UNIVERSITY OF CAMBRIDGE

The modern-day blacksmith

Gareth Conduit

Machine learning for engineering faces the challenge that

not everything has been measured so data is sparse

Actively pursue three approaches to empower machine learning

not everything has been measured so data is sparse

Exploit property-property relationships to merge data, simulations, and physical laws

Adaptive design of experiments to accelerate discovery

Probabalistic formulation design

Black box machine learning for materials design

Properties

Defects

Composition

Fatigue

Strength

Train the machine learning

Machine learning predicts material properties

Composition

Properties

Defects

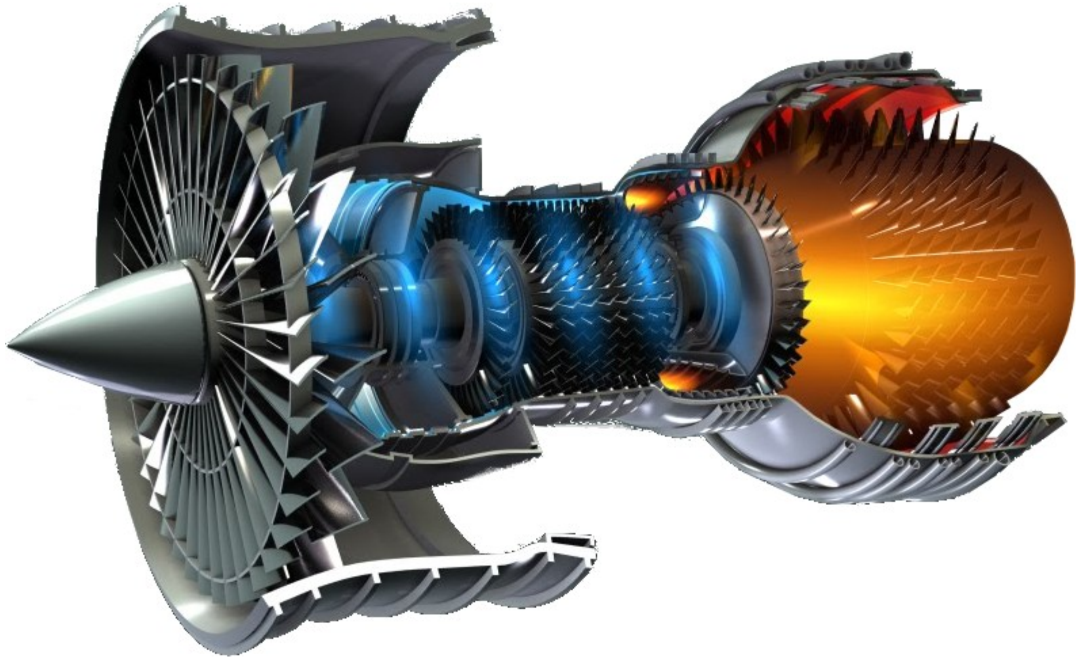
Fatigue

Strength

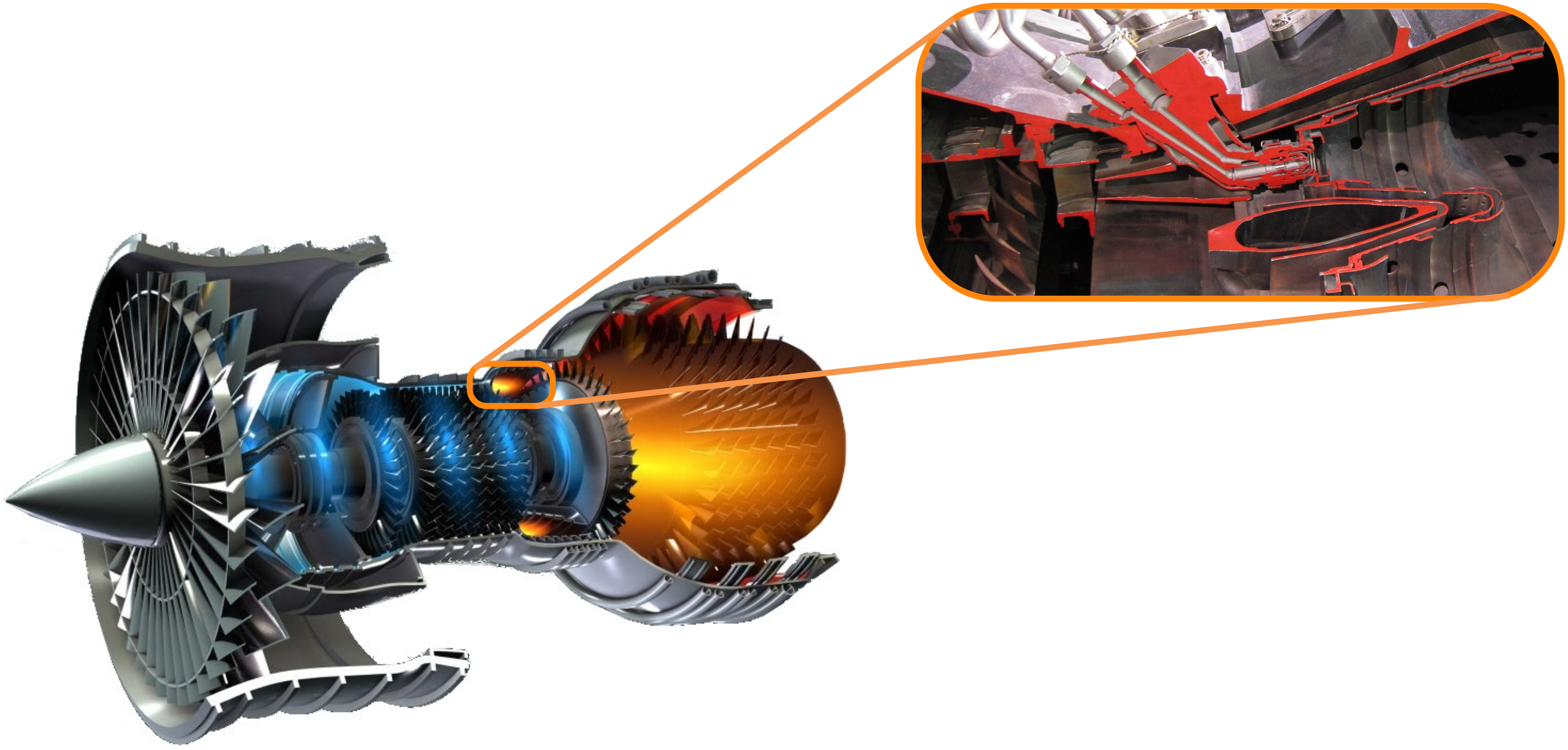
Exploit property-property relations

to circumvent sparse data

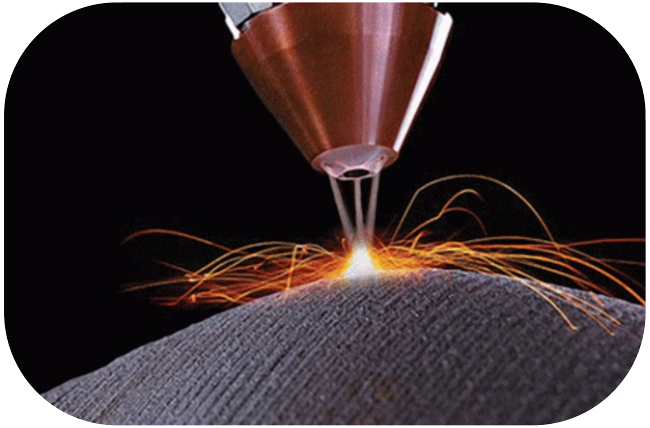
Jet engine schematic



Combustor in a jet engine



Direct laser deposition



Data available to model defect density

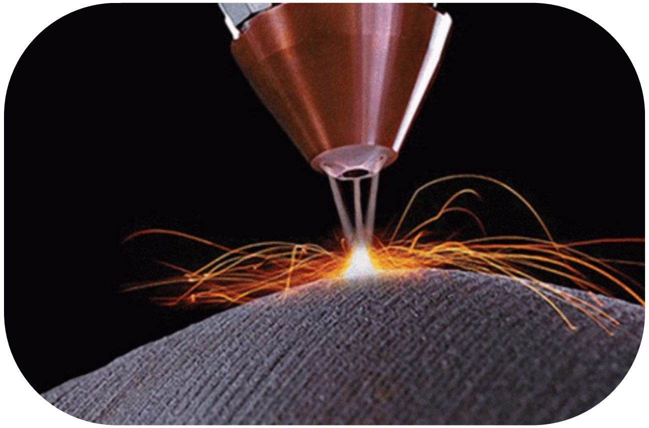
10 entries

Composition and heat treatment space 30 dimensions

Requires 31 points to fit a hyperplane

Just 10 data entries available to model defect density

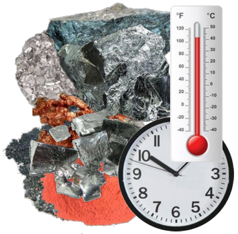
Ability for printing and welding are strongly correlated



Laser

Electricity

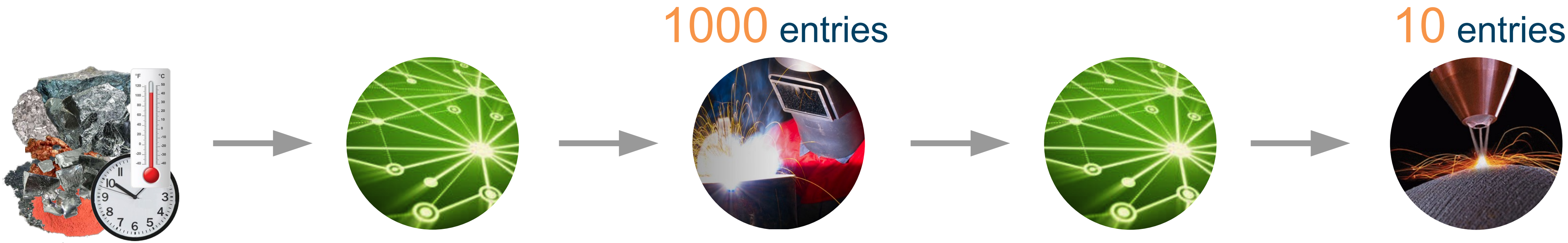
First predict weldability



1000 entries

Use 1000 weldability entries to understand complex composition → weldability model

Use weldability to predict defects formed



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

Target properties

Elemental cost	$< 25\ \$\mathrm{kg}^{-1}$
Density	$< 8500\ \mathrm{kgm}^{-3}$
γ’ content	< 25 wt%
Oxidation resistance	$< 0.3\ \mathrm{mgcm}^{-2}$
Defects	$< 0.15\%$ defects
Phase stability	> 99.0 wt%
γ’ solvus	$> 1000^{\circ}\mathrm{C}$
Thermal resistance	$> 0.04\ \mathrm{K}\Omega^{-1}\mathrm{m}^{-3}$
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%

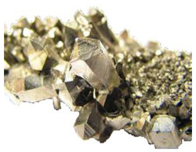
Co 4%

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

Phase behavior targets

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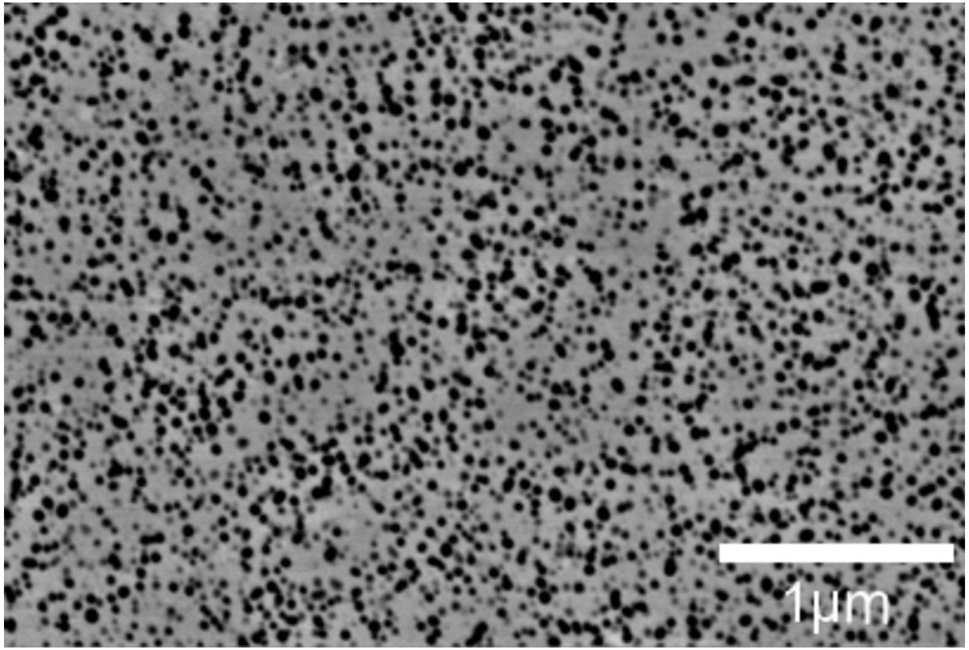
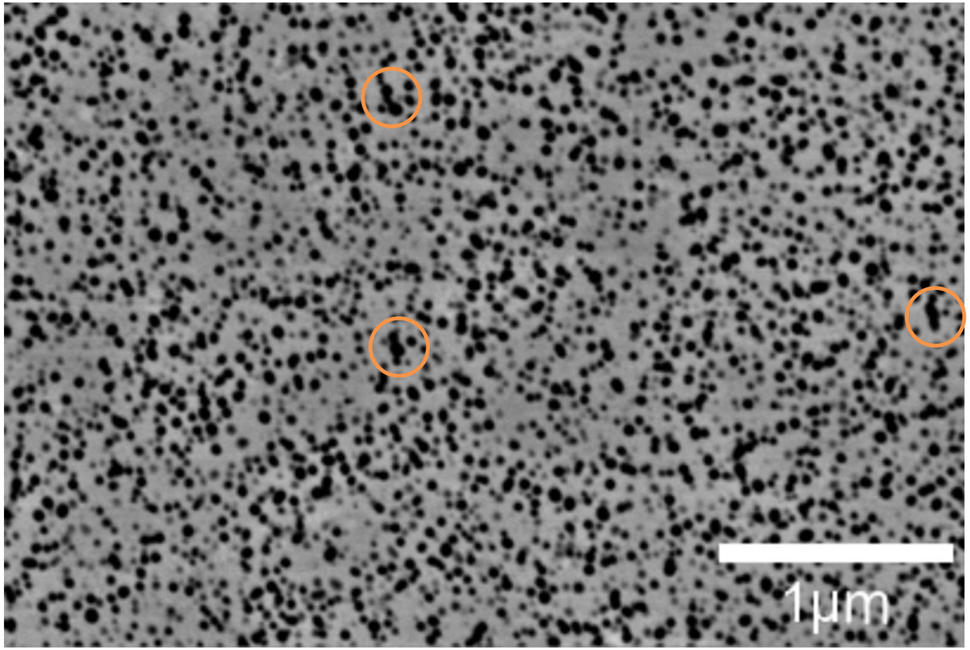
Microstructure



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

Microstructure



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

Defects target

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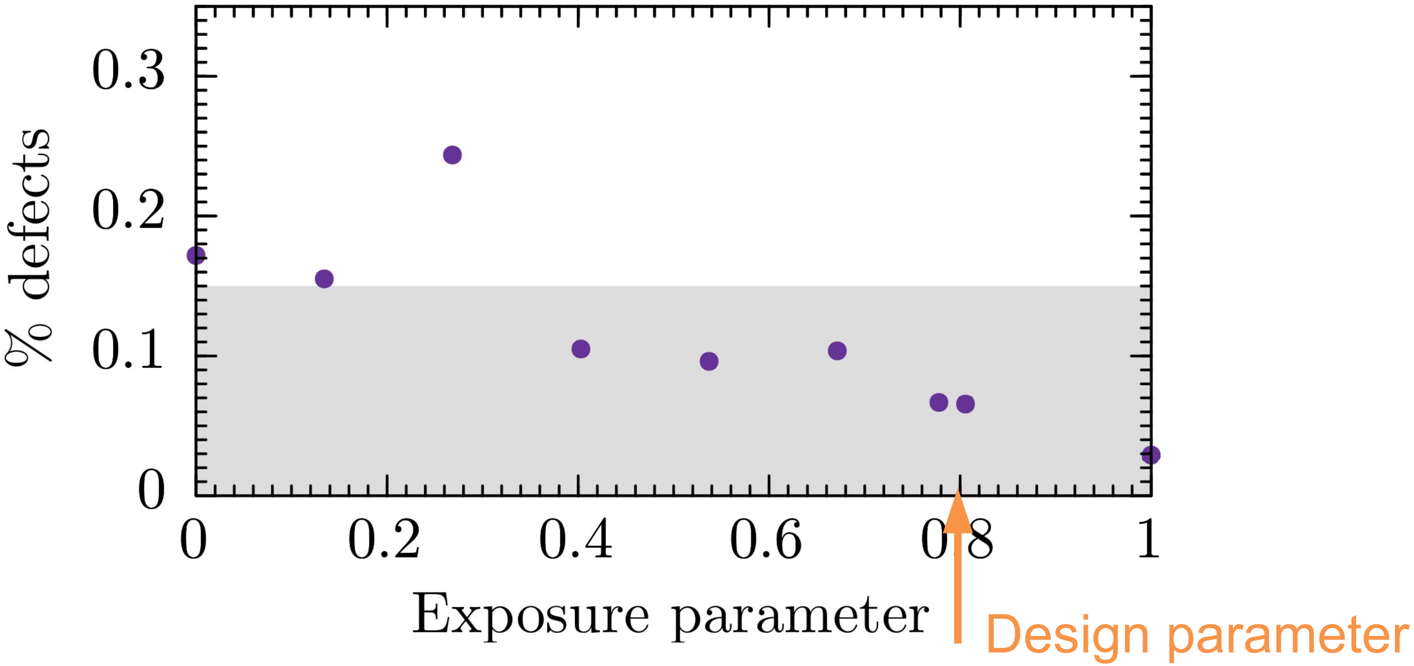
Testing the defect density



Probabilistic neural network identification of an alloy for direct laser deposition
B. Conduit, T. Illston, S. Baker, D. Vadegadde Duggappa, S. Harding, H. Stone & GJC
Materials & Design **168**, 107644 (2019)

Maximize uncertainty

in design of experiments

Project MEDAL

Commissioning an
additive manufacturing machine
is time consuming

Propose process parameters for the
400W M2 from GE Additive
with the new additive-specific
Aheadd® CP1 powder from Constellium

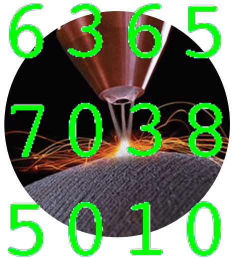
The University Of Sheffield. AMRC Advanced Manufacturing Research Centre
BOEING
Constellium
GE Additive

Train machine learning on initial data set

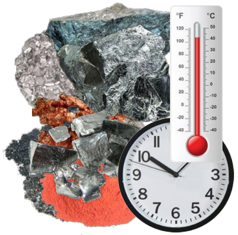
Train machine learning on initial data set

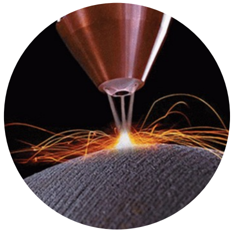
Machine learning proposes additional data to collect

Train machine learning on initial data set



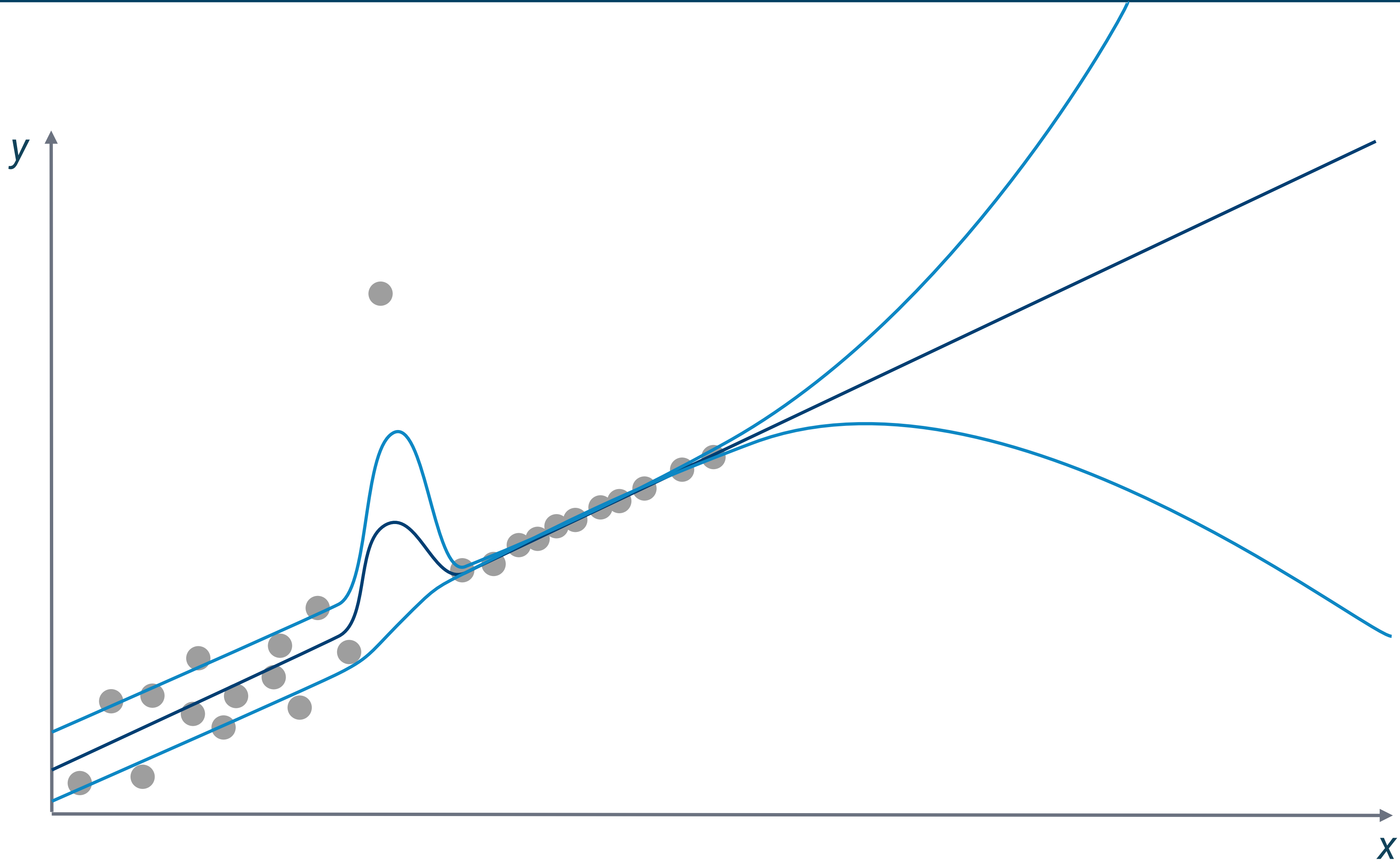
Machine learning proposes additional data to collect



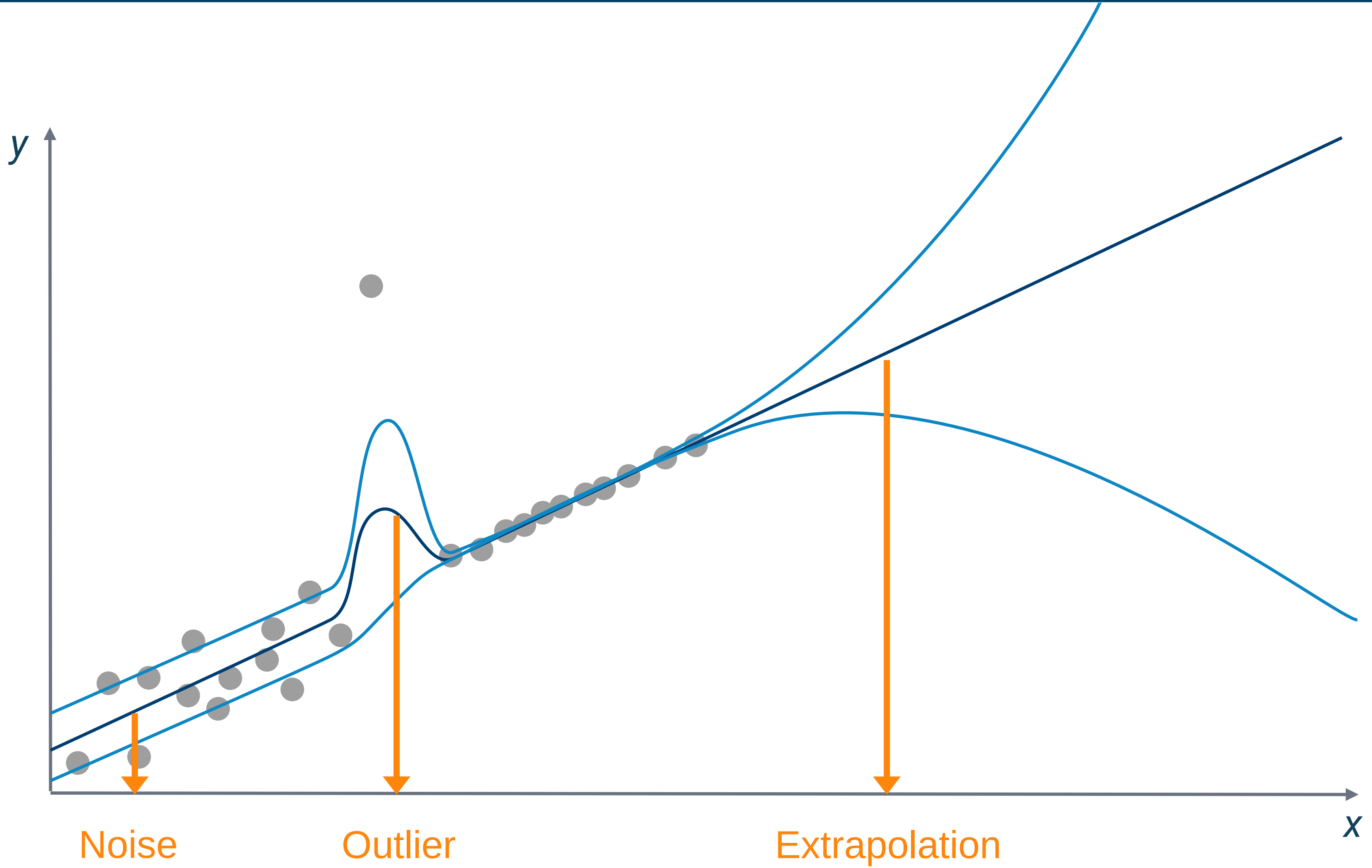


3 3 3 2 7 2 1
6 5 7 9 3 4 2
4 0 4 6 7 0 3
7 6 9 2 8 6 8
6 4 1 3 4 3 9

Uncertainty estimated with machine learning



Interrogate machine learning of where to collect data

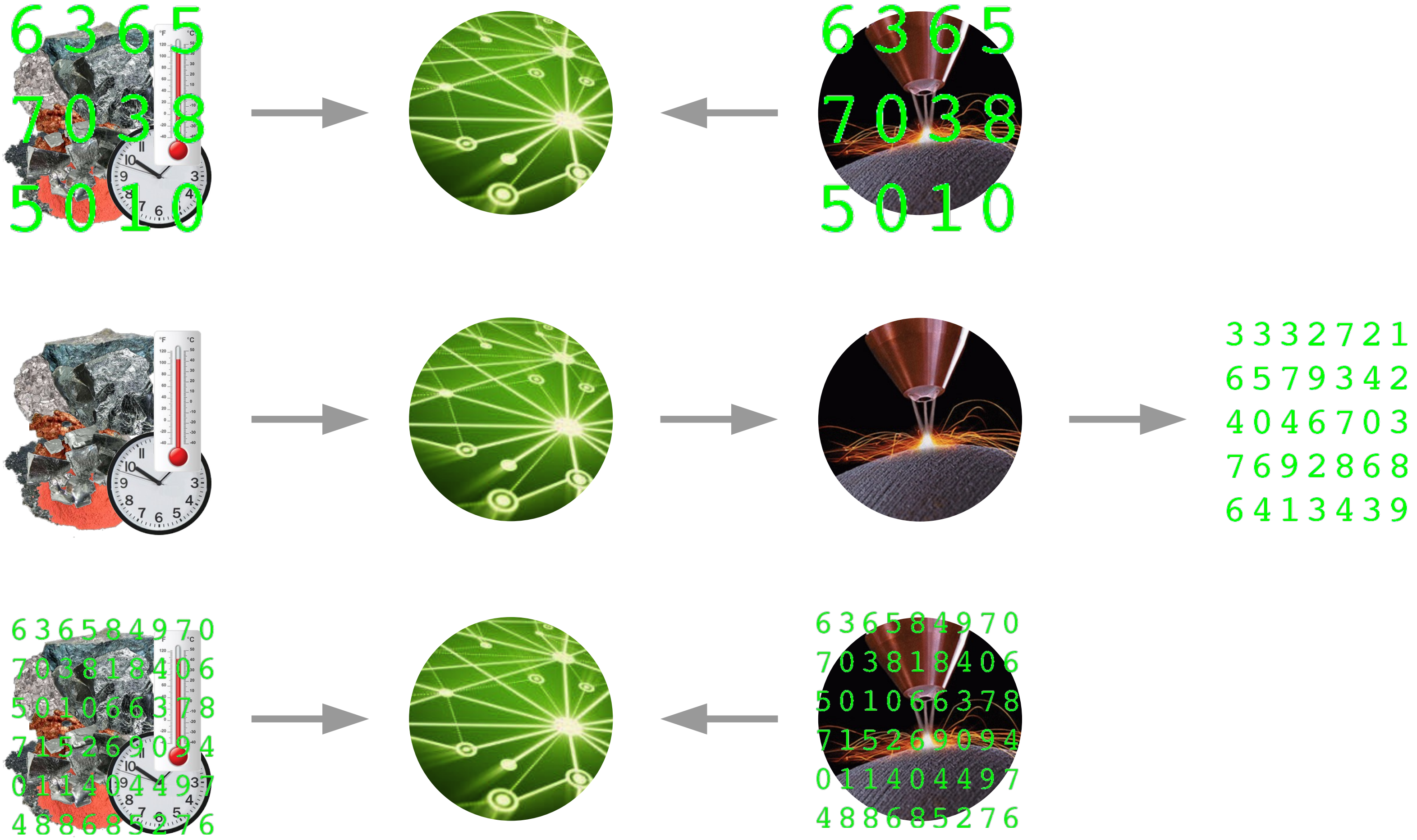


Train machine learning on larger data set

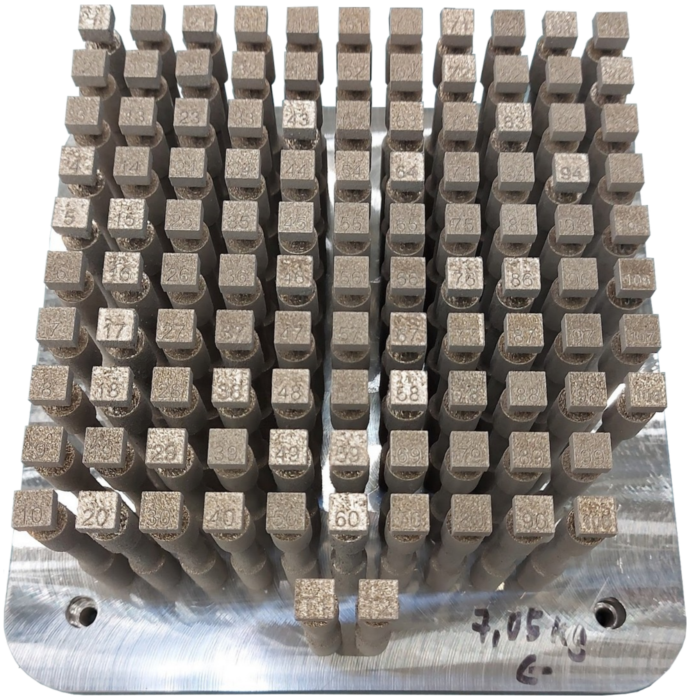
Train machine learning on initial data set

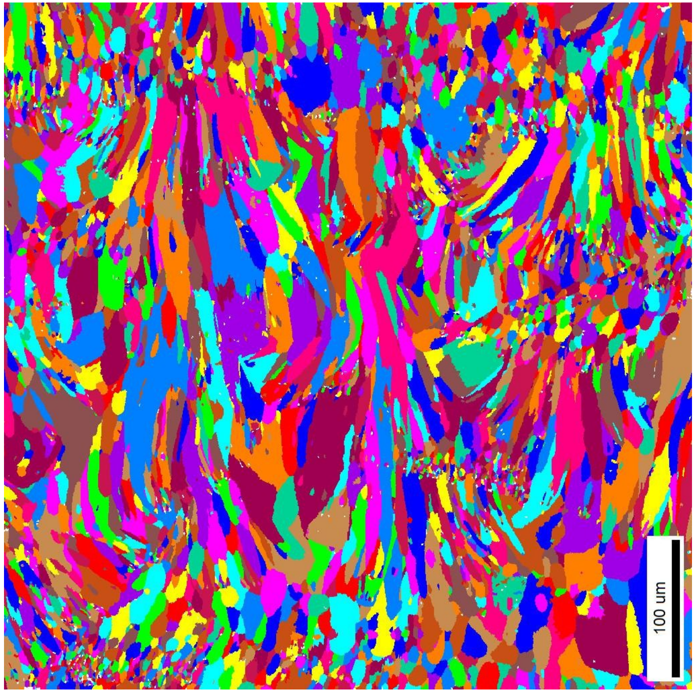
Machine learning proposes additional data to collect

Train machine learning on larger data set

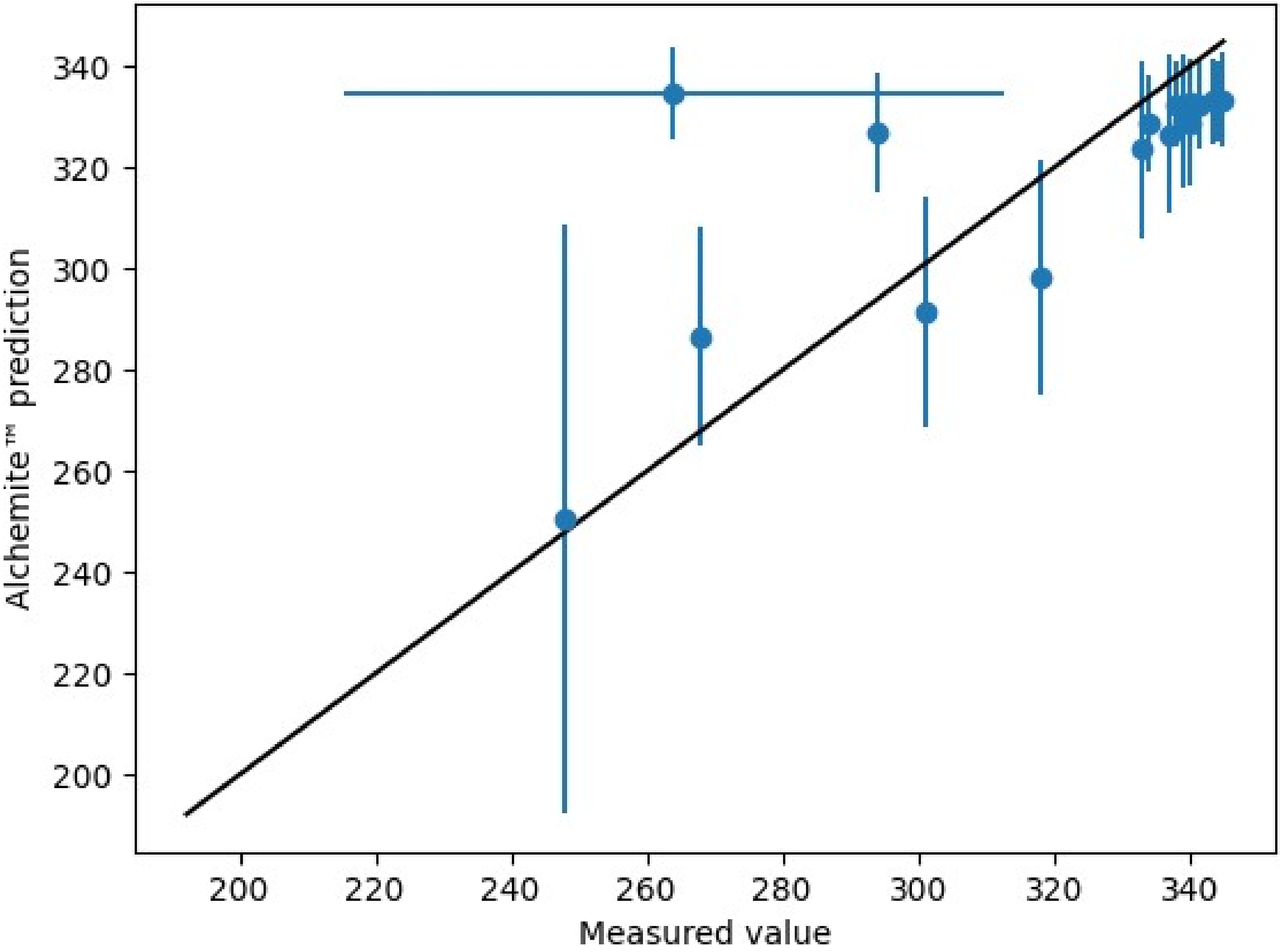


Project MEDAL proposed samples

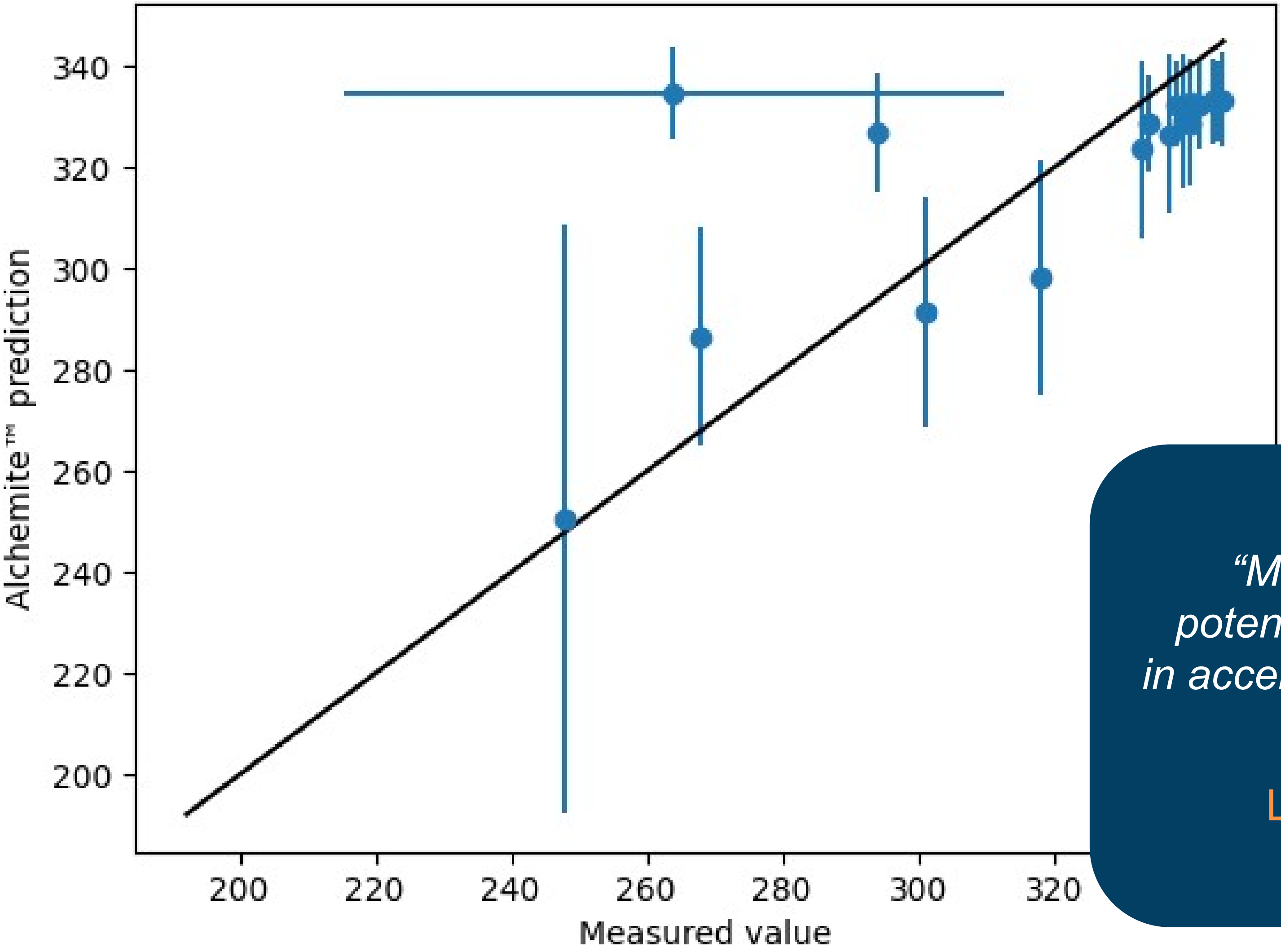




Project MEDAL model performance



Project MEDAL outcome



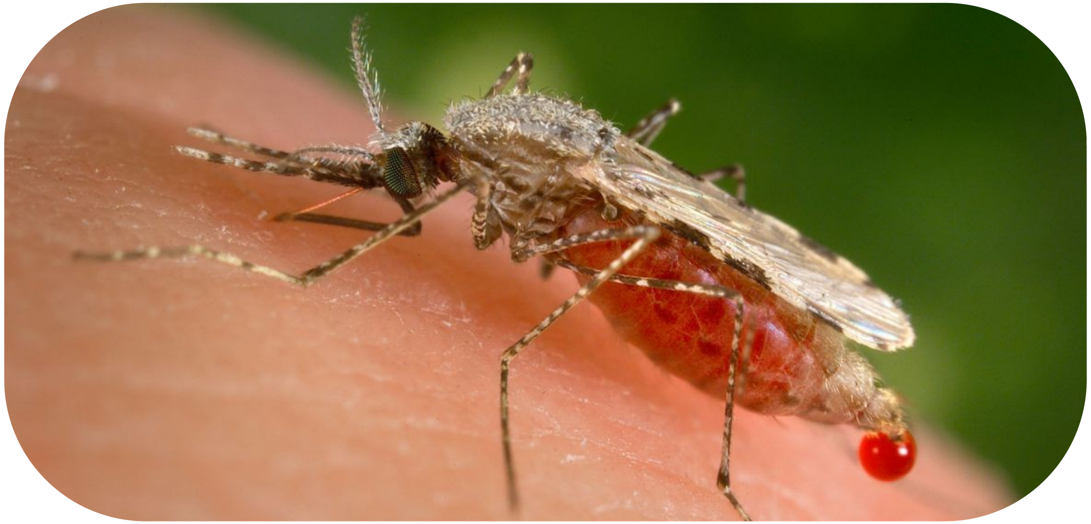
“Machine learning has the potential to be a key technology in accelerating further development and adoption of AM”

Lukas Jiranek, Boeing

Minimize uncertainty

in formulation design

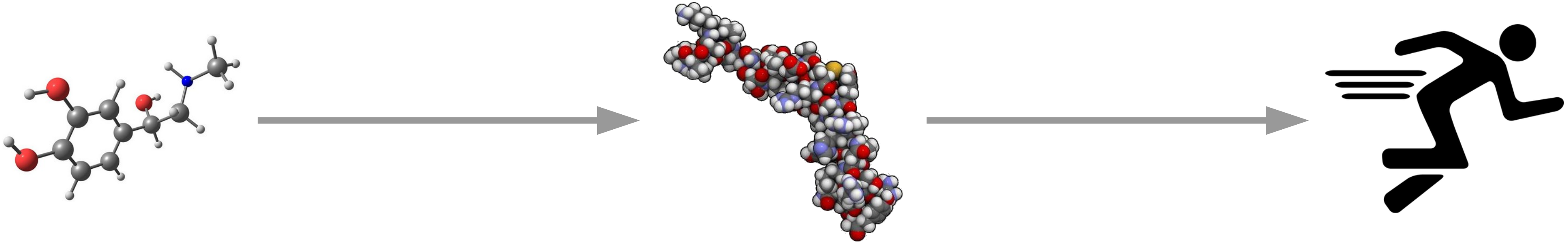
Open Source Malaria contest



OPEN SOURCE MALARIA

Looking for New Medicines

Action of a drug

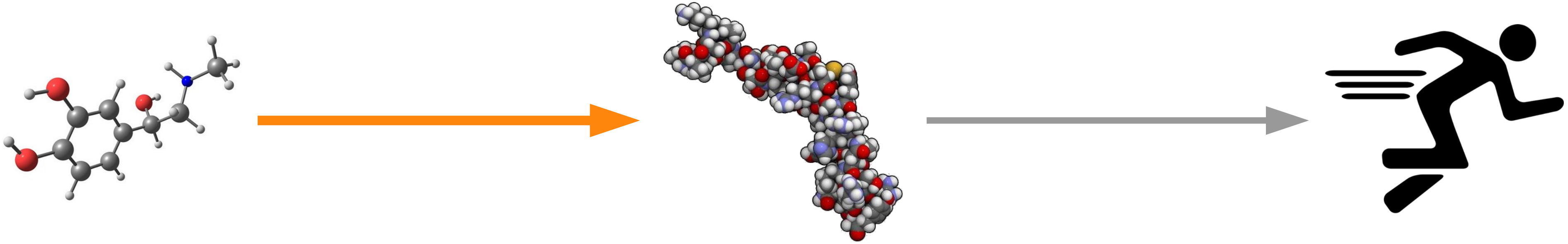


Drug

Protein

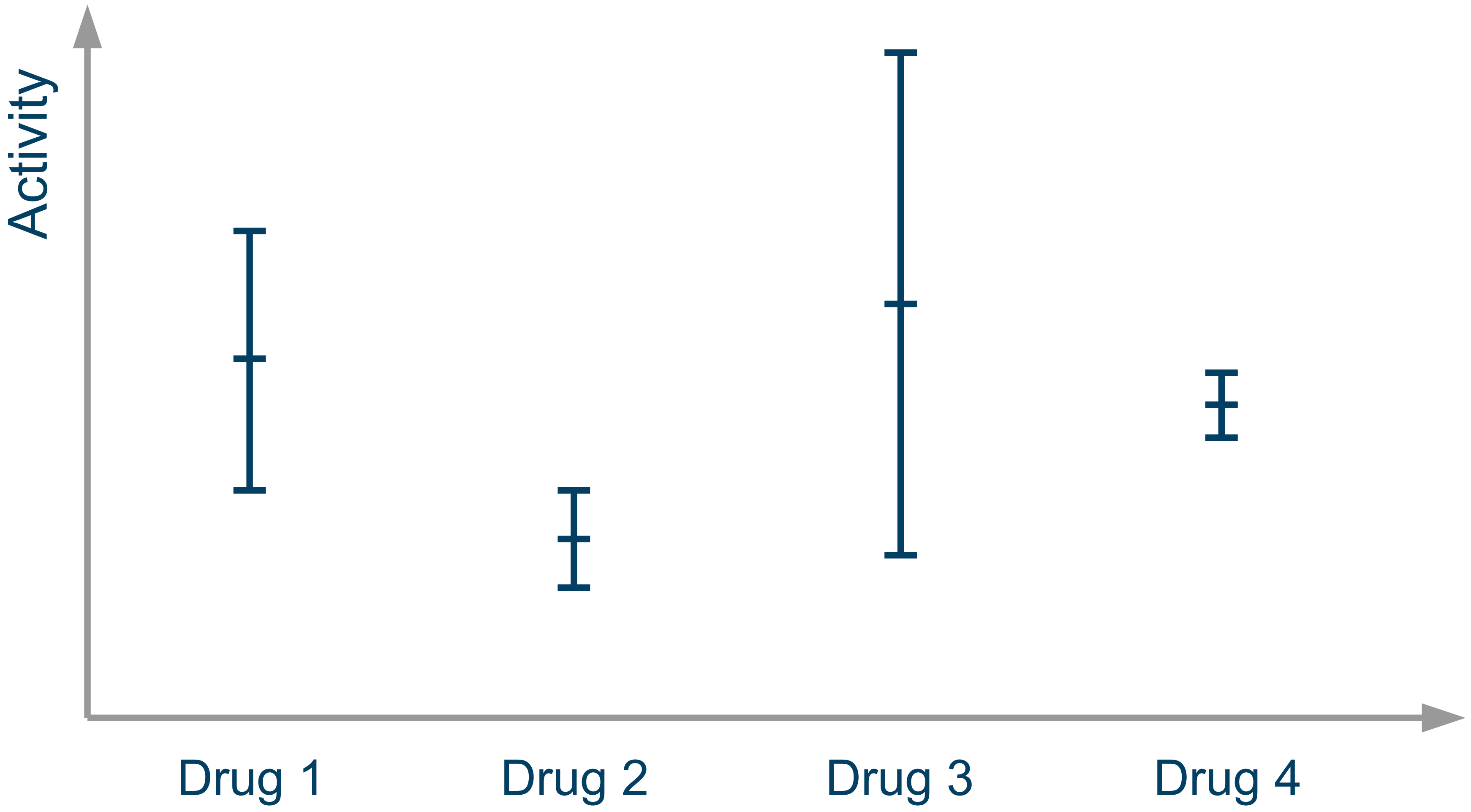
Effect

Action of a drug

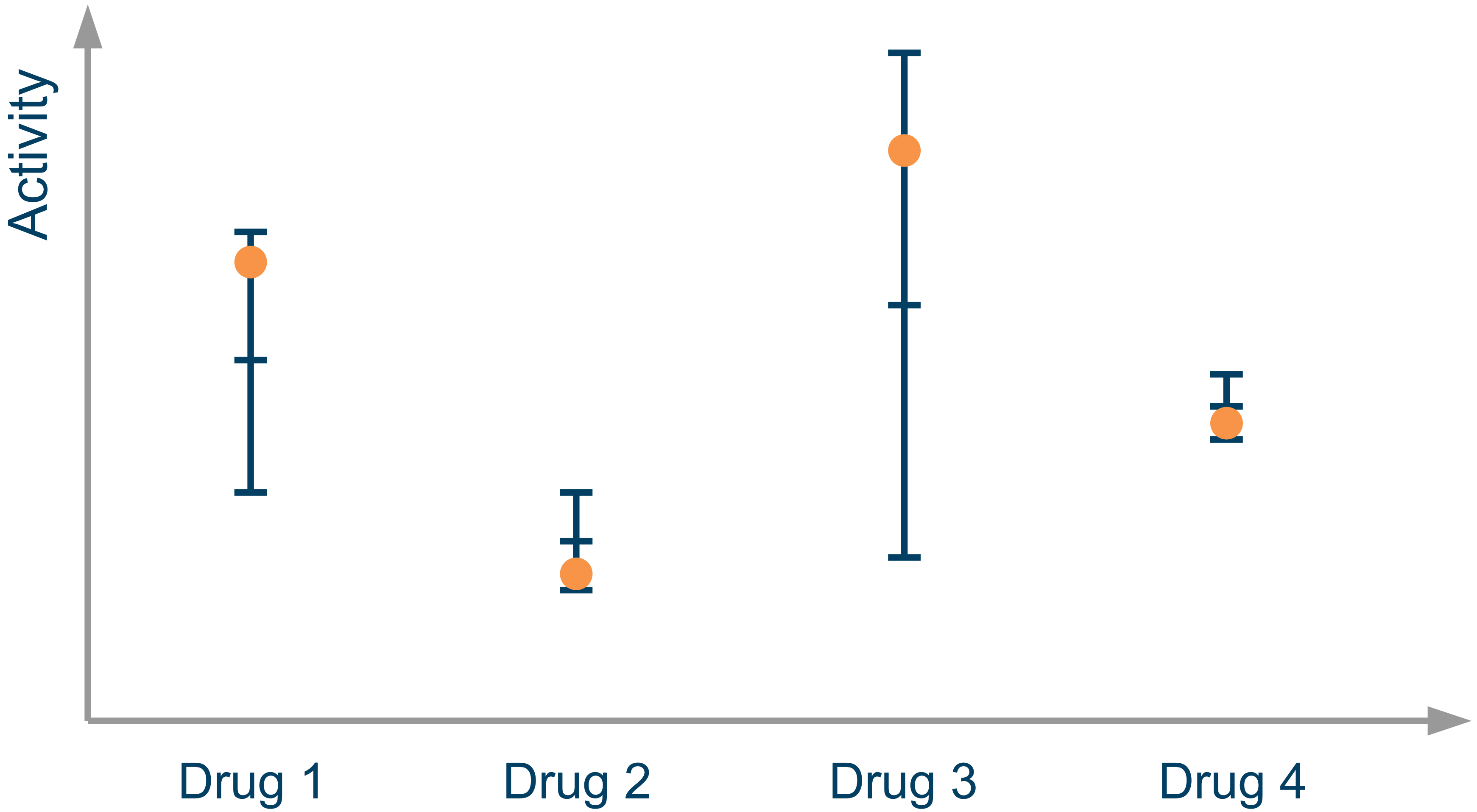


Drug Protein Effect

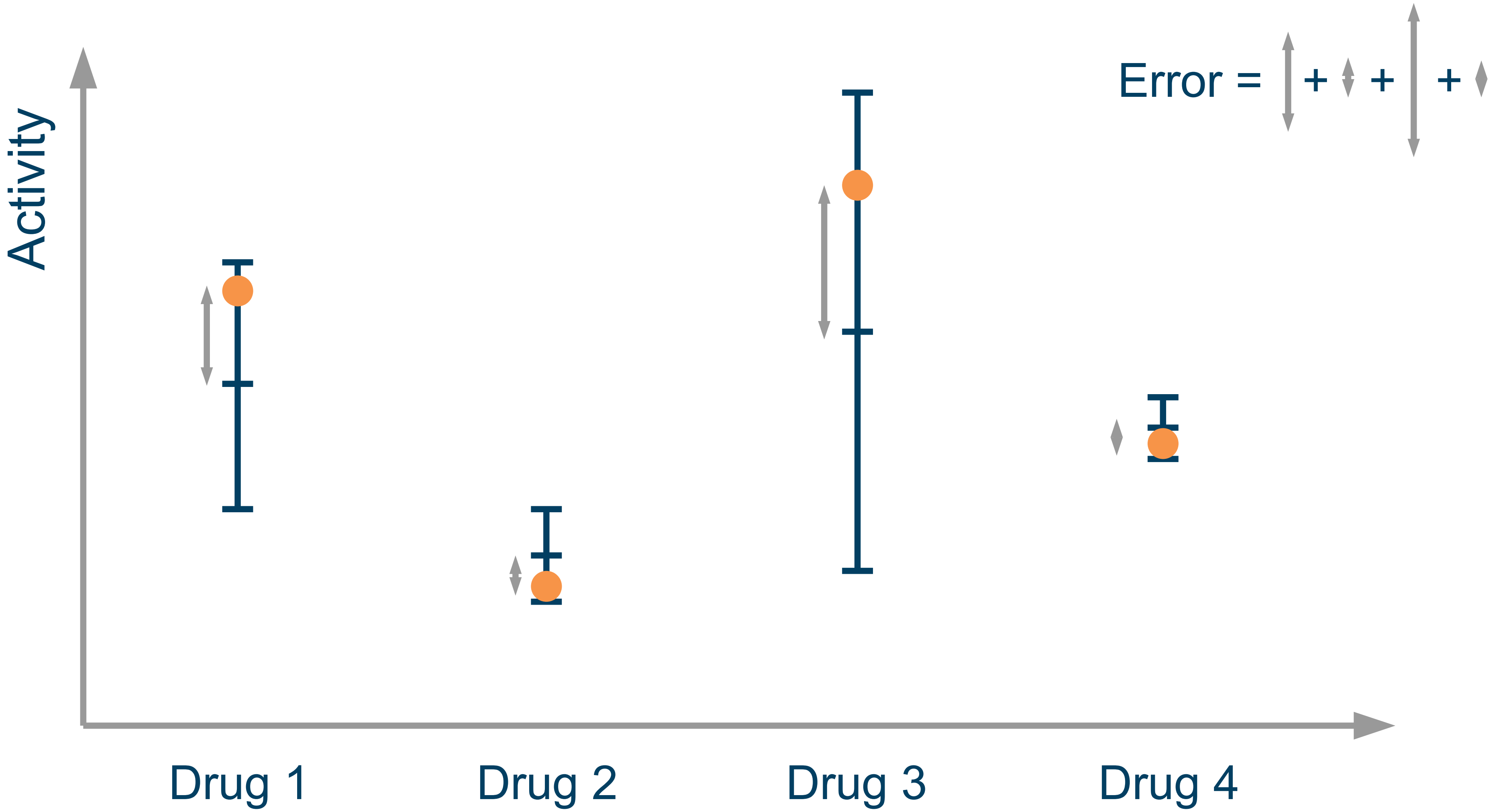
Predictions have an uncertainty



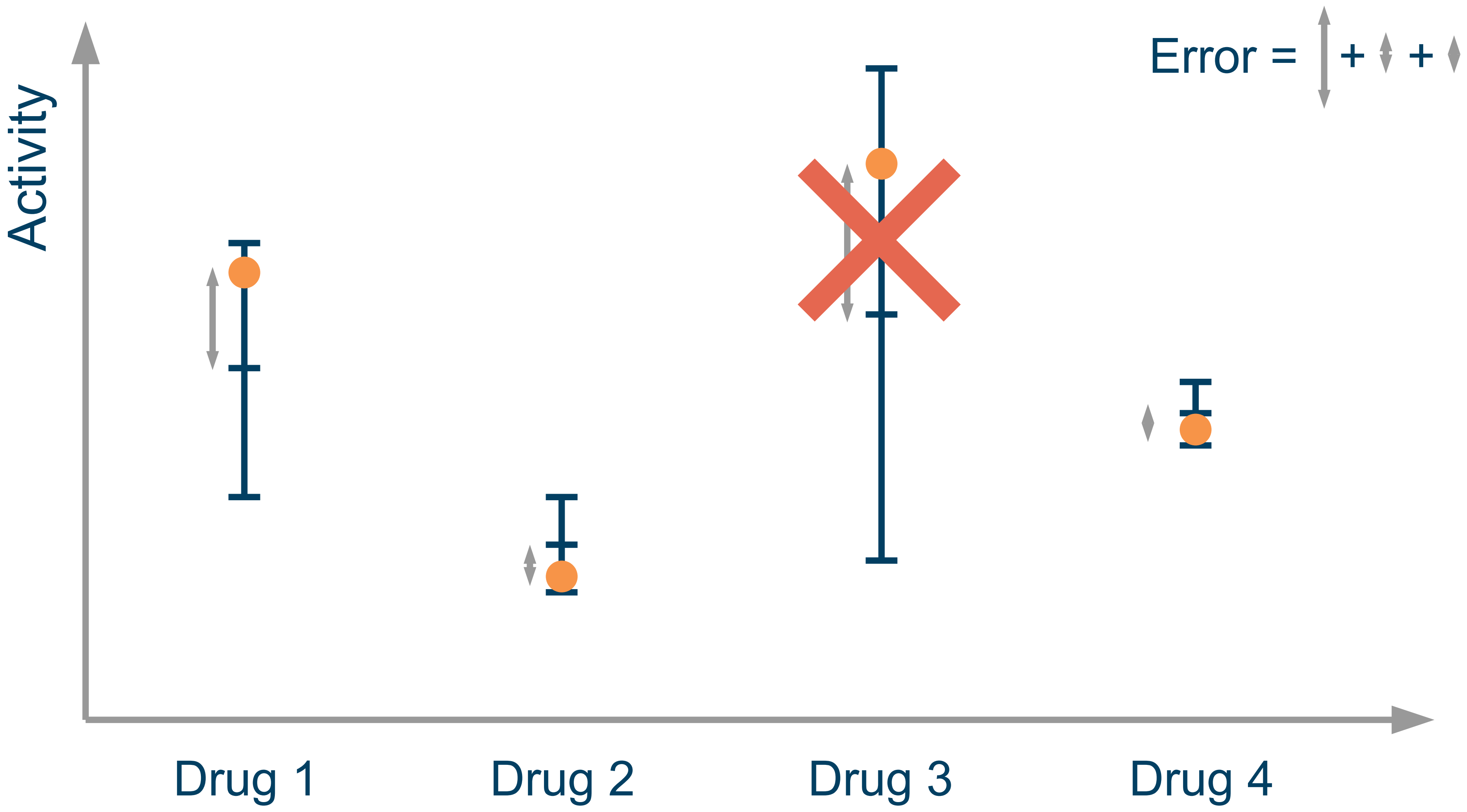
Validation data typically within one standard deviation



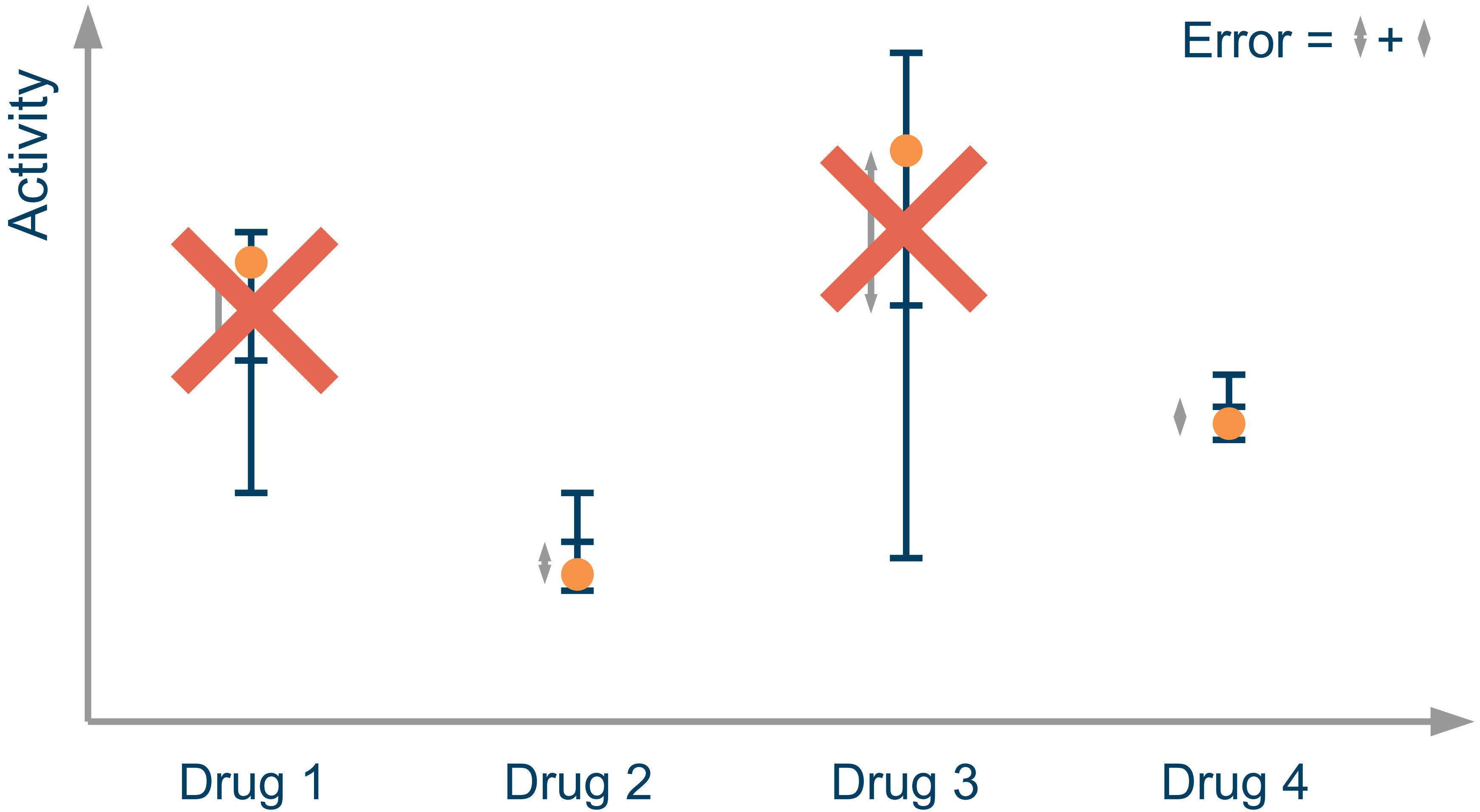
Accuracy R^2 metric calculated with difference from mean



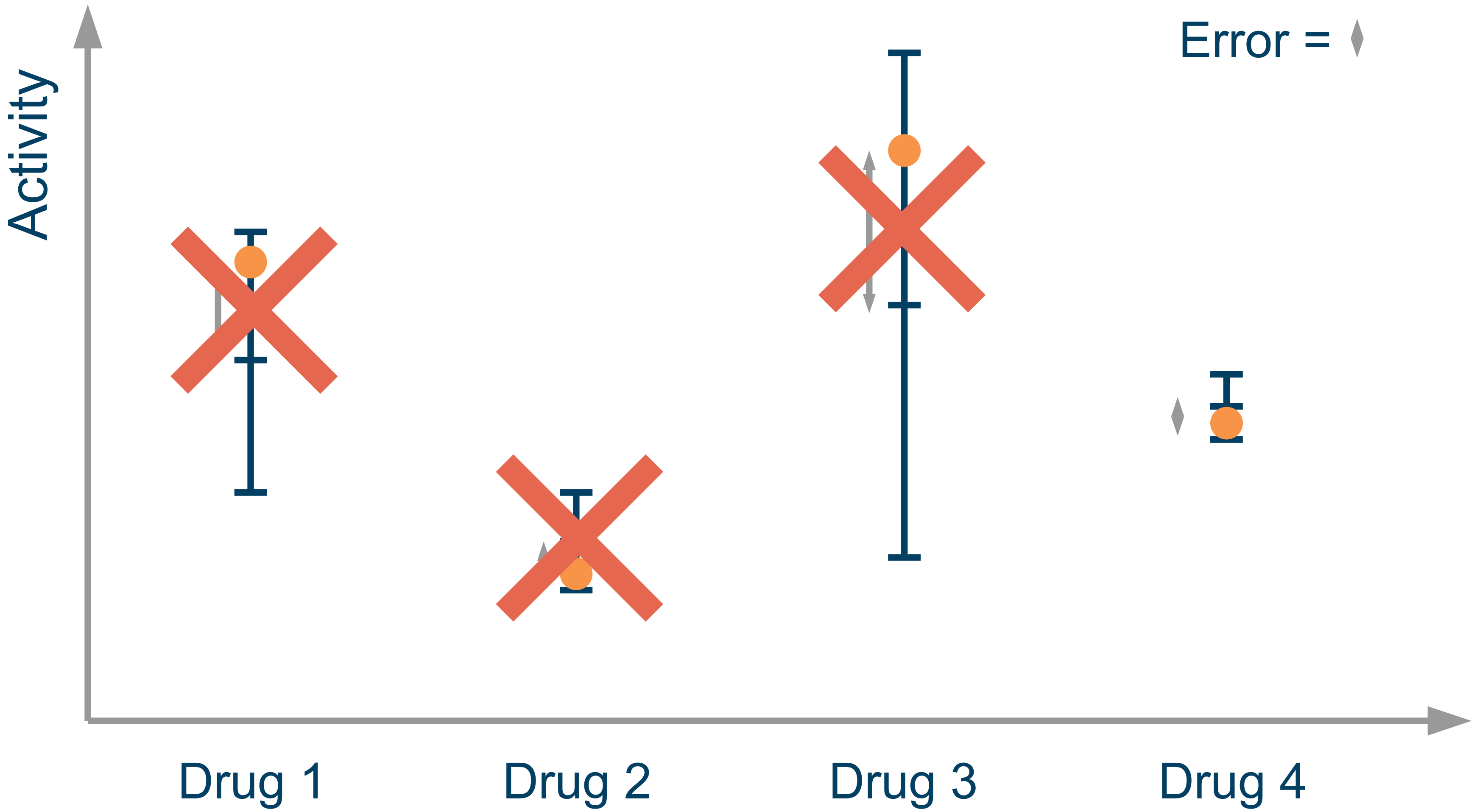
Impute 75% of data with smallest uncertainty



Impute 50% of data with smallest uncertainty



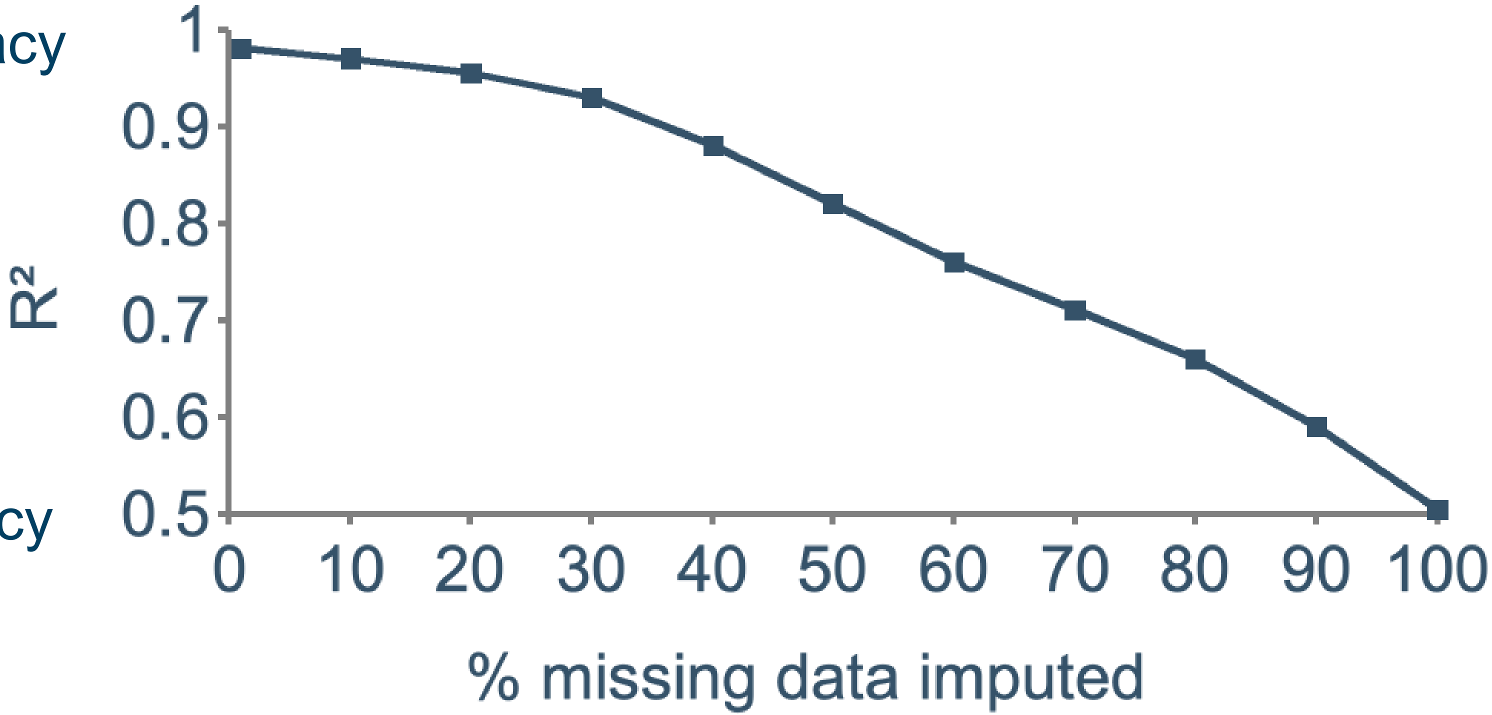
Impute 25% of data with smallest uncertainty



Improved performance by exploiting uncertainty

High accuracy

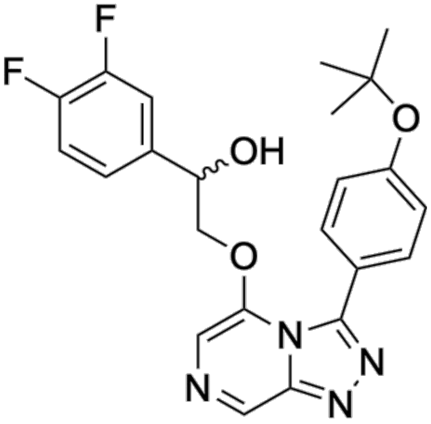
Low accuracy



Different drugs can treat the same ailment

Focus on compounds with low uncertainty

Open Source Malaria experimental validation

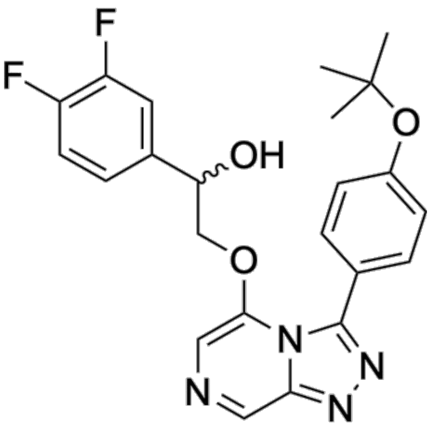


Optibrium & Intellegens

0.647 μM

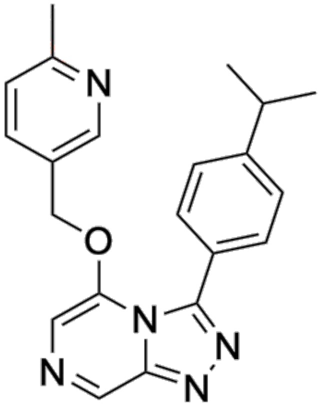
Journal of Medicinal Chemistry **64**, 16450 (2021)

Open Source Malaria other compounds



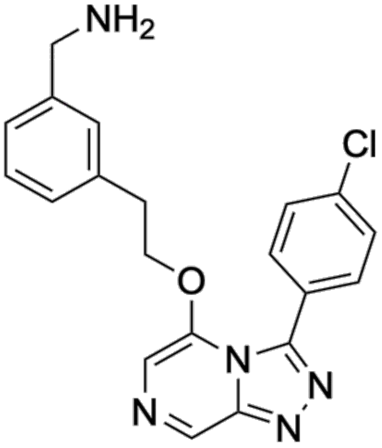
Optibrium & Intellegens

0.647 μM



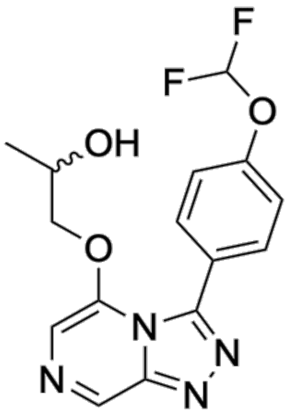
Davy Guan

>25 μM



Exscientia

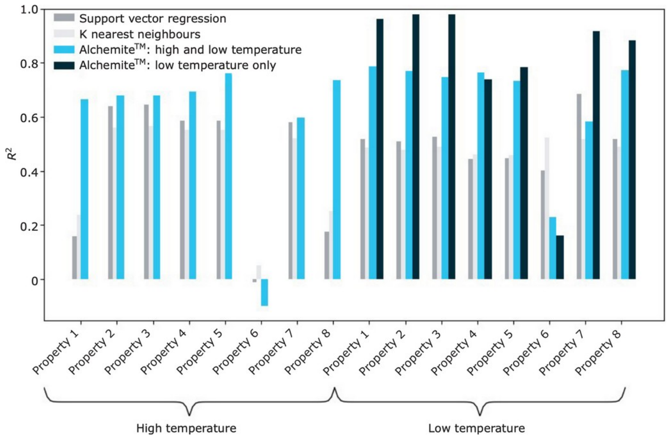
10.9 μM



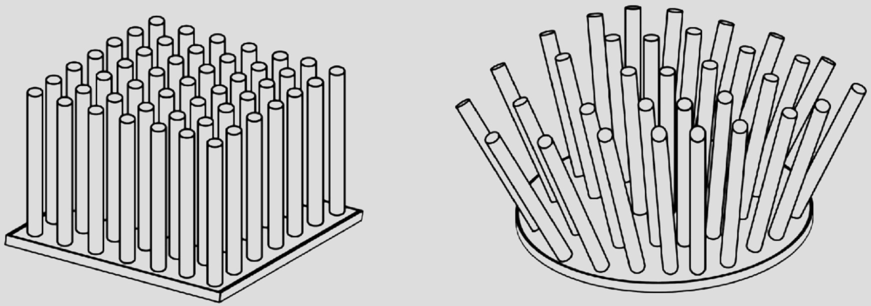
Molomics

>25 μM

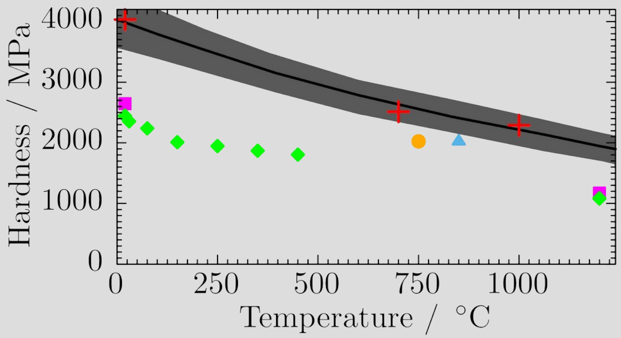
Journal of Medicinal Chemistry **64**, 16450 (2021)



Johnson Matthey Technology Review
66, 130 (2022)



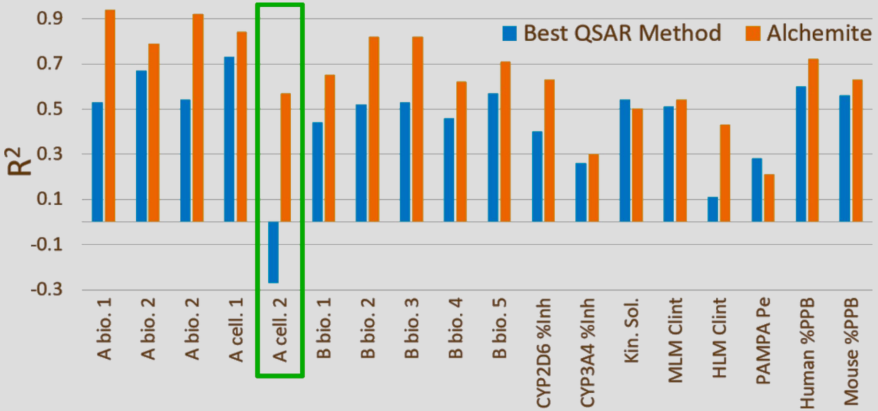
NASA Technical Memorandum
20220008637



Materials & Design **131**, 358 (2017)
Scripta Materialia **146**, 82 (2018)
Data Centric Engineering **3**, e30 (2022)

Alloy	Source	ANN	Δ_σ	Actual
Steel AISI 301L	193	269	5	238[23]
Steel AISI 301	193	267	5	221[23]
Al 1080 H18	51	124	5	120[23]
Al 5083 wrought	117	191	14	300,190[4, 23]
Al 5086 wrought	110	172	11	269,131[4, 23]
Al 5454 wrought	102	149	14	124[23]
Al 5456 wrought	130	201	11	165[23]
INCONEL600	223	278	10	≥550[23]

Computational Materials Science **147**, 176 (2018)

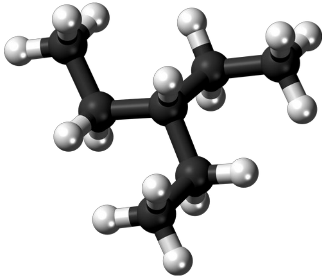


J. of Chem. Info. & Model. **60**, 2848 (2020)
Applied AI Letters **2**, e31 (2021)
Molecular Pharmaceutics **19**, 1488 (2022)

Constellation
PHARMACEUTICALS
Takeda
AstraZeneca

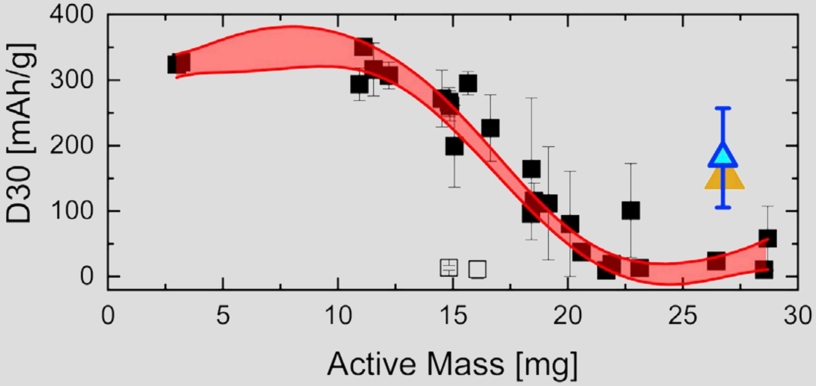
optibrium™
iff

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



Fluid Phase Equilibria **501**, 112259 (2019)
Journal of Chemical Physics **153**, 014102 (2020)

bp



Cell Reports
Physical Science
2, 100683 (2021)

UNIVERSITY OF
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Ansys
GRANTA

Summary

Exploit property-property relationships to improve predictions

Machine learning guided design of experiments

Probabilistic design improves success rate

Taken to market through Intellegens