

# Commercialisation of research in bioinformatics

Gareth Conduit

# Alchemite™ machine learning tool to

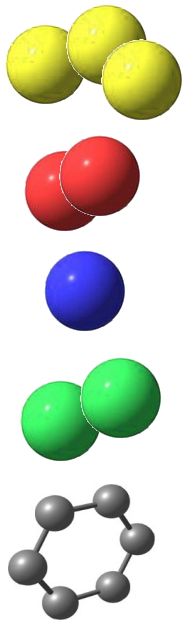


Utilise **all available** information: computer simulations and real-life measurements

**Reduce** the need for experiments and **accelerate** discovery

**Broadly applicable** with **proven** applications in drug design, industrial chemicals, and materials

# Machine learning as a black box



# Train from historical data



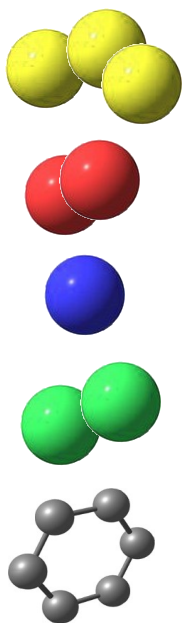
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# Predict new chemicals



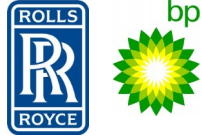
# First foray into machine learning at University of Cambridge



2013

Multiple  
properties for  
Rolls Royce  
engines

# Development of core machine learning ideas



2013

Multiple properties for Rolls Royce engines

2014

Property-property correlations with Rolls Royce and BP

# Realign research focus to machine learning



*Concurrent materials design*



2013

Multiple properties for Rolls Royce engines

2014

Property-property correlations with Rolls Royce and BP

2015

Royal Society University Research Fellowship



# First large machine learning contract as principal investigator



*Concurrent  
materials design*



2013

Multiple  
properties for  
Rolls Royce  
engines

2014

Property-  
property  
correlations  
with Rolls  
Royce and BP

2015

Royal Society  
University  
Research  
Fellowship

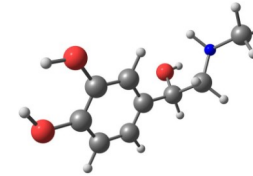
2016

Experiment-  
simulation  
correlations  
with Samsung  
Electronics

# Initial application of machine learning to drug discovery



*Concurrent  
materials design*



2013

Multiple properties for Rolls Royce engines

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Property-property correlations with Rolls Royce and BP

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2016

Experiment-simulation correlations with Samsung Electronics

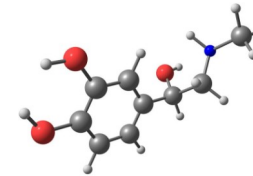
2017

Drug discovery study with e-therapeutics

# Commercializing the methodology



*Concurrent materials design*



2013

Multiple properties for Rolls Royce engines

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Experiment-simulation correlations with Samsung Electronics

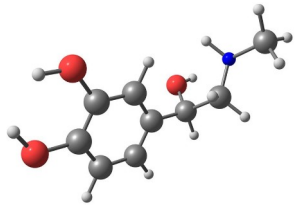
2017

Drug discovery study with e-therapeutics

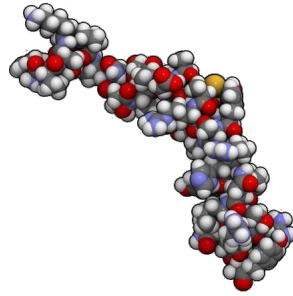
2018

Founding of Intellegens

# Action of a drug



Drug

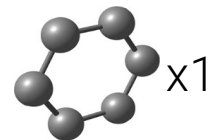
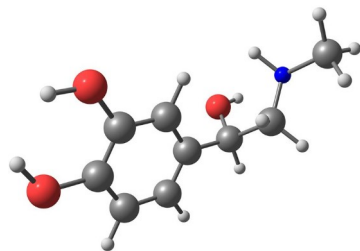


Protein

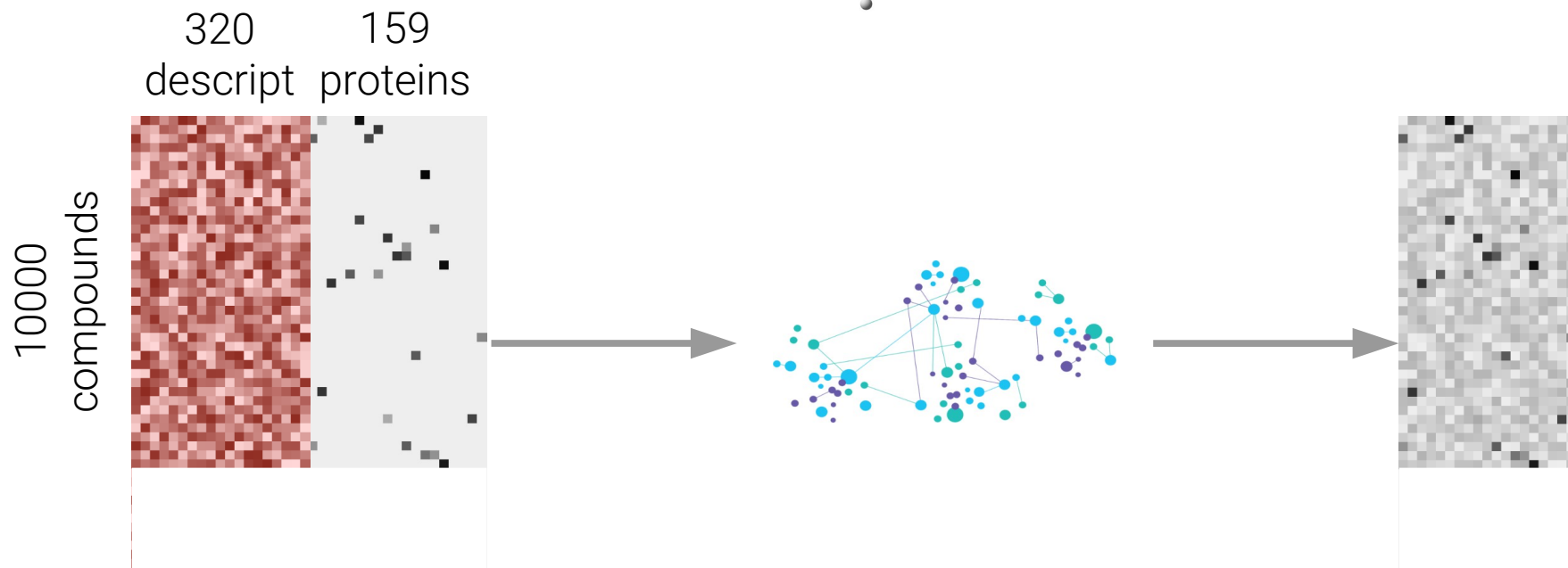


Effect

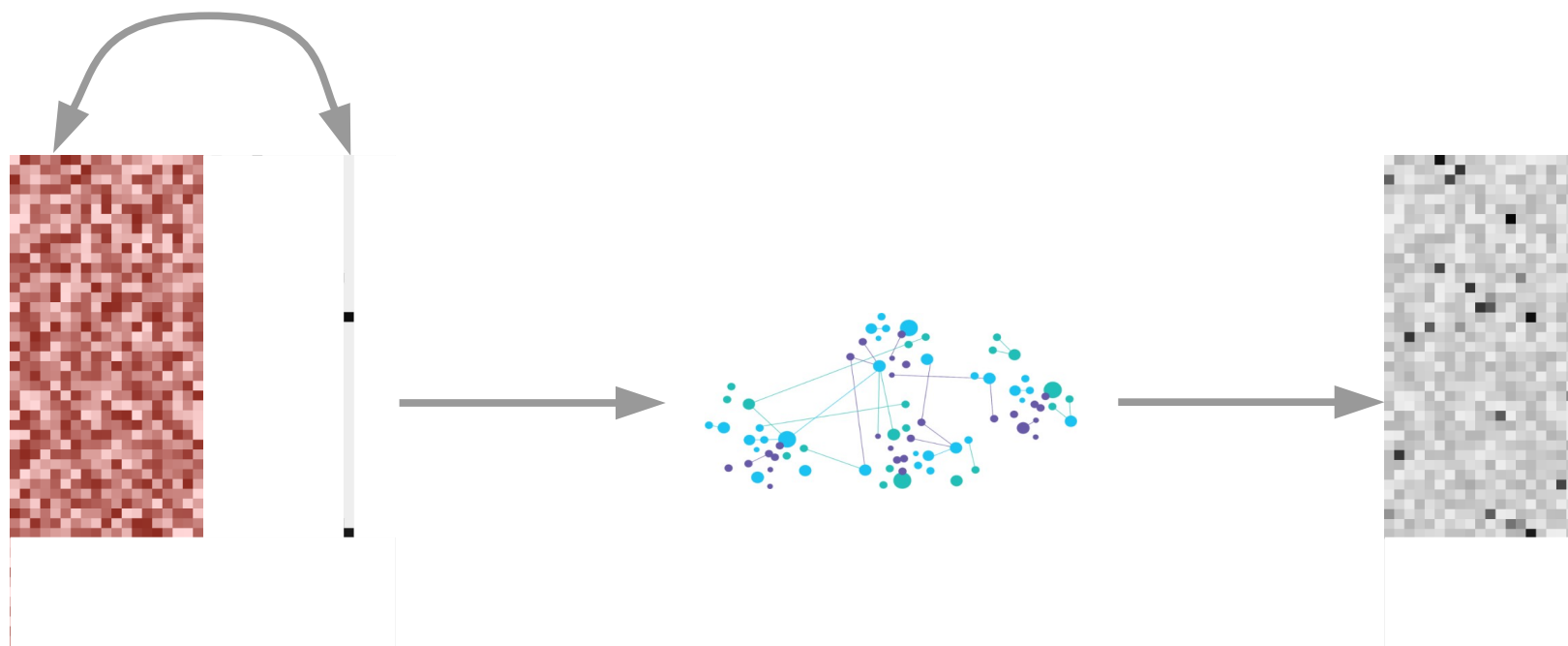
# QSAR: quantitative structure-activity relationships



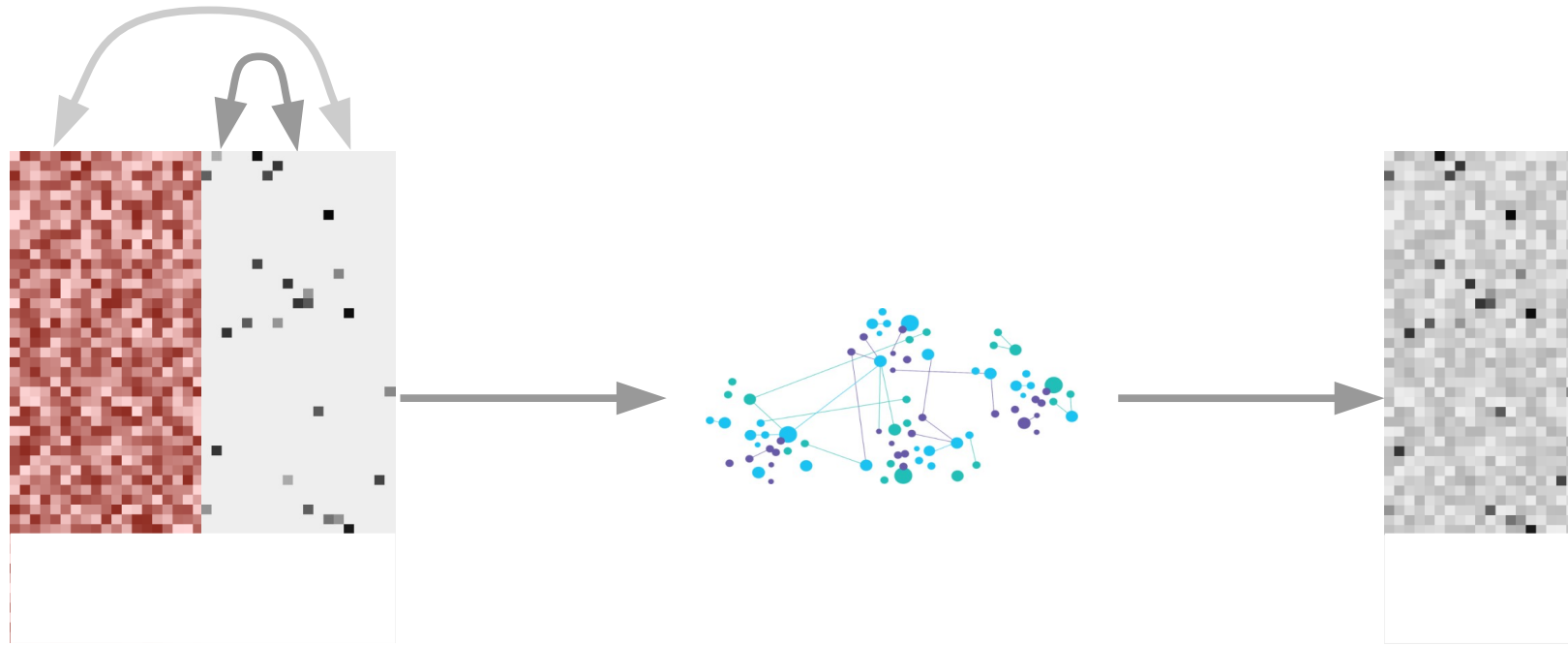
Molecular weight=183 Da



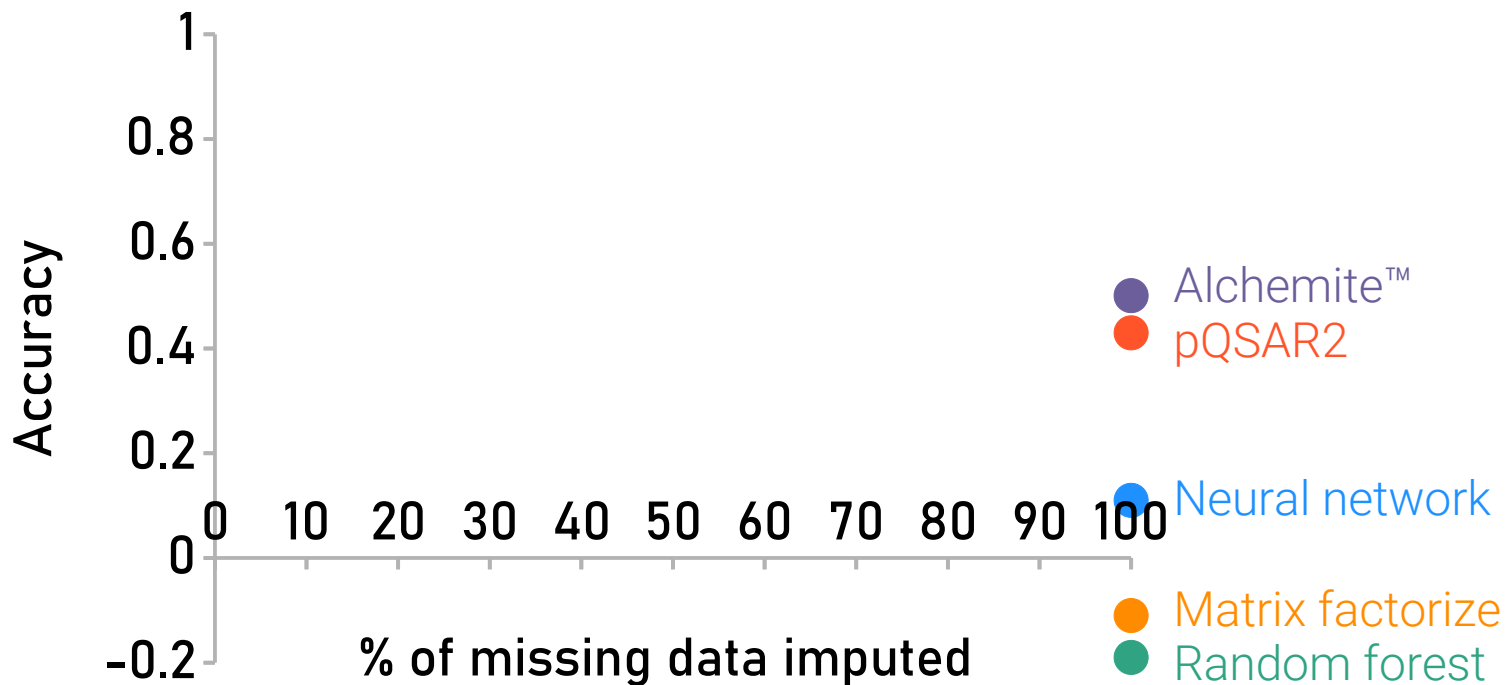
# Train off one column at a time: descriptor-protein correlations



# Alchemite™ uses all available data: protein-protein correlations

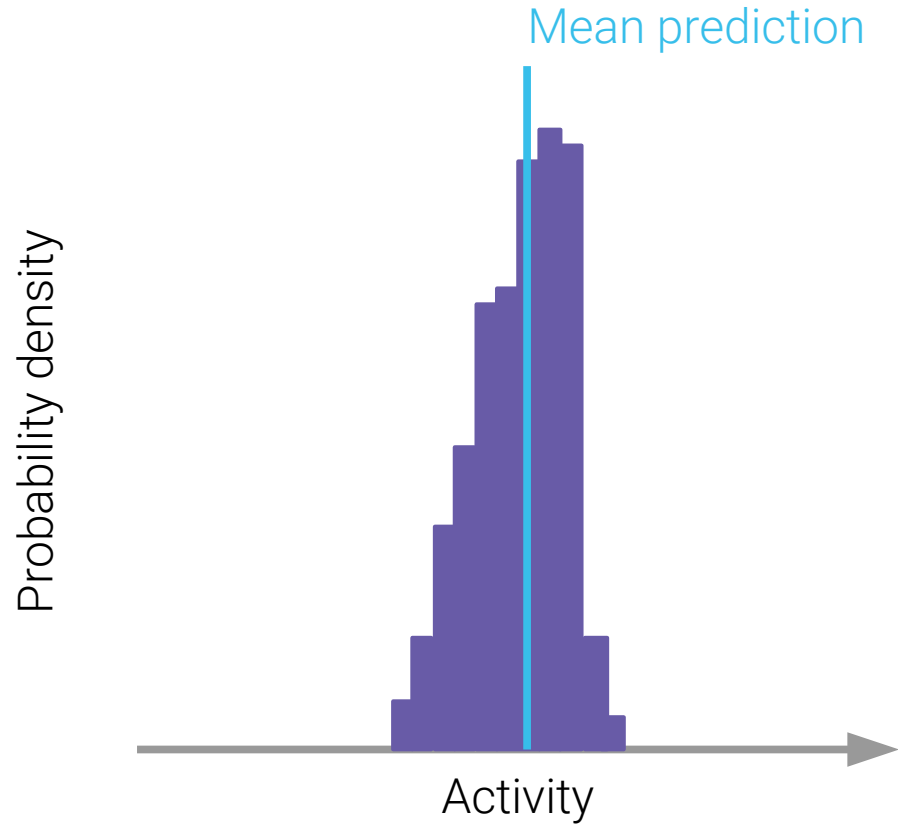


# Alchemite™ outperforms other methods

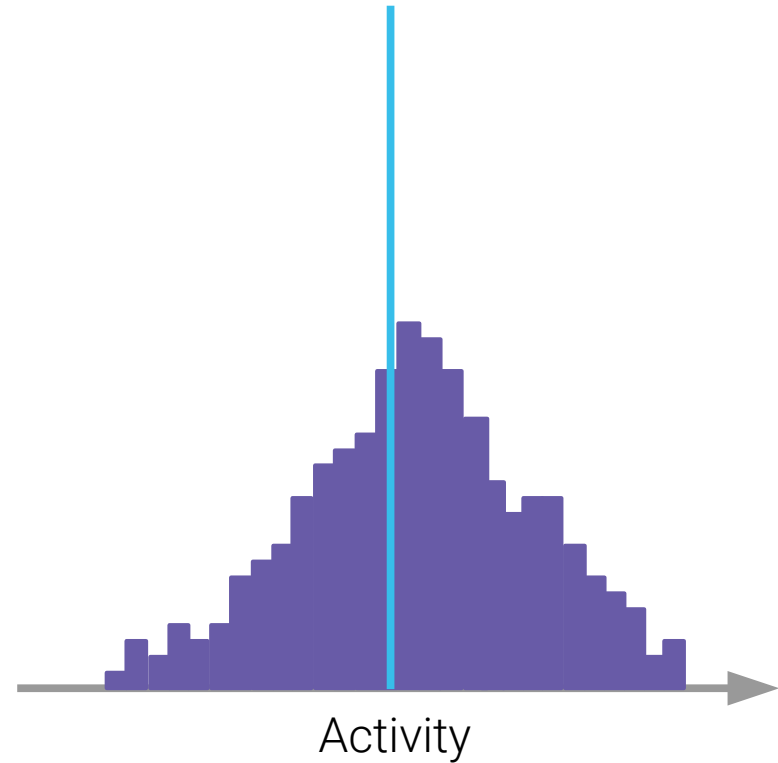
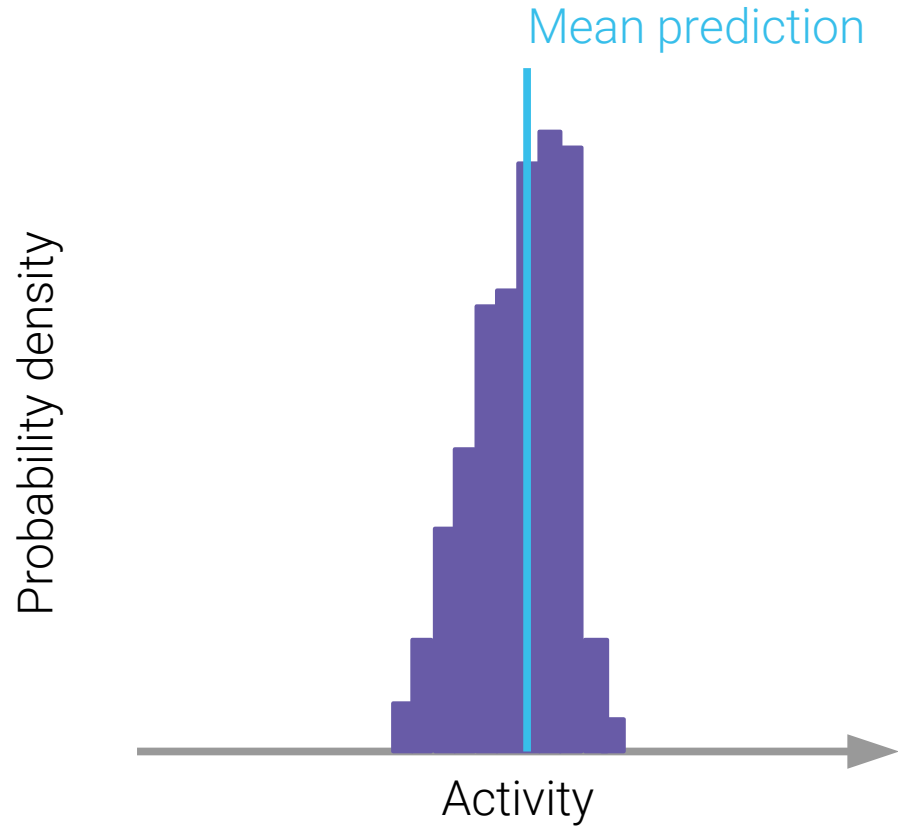




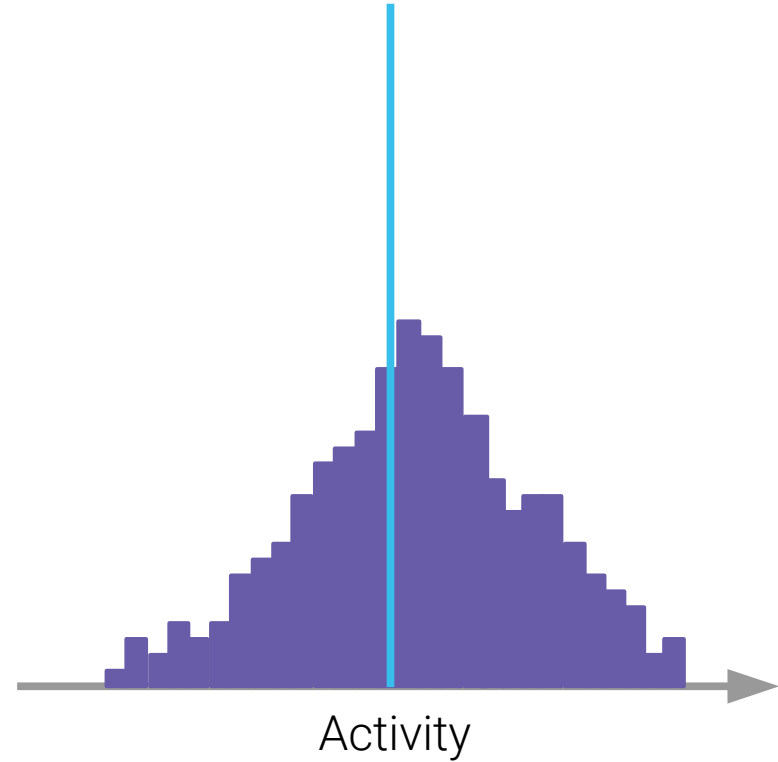
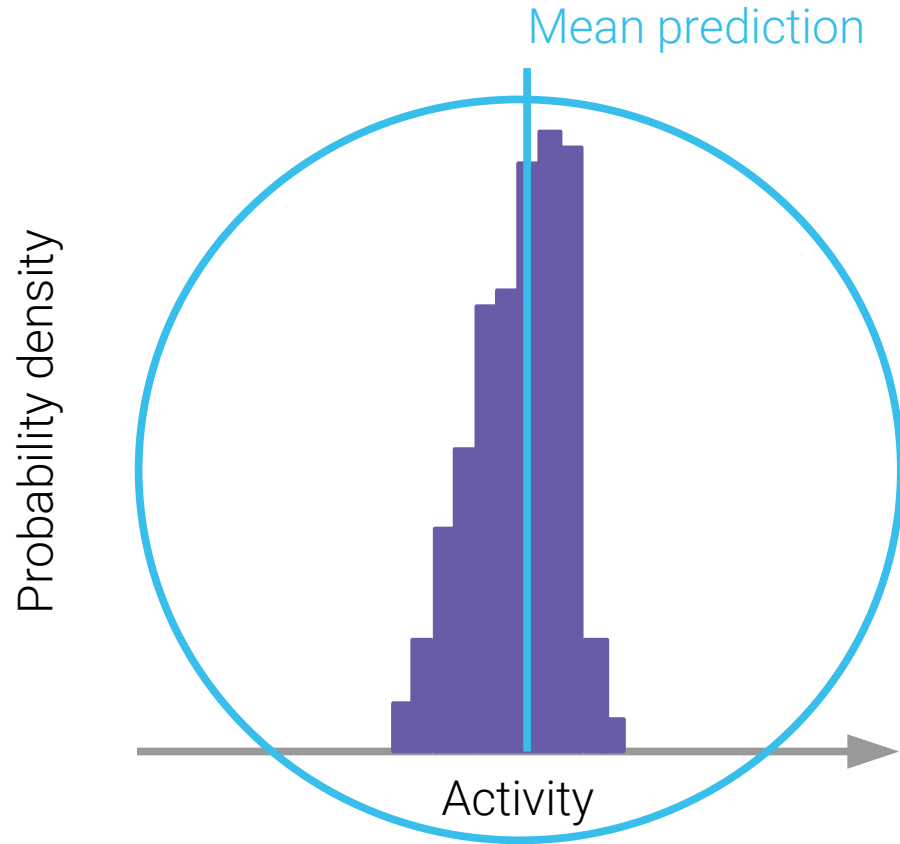
# Calculate probability distribution



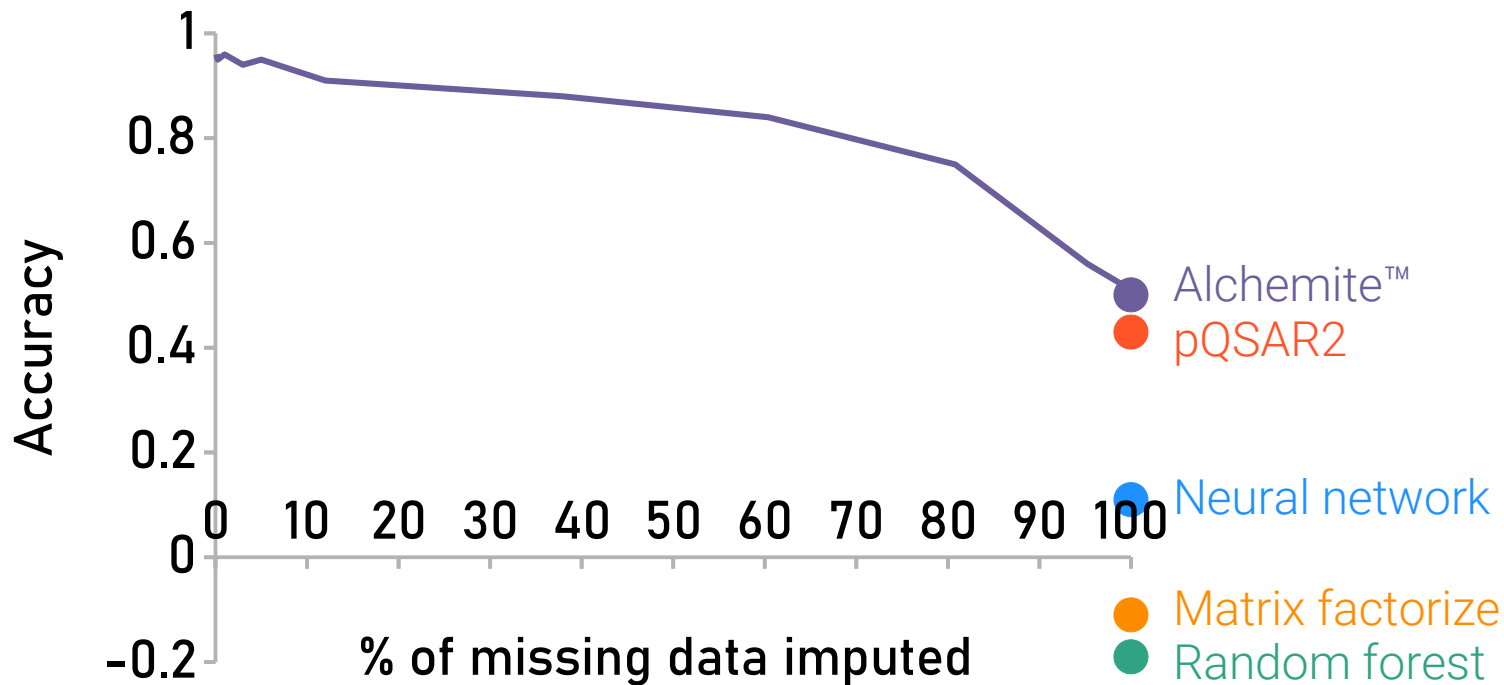
# Less confident prediction



# Focus on most confident predictions



# Reporting on only most confident predictions



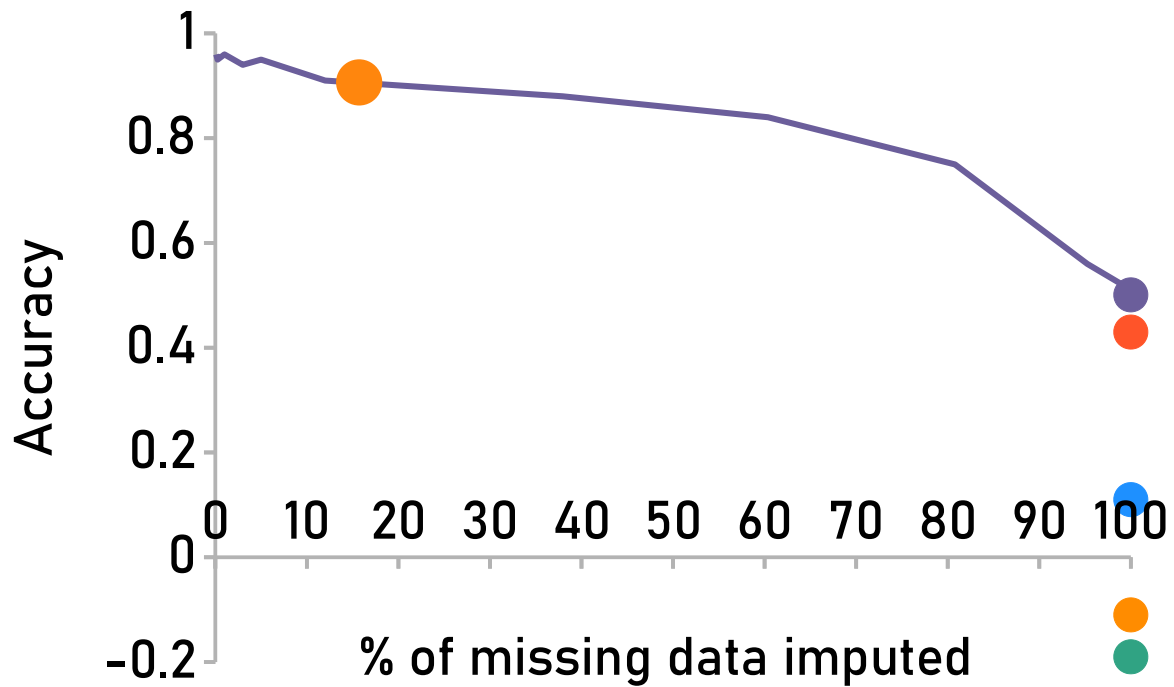
# Open Source Malaria competition



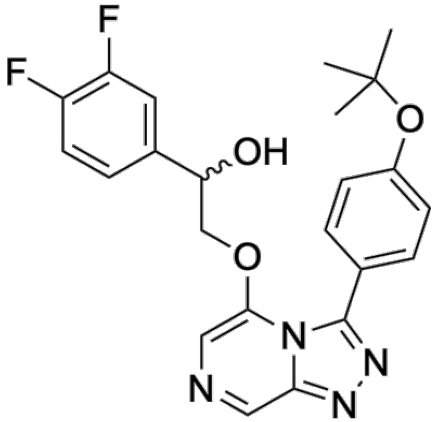
**OPEN SOURCE MALARIA**

Looking for New Medicines

# Focus on compounds with low uncertainty



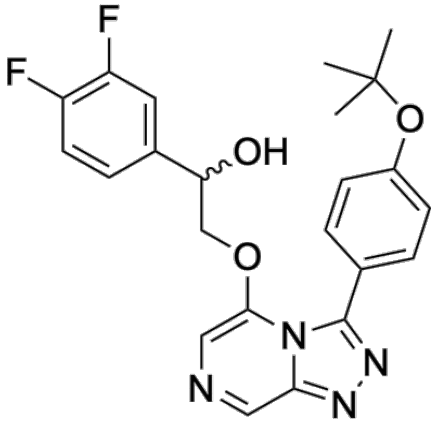
# Open Source Malaria experimental validation



Optibrium & Intellegens

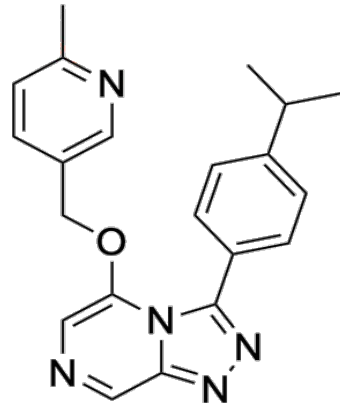
0.647  $\mu\text{M}$

# Open Source Malaria other compounds



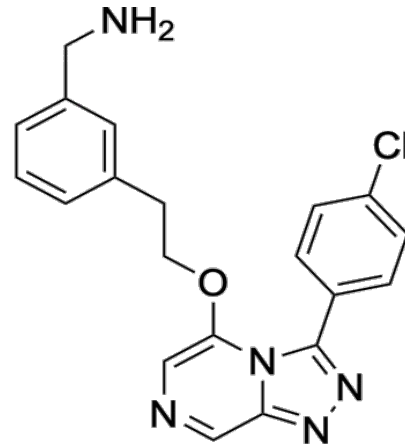
Optibrium & Intellegens

0.647  $\mu\text{M}$



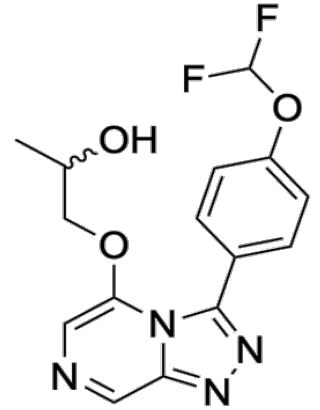
Davy Guan

>25  $\mu\text{M}$



Exscientia

10.9  $\mu\text{M}$



Molomics

>25  $\mu\text{M}$



# Initial contracts for Intellegens



2018

Bring across  
contracts from  
University

# Starting the development of a product



therapeutics



*Demonstrator for  
application of AI  
to experimental  
data*

2018

2018

Bring across  
contracts from  
University

InnovateUK  
grant

# Enter the market as a reseller



*Demonstrator for  
application of AI  
to experimental  
data*

2018

Bring across  
contracts from  
University

2018

InnovateUK  
grant

2018

Reseller  
agreement  
with Optibrium

# Build out technology through consultancy projects



Innovate UK



*Demonstrator for application of AI to experimental data*



2018

2018

2018

2019

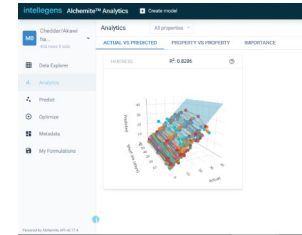
Bring across contracts from University

InnovateUK grant

Reseller agreement with Optibrium

Consultancy work

# Launch Intellegens generic industrial formulations product



*Demonstrator for application of AI to experimental data*

2018

2018

2018

2019

2020

Bring across contracts from University

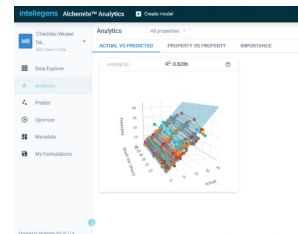
InnovateUK grant

Reseller agreement with Optibrium

Consultancy work

Release Alchemite Analytics

# Launch drug design product



*Demonstrator for application of AI to experimental data*

2018

2018

2018

2019

2020

2020

Bring across contracts from University

InnovateUK grant

Reseller agreement with Optibrium

Consultancy work

Release Alchemite Analytics

Release Cerella product with Optibrium

# Questions for commercialization of research



- Investment**      Organic growth or seek venture capital
- Breadth**      Generic technology, but how many verticals should we enter?
- Sales**      Enter a vertical directly or through a reseller?
- Exit strategy**      Seek maximum impact but opportunity to develop next idea

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**Website**      <https://intellegens.ai>  
**Demo**      [https://app.intellegens.ai/steel\\_optimise](https://app.intellegens.ai/steel_optimise)  
**Papers**      <https://www.intellegens.ai/paper.html>