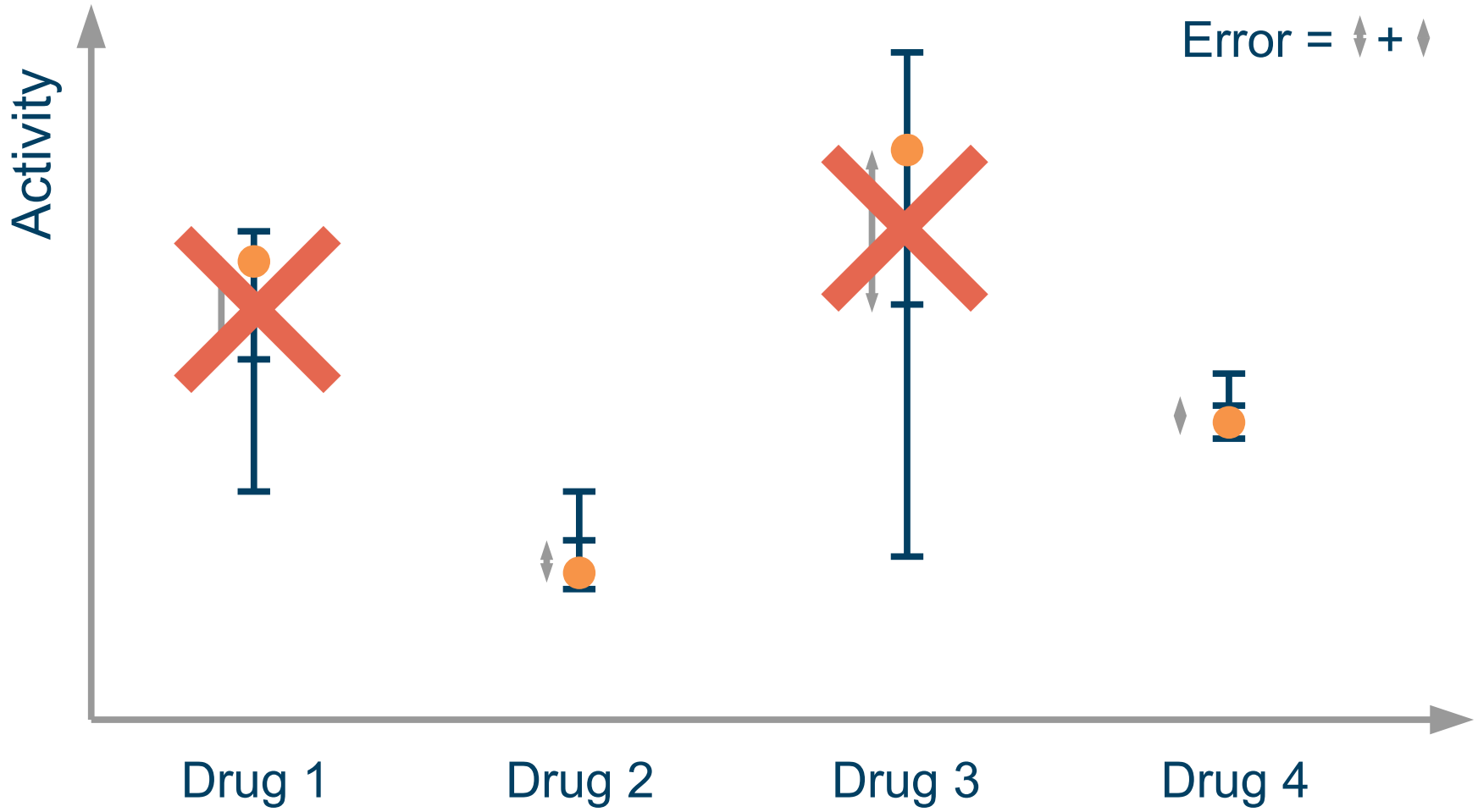
Accuracy R^2 metric calculated with difference from mean



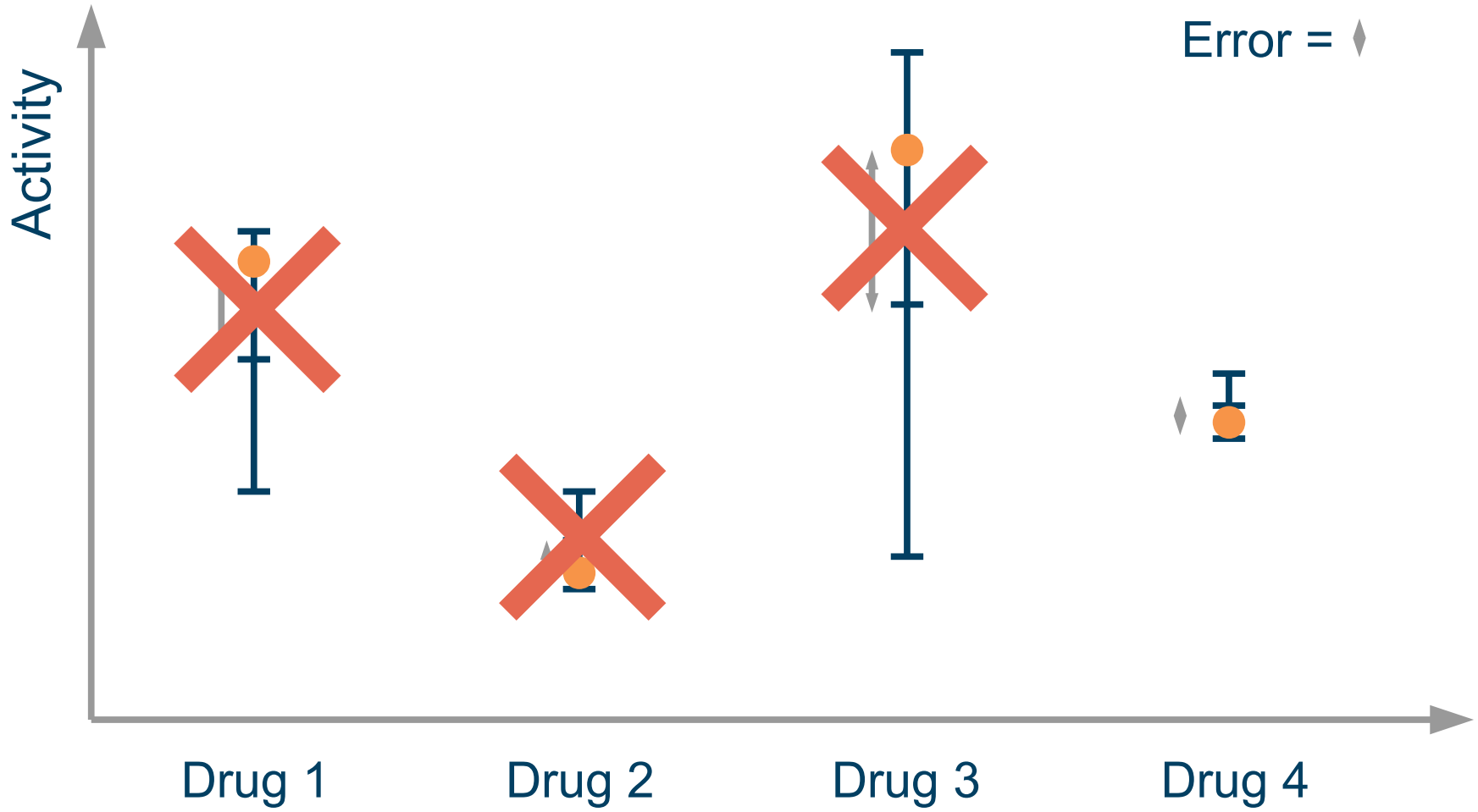
Impute 75% of data with smallest uncertainty



Impute 50% of data with smallest uncertainty



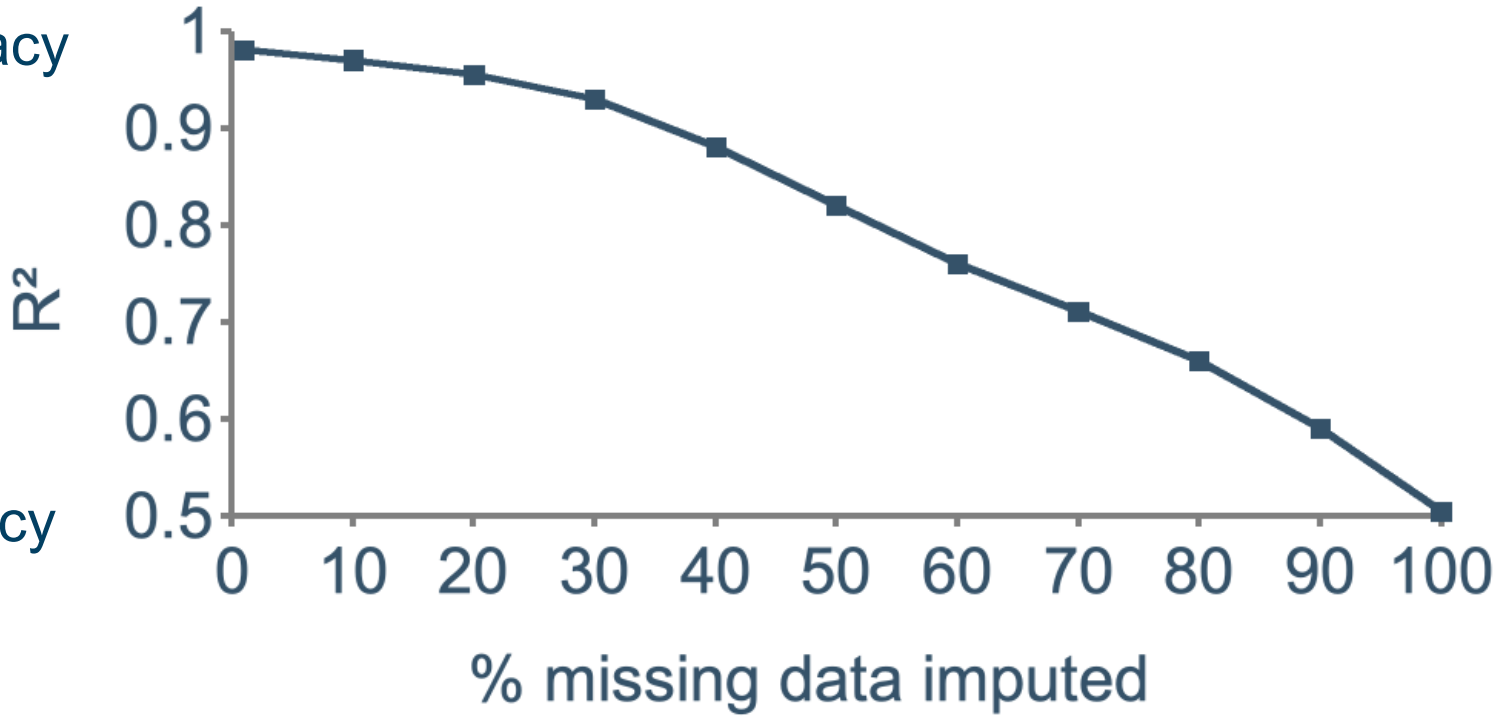
Impute 25% of data with smallest uncertainty



Improved performance by exploiting uncertainty

High accuracy

Low accuracy

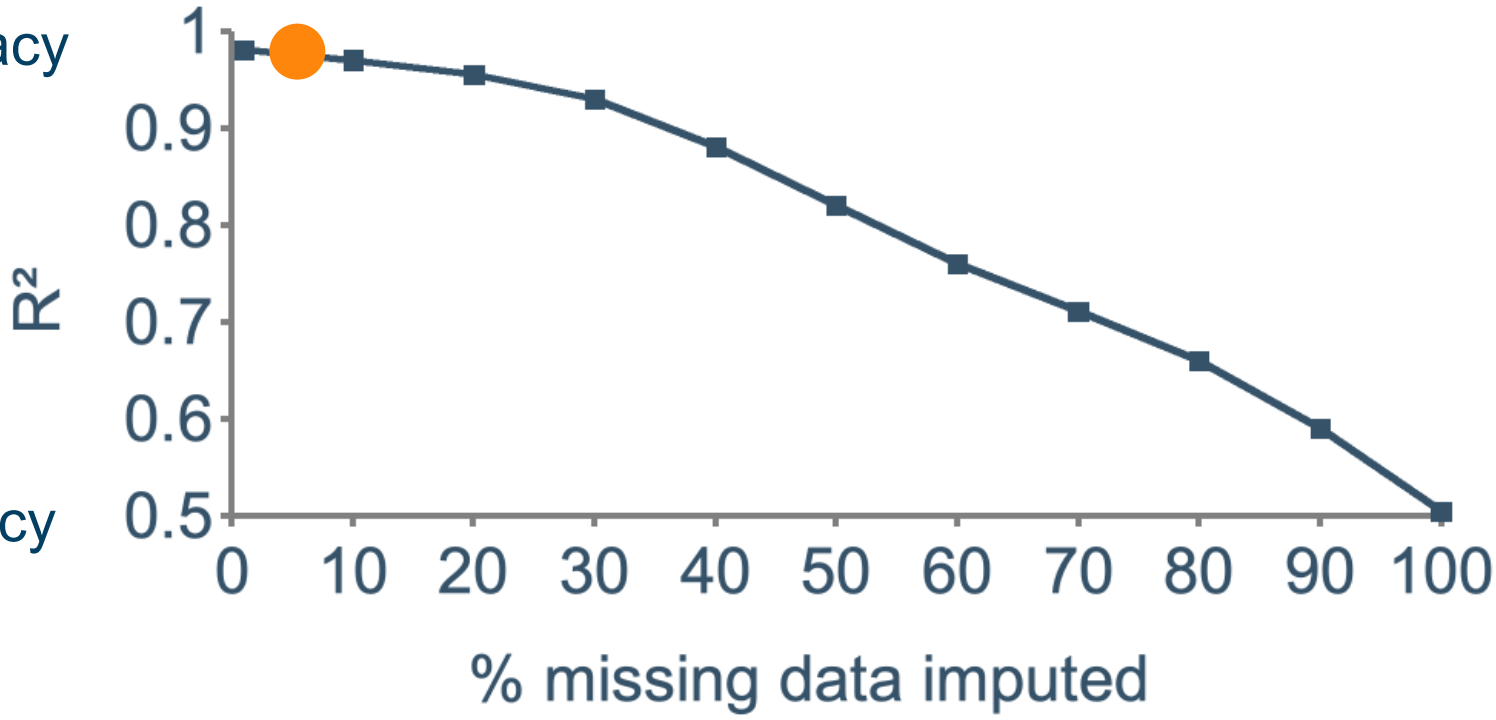


Different drugs can treat the same ailment

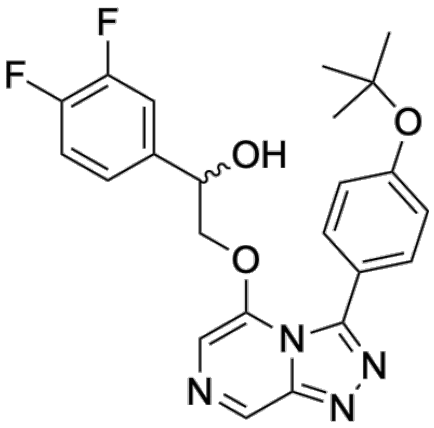
Focus on compounds with low uncertainty

High accuracy

Low accuracy



Open Source Malaria experimental validation

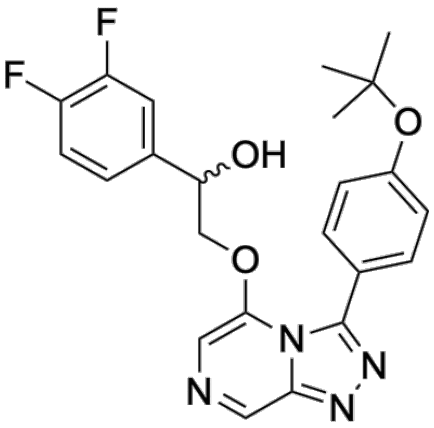


Optibrium & Intellegens

0.647 µM

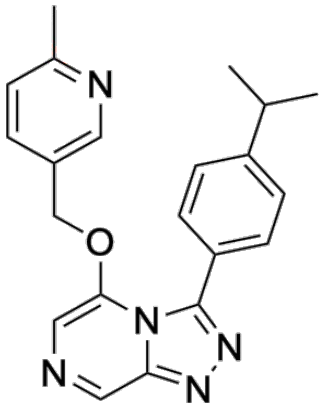
Journal of Medicinal Chemistry 64, 16450 (2021)

Open Source Malaria other compounds



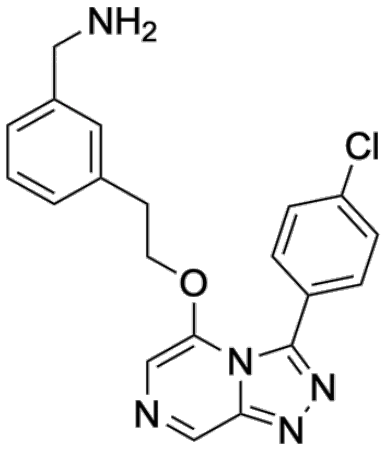
Optibrium & Intellegens

0.647 µM



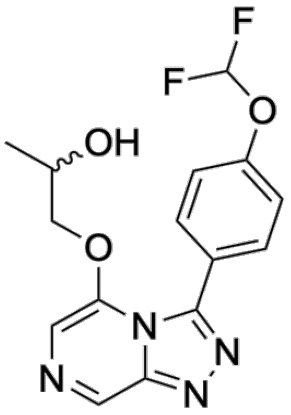
Davy Guan

>25 µM



Exscientia

10.9 µM



Molomics

>25 µM

Journal of Medicinal Chemistry 64, 16450 (2021)

Commercialization

therapeutics

bp

2018

Transfer contracts from University

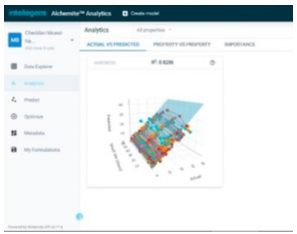
Commercialization

2018 | 2019

Transfer contracts from University

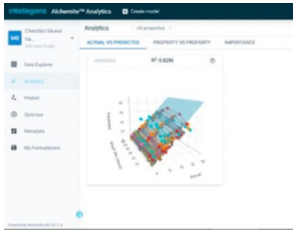
Consultancy work

Commercialization



2018	2019	2020
Transfer contracts from University	Consultancy work	Launch Alchemite Analytics™ product

Commercialization

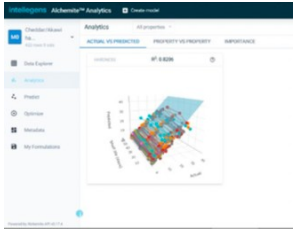


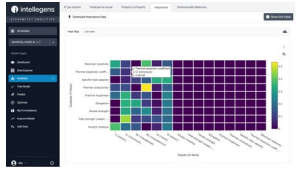
2018	2019	2020	2021
Transfer contracts from University	Consultancy work	Launch Alchemite Analytics™ product	Launch Cerella™ product with Optibrium

Commercialization

2018	2019	2020	2021	2021
Transfer contracts from University	Consultancy work	Launch Alchemite Analytics™ product	Launch Cerella™ product with Optibrium	Enterprise licenses & many case studies

Commercialization





2018	2019	2020	2021	2021	2022
Transfer contracts from University	Consultancy work	Launch Alchemite Analytics™ product	Launch Cerella™ product with Optibrium	Enterprise licenses & many case studies	Launch product with ANSYS Granta

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 most probable drug

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

Commercialized as Alchemite™ by Intellegens