intellegens

Applied machine learning

Synthetic alchemy: unleash the power of multimodal machine learning for materials design

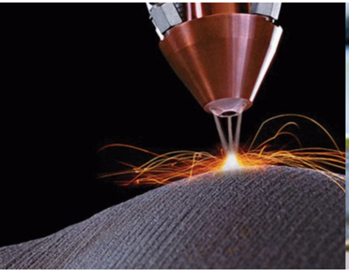
Dr Gareth Conduit

Alchemite™ machine learning

Use case of machine learning to extract information beyond data

Applications of generic Alchemite™ to materials design

Introducing Alchemite™ applied machine learning






Developed at University of Cambridge

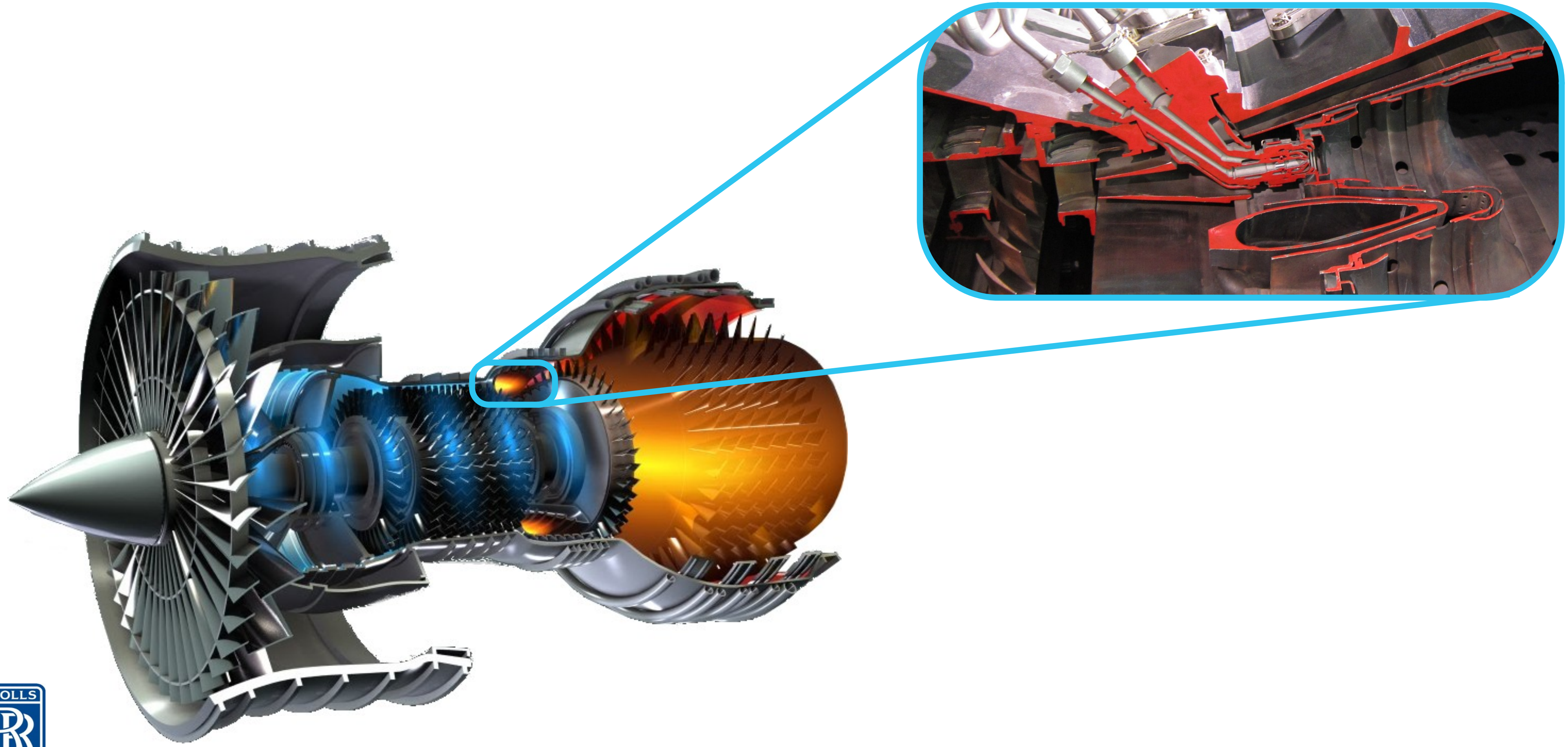
Key use cases: chemicals, materials, life sciences, and manufacturing

Innovative method extracts value from sparse, noisy data to solve complex, high-dimensional problems

Focus on ease-of-deployment for immediate return on investment

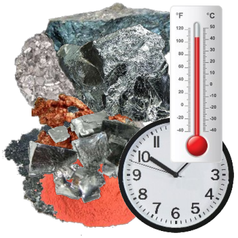
Machine learning beyond data

Combustor in a jet engine



Strength and phase behavior are correlated

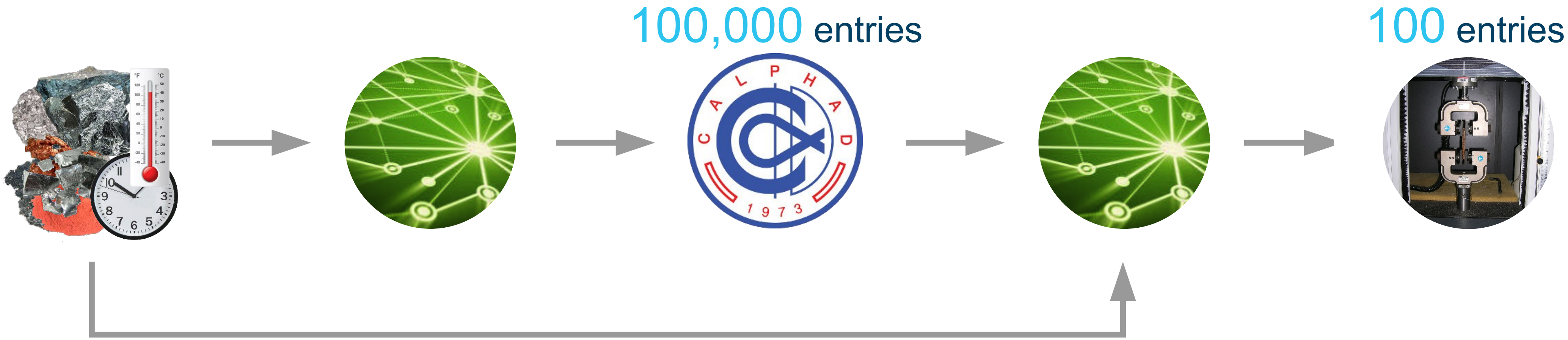
First predict phase behavior



100,000 entries

Use 100,000 CALPHAD results to model complex composition → phase behavior

Use CALPHAD to predict strength



Use 100,000 CALPHAD results to model complex composition → phase behavior

100 strength entries capture the phase behavior → strength relationship

Two interpolations aid the composition → strength 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	$> 0.04\ \mathrm{K\Omega^{-1}m^{-3}}$
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%

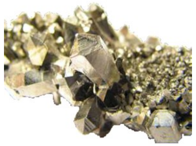
Co 4%

Mo 4.9%

W 1.2%

Zr 0.05%

Nb 3%



Al 2.9%

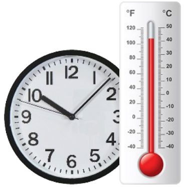
C 0.04%

B 0.01%

Ni

Expose 0.8

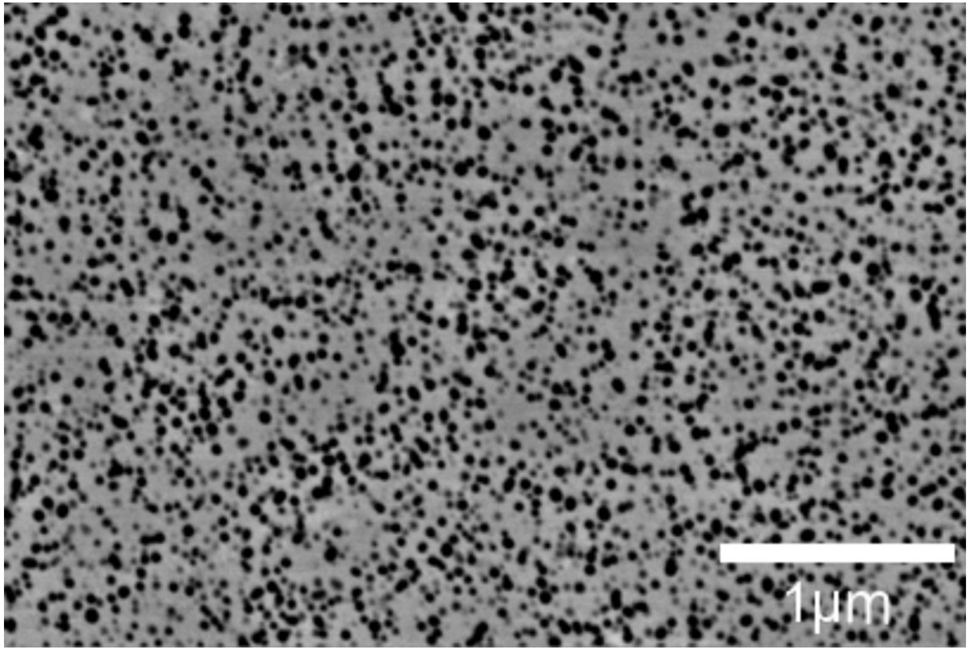
T_{HT} 1300ºC



Phase behavior targets

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

Microstructure

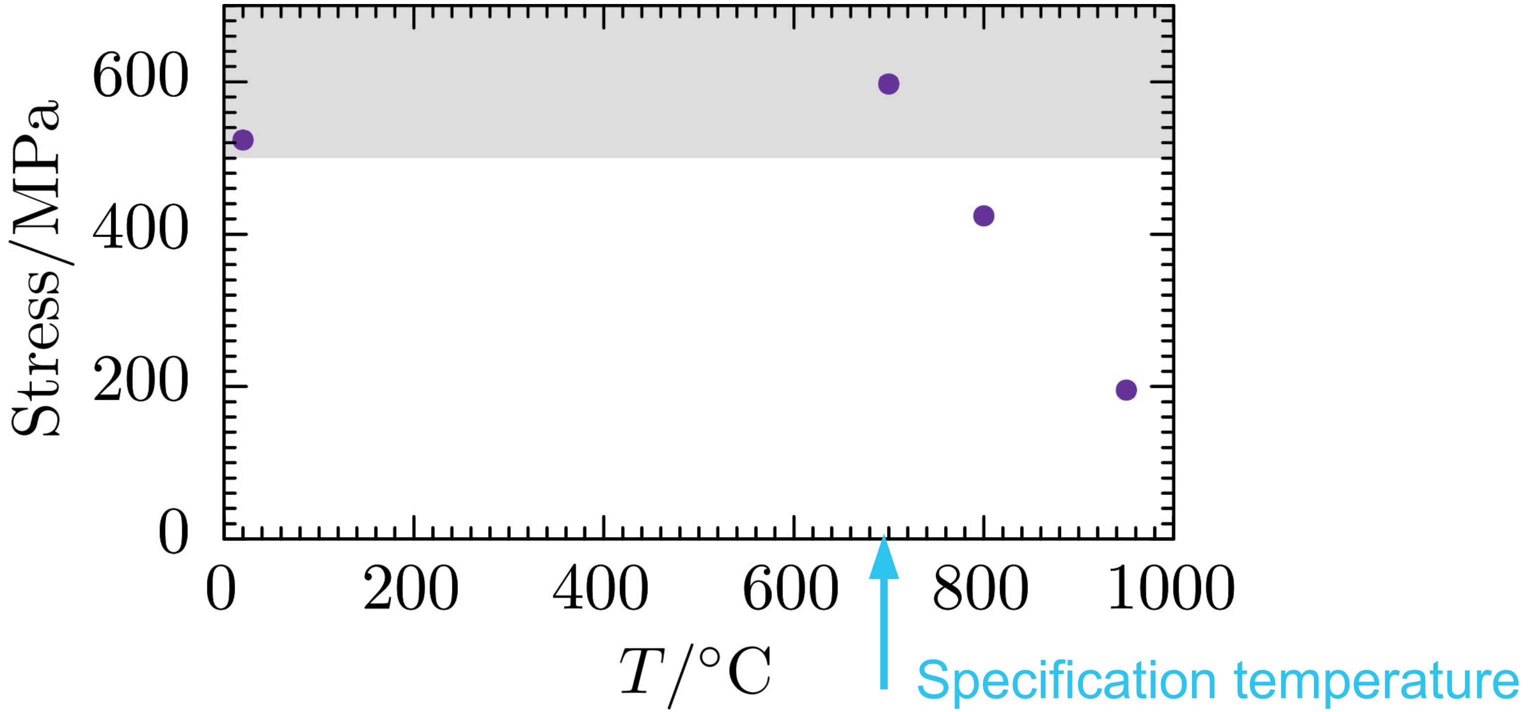


Probabilistic neural network identification of an alloy for direct laser deposition
B. Conduit, T. Illston, S. Baker, D. Vadegadde Duggappa, S. Harding, H. Stone & GJC
Materials & Design **168**, 107644 (2019)

Strength target

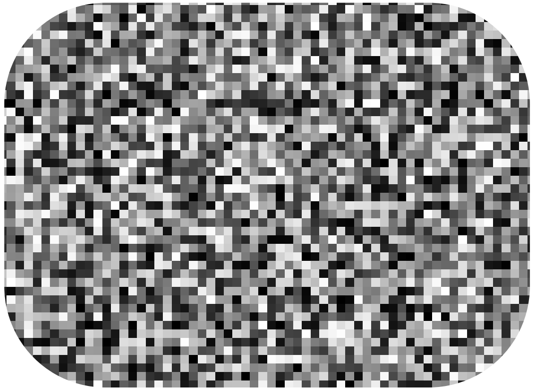
Elemental cost	< 25 $\$kg^{-1}$
Density	< 8500 kgm^{-3}
γ’ content	< 25 wt%
Oxidation resistance	< 0.3 $mgcm^{-2}$
Defects	< 0.15% defects
Phase stability	> 99.0 wt%
γ’ solvus	> 1000˚C
Thermal resistance	> 0.04 $K\Omega^{-1}m^{-3}$
Yield stress at 900˚C	> 200 MPa
Tensile strength at 900˚C	> 300 MPa
Tensile elongation at 700˚C	> 8%
1000hr stress rupture at 800˚C	> 100 MPa
Fatigue life at 500 MPa, 700˚C	> 10^5 cycles

Test the high cycle fatigue stress



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)

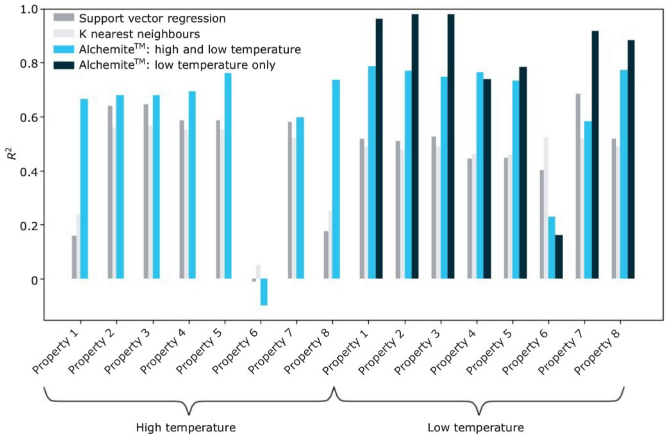
Extract information from noise



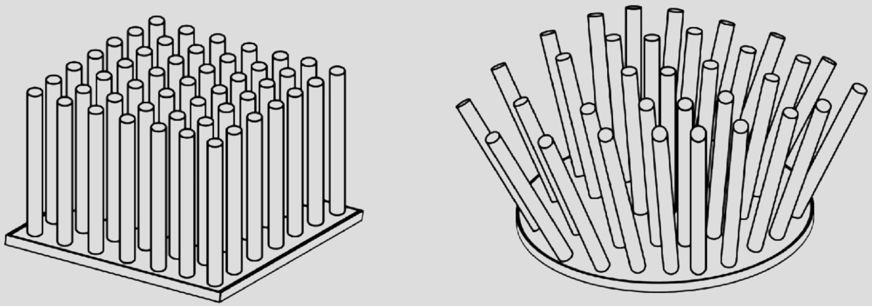
Machine learning approach to the formulation problem

Probabilistic selection and design of concrete using machine learning
Data-Centric Engineering **4**, e9 (2023)

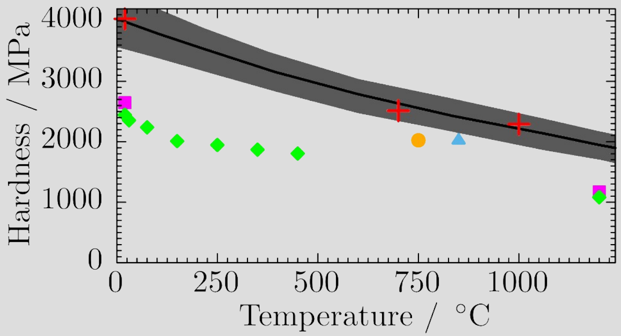
Real-life use of Alchemite™



Johnson Matthey Technology Review
66, 130 (2022)



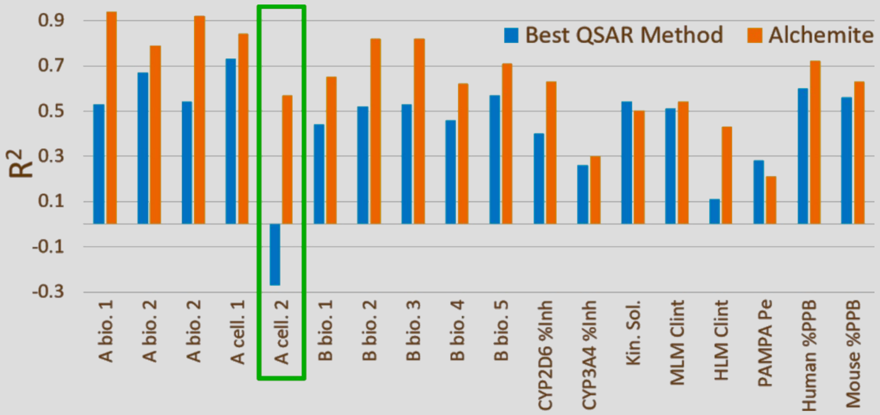
NASA Technical Memorandum
20220008637



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)



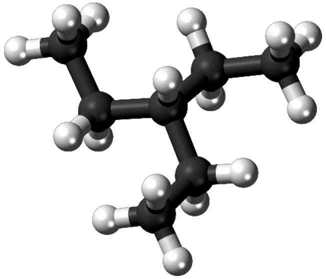
J. of Chem. Info. & Model. **60**, 2848 (2020)
Applied AI Letters **2**, e31 (2021)
Molecular Pharmaceutics **19**, 1488 (2022)

Constellation PHARMACEUTICALS
Takeda
AstraZeneca

optibrium

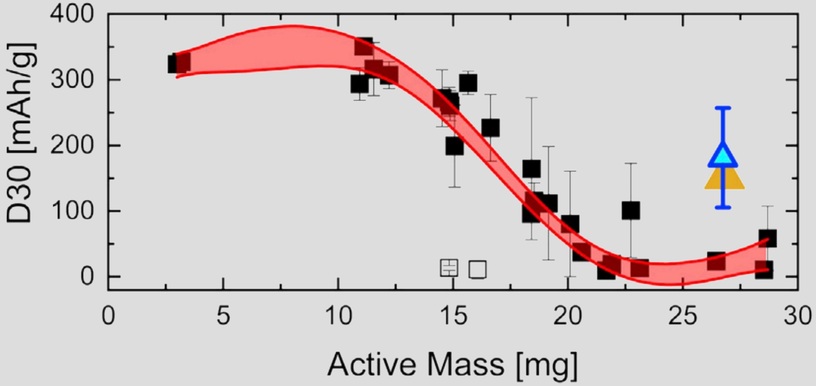
iff

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



bp

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

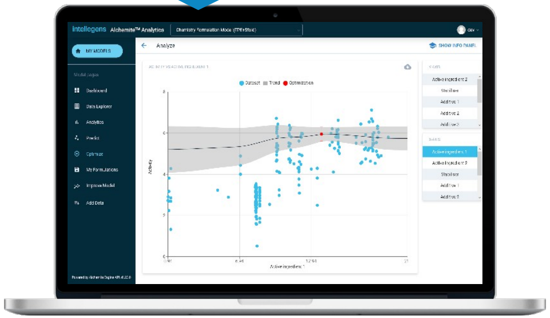


UNIVERSITY OF BIRMINGHAM
Ansys GRANTA

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

Intellegens offers the Alchemite™ product family

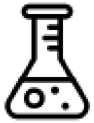
Scientists & engineers
Fast start, easy-to-use, visual



Option to deploy models

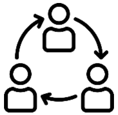
Data scientists
Add to your ML toolkit

Optional connectors



Lab systems

Software & scripts



Sharing & collaboration

Alchemite™ Analytics

Deep data insights on your desktop
Guide experiments, predict, design, optimize

Alchemite™ Engine

Integrate into your workflow (API, Python)
Advanced configuration, enterprise deployment

Alchemite™ Success

Apply Intellegens deep learning expertise
Advice to your data science team or full project management

Alchemite™ enables machine learning beyond data

Include first principles simulations and extract information from noise

Generic approach applied to many physical, chemical, and biological sciences