UNIVERSITY OF CAMBRIDGE

# The modern-day blacksmith

Gareth Conduit

# Machine learning to

Model systems where the data is sparse

Merge data, images, computer simulations, and physical laws

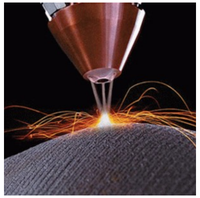
Reduce costly experiments to accelerate discovery

# Black box machine learning for materials design

Properties

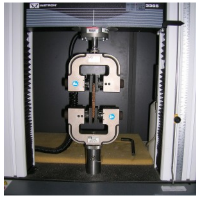
Composition

Defects



Fatigue

Strength

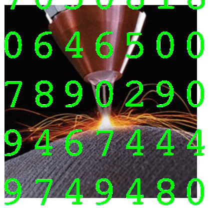


# Train the machine learning

Composition

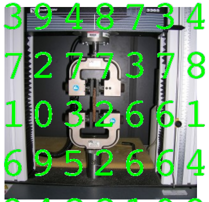
Properties

Defects



Fatigue

Strength

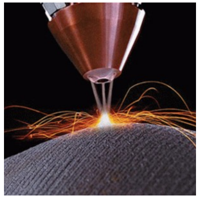


# Machine learning predicts material properties

Composition

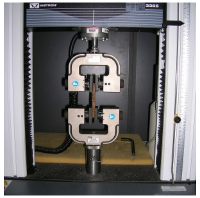
Properties

Defects

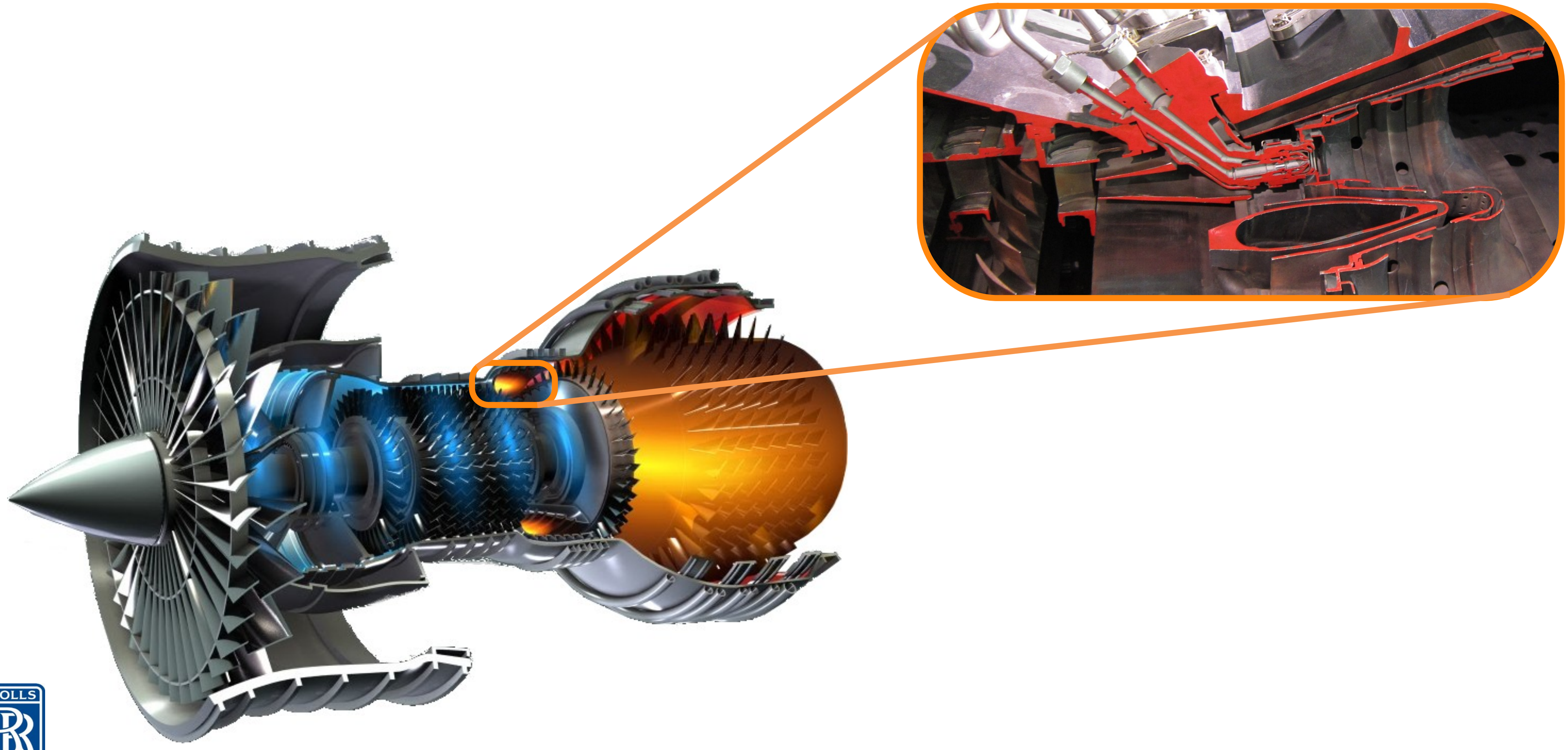


Fatigue

Strength



# Combustor in a jet engine



# Data available to model defect density

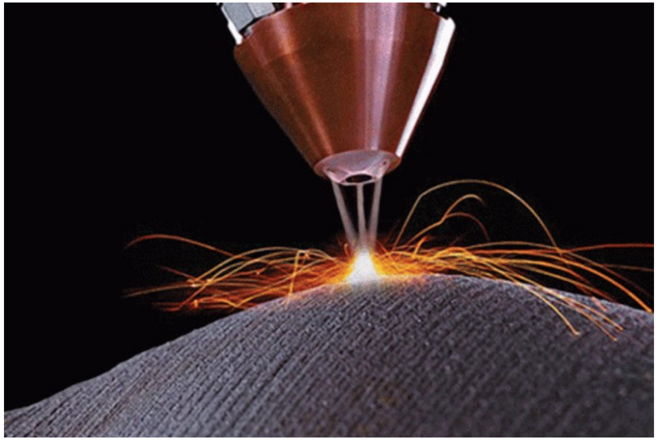
10 entries

Composition and heat treatment space 30 dimensions

Requires 31 points to fit a hyperplane

Just 10 data entries available to model defect density

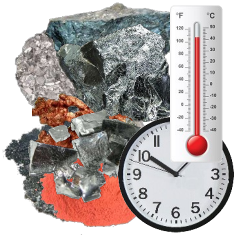
# Ability for printing and welding are strongly correlated



Laser

Electricity

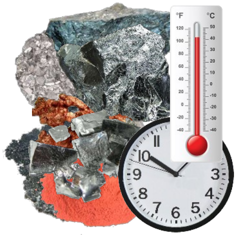
# First predict weldability



1000 entries

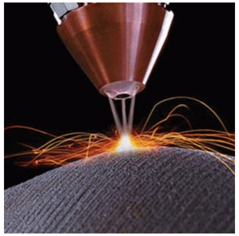
Use 1000 weldability entries to understand complex composition → weldability model

# 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 give composition → defects extrapolation

# Target properties

| | |
|---|---|
| Elemental cost | < 25 $\$kg^{-1}$ |
| Density | < 8500 $kgm^{-3}$ |
| Defects | < 0.15% defects |
| Oxidation resistance | < 0.3 $mgcm^{-2}$ |
| γ content | > 75 wt% |
| Phase stability | > 99 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%

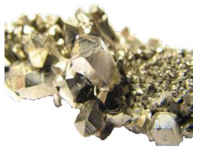
Co 4%

Mo 4.9%

W 1.2%

Zr 0.05%

Nb 3%



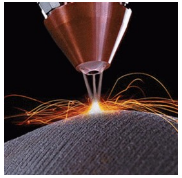
Al 2.9%

C 0.04%

B 0.01%

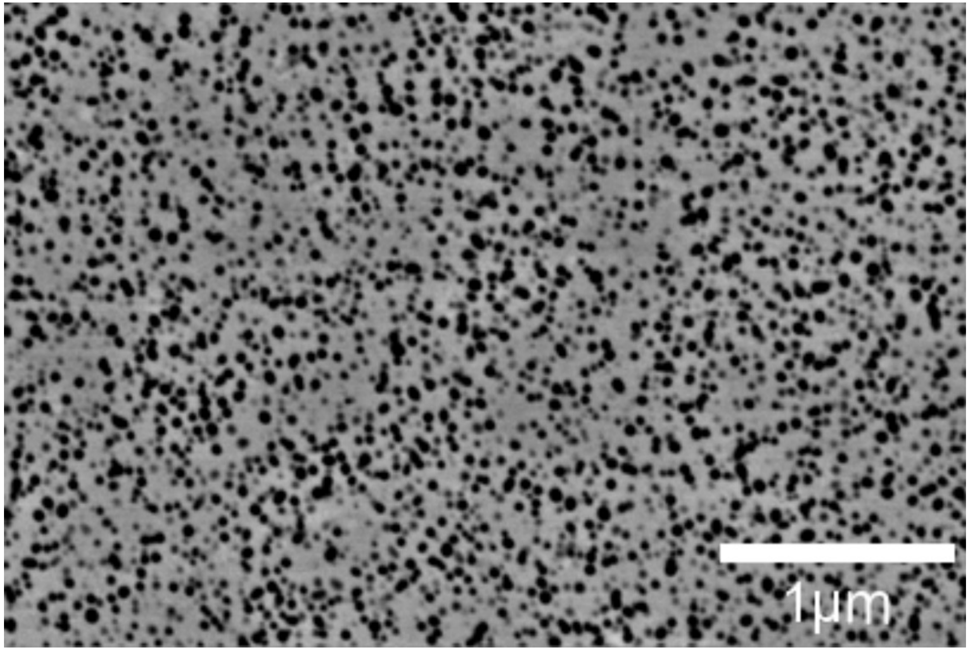
Ni

Expose 0.8



$T_{HT}$ 1300ºC

# Microstructure




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

# Target γ content

Elemental cost < 25 $\$kg^{-1}$

Density < 8500 $kgm^{-3}$

Defects < 0.15% defects

Oxidation resistance < 0.3 $mgcm^{-2}$

γ content > 75 wt%

Phase stability > 99 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%

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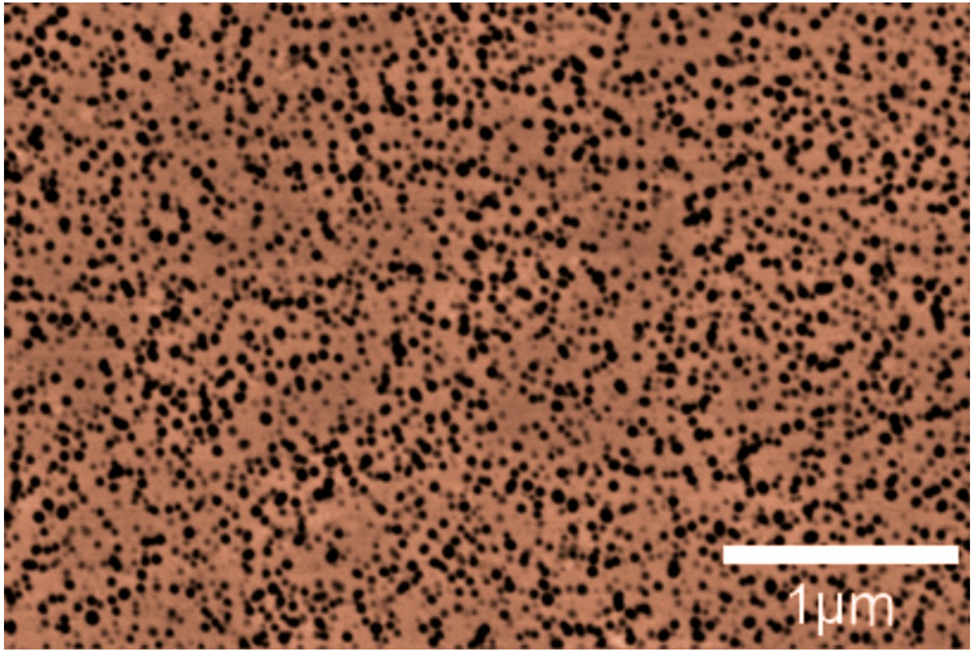
# Microstructure

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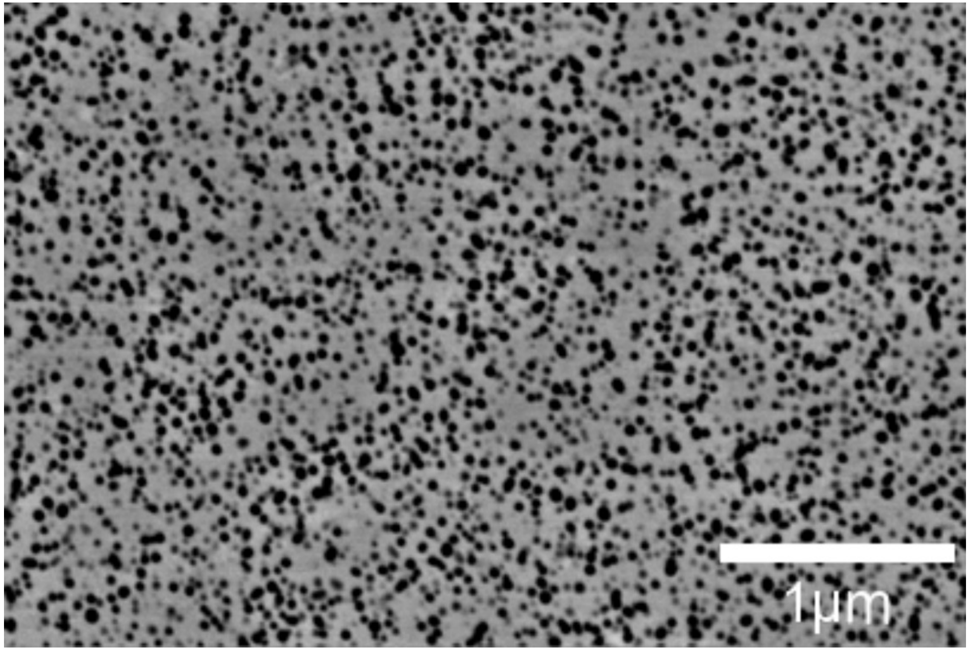
Fatigue life at 500 MPa, 700˚C > $10^5$ cycles

# Deleterious phases formed

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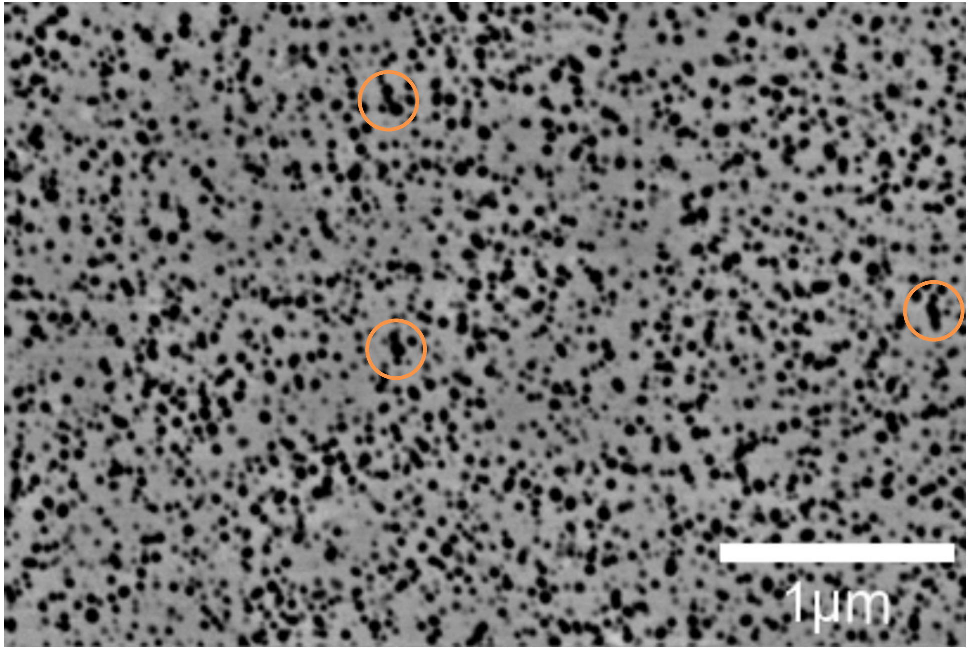
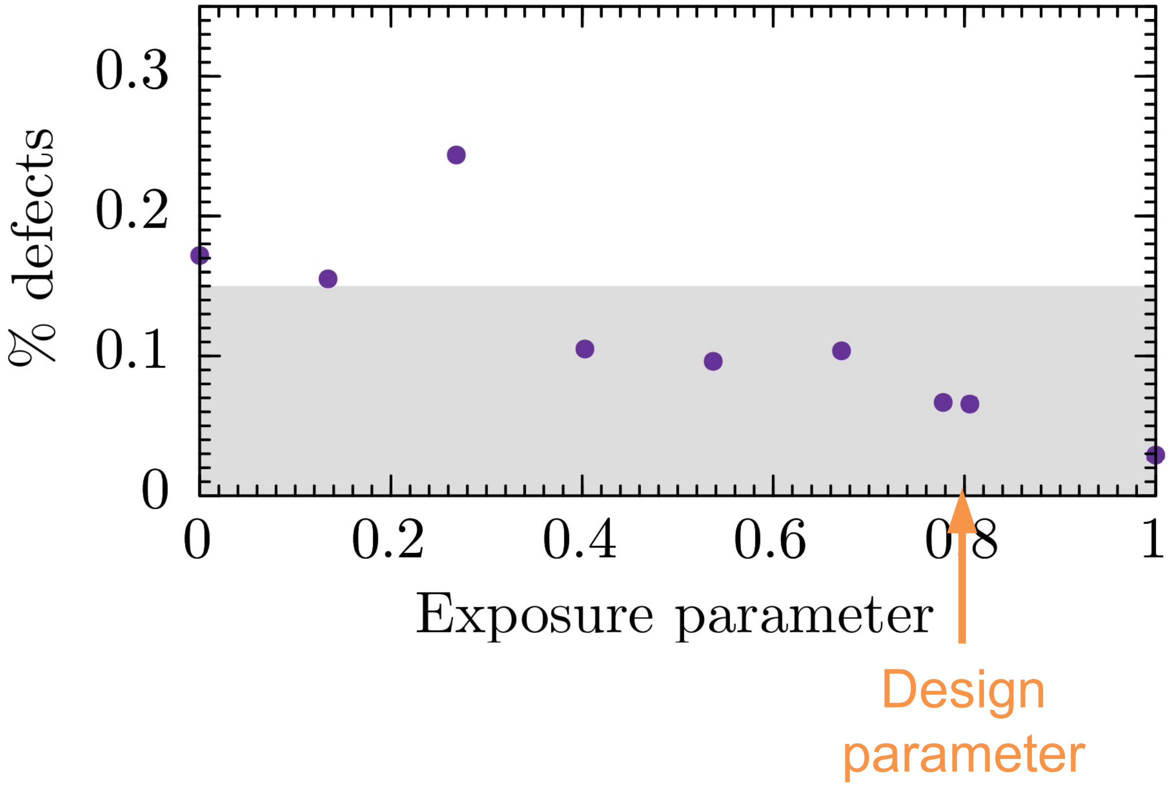
# Defect detection




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

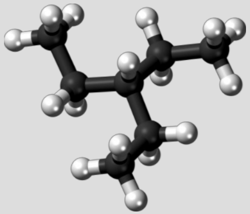
Ordnance Survey

The University Of Sheffield. AMRC Advanced Manufacturing Research Centre

BOEING

GKN

Agency for Science, Technology and Research SINGAPORE



bp

Lubricants
for electric cars

nature machine intelligence

REVIEW ARTICLE

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

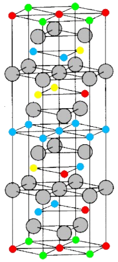
Check for updates

# 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]✉

Agency for Science, Technology and Research SINGAPORE

SAMSUNG



NASA

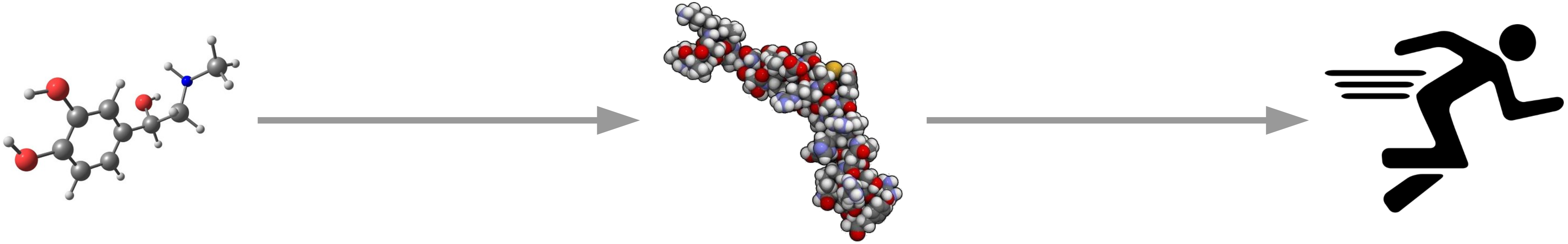
Heat exchanger
& shape memory
alloy applications

# Open Source Malaria contest

OPEN SOURCE MALARIA

Looking for New Medicines

# Action of a drug

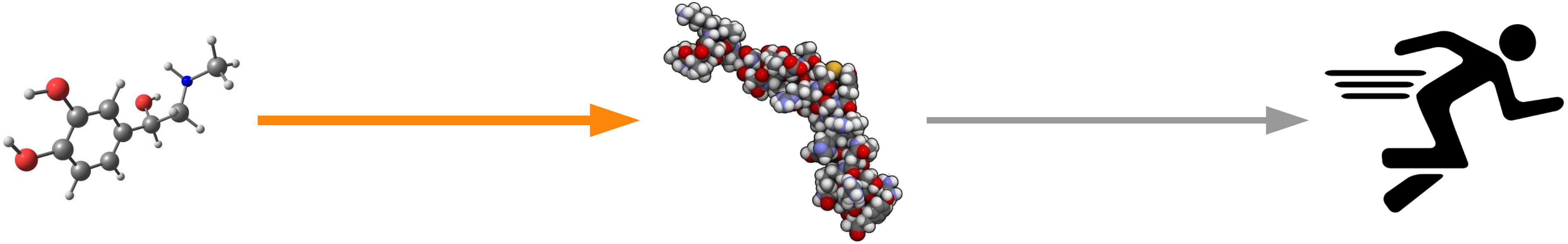


Drug

Protein

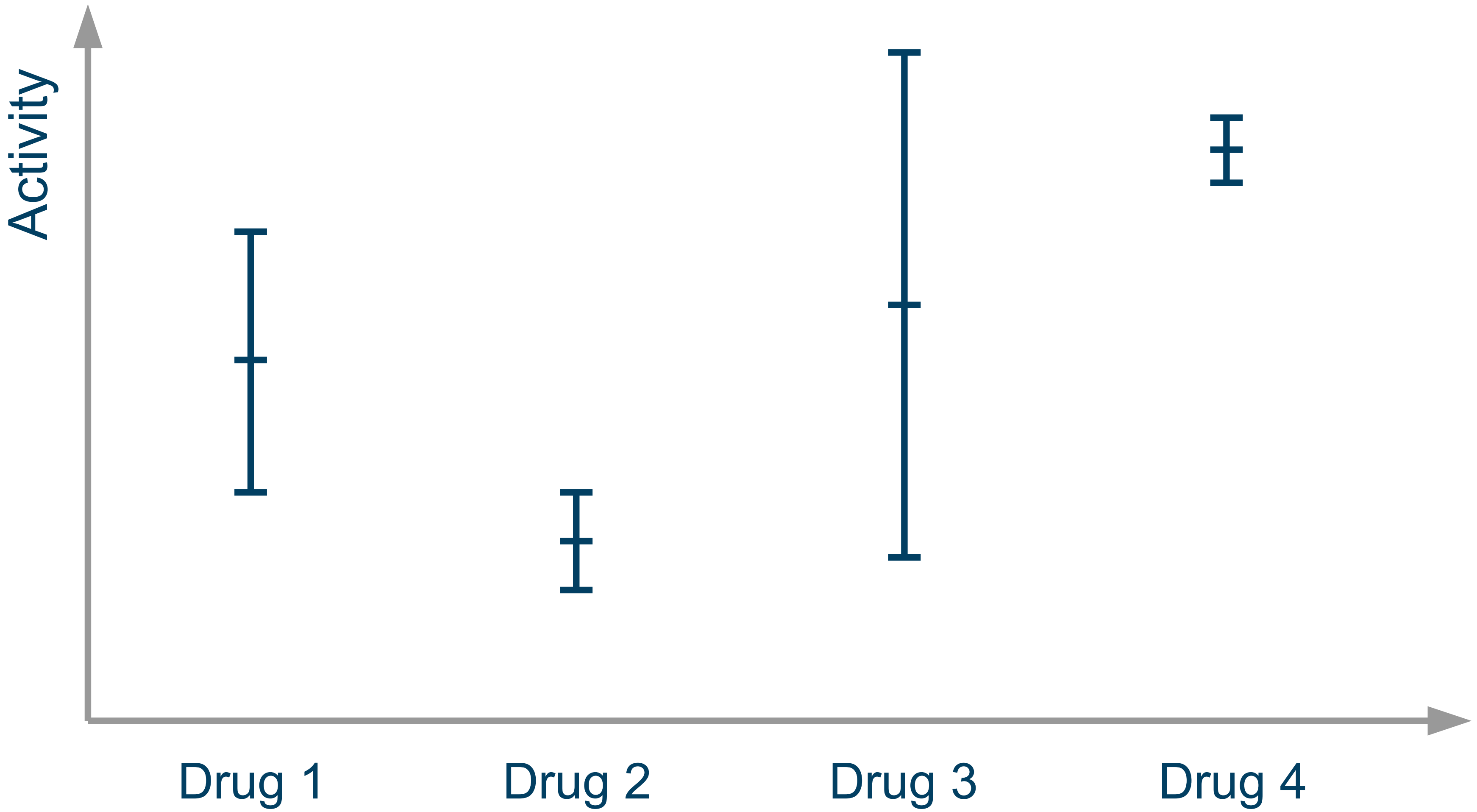
Effect

# Action of a drug

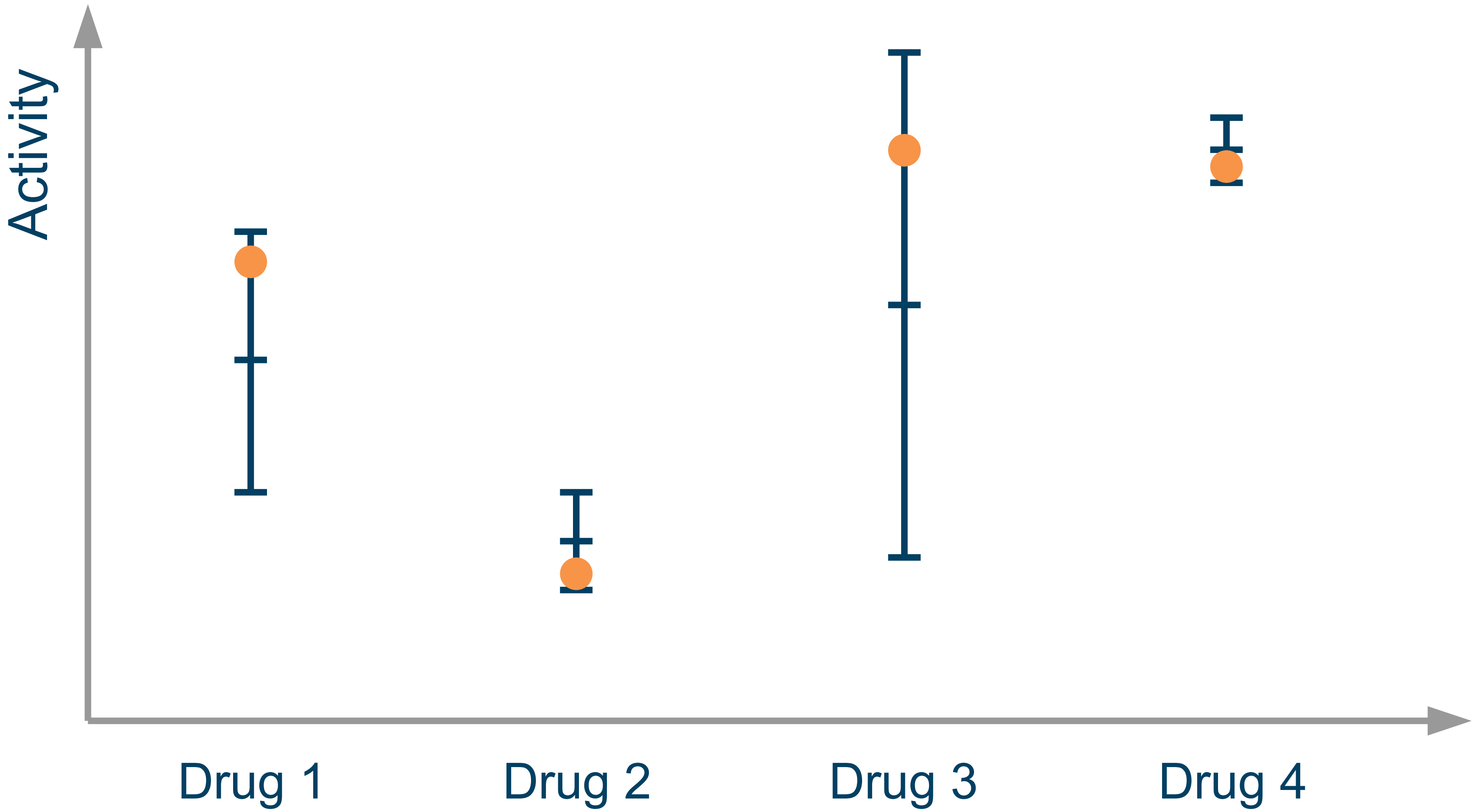


Drug Protein Effect

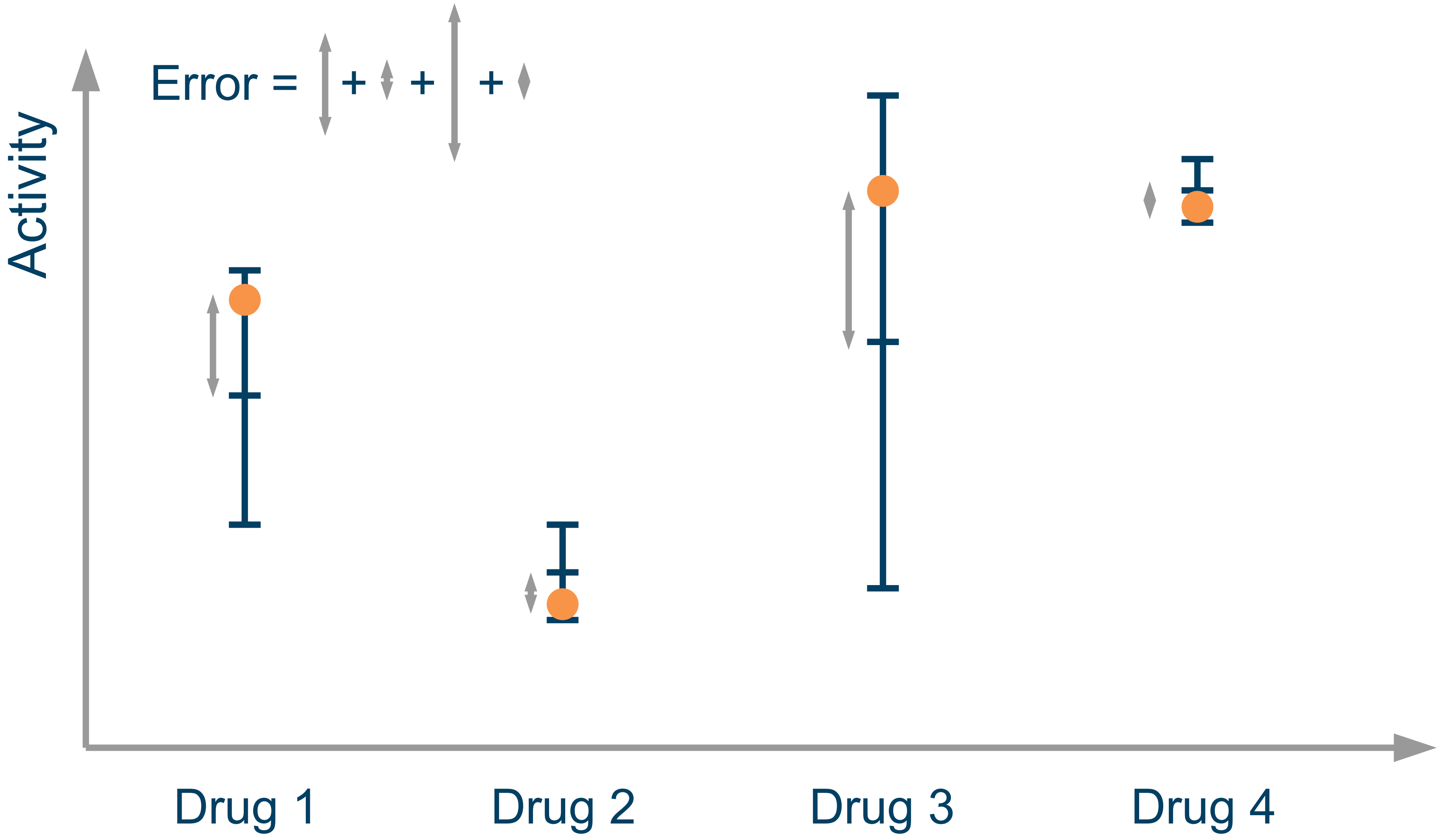
# Predictions have an uncertainty



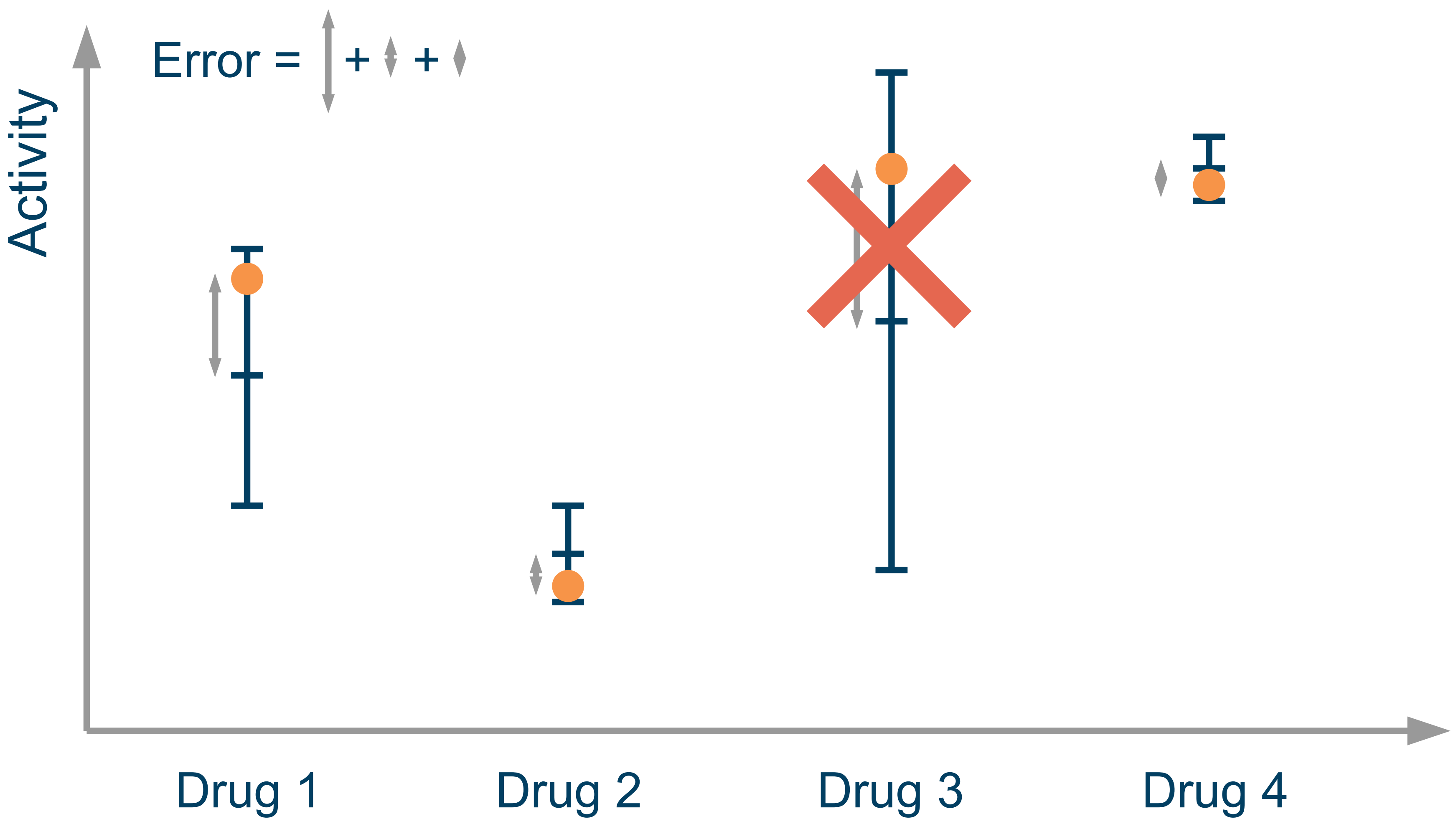
# Validation data typically within one standard deviation



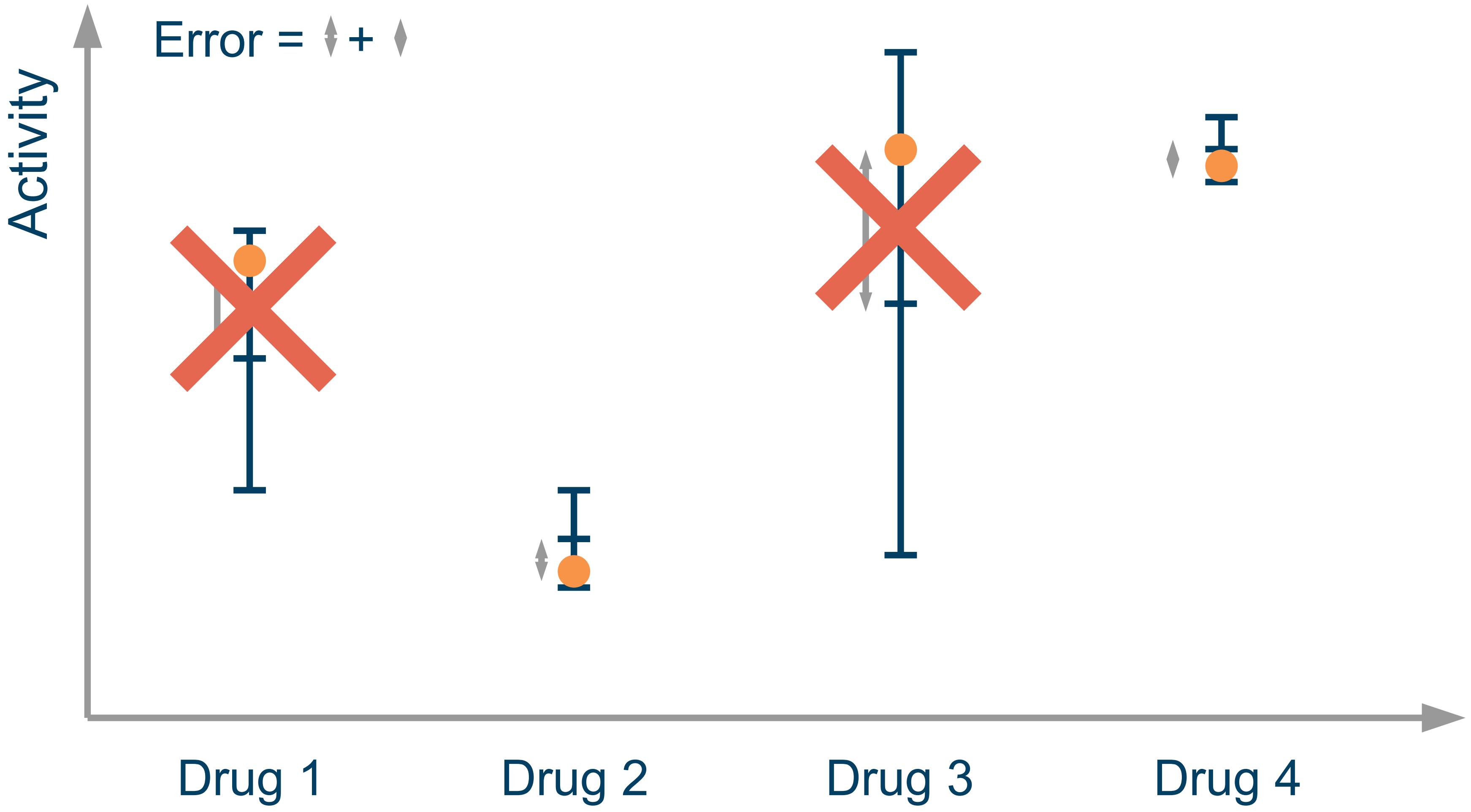
# $R^2$ metric calculated with difference from mean



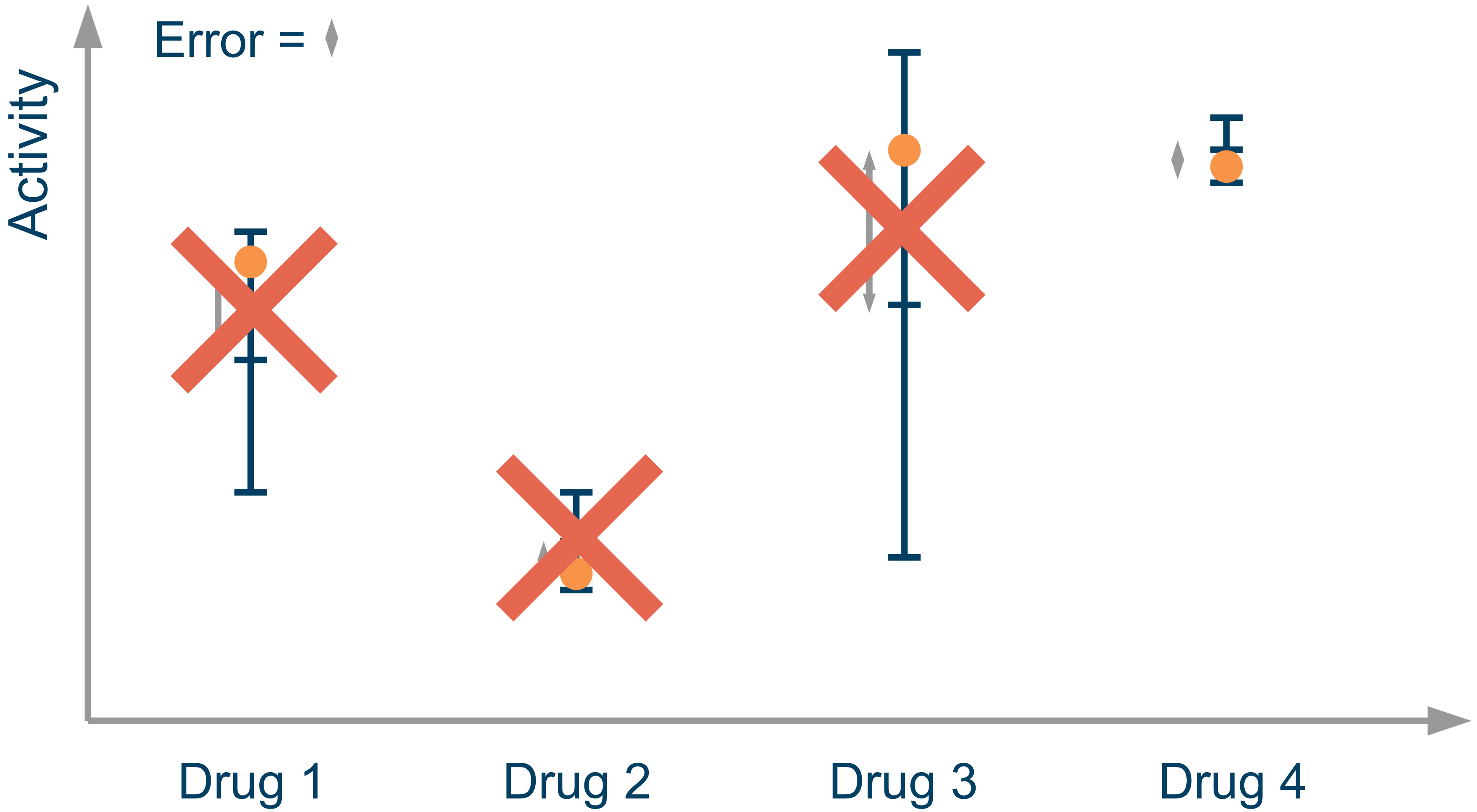
# Impute 75% of data with smallest uncertainty



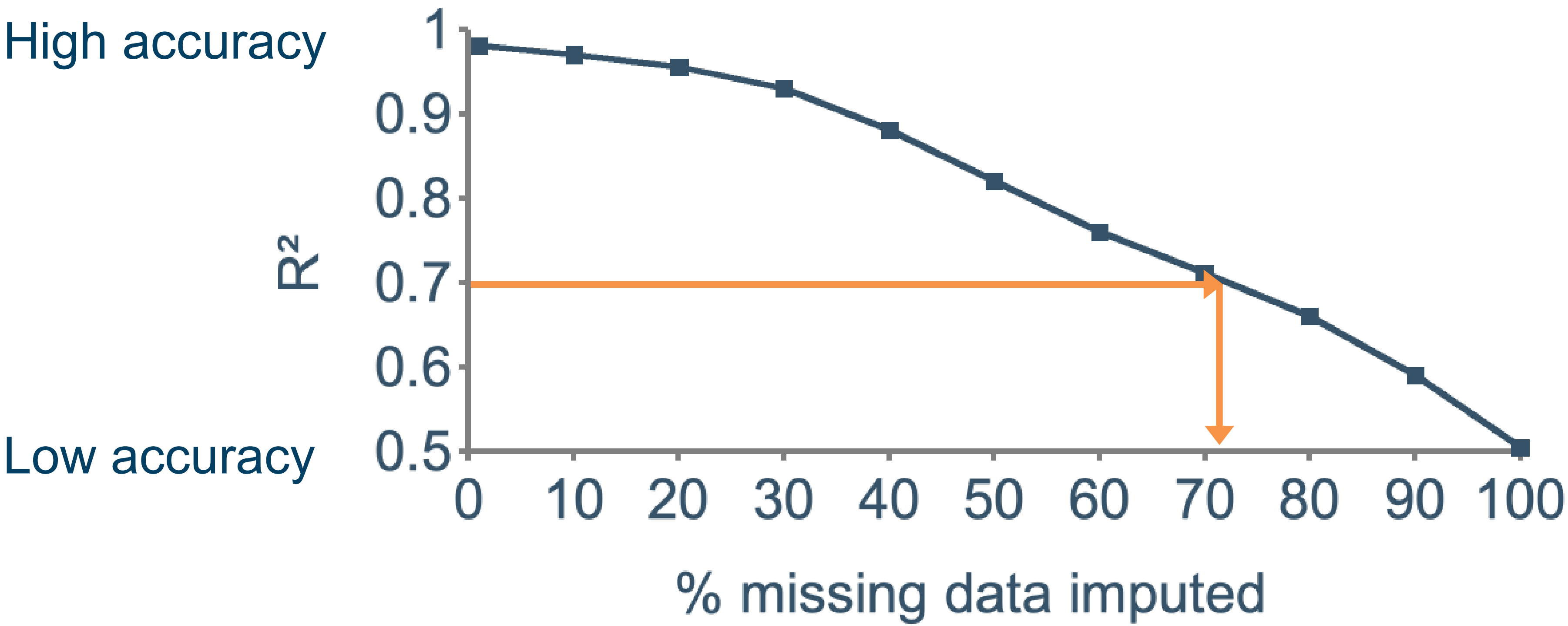
# Impute 50% of data with smallest uncertainty



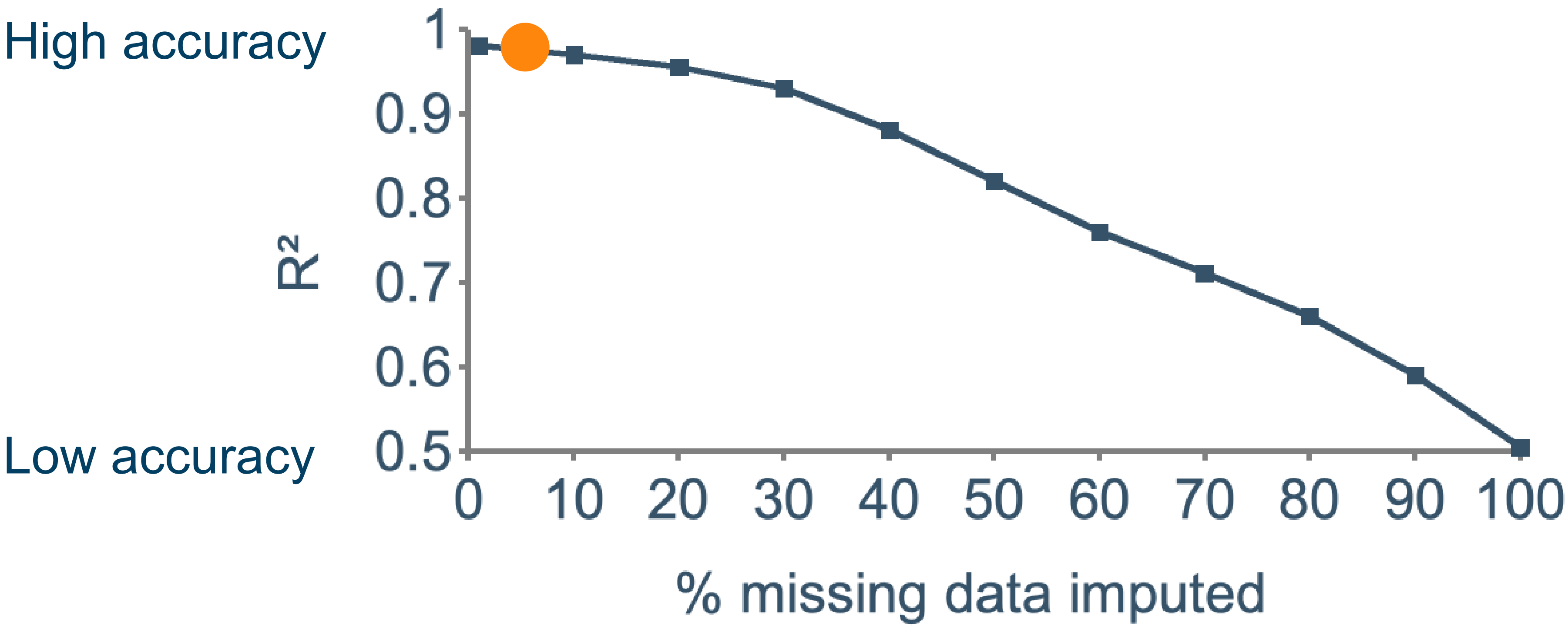
# Impute 25% of data with smallest uncertainty



# Improved performance by exploiting uncertainty

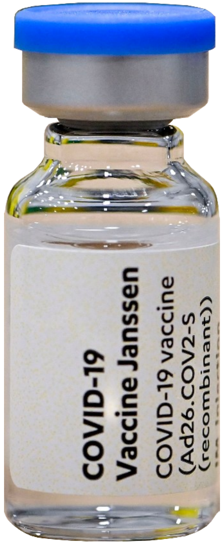


# Focus on compounds with low uncertainty

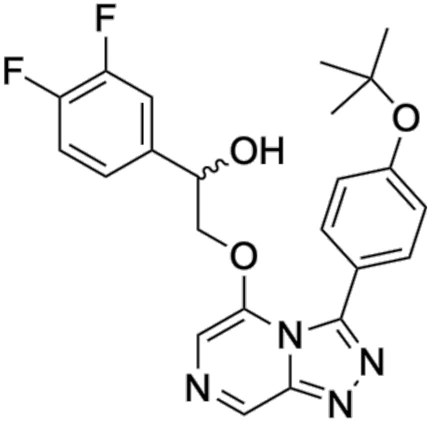


# Different drugs can treat the same ailment






# Open Source Malaria experimental validation



Optibrium & Intellegens

Davy Guan

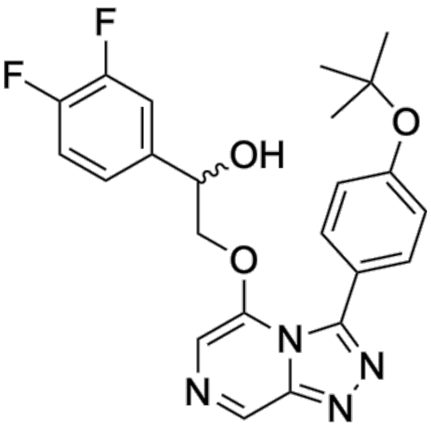
Exscientia

Molomics

0.647 μM

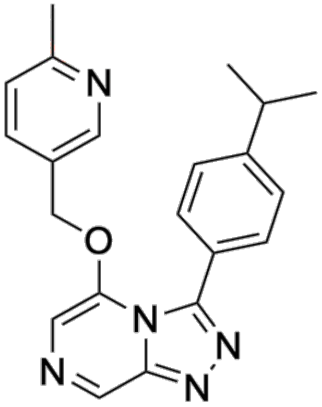
Journal of Medicinal Chemistry 64, 16450 (2021)

# Open Source Malaria other compounds



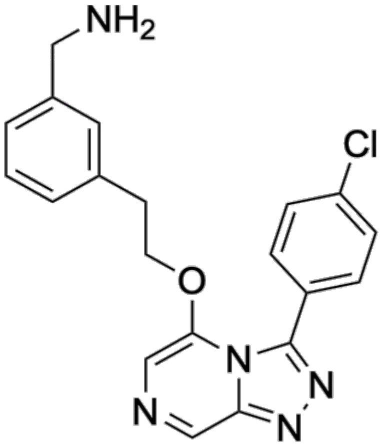

Optibrium & Intellegens

0.647 µM



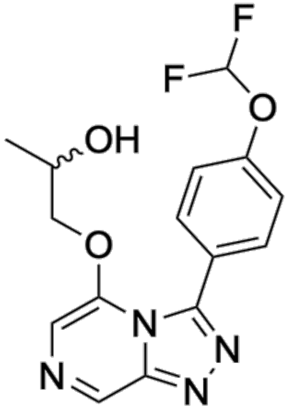

Davy Guan

>25 µM




Exscientia

10.9 µM




Molomics

>25 µM

Journal of Medicinal Chemistry 64, 16450 (2021)

OPEN SOURCE MALARIA
Looking for New Medicines

# Summary

Merge simulation with experimental data and exploit property-property relationships to circumvent missing data, designed an experimentally verified alloy for 3d printing

Exploited uncertainty to predict drug most probable drug

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

Taken to market through startup Intellegens as Alchemite Analytics™ and with partners Optibrium and Ansys

intellegens

optibrium

Ansys / GRANTA