UNIVERSITY OF CAMBRIDGE

Artificial intelligence – a tool for the modern-day blacksmith

Gareth Conduit

Model **sparse** datasets

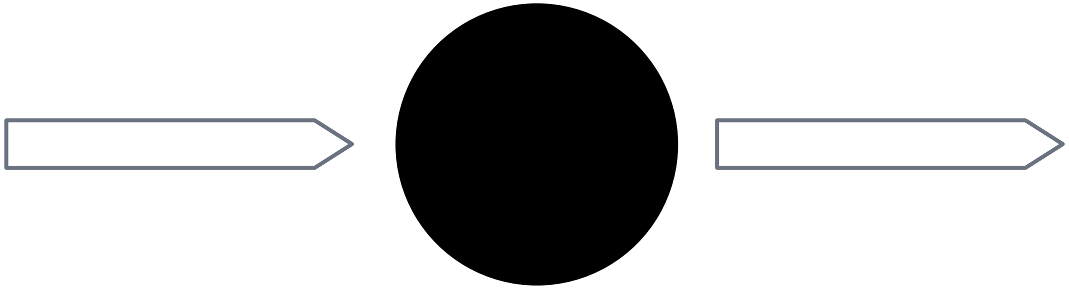
Exploit **property-property** relationships

Merge data, computer simulations, and physical laws

Exploit **uncertainties** to deliver most robust predictions

Black box machine learning for materials design

Composition



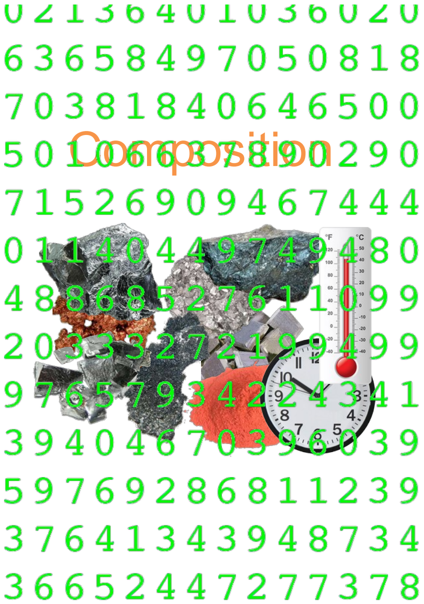
Properties

Defects

Fatigue

Strength

Train the machine learning



Machine learning predicts material properties

Composition

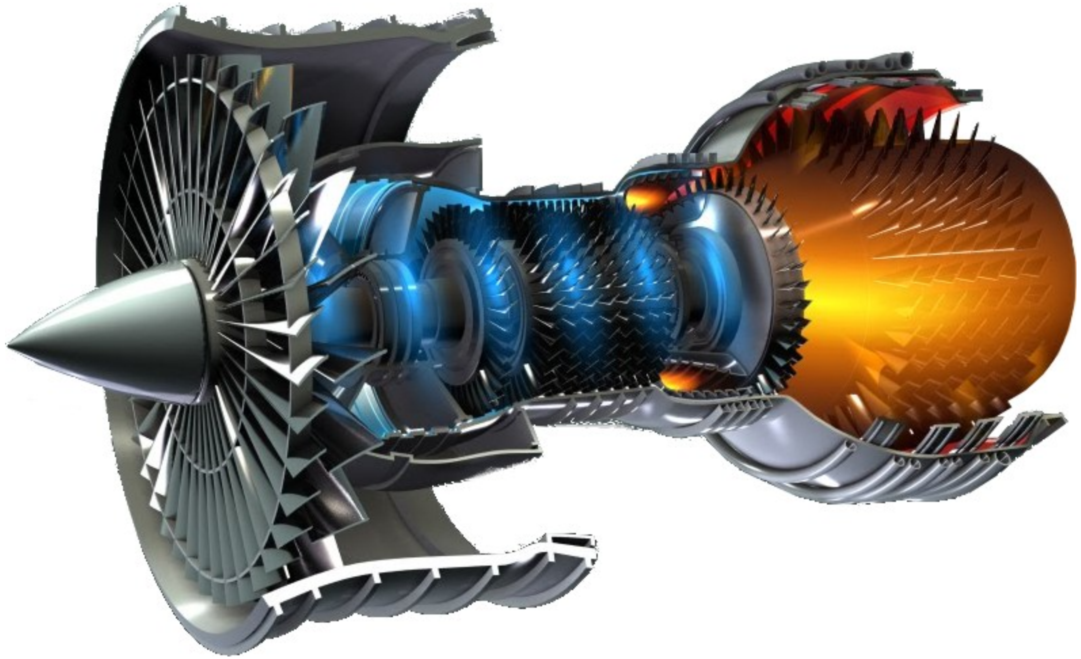
Properties

Defects

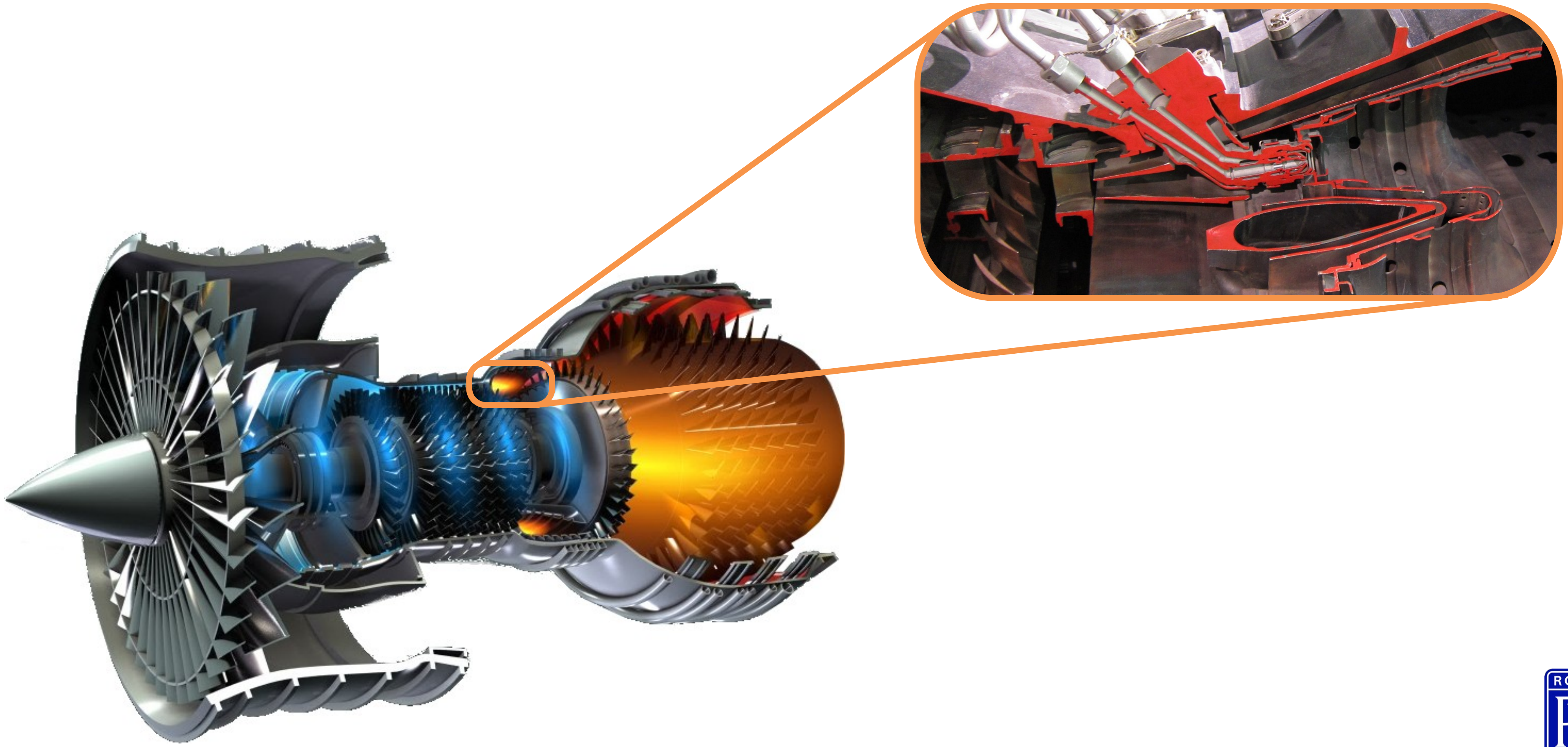
Fatigue

Strength

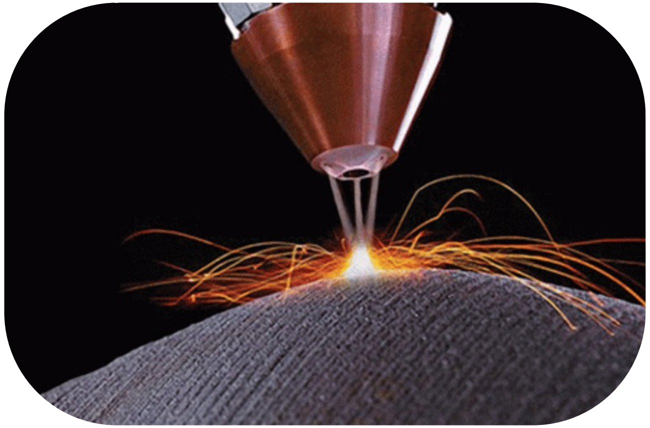
Jet engine schematic



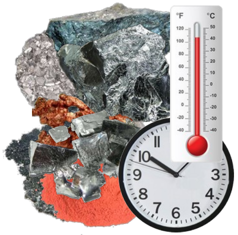
Combustor in a jet engine



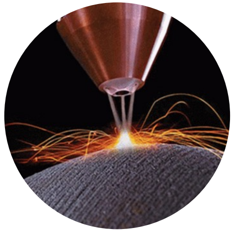
Direct laser deposition



Data available to model defect density



10 entries

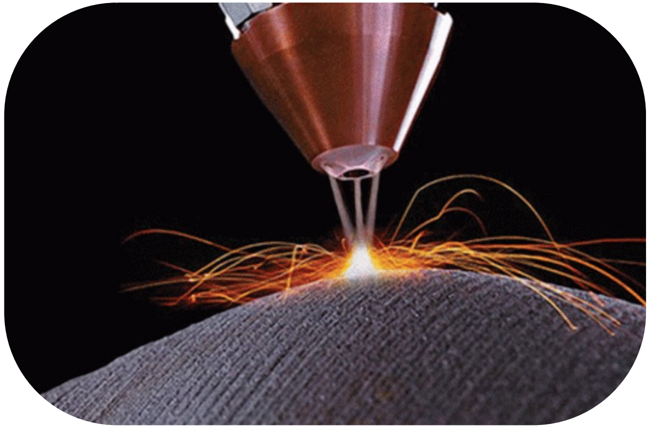


Composition and heat treatment space 30 dimensions

Requires 31 points to fit a hyperplane

Just 10 data entries available to model defect density

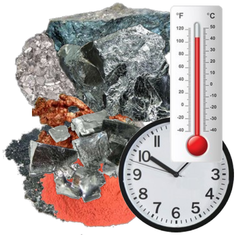
Ability for printing and welding are strongly correlated



Laser

Electricity

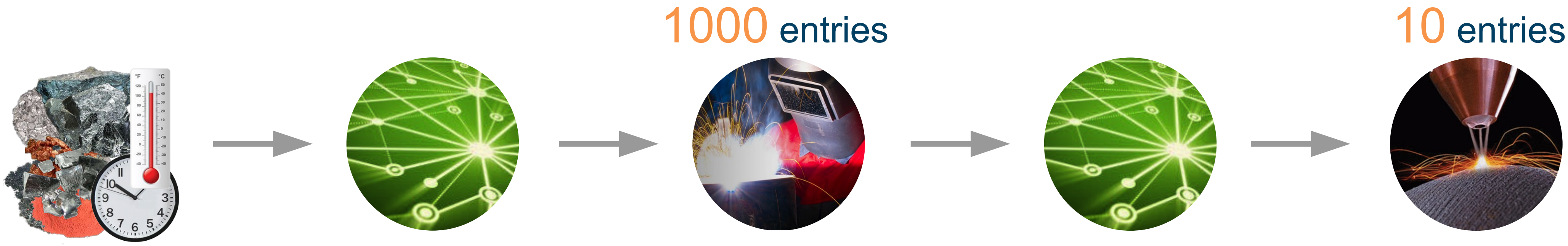
First predict weldability



1000 entries

Use 1000 weldability entries to understand complex composition → weldability model

Use weldability to predict defects formed



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 $\$kg^{-1}$
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%

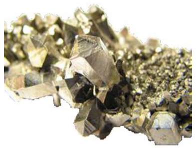
Co 4%

Mo 4.9%

W 1.2%

Zr 0.05%

Nb 3%



Al 2.9%

C 0.04%

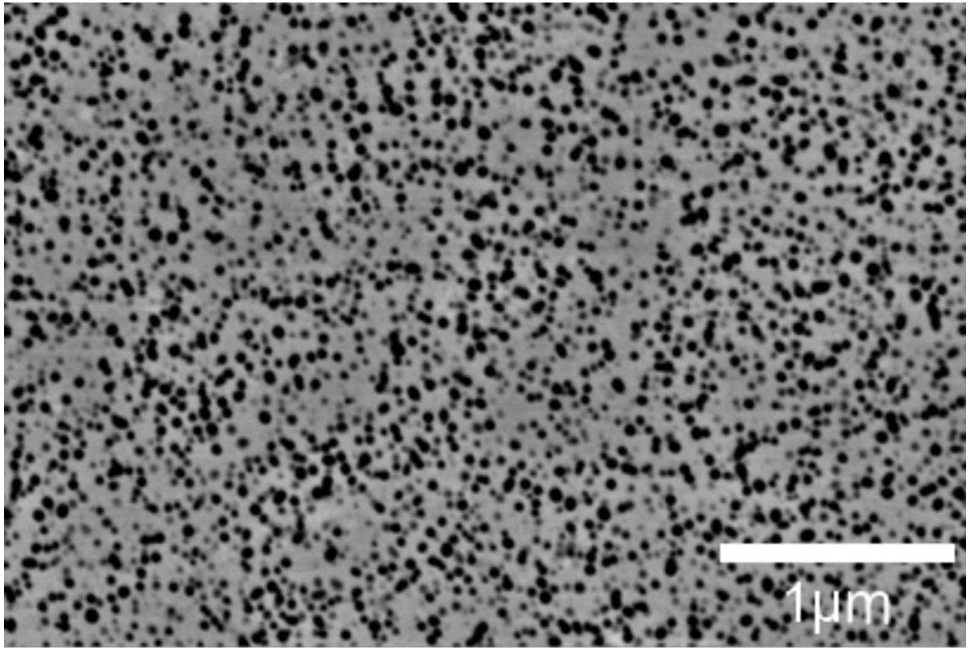
B 0.01%

Ni

Expose 0.8

T_{HT} 1300ºC

Microstructure



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

Defects target

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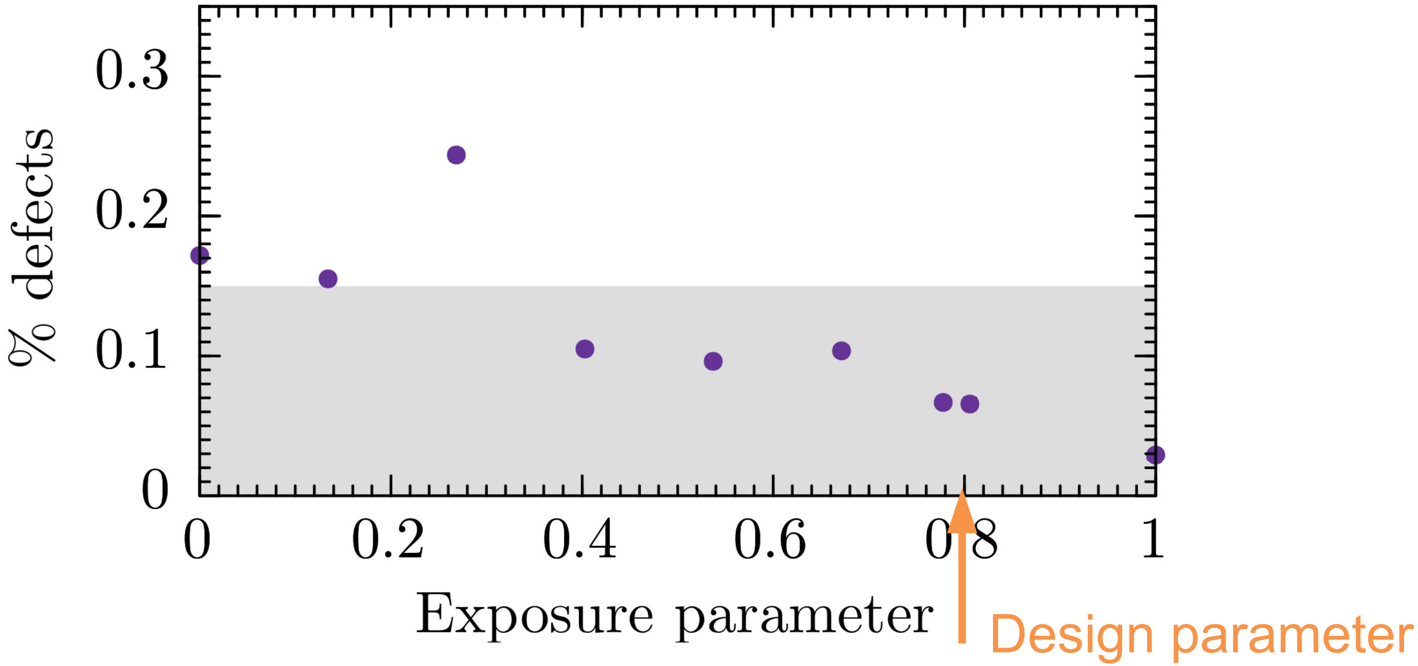
Testing the defect density



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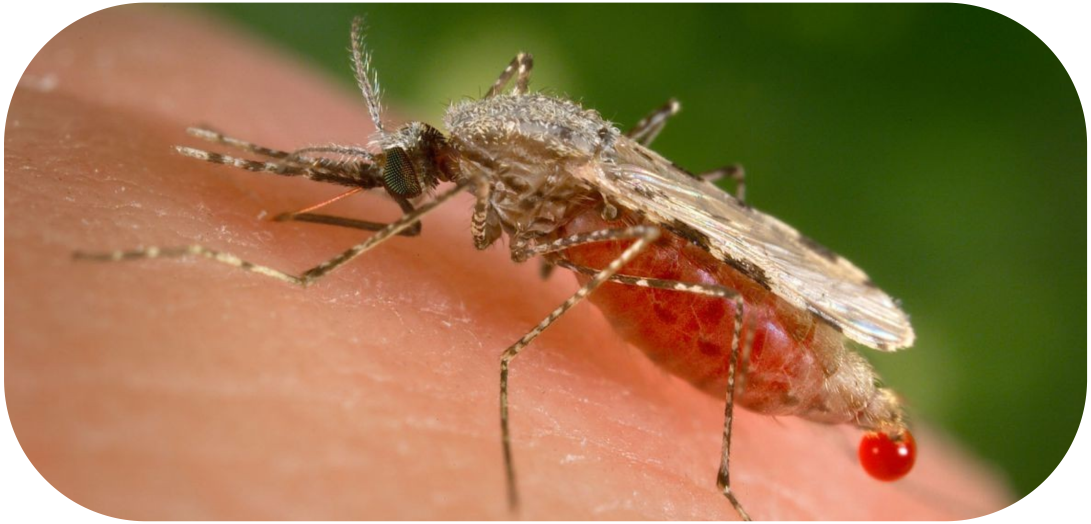
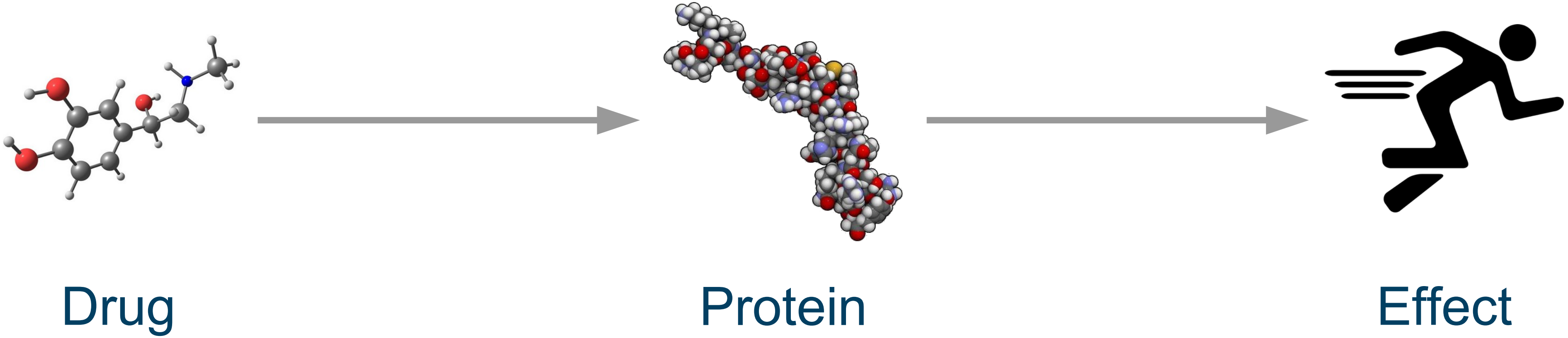
Open Source Malaria contest



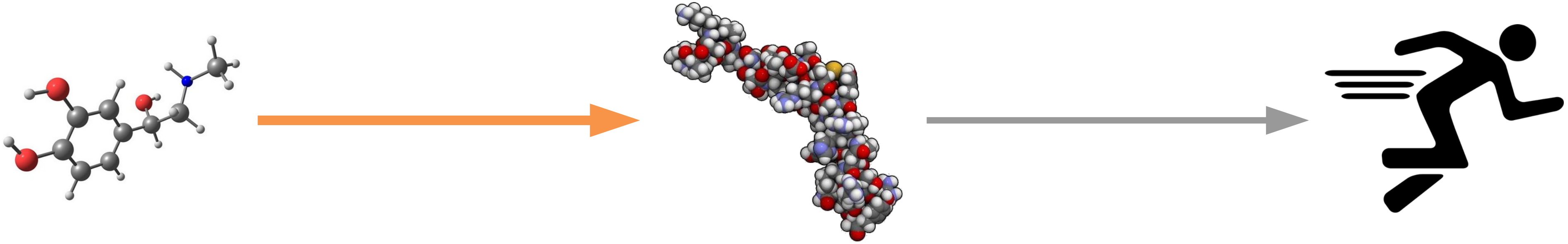
OPEN SOURCE MALARIA

Looking for New Medicines

Action of a drug

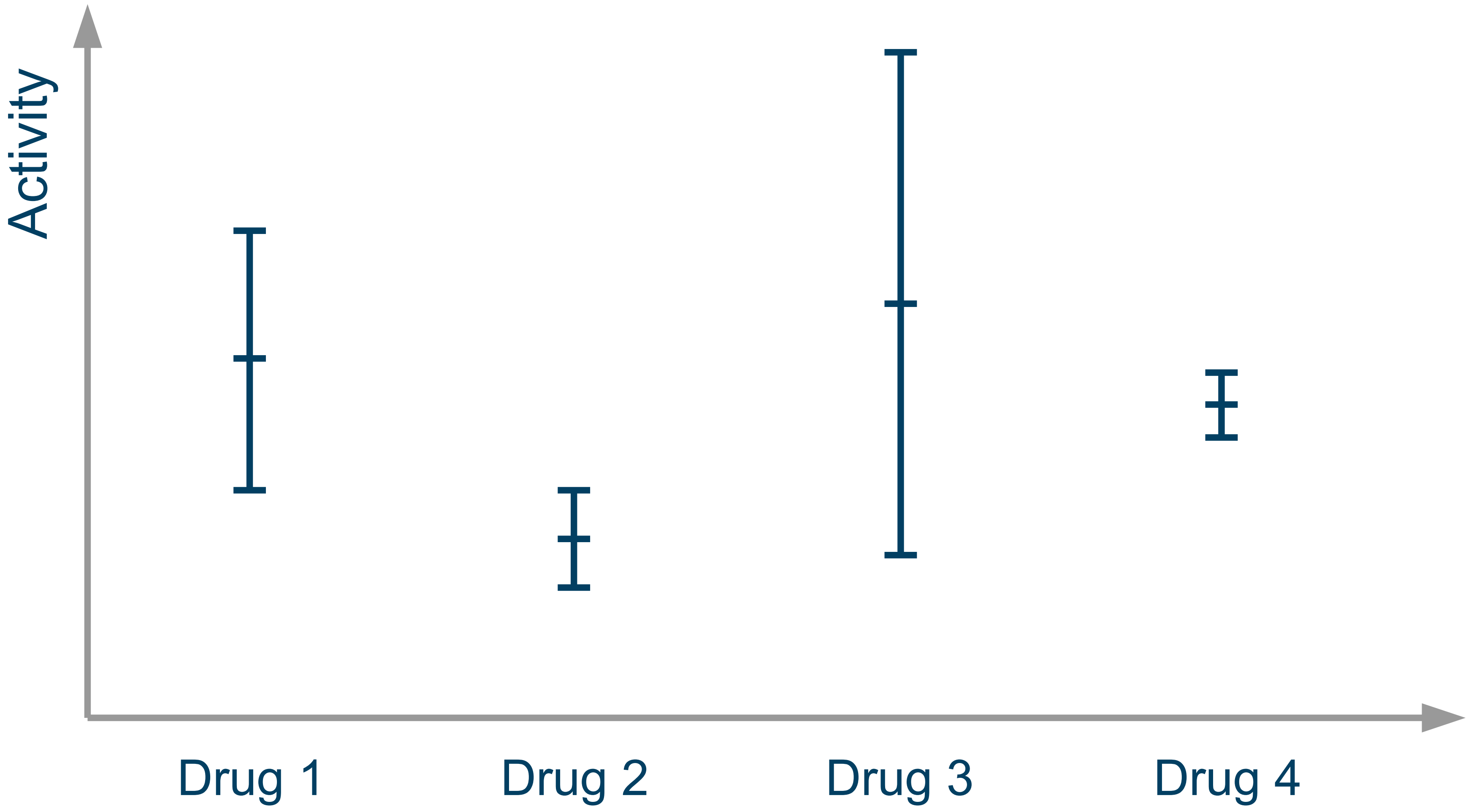


Action of a drug

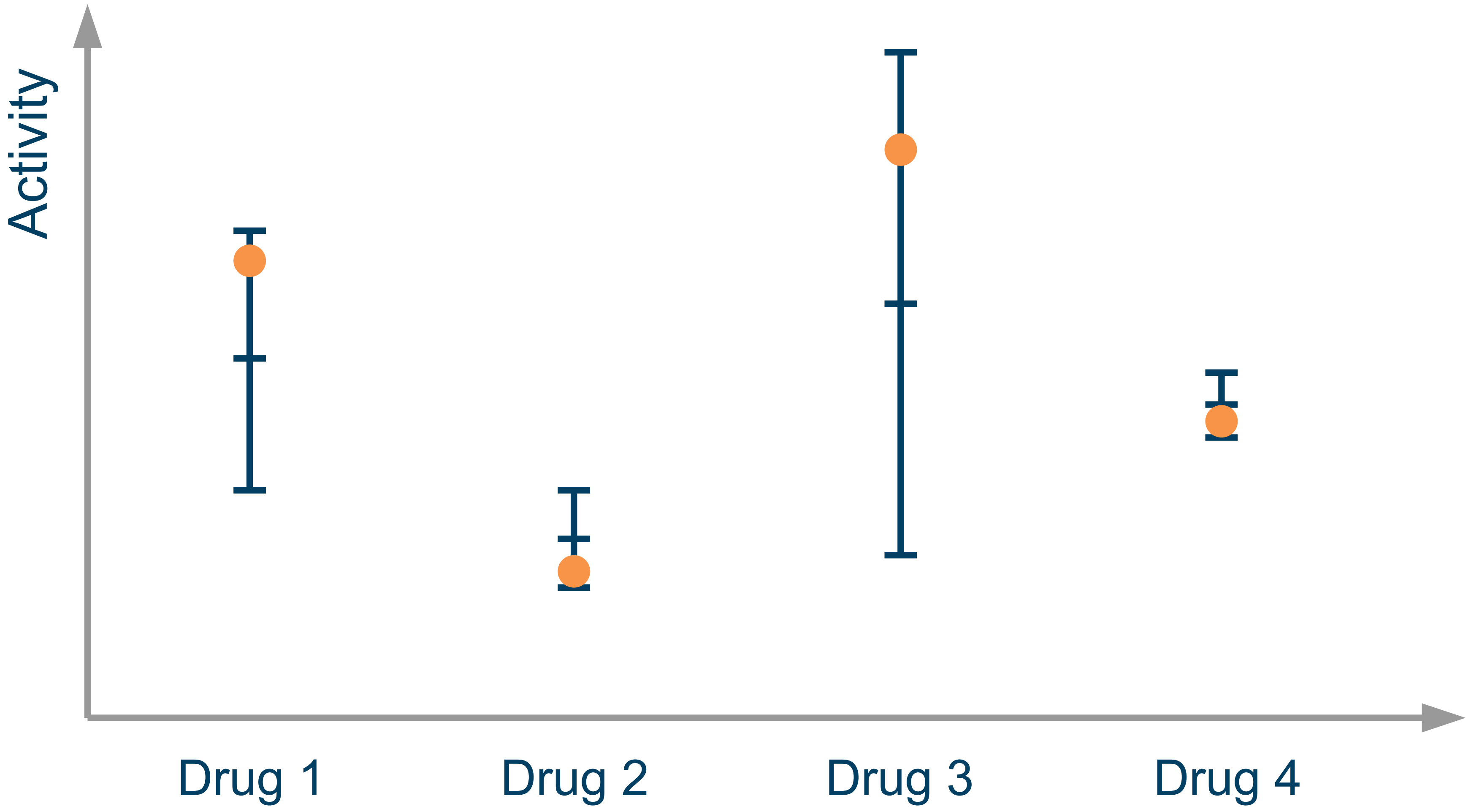


Drug Protein Effect

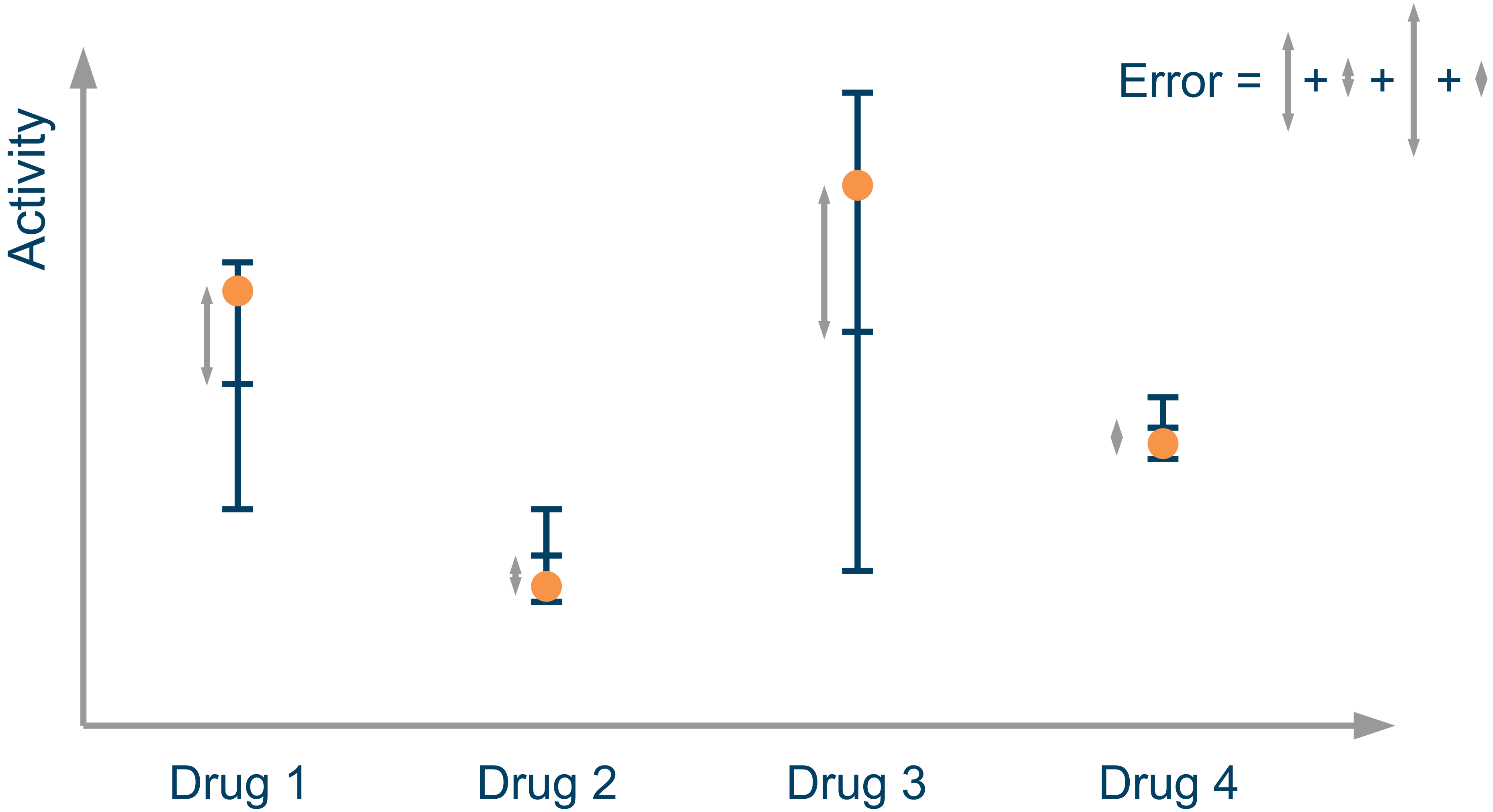
Predictions have an uncertainty



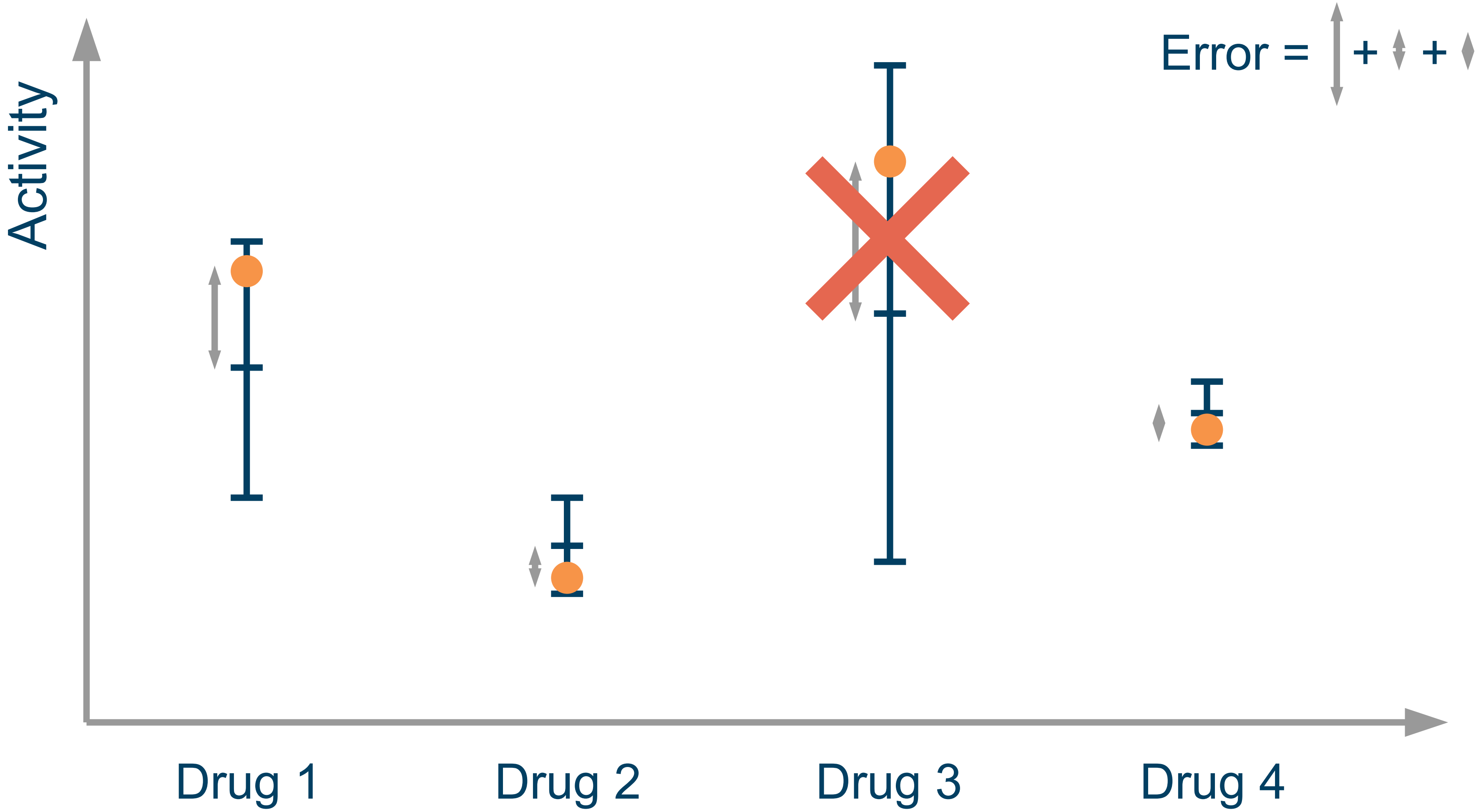
Validation data typically within one standard deviation



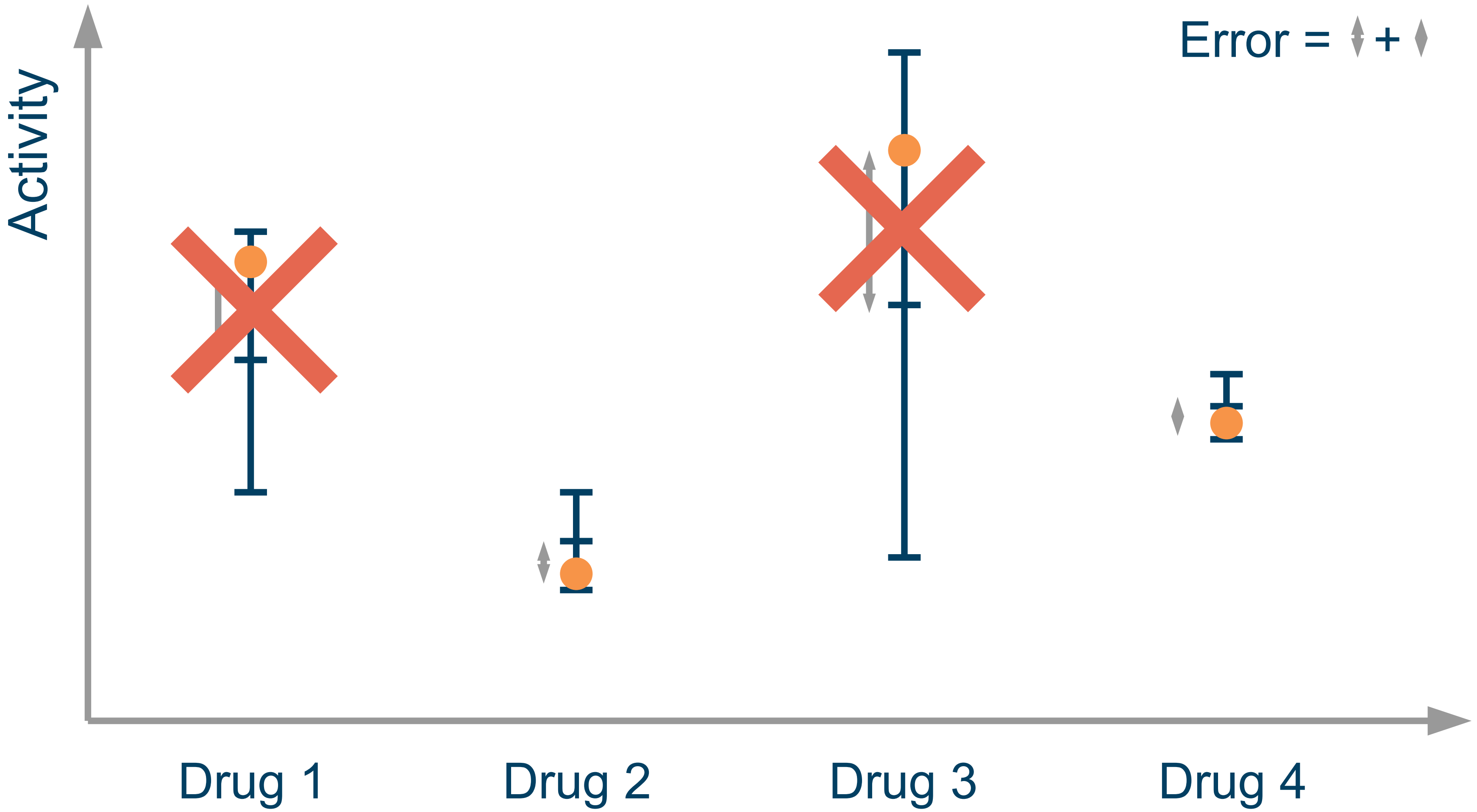
Accuracy R^2 metric calculated with difference from mean



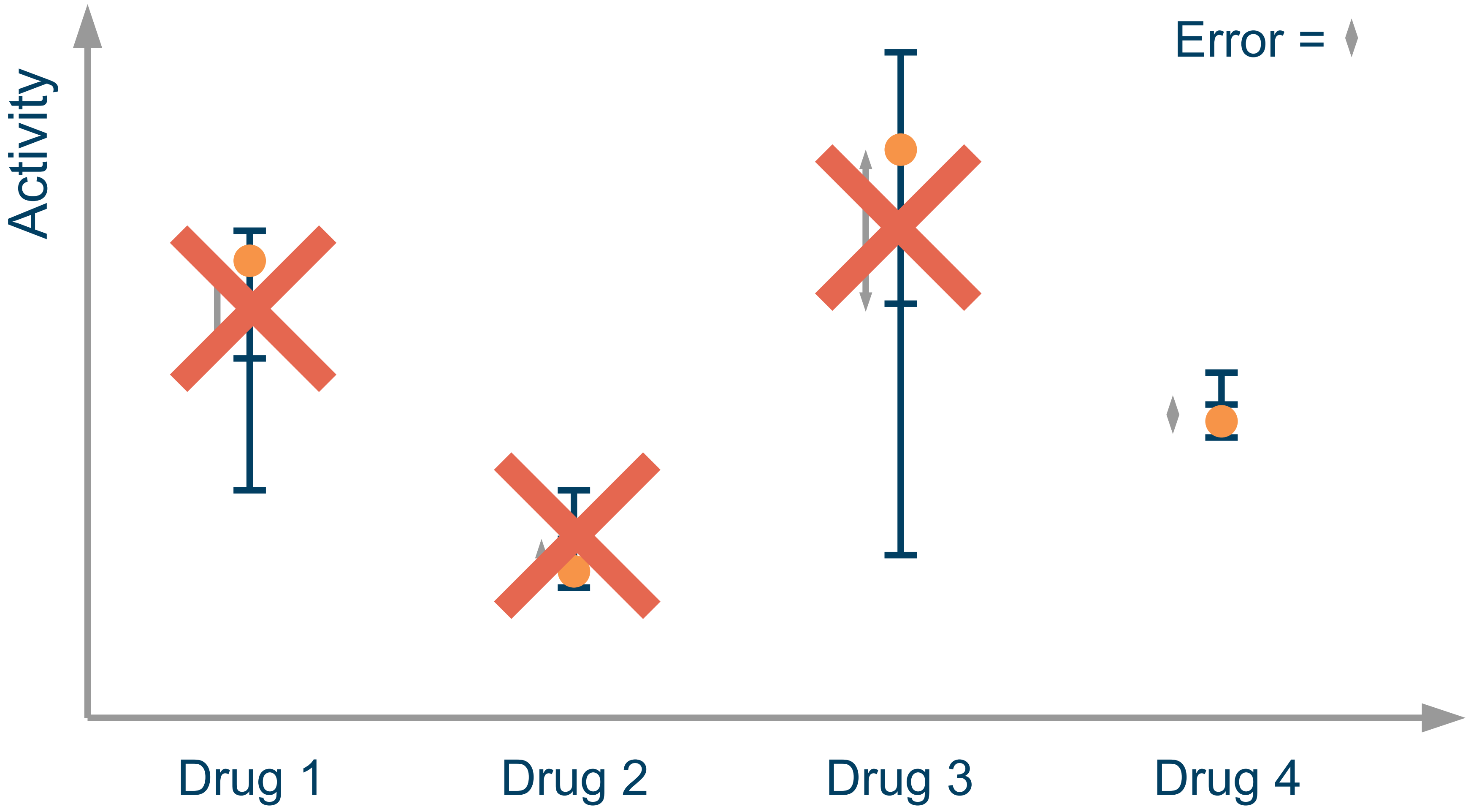
Impute 75% of data with smallest uncertainty



Impute 50% of data with smallest uncertainty

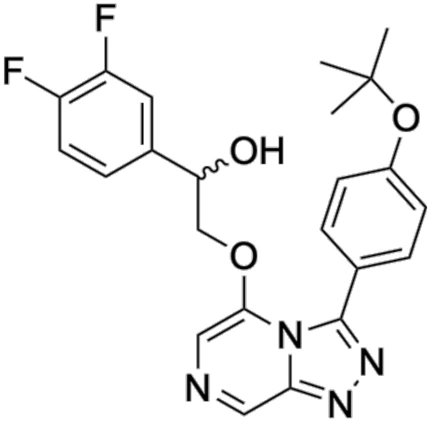


Impute 25% of data with smallest uncertainty



Different drugs can treat the same ailment

Open Source Malaria experimental validation

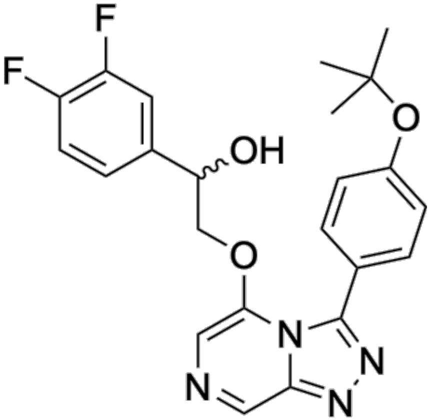
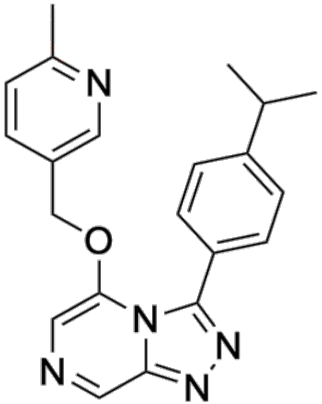
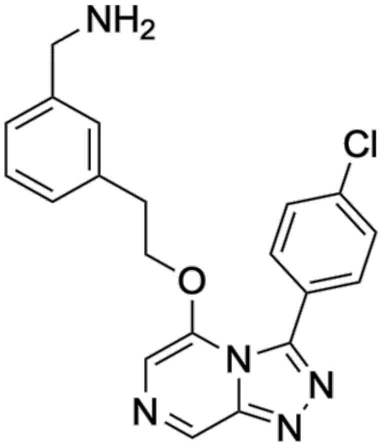
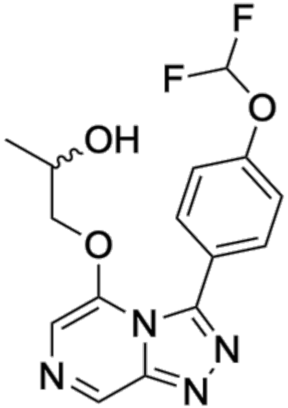


Optibrium & Intellegens

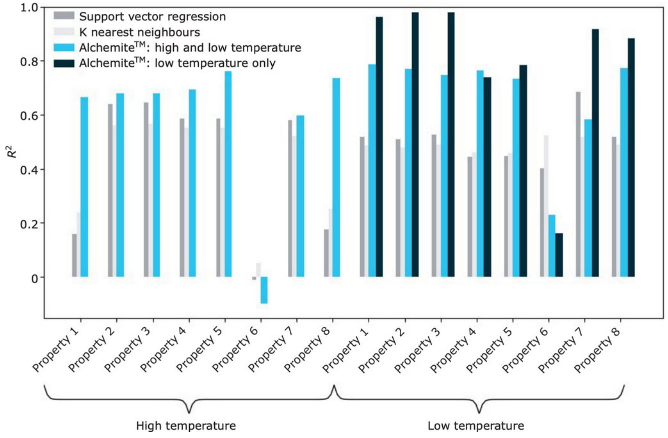
0.647 μM

Journal of Medicinal Chemistry 64, 16450 (2021)

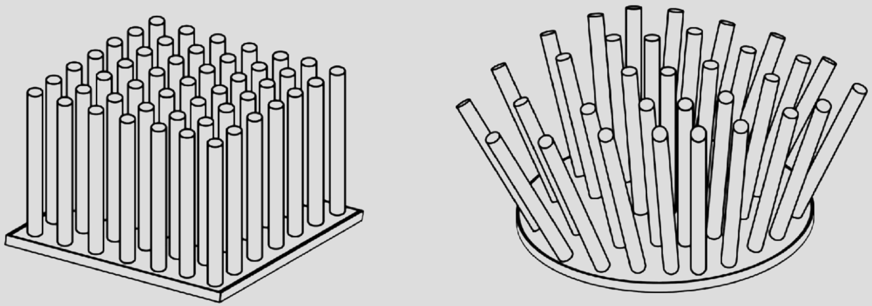
Open Source Malaria other compounds

			
Optibrium & Intellegens	Davy Guan	Exscientia	Molomics
0.647 µM	>25 µM	10.9 µM	>25 µM

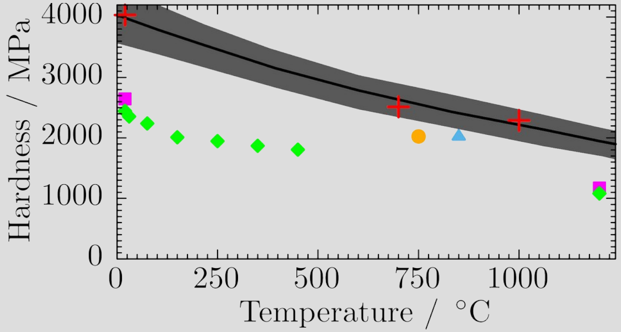
Journal of Medicinal Chemistry 64, 16450 (2021)



Johnson Matthey Technology Review
66, 130 (2022)



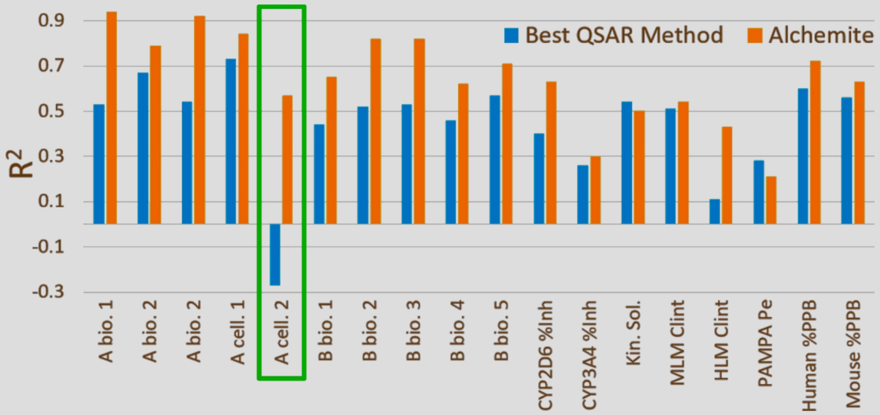
NASA Technical Memorandum
20220008637



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

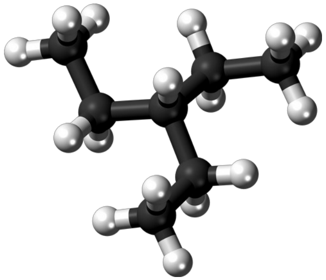
Alloy	Source	ANN	Δ_σ	Actual
Steel AISI 301L	193	269	5	238[23]
Steel AISI 301	193	267	5	221[23]
Al 1080 H18	51	124	5	120[23]
Al 5083 wrought	117	191	14	300,190[4, 23]
Al 5086 wrought	110	172	11	269,131[4, 23]
Al 5454 wrought	102	149	14	124[23]
Al 5456 wrought	130	201	11	165[23]
INCONEL600	223	278	10	≥550[23]

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

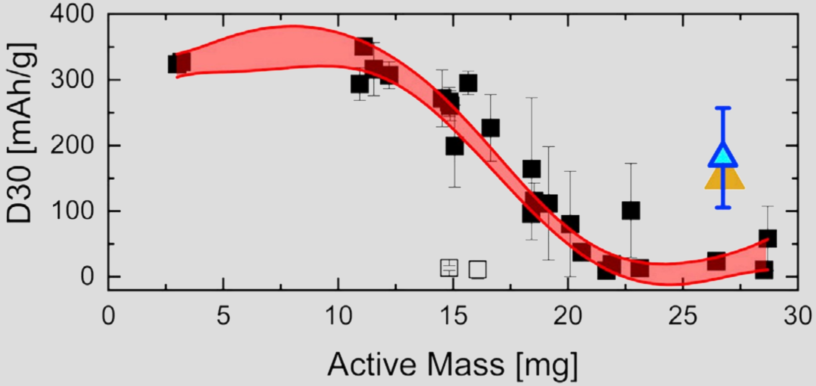


J. of Chem. Info. & Model. **60**, 2848 (2020)
Applied AI Letters **2**, e31 (2021)
Molecular Pharmaceutics **19**, 1488 (2022)

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



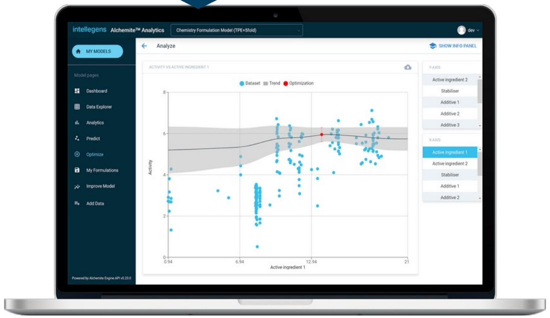
Fluid Phase Equilibria **501**, 112259 (2019)
Journal of Chemical Physics **153**, 014102 (2020)



Nature Machine Intelligence **2**, 161 (2020)
Cell Reports Physical Science **2**, 100683 (2021)

Intellegens offers the Alchemite™ product family

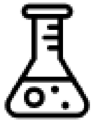
Scientists & engineers
Fast start, easy-to-use, visual



Option to deploy models

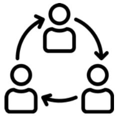
Data scientists
Add to your ML toolkit

Optional connectors



Lab systems

Software & scripts



Sharing & collaboration

Alchemite™ Analytics

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Alchemite™ Engine

Integrate into your workflow (API, Python)

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Alchemite™ Academic Programme

Access Alchemite™ for academic research

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 uncertainties to propose anti-malarial drug

Software product taken to market through startup Intellegens