UNIVERSITY OF CAMBRIDGE

# The modern day blacksmith

Gareth Conduit

Theory of Condensed Matter group

# Machine learning algorithm to

Train from sparse datasets

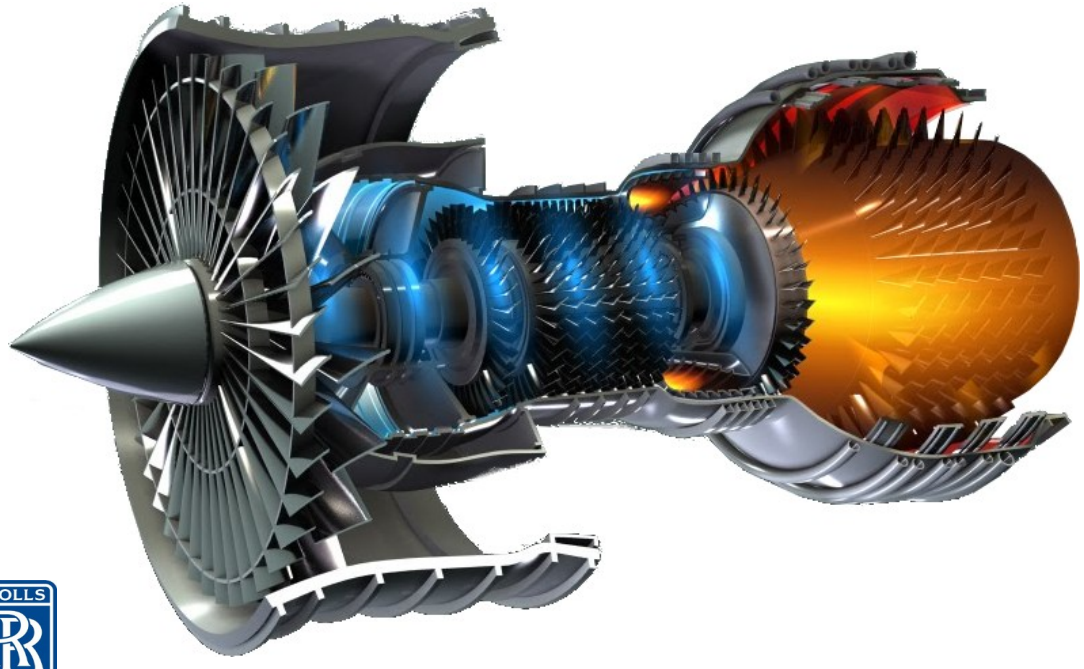
Merge simulations, physical laws, and experimental data

Reduce the need for expensive experimental development

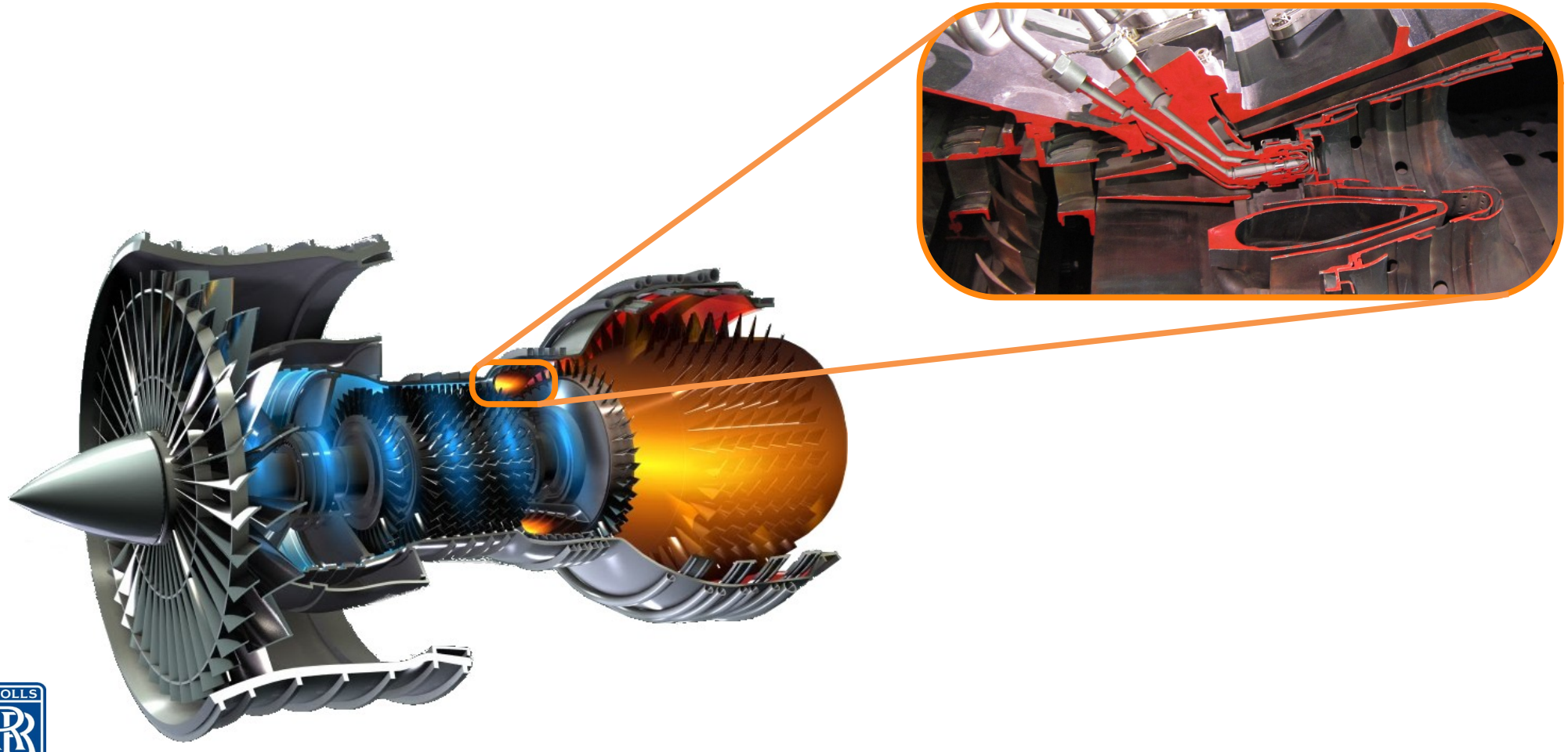
Accelerate materials and drugs discovery

Generic with proven applications in materials discovery and drug design

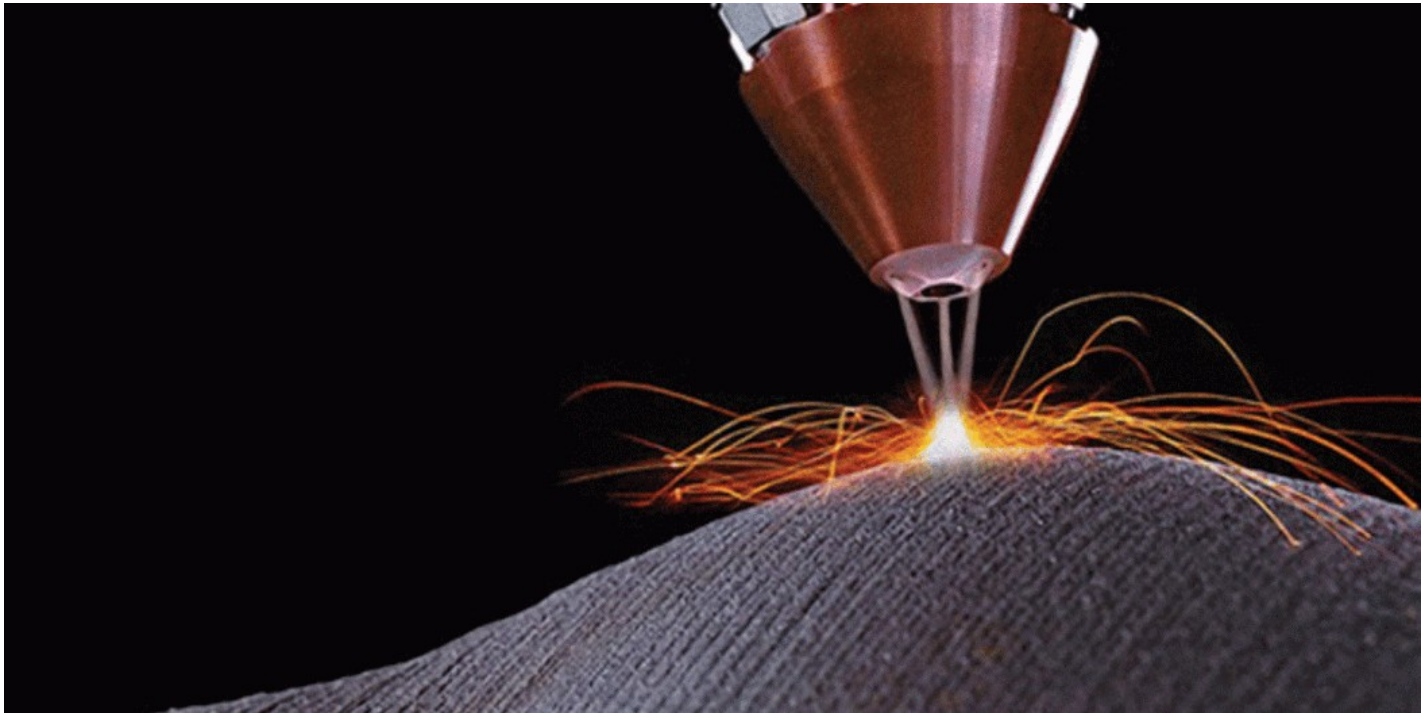
# Schematic of a jet engine



# Combustor in a jet engine



# Direct laser deposition requires new alloys

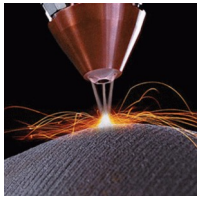


# *A posteriori* black box machine learning for materials design

Composition

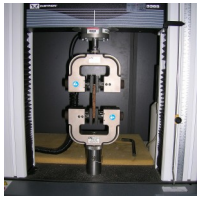
Properties

Defects

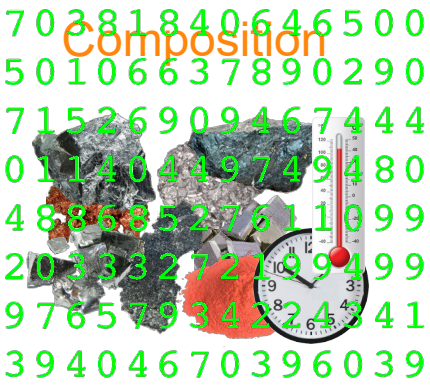


Fatigue

Strength



# Train the *a posteriori* machine learning

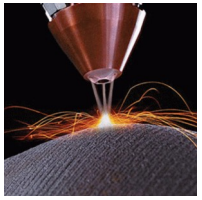



# *A posteriori* machine learning predicts material properties

Composition

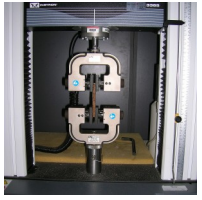
Properties

Defects

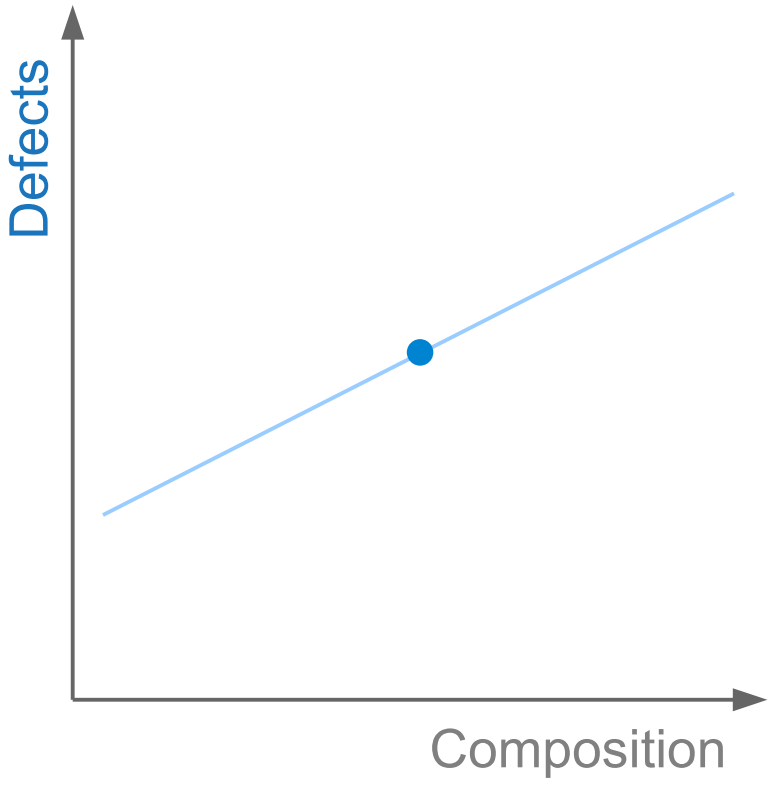


Fatigue

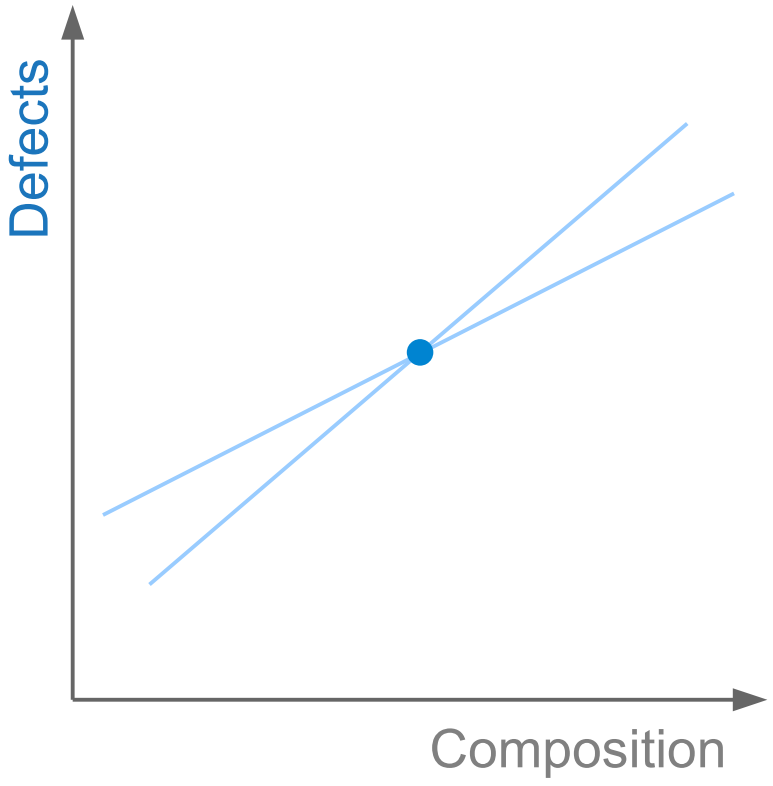
Strength



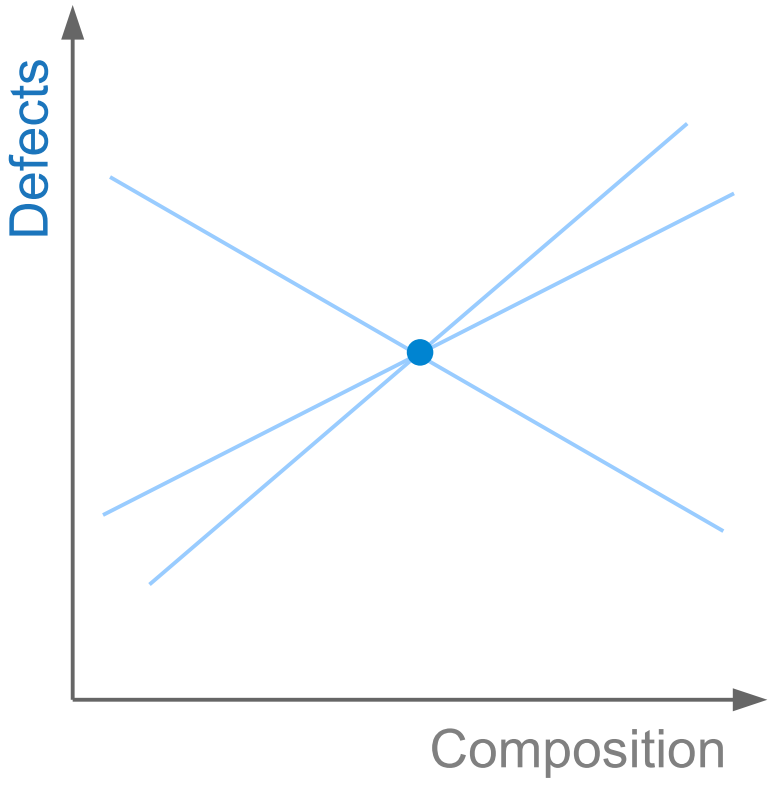
# One point cannot define a straight line



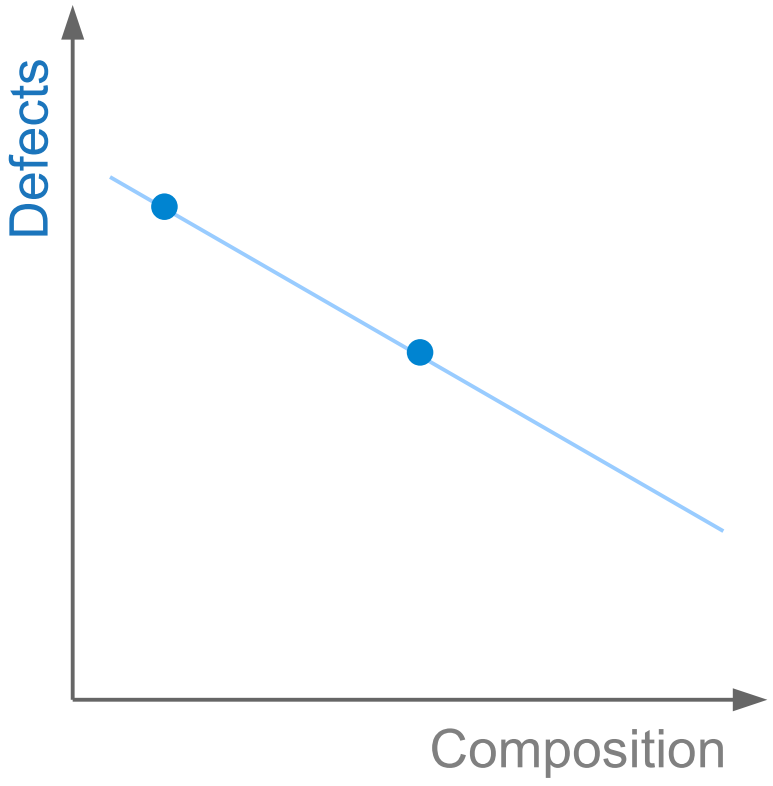
# One point cannot define a straight line



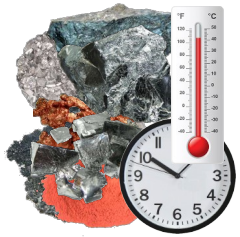
# One point cannot define a straight line

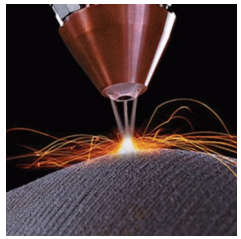


# Need at least two points to define a straight line



# Data available to model defect density



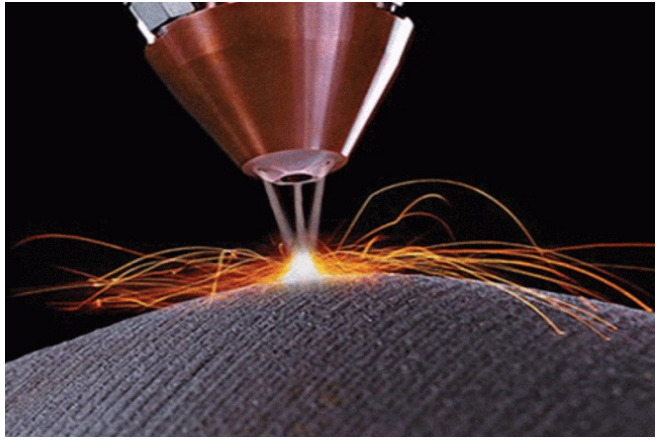


Composition and heat treatment space 30 dimensions

Requires 31 points to fit a hyperplane

Just 10 data entries available to model defect density

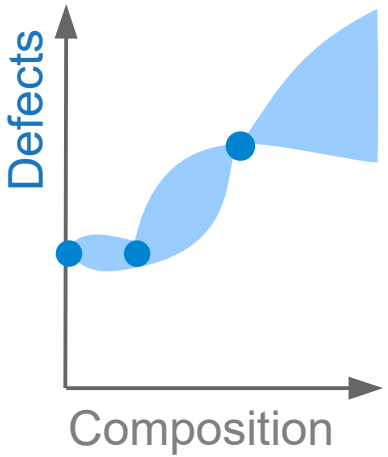
# Neural networks for materials design



Laser

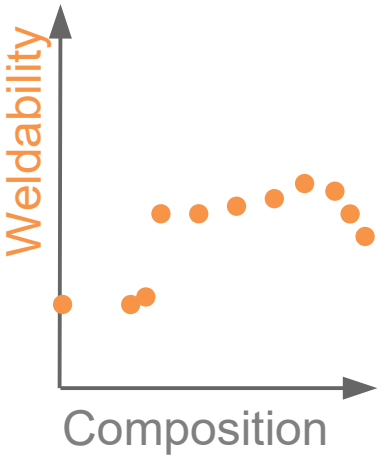
Electricity

# Insufficient data for processability

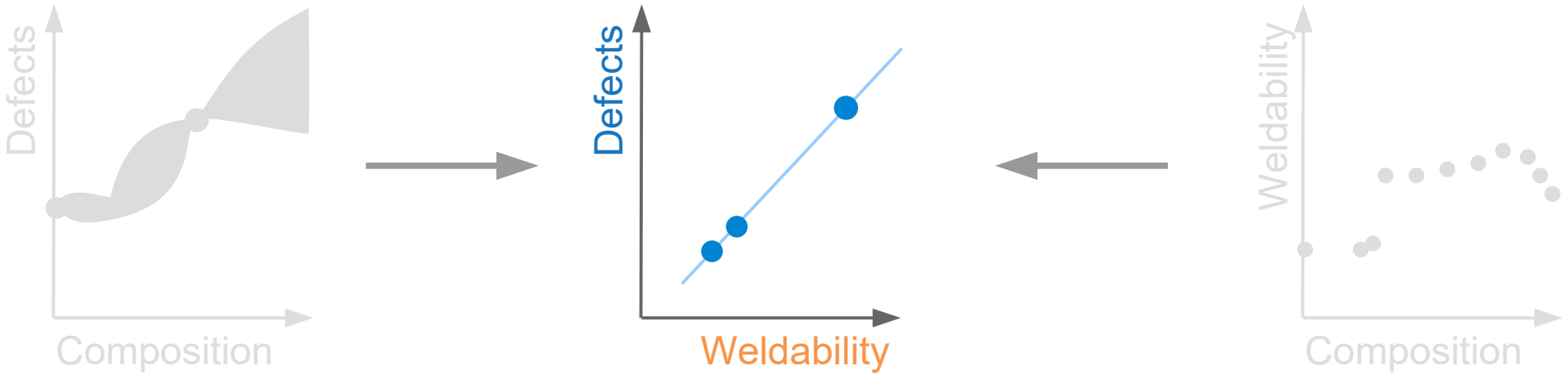


# Welding is analogous to direct laser deposition

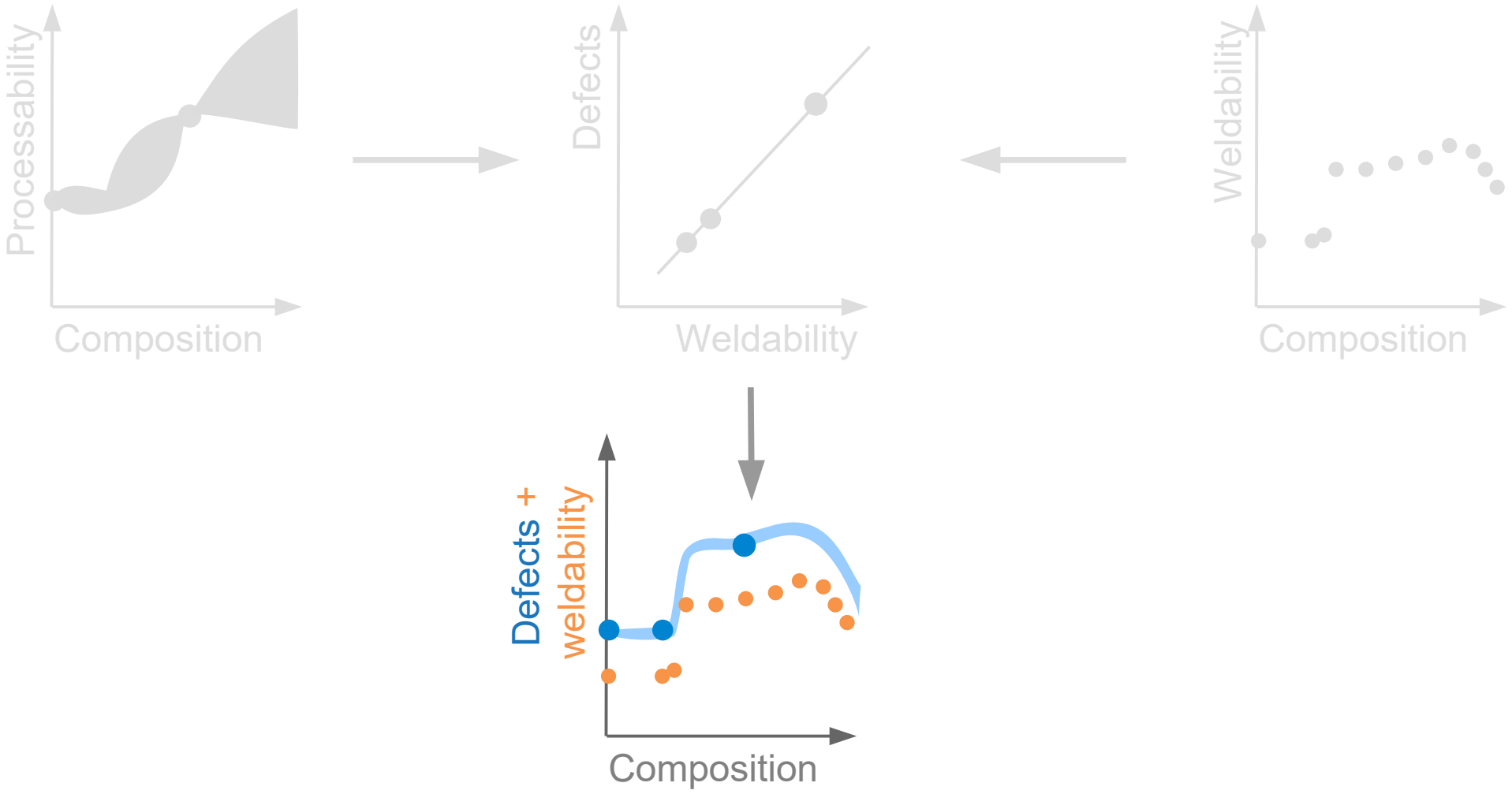


# Simple processability-welding relationship

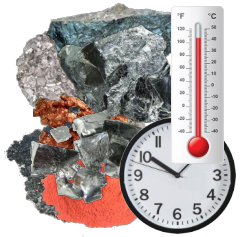


# Merging properties with the neural network



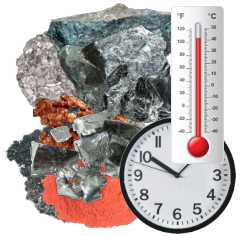
# First predict weldability

1000 entries



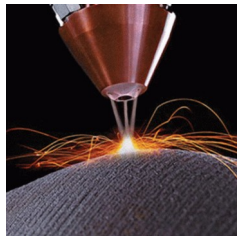
Use 1000 weldability entries to understand complex composition → weldability model

# Use weldability to predict defects formed



1000 entries

10 entries

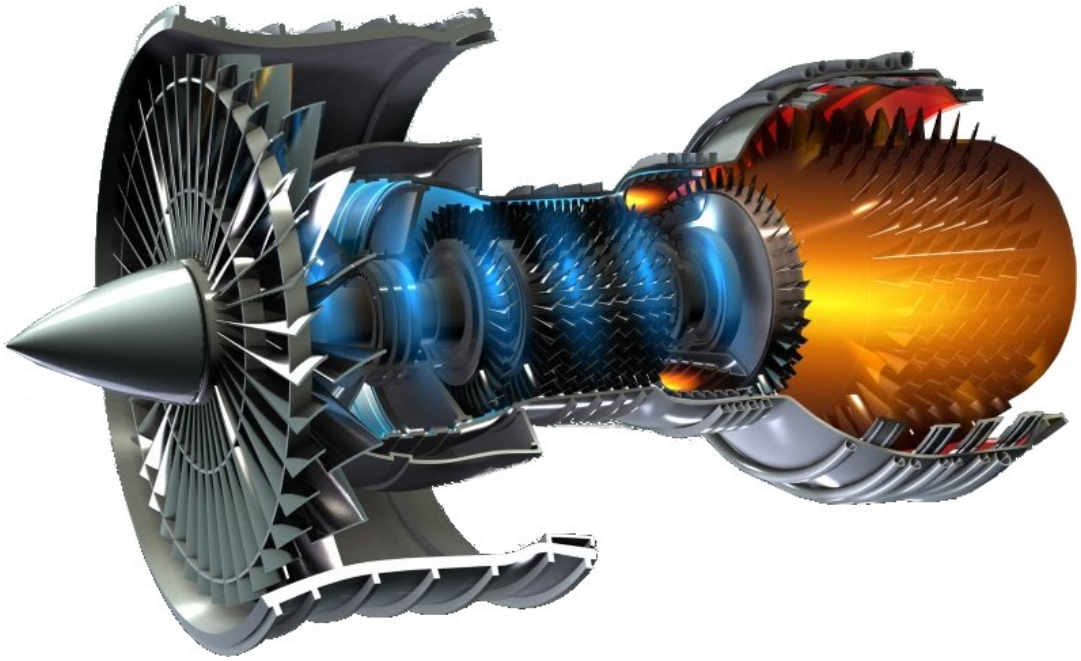


Use 1000 weldability entries to model complex composition → weldability

10 defects entries capture the simple weldability → defect relationship

Two interpolations give composition → defects extrapolation

# Schematic of a jet engine



# 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

Cr 19%

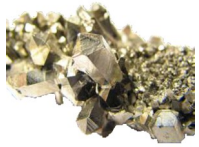
Co 4%

Mo 4.9%

W 1.2%

Zr 0.05%

Nb 3%



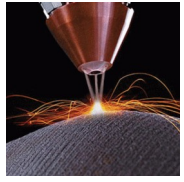
Al 2.9%

C 0.04%

B 0.01%

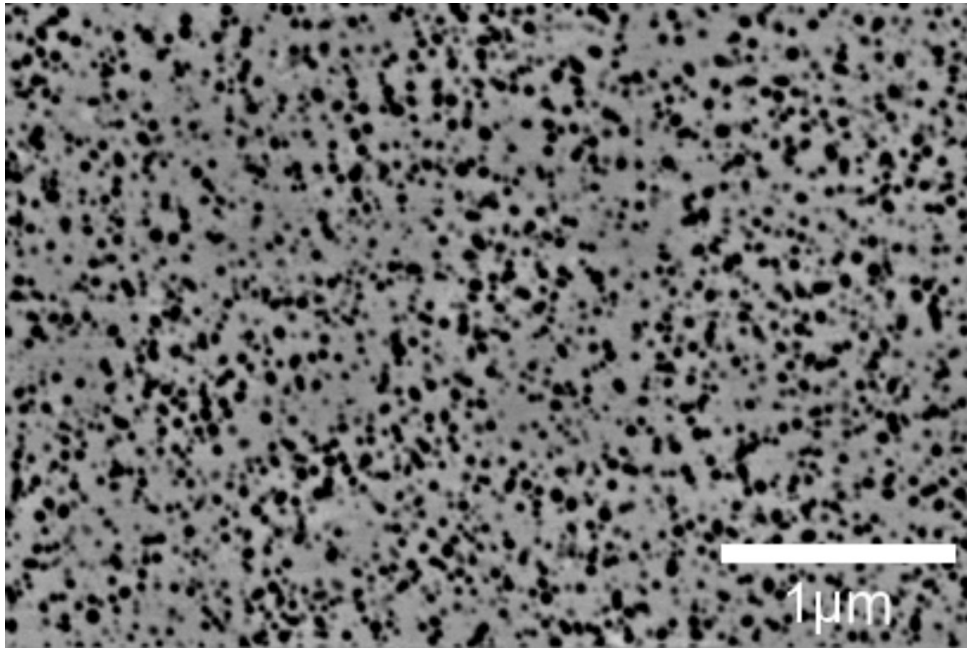
Ni

Expose 0.8



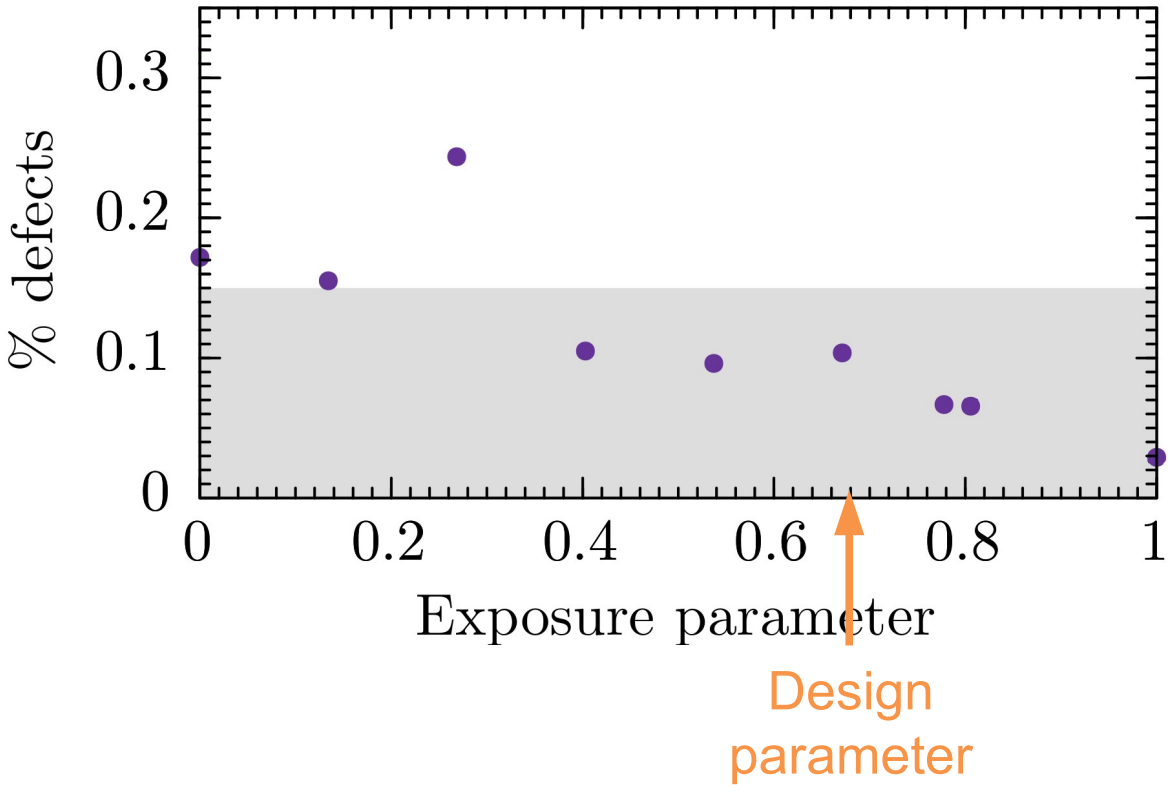
$T_{HT}$ 1300ºC

# Microstructure



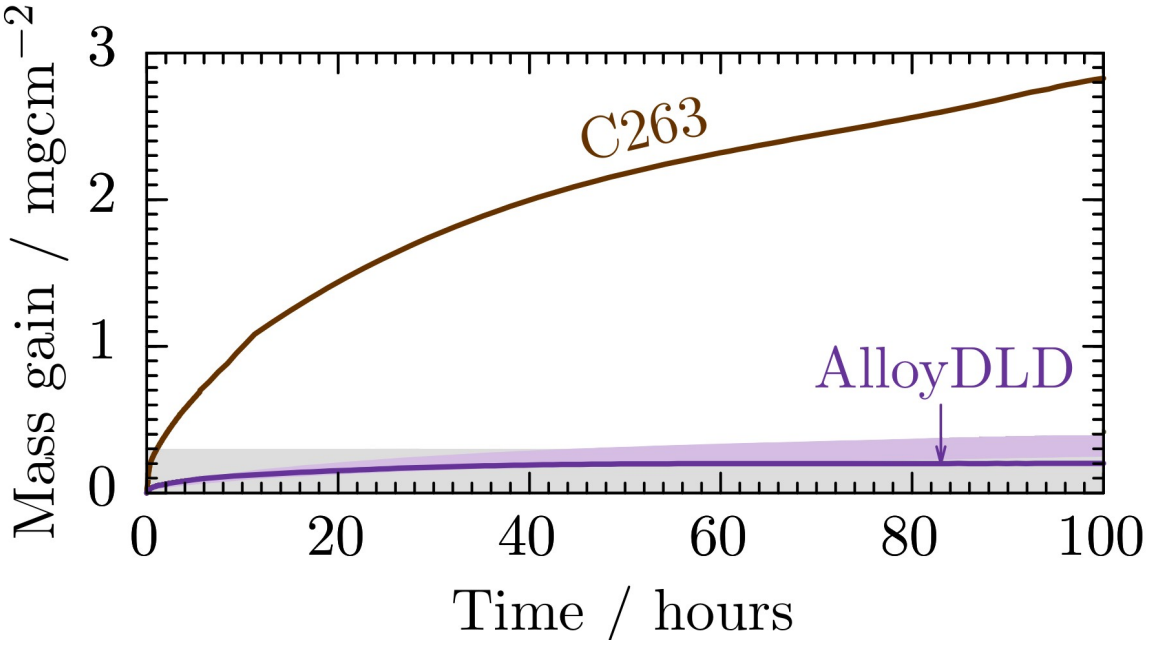

Probabilistic neural network identification of an alloy for direct laser deposition
Materials & Design 168, 107644 (2019)

# Testing the defect density




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

# Testing the oxidation resistance

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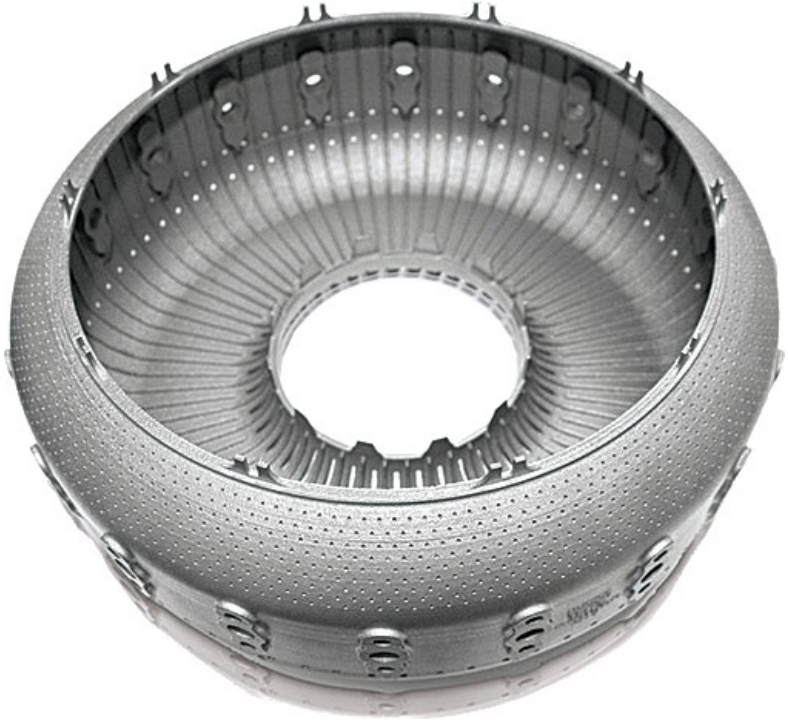
# Printing components for an engine



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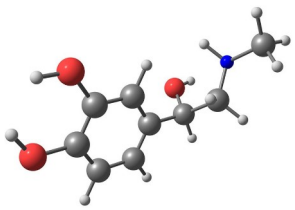
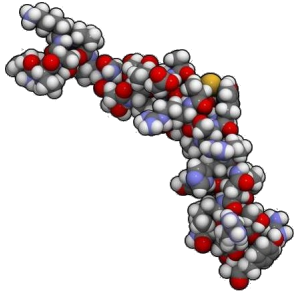
# Action of a drug



Drug

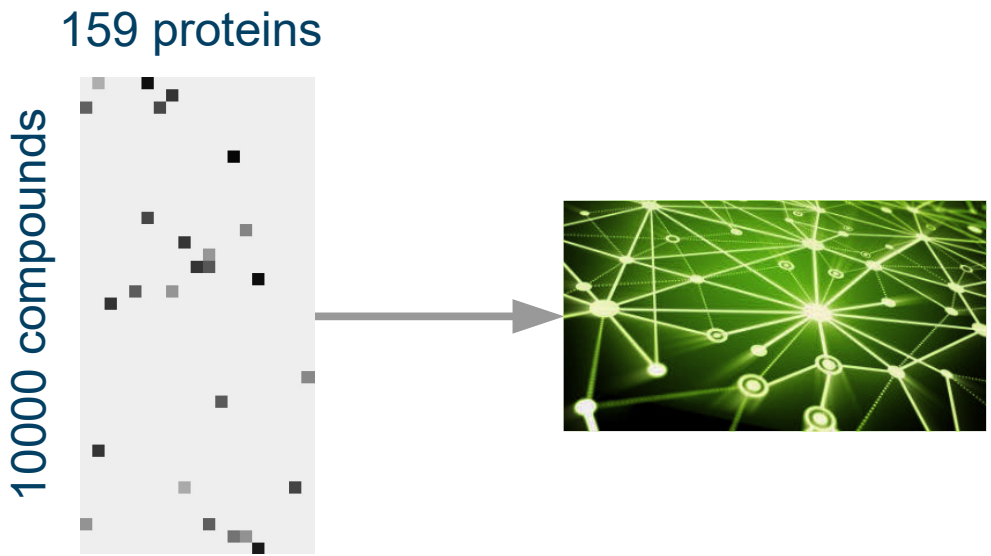


Protein

Effect

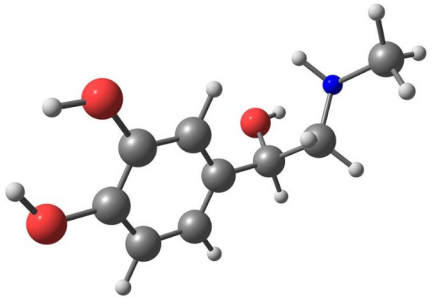
# Novartis dataset to benchmark machine learning

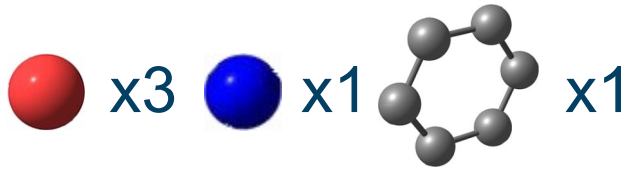
159 kinase proteins, 10000 compounds, data 5% complete



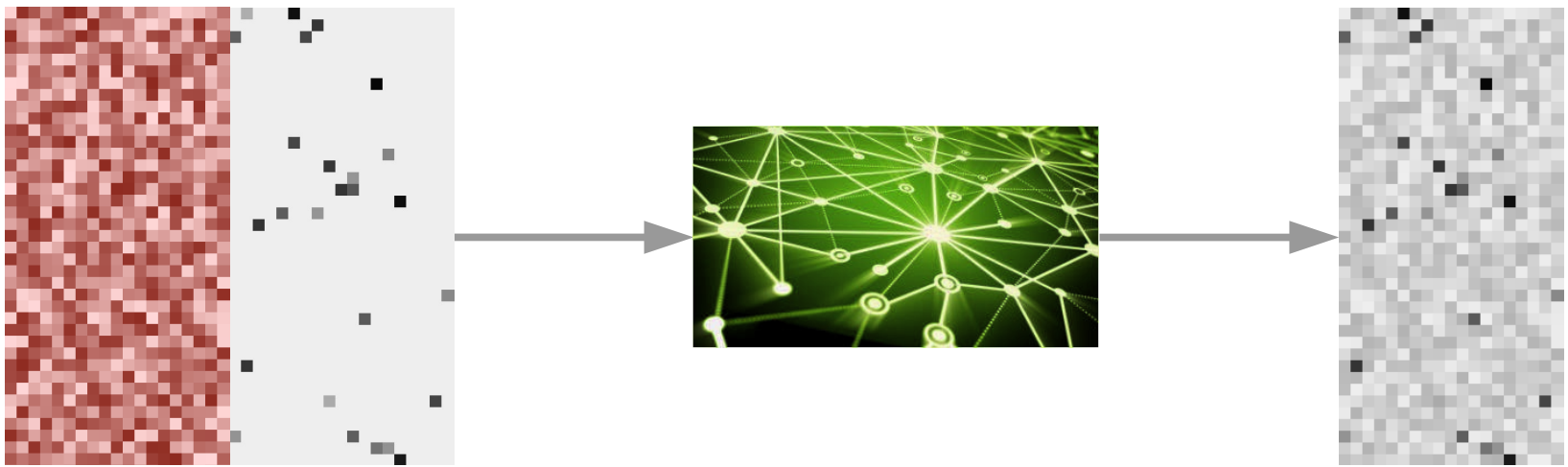

Imputation of Assay Bioactivity Data using Deep Learning
Journal of Chemical Information and Modeling, 59, 1197 (2019)

# Quantitative structure-activity relationships






Molecular weight=183 Da



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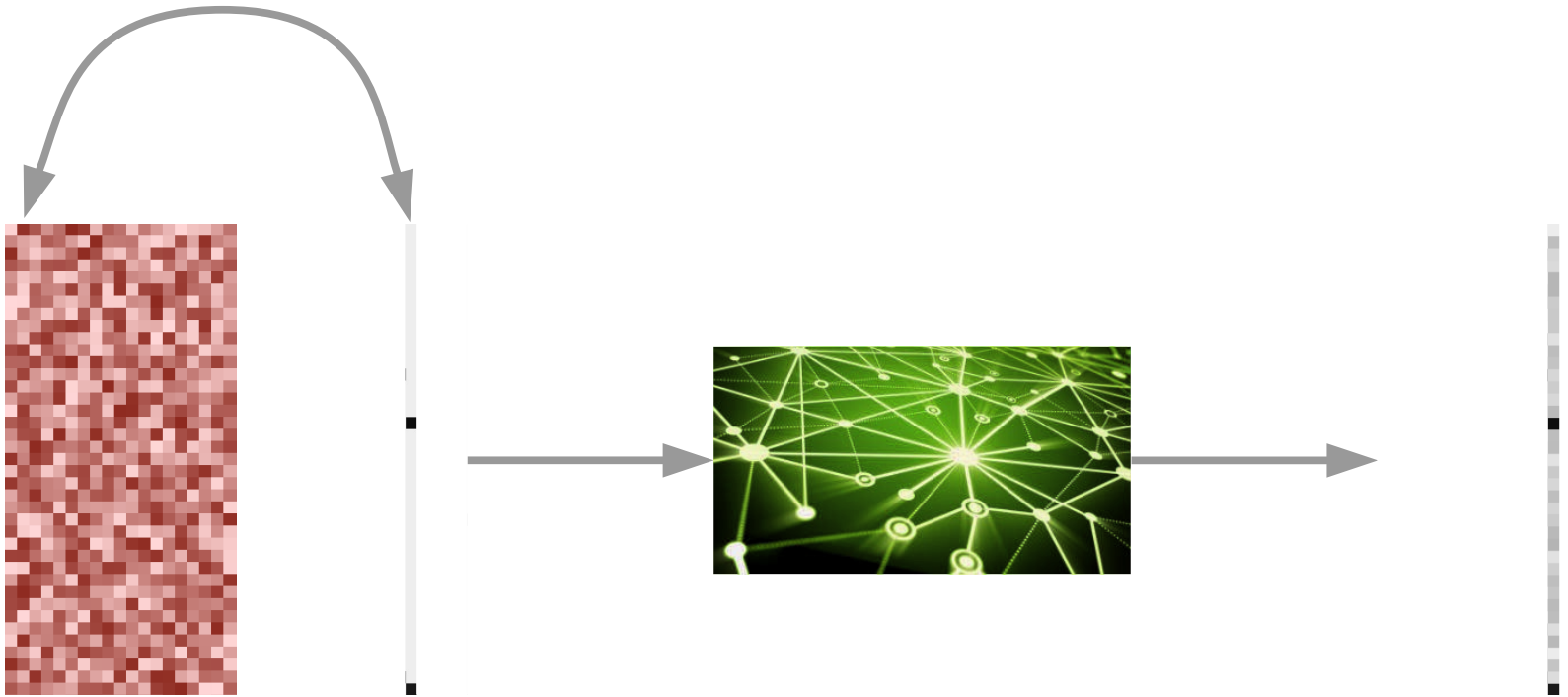

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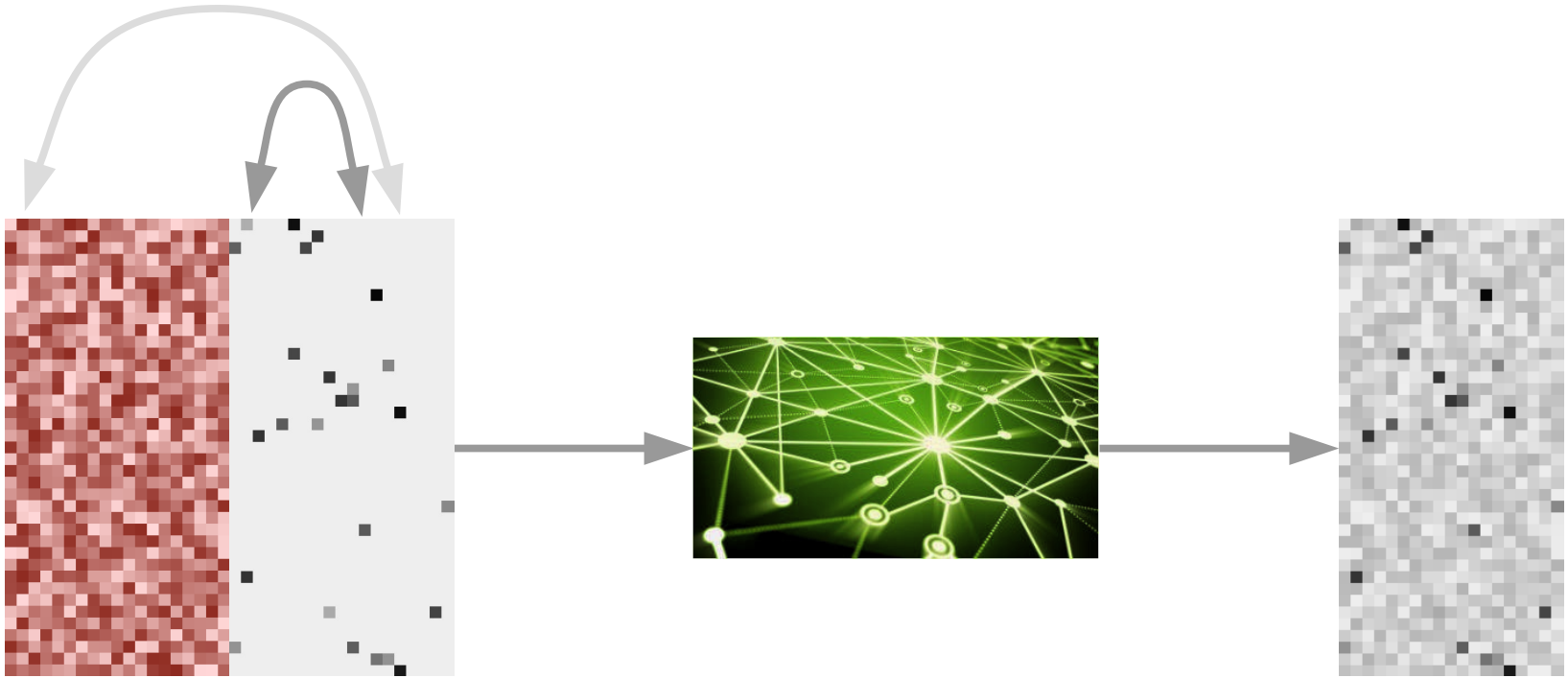
Journal of Chemical Information and Modeling, 59, 1197 (2019)

# Exploit protein-protein correlations



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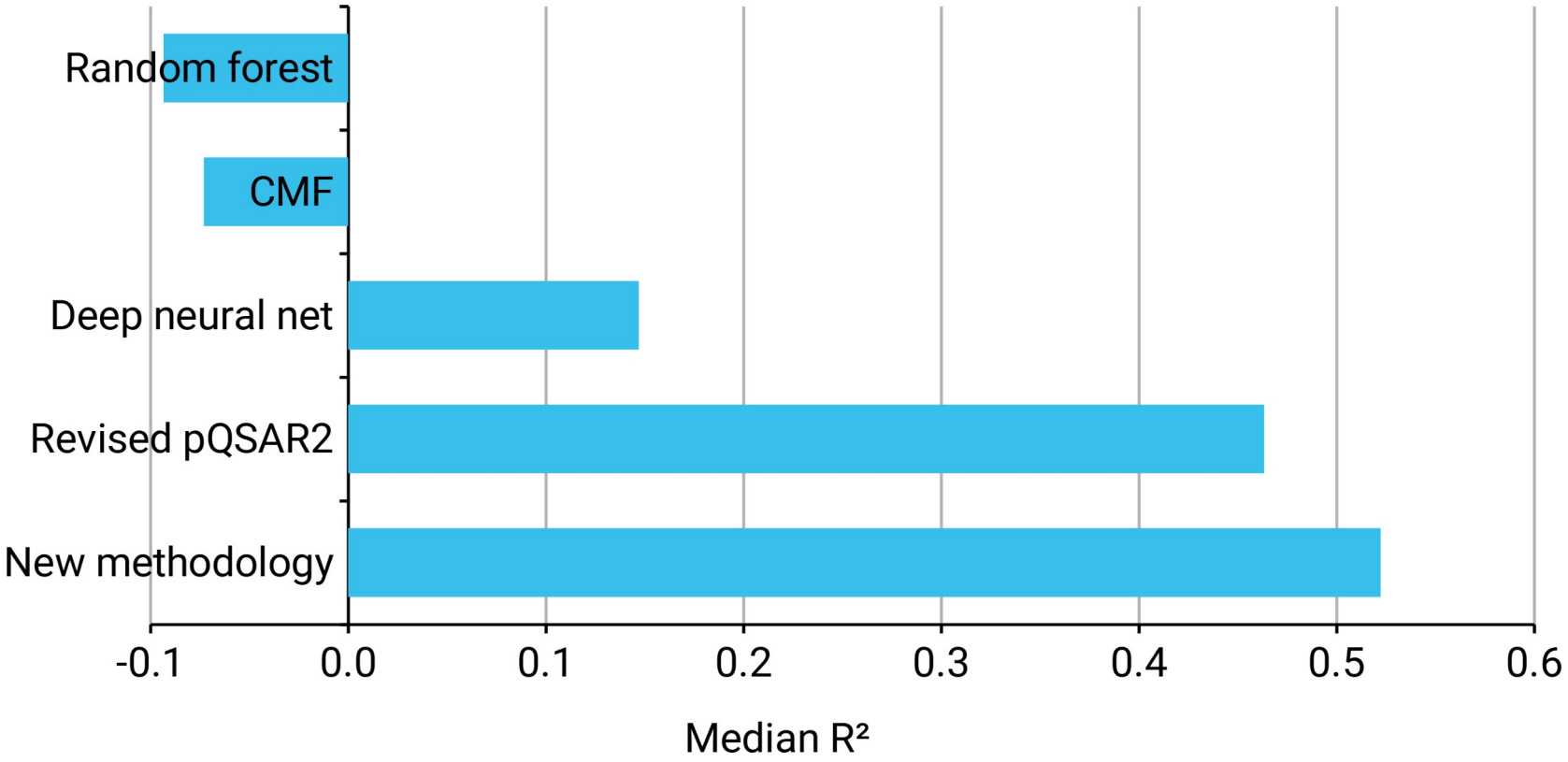
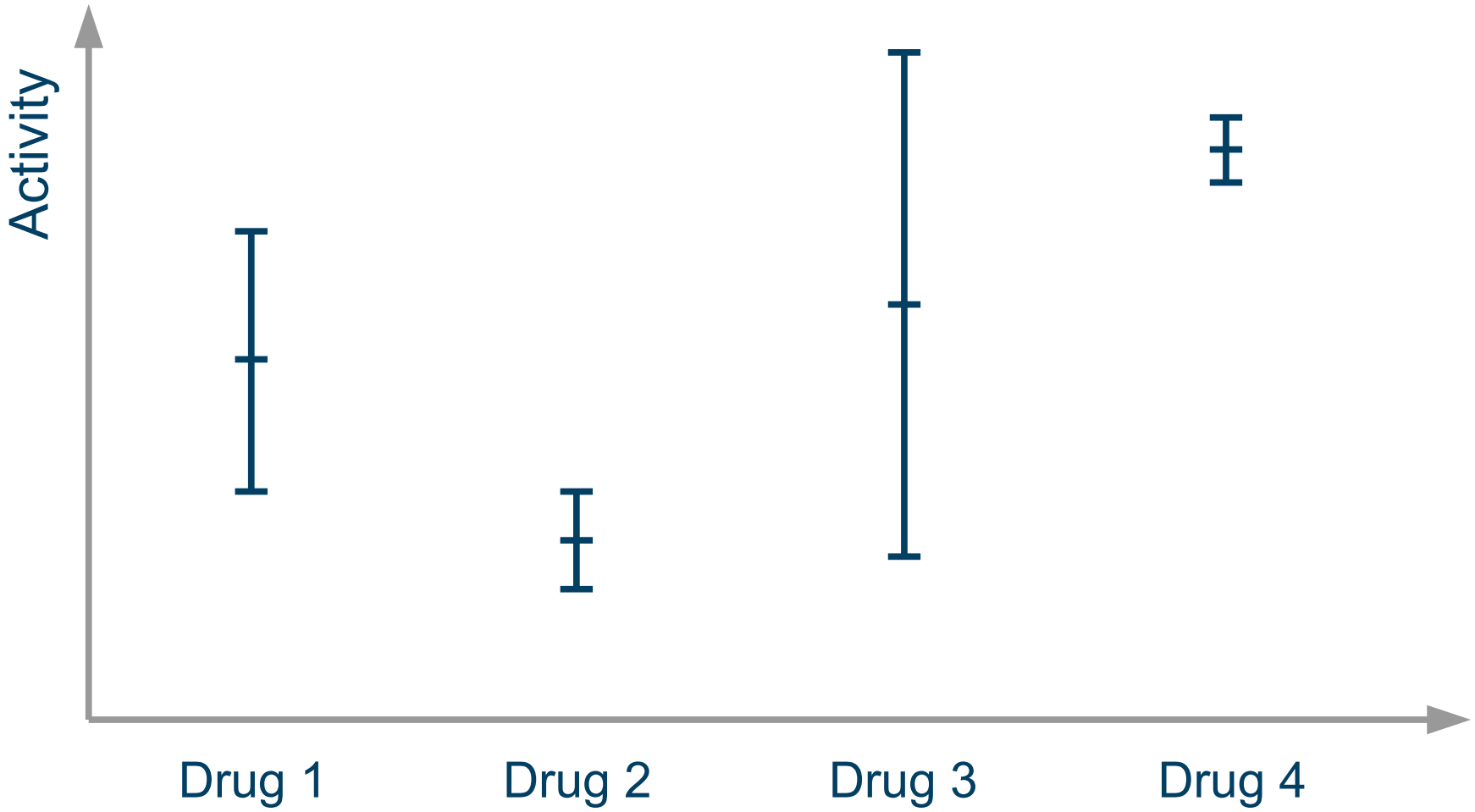
Journal of Chemical Information and Modeling, 59, 1197 (2019)

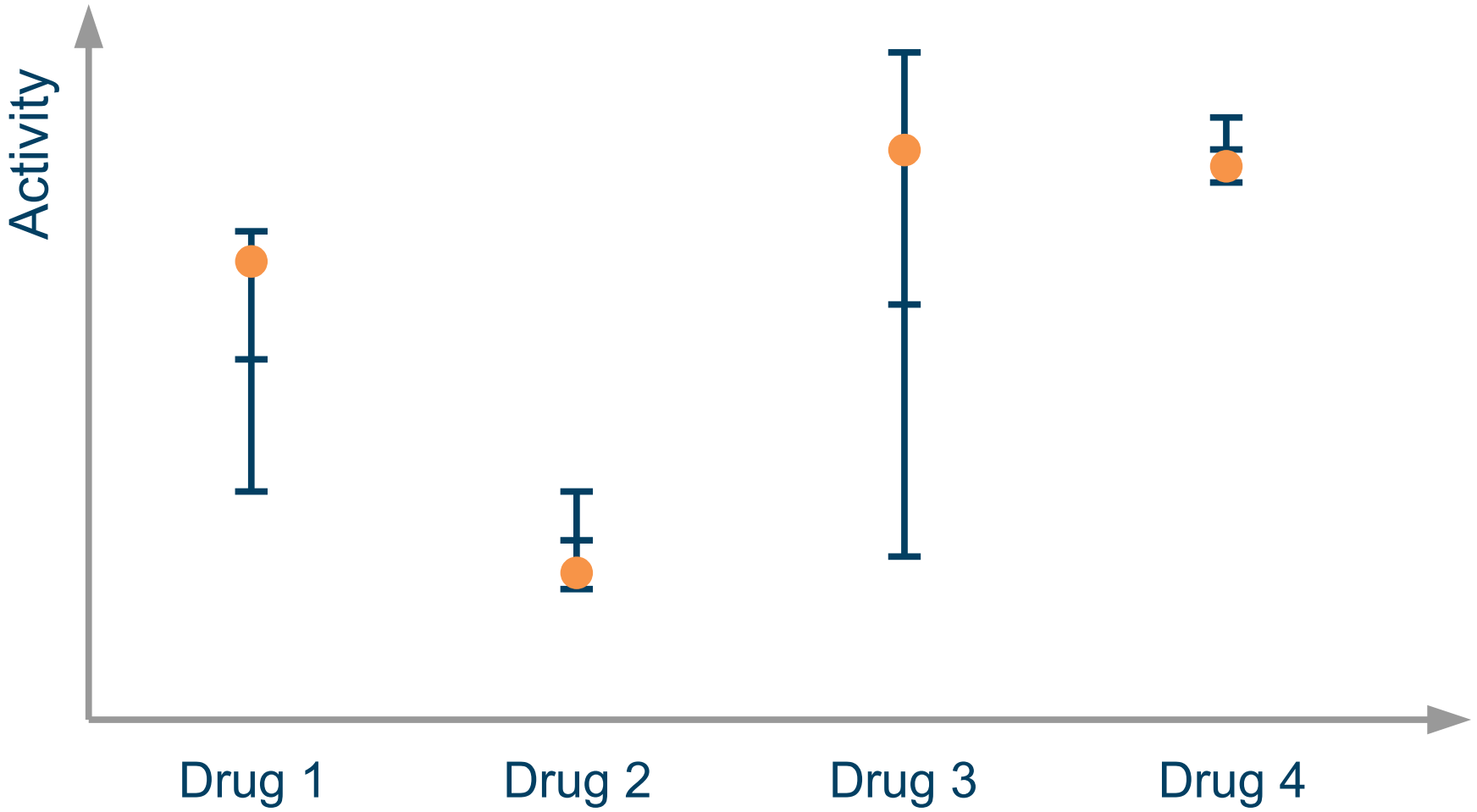
# Comparison of techniques



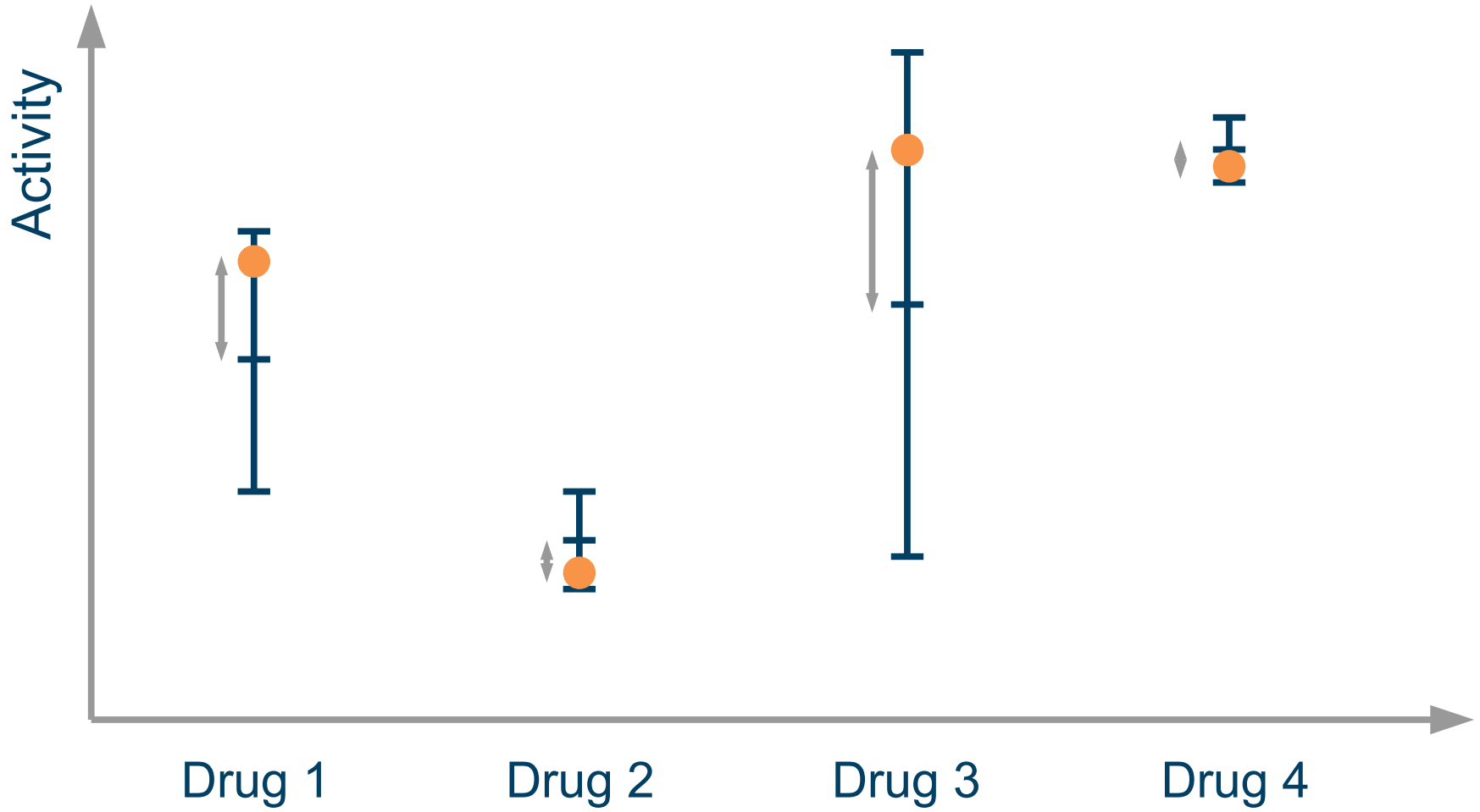
# Predictions have an uncertainty



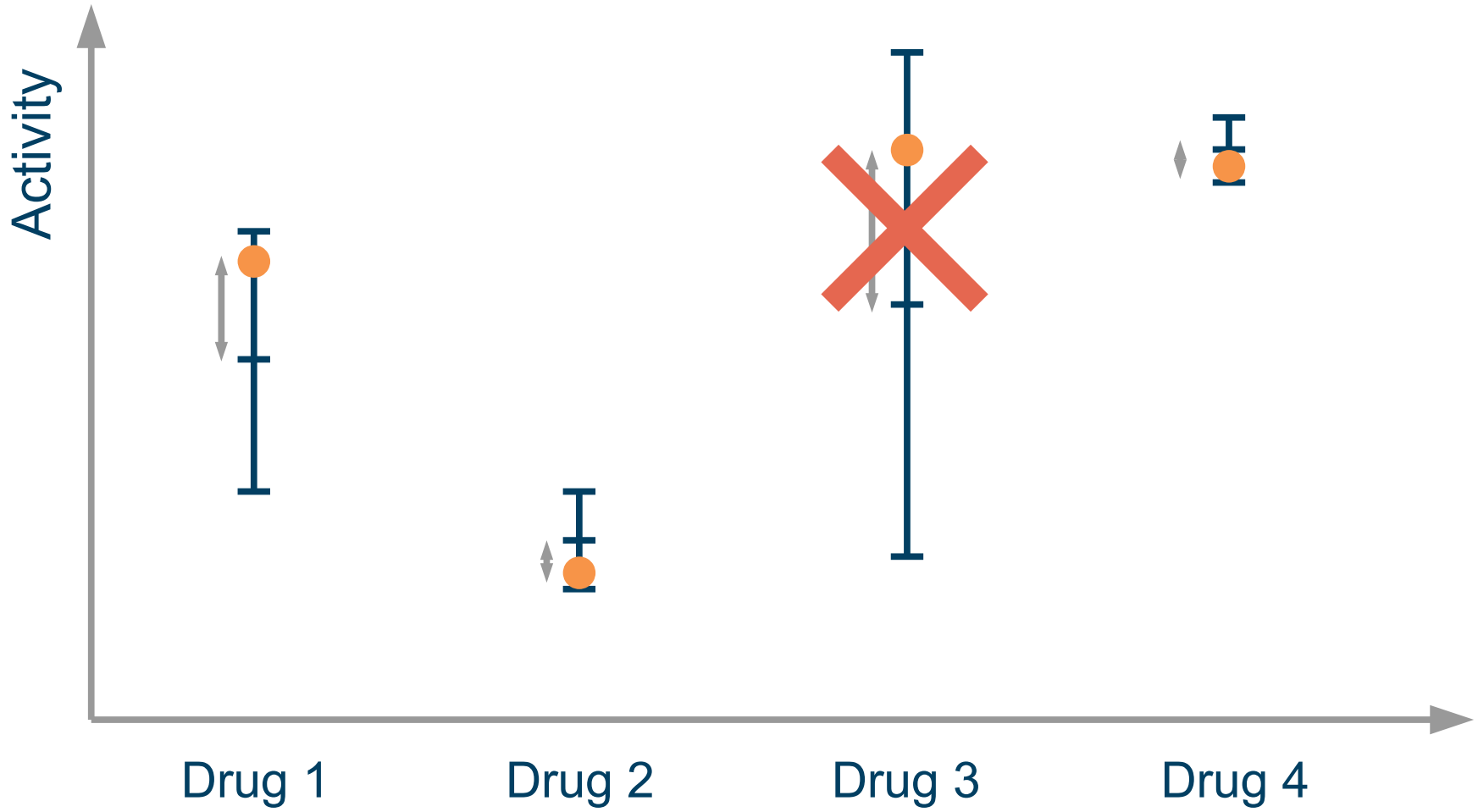
# Validation data typically within one standard deviation



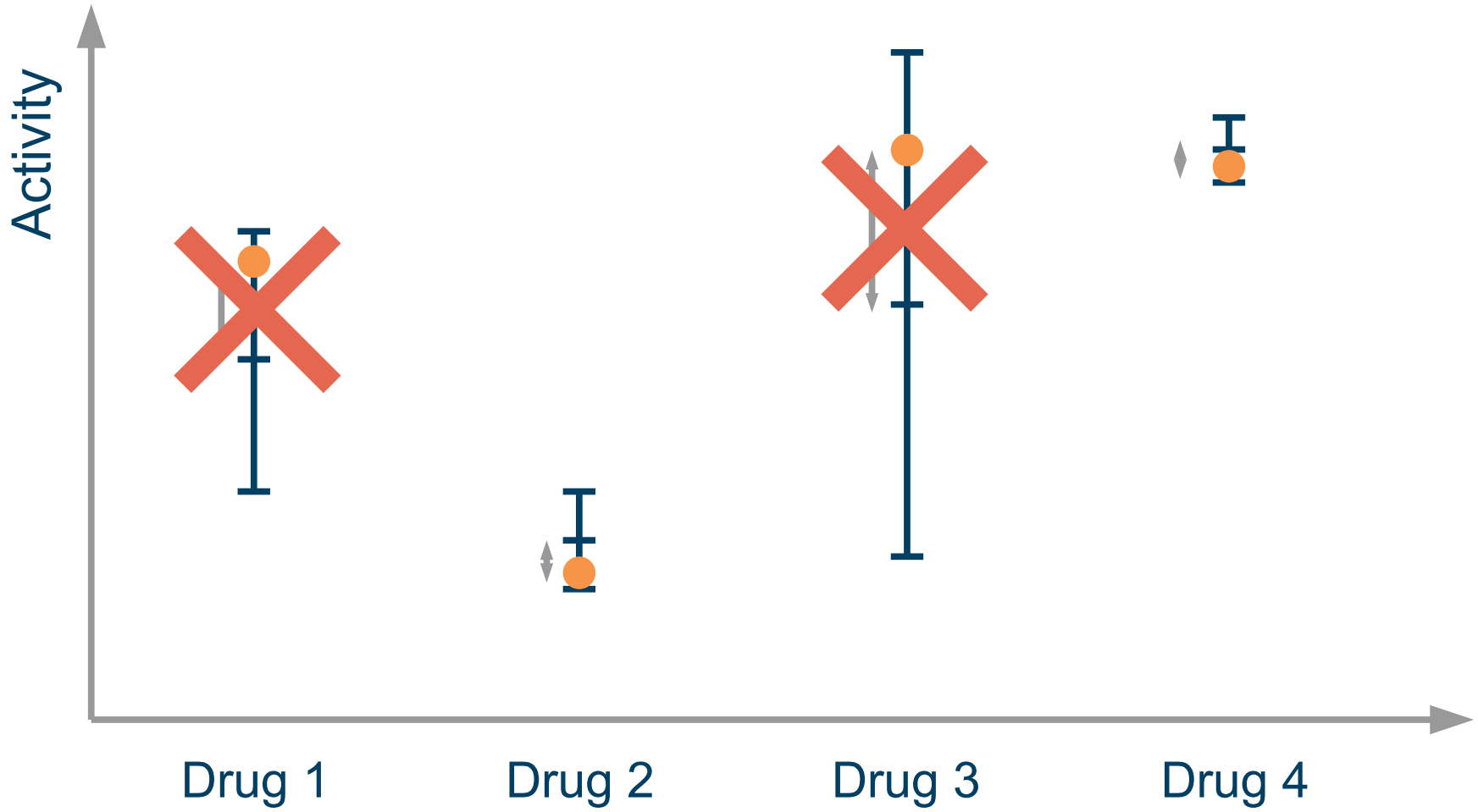
# $R^2$ metric calculated with difference from mean



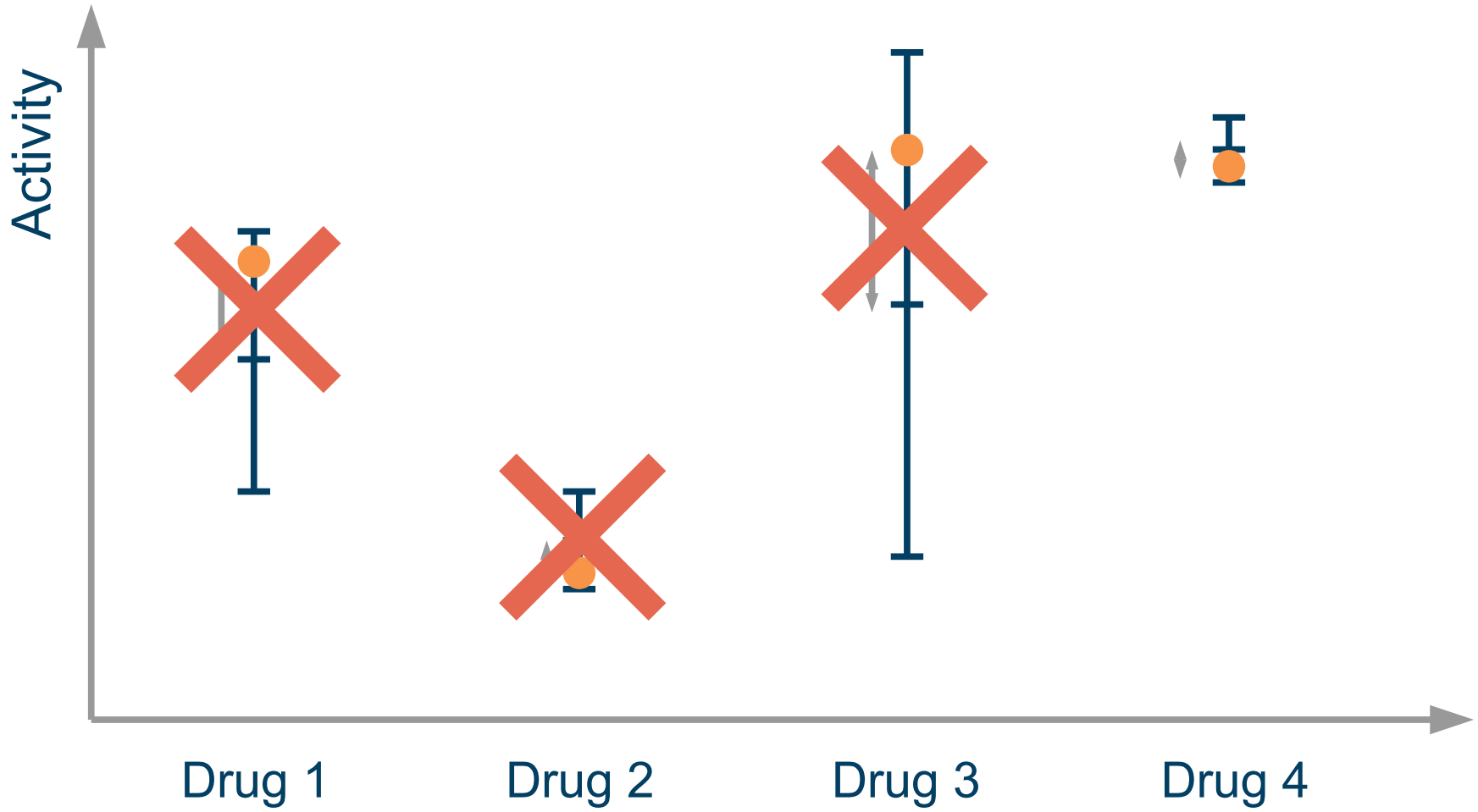
# Impute 75% of data with smallest uncertainty



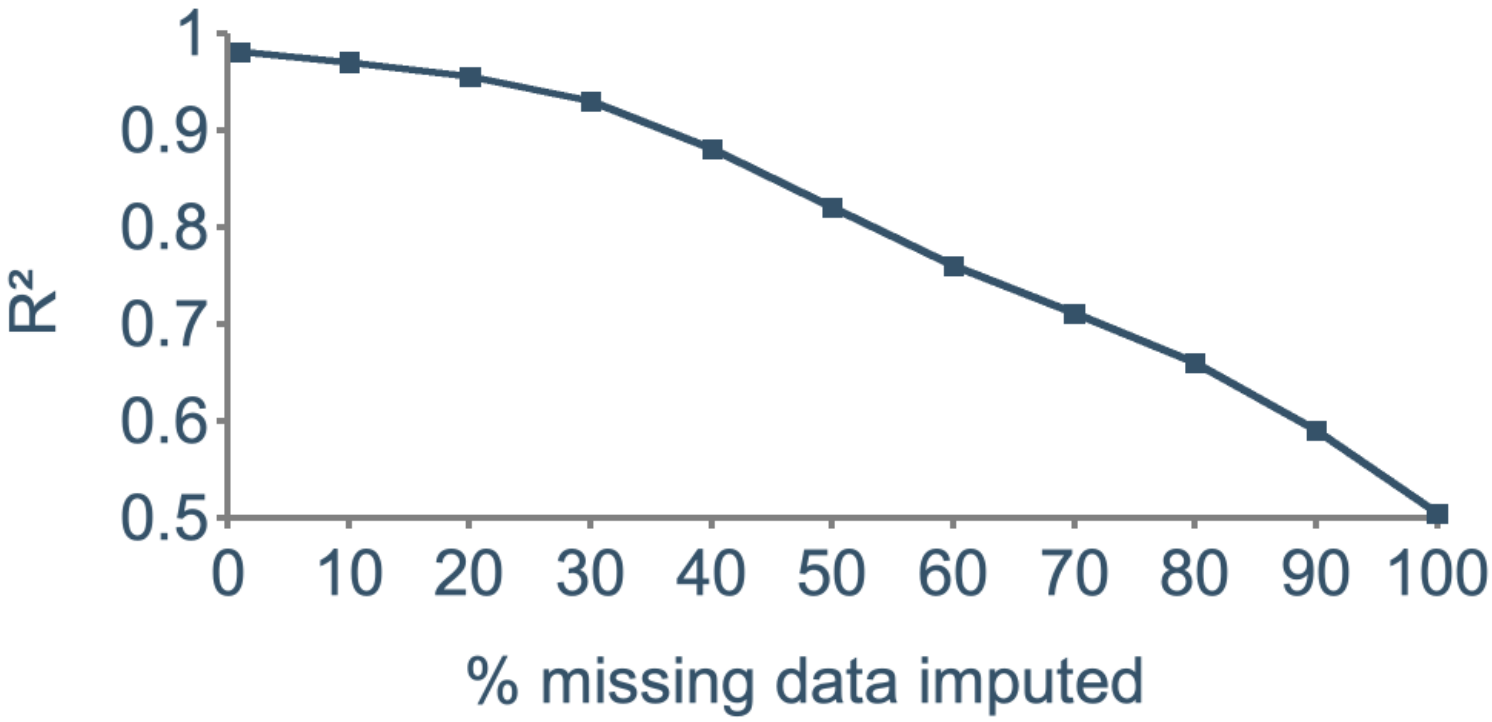
# Impute 50% of data with smallest uncertainty



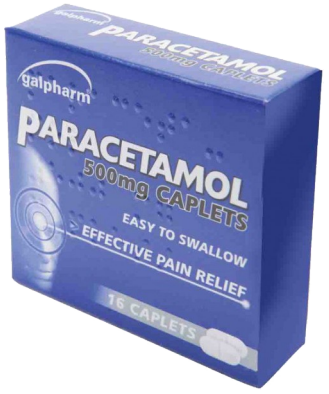
# Impute 25% of data with smallest uncertainty



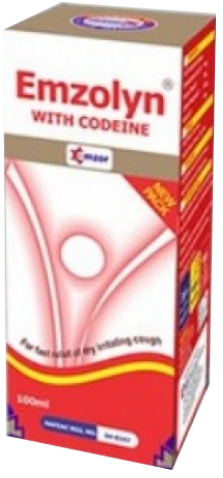
# Improved performance by exploiting uncertainty



# Different drugs can treat the same ailment



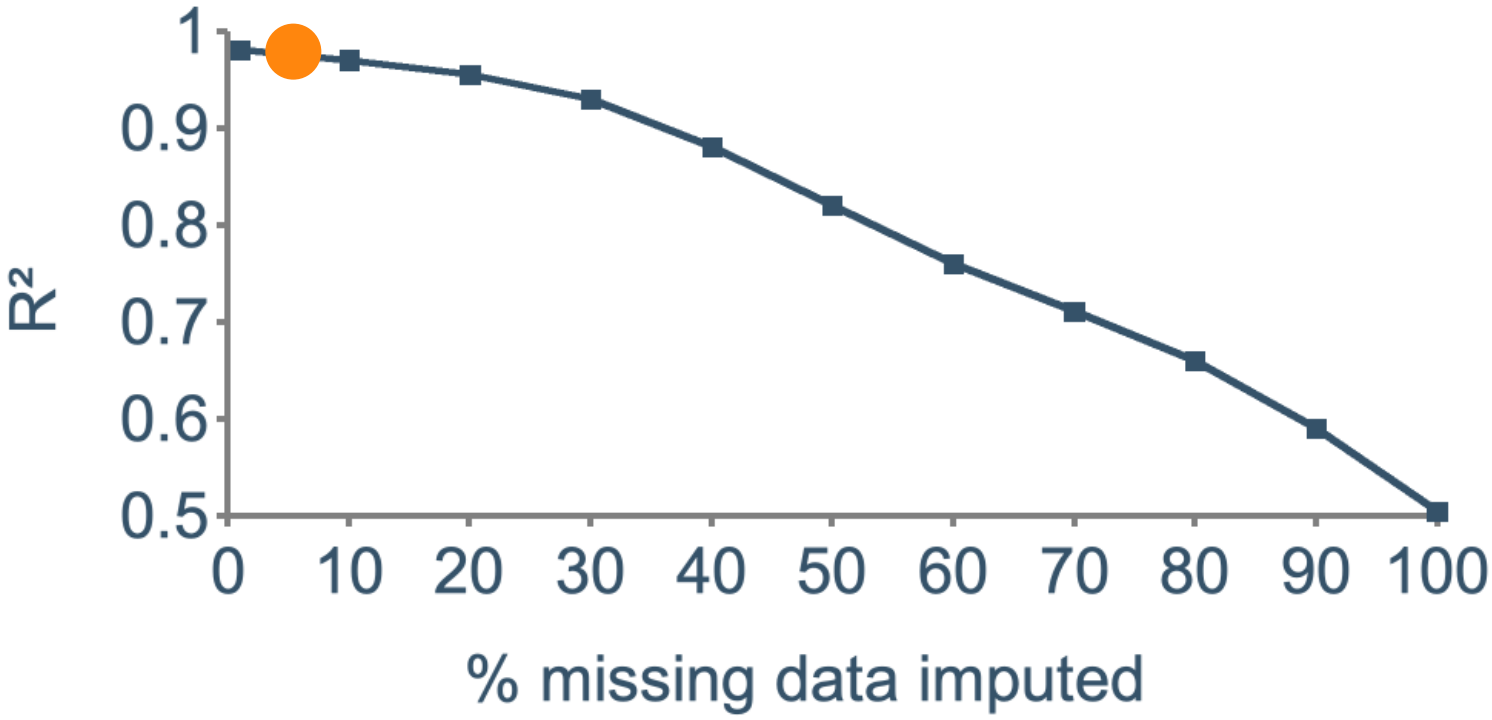


# Open Source Malaria contest

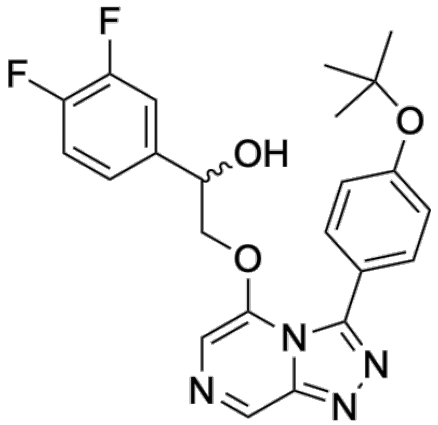
OPEN SOURCE MALARIA

Looking for New Medicines

# Focus on compounds with low uncertainty



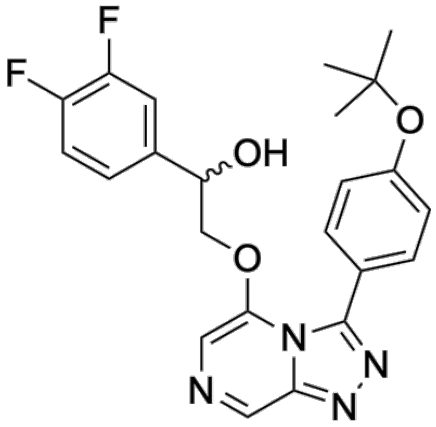
# Open Source Malaria experimental validation




Irwin, Whitehead, Wade,
Segall, Conduit

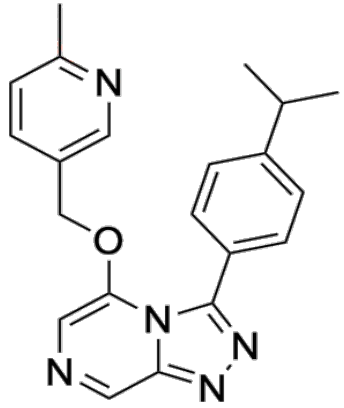
0.647 µM

# Open Source Malaria other compounds



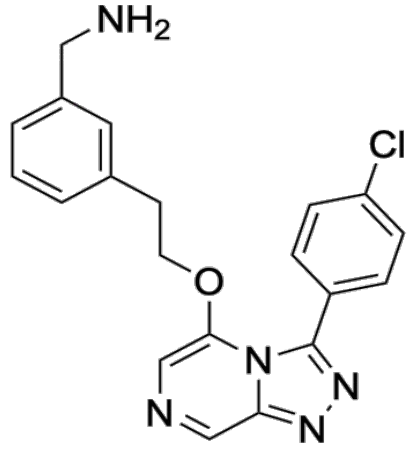

Irwin, Whitehead, Wade, Segall, Conduit

0.647 µM



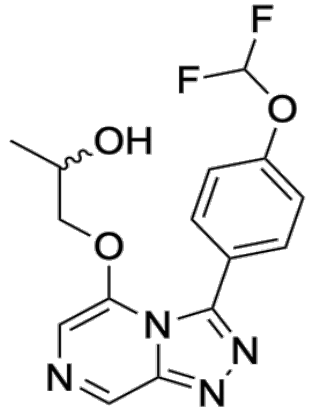

Davy Guan

>25 µM




Exscientia

10.9 µM




Molomics

>25 µM

# Commercialization

intellegens

Alchemite Analytics™ platform for materials and chemicals with Intellegens released in September 2020

optibrium

Machine learning tool embedded into Cerella™ released in October 2020

Ansys / GRANTA

Integrate machine learning into Granta MI™

# Summary

Merge different experimental quantities and computer simulations into a holistic design tool

Designed and experimentally verified alloy for direct laser deposition

Designed experimentally verified drug in Open Source Malaria competition

Taken to market through startup Intellegens