UNIVERSITY OF CAMBRIDGE

The modern day blacksmith

Gareth Conduit

Theory of Condensed Matter group

Neural network algorithm to

Train from sparse datasets

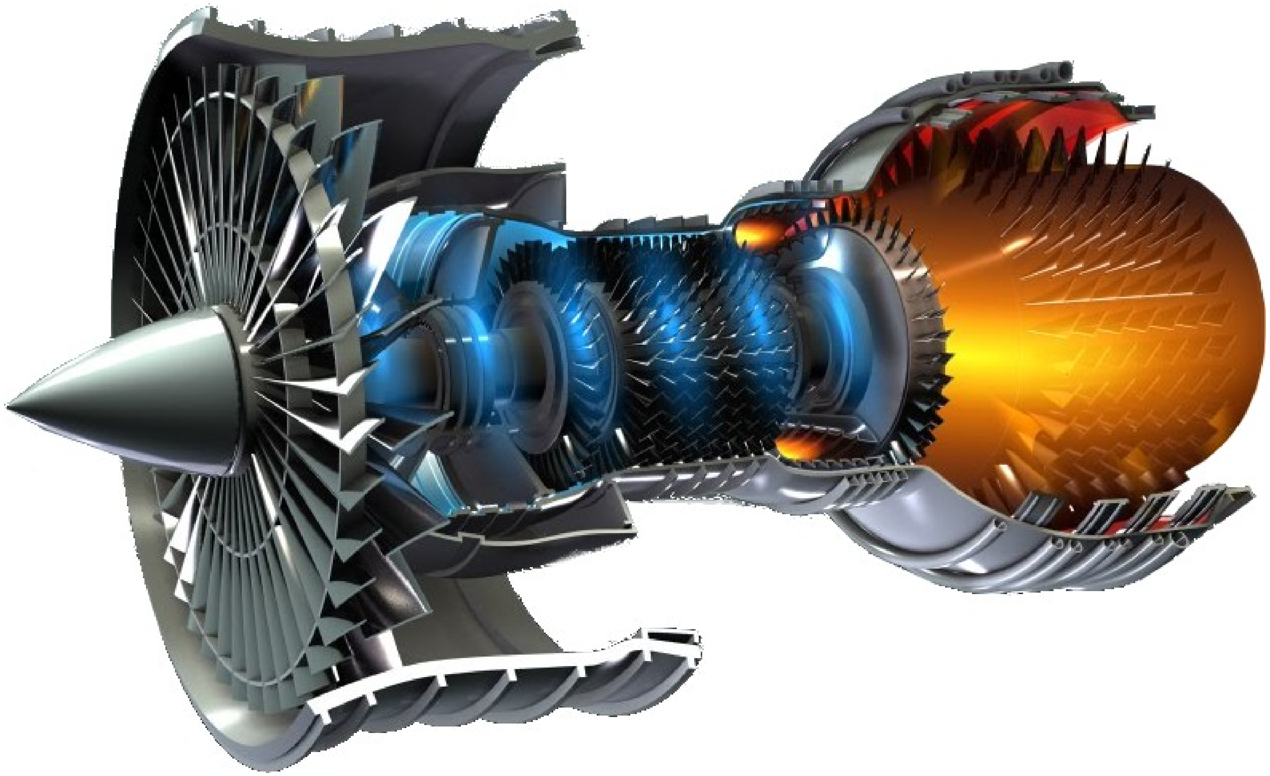
Merge simulations, physical laws, and experimental data

Reduce the need for expensive experimental development

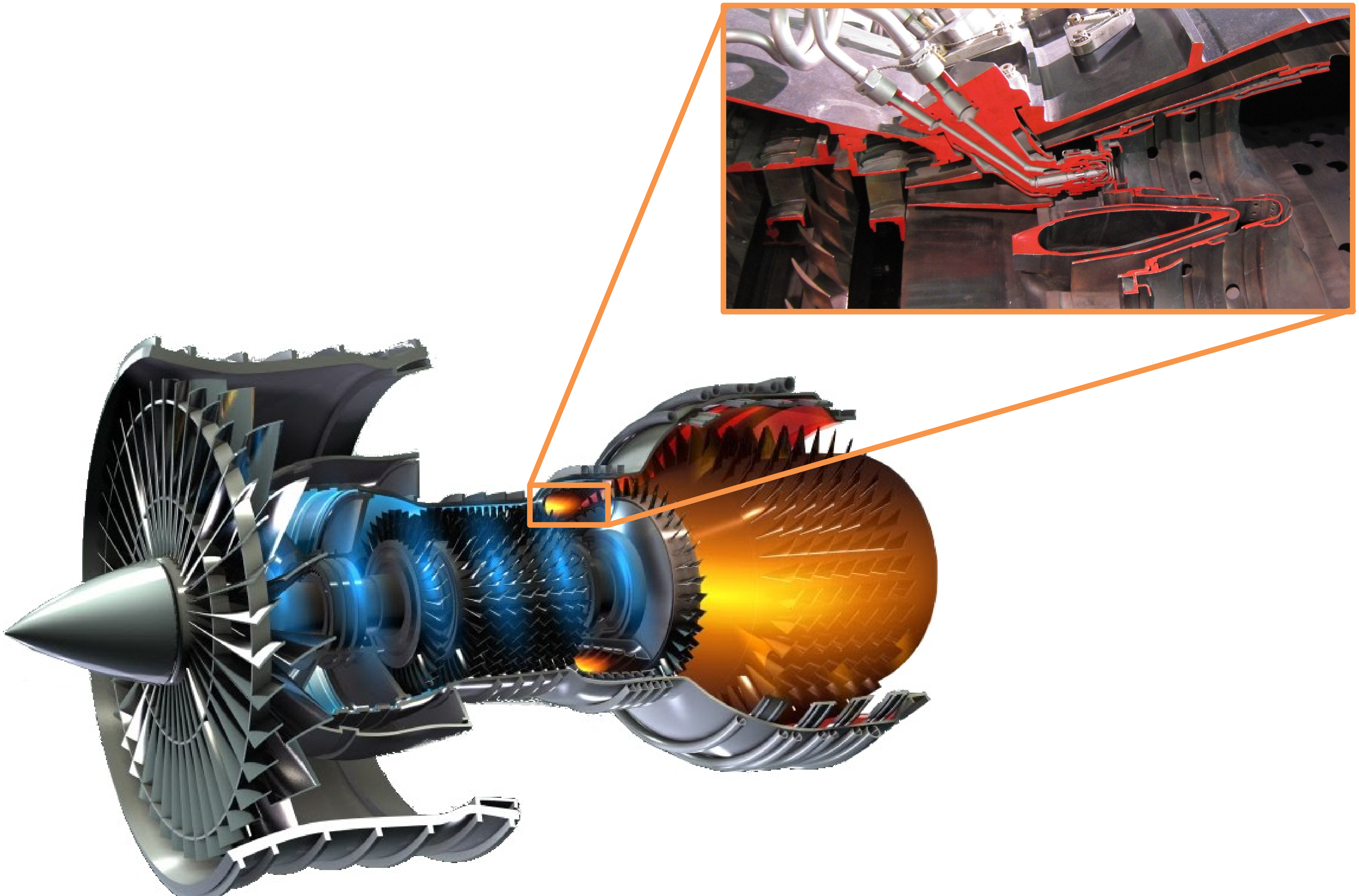
Accelerate materials and drugs discovery

Generic with proven applications in materials discovery and drug design

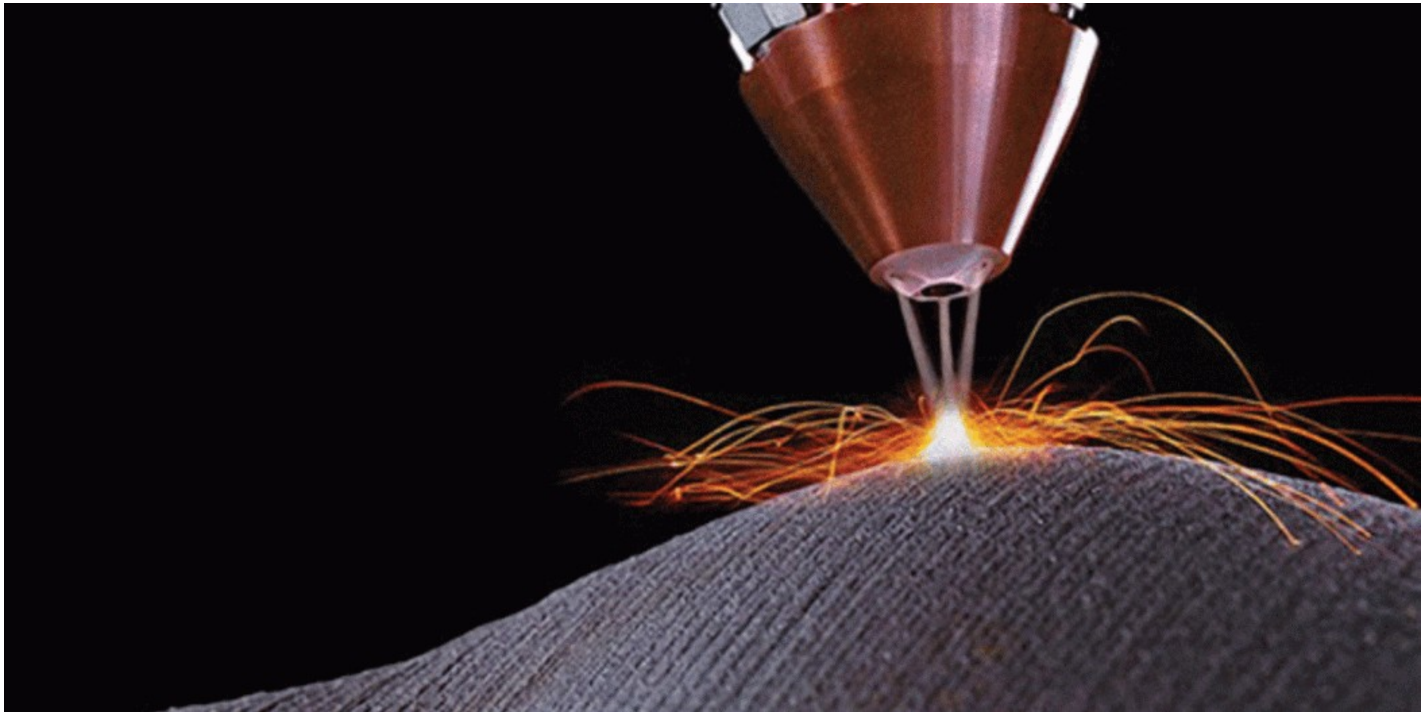
Schematic of a jet engine



Combustor in a jet engine



Direct laser deposition requires new alloys

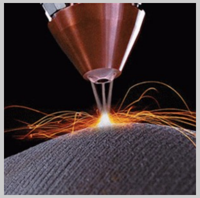


Neural networks for materials design

Composition

Properties

Process



Fatigue

Welding

Neural networks for materials design

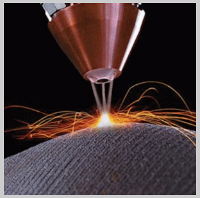
Composition

Neural networks for materials design

Composition

Properties

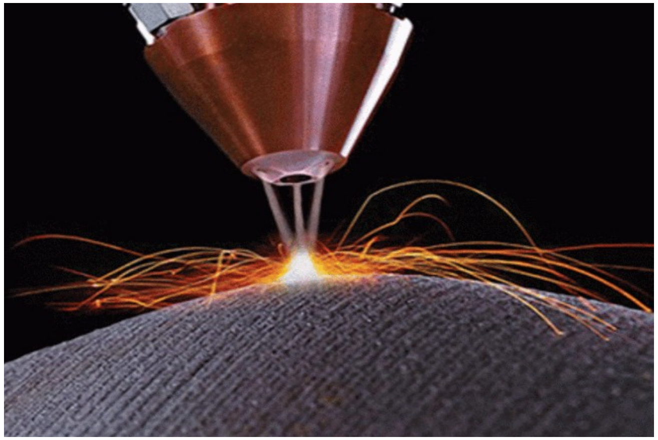
Process



Fatigue

Welding

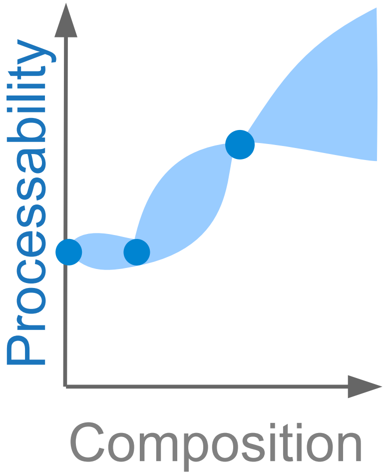
Neural networks for materials design



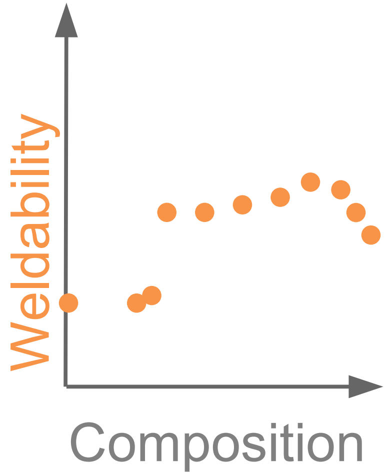
Laser

Electricity

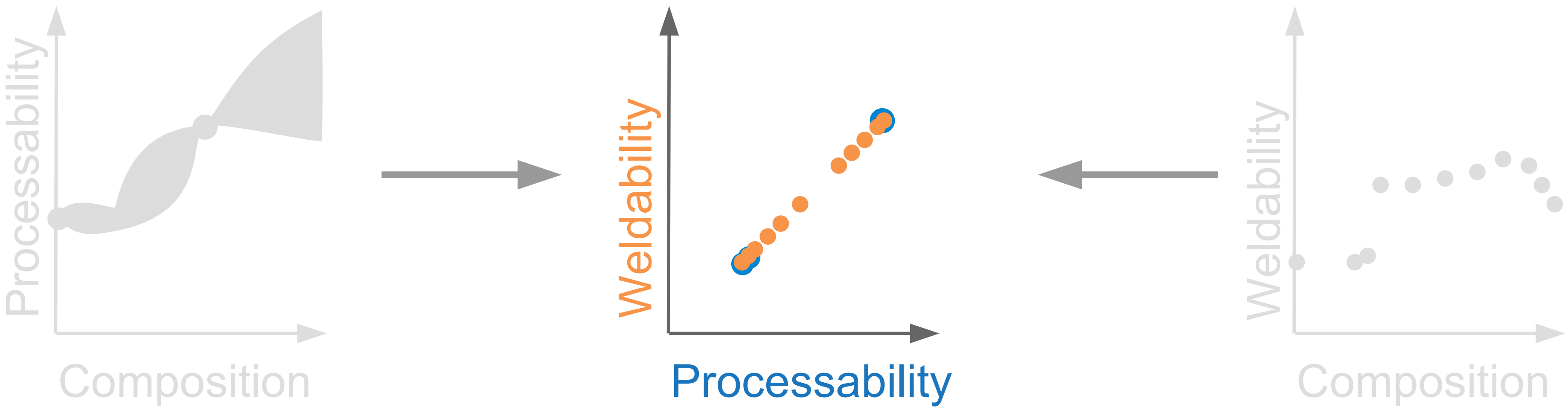
Insufficient data for processability



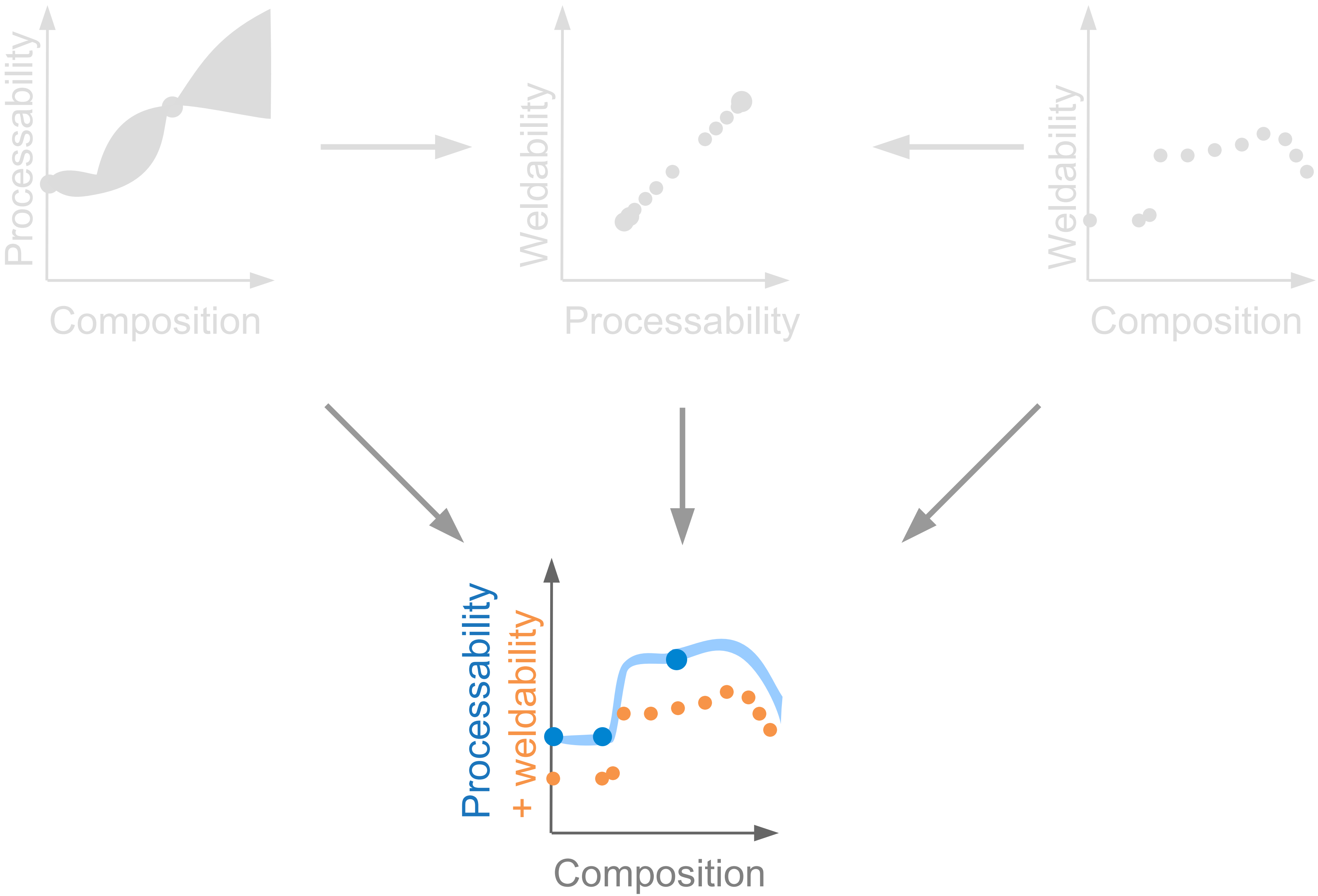
Welding is analogous to direct laser deposition



Simple processability-welding relationship



Merging properties with the neural network

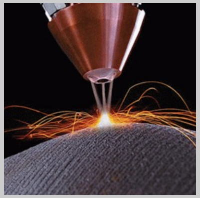


Neural networks for materials design

Composition

Properties

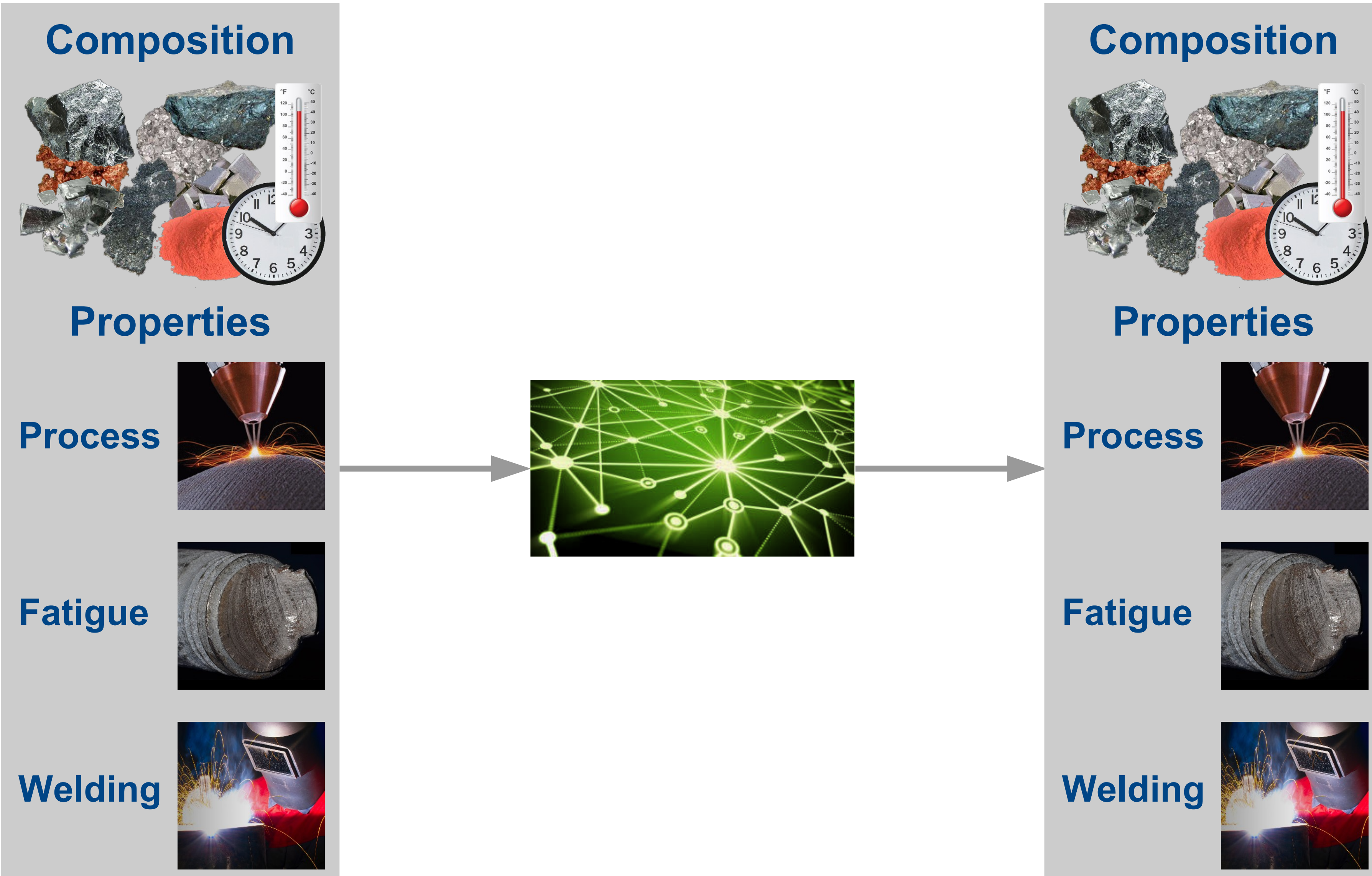
Process



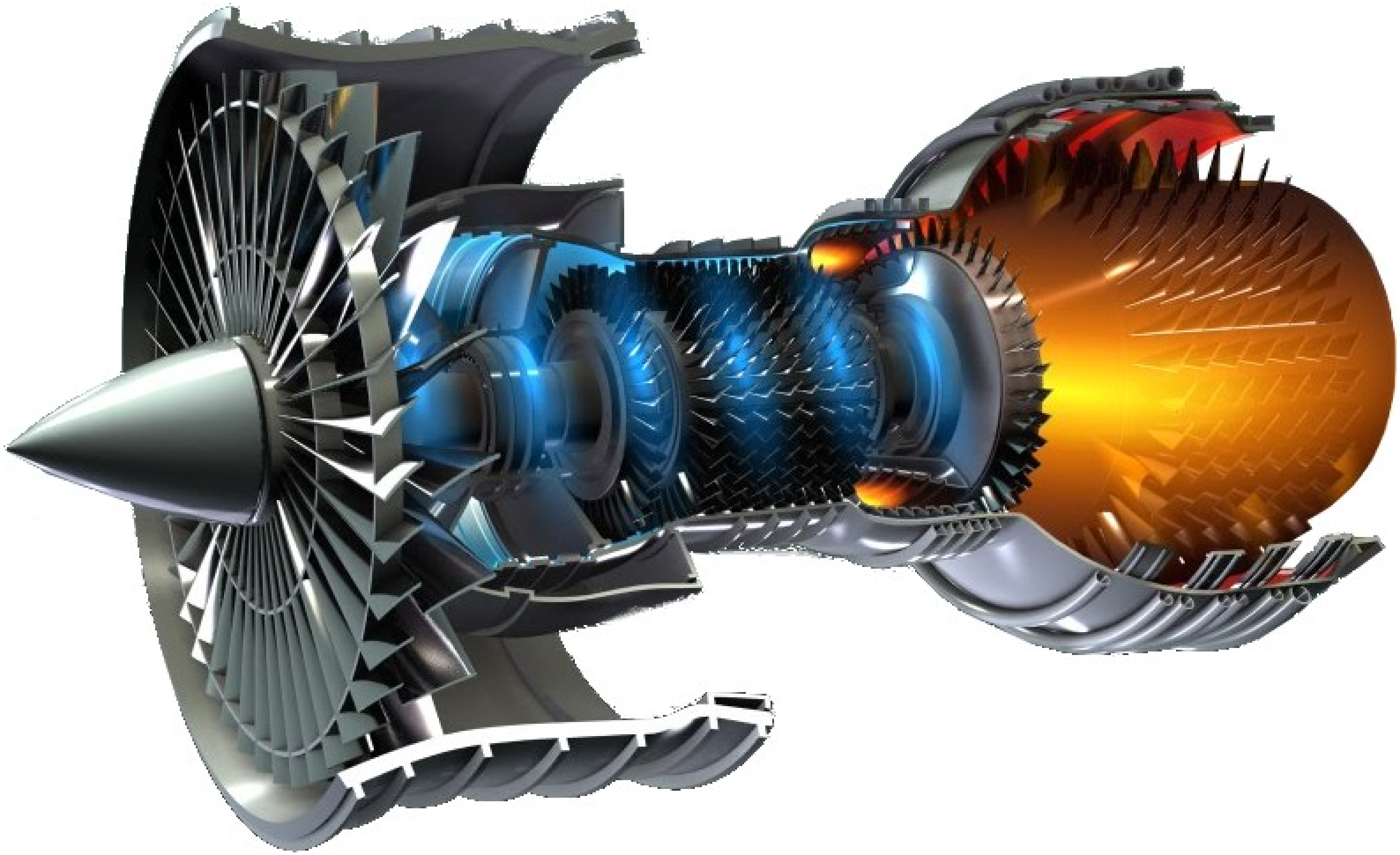
Fatigue

Welding

Neural networks for materials design



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}
Processability	< 0.15% defects
Phase stability	> 99.0 wt%
γ' solvus	> 1000˚C
Thermal resistance	> 0.04 KΩ^{-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%

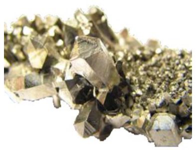
Co: 4%

Mo: 4.9%

W: 1.2%

Zr: 0.05%

Nb: 3%



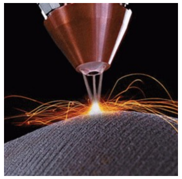
Al: 2.9%

C: 0.04%

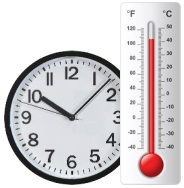
B: 0.01%

Ni

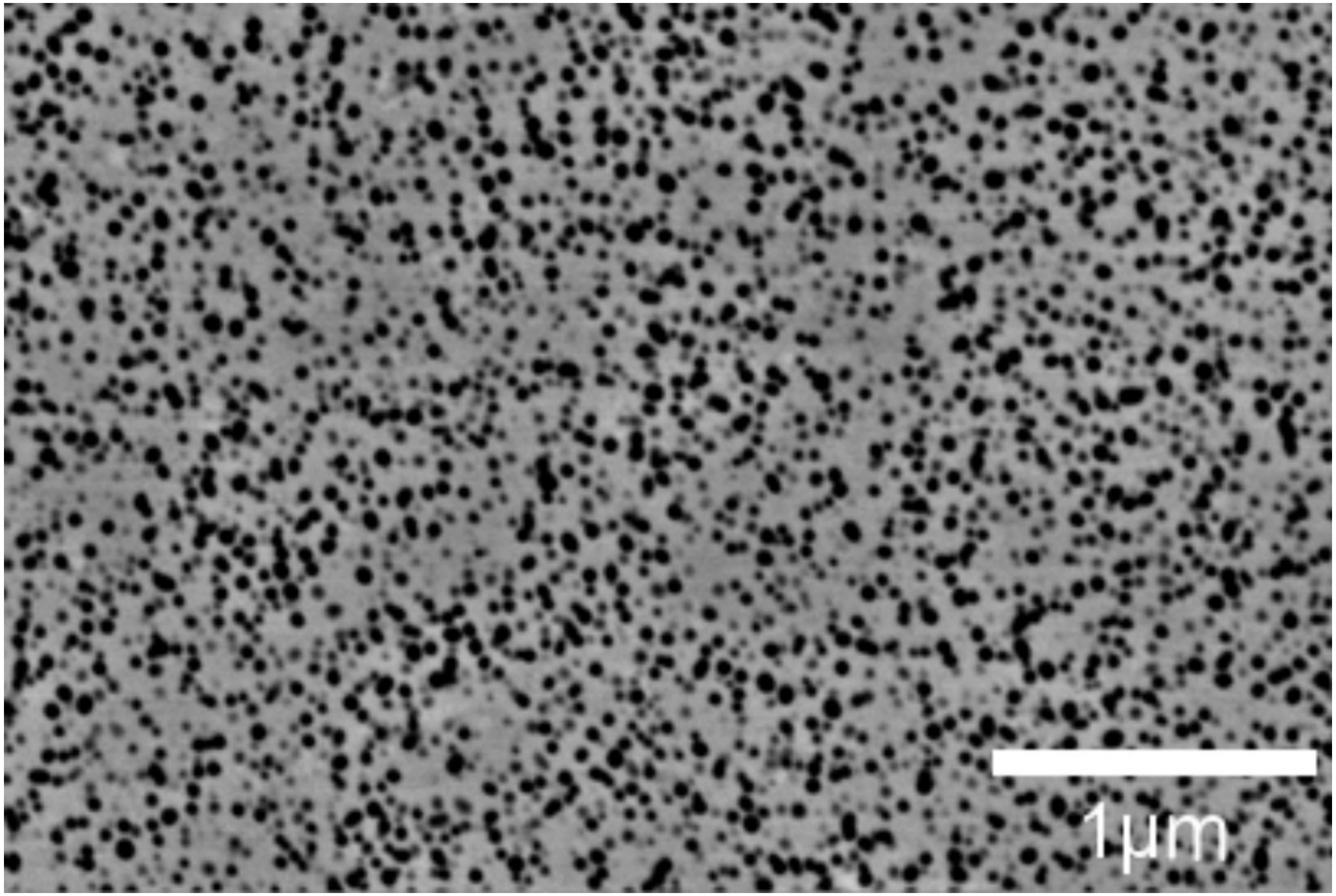
Expose 0.8



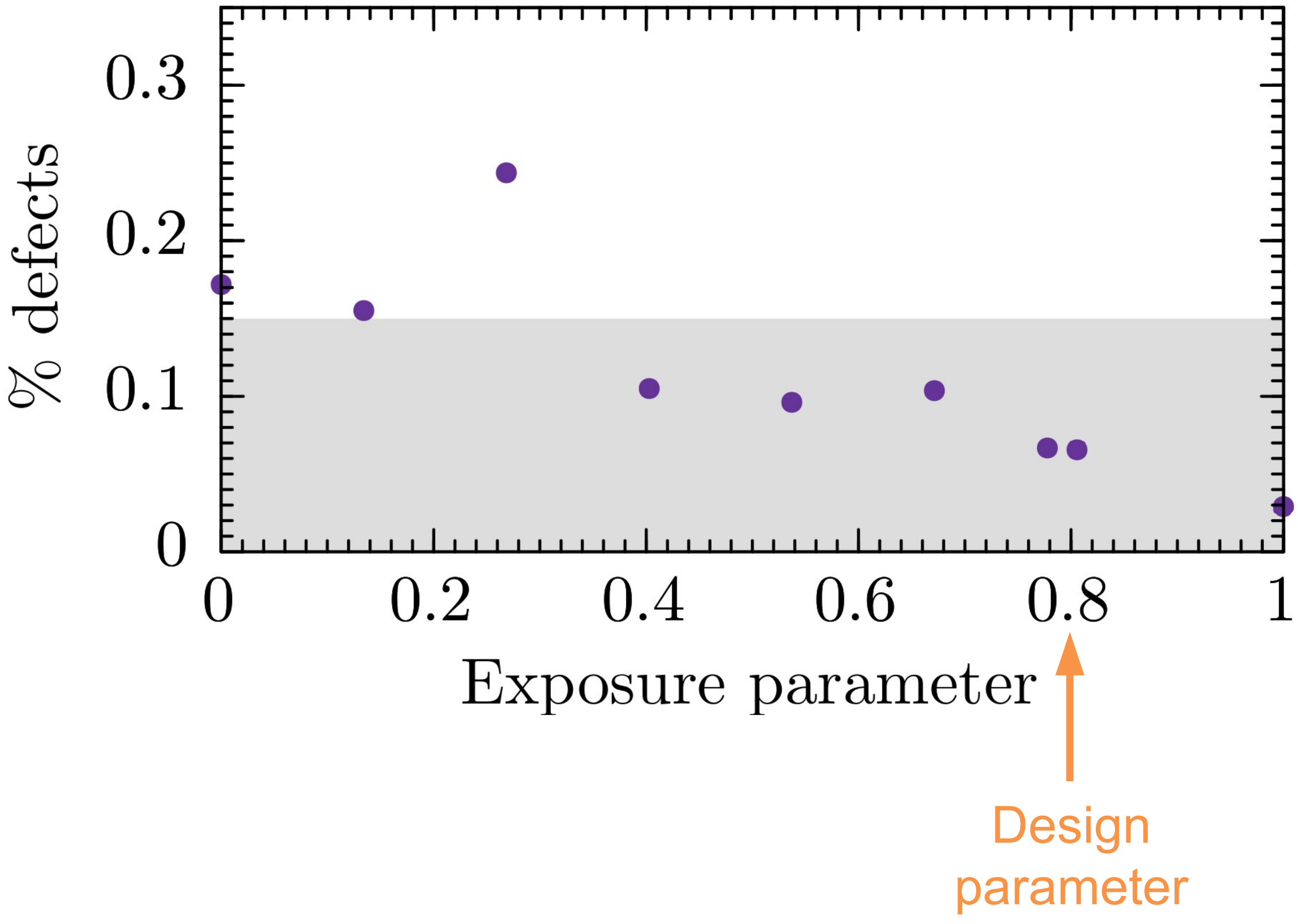
T_{HT} 1300ºC



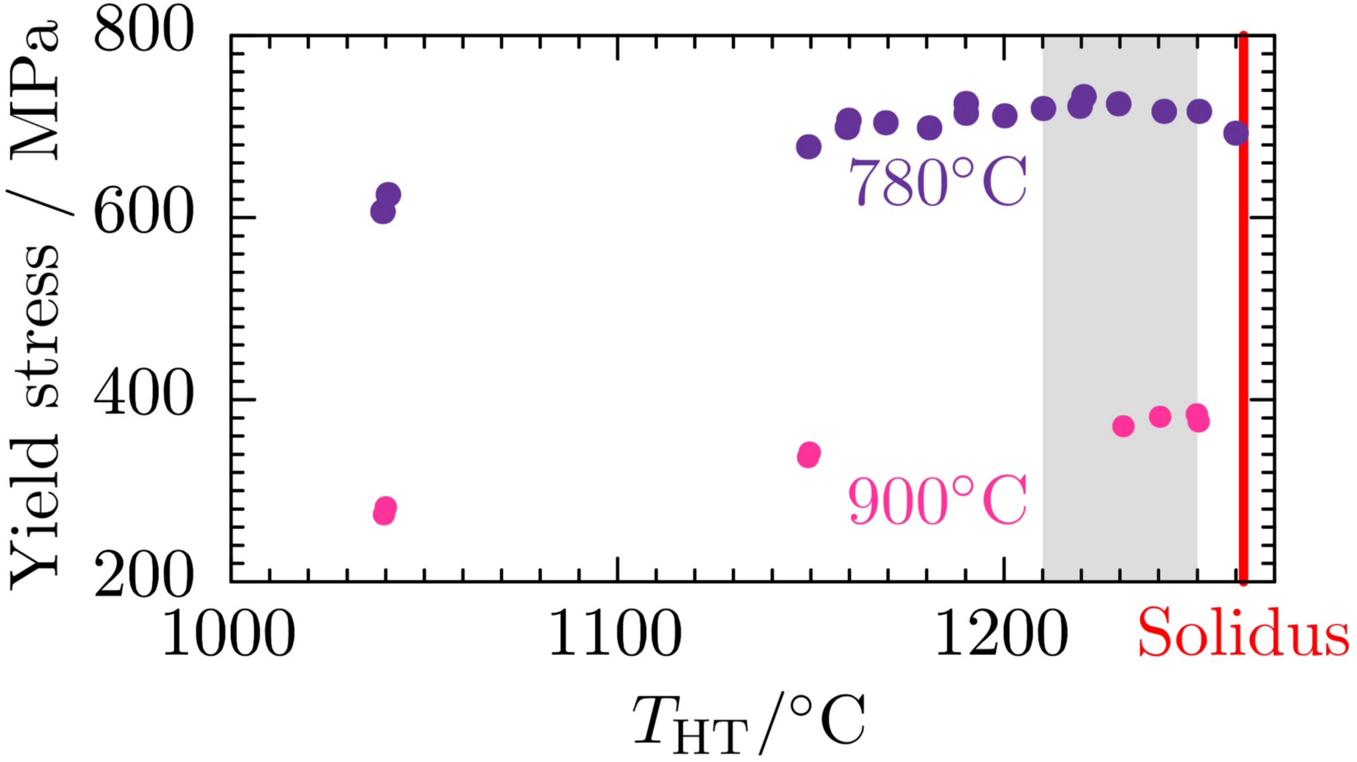
Microstructure



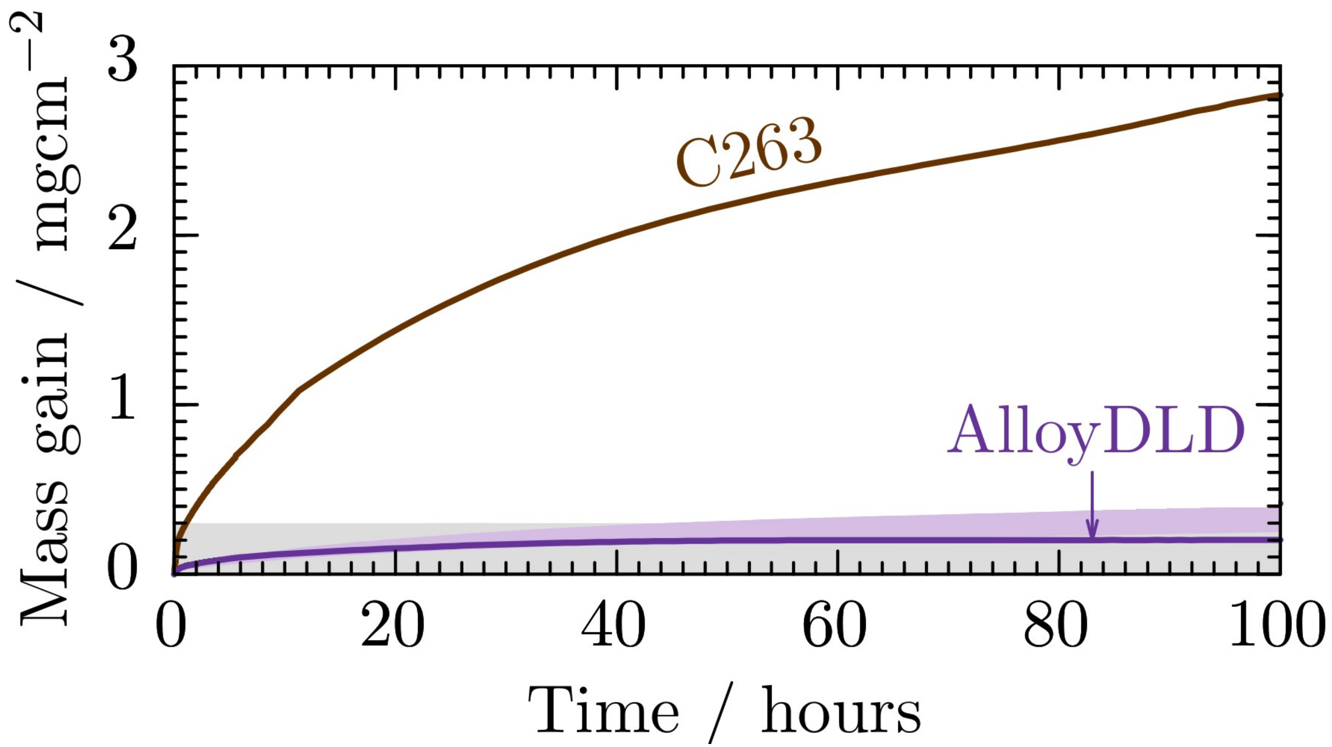
Testing the processability: horizontal printing



Testing the processability: horizontal printing



Testing the oxidation resistance

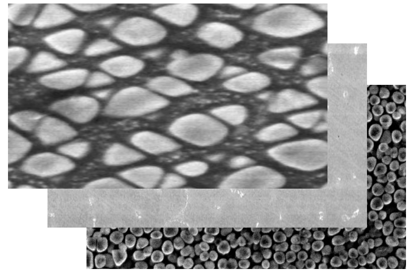


Printing components for an engine

Materials & Design 168, 107644 (2019)

More materials designed

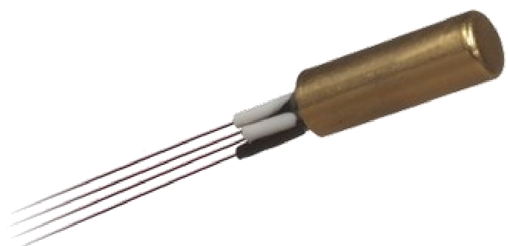
Nickel and molybdenum



ROLLS ROYCE

Steel for welding

Steel for turbos



UNIVERSITY OF CAMBRIDGE

Experiment and DFT for batteries

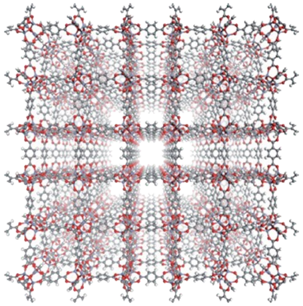
SAMSUNG

Application to chemicals and drugs

Design concrete mixtures on site

BASF
We create chemistry

Metal organic framework



UNIVERSITY OF CAMBRIDGE

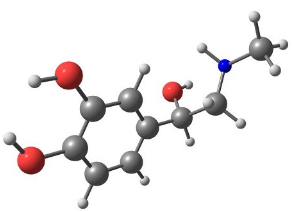
Lubricants with molecular dynamics and experiments

bp

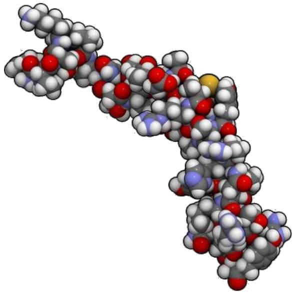
Drug design

e-therapeutics
optibrium
AstraZeneca
Celgene
Takeda
Constellation
PHARMACEUTICALS

Action of a drug



Drug

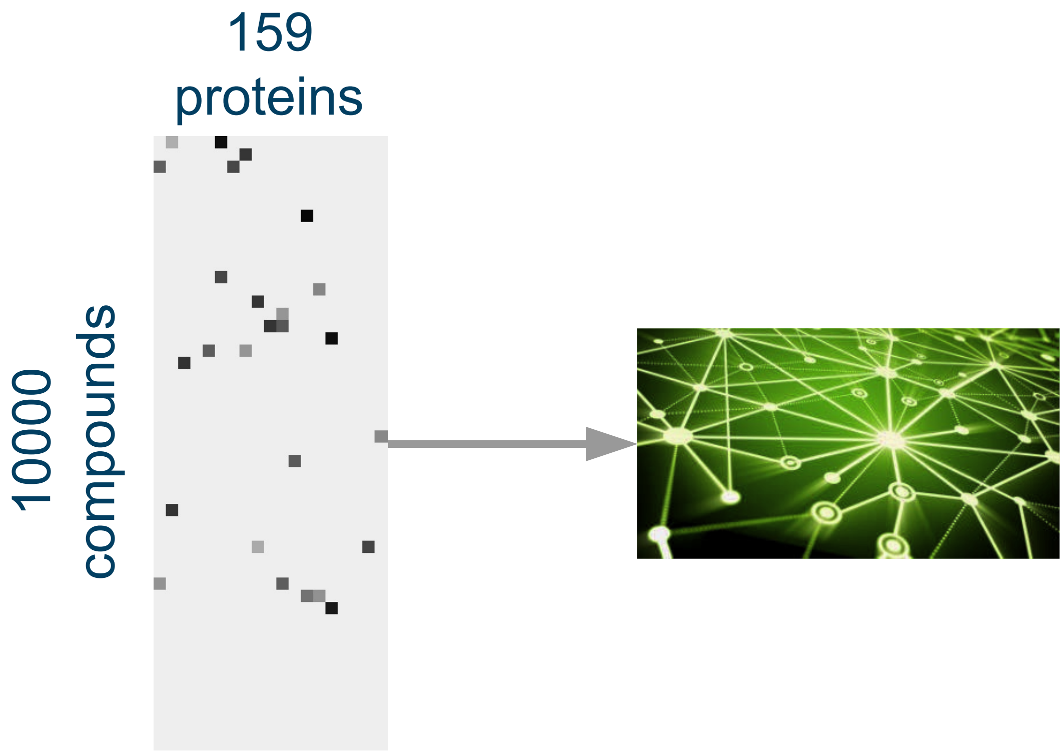


Protein

Effect

Novartis dataset to benchmark machine learning

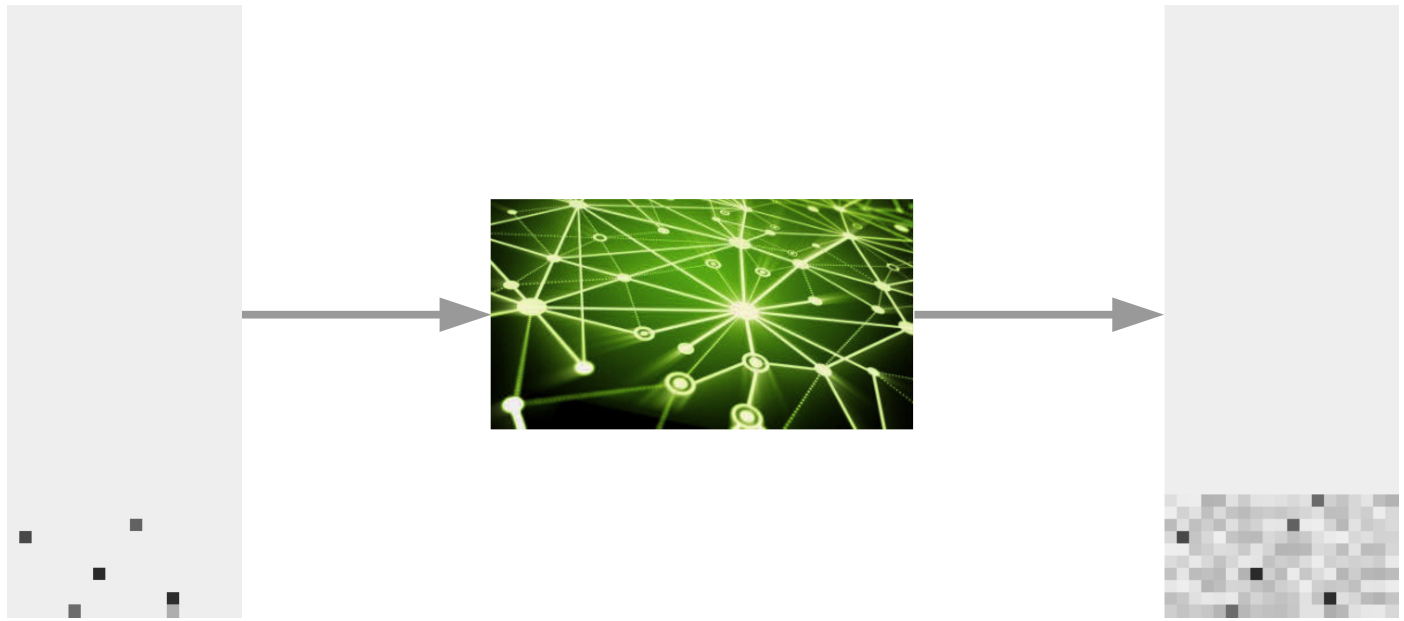
159 kinase proteins, 10000 compounds, data 5% complete



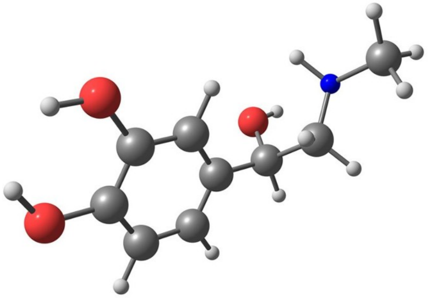
Data from ChEMBL
Martin, Polyakov, Tian, and Perez,
J. Chem. Inf. Model. 57, 2077 (2017)

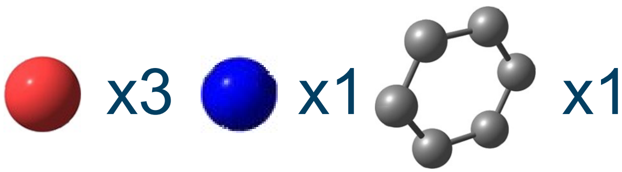
Impute missing entries to validate

Validate using a realistically split holdout data set, extrapolate to new chemical space

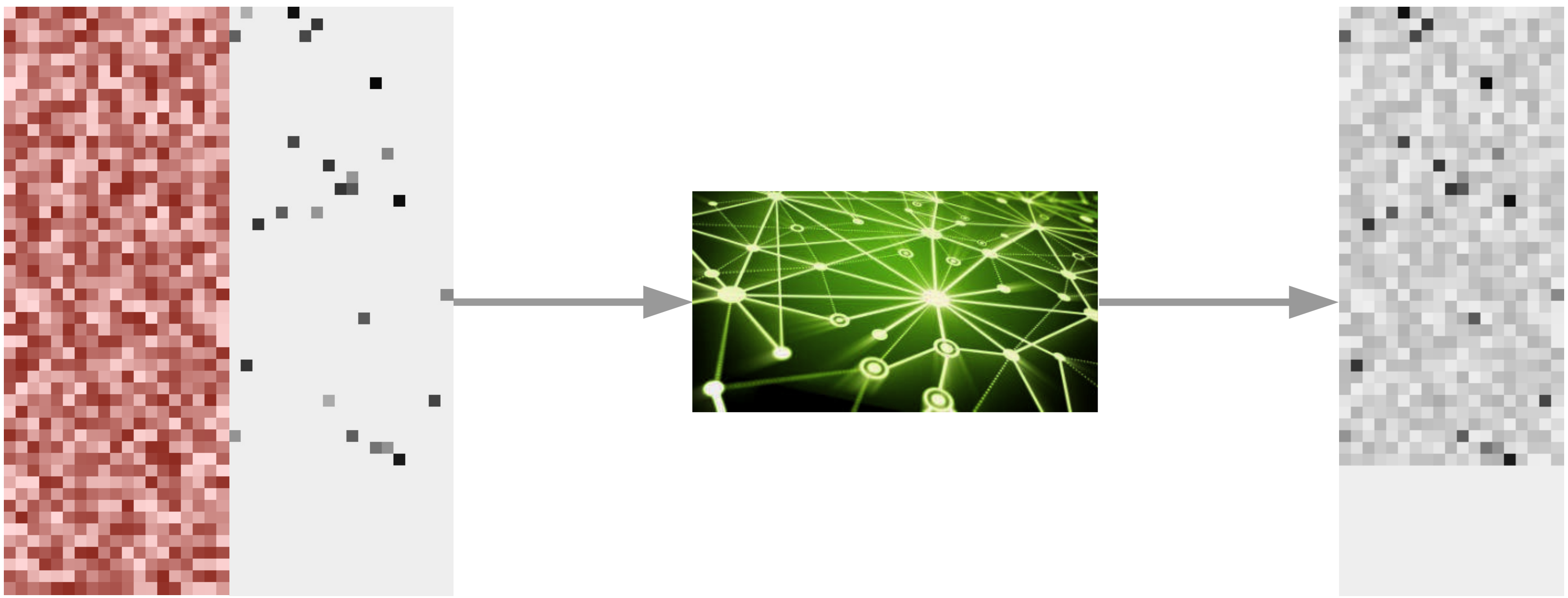


Quantitative structure-activity relationships

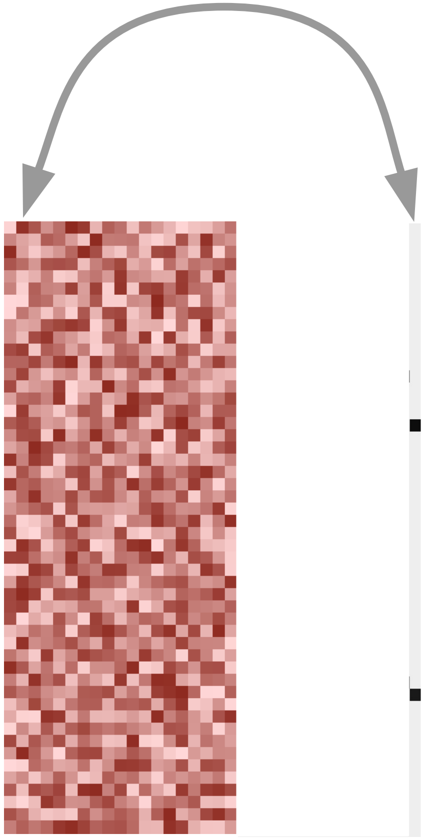




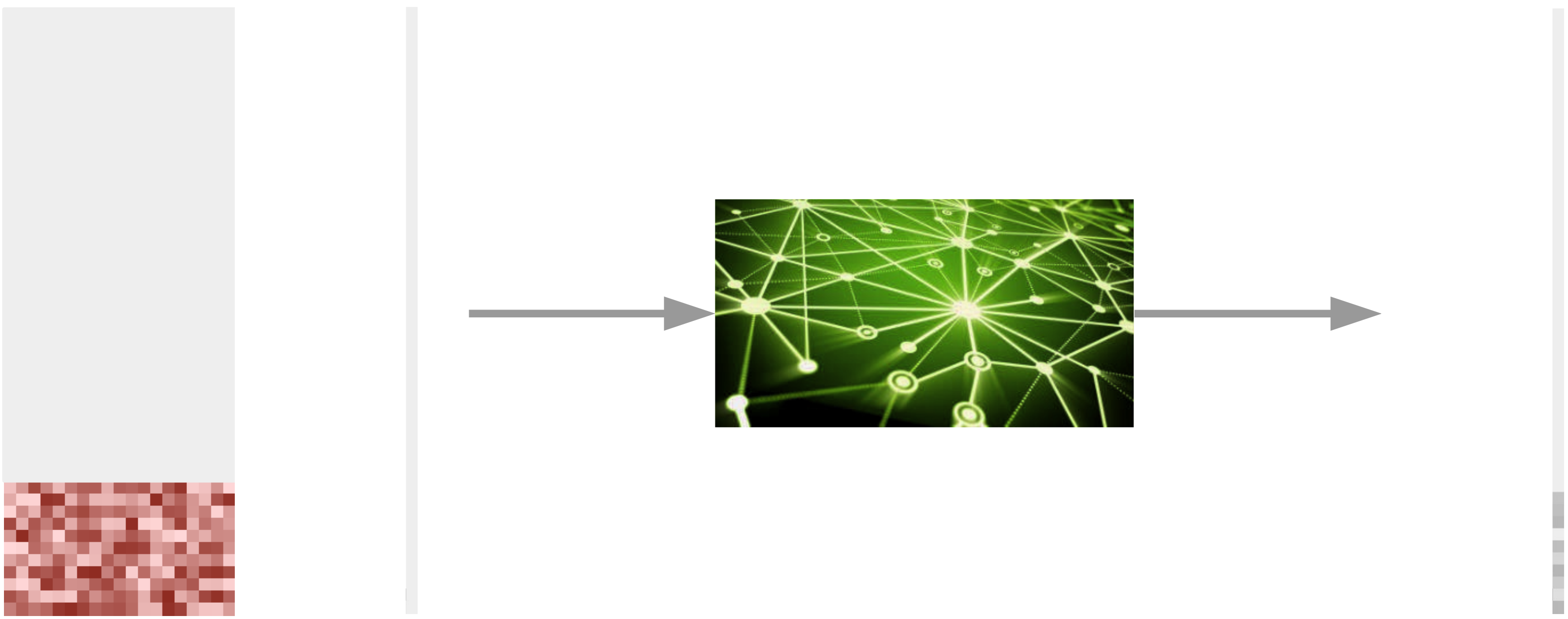
Molecular weight=183 Da



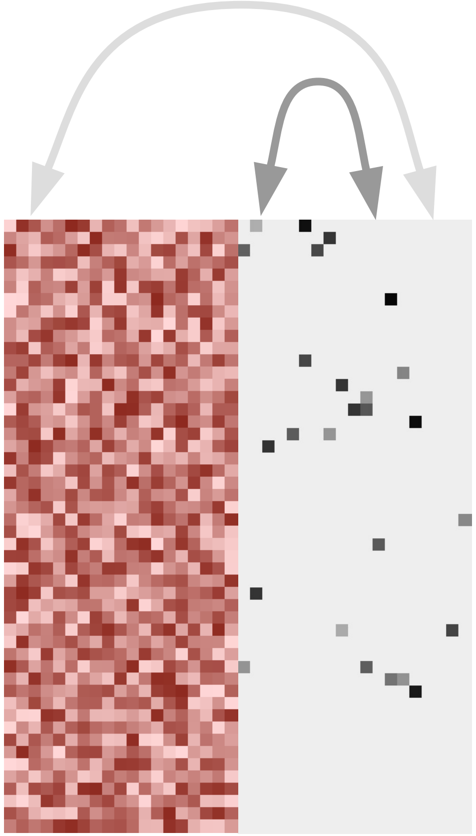
Quantitative structure-activity relationships



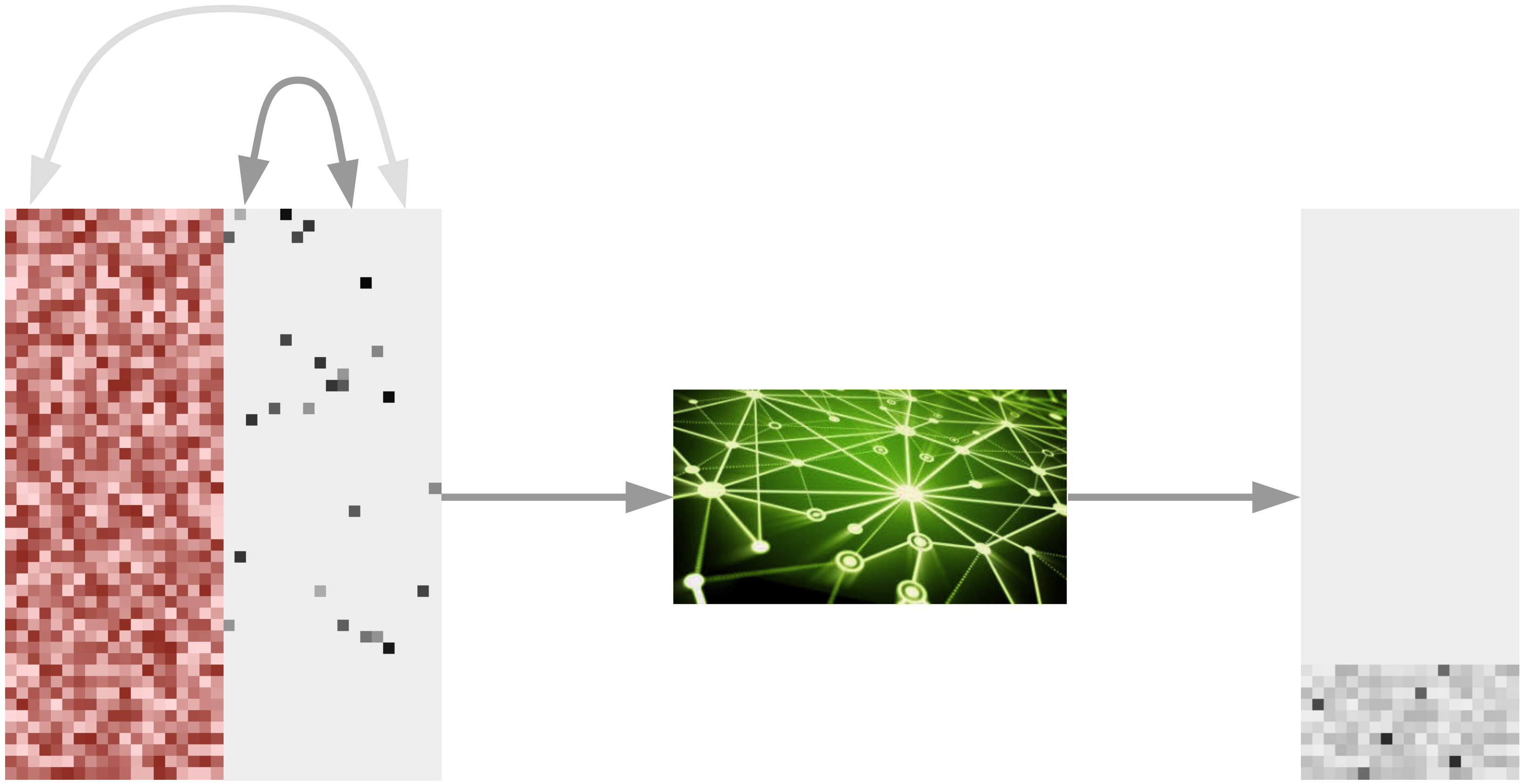
Predict one column at a time



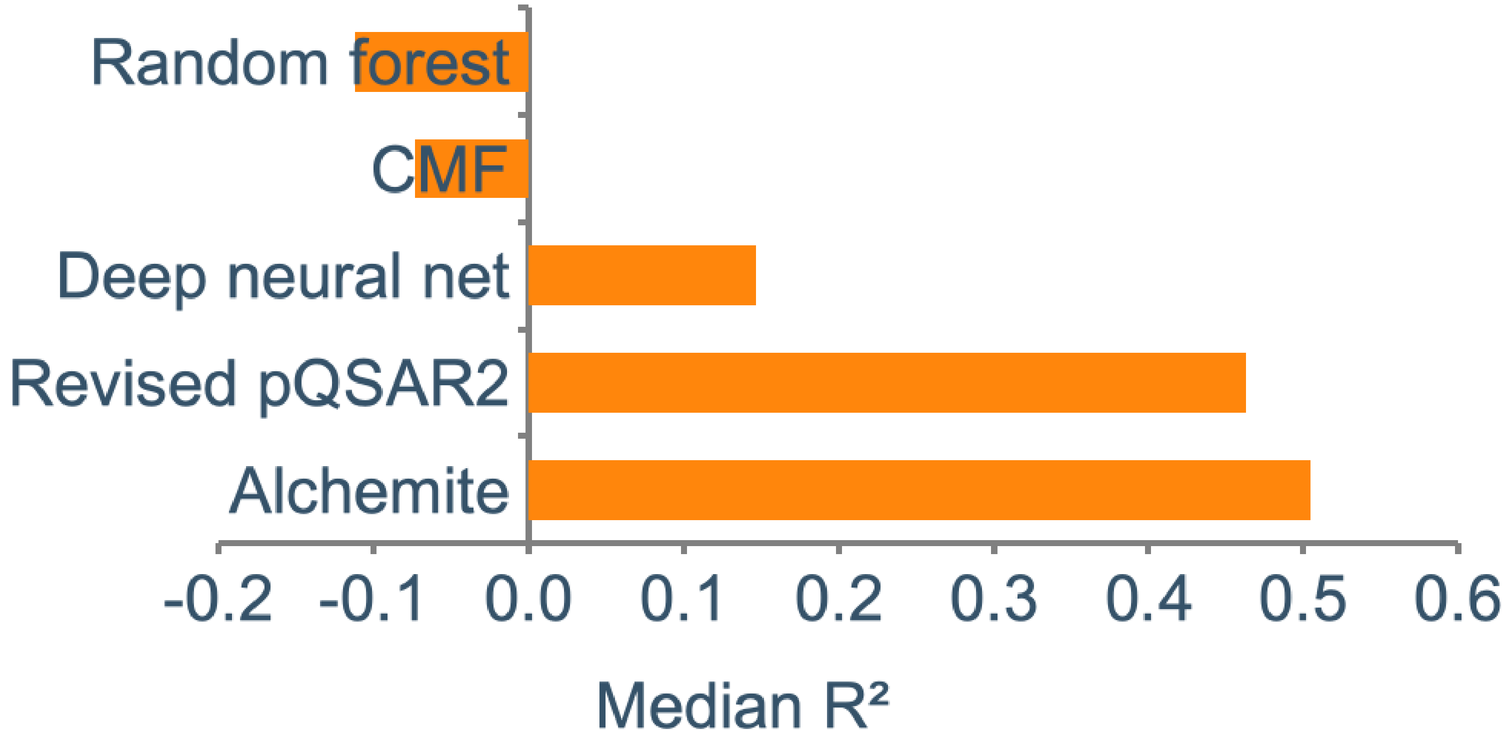
Learn protein-protein correlations



Learn protein-protein correlations

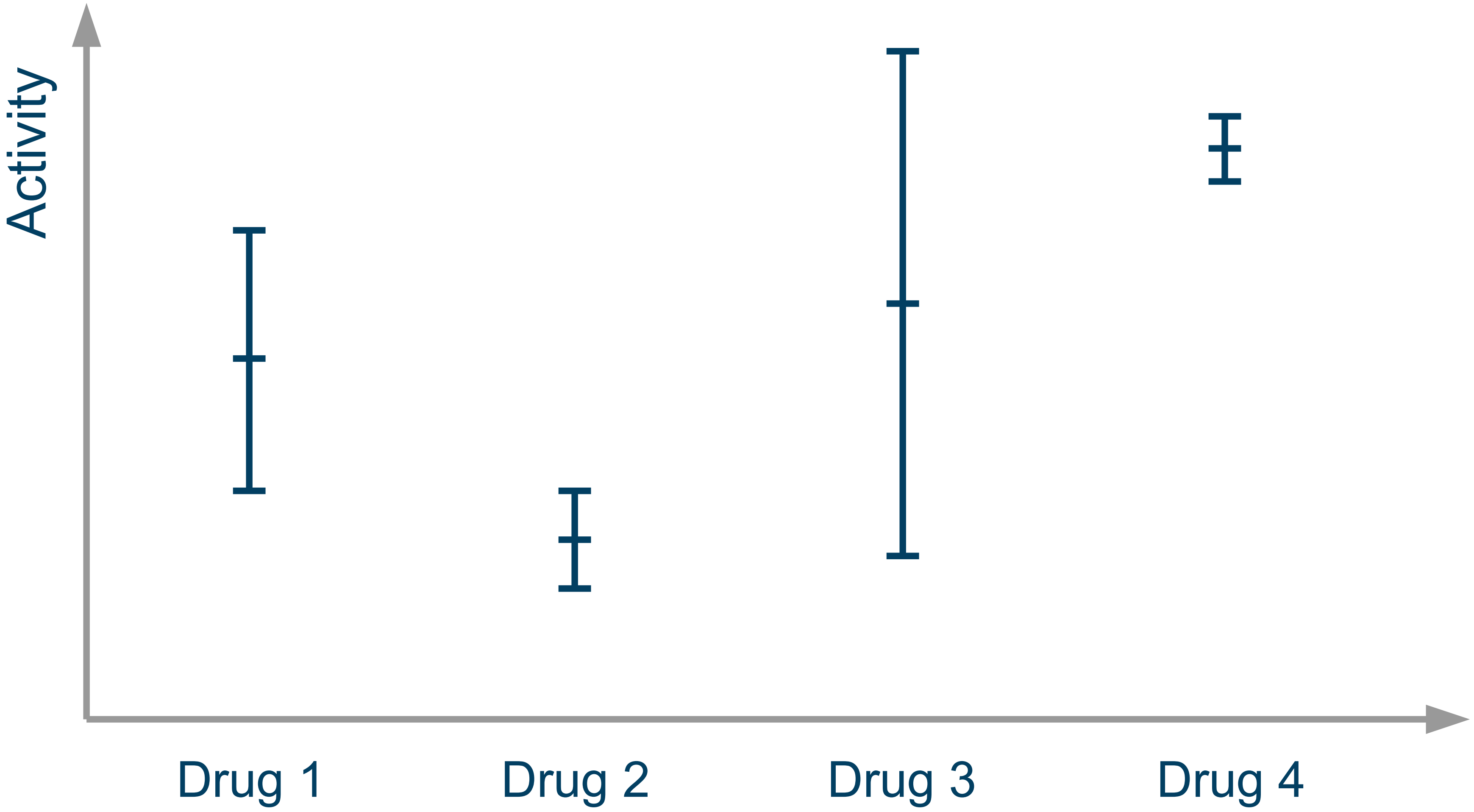


Comparison of techniques

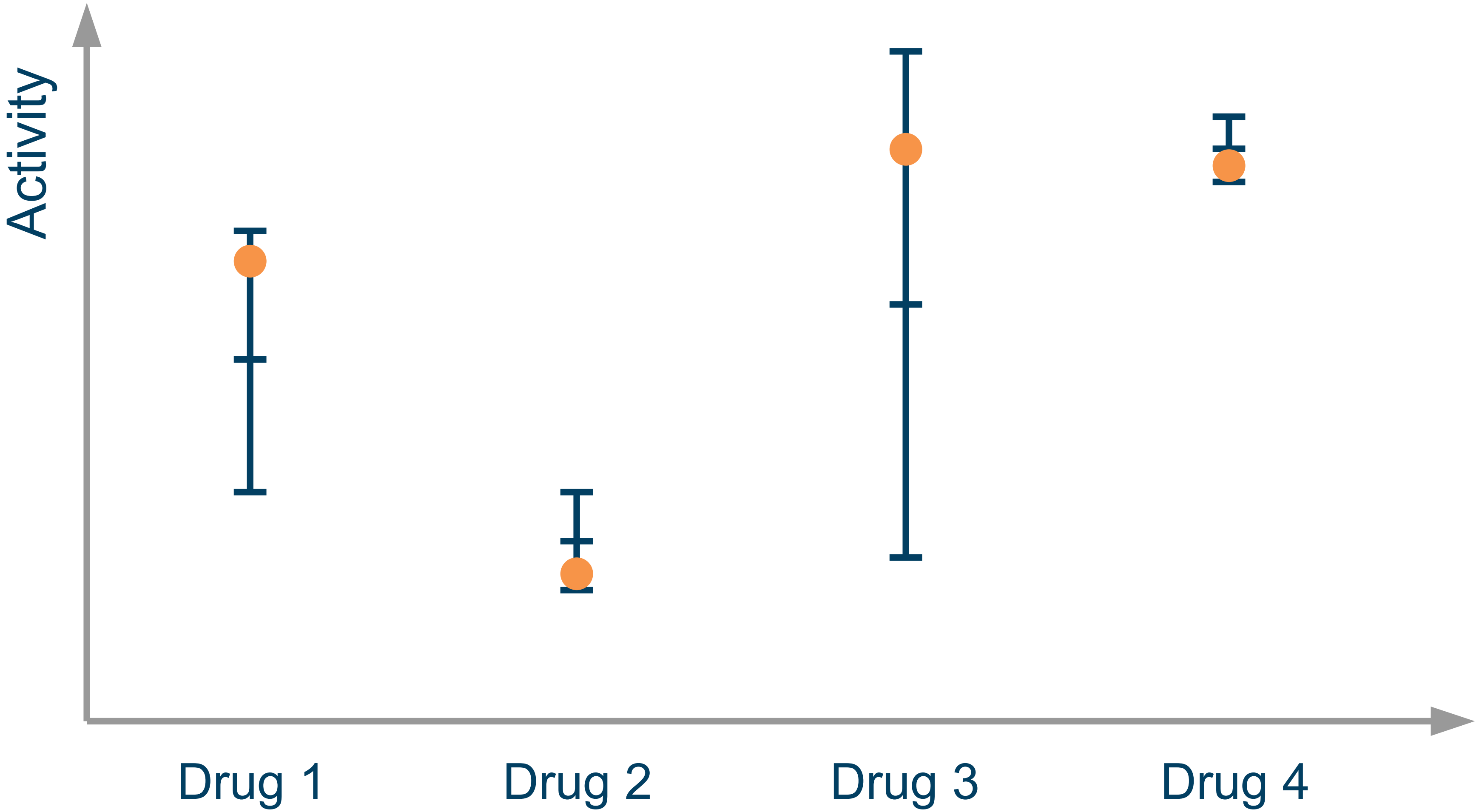


Journal of Chemical Information and Modeling, 59, 1197 (2019)

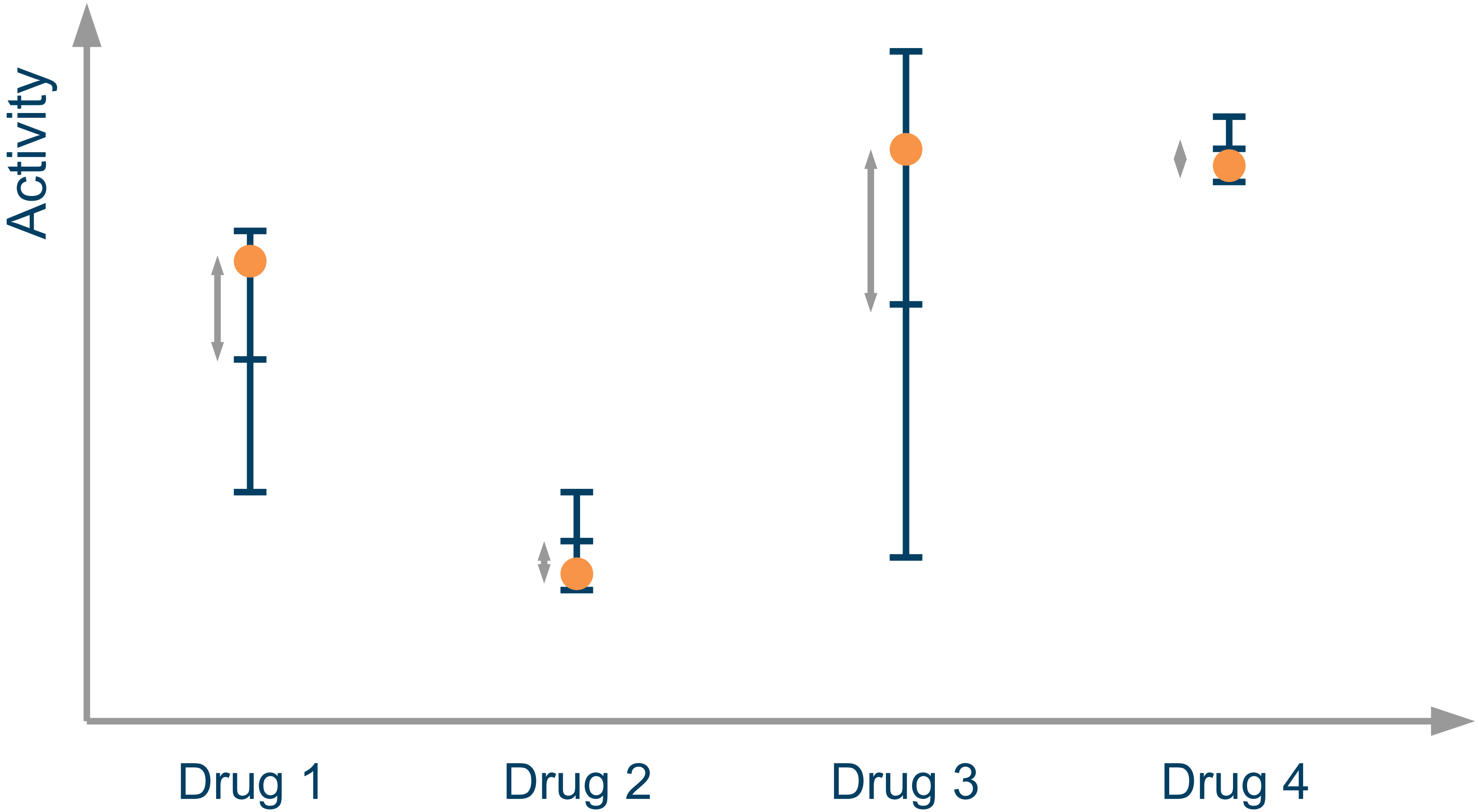
Predictions have an uncertainty



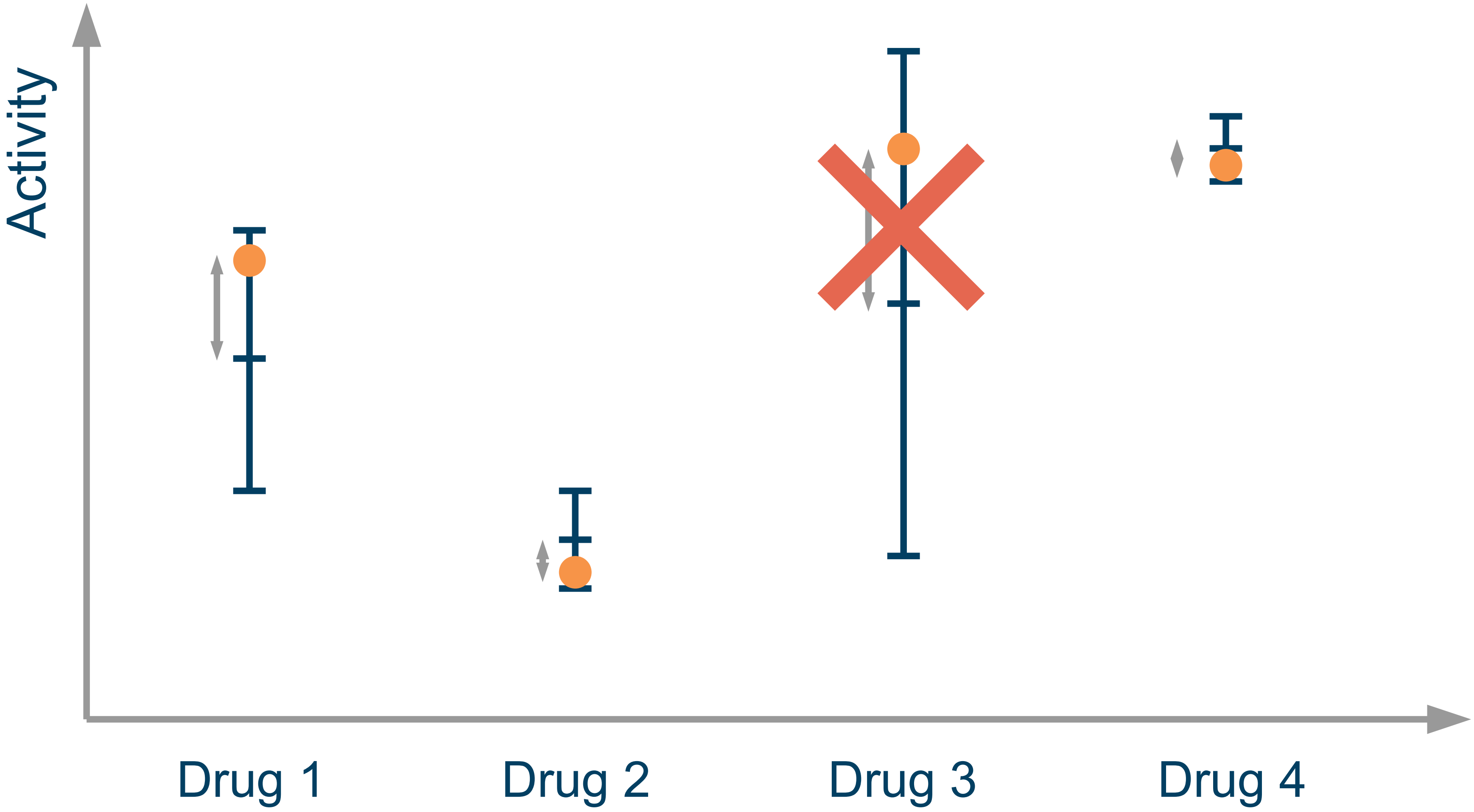
Validation data typically within one standard deviation



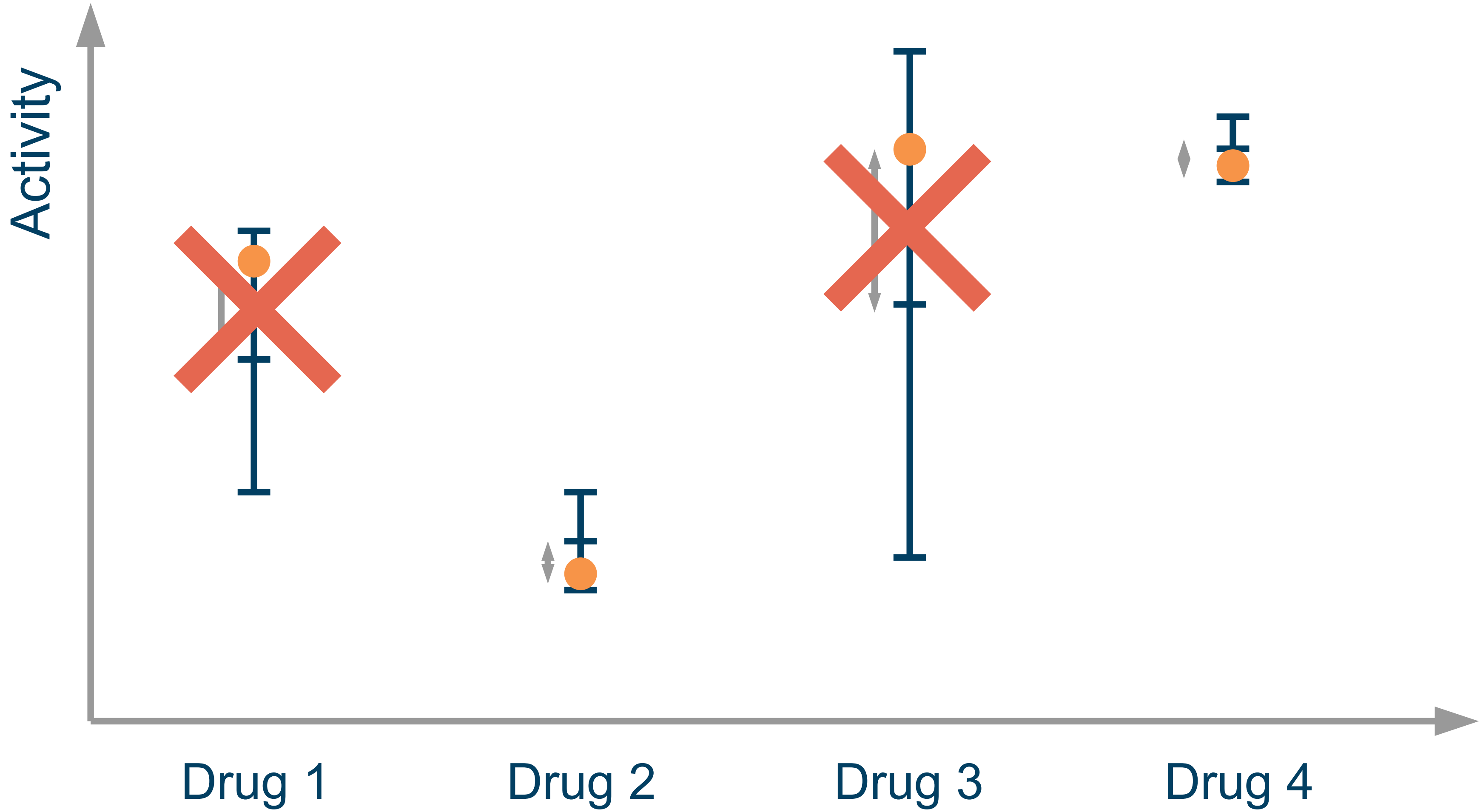
R^2 metric calculated with difference from mean



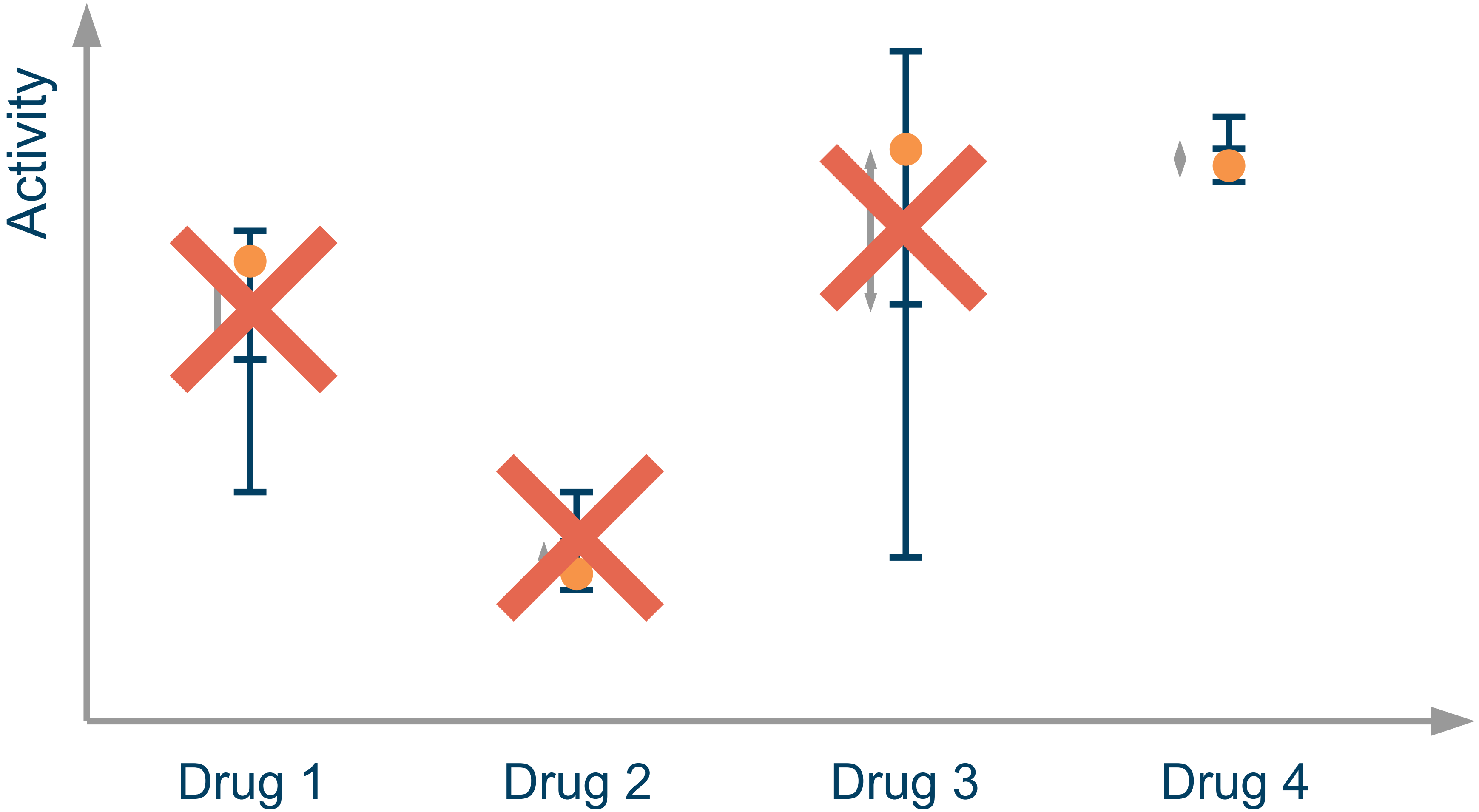
Impute 75% of data with smallest uncertainty



Impute 50% of data with smallest uncertainty

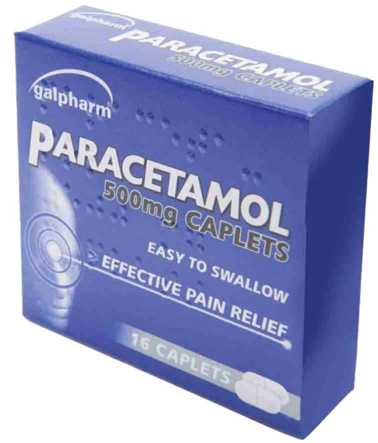


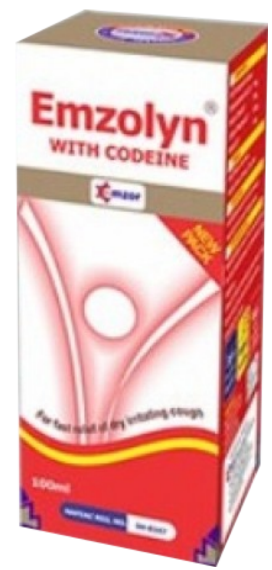
Impute 25% of data with smallest uncertainty



Improved performance by exploiting uncertainty

Different drugs can treat the same ailment





Open Source Malaria contest

OPEN SOURCE MALARIA

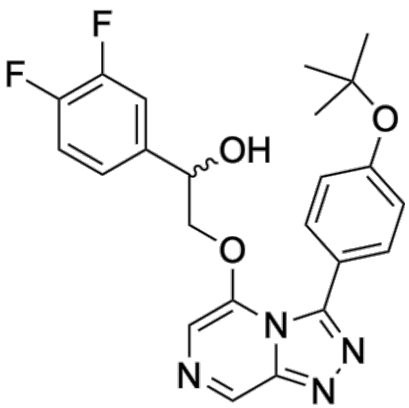
Looking for New Medicines

Open Source Malaria entrants

Entrant	Precision	Result
Molomics	82%	**Winner (company)**
Davy Guan	82%	**Winner (non-company)**
Optibrium/Intellegens	81%	**Second place**
Exscientia	81%	**Second place**
Slade Matthews	64%	Runner-up
Auromind	58%	Runner-up
Raymond Lui	58%	Runner-up
KCL	36%	Runner-up
Interlinked TX	36%	Runner-up

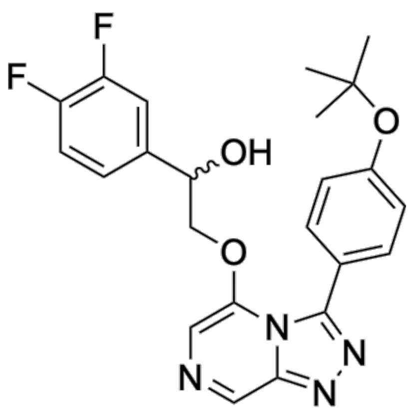
Focus on compounds with low uncertainty

Open Source Malaria experimental validation

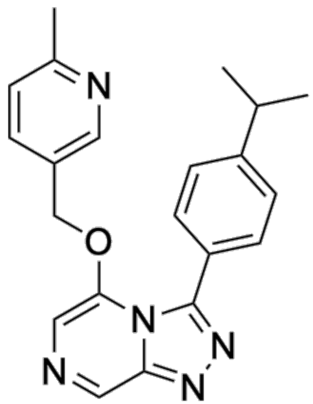


Optibrium/Intellegens
0.647 µM

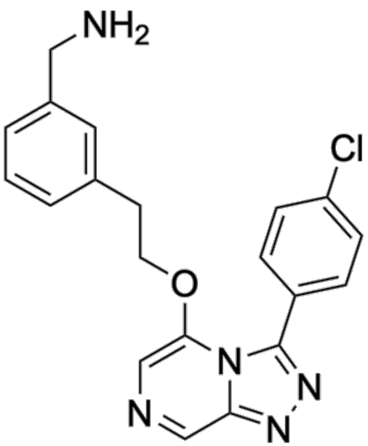
Open Source Malaria other compounds



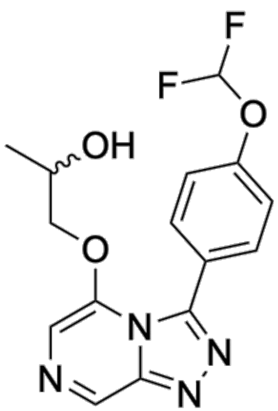
Optibrium/Intellegens
0.647 μM



Davy Guan
>25 μM



Exscientia
10.9 μM



Molomics
>25 μM

Other compounds have large uncertainty

Commercialization

Products and consultancy projects for materials and chemicals with Intellegens

Reseller agreement with drug discovery software company Optibrium

Machine learning tool embedded into next generation of Optibrium software for release in October 2020

intellegens

optibrium

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